

UNIVERSIDADE ESTADUAL PAULISTA "JÚLIO DE MESQUITA FILHO"  
INSTITUTO DE QUÍMICA

**ALEXANDER ALVES DA SILVA**

**Estudo lipidômico em folhas de cultivares de cana-  
de-açúcar e avaliação do papel desses metabólitos  
na ferrugem alaranjada**

Orientador: Prof. Dr. Alberto José Cavalheiro

ARARAQUARA - SP

2014

UNIVERSIDADE ESTADUAL PAULISTA "JÚLIO DE MESQUITA FILHO"  
INSTITUTO DE QUÍMICA

**ALEXANDER ALVES DA SILVA**

**Estudo lipidômico em folhas de cultivares de cana-  
de-açúcar e avaliação do papel desses metabólitos  
na ferrugem alaranjada**

Tese de Doutorado apresentada ao  
Instituto de Química, Universidade  
Estadual Paulista, como parte dos  
requisitos para obtenção do título de  
Doutor em Química.

Orientador: Prof. Dr. Alberto José Cavalheiro

ARARAQUARA - SP

2014

FICHA CATALOGRÁFICA

S586c Silva, Alexander Alves da  
Estudo lipidômico em folhas de cultivares de cana-de-  
açúcar e avaliação do papel desses metabólitos na ferrugem  
alaranjada / Alexander Alves da Silva. –  
Araraquara : [s.n], 2014  
183 f. : il.

Tese (doutorado) – Universidade Estadual Paulista,  
Instituto de Química  
Orientador: Alberto José Cavalheiro

1. Cana-de-açúcar. 2. Cromatografia a gás.  
3. Espectrometria de massa. 4. *Puccinia*. 5. Fungos  
fitopatogênicos. I. Título.

## DADOS CURRICULARES

### DADOS PESSOAIS

Nome: Alexander Alves da Silva

Filiação: Antonio Joaquim da Silva e Maria Aparecida Alves da Silva

e-mail: alexanderquimico@yahoo.com.br

### FORMAÇÃO ACADÊMICA/TITULAÇÃO

#### **2010 - 2014 Doutorado em Química.**

Universidade Estadual Paulista “Júlio de Mesquita Filho”, UNESP, Araraquara - São Paulo, Brasil. Bolsista da: Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (Capes), Brasil.

#### **2007 - 2009 Mestrado em Química.**

Instituto de Química de Araraquara, Universidade Estadual Paulista “Júlio de Mesquita Filho” - UNESP, São Paulo, Brasil.

Título: Caracterização de organossulfurados em diferentes cultivares de alho (*allium sativum* L.) e cebola (*allium cepa* L.) Orientador: Dr Alberto José Cavalheiro.

#### **2002 - 2006 Graduação em Química Tecnológica.**

Instituto de Química de Araraquara, Universidade Estadual Paulista “Júlio de Mesquita Filho” - UNESP, São Paulo, Brasil.

### FORMAÇÃO COMPLEMENTAR

#### **2011 - 2011** Extensão universitária em Introdução à Quimiometria.

Universidade Federal de São Carlos, UFSCAR, São Carlos, São Paulo, Brasil.

#### **2010 - 2010** Extensão universitária em I Escola de Inverno de Separações.

Universidade Estadual de Campinas, UNICAMP, Campinas, Brasil.

#### **2001 - 2001** Extensão Universitária em Tecnologia de Fabricação de Shampoos e Condicionadores, Universidade de Franca - UNIFRAN, Franca, São Paulo, Brasil.

#### **2001 - 2001** Extensão Universitária em Análises de Solos, Universidade de Franca - UNIFRAN, Franca, São Paulo, Brasil.

#### **2001 - 2001** Extensão Universitária em Polímeros, Universidade de Franca - UNIFRAN, Franca, São Paulo, Brasil.

#### **1999 - 2001** Curso técnico em Desenho de Construção Civil, ETEc Coronel Raphael Brandão de Barretos, São Paulo, Brasil.

### ATUAÇÃO PROFISSIONAL

**2008-2010** Participação no projeto: "Produção de Plásticos Biodegradáveis a partir da cana de açúcar por via Biotecnológica" desenvolvido mediante convênio estabelecido entre a FACTE (Fundação de Apoio à Ciência, Tecnologia e Educação) e a empresa PHB – Industrial, Instituto de Química de Araraquara, Universidade Estadual Paulista “Júlio de Mesquita Filho” - UNESP, São Paulo, Brasil.

**2008-2010** Estágio supervisionado na empresa: Centro de Monitoramento e Pesquisa da Qualidade de Combustíveis, Petróleo e Derivados – CEMPEQC - Fundação para o Desenvolvimento da UNESP – FUNDUNESP – Situado no Instituto de Química de Araraquara, Universidade Estadual Paulista “Júlio de Mesquita Filho” - UNESP, São Paulo, Brasil.

**2003-2004** Estágio supervisionado na empresa: Departamento de Esgoto e Água de Guaíra - DEAGUA, Guaíra, São Paulo, Brasil.



## **PRODUÇÃO BIBLIOGRÁFICA**

### **Artigos completos publicados em periódicos**

BRITO, J. F.; SILVA, A. A. ; CAVALHEIRO, A. J. ; ZANONI, M. V. B. . Evaluation of the Parameters Affecting the Photoelectrocatalytic Reduction of CO<sub>2</sub> to CH<sub>3</sub>OH at Cu/Cu<sub>2</sub>O Electrode. International Journal of Electrochemical Science, v. 9, p. 5961-5973, 2014.

### **Capítulos de livros publicados**

CAVALHEIRO, J. A.; COUTINHO, I. D.; LEME, G. M. ; **SILVA, A. A.** ; SILVA, A. P. D. Metabolômica de cana-de-açúcar e sua relação com a produção de biomassa vegetal para bioenergia. In: Nelson R. Stradiotto; Eliana G. M. Lemos;. (Org.). BIOENERGIA: DESENVOLVIMENTO, PESQUISA E INOVAÇÃO. 1ed. São Paulo: Cultura Acadêmica, 2012, v. 1, p. 15-34.

### **Trabalhos publicados em anais de eventos (resumo)**

**SILVA, A. A.**; CAVALHEIRO, A. J.; COUTINHO, I.D.; CRESTE, S.; TURATTI, I. C. C.. Análise da Composição Química da Cera Epicuticular de Folhas de Cana-de-açúcar por Cromatografia Gasosa. COLACRO XII - Congresso Latino-americano de Cromatografia e Técnicas Relacionadas, 2012, Florianópolis. COLACRO XVI.

### **Participação em eventos**

SILVA, A. A.; CRESTE, S.; TURATTI, I. C. C.; BRONZEL, J. J. L.; CAVALHEIRO, A. J. Identification of chemical composition of epicuticular wax from leaves of sugarcane varieties. In: 4nd. BCNP - Brazilian Conference on Natural Products, 2013, Natal - RN. 4nd. BCNP - Brazilian Conference on Natural Products, 2013.

SILVA, A. A.; COUTINHO, I. D.; ZOCCOLO, G. J.; ALVES, P. L. C. A.; NEPOMUCENO, M. P.; CRESTE, S.; TURATTI, I. C. C.; Cavalheiro, A. J.. COLACRO XIV - Congresso Latino-Americano de Cromatografia e Técnicas Relacionadas. Análise da composição química da cera epicuticular de folhas de cana-de-açúcar por cromatografia gasosa. 2012.

SILVA, A. A.; COUTINHO, I. D.; ZOCCOLO, G. J.; ALVES, P. L. C. A.; NEPOMUCENO, M. P.; CRESTE, S.; TURATTI, I. C. C.; Cavalheiro, A. J.. Analysis of apolar metabolites in sugarcane leaves by gas chromatography. In: 3nd. BCNP - Brazilian Conference on Natural Products, 2011, Ouro Preto - MG. 3nd. BCNP - Brazilian Conference on Natural Products, 2011.

SILVA, A. A. ; CAVALHEIRO, A. J. . Extração e análise de organossulfurados em diferentes cultivares de alho (*allium sativum* L.) E CEBOLA (*allium cepa* L.). In: XII Congresso Latino-Americano de Cromatografia e Técnicas Relacionadas (COLACRO XII), 2008, Florianópolis/SC. In: XII Congresso Latino-Americano de Cromatografia e Técnicas Relacionadas (COLACRO XII), 2008.

ALEXANDER ALVES DA SILVA


Tese de Doutorado apresentada ao Instituto de Química, Universidade Estadual Paulista, como parte dos requisitos para obtenção do título de Doutor em Química.

Araraquara, 24 de outubro de 2014.


BANCA EXAMINADORA



Prof. Dr. ALBERTO JOSÉ CAVALHEIRO (Orientador)  
Instituto de Química / UNESP / Araraquara – SP



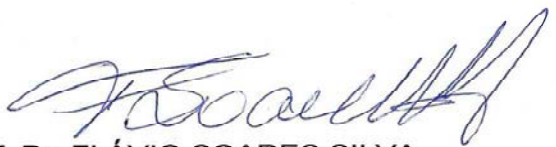
Prof.ª Dr.ª CÍNTIA DUARTE DE FREITAS MILAGRE  
Instituto de Química / UNESP / Araraquara - SP



Prof. Dr. ANDRÉ GONZAGA DOS SANTOS  
Faculdade de Ciências Farmacêuticas / UNESP/ Araraquara – SP



Prof. Dr. MARCELO TELASCRÊA  
Centro de Ciências Exatas e Sociais Aplicadas / USC / Bauru - SP



Prof. Dr. FLÁVIO SOARES SILVA  
Instituto de Física e Química / UNIFEI / Itajubá - MG

*Dedico esse trabalho aos meus pais Antonio e Maria,  
aos meus irmãos Elisangela, Anderson e Patrícia  
e a Carine pelo carinho, apoio e confiança que  
tiveram em mim no decorrer do curso.*

## AGRADECIMENTOS

*Primeiramente agradeço a Deus, por me dar forças e vontade de vencer todos os obstáculos.*

*A Carine pela paciência, carinho, companheirismo, e pela ajuda durante o desenvolvimento deste trabalho e principalmente nos momentos mais difíceis.*

*Ao meu orientador, Prof. Dr. Alberto José Cavalheiro pela atenção, dedicação, paciência, amizade, e incentivo no decorrer dos trabalhos.*

*A Professora Mary Rosa Rodrigues de Marchi, pela co-orientação, ensinamentos, amizade, colaboração e pela bolsa indústria concedida.*

*Aos meus amigos Alam, Rafael, Matheus, Fernando e Tiago pela amizade e pelos bons momentos de convivência e diversão.*

*Ao meu amigo Guilherme Julião Zocolo pela amizade, atenção, paciência e pela motivação e conselhos.*

*Aos técnicos e grandes amigos do peito João Bronzel e Juliana Rodrigues pela amizade, atenção, colaboração, conselhos, descontração, incentivos e pelos momentos de diversão.*

*Aos meus amigos e compadres Marcelo e Gabriela e as demais amigos de Guaíra.*

*Ao meu grande amigo Christiann pelos ensinamentos, conselhos e incentivos nos momentos mais difíceis.*

*Aos meus “irmãos” grandes amigos Amauri, Doni e Juliano, obrigado pela amizade, colaboração, conselhos, incentivos e pelos momentos de diversão e claro pelos churrascos de última hora....*

*Ao Prof. Dr. Norberto Peporine Lopes pela amizade e confiança em mim depositada e pelo espaço cedido para a realização das análises no Departamento de Física e Química da FCFRP - USP.*

*Aos técnicos Cristina e Tomaz do Departamento de Física e Química da FCFRP – USP pela amizade, contribuições, conselhos e incentivos.*

*Aos meus amigos de grupo Paula, Gabriel, Fernando, Vinicius, Cristiano, Livia, Naira, Raquel e Isabel obrigado pelas contribuições, incentivos e momentos de descontração.*

*Ao Rafael Freire pela amizade e pela colaboração durante no decorrer do trabalho.*

*A todos os amigos do Nubbe em especial a Alessandra, Gislaine, Rebeca, Vânia e Teresinha.*

*Ao Rafael (Para) pelas colaborações, atenção, disponibilidade e amizade.*

*Aos meus amigos Fernando (Fernandim), Lucy e Carlos pela amizade e incentivo e colaborações.*

*A todos os professores do Nubbe pelas colaborações diretas e indiretas.*

*Ao técnico Nivaldo pela amizade, conselhos e pelo sofrimento com a ferrinha...*

*A todas as bibliotecárias, em especial a Isabel, Valéria, Marilda e Catia pela amizade e eficiência no atendimento.*

*Agradeço a Capes, Fapce pelas bolsas e Fapesp pelos auxílios.*

A banca examinadora deste trabalho pela disponibilização e contribuições.

Ao Programa de Pós-graduação em Química, bem como, a todos deste Instituto (professores, equipe administrativa, seguranças e as faxineiras).

*Há apenas uma maneira de evitar as críticas:  
não faça nada, não diga nada,  
e não seja nada".  
Aristóteles.*

*“Nunca tenha certeza de nada,  
por que a sabedoria começa com a dúvida.”*

*Sigmund Freud*

## Resumo

A cana-de-açúcar (*Sacharum spp.*) é uma planta de grande importância econômica para o Brasil, usada principalmente na produção de açúcar e etanol, mas que está sujeita ao ataque de diversas doenças, tais como aquelas associadas à proliferação de vírus, bactérias e fungos, que comprometem a produtividade, impactando a produção de biomassa. Estudos que visam estabelecer uma correlação entre a composição micromolecular e a resistência hospedeiro/patógeno ainda são pouco explorados, mas podem auxiliar na investigação dessas interações. Portanto, o objetivo deste estudo foi analisar e comparar os perfis metabólicos da cera epicuticular e de outros metabólitos lipofílicos de folhas de diversas variedades de cana-de-açúcar, por cromatografia a gás acoplada à espectrometria de massas (GC-MS). As análises qualitativas resultaram na identificação de 58 compostos na cera epicuticular (138 observados), 41 no extrato hexânico (65 observados) de folhas de cana-de-açúcar. Essas análises foram realizadas por GC-MS após sililação das amostras e alicerçadas principalmente na comparação de índices de retenção e espectros de massas experimentais com dados da literatura e de biblioteca de espectros. Algumas propostas foram também reforçadas pela análise do padrão de fragmentação, entre as quais incluem-se séries homólogas de hidrocarbonetos, ácidos e álcoois graxos e alquilresorcinóis, além de esteroides e triterpenos. A identificação de alquilresorcinóis e do triterpeno simiarenol foi confirmada por análise de frações de cera epicuticular por RMN de  $^1\text{H}$  e  $^{13}\text{C}$ . A julgar pelas massas de cada fração obtida no fracionamento da cera epicuticular de folhas, por cromatografia em camada delgada preparativa, e respectivos espectro de RMN de  $^1\text{H}$ , conclui-se que os constituintes principais da cera são 5-nonadecil resorcinol, heneicosil resorcinol e o triterpeno simiarenol. Na comparação dos perfis químicos de ceras epicuticulares e do extrato hexânico de folhas dos diversos cultivares de cana-de-açúcar acessados, observou-se variações qualitativas e quantitativas significativas mas aleatórias entre as amostras, inviabilizando o agrupamento de cultivares por similaridade química. No estudo preliminar realizado com cultivares susceptíveis e resistentes à ferrugem alaranjada (*Puccinia kuehnii*), inoculados ou não com o patógeno, os perfis químicos de compostos lipofílicos (extrato hexânico) de folhas foram comparados após sililação e análise por GC-MS. Os dados obtidos não indicaram diferenças nítidas entre os cultivares susceptível e resistente, nem entre as amostras testemunha e inoculadas, indicando que a resistência a este patógeno não deve estar associada à compostos lipofílicos.

**Palavras-chave:** cana-de-açúcar, *Puccinia kuehnii*, ferrugem alaranjada, índice de retenção, cromatografia a gás, espectrometria de massas, simiarenol, alquil resorcinol.



## Abstract

Sugarcane (*Sacharam* spp.) is a plant of great importance to Brazil, used mainly in the production of sugar and ethanol, but is subject to several diseases, such as those associated with the proliferation of viruses, bacteria and fungi, that compromise productivity and impacting the production of biomass.

Studies aimed to establish the correlation between the micromolecula composition and the host / pathogen resistance are underexplored, but may assist in the understanding of these interactions. Therefore, the aim of this study was to analyze and compare the metabolic profiles of epicuticular wax and other lipophilic metabolites from leaves of different varieties of sugarcane by gas chromatography coupled to mass spectrometry (GC-MS). The qualitative analysis resulted in the identification of 58 compounds in epicuticular wax (seen 138) and 41 compounds in the hexane extract (seen 65) of leaves of sugarcane. These analyzes were performed by GC-MS after sample silylation, and the compound identification was grounded mainly on comparison of retention indices and mass spectra with experimental literature data and spectra libraries. Some proposals have also been enhanced by the fragmentation pattern analysis. The identified compounds include homologous series of hydrocarbons, fatty acids, policosanols and alkyl resorcinols, triterpenes and steroids. The identification of alkyl resorcinols and the triterpene simiarenol was confirmed by  $^1\text{H}$  NMR and  $^{13}\text{C}$ . Judging by the masses of fractions obtained from analysis of the epicuticular wax by preparative TLC, and its  $^1\text{H}$  NMR spectrum, it was concluded that the main constituents of wax are 5-nonadecyl resorcinol, 5-heneicosil resorcinol and simiarenol. The comparison of the chemical profiles of epicuticular waxes and the hexane extract of leaves from different sugarcane cultivars showed random qualitative and quantitative variations between the samples, but without statistical significance, preventing the grouping of cultivars by chemical similarity. Additionally, a preliminary study involving pathogen inoculation (*Puccinia kuehnii*) in cultivars susceptible and resistant to orange rust showed again no differentiation between the lipophilic compounds from leaves, indicating that resistance to this pathogen is not associated with lipophilic compounds.

**Keywords:** sugarcane, *Puccinia kuehnii*, orange rust, retention index, gas chromatography, mass spectrometry, simiarenol, alkylresorcinol.

## **LISTA DE FIGURAS**

---

<b>Figura 1: Nomenclatura específica de híbridos de cana-de-açúcar. ....</b>	<b>19</b>
<b>Figura 2: Produção mundial em 2012 (em milhões de toneladas).....</b>	<b>20</b>
<b>Figura 3: Projeção da produção de açúcar para safra de 2018/19.....</b>	<b>21</b>
<b>Figura 4: Projeção da produção de etanol para safra de 2018/19.....</b>	<b>21</b>
<b>Figura 5: Sintomas da ferrugem alaranjada em cana-de-açúcar. ....</b>	<b>23</b>
<b>Figura 6: Comparação da ferrugem alaranjada (a, b) com a ferrugem marrom (c, d).....</b>	<b>25</b>
<b>Figura 7: Escala diagramática para avaliação da severidade da ferrugem marrom.....</b>	<b>26</b>
<b>Figura 8: Esquema de numeração de folhas pelo sistema de Kuijper. ....</b>	<b>26</b>
<b>Figura 9: Representação clássica dos fatores que interagem para a ocorrência de doenças em plantas.....</b>	<b>27</b>
<b>Figura 10: Vias de penetrações dos fungos. ....</b>	<b>28</b>
<b>Figura 11: Representação esquemática da estrutura da cutícula em tecido foliar. ....</b>	<b>31</b>
<b>Figura 12: Estrutura de alquilresorcinol.....</b>	<b>32</b>
<b>Figura 13: Alguns constituintes identificados em cana-de-açúcar. ....</b>	<b>34</b>
<b>Figura 14: Extração da cera epicuticular.....</b>	<b>41</b>
<b>Figura 15: Mecanismo de reação geral de sililação. ....</b>	<b>41</b>
<b>Figura 16: Fluxograma da extração de metabolitos apolares em folhas de cana-de-açúcar .....</b>	<b>42</b>
<b>Figura 17: Fluxograma da extração da cera epicuticular de folhas de cana-de-açúcar.....</b>	<b>43</b>
<b>Figura 18: Exemplo de perfil cromatográfico de cera epicuticular (TMS) de folhas de cana-de-açúcar obtidos por GC-FID e GC-MS.....</b>	<b>48</b>
<b>Figura 19: Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 10 a 30 minutos. ....</b>	<b>49</b>
<b>Figura 20: Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 10 a 30 minutos.....</b>	<b>50</b>
<b>Figura 21: Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 30 a 65 minutos. ....</b>	<b>51</b>
<b>Figura 22: Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 30 a 65 minutos.....</b>	<b>52</b>

## **LISTA DE FIGURAS**

---

Figura 23: Análise de séries homólogas de hidrocarboneto C8-C40 em GC-FID e GC-MS. ....	53
Figura 24: Exemplo do cálculo do IR do ácido pentadecanóico (TMS) utilizando a equação de Van Den Dool e Kratz. ....	54
Figura 25: Comparação dos espectros de massas de amostras de cana-de-açúcar com os espectros das bibliotecas.....	55
Figura 26: Comparação do perfil cromatográfico e do IR entre os tempos de retenção de 10 a 45 minutos (a) e de 45 a 65 minutos (b) das análises de cera epicuticular (TMS) GC-FID com GC-MS.....	57
Figura 27: Proposta de fragmentação do octacosano.....	60
Figura 28: Proposta de fragmentação do ácido hexacosanóico (TMS).....	61
Figura 29: Proposta de fragmentação do dotriacontanol (TMS). ....	61
Figura 30: Proposta de fragmentação do $\beta$ -Sitosterol, (TMS). ....	62
Figura 31: Proposta de fragmentação do heneicosanilresorcinol, (TMS). ....	62
Figura 32: Estruturas das colunas capilares: DB-5 (5% difenil-95-dimetil polissiloxano) e DB-5MS (5% fenil arileno-95% dimetil polissiloxano). ....	65
Figura 33: Comparação do pico em $t_R=41$ minutos do cromatograma da análise de cera epicuticular de cana-de-açúcar com o padrão heptacosano.....	66
Figura 34: Comparação dos constituintes com $t_R = 54,172$ minutos dos cromatogramas das análises de cera epicuticular de cana-de-açúcar das amostras IAC95-5000, IACSP94-2094 e do padrão tritriacontano.....	67
Figura 35: Indicação da série homóloga de hidrocarbonetos identificada em amostras de cera epicuticular de cana-de-açúcar. ....	69
Figura 36: Comparação do teor relativo da série homóloga de hidrocarbonetos identificados na análise de cera epicuticular de folha de cana-de-açúcar. ....	69
Figura 37: Indicação da série homóloga de alcoóis identificado em amostras de cera epicuticular de cana-de-açúcar. ....	70
Figura 38: Comparação do teor relativo da série homóloga de alcoóis identificados na análise de cera epicuticular de folha de cana-de-açúcar. ....	70
Figura 39: Indicação da série homóloga de ácidos graxos identificado em amostras de cera epicuticular de cana-de-açúcar. ....	71
Figura 40: Comparação do teor relativo da série homóloga de ácidos graxos identificados na análise de cera epicuticular de folha de cana-de-açúcar. ....	71

## **LISTA DE FIGURAS**

---

<b>Figura 41: Indicação da série homóloga de alquilresorcinóis identificado em amostras de cera epicuticular de cana-de-açúcar. ....</b>	<b>72</b>
<b>Figura 42: Comparação do teor relativo da série homóloga de alquilresorcinol identificados na análise de cera epicuticular de folha de cana-de-açúcar. ....</b>	<b>73</b>
<b>Figura 43: Comparação do teor relativo de compostos com proposta de identificação da análise de cera epicuticular de folha de cana-de-açúcar.....</b>	<b>73</b>
<b>Figura 44: Comparação do teor relativo de compostos não identificados em cera epicuticular (TMS) de folha de cana-de-açúcar.....</b>	<b>74</b>
<b>Figura 45: Gráfico de 3D scores da PCA das análises da cera epicuticular de folhas de cana-de-açúcar de 13 cultivares analisados em GC-MS.....</b>	<b>75</b>
<b>Figura 46: Exemplo de perfil cromatográfico de extrato hexânico (TMS) de folhas de cana-de-açúcar obtidos por GC-FID e GC-MS.....</b>	<b>76</b>
<b>Figura 47: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 10 a 30 minutos. ....</b>	<b>77</b>
<b>Figura 48: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 10 a 30 minutos.....</b>	<b>79</b>
<b>Figura 49: Cromatogramas ampliados da análise extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 30 a 65 minutos. ....</b>	<b>81</b>
<b>Figura 50: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 30 a 65 minutos.....</b>	<b>83</b>
<b>Figura 51: Comparação do perfil cromatográfico e do IR entre os tempos de retenção de 10 a 30 minutos (a) e de 30 a 65 minutos (b) das análises do extrato hexânico (TMS) de GC-FID com GC-MS. ....</b>	<b>86</b>
<b>Figura 52: Indicação dos ácidos graxos identificados em amostras dos extratos hexânicos (TMS) de folhas de cana-de-açúcar.....</b>	<b>89</b>
<b>Figura 53: Comparação do teor relativo da série homóloga de ácidos graxos identificados na análise de extrato hexânico (TMS) de folhas de cana-de-açúcar.....</b>	<b>90</b>
<b>Figura 54: Comparação do teor relativo da série homóloga de alcoóis identificados na análise de extrato hexânico (TMS) de folhas de cana-de-açúcar.....</b>	<b>90</b>
<b>Figura 55: Comparação do teor relativo de outros constituintes identificados em extrato hexânicos (TMS) de folhas de cana-de-açúcar.....</b>	<b>91</b>

## **LISTA DE FIGURAS**

---

Figura 56: Gráfico de 3D scores da PCA das análises de extrato hexânico (TMS) de folhas de cana-de-açúcar analisados em GC-MS.....	92
Figura 57: Cromatografia em camada delgada comparativa da cera epicuticular. .....	93
Figura 58: Análise da cera epicuticular por CCDP e análises das frações por GC-FID.....	94
Figura 59: Identificação de série homóloga de alquilresorcinol por GC-MS (a) e MS-APCI (b).....	95
Figura 60: Estruturas de (a) nonadecilresorcinol (nonadecildiidroxi-benzeno) e (b) heneicosilresorcinol (heneicosildiidroxi-benzeno) identificados em cera epicuticular de cana-de-açúcar.....	96
Figura 61: Espectro de RMN de $^1\text{H}$ do Alquilresorcinol ( $\text{CDCl}_3$ , 7,0 T). ....	97
Figura 62: Espectro de RMN de $^{13}\text{C}$ do Alquilresorcinol ( $\text{CDCl}_3$ , 7,0 T). ....	97
Figura 63: Experimento de MS-APCI da Fr3 obtido no modo positivo.....	99
Figura 64: Estrutura do simiarenol identificado em cera epiicuticular. ....	99
Figura 65: Espectro de RMN de $^1\text{H}$ de simiarenol ( $\text{CDCl}_3$ , 14,1 T).....	101
Figura 66: Ampliação do espectro de RMN de $^1\text{H}$ de simiarenol ( $\text{CDCl}_3$ , 14,1 T). .....	101
Figura 67: Espectro de RMN de $^{13}\text{C}$ de simiarenol ( $\text{CHCl}_3$ , 14,1 T).....	102
Figura 68: Ampliação do espectro de RMN de $^{13}\text{C}$ de simiarenol ( $\text{CDCl}_3$ , 14,1 T). .....	102
Figura 69: Análise de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares SP89-1115 e IACSP95-5000 testemunha e inoculada analisadas por GC-FID.....	104
Figura 70: Gráfico de barra da área normalizada dos ácidos graxos de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS. ....	105
Figura 71: Gráfico de barra da área normalizada de hidrocarbonetos de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS. ....	106
Figura 72: Gráfico de barra da área normalizada do álcool de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS. ....	107

## **LISTA DE FIGURAS**

---

<b>Figura 73: Gráfico de barra da área normalizada do alquilresorcinol de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS. ....</b>	<b>108</b>
<b>Figura 74: Gráfico de barra da área de esteroides de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS.....</b>	<b>108</b>
<b>Figura 75: Gráfico de barra da área de compostos com propostas de identificação de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisados em GC-MS.....</b>	<b>109</b>
<b>Figura 76: Gráfico de barra da média da área normalizada de extrato hexânico (TMS) de folhas de cana-de-açúcar do cultivar SP89-1115 (a) testemunha e (b) inoculada analisados por GC-FID. ....</b>	<b>110</b>
<b>Figura 77: Gráfico de barra da média da área normalizada de extrato hexânico (TMS) de folhas de cana-de-açúcar do cultivar IACSP95-5000 (a) testemunha e (b) inoculada analisados por GC-FID. ....</b>	<b>111</b>

## **LISTA DE TABELAS**

---

<b>Tabela 1: Siglas de algumas Instituições responsáveis pelo cruzamento e desenvolvimento de cultivares de cana-de-açúcar do Brasil.....</b>	<b>19</b>
<b>Tabela 2: Variedades de cana-de-açúcar com resistência diferenciada à ferrugem.....</b>	<b>38</b>
<b>Tabela 3: Proposta de identificação dos constituintes da cera epicuticular (TMS) de folhas de cana-de-açúcar por comparação do IR das análises de GC-MS e GC-FID. Espectros de massas disponíveis no anexo 3, colocados em ordem crescente de ordem retenção.....</b>	<b>58</b>
<b>Tabela 4: Fragmentos de massas característicos das principais classes de compostos identificados em cera epicuticular de folhas de cana-de-açúcar....</b>	<b>63</b>
<b>Tabela 5: Proposta de identificação dos constituintes do extrato hexânico (TMS) de folhas de cana-de-açúcar por comparação do IR das análises de GC-MS e GC-FID. Espectros de massas disponíveis no anexo 4, colocados em ordem crescente de retenção. Tabela contento área de cada constituintes nos cultivares estudados esta disponível no anexo 2. ....</b>	<b>87</b>
<b>Tabela 6: Massas das frações de cera epicuticular analisadas por CCDP. ....</b>	<b>93</b>
<b>Tabela 7: Dados de RMN de <sup>1</sup>H e <sup>13</sup>C (CDCl<sub>3</sub>, 7,0 T) de alquilresorcinol.....</b>	<b>98</b>
<b>Tabela 8: Dados de RMN de <sup>1</sup>H e <sup>13</sup>C (CDCl<sub>3</sub>, 14,1 T) de simiarenol.....</b>	<b>100</b>

## **LISTA DE ABREVIATURAS E SIGLAS**

---

$^{13}\text{C}$  NMR - ressonância magnética nuclear de carbono  
 $^1\text{H}$  NMR - ressonância magnética nuclear de hidrogênio  
APCI - Ionização Química a Pressão Atmosférica  
AR - alquilresorcionol  
BOD - demanda bioquímica de oxigênio  
CCDC - cromatografia em camada delgada comparativa  
CCDP - cromatografia em camada delgada preparativa  
 $\text{CDCl}_3$  – clorofórmio deuterado  
FID - detector de ionização em chama  
GC - cromatógrafo a gás  
GMD - Golm Metabolome Database  
IR - índice de retenção  
 $m/z$  - razão massa/carga  
MS - espectrometria massa  
MSTFA - N-metil-N-(trimetilsilil) trifluoroacetamida  
NIST - Instituto nacional de normas e tecnologia  
PC - componente principal  
PCA - análise da componente principal  
TMS - trimetilsililano  
tR - tempo de retenção



## SUMÁRIO

---

<b>1</b>	<b>Introdução .....</b>	<b>18</b>
1.1	A cana-de-açúcar .....	18
1.2	Importância econômica da cana-de-açúcar .....	19
1.3	Doenças da Cana-de-açúcar .....	21
1.3.1	Ferrugem alaranjada .....	22
1.3.2	Influência do clima .....	25
1.3.3	Controle .....	25
1.4	Interação hospedeiro - patógeno .....	26
1.5	Defesa das plantas aos patógenos .....	29
1.6	Análises dos metabólitos apolares .....	30
1.6.1	Análises do extrato hexânico .....	30
1.6.2	Cera epicuticular - superfície foliar .....	30
1.6.3	Composição química da cana-de-açúcar .....	33
<b>2</b>	<b>Objetivos .....</b>	<b>37</b>
<b>3</b>	<b>PROCEDIMENTO EXPERIMENTAL .....</b>	<b>38</b>
3.1	Material vegetal .....	38
3.2	Experimento de cultivo com inoculação de ferrugem alaranjada .....	39
3.3	Preparo de amostra .....	40
3.3.1	Extração .....	40
3.3.2	Tratamentos dos extratos - Reação de derivação (sililação) .....	41
3.4	Análises Cromatográficas .....	43
3.4.1	Análises GC-FID .....	43
3.4.2	Análises GC-MS .....	44
3.4.3	Tratamento e análise de dados .....	44
3.4.4	Análises quimiométricas .....	45
3.5	Fracionamentos da cera epicuticular .....	46
3.6	Análises das frações da cera epicuticular .....	46
3.6.1	Análises Cromatográficas .....	46

## **SUMÁRIO**

---

3.6.2	Análises Espectrométricas.....	46
3.7	Identificação .....	47
4	Resultados e discussão .....	48
4.1	Análises do perfis cromatográfico de cera epicuticular de folhas de cana-de-açúcar.....	48
4.1.1	Identificação dos constituintes apolares da cera epicuticular por índice de retenção (IR) e espectrometria de massas (EM).....	53
4.1.2	Dificuldades encontradas nas análises por GC-MS e GC-FID.....	64
4.1.3	Comparação de alguns cultivares de cana-de-açúcar em relação composição da cera epicuticular de folhas.....	68
4.2	Análises qualitativas do extrato hexânico de folhas de cana-de-açúcar.....	75
4.2.1	Identificação dos constituintes apolares do extrato hexânico por índice de retenção (IR) e espectrometria de massas (EM).....	85
4.2.2	Comparação de alguns cultivares de cana-de-açúcar em relação composição do extrato hexânico de folhas. ....	88
4.2.3	Classificação dos cultivares estudados por PCA em função da composição química do extrato hexânico.....	92
4.3	Fracionamento cera epicuticular por CCD preparativa e análises da frações por GC-MS, MS-APCI e RMN. ....	92
4.4	Análises de metabolitos apolares em folhas de cana-de-açúcar inoculadas com ferrugem alaranjada.....	103
5	Conclusão .....	112

### 1 Introdução

#### 1.1 A cana-de-açúcar

Canas-de-açúcar (*Saccharum* spp.) são gramíneas híbridas derivadas de *Saccharum officinarum* (cana-nobre), *S. sinense* (cana chinesa), *S. barberi* (cana indiana) e *S. spontaneum* (espécie selvagem), pertencentes à família Gramineae (Poaceae) (ARCENEUX, 1968; ROACH, 1972; DANIELS; ROACH; DON, 1987).

A sua origem é relatada por diversas fontes controversas. Para alguns autores a origem da cana-de-açúcar data de 10.000 anos a.C., nas regiões de Papua Nova Guiné, Oceania e Polinésia, onde se expandiu. Outras pesquisas indicam que é procedente do continente Asiático, incluindo Índia, Indonésia e Filipinas, além do Norte do continente Africano (D'AGOSTINI, 2010).

A palavra que originou o termo açúcar vem do sânscrito “sarkar” que significa grão de areia. No leste da Índia, o açúcar era chamado “shekar”. Os povos árabes o denominavam “al zucar”, que se transformou no espanhol “azucar” e no português “açúcar”. Na França, o termo usado é “sucre” e na Alemanha “zucker”, passando para o inglês “sugar” (D'AGOSTINI, 2010).

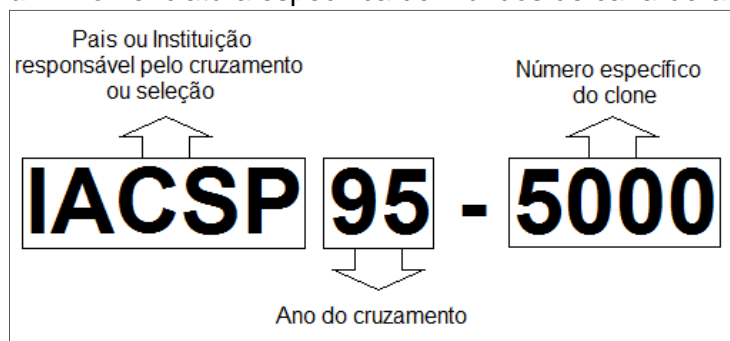
A introdução da cana-de-açúcar nas Américas ocorreu por volta de 1493, quando colmos de cana-de-açúcar foram levados para a atual República Dominicana e imediações, na segunda viagem de Cristovão Colombo ao Novo Mundo. Alguns anos mais tarde (1532) foi introduzida no Brasil, em São Vicente-SP, por Martim Afonso de Souza em suas primeiras viagens ao Brasil (FIGUEIREDO, 2008).

Variedades modernas de cana-de-açúcar são derivadas principalmente de cruzamento interespecífico entre a espécie nobre *S. officinarum* e a espécie selvagem *S. spontaneum*. O melhoramento genético da espécie teve início antes de 1950, com o desenvolvimento de diversas cultivares a partir do cruzamento dessas espécies, com o objetivo de obter-se variedades com características agronômicas melhoradas, incluindo resistência a doenças. Como resultado, as variedades atuais de cana possuem um genoma interespecífico complexo, com o número de cromossomos variando de 100 a 130 (HOARAU et al., 2001). Esta complexidade genômica juntamente com a natureza multi-alélica e multigênica da maioria das variedades agronômicas torna o melhoramento da cana-de-açúcar uma tarefa muito difícil (CASU et al., 2004).

## INTRODUÇÃO

Os híbridos de cana-de-açúcar atualmente cultivados no Brasil recebem uma nomenclatura específica, que informa a instituição responsável pelo cruzamento ou seleção, ano do cruzamento e o número específico do clone (**Figura 1 e Tabela 1**).

**Figura 1:** Nomenclatura específica de híbridos de cana-de-açúcar.



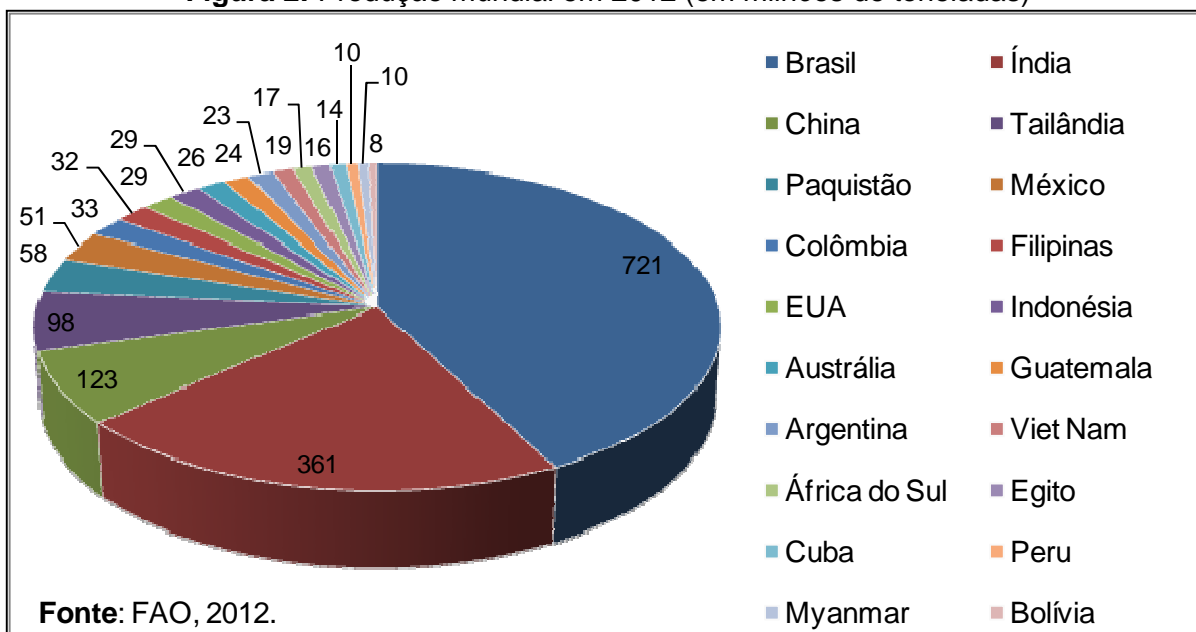
**Tabela 1:** Siglas de algumas Instituições responsáveis pelo cruzamento e desenvolvimento de cultivares de cana-de-açúcar do Brasil.

CB	Campos
IAC	Instituto Agrônomo de Campinas
RB	República Federativa do Brasil (RIDESA)
SP	São Paulo (Copersucar)
CTC	Centro de Tecnologia Canavieira
PO	Pedro Ometto (Usina da Barra)
PB	Pernambuco

### 1.2 Importância econômica da cana-de-açúcar

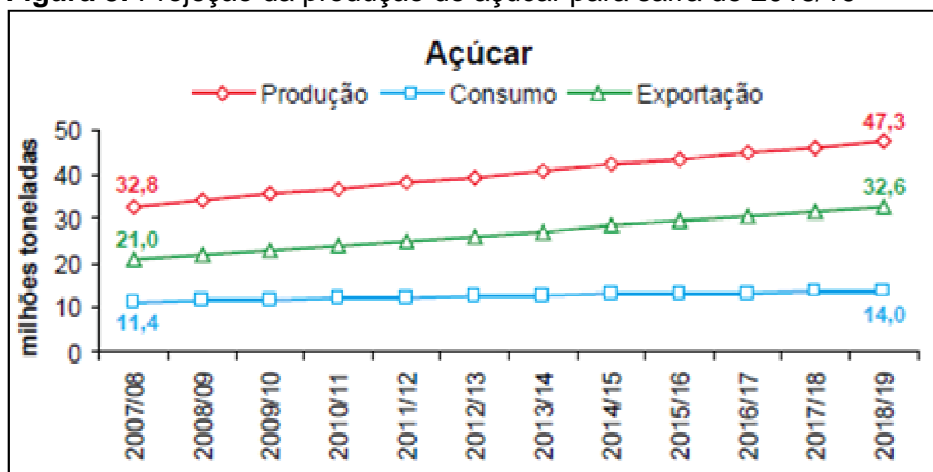
O Brasil é o líder mundial na produção de cana-de-açúcar, com cerca de 9 milhões de hectares plantados, seguido pela Índia, China, Paquistão e Tailândia (**Figura 2**). A extensa área territorial brasileira facilita a produção contínua de cana-de-açúcar durante todo o ano no país, principalmente nas regiões Sudeste, Centro-Oeste, Sul e Nordeste (UNICA, 2012).

**Figura 2:** Produção mundial em 2012 (em milhões de toneladas)



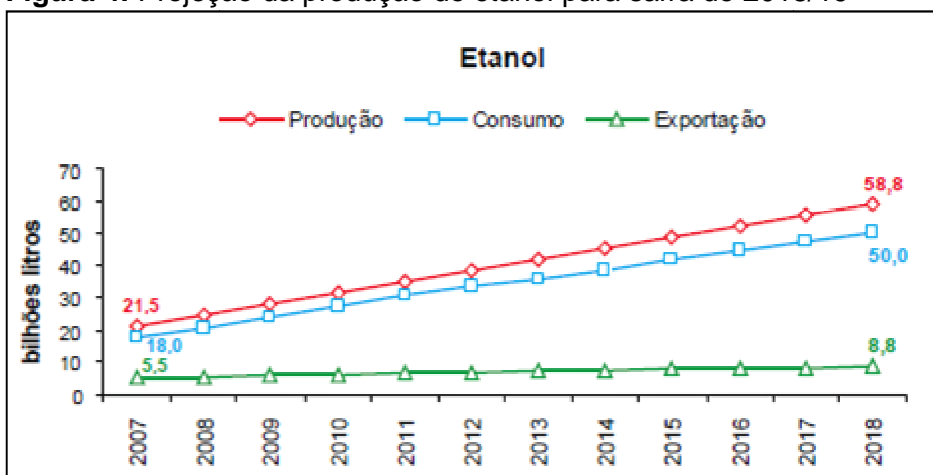
O Brasil também é o primeiro do mundo na produção de açúcar e o segundo de na produção de etanol (UNICA, 2012), e conquista cada vez mais o mercado externo com o uso do biocombustível como alternativa energética. Responsável por mais da metade do açúcar comercializado no mundo, a projeção para a safra de 2018/19 indica uma taxa de aumento de 3,25%, o que corresponde a um acréscimo de 14,6 milhões de toneladas em relação ao período de 2007/2008 (**Figura 3**) (BRASIL, 2009). Além disso, a projeção para a produção de etanol a partir da cana-de-açúcar para 2019 será de 58,8 bilhões de litros (**Figura 4**), dos quais 50 bilhões de litros são projetados para consumo interno e 8,8 bilhões de litros para exportação (BRASIL, 2009).

Figura 3: Projeção da produção de açúcar para safra de 2018/19



Fonte: BRASIL, 2009.

Figura 4: Projeção da produção de etanol para safra de 2018/19



Fonte: BRASIL, 2009

### 1.3 Doenças da Cana-de-açúcar

Um dos aspectos importantes a serem considerados sobre a produção da cana-de-açúcar é a ocorrência de doenças, bem como a severidade das mesmas, capazes de trazer prejuízo à biodiversidade e a economia do país. Das doenças atualmente mais importantes, destacam-se a doença de Fiji, amarelinho e mosaico (vírus); escaldadura e raquitismo (bactérias); carvão, ferrugem marrom e ferrugem alaranjada (fungos). Destas, a cana-de-açúcar brasileira vem sofrendo com a ocorrência de ferrugem alaranjada, que tem elevado potencial destrutivo (FERRARI et al., 2010; CARVALHO; FURTADO, 2013).

### 1.3.1 Ferrugem alaranjada

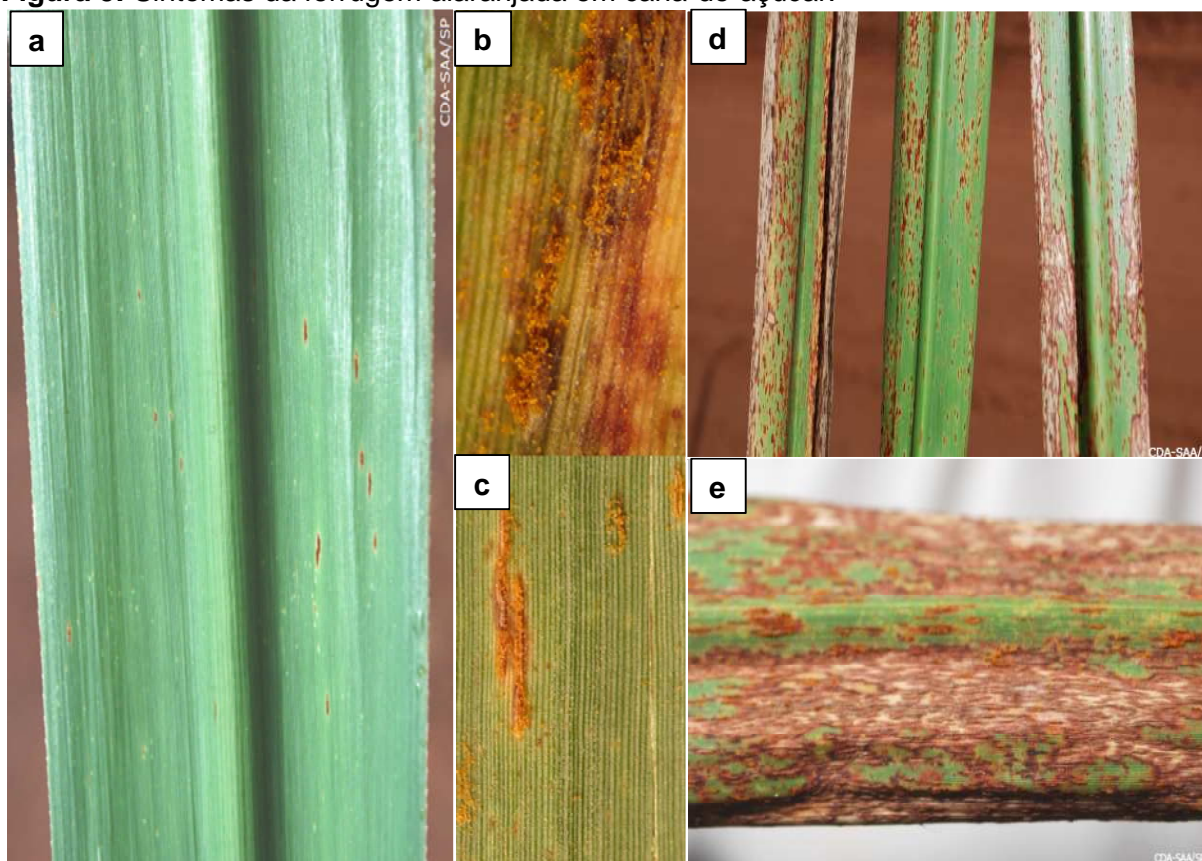
A ferrugem alaranjada é causada pelo fungo *Puccinia kuehnii* pertence à ordem Uredinales, família Pucciniaceae e ao gênero *Puccinia*. Esse é um biotrófico (somente coloniza em plantas vivas), com baixa gama de hospedeiros que ataca principalmente as plantas do gênero *Saccharum* (*S. arundinaceum*, *S. nargenga*, *S. officinarum*, *S.spontaneum*, *S. robustum*, *S. munja*, *S. edule* e *S. bengalense*, além de *Sclerostachya fusca*) (FERRARI et al., 2010; SÃO PAULO, 2010).

A ferrugem alaranjada é disseminada pelo ar, podendo alcançar longas distâncias. Além disso, os esporos dos fungos também podem ser dispersos pelo homem através das roupas, calçados e transporte de material vegetal (FERRARI et al., 2010).

Os sintomas da doença são pequenas manchas amareladas nas folhas jovens, que formam as urédias (pústulas) (**Figura 5a**). As urédias são hipófilas (parte inferior da folha ou abaxial) e às vezes anfígenas com até 4 mm e coloração laranja a castanho avermelhado (**Figura 5b e 5c**). Além disso, as pústulas podem ocorrer distribuídas por toda a superfície da folha levando a necrose (**Figuras 5d e 5e**) (FERRARI et al., 2010; SÃO PAULO, 2010).



**Figura 5:** Sintomas da ferrugem alaranjada em cana-de-açúcar.



**Legenda:** (a): Primeiros sintomas da ferrugem alaranjada, (b e c): Urédias de *Puccinia kuehnii* observadas em folhas de cana-de-açúcar, (d): Pústulas e necrose, (e): Coalescência das pústulas e necrose.

### 1.3.1.1 Relatos de contaminação da ferrugem alaranjada

A primeira descrição da ferrugem alaranjada da cana-de-açúcar foi datada em 1880, e a primeira epidemia notificada na Austrália, em 2000. A variedade mais plantada, Q124, representava 45% da área plantada na Austrália, ocasionando prejuízos da ordem de 210 milhões de dólares australiano. Entre 2007 e 2009, a doença foi relatada na Flórida, Costa Rica, Guatemala, Nicarágua, Panamá e México. No Brasil, os primeiros relatos da doença ocorreram em dezembro de 2009, no município de Araraquara, interior do estado de São Paulo. No ano seguinte, (2010), a ferrugem alaranjada foi detectada na região central do estado de São Paulo, e nos estados do Paraná, Mato Grosso do Sul, Espírito Santo e Minas Gerais, sendo relatadas nos estados de Pernambuco e Rio Grande do Norte no ano de 2012 (FERRARI et al., 2010; SÃO PAULO, 2010; CHAVES et al., 2013). Esses dados, confirmam que a ferrugem alaranjada está se espalhando rapidamente nos canaviais brasileiros. O Diário Oficial da União publicou, no dia 19 de dezembro de



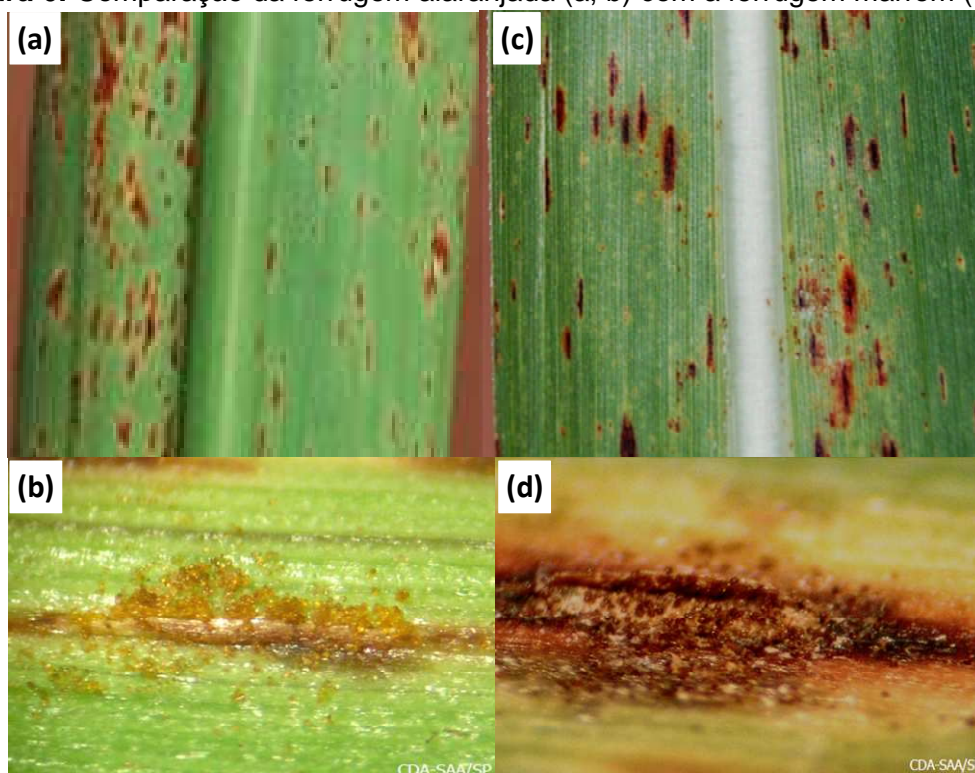
2013 uma Instrução Normativa do Ministério da Agricultura atualizando a lista de pragas quarentenárias, onde a Instrução Normativa excluiu dessa relação o fungo *Puccinia kuehni*, mudando seu estatus de praga quarentenária para doença importante (BRASIL, 2013).

### 1.3.1.2 Ferrugem alaranjada x Ferrugem marrom

Em campo, é normal confundir ferrugem alaranjada (*P. kuehni*) com ferrugem marrom (*Puccinia melanocephalla*). Na ferrugem marrom as pústulas são maiores e mais alongadas, ocorrendo em maior número do centro para as pontas das folhas. Além disso, no início da doença a coloração das folhas varia de laranja a castanho-avermelhado, alterando sua coloração para marrom-escuro, com o desenvolvimento da doença (**Figura 6**). Diferentemente, na ferrugem alaranjada os sintomas nas folhas são caracterizados por pequenas pontuações alongadas, com halo amarelo no início da doença que evoluem para a formação de pústulas alaranjadas. Em geral, essas pústulas ocorrem agrupadas e próximas ao ponto de inserção da folha ao colmo, porém, podem ocorrer distribuídas por toda superfície das folhas (FERRARI et al., 2010; SÃO PAULO, 2010).

As ferrugens, como são nomeadas devido ao aspecto ferruginoso e às lesões alaranjadas (pústulas) que aparecem no hospedeiro atacado, são constituídas por estruturas reprodutivas do fungo que emergem do tecido vegetal doente através do rompimento da epiderme do hospedeiro. A ferrugem encontra-se entre as doenças mais destrutivas, de grande importância para algumas culturas como no caso de gramíneas, tais como, trigo, cevada, milho e cana-de-açúcar. Além disso, pode afetar culturas de café, soja, feijão, frutíferas, hortícolas e plantas ornamentais. As ferrugens atacam predominantemente as folhas, podendo também atacar outras partes do vegetal, como bainhas, colmos, ramos, frutos e órgãos florais. Os principais gêneros causadores de doenças, em frequência e importância, são: *Puccinia*, *Hemileia*, *Uromyces*, *Phakopsora* e *Melampsora* (BEDENDO, 2011).

**Figura 6:** Comparação da ferrugem alaranjada (a, b) com a ferrugem marrom (c, d).



**Legenda:** Ferrugem alaranjada: (a): pústula, (b): esporulação na pústula; Ferrugem marrom: (c): pústula, (d): esporulação na pústula.

### 1.3.2 Influência do clima

A germinação dos esporos do fungo *P. kuehni* pode ocorrer sob condições de alta umidade relativa e de temperaturas amenas a quentes. Assim, temperaturas entre 19° e 26°C e umidade relativa entre 98% e 99% são as condições ótimas para germinação dos esporos (MAGAREY et al., 2004; SÃO PAULO, 2010).

### 1.3.3 Controle

O controle da ferrugem alaranjada mais eficiente e economicamente viável é a utilização de variedades resistentes e intermediárias. O emprego de fungicidas é uma alternativa para variedades suscetíveis, mas nesse caso o custo final de produção será afetado (BEDENDO, 2011).

A avaliação do grau de resistência dos cultivares a ferrugem alaranjada é feita pela escala diagramática de Amorim et al. (1987) (**Figura 7**), sendo realizada na folha +3 (**Figura 8**). As variedades resistentes são aquelas avaliadas com notas entre 1 a 3, as intermediárias com notas entre 4 e 6 e suscetíveis com nota 7 a 9 (SÃO PAULO, 2010).

Figura 7: Escala diagramática para avaliação da severidade da ferrugem marrom.

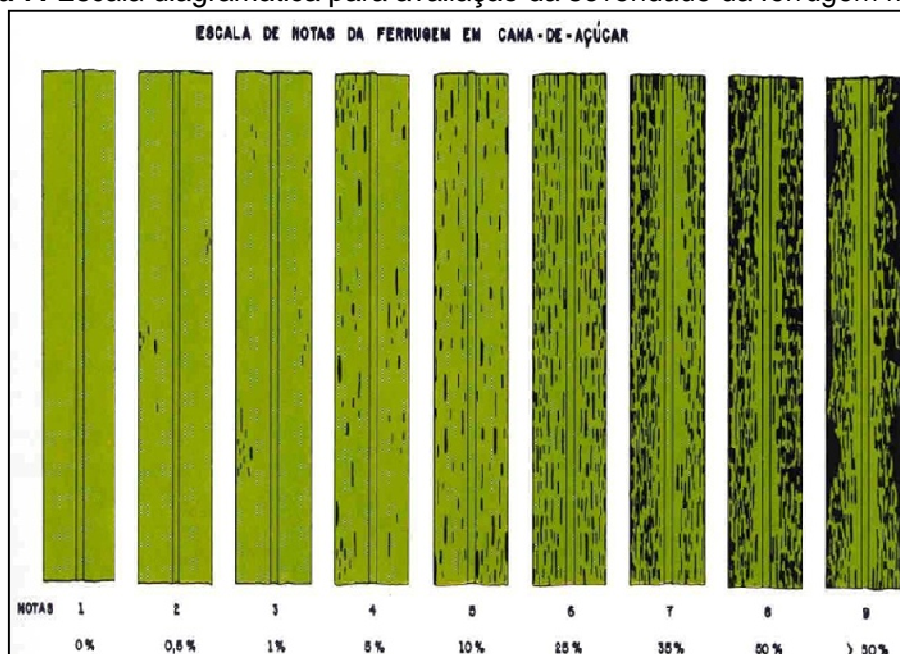
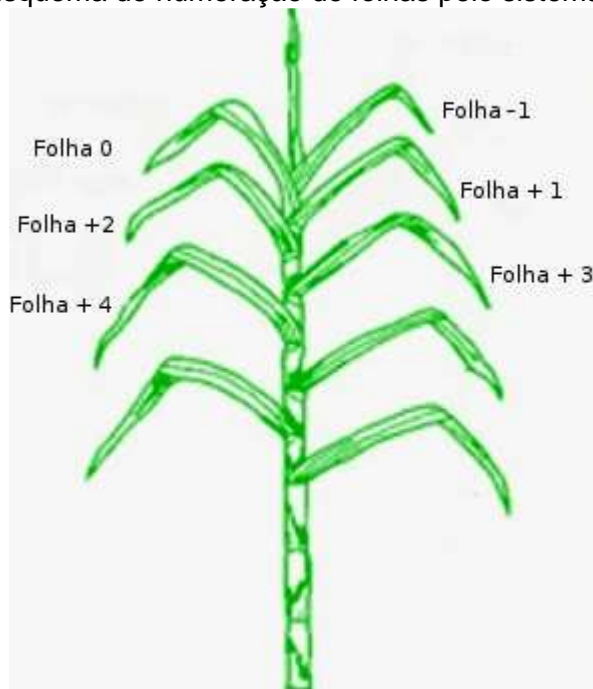


Figura 8: Esquema de numeração de folhas pelo sistema de Kuijper.



Fonte: ROSSETTO, 2011.

### 1.4 Interação hospedeiro - patógeno

Para ocorrer a doença é necessário um conjunto de fatores, tais como: o patógeno com capacidade de causar a doença (agente causal), a planta suscetível ao patógeno (hospedeiro) e ambiente favorável para o desenvolvimento do patógeno

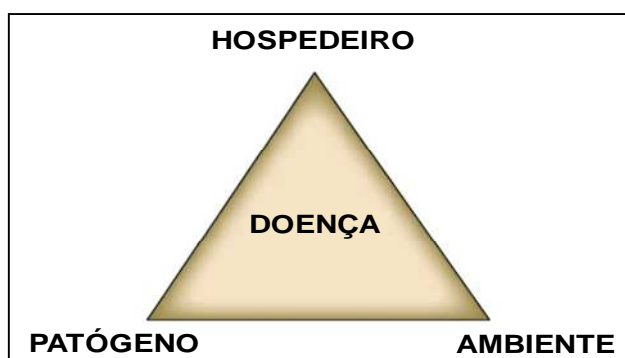
## INTRODUÇÃO

---

e da doença (AGRIOS, 2005). A interação desses fatores é representada pelo “Triângulo da Doença” (**Figura 9**).

Na planta a primeira defesa ao ataque de patógenos é a superfície onde esses patógenos tendem a se alojar. A função das barreiras de proteção são dificultar e/ou impedir a colonização do patógeno nos tecidos, sendo essas barreiras: as cutículas, os estômatos, lenticelas e células epidérmicas (AGRIOS, 2005).

**Figura 9:** Representação clássica dos fatores que interagem para a ocorrência de doenças em plantas.



Fonte: Adaptado de AGRIOS, 2005.

A penetração dos patógenos em seus hospedeiros na planta pode se dar por três vias: direta, aberturas naturais e ferimentos (**Figura 10**) (AGRIOS, 2005; AMORIM; PASCHOLATI, 2011).

A penetração direta dos patógenos no hospedeiro ocorre através da superfície intacta, assim os patógenos precisam romper as barreiras naturais que são formadas pela cutícula e epiderme na parte aérea e pela periderme em raízes e ramos lenhosos. Para penetrar diretamente pela cutícula os fungos fixam-se firmemente na superfície através do apressório e lançam no meio intracelular uma pequena hifa denominada “peg de penetração” que possui diâmetro menor que o tubo germinativo, capaz de perfurar a cutícula do hospedeiro até atingir o lúmen da célula (AGRIOS, 2005; AMORIM; PASCHOLATI, 2011).

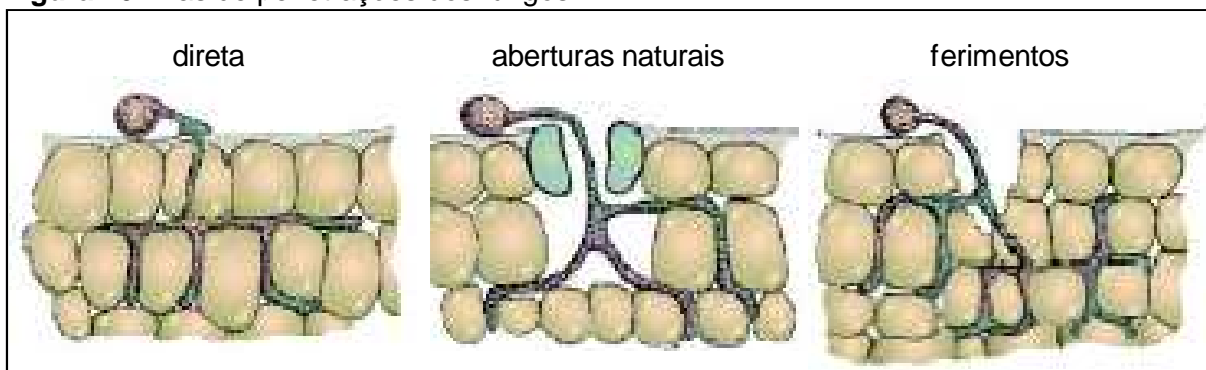
Já a penetração por aberturas naturais são as principais portas de entrada para muitos fungos, principalmente os causadores de ferrugem e de bactérias fitopatogênicas. Os principais alvos de penetração por aberturas naturais nos hospedeiros são os estômatos e hidatódios nas folhas, estigmas e nectários nas flores e lenticelas em órgãos suberificados.

## INTRODUÇÃO

---

Da mesma maneira que as aberturas naturais, os ferimentos servem como portas de entrada para bactérias, fungos, vírus, viróides e outros. Nesse caso, os ferimentos podem ocorrer por picadas de pulgões, partículas de solo, espinhos dispersos pelo vento e podas em plantas elaboradas pelo homem (AGRIOS, 2005; AMORIM; PASCHOLATI, 2011).

**Figura 10:** Vias de penetrações dos fungos.



**Fonte:** AGRIOS, 2005

A ferrugem é causada por fungos que são parasitas obrigatórios, não sendo saprófitos eles necessitam do hospedeiro para o crescimento e reprodução. No entanto, eles sobrevivem como esporos na ausência do hospedeiro. Nesse caso, os teliósporos (esporo) são adaptados para sobreviver fora do hospedeiro vivo, podendo chegar a vários meses em condições de campo (MASSOLA; KRUGNER, 2011; BEDENDO, 2011).

Os agentes causadores de ferrugens produzem vários tipos de estruturas de frutificação, cada uma correspondendo a uma fase do ciclo patogênico. Nesse contexto, o ciclo envolvido em *Puccinales* geralmente é complexo, podendo ter até cinco estágios diferentes denominados de autoécia e heteroécias, com um e dois hospedeiros, respectivamente. Quando o ciclo da ferrugem compreende cinco fases é chamada de macrocíclica ou de ciclo longo, enquanto aquelas que não apresentam as cinco fases são denominadas de microcíclica ou de ciclo curto (MASSOLA; KRUGNER, 2011; BEDENDO, 2011).

As cinco fases compreendem a fase 0: espermogônia, fase I: ecial, fase II: urédinial, fase III: télial e fase IV: basídial, de maneira que a formação dos esporos segue a seguinte ordem: espermogônio, écio, uredínio, télcio e basídio, respectivamente. Contudo, apenas o estado anamorfo é conhecido no caso do fungo

*P. kuehnii* e, conseqüentemente, o patógeno tem ciclo assexual curto (MASSOLA; KRUGNER, 2011; BEDENDO, 2011).

### 1.5 Defesa das plantas aos patógenos

As plantas podem “defender-se” dos patógenos de forma passiva ou ativa. Os mecanismos de defesa são divididos em duas categorias: pré-formados (passivos e constituídos) e pós-formados (ativos e induzíveis). Os mecanismos pré-formados são aqueles presentes na planta antes do contato com o patógeno, enquanto que os mecanismos pós-formados estão presentes em baixos níveis ou ausentes antes da infecção, sendo ativados ou produzidos após o contato com o patógeno (AGRIOS, 2005; PASCHOLATI, 2011).

Em ambos os mecanismos, pré- e pós-formados, os fatores envolvidos na resistência podem ser subdivididos em estruturais e bioquímicos (AGRIOS, 2005; PASCHOLATI, 2011).

Os fatores estruturais pré-formados da planta são: cutícula, tricomas, estômatos e paredes celulares espessas que atuam como barreiras físicas, ou seja, impedem a entrada do patógeno e a colonização dos tecidos. Já os fatores estruturais pós-formados são decorrentes de processos de defesa contra invasores que conseguiram o acesso ao interior da planta, nesse tipo de processo de defesa ocorre à formação de novas barreiras estruturais nos tecidos (AGRIOS, 2005; PASCHOLATI, 2011).

Esses fatores estruturais pós-formados também podem ser agrupados em estruturas de defesa celular e defesa histológica. Os mecanismos envolvidos nas estruturas de defesa celular ocorrem em células individuais sob ataque do patógeno. Diferentemente, os mecanismos que atuam nas estruturas de defesa histológica envolvem tecidos de planta que normalmente encontram-se distante do sítio de penetração (AGRIOS, 2005; PASCHOLATI, 2011).

Os fatores bioquímicos são dirigidos por reações bioquímicas que ocorrem nas células dos hospedeiros, as quais são responsáveis por produzir substâncias tóxicas, e conseqüentemente, gerar condições que impeça o desenvolvimento do patógeno no interior da planta.

Os fatores bioquímicos pré-formados são provenientes de substâncias presentes nos tecidos sadios da planta, incluindo compostos fenólicos, saponinas,



glicosídeos cianogênicos, glicosídeos sulfurados, ácidos hidroxicarboxílicos, proteínas, peptídeos antimicrobianos e as fototoxinas (AGRIOS, 2005; PASCHOLATI, 2011).

No caso dos fatores bioquímicos pós-formados, as substâncias estão presentes em baixa concentração, ou até mesmo ausentes no período que antecede a ação do patógeno, sendo ativadas com o ataque do mesmo. Exemplo disso são as fitoalexinas, compostos antimicrobianos que são biossintetizadas pelas plantas em resposta à infecção, se acumulando nas células vegetais (AGRIOS, 2005; PASCHOLATI, 2011).

### 1.6 Análises dos metabólitos apolares

#### 1.6.1 Análises do extrato hexânico

A lipidômica é definida como a caracterização e quantificação dos lípidos nas células/organismos. Os lipídios são grupos numerosos de moléculas que ocorrem naturalmente, incluindo as gorduras, ceras, esteróis, monoglicerídeos, diglicerídeos, fosfolípidos e vitaminas solúveis em gordura (tais como, vitaminas A, D, E e K). As principais funções biológicas dos lipídios incluem o armazenamento de energia, como componentes estruturais das membranas celulares, e importantes moléculas sinalizadoras. Os lipídios podem ser definidos como hidrofóbicos ou pequenas moléculas anfipáticas que podem ser divididos nas seguintes classes: ácidos graxos, glicerolipídeos (triglicerídeos), glicerofosfolipídeos, esfingolipídeos, sacarolipídeos, policetídeos e esteróides (BOU KHALIL, 2010).

Análise por espectrometria massa (MS), ressonância magnética nuclear (NMR) e espectroscopia de fluorescência estão sendo utilizadas em lipidômica com objetivo de identificar, quantificar e compreender a relação estrutural e funcional dos lípidos nos sistemas biológicos (WENK, 2010).

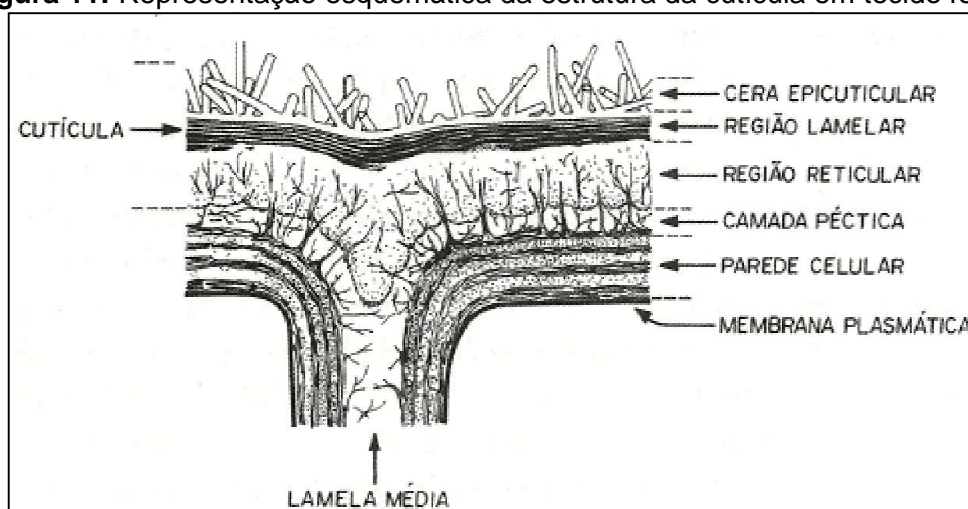
#### 1.6.2 Cera epicuticular - superfície foliar

As superfícies das plantas superiores são cobertas por uma membrana lipídica extracelular, a qual é sintetizada pelas células epidérmicas, e denominada de cutícula ou cera cuticular (**Figura 11**). Em geral, as células epidérmicas podem apresentar a cutina e ceras. A cutina pode estar impregnada na parede celular ou formando uma camada na superfície externa da célula, sua composição é

## INTRODUÇÃO

basicamente de polímeros de ácidos graxos di- e trihidroxilados. Já as ceras, encontram-se na superfície externa da cutícula, denominada de cera epicuticular, ou dentro da matriz da cutícula na forma de partículas, a qual é denominada de cera intracuticular (JETTER, 2000; EGLINTON; HAMILTON, 1967).

**Figura 11:** Representação esquemática da estrutura da cutícula em tecido foliar.



Fonte: PASCHOLATI, 2011

A cera se destaca como a principal barreira protetora contra perdas de água por transpiração excessiva, ação de patógenos, radiações solares, contaminantes e produtos químicos (HEREDIA et al., 1998). Além disso, as ceras influenciam a molhabilidade, o comportamento de auto-limpeza e a reflexão da luz na interface da cutícula (BARGEL et al., 2006). A quantidade e a composição da cera epicuticular podem variar entre espécies, cultivares e até mesmo dentro da mesma população de uma espécie, bem como a partir da fenologia da planta e condições climáticas (PURCELL et al., 2005).

### 1.6.2.1 Composição química da cera epicuticular

A cera epicuticular é uma mistura de vários compostos, incluindo os ácidos graxos de cadeias longas, aldeídos, alcoóis primários e secundários, cetonas, ésteres e alcanos (JETTER, 2000; EGLINTON; HAMILTON, 1967).

Uma característica da composição química da cera epicuticular é a sua variabilidade intraspecífica, por exemplo, a concentração de alcanos na cera epicuticular varia de acordo com a espécie (EGLINTON; HAMILTON, 1967).

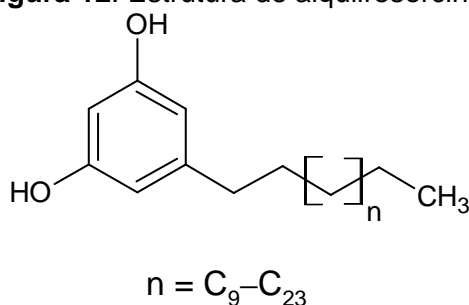


No entanto, a composição química da cera epicuticular é parâmetro importante em diversos estudos cujo objetivo é avaliar as respostas dos indivíduos frente a perturbações bióticas ou abióticas. Nesse contexto, em um trabalho publicado por Oliveira et al. (2003) foi avaliada a cera epicuticular de algumas espécies nativas das regiões da caatinga e do cerrado, com vistas a determinar a resistência da planta em função da perda de água. Nesse trabalho foi constatado que espécies provenientes da caatinga são mais eficientes em relação às espécies do cerrado em relação à essa função, visto que as espécies da caatinga apresentam elevada proporção de hidrocarbonetos. Já nas espécies do cerrado, os triterpenoides são preponderantes, os quais podem atuar na proteção frente à ação de patógenos (OLIVEIRA; MEIRELLES; SALATINO, 2003).

### 1.6.2.2 Alquilresorcionóis em cera epicuticular

Os alquilresorcionóis (AR) são lipídios fenólicos derivados do resorcinol com cadeia alquílica longa, com 13 a 27 átomos de carbono e inseridas na posição 5 do anel fenólico (**Figura 12**). Numerosos estudos foram realizados com diversas famílias de plantas superiores e demonstraram a ocorrência de ARs em Anacardiaceae, Ginkgoaceae, Proteaceae, Myrsinaceae, Primulaceae, Myristicaceae, Iridaceae, Compositae, Leguminosae e Gramineae (KOZUBEK, 1998; MADRIGAL, 1977).

**Figura 12:** Estrutura de alquilresorcinol.



Os ARs compreendem uma classe de lipídios fenólicos com crescente interesse, visto que diversos estudos realizados com AR demonstraram que estes possuem uma ampla faixa de atividades biológicas, incluindo antimicrobiana, antibacteriana, antifúngica e antitumoral (KOZUBEK, 1998; MADRIGAL, 1977).

Nessa óptica de estudos lipidômicos, os AR presentes na cera epicuticular da semente de cevada foram responsáveis pela resistência contra ação dos fungos

patogênicos *Aspergillus niger* e *Penicillium crysogenum* (GARCÍA, 1997). Além disso, outros estudos demonstraram que o 5-heptadecenil resorcinol e o 5-pentadecil resorcinol, presentes na casca de manga, são responsáveis pela resistência dos frutos de manga frente às infecções causadas pelos fungos *Alternaria alternata* e *Colletotrichum gloeosporioides* (KNÖDLER et al. 2007; HASSAN et al. 2007; DROBY et al. 1986).

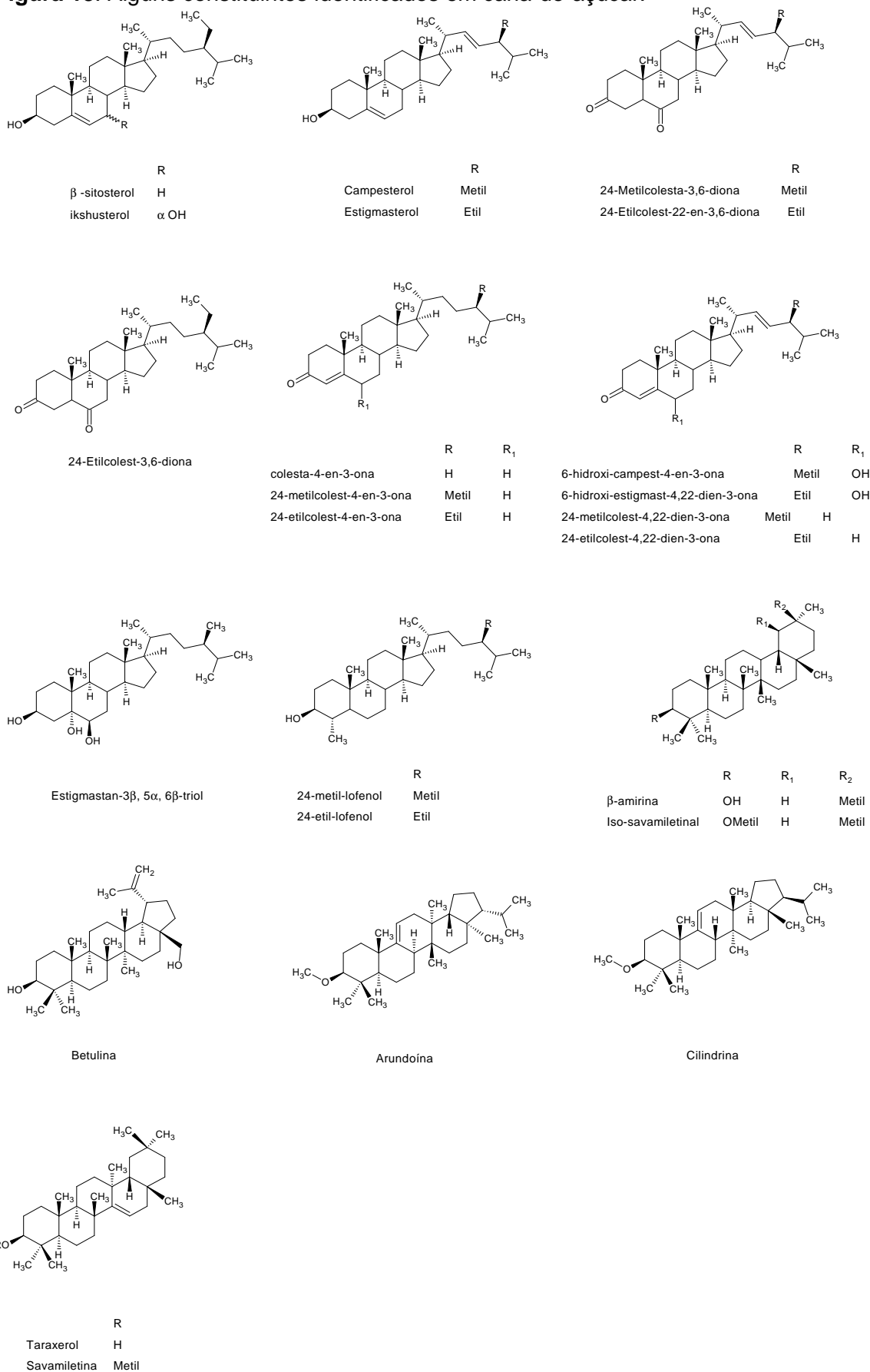
### 1.6.3 Composição química da cana-de-açúcar

Os primeiros relatos de constituintes químicos surgiram no ano de 1930, publicados por Burr e colaboradores, que apontaram a ocorrência de pirogalol, ácido protocatêquico e vanilina na fração lignínica; vitamina A, inositol, fitina e os ácidos aconítico, cítrico, fumárico, glicólico, málico, mesacônico, oxálico, succínico, siríngico e ascórbico na garapa; tiamina, riboflavina, ácido pantotênico, niacina e biotina nos colmos; ácido fólico no melaço; piridoxina e ácido ascórbico nas folhas (BURR et al., 1957).

Em revisão recente sobre esse tema (CAVALHEIRO et al., 2012), são listados estudos que identificaram inúmeros metabólitos em cana-de-açúcar. Na cera dos colmos foram encontrados álcool miricílico e hidrocarbonetos, enquanto nos extratos da cana foram obtidos ácidos palmítico e linoleico, estigmasterol, sitostetol, glicerol, clorofila e caroteno. Os primeiros triterpenos relatados nas folhas de *Sacharam officinarum* L. foram a arundoína (fernenol metil éter) e taraxerol metil éter (savamiletina). Posteriormente, foram caracterizados  $\beta$ -sitosterol, estigmasterol e os compostos minoritários taraxerol,  $\beta$ -amirina, betulina,  $\beta$ -amirina metil éter (iso-savamiletina), fernenol, cilindrina, 24-metil-lofenol, 24-etil-lofenol, estigmasten-5-en-3  $\beta$ -diol (ikshusterol), estigmasten-5-en-3 $\beta$ -diol (epi-ikshusterol) e estigmastan-3 $\beta$ , 5 $\alpha$ , 6 $\beta$ -triol (DESHMANE; DEV, 1971). Além disso, triterpenos e esteroides foram isolados da torta de filtro da cana-de-açúcar, incluindo campesterol;  $\beta$ -sitosterol; estigmasterol; 24-metilcolesta-3,6-diona; 24-etilcolesta-22-3,6-diona; 24-etilcolest-22-en-3,6-diona; 6-hidroxi-campest-4-en-3-ona; 6-hidroxiestigmast-4,22-dien-3-ona; colesta-4-en-3-ona; 24-metilcolest-4-en-3-ona; 24-metilcolest-4,22-dien-3-ona; 24-etilcolest-4-en-3-ona e 24-etilcolesta-4,22-dien-3-ona (GEORGES et al., 2006; CAVALHEIRO et al., 2012).

# INTRODUÇÃO

Figura 13: Alguns constituintes identificados em cana-de-açúcar.



## INTRODUÇÃO

---

Feng (2014) avaliou os triterpenoides, flavonoides, compostos fenólicos e fitoesteroides de diferentes partes de duas variedades de cana-de-açúcar (casca, medula, nó e ponta), sendo uma variedade de casca vermelha e a outra verde. Feng et al. concluíram que na casca da cana se encontram os maiores teores de compostos fenólicos, flavonoides e fitoesteroides. Na medula foram encontrados os maiores teores de triterpenoides. Comparando a cana-de-açúcar de casca vermelha e verde, concluiu que a cana com casca vermelha apresentou maior atividade antioxidante do que a cana de casca verde devido os maiores teores de flavonoides e compostos fenólicos. O estigmasterol e  $\beta$ -sitosterol foram os principais fitoesteroides com variações do conteúdo entre as diferentes partes da cana-de-açúcar.

A cana-de-açúcar pode trazer vários benefícios a saúde, devidos a sua riqueza em componentes ativos, incluindo triterpenoides, flavonoides, compostos fenólicos e fitoesteroides. Ademais, constitui uma cultura com alto potencial econômico para o Brasil e o mundo. No entanto, está sujeita ao ataque de diversas doenças, tais como aquelas associadas à proliferação de vírus, bactérias e fungos. A ferrugem alaranjada, doença causada pelo fungo *Puccinia kuehnii*, é responsável por comprometer o desenvolvimento das variedades, consequentemente, afetando a biodiversidade e ocasionando danos econômicos, tais como, diminuir a capacidade fotossintética acarretando na redução da produção de sacarose. Com a finalidade de contornar esse problema, estudos realizados com ênfase no melhoramento genético foram conduzidos com a finalidade de desenvolver variedades resistentes ao patógeno *P. kuehnii*. Apesar disso, estudos com vistas a estabelecer uma correlação entre a composição micromolecular e a resistência hospedeiro/patógeno não foram descritos. Adicionalmente, análises metabolômicas constituem-se em uma ferramenta robusta para a investigação holística da composição micromolecular de variedades de cana, uma vez que permitem obter uma extensa visão de perfil metabólico do vegetal e sua rede regulatória. Além disso, essas abordagens metabolômicas podem subsidiar a identificação de fatores que possam ser manipulados com intuito de aumentar a produtividade de compostos energéticos e também na identificação de características moleculares que possibilitem à espécie vegetal uma maior resistência a situações de estresse. Portanto, o entendimento das respostas metabólicas poderão trazer subsídios importantes para o planejamento

## **INTRODUÇÃO**

---

mais específico e manejo de espécies selecionadas, visando o desenvolvimento de variedades com maior potencial econômico.

### 2 Objetivos

Considerando o exposto anteriormente e o reconhecimento de que a descrição detalhada da composição química micromolecular de cana-de-açúcar pode contribuir para estudos metabolômicos futuros, complementares às abordagens genômicas e proteômicas, que busquem melhorar a produtividade dessa cultivar de enorme importância econômica, estabeleceu-se alguns objetivos para esse trabalho:

1. Estabelecer/implantar um método para análise de metabólitos apolares em variedades de folhas de cana-de-açúcar;
2. Descrever a constituição química de folhas de cana-de-açúcar, no que diz respeito aos compostos lipofílicos presentes em cera epicuticular e no extrato hexânico de folhas;
3. Comparar o perfil químico da cera epicuticular e extrato hexânico de folhas de cultivares de cana-de-açúcar;
4. Avaliar eventuais alterações na composição química do extrato hexânico de folhas de dois cultivares cana-de-açúcar com resistência diferenciada em relação ao patógeno fúngico *Puccinia kuehnii* (ferrugem alaranjada), buscando identificar marcadores (indicadores) micromoleculares de resistência.

**3 PROCEDIMENTO EXPERIMENTAL****3.1 Material vegetal**

Folhas de diferentes variedades de cana-de-açúcar (**Tabela 2**) com resistência diferenciada à ferrugem alaranjada foram coletadas no Instituto Agrônomo de Campinas (IAC) - Centro de Cana – Ribeirão Preto - SP e CTC (Centro de Tecnologia Canavieira) e UFSCar (Universidade Federal São Carlos - Araras). Foram realizados experimentos nas diferentes variedades coletando amostras para análises da cera (1), análises de extrato hexânico (2), e para experimentos de inoculação e análises de extrato hexânico (3). Os experimentos foram realizados de acordo com a numeração da **tabela 2**, esses experimentos foram realizados em épocas diferentes não sendo possível a realização de todos os experimentos para as mesmas variedades.

**Tabela 2:** Variedades de cana-de-açúcar com resistência diferenciada à ferrugem alaranjada

<b>Variedades</b>			
IACSP95-5000	<b>1</b>	<b>2</b>	<b>3</b>
IACSP96-2042	<b>1</b>	-	-
IACSP95-3028	<b>1</b>	-	-
IACSP94-2094	<b>1</b>	<b>2</b>	-
IACSP96-3060	<b>1</b>	-	-
IACSP95-5094	<b>1</b>	-	-
IACSP93-3046	<b>1</b>	<b>2</b>	-
IACSP94-2101	<b>1</b>	<b>2</b>	-
IAC87-3396	<b>1</b>	-	-
RB72454	<b>1</b>	-	-
RB83-5486	<b>1</b>	-	-
RB84-5210	<b>1</b>	-	-
SP89-1115	<b>1</b>	<b>2</b>	<b>3</b>
IAC 91-5155	-	<b>2</b>	-
IAC 91-2218	-	<b>2</b>	-
IAC 91-2195	-	<b>2</b>	-
IAC 91-1099	-	<b>2</b>	-
IACSP 93-6006	-	<b>2</b>	-
pora	-	<b>2</b>	-
RB 93-1530	-	<b>2</b>	-
RB 85-5453	-	<b>2</b>	-
<i>Sacharam officinarum x S. barberi</i>	-	<b>2</b>	-
<i>Saccharum robustum</i>	-	<b>2</b>	-
<i>Saccharum officinarum x S. cheming cemis</i>	-	<b>2</b>	-

**Legenda:** **1 e 2:** Amostras coletadas no IAC, **3:** Amostras coletadas no CTC e UFSCar.

A coleta foi executada de acordo com o sistema de numeração de folhas estabelecido por Kuijper, onde apenas as folhas +1 e +2 foram utilizadas. Nesse sistema numera-se as folhas a partir do primeiro colarinho visível, considerando-a a folha +1; as folhas acima da +1 decrescem uma unidade cada (0, -1...), enquanto as folhas abaixo da +1 aumentam uma a uma (+2, +3, +4...) **Figura 8.**

### 3.2 Experimento de cultivo com inoculação de ferrugem alaranjada

Os experimentos foram realizados no Departamento de Fitopatologia e Nematologia da Escola Superior de Agricultura “Luiz de Queiroz” da Universidade de São Paulo, de Piracicaba, estado de São Paulo entre os meses de Setembro de 2011 e junho de 2012. Para tal experimento, foram utilizadas as variedades SP 89-1115 e IACSP 95-5000, consideradas, respectivamente, altamente suscetível e resistente à ferrugem alaranjada (BARBASSO et al., 2010; MOREIRA, 2012). As variedades foram cedidas pelo CTC (Centro de Tecnologia Canavieira) e UFSCar (Universidade Federal São Carlos - Araras). As gemas das variedades foram plantadas individualmente em copos plásticos descartáveis de 500 mL contendo substrato autoclavado. As mudas foram mantidas em estufa durante 40 dias e foram irrigadas sempre que necessário. Dez dias antes da inoculação foram adubadas com uma solução de sulfato de amônio (30g/L).

Para a inoculação do fungo causador da ferrugem alaranjada (*Puccinia kuehnii*), o inóculo foi obtido a partir de folhas doentes com pústulas abertas coletadas no CTC utilizando uma bomba de vácuo (Primatec Mod. 131). Os esporos foram mantidos em câmara incubadora tipo BOD (demanda bioquímica de oxigênio) para garantir maior pureza e qualidade do inóculo (MACLEAN, 1982). A coleta foi feita um dia antes da inoculação e os esporos foram mantidos em temperatura ambiente. Uma suspensão de esporos foi preparada a fim de obter uma concentração de  $10^4$  esporos por mL. As plantas foram pulverizadas com aproximadamente 4 mL dessa suspensão, com prioridade a atingir a face abaxial das folhas, essa pulverização foi feita por meio de borrifador manual de distribuição regular de gotas pequenas. A viabilidade média dos esporos utilizados como inóculo foi de 54%. A avaliação foi feita com microscópio com observações diretas nas placas 12 horas após a semeadura. As plantas foram imediatamente transferidas para câmara de orvalho após a inoculação. Nas primeiras 24 horas, as planta



inoculadas permaneceram a temperatura média de 22°C , com umidade controlada próxima a saturação por meio de um umidificador de ar (Waterclear Max) que ligava durante 15 minutos a cada 2 horas.

As plantas permaneceram durante 24 horas na câmara de orvalho, sendo transferidas para câmaras de crescimento até o encerramento dos experimentos. Metade das plantas de cada variedade foi acondicionada a 18 °C e a outra metade permaneceu a 25 °C, com a finalidade de testar o efeito da temperatura no desenvolvimento da ferrugem. As condições de luminosidade nas câmaras de crescimento foram ajustadas para manter um fotoperíodo de 12 horas de luz branca fluorescente e 12 horas de escuro.

### **3.3 Preparo de amostra**

#### **3.3.1 Extração**

##### **3.3.1.1 Análise de metabolitos apolares em folhas de cana-de-açúcar**

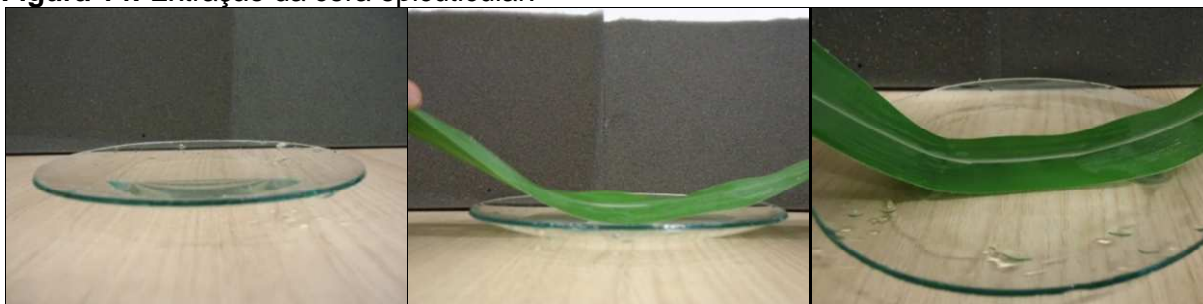
As coletas foram realizadas em 5 indivíduos diferentes (quintuplicata), a atividade enzimática foi imediatamente inibida por congelamento com nitrogênio líquido e o material vegetal armazenado em freezer -80°C. Depois de seco por liofilização (Liofilizador CHRIST ALPHA 2-4 LD Plus), o material vegetal foi triturado em moinho criogênico (Spex model 6800-115) durante 10 minutos. O procedimento de moagem consistiu de congelamento da amostra seguida por 1 ciclo com dois estágios de pulverização e resfriamento, respectivamente, para obter partículas < 60 µm. Após a moagem a amostra triturada foi armazenada em freezer -80°C.

Para a extração: 4 mg de folhas trituradas foram submetidas a extração com 4 mL de hexano (n-hexano 95% - Tédia, grau HPLC) por sonicação durante 15 minutos (Banho ultra-som Elmasonic S 60/(H)), esse procedimento foi repetido por 3 vezes (**Figura 16**).

### 3.3.1.2 Extração da cera epicuticular da superfície superior da folha de cana-de-açúcar

Para a extração da cera epicuticular, 20 cm de folhas de cana-de-açúcar recém-coletadas foram imediatamente imersas (lavadas) em 10 mL de clorofórmio (Clorofórmio - PA ACS J T Baker) durante 15 segundos, sendo o extrato clorofórmico seco a temperatura ambiente, para a extração foram coletados 5 indivíduos diferentes (**Figura 14 e 17**).

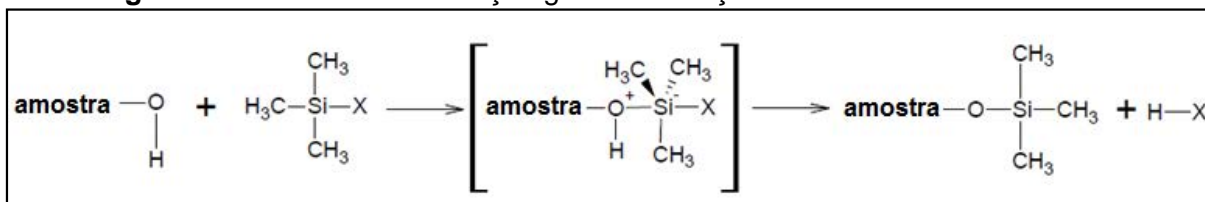
**Figura 14:** Extração da cera epicuticular.



### 3.3.2 Tratamentos dos extratos - Reação de derivação (sililação)

A análise por cromatografia gasosa da cera epicuticular e do extrato hexânico de folhas de cana-de-açúcar pode ter baixa resolução cromatográfica, isso devido à elevada polaridade, baixa volatilidade e instabilidade térmica de alguns constituintes (PELLATI e BENVENUTI, 2007). Esse problema pode ser solucionado pela reação de derivação (sililação). Essa é a etapa final da preparação da amostra, que consiste na substituição dos hidrogênios ativos presentes nos grupos –OH, –SH, –NH e –COOH por grupos trimetilsilanos (TMS) ou *tert*-butildimetilsililanos (TBDMS) (**Figura 15**), de forma a se obter derivados com maior volatilidade e estabilidade térmica.

**Figura 15:** Mecanismo de reação geral de sililação.



O extrato hexânico bruto (~ 3 mg) foi solubilizado em 200 µL de piridina (PA ACS - Tedia), juntamente com 200 µL de N-metil-N-(trimetilsilil) trifluoroacetamida

## PROCEDIMENTO EXPERIMENTAL

(MSTFA, Sigma). Essa foi mantida a 37° C por 30 minutos em banho-maria (Banho de aquecimento - marca IKA modelo H 0.5 0.6 CN). A seguir as amostras derivadas foram filtradas em filtros de membranas de nylon de 13 mm x 0,22 µm (ALLCROM). Os filtrados permaneceram em repouso a uma temperatura de ~3° C em freezer por 24 horas, sendo então analisadas por GC-FID e GC-MS.

O mesmo procedimento de derivação (silação) foi feito com as amostras de cera epicuticular, sendo utilizado 3 mg de extrato clorofórmico.

**Figura 16:** Fluxograma da extração de metabolitos apolares em folhas de cana-de-açúcar

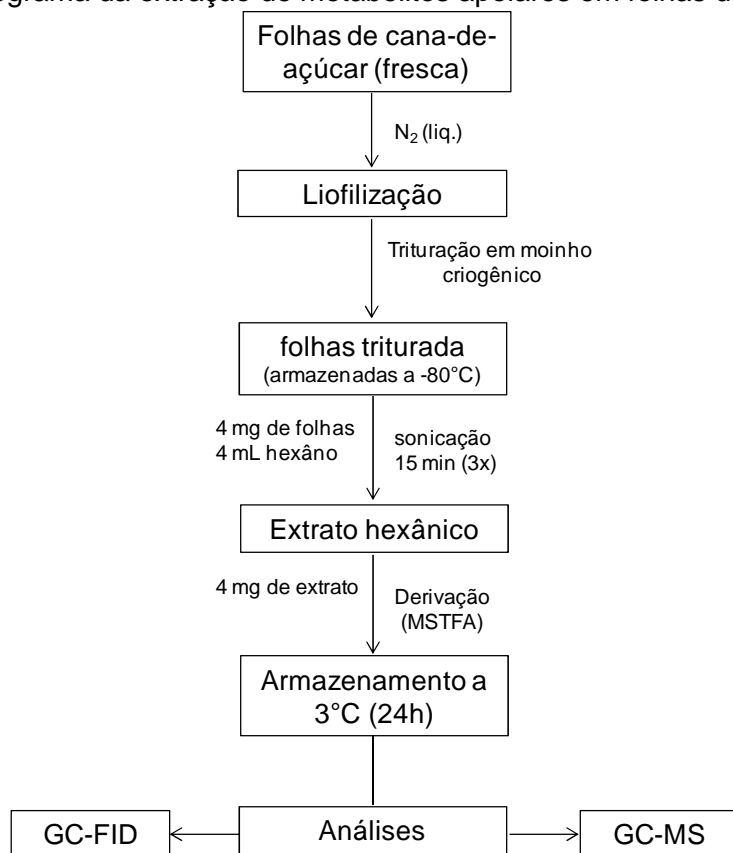
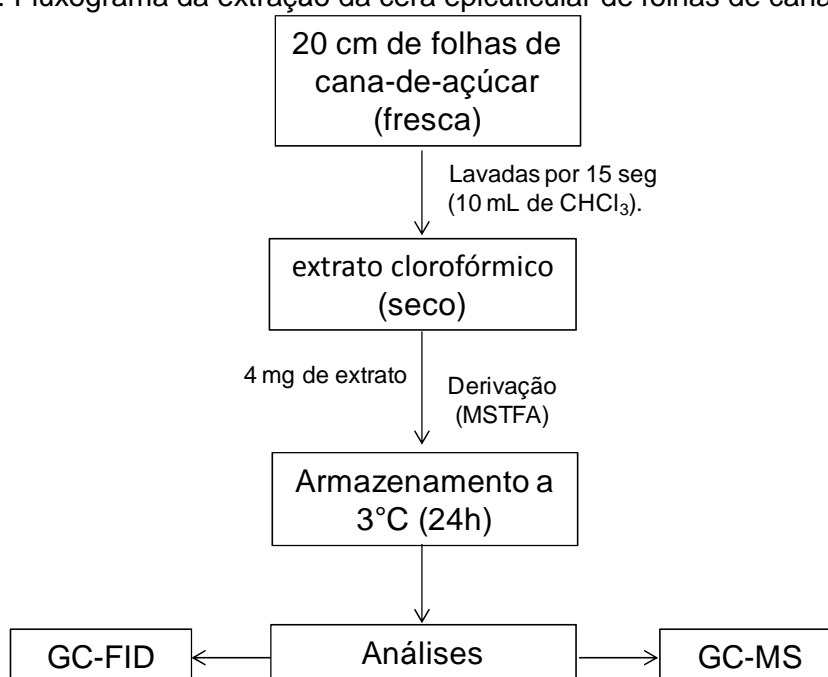


Figura 17: Fluxograma da extração da cera epicuticular de folhas de cana-de-açúcar.



### 3.4 Análises Cromatográficas

#### 3.4.1 Análises GC-FID

Para as análises por GC-FID utilizou-se um Cromatógrafo a Gás Varian CP - 3800, equipado com injetor automático Varian 8200 e detector de ionização em chama (FID). A coluna capilar utilizada foi Supelco SPB-5 (5% fenil polimetilsiloxano) de 30 m x 0,25 mm x 0,25 µm.

A temperatura do forno foi assim programada:

$$140\text{ °C (3 min)} \xrightarrow{3\text{ °C/min}} 320\text{ °C (10 min)}$$

Temperatura do injetor 260 °C.

Modo de injeção: *splitless/split* (modo de Grob). Início *splitless*, 0,75 min *split* (1/50) e 2 min *split* 1/20.

Temperatura do detetor: 320 °C

Volume de amostra injetado: 1 µL.

Vazão do gás de arraste (N<sub>2</sub>): 1.0 mL/min, gás de *make up* (N<sub>2</sub>): 29 mL/min, ar sintético: 10 mL/min e hidrogênio: 1 mL/min.

O tratamento dos dados foi efetuado no software Galaxie Chromaography Data System - Version 1.9.302.530

### 3.4.2 Análises GC-MS

Para as análises por GC-MS utilizou-se cromatógrafo a gás Shimadzu QP-2010 equipado com *injetor automático AOC-5000 Shimadzu* e interface com um espectrômetro de massas. A coluna utilizada foi uma Phenomenex ZB-5MS (30 m x 0,25 x 0,25 mm), *GCMS solutions Ver. 2.5*.

A temperatura do forno foi assim programada:

$$140\text{ °C (3 min)} \xrightarrow{3\text{ °C/min}} 320\text{ °C (10 min)}$$

A temperatura do injetor foi 260 °C.

Modo de injeção: *splitless/split* (Grob). Início *splitless*, 0,75 min *split* (1/50), 2 min *split* 1/20, gás de arraste hélio (99,999%) a um fluxo constante de 1,3 mL/min, o volume de amostra injetado foi de 1 µL. Pressão: 114.9 kPa, velocidade linear: 43.1 cm/sec., fluxo total: 17.3. Condições MS: temperatura da fonte de íons e interface de 250 °C, modo de impacto de eletrons a 70 eV, faixa da massas de aquisição de *m/z* 40-650 Daltons.

### 3.4.3 Tratamento e análise de dados

Os cromatogramas das análises por GC-MS e GC-FID foram integrados e os *tR* (tempo de retenção) e áreas dos picos tabulados. O cálculo do índice de retenção linear foi calculado utilizando série homóloga de *n*-alcanos C<sub>8</sub>-C<sub>40</sub> (Sigma-Aldrich). O índice de retenção de um analito é um número, obtido por interpolação, relacionando o tempo de retenção do analito de interesse com o tempo de retenção de dois padrões (séries homologas de hidrocarbonetos) eluídos antes e após o pico do composto de interesse (VAN DEN DOOL AND KRATZ, 1963). Para o cálculo do índice de retenção linear foi utilizada a equação de Van Den Dool e Kratz:

$$IR = 100.n + 100.\left(\frac{tR_x - tR_n}{tR_{n+1} - tR_n}\right) \quad \text{(equação 1)}$$

onde *n* é número de carbonos do *n*-alcano anterior ao analito, *t<sub>x</sub>* é o tempo de retenção do analito de interesse, *t<sub>n</sub>* é o tempo de retenção do *n*-alcano eluído antes do analito e *t<sub>n+1</sub>* é o tempo de retenção do *n*-alcano eluído após o analito. Os índices de retenção do GC-FID foram comparados com os do GC-MS, que foram

comparados com o banco de dados NIST e Golm Metabolome Database (Max Planck Institute).

### **3.4.4 Análises quimiométricas**

A análise quimiométrica foi realizada a fim de se identificar diferenças entre amostras de cana-de-açúcar com resistência diferenciada à ferrugem alaranjada. Foi usado para estas análises o software Matlab® (MATHWORKS) e pacote computacional PLS-toolbox (Eigenvector Reserach, Inc.).

#### **3.4.4.1 Pré-processamento dos dados brutos**

Os cromatogramas obtidos foram submetidos a uma etapa de pré-processamento. A etapa de pré-processamento consistiu no alinhamento dos cromatogramas empregando o algoritmo COW – Correlation optimized warning (NIELSEN; CARTENSEN; SMEDSGAARD, 1998; TOMASI; BERG; ANDERSON, 2004) disponível na página <http://www.models.kvl.dk/users/rasmus/>. O alinhamento é necessário, devido ao deslocamento dos picos (tempo de retenção) por possíveis variações dentro do sistema cromatográfico, tais como: variações na temperatura, coluna, pequenas variações na vazão da fase móvel, diferentes maneiras de injeção da amostra e origem da amostra. Após o alinhamento os cromatogramas foram normalizados e centrados na média e então os dados foram submetidos a análises estatísticas por métodos supervisionados e não supervisionado.

#### **3.4.4.2 PCA - Análise de componentes principais**

A PCA é um método não supervisionado de caráter exploratório que visa buscar similaridades ou diferenças entre as amostras, agrupando-as em um gráfico de *scores* que representa as amostras com sua dimensionalidade reduzida (BRERETON, 2000). Os valores de *loadings* que são gerados pela PCA caracterizam através de pesos as variáveis responsáveis para esta separação em um espaço ortogonal. Este conjunto de dados é organizado na forma de uma matriz (dados bidimensionais), onde as linhas devem ser as amostras e as colunas as variáveis (FERREIRA et al., 1999). Dentre as informações coletas para as diferentes variedades de amostras de cana-de-açúcar, as variáveis exploradas foram às

intensidades e os respectivos tempo de retenção relativos das substâncias separadas na análise cromatográfica empregando o detector FID.

### 3.5 Fracionamentos da cera epicuticular

A cera epicuticular obtida de folhas de cana-de-açúcar foi analisada por cromatografia em camada delgada comparativa (CCDC) e fracionada por cromatografia em camada delgada preparativa (CCDP). Para CCDC foram utilizadas placas comerciais de sílica de sílica G (2-25  $\mu\text{m}$ , 60  $\text{\AA}$ , Sigma-Aldrich<sup>®</sup>) e sílica gel 60H (Merck<sup>®</sup>). A placa preparativa (espessura indeterminada) foi preparada manualmente espalhando-se uma suspensão de sílica (16,9 g) em água deionizada (37,0 mL) sobre uma placa de vidro de 20 cm x 20 cm, eluídas com [Hex/AcOEt (7:3)]. As revelações das cromatoplasmas foram efetuadas mediante irradiação na região de absorção no UV (254 e 366 nm) e nebulizada com *para*-anisaldeído seguido de aquecimento em estufa a 100° C. Após a revelação das CCDC e detecção das frações, as CCDP foram raspadas e cada fração foi lavada com clorofórmio. Essas frações foram analisadas por GC-FID, GC-MS, MS-APCI e espectroscopia de RMN.

### 3.6 Análises das frações da cera epicuticular

#### 3.6.1 Análises Cromatográficas

As frações da cera epicuticular (~ 3mg) foram submetidas ao mesmo procedimento de derivação (sililação), **item 3.3.2** e analisadas por GC-FID e GC-MS

#### 3.6.2 Análises Espectrométricas

Alíquotas das frações da cera (~5 mg/0,7 mL de  $\text{CDCl}_3$ ) foram analisadas por espectroscopia de RMN.

Os espectros de RMN uni ( $^1\text{H}$ ,  $^{13}\text{C}$ , DEPT) e bidimensionais ( $^1\text{H}$ - $^1\text{H}$  gCOSY, gHMQC, gHMBC) foram adquiridos em espectrômetros Bruker Avance III 600 (14,2 T) a 600 MHz ( $^1\text{H}$ ) e 151 MHz ( $^{13}\text{C}$ ).

Após análises das frações por GC-FID, duas frações de cera epicuticular foram selecionadas: Fr3 e Fr6. Cerca de 0,02 mg/mL dessas frações de cera epicuticular foram analisadas por MS-APCI. Os espectros de massas foram adquiridos em espectrômetro Thermo Scientific<sup>™</sup> LCQ Fleet LC/MS operando a

baixa resolução, injeção direta e Ionização Química a Pressão Atmosférica (APCI) utilizando nitrogênio como gás de nebulização.

### **3.7 Identificação**

A identificação dos constituintes dos extratos (cera e hexânico) analisados por cromatografia gasosa foi realizada por meio de análise e comparação dos espectros de massas com dados das bibliotecas Wiley 7 e Nist através do software *GCMS solutions* Ver. 2.61. Para tal comparação estabeleceu-se um limite de 70% de similaridade entre o espectro da amostra e o espectro da biblioteca. A proposta de identificação também foi confirmada pela comparação do índice de retenção calculado (usando séries homologas de hidrocarbonetos) com os índices de retenção da literatura (NIST e GMD). A fim de diminuir as incertezas entre as comparações, foi proposta um limite  $\pm 5$  unidade para comparação dos índices de retenção.

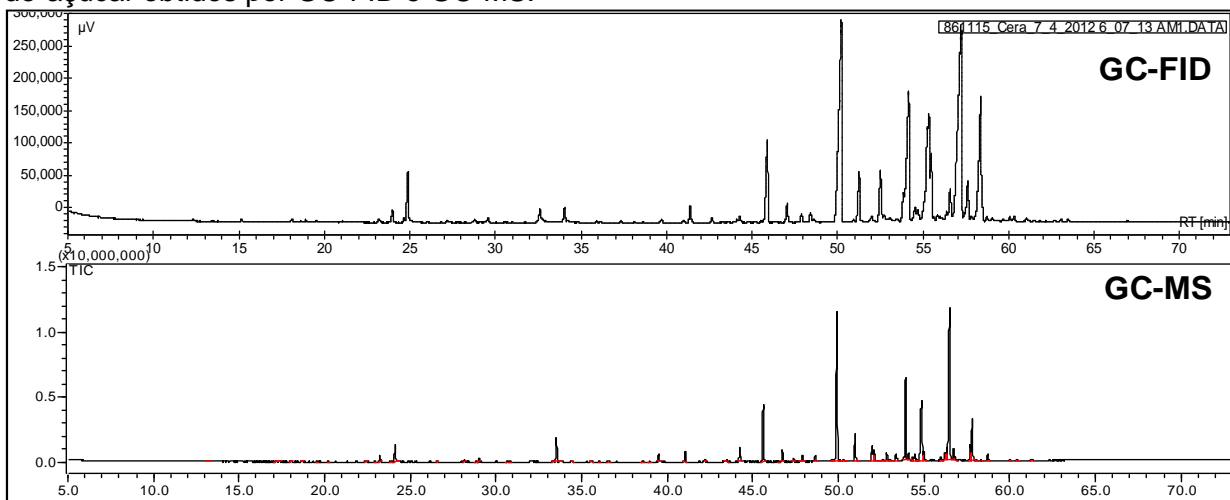


### 4 Resultados e discussão

#### 4.1 Análises do perfil cromatográfico de cera epicuticular de folhas de cana-de-açúcar

A análise do perfil cromatográfico da cera epicuticular de folhas de cana-de-açúcar foi feita comparativamente com 13 cultivares (**Tabela 2**). Todos os cultivares foram analisados em duplicatas. As análises foram realizadas inicialmente por GC-FID para ajustes das condições cromatográficas e posteriormente por GC-MS para obtenção de dados de retenção e espectros de massas dos constituintes da cera (**Figura 18**).

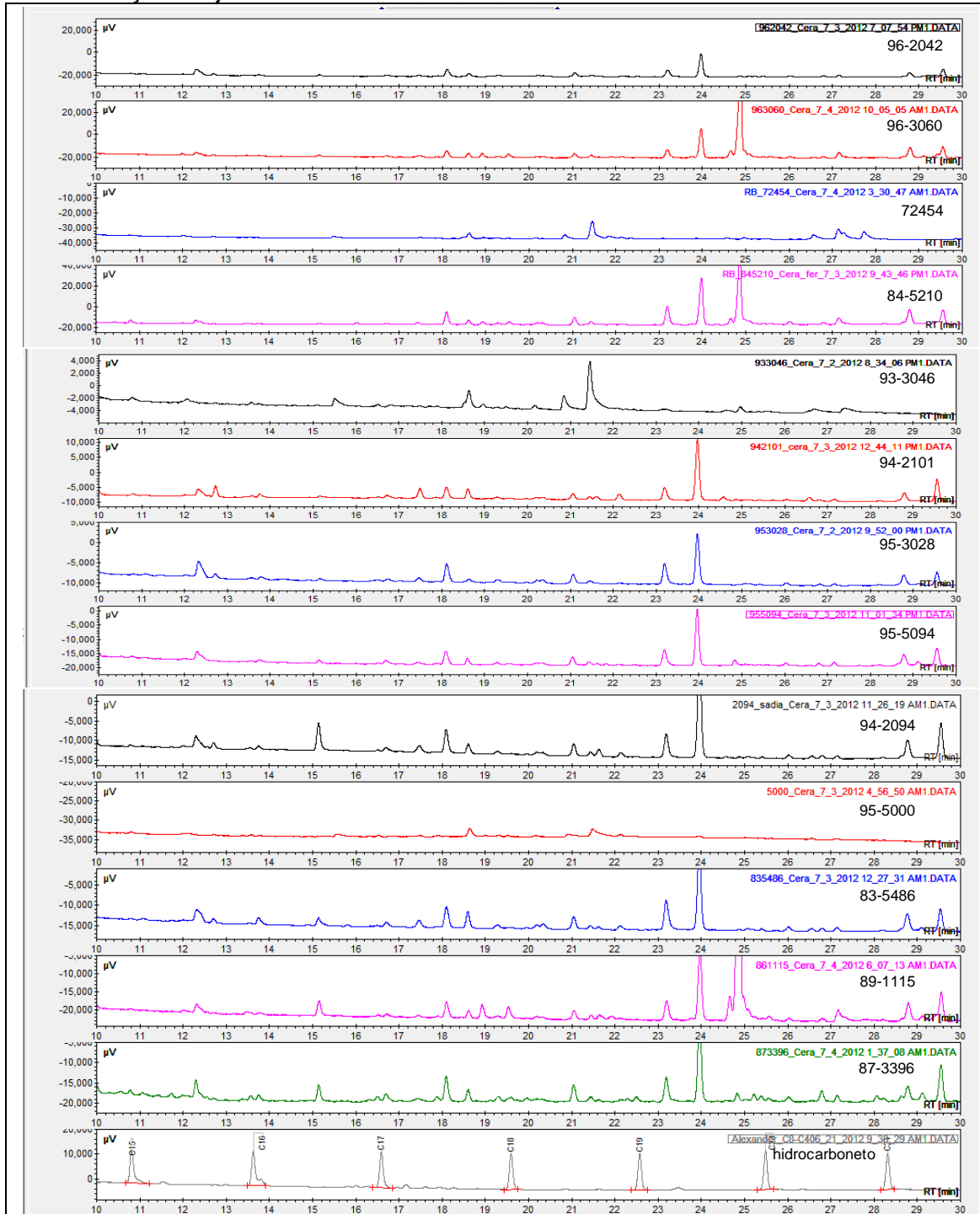
**Figura 18:** Exemplo de perfil cromatográfico de cera epicuticular (TMS) de folhas de cana-de-açúcar obtidos por GC-FID e GC-MS.



Os cromatogramas dos 13 cultivares analisados por GC-FID e GC-MS foram comparados (**Figura 19** e **Figura 20**), sendo observadas diferenças significativas nos perfis cromatográficos. Para facilitar a avaliação dos diversos constituintes presentes nas amostras, os cromatogramas foram ampliados e divididos em duas partes: parte 1 de 10 a 30 minutos (**Figura 19** e **Figura 20**) e parte 2 de 30 a 65 minutos (**Figura 21** e **Figura 22**).

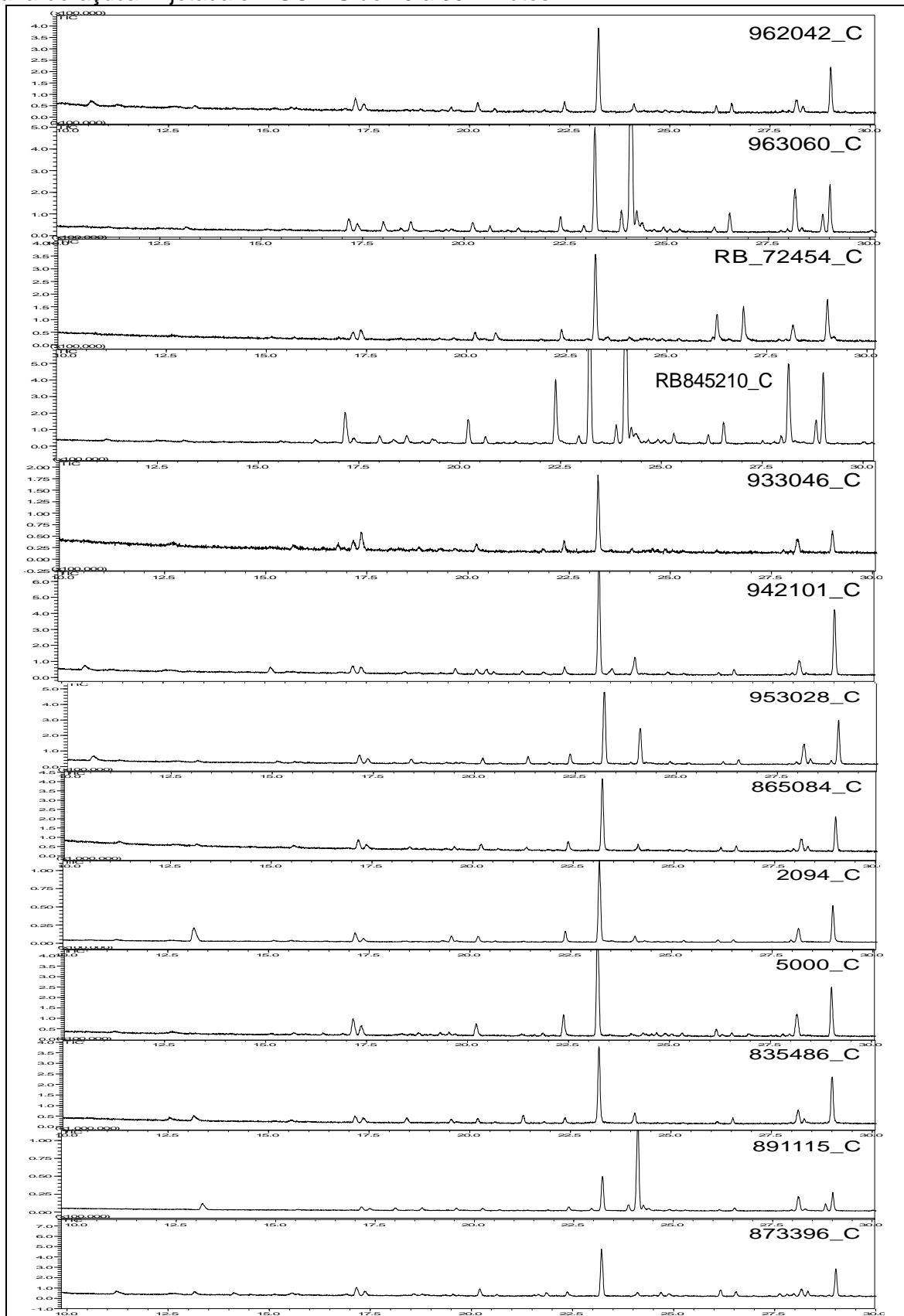
## Resultados

**Figura 19:** Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 10 a 30 minutos.



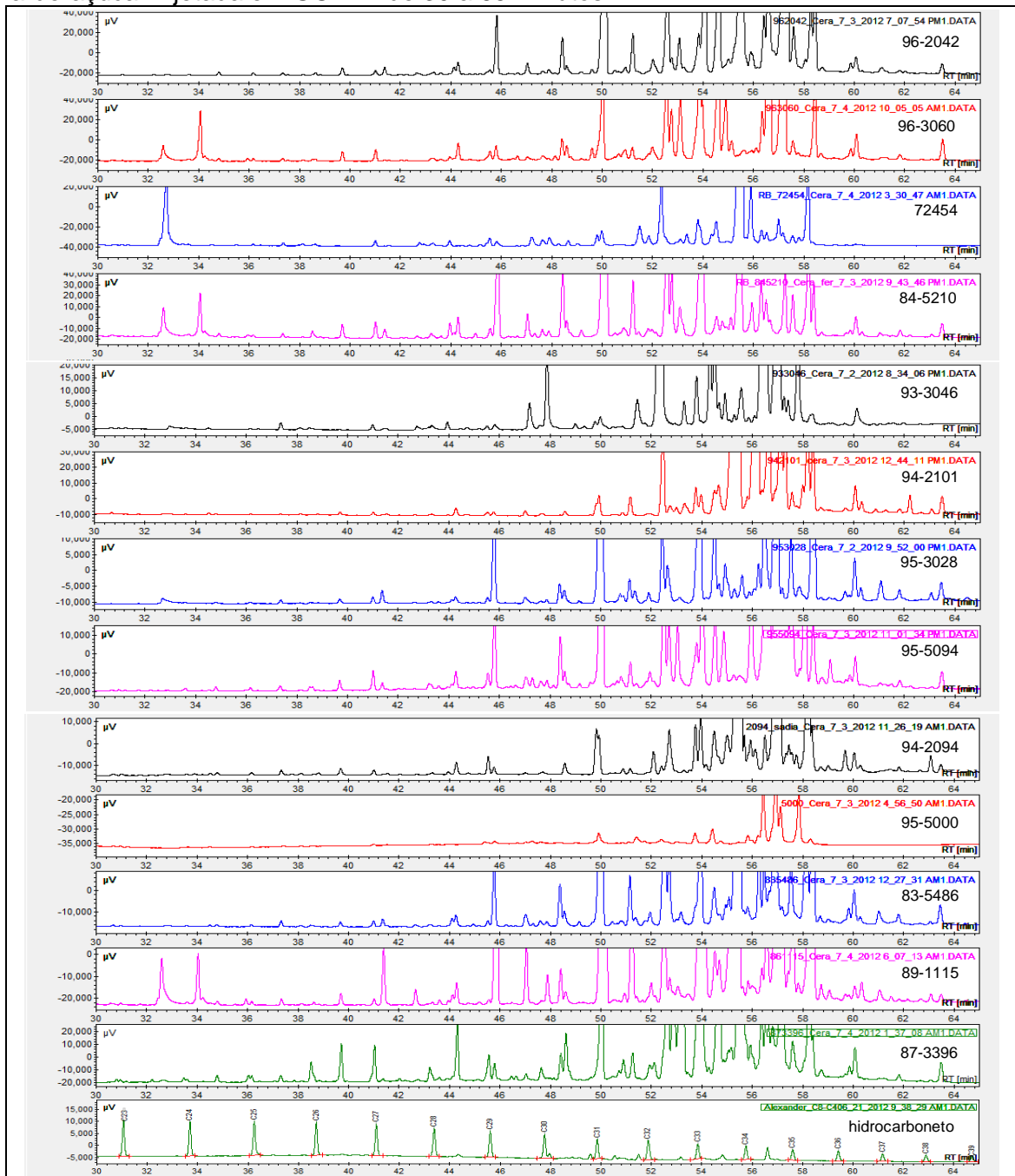
## Resultados

Figura 20: Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 10 a 30 minutos.



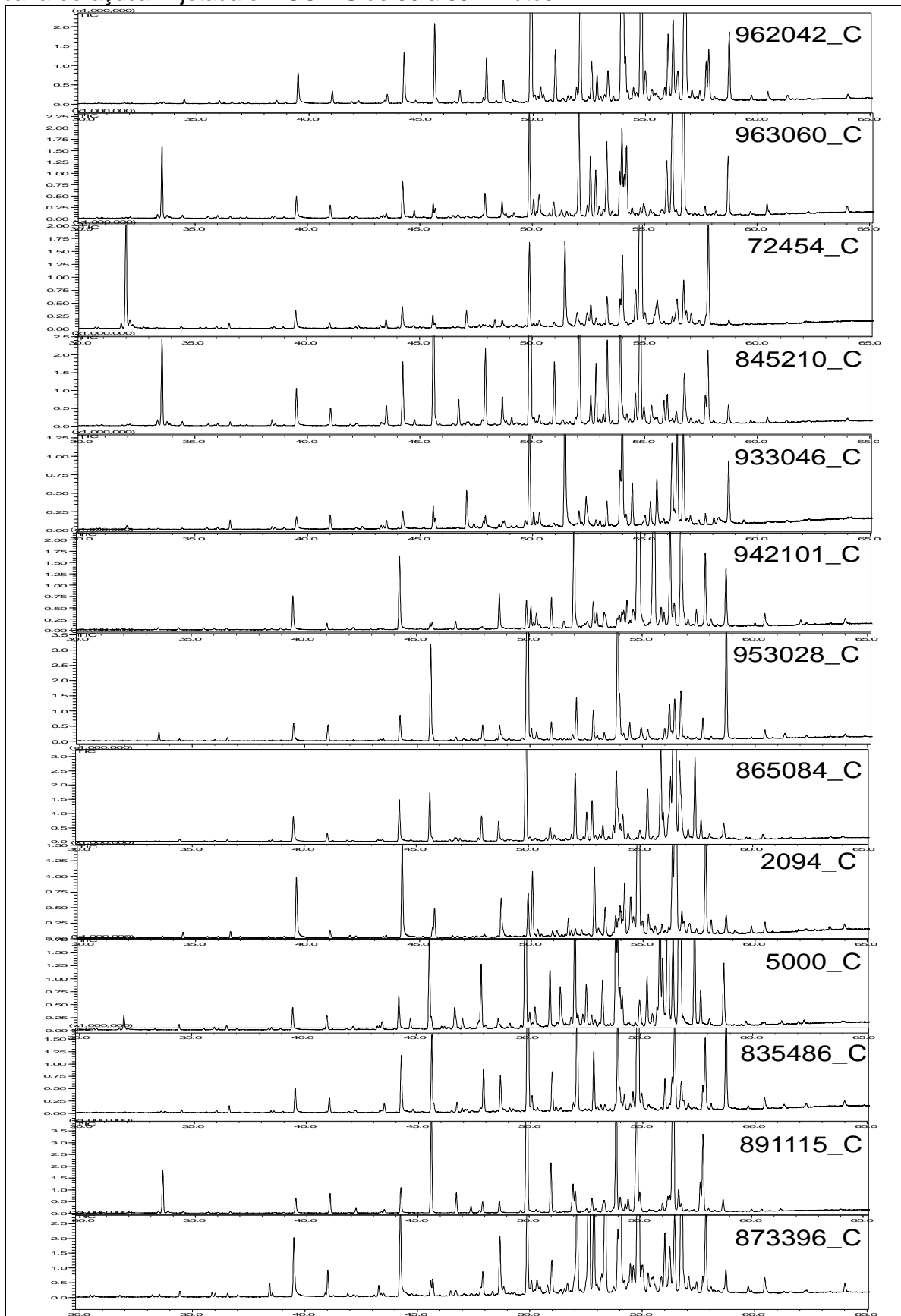
## Resultados

Figura 21: Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 30 a 65 minutos.



## Resultados

**Figura 22:** Cromatogramas ampliados da análise da cera epicuticular (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 30 a 65 minutos.



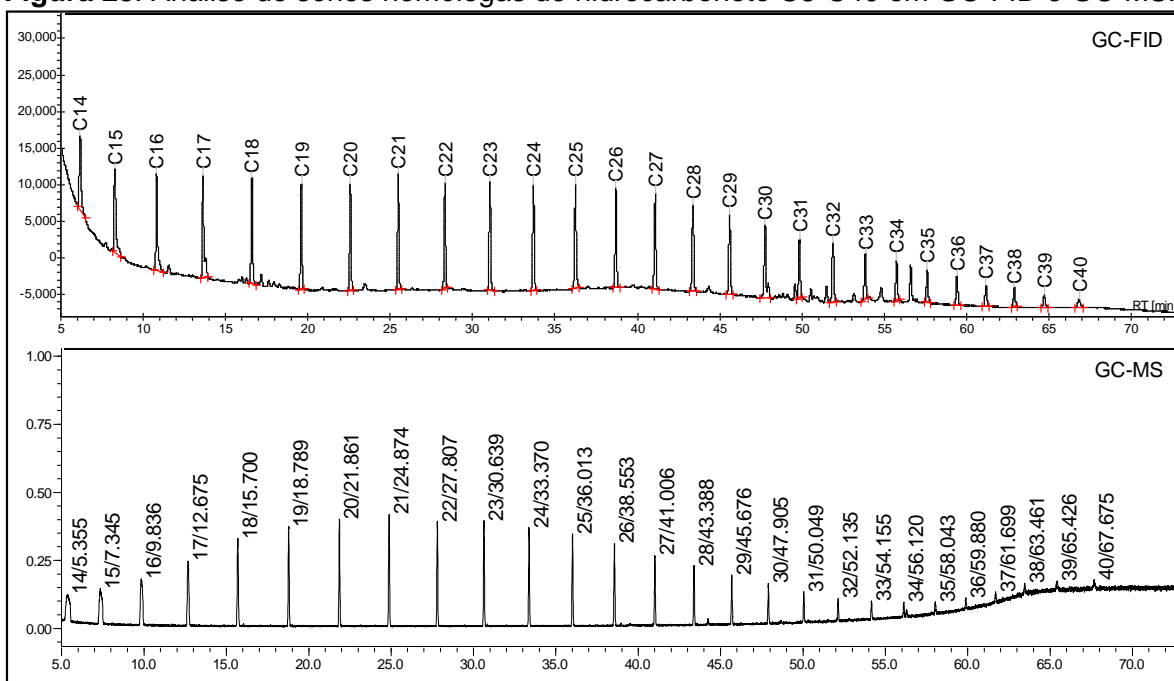
## Resultados

### 4.1.1 Identificação dos constituintes apolares da cera epicuticular por índice de retenção (IR) e espectrometria de massas (EM).

Para a identificação dos constituintes da cera epicuticular inicialmente foi calculado o índice de retenção de cada constituinte usando a equação de VAN DEN DOOL E KRATZ (**equação 1**), tendo como referencia uma série homóloga de alcanos ( $C_8$ - $C_{40}$ ). Nas condições cromatográficas utilizadas os alcanos  $C_8$ - $C_{13}$  coeluíram com o pico do solvente.

Os cromatogramas das séries homólogas de hidrocarbonetos analisados por GC-FID e GC-MS foram comparados, a fim de confirmar a ordem de eluição e eliminar um possível erro na contagem dos hidrocarbonetos e consequentemente influenciar no cálculo do IR. No cromatograma da análise por GC-FID, observa-se um possível contaminante no tR = 56 minutos, entre os hidrocarbonetos  $C_{34}$  e  $C_{35}$ . Tal contaminação foi confirmada observando-se a ordem de eluição dos hidrocarbonetos na análise por GC-MS, onde esse contaminante não foi observado (**Figura 23**).

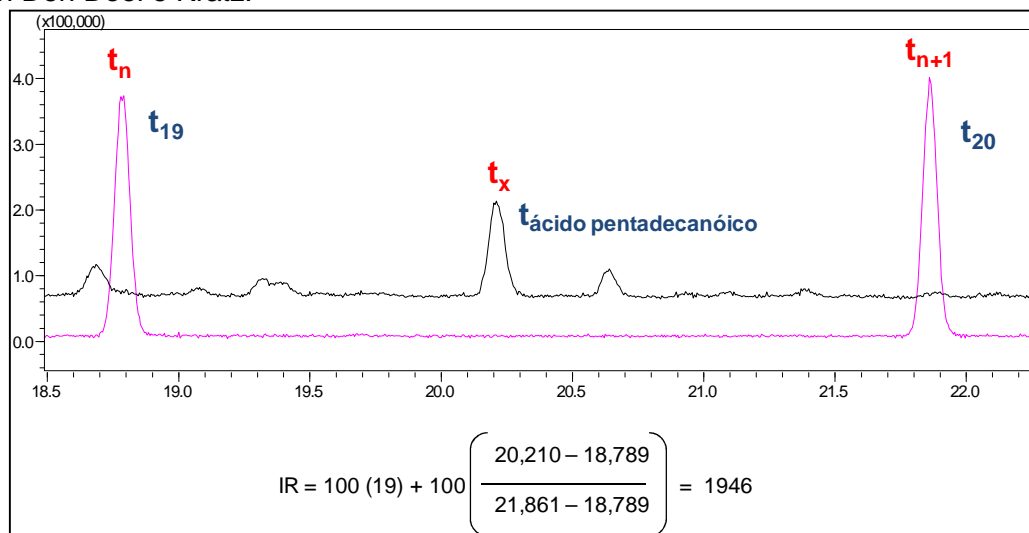
**Figura 23:** Análise de séries homólogas de hidrocarboneto  $C_8$ - $C_{40}$  em GC-FID e GC-MS.



## Resultados

O índice de retenção é o número obtido pela interpolação do tempo de retenção do componente de interesse com os tempos de retenção de dois padrões da série homóloga de alcanos eluídos imediatamente antes e após o componente de interesse, como exemplificado na **figura 24**.

**Figura 24:** Exemplo do cálculo do IR do ácido pentadecanóico (TMS) utilizando a equação de Van Den Dool e Kratz.

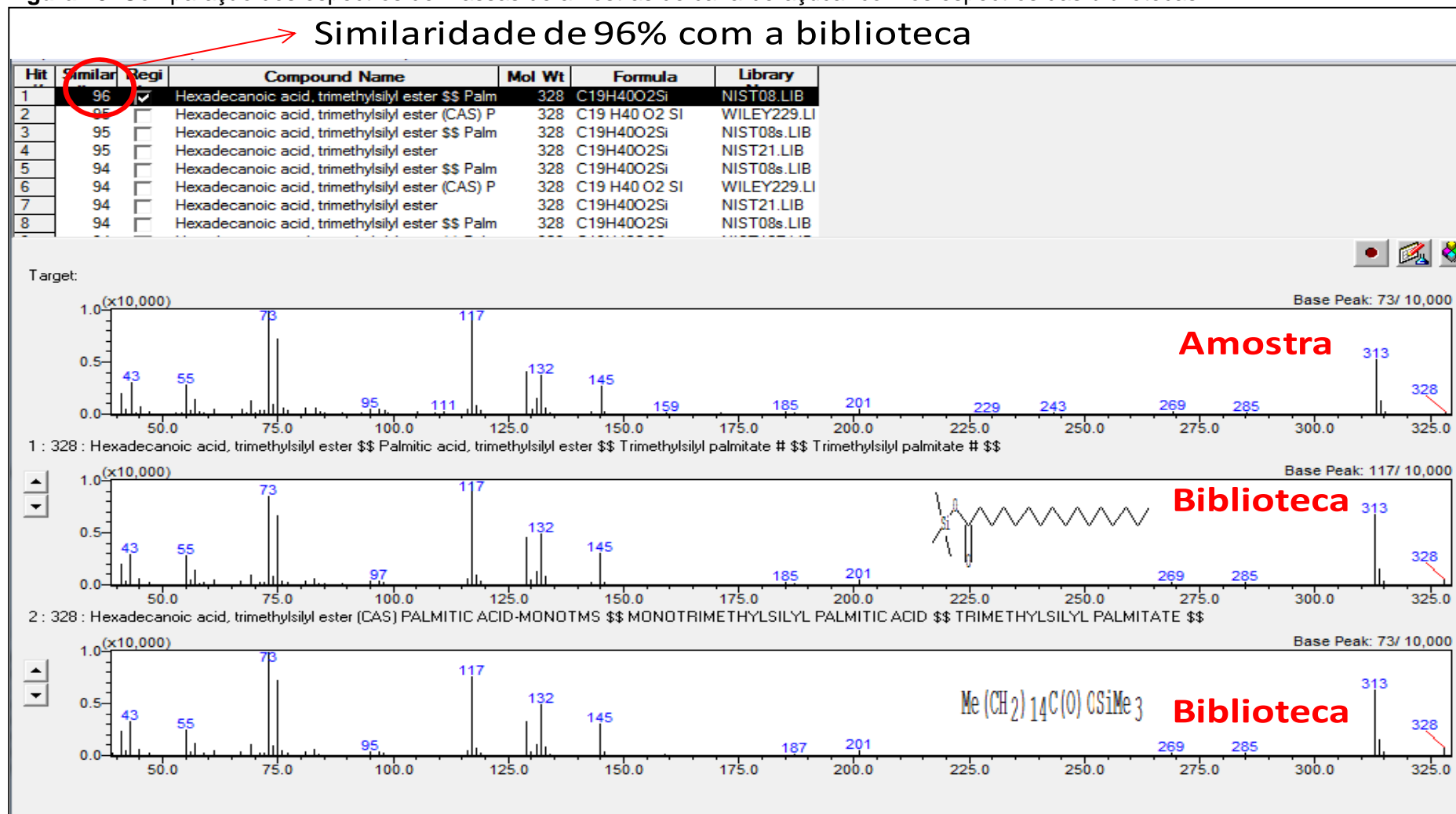


**Legenda:**  $t_{19}$ = tempo de retenção do nonacosano;  $t_{\text{ácido pentadecanóico}}$ = tempo de retenção do ácido pentadecanóico;  $t_{20}$ = tempo de retenção do eicosano.

Calculado o IR ( $IR_{\text{cal}} = 1946$ ), a identificação do ácido pentadecanóico foi proposta pela comparação com o índice de retenção da literatura,  $IR = 1943$  (NIST e GMD), e confirmada quando a comparação do espectro de massas obtida por EI com espectros da literatura e/ou de biblioteca de espectros (Wiley 7 e NIST), como exemplificado para o ácido hexadecanóico (TMS) (**Figura 25**), resultou em pelo menos 70% de similaridade.

## Resultados

Figura 25: Comparação dos espectros de massas de amostras de cana-de-açúcar com os espectros das bibliotecas.





## **Resultados**

---

A comparação dos dados de retenção e espectros de massas experimentais com os dados da literatura possibilitaram a identificação tentativa de 58 constituintes dos 138 detectados por GC-MS (**Figura 26**). Entre estes constituintes encontram-se vários homólogos de alcanos de cadeia linear, alcoóis e ácidos graxos, alquil diidroxibenzenos, além de alguns esteroides e triterpenos (**Tabela 3 e Anexo 1**). Fragmentos característicos de algumas dessas substâncias estão listados na **tabela 4**. Para reforçar a identificação de constituintes majoritários e definir o padrão de substituição no anel aromáticos dos alquil diidroxibenzenos, uma alíquota de cera epicuticular foi submetida a fracionamento em CCD preparativa e análises por RMN e MS-APCI (**Item 4.3.1.1**), concluindo-se que são 5-alquil-1,3-diidroxibenzenos, isto é, 5-alquil resorcinois. Da mesma forma, em outra fração obtida nesta mesma análise preparativa foi possível identificar o triterpeno pentacíclico simiarenol (**Item 4.3.1.2**).

## Resultados

**Figura 26:** Comparação do perfil cromatográfico e do IR entre os tempos de retenção de 10 a 45 minutos (a) e de 45 a 65 minutos (b) das análises de cera epicuticular (TMS) GC-FID com GC-MS.



## Resultados

**Tabela 3:** Proposta de identificação dos constituintes da cera epicuticular (TMS) de folhas de cana-de-açúcar por comparação do IR das análises de GC-MS e GC-FID. Espectros de massas disponíveis no anexo 3, colocados em ordem crescente de ordem retenção.

GC-MS (coluna ZB-5ms)				GC-FID (coluna SPB-5)			$\Delta$ IR	Identificação
PICOS	tR (min)	IR exp.	IR lit.	tR (min)	IR exp.	IR lit.		
1	11.211	1648	1645	12.290	1652	1650	4	ácido láurico*
2	13.150	1716	-	-	-	-	-	-
3	14.115	1748	1745	15.140	1751	1749	3	ácido tridecanóico*
4	17.155	1847	1843	18.090	1850	1845	3	ácido mirístico*
5	20.204	1946	1943	21.040	1948	1945	2	ácido pentadecanóico*
6	20.624	1960	1955	21.430	1961	-	1	1-hexadecanol*
7	22.366	2017	2023	23.190	2021	2029	4	ácido palmitoleico*
8	22.949	2036	-	-	-	-	-	-
9	23.215	2045	2040	23.990	2048	2047	3	ácido palmítico*
10	24.694	2094	-	-	-	-	-	-
11	24.875	2100	2100	-	-	-	-	heneicosano
12	25.316	2115	2126	-	-	-	-	cis-10-ácido heptadecanoico*
13	26.153	2144	2148	26.790	2146	2148	2	ácido margárico*
14	26.540	2157	2149/2165	27.160	2159	-	2	1-octadecanol*
15	27.620	2194	-	-	-	-	-	-
16	27.968	2206	2208	28.680	2213	2212	7	ácido linoleico*
17	28.153	2212	2215	28.790	2217	2216	5	ácido oléico*
18	28.322	2218	-	-	-	-	-	-
19	28.831	2236	-	-	-	-	-	-
20	29.009	2243	2248	29.560	2245	2243	2	ácido esteárico*
21	30.475	2294	-	-	-	-	-	-
22	30.625	2300	2300	30.960	2296	2300	4	tricosano
23	30.771	2342	-	-	-	-	-	-
24	31.783	2342	2338	32.220	2344	2351	2	ácido nonadecanóico*
25	32.107	2354	2349	-	-	-	-	eicosanol*
26	33.375	2400	2400	33.590	2397	2400	3	tetracosano
27	34.434	2440	2447	34.800	2443	2447	3	ácido araquídico*
28	36.001	2500	2500	36.160	2496	2500	4	pentacosano
29	36.995	2539	2534	37.340	2544	2552	5	ácido heneicosanóico*
30	37.300	2551	2543	37.550	2553	-	2	1-docosanol*
31	38.255	2589	2583/2006	38.510	2592	2583/2606	3	monopalmitina*
32	38.556	2601	2600	38.820	2605	2600	4	hexacosano
33	39.509	2639	2632	39.700	2642	2644	3	ácido behênico*
34	41.011	2700	2700	41.020	2697	2700	3	heptacosano
35	41.035	2701	-	41.380	2713	-	12	5-n-pentadecil resorcinol*
36	41.904	2738	2731	-	-	-	-	ácido tricosanóico*
37	42.203	2750	-	-	-	-	-	-
38	43.280	2796	-	-	-	-	-	-
39	43.364	2800	-	43.290	2796	-	4	5-n-hexadecil resorcinol*
40	43.374	2800	2800	-	-	-	-	octacosano
41	43.491	2805	-	-	-	-	-	-
42	43.502	2806	2812	43.610	2810	2808	4	esqualeno
43	44.229	2837	2834	44.290	2841	2834	4	ácido tetracosanóico*
44	44.750	2860	-	-	-	-	-	-
45	44.759	2860	-	-	-	-	-	-
46	45.160	2877	-	-	-	-	-	-
47	45.582	2897	-	45.890	2913	-	16	Ar:c17*
48	45.673	2900	2900	45.560	2898	2900	2	nonacosano
49	46.131	2920	-	-	-	-	-	-
50	46.274	2927	-	-	-	-	-	-
51	46.476	2936	2937	46.470	2940	2937	4	ácido pentacosanóico*
52	46.708	2947	-	47.050	2967	-	20	-
53	46.951	2957	-	-	-	-	-	alquilresorcinol
54	47.071	2963	-	-	-	-	-	-
55	47.161	2967	-	-	-	-	-	alquilresorcinol

## Resultados

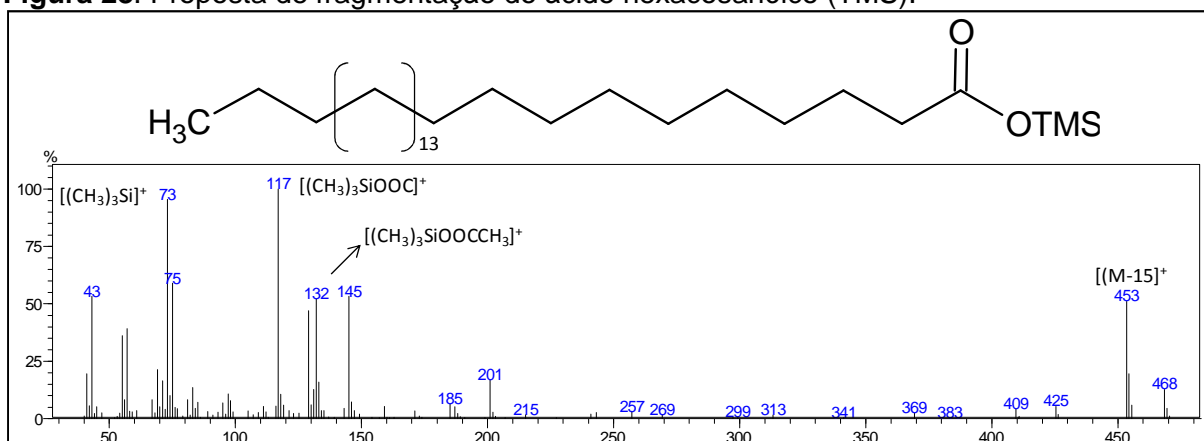
56	47.395	<b>2977</b>	-	-	-	-	-	esteroide
57	47.765	<b>2995</b>	-	48.600	<b>3040</b>	-	45	Ar:C18*
58	47.826	<b>2996</b>	-	-	-	-	-	-
59	47.902	<b>3000</b>	-	48.460	<b>3033</b>	-	33	-
60	48.114	<b>3010</b>	-	-	-	-	-	-
61	48.348	<b>3021</b>	-	-	-	-	-	triterpenoide
62	48.657	<b>3035</b>	<b>3035</b>	48.600	<b>3040</b>	<b>3036</b>	5	ácido hexacosanóico*
63	48.838	<b>3044</b>	<b>3037</b>	48.600	<b>3040</b>	<b>3037</b>	4	1-Heptacosanol*
64	49.076	<b>3055</b>	-	-	-	-	-	alquilresorcinol
65	49.179	<b>3094</b>	-	-	-	-	-	-
66	49.224	<b>3062</b>	-	-	-	-	-	-
67	49.440	<b>3072</b>	-	-	-	-	-	-
68	49.668	<b>3082</b>	-	-	-	-	-	-
69	49.856	<b>3091</b>	-	50.520	<b>3133</b>	-	42	Ar:C19*
70	50.051	<b>3100</b>	<b>3100</b>	49.830	<b>3100</b>	-	0	hentriacontano
71	50.190	<b>3108</b>	-	-	-	-	-	-
72	50.291	<b>3112</b>	-	-	-	-	-	colesterol*
73	50.455	<b>3120</b>	<b>3136</b>	-	-	-	-	$\alpha$ -tocoferol*
74	50.787	<b>3135</b>	<b>3120</b>	50.500	<b>3132</b>	-	3	ácido heptacosanóico*
75	50.961	<b>3145</b>	-	51.240	<b>3168</b>	-	23	-
76	51.155	<b>3153</b>	-	-	-	-	-	alquilresorcinol
77	51.146	<b>3153</b>	-	-	-	-	-	-
78	51.357	<b>3163</b>	-	-	-	-	-	alquilresorcinol
79	51.426	<b>3166</b>	-	-	-	-	-	-
80	51.545	<b>3171</b>	-	-	-	-	-	-
81	51.655	<b>3178</b>	-	-	-	-	-	-
82	51.784	<b>3183</b>	-	-	-	-	-	-
83	51.910	<b>3190</b>	-	-	-	-	-	Ar C20:0*
84	51.971	<b>3192</b>	-	-	-	-	-	-
85	52.087	<b>3198</b>	-	52.590	<b>3236</b>	-	38	-
86	52.205	<b>3203</b>	-	-	-	-	-	-
87	52.251	<b>3206</b>	-	-	-	-	-	-
88	52.380	<b>3212</b>	-	-	-	-	-	-
89	52.426	<b>3214</b>	-	-	-	-	-	-
90	52.451	<b>3216</b>	<b>3204/ 3253</b>	-	-	-	-	campesterol*
91	52.588	<b>3223</b>	-	-	-	-	-	-
92	52.822	<b>3234</b>	-	-	-	<b>3232</b>	-	ácido octacosanóico*
93	52.993	<b>3292</b>	<b>3286</b>	-	-	-	-	estigmasterol*
94	53.180	<b>3251</b>	-	-	-	-	-	alquilresorcinol
95	53.300	<b>3259</b>	-	-	-	-	-	-
96	53.381	<b>3262</b>	-	-	-	-	-	-
97	53.551	<b>3270</b>	-	-	-	-	-	alquilresocinol
98	53.740	<b>3279</b>	-	-	-	-	-	-
99	53.774	<b>3281</b>	-	-	-	-	-	-
100	53.896	<b>3288</b>	-	-	-	-	-	Ar:C21*
101	53.968	<b>3291</b>	-	-	-	-	-	triterpenoide
102	54.076	<b>3296</b>	-	-	-	-	-	esteroide
103	54.095	<b>3297</b>	-	-	-	-	-	-
104	54.164	<b>3300</b>	<b>3300</b>	-	-	-	-	tritriacontano
105	54.200	<b>3302</b>	<b>3348/3296</b>	-	-	<b>3348</b>	-	$\beta$ -sitosterol*
106	54.321	<b>3308</b>	-	-	-	-	-	arundoina
107	54.443	<b>3315</b>	-	-	-	-	-	-
108	54.551	<b>3320</b>	-	-	-	-	-	-
109	54.799	<b>3333</b>	-	-	-	-	-	-
110	54.861	<b>3336</b>	-	-	-	-	-	-
111	54.969	<b>3341</b>	-	-	-	-	-	-
112	55.228	<b>3355</b>	<b>3348</b>	-	-	-	-	$\beta$ -amirina*
113	55.312	<b>3359</b>	-	-	-	-	-	-
114	55.530	<b>3370</b>	-	-	-	-	-	-
115	55.540	<b>3370</b>	-	-	-	-	-	-
116	55.735	<b>3380</b>	-	-	-	-	-	-



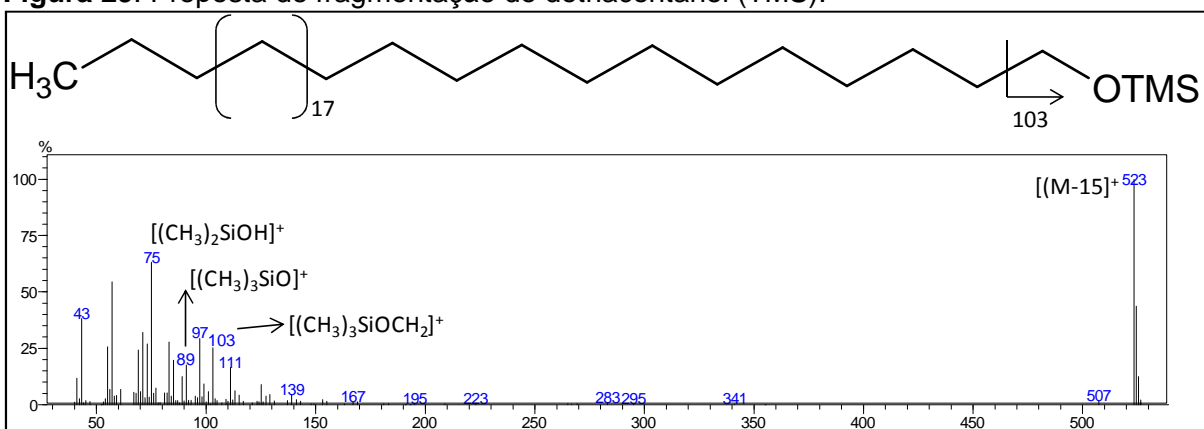
## Resultados

$[(\text{CH}_3)_2\text{SiOH}^+]$ . Adicionalmente os fragmentos característicos de ácidos graxos são:  $m/z$  117  $[(\text{CH}_3)_3\text{SiOOC}^+]$ , 129, 132 e 145, sendo que os fragmentos 132 e 145 são formados devido ao rearranjo de McLafferty (**Figura 28**). Os fragmentos característicos de alcoóis alifáticos são:  $m/z$  75, 89  $[(\text{CH}_3)_3\text{SiO}^+]$  e 103  $[(\text{CH}_3)_3\text{SiOCH}_2^+]$  (**Figura 29**). Aqueles típicos de esteroides são:  $m/z$  129,  $m/z$  396, que corresponde à perda de um grupo TMS com um fragmento de três carbonos que contém o anel A, C1, C2 e C3, favorecida pela ligação dupla no C5- $\beta$ , (**Figura 30**). Para os alquilresorcinóis, os fragmentos característicos são  $m/z$  73, 268  $[(\text{TMSO})$  2  $\text{C}_6\text{H}_3\text{CH}_3^+$ ] e 281, sendo que o fragmento  $m/z$  268 é formado devido ao rearranjo de McLafferty (**Figura 31**) (McLAFFERTY, 1993; KITSON; LARSEN; MCEWEN, 1996).

**Figura 28:** Proposta de fragmentação do ácido hexacosanóico (TMS).



**Figura 29:** Proposta de fragmentação do dotriacontanol (TMS).



## Resultados

Figura 30: Proposta de fragmentação do  $\beta$ -Sitosterol, (TMS).

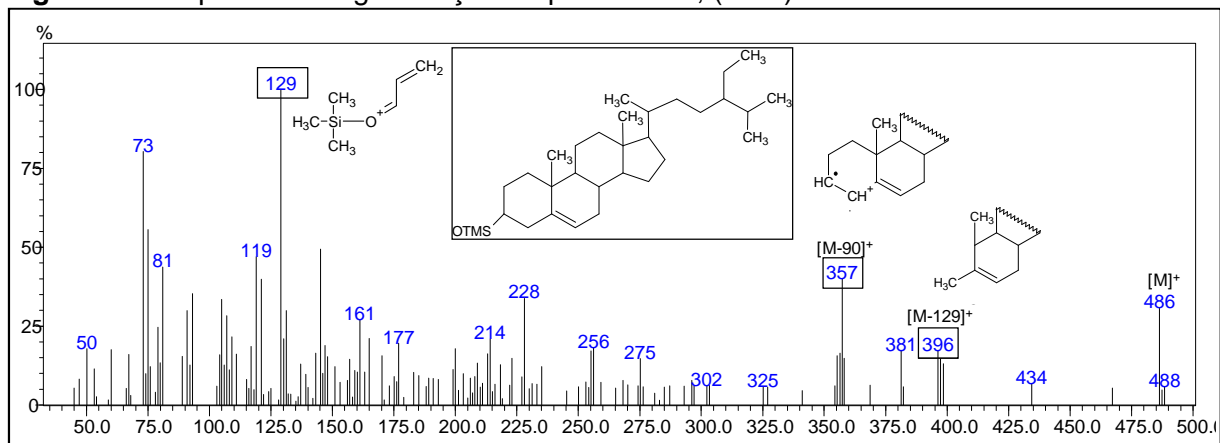
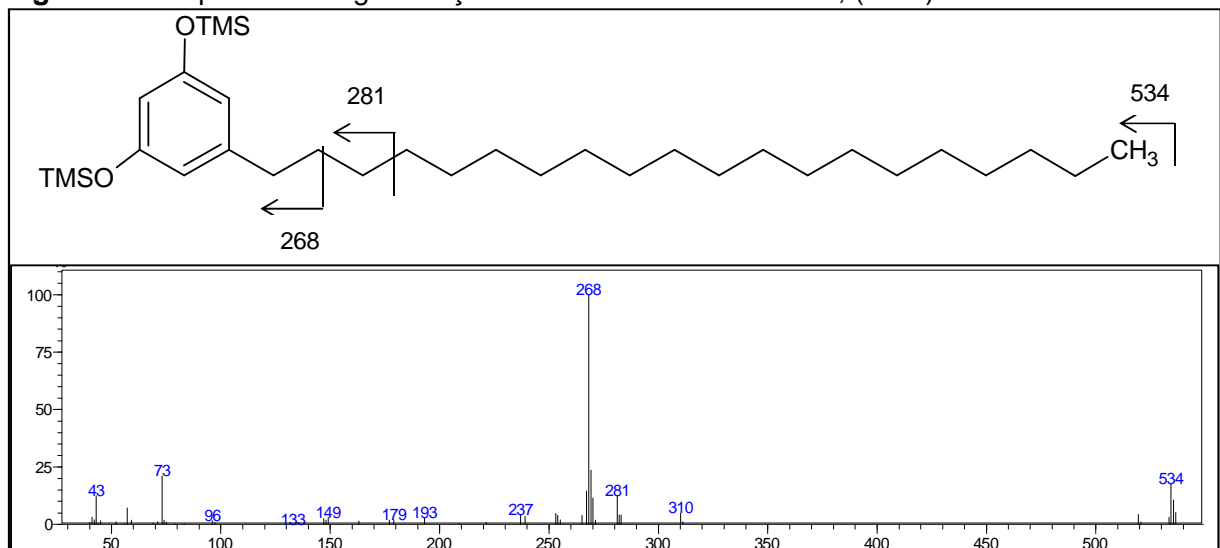


Figura 31: Proposta de fragmentação do heneicosanilresorcinol, (TMS).



## Resultados

**Tabela 4:** Fragmentos de massas característicos das principais classes de compostos identificados em cera epicuticular de folhas de cana-de-açúcar.

						M-15	M <sup>+</sup>
<b>alcanos</b>							
n heneicosano	43	57	71	85	99		296
n-tricosano	43	57	71	85	99		324
n-tetracosano	43	57	71	85	99		338
n-pentacosano	43	57	71	85	99		352
n-hexacosano	43	57	71	85	99		366
n-heptacosano	43	57	71	85	99		380
n-octacosano	43	57	71	85	99		394
n-nonacosano	43	57	71	85	99		408
n-hentriacontano	43	57	71	85	99		436
n-tritriacontano	43	57	71	85	99		464
<b>álcoois</b>							
n-hexadecanol	75	89	103	299			314
n-octadecanol	75	89	103	327			341
n-eneicosanol	75	89	103	355			370
n-docosanol	75	89	103	383			398
n-heptacosanol	75	89	103	453			468
n-dotriacontanol	75	89	103	523			538
n-tetratriacontanol	75	89	103	551			566
<b>ácidos graxos</b>							
Ácido Laurico	73	117	132	145	257		272
Ácido n-tridecanóico	73	117	132	145	271		286
Ácido mirístico	73	117	132	145	285		300
Ácido n-pentadecanóico	73	117	132	145	299		314
Ácido palmítoleico	73	117	132	145	311		326
Ácido palmítico	73	117	132	145	313		328
Ácido margárico	73	117	132	145	327		342
Ácido esteárico	73	117	132	145	341		356
Ácido n-nonadecanóico	73	117	132	145	355		370
Ácido araquídico	73	117	132	145	369		384
Ácido n-heneicosanoico	73	117	132	145	383		398
Ácido behênico	73	117	132	145	397		412
Ácido n-tricosanoico	73	117	132	145	411		426
Ácido n-tetracosanoico	73	117	132	145	425		440
Ácido n-pentacosanoico	73	117	132	145	439		454
Ácido n-hexacosanoico	73	117	132	145	453		468
Ácido n-heptacosanoico	73	117	132	145	467		482
Ácido n-octacosanoico	73	117	132	145	481		496
Ácido n-triacontanoico	73	117	132	145	509		524
Ácido n-dotriacontanoico	73	117	132	145	537		552
Ácido n-tetratriacontanoico	73	117	132	145	565		580
<b>Alquilresorcionol</b>							
AR C15:0	73	268	281				464
AR C16:0	73	268	281				478
AR C17:0	73	268	281				492
AR C18:0	73	268	281				506
AR C19:0	73	268	281				520
AR C20:0	73	268	281				534
AR C21:0	73	268	281				548
AR C23:0	73	268	281				576
AR C25:0	73	268	281				604
<b>Esteróides</b>							
colesterol	73	129	329	353	368	443	458
campesterol	73	129	255	343	382	457	472
estigmasterol	73	83	129	255	394	469	484
$\beta$ -sitosterol*	73	129	255	381	396	471	486

**Legenda:** TMS: trimetilsililano.



### 4.1.2 Dificuldades encontradas nas análises por GC-MS e GC-FID

Vários contaminantes foram identificados nas amostras analisadas. Entre eles destacam-se ftalatos, que podem ser oriundos de solventes e acessórios de plásticos utilizados na preparação das amostras, bem como alquilnitrilas e alquilamidas homologas, possivelmente decorrentes da contaminação das amostras por óleos lubrificantes utilizados em compressores de ar, moinhos e liofilizadores utilizados na preparação de amostras, ou até mesmo resultantes da contaminação da planta no campo por fumaça de escapamento de maquinário agrícola. Os picos cromatográficos relacionados a esses contaminantes estão indicados na **figura 26** pelos índices 1, 2 e 3, respectivamente. Estes constituintes foram removidos da planilha de dados utilizada na comparação do perfil químico de cera epicuticulares de cana-de-açúcar.

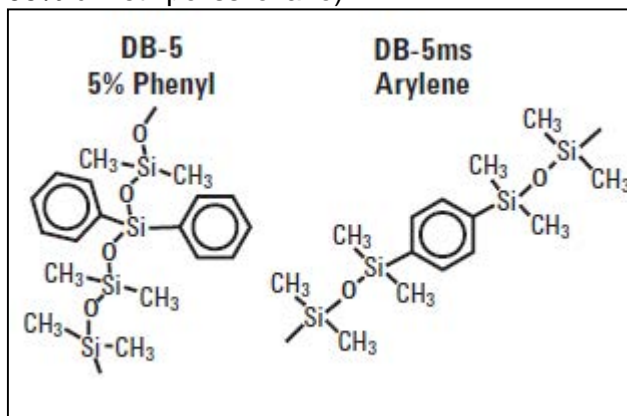
Após os cálculos, os índices de retenção obtidos nos dois sistemas cromatográficos foram comparados. Nessa comparação, de modo geral, foi possível relacionar os picos cromatográficos observados nos dois sistemas, com variação no  $IR \leq 5$  para alcanos, alcoóis e ácidos graxos homólogos. No entanto, quando comparados os IR obtidos para 5-alkil resorcinois, esteroides e triterpenos, foram encontradas diferenças de até 45 unidades (**Tabela 3**). Essas diferenças dificultaram uma transferência direta da identificação dos picos obtida por GC-MS para o GC-FID para análises de rotina. Para justificar essas diferenças foram averiguada diferenças/erros nas condições cromatográficas (temperatura do injetor e detector, modo de injeção, rampa de aquecimento e vazão do gás de arraste) entre o GC-FID e GC-MS, mesmo sabendo que essas diferenças deveriam ser corrigidas pelo IR, uma vez que as condições cromatográficas foram idênticas para os dois sistemas. Nenhum dessas hipóteses pode explicar as variações observadas no IR de alguns constituintes.

Outra hipótese verificada foi da coluna cromatográfica. Foram utilizadas colunas capilares: Supelco SPB-5 para o GC-FID e Phenomenex ZB-5MS para o GC-MS, as duas com 30 m de comprimento, 0,25 mm de diâmetro e 0,25  $\mu$ m de espessura de filme. As duas colunas são citadas em alguns catálogos como similares (5% difenil 95 dimetil polissiloxano), sendo a ZB-5MS utilizada para uso exclusivo em GC-MS, com baixo sangramento e melhoria no sinal-ruído. Entretanto as duas colunas são ligeiramente diferentes. As colunas ZB-5MS ou de marcas

## Resultados

diferentes como DB-5MS, HP-5MS, dentre outras possuem os grupos fenila inseridos no polímero de siloxano, enquanto nas colunas ZB-5, DB-5, HP-5 ou similares compostas por 5% difenil 95% dimetil polissiloxano, o grupo fenila aparece como uma ramificação na cadeia siloxanicas (**Figura 32**). Isso garante seletividade similar, mas não equivalente (AGILENT, 2010). As diferenças de resolução entre as colunas ZB-5MS e DB-5 são frequentemente observadas quando são analisados compostos aromáticos e compostos aromáticos com múltiplos anéis. Isso se deve ao fato da coluna ZB-5MS possuir melhor estabilidade térmica, menor sangramento, ligeiro aumento na seletividade para compostos aromáticos e conseqüentemente melhor resolução cromatográfica, como pode ser observado comparando-se os cromatogramas na região entre 45 e 60 minutos (**Figura 26**). Assim, conclui-se que as variações dos IR maiores que o limite de  $\pm 5$  unidades estabelecido na **Tabelas 3** são de fato ocorridos devido à coluna.

**Figura 32:** Estruturas das colunas capilares: DB-5 (5% difenil-95-dimetil polissiloxano) e DB-5MS (5% fenil arileno-95% dimetil polissiloxano).



Fonte: AGILENT, 2010

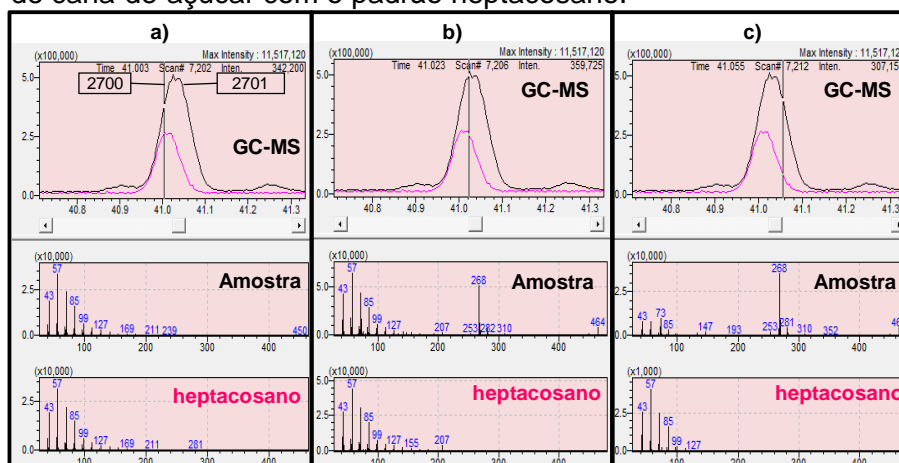
Outro problema encontrado foi na etapa de comparação dos IR experimentais com os IR da literatura. Em vários artigos verificam-se diferenças significativas nos valores dos IR experimentais com os da literatura, provavelmente devido à comparação de dados de colunas distintas, ou até mesmo a utilização da equação de IR Kovatz quando deveria ser utilizada a equação de VAN DEN DOOL E KRATZ ou vice-versa. Por isso recomenda-se atenção redobrada na comparação de índice de retenção.

Em amostras complexas, a comparação espectral deve atentar para a co-eluição de constituintes sob uma mesma banda cromatográfica. Na **Figura 33** é um

## Resultados

exemplo desse problema. O espectro de massas obtido no início do pico é idêntico ao do padrão heptacosano (**Figura 33a**), enquanto que o espectro de massas obtido no centro do pico é visivelmente resultante da sobreposição do espectro heptacosano com de outro constituinte (**Figura 33b**), sendo que o espectro deste ultimo pode ser observado no final do pico e corresponde possivelmente pentadecil diidroxibenzeno (**Figura 33c**). Para tentar caracterizar e eliminar esses possíveis problemas da coeluição e sobreposição dos espectros de massas e, assim diminuir a dificuldade de análise comparativa dos espectros de massas, é essencial nos futuros trabalhos a utilização de técnicas de deconvolução.

**Figura 33:** Comparação do pico em tR=41 minutos do cromatograma da análise de cera epicuticular de cana-de-açúcar com o padrão heptacosano.

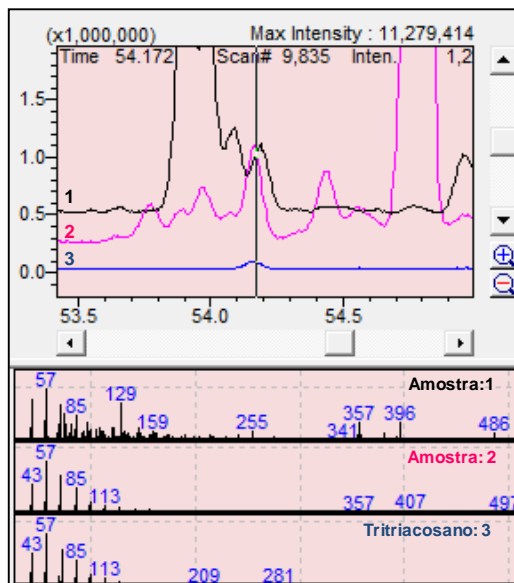


**Legenda:** a) espectro massas com cursor no início do pico; b) espectro de massa com cursor no meio do pico; c) espectro de massas com cursor no fim do pico.

Finalmente, observou-se constituintes distintos com o mesmo IR ocorrendo em amostras diferente. Por exemplo, as amostras IAC95-5000, IACSP94-2094 possuem constituinte que elui no tempo de retenção 54,175 minutos (IR = 3300), mas que apresentam espectros de massas diferentes (**Figura 34**). O constituinte relacionado a estas bandas foi  $\beta$ -sitosterol para a IAC95-5000 e triacotano para IACSP94-2094.

## Resultados

**Figura 34:** Comparação dos constituintes com tR = 54,172 minutos dos cromatogramas das análises de cera epicuticular de cana-de-açúcar das amostras IAC95-5000, IACSP94-2094 e do padrão tritriacontano.



**Legenda:** 1: Espectro de massas da amostra IAC95-5000; 2: espectro de massas da amostra IACSP94-2094; 3: espectro de massas do padrão tritriacontano.

Considerando o exposto acima, é importante destacar que a análise qualitativa de constituintes orgânicos em amostras complexas demanda alguns cuidados:

- utilizar pelo menos dois parâmetros distintos, sendo pelo menos uma informação de retenção e uma espectral;
- na informação de retenção, usar índices de retenção validados para minimizar erros derivados de oscilações nos parâmetros cromatográficos;
- a comparação de índices de retenção só pode ser feita se as colunas cromatográficas (experimental x literatura) tiverem as mesmas características no que diz respeito a FE, dimensões e modo de eluição (isotérmico ou gradiente de temperatura).
- certificar-se de que os constituintes não são resultados de contaminações da amostra;
- na informação espectral, verificar-se a similaridade com a base de dados utilizada, diferentes bases de dados podem dar informações espectrais distintas, como a faixa da massa de aquisição e intensidade dos fragmentos resultando em menor similaridade com o constituinte comparado.

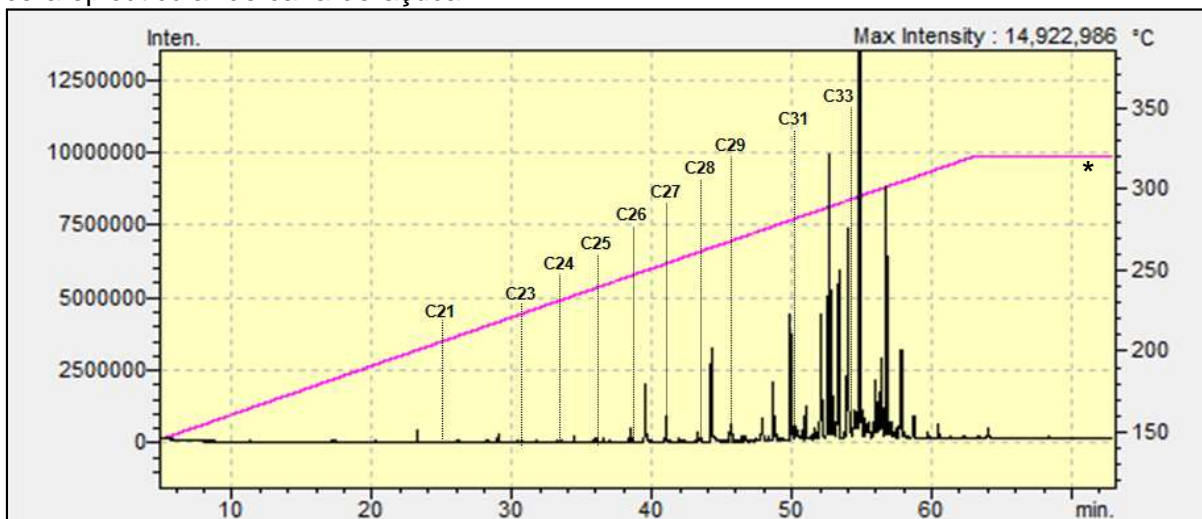
### 4.1.3 Comparação de alguns cultivares de cana-de-açúcar em relação composição da cera epicuticular de folhas.

Para visualizar melhor a distribuição e variação dos constituintes identificados nos vários cultivares estudados, construiu-se o gráfico de barra das áreas normalizadas para cada série homóloga.

Os hidrocarbonetos identificados foram todos de cadeias longas C21, C23, C24, C25, C26, C27, C28, C29, C31 e C33 (**Figura 35**). Observa-se grande variação na área normalizada da série homóloga dos hidrocarbonetos de cada amostra e nas séries de diferentes cultivares. Os hidrocarbonetos majoritários variaram de acordo com a amostra, sendo o heptacosano (C27) majoritário para as amostras IAC87-3396, IACSP93-3046, IACSP95-3028, RB845210 e RB72454, enquanto que o hentriacontano (C31) foi majoritário para as amostras IACSP95-5000, IACSP94-2094, SP89-1115, IACSP95-5094, IACSP94-2101, IACSP96-2042 e IACSP96-3060; e o hidrocarboneto tritriacontano (C33) foi majoritário para a amostra RB83-5486 (**Figura 36**). Há relatos na literatura que componentes de cera são diferentes para diferentes espécies de plantas. Por exemplo, a cera de cana-de-açúcar contém pequenas proporções de alcanos (cerca de 10 %) enquanto que ceras de folhas de *Cotyledon orbicularis* possuem grandes quantidades de alcanos. Em outro estudo, a análises de cera de pétalas e de folhas de diferentes espécies demonstraram que há variações nos constituintes majoritários, sendo que em algumas espécies os constituintes majoritários foram C27 e C29 e em outras espécies o C31 (EGLINTON; HAMILTON, 1967).

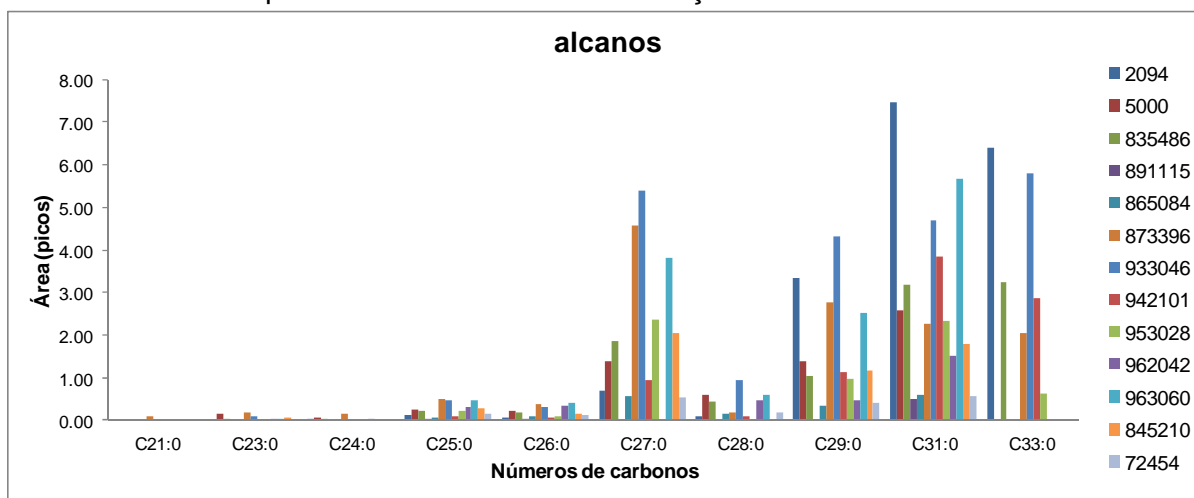
## Resultados

**Figura 35:** Indicação da série homóloga de hidrocarbonetos identificada em amostras de cera epicuticular de cana-de-açúcar.



**Legenda:** C<sub>n+1</sub>: número de átomos de carbono dos hidrocarbonetos. \*: rampa de programação linear de temperatura.

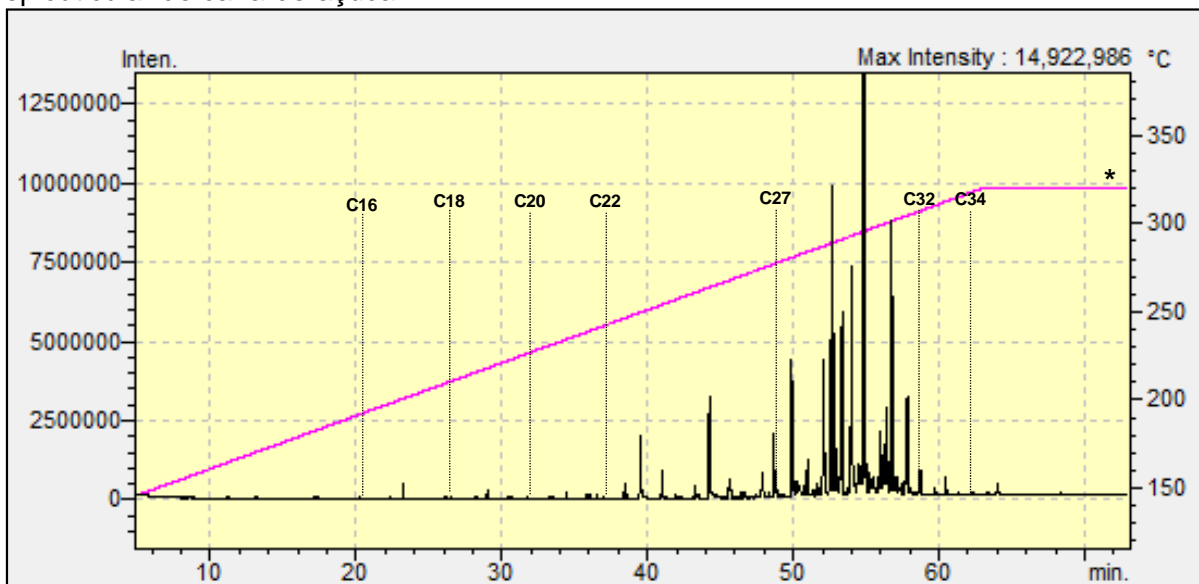
**Figura 36:** Comparação do teor relativo da série homóloga de hidrocarbonetos identificados na análise de cera epicuticular de folha de cana-de-açúcar.



Os alcoóis graxos homólogos (policosanóis) identificados foram C16, C18, C20, C22, C27, C32 e C34 (**Figura 37**), sendo que o dotriacontanol (C32) é o policosanol presente em maior teor na maioria das amostras analisadas (**Figura 38**). Irmak et al (2006) identificaram série homóloga de policosanóis de C20 a C30 em cera de casca, folha e palha de cana-de-açúcar, relatando o policosanol C28 como constituinte majoritário. A quantidade de cera extraída variou de 270 mg/kg em casca a 181 mg/kg para folhas e palhas.

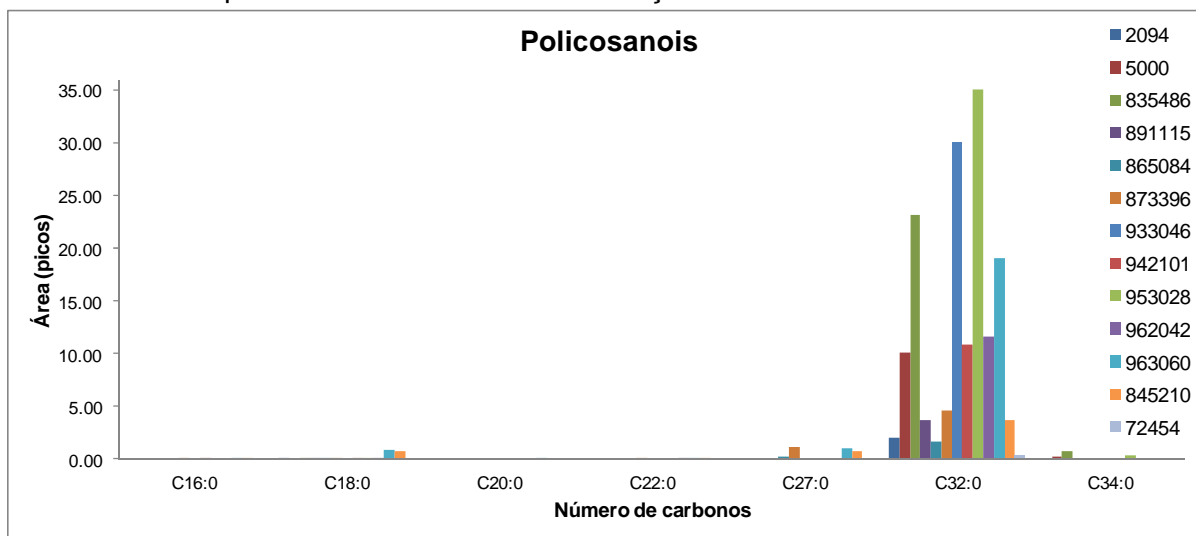
## Resultados

**Figura 37:** Indicação da série homóloga de alcoóis identificado em amostras de cera epicuticular de cana-de-açúcar.



**Legenda:** C<sub>n+1</sub>: número de átomos de carbono do álcool. \*: rampa de programação linear de temperatura.

**Figura 38:** Comparação do teor relativo da série homóloga de alcoóis identificados na análise de cera epicuticular de folha de cana-de-açúcar.



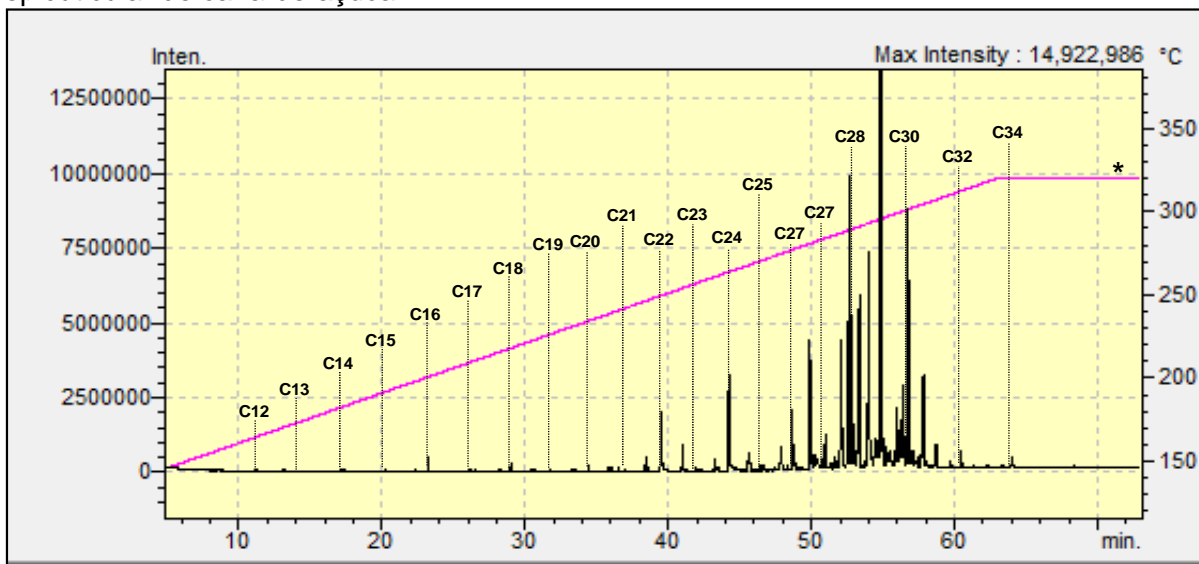
Vários ácidos graxos homólogos foram identificados na cera epicuticular (**Figura 39**). Os ácidos graxos majoritários variam de acordo com o cultivar, sendo o ácido tetracosanóico majoritário em: IACSP95-5000, IACSP94-2094, SP89-1115, IACSP95-5094, IACSP93-3046, IACSP94-2101, IACSP96-2042, RB845210, RB72454 e o ácido octacosanóico majoritário em: IACSP95-3028, IACSP96-3060, IAC87-3396 e RB83-5486 (**Figura 40**). Gonzalez et al (1997) desenvolveu



## Resultados

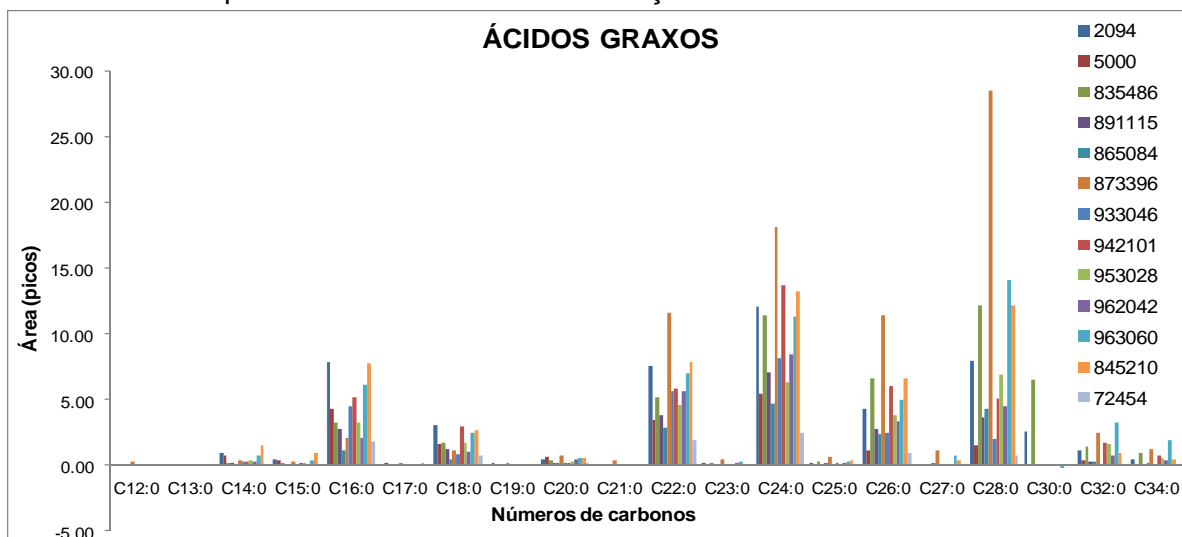
(patenteou) um método para a obtenção de misturas de ácidos graxos a partir da cera de cana-de-açúcar.

**Figura 39:** Indicação da série homóloga de ácidos graxos identificado em amostras de cera epicuticular de cana-de-açúcar.



**Legenda:** C<sub>n+1</sub>: número de átomos de carbono do álcool. \*: rampa de programação linear de temperatura.

**Figura 40:** Comparação do teor relativo da série homóloga de ácidos graxos identificados na análise de cera epicuticular de folha de cana-de-açúcar.



Os alquilresorcinóis homólogos identificados nos cultivares de cana-de-açúcar estudados possuem cadeias alifáticas longas com C15, C16, C17, C18, C19, C20, C21, C23, C25 (**Figura 41**), sendo que 5-heptadecilresorcinol, 5-heneicosilresorcinol

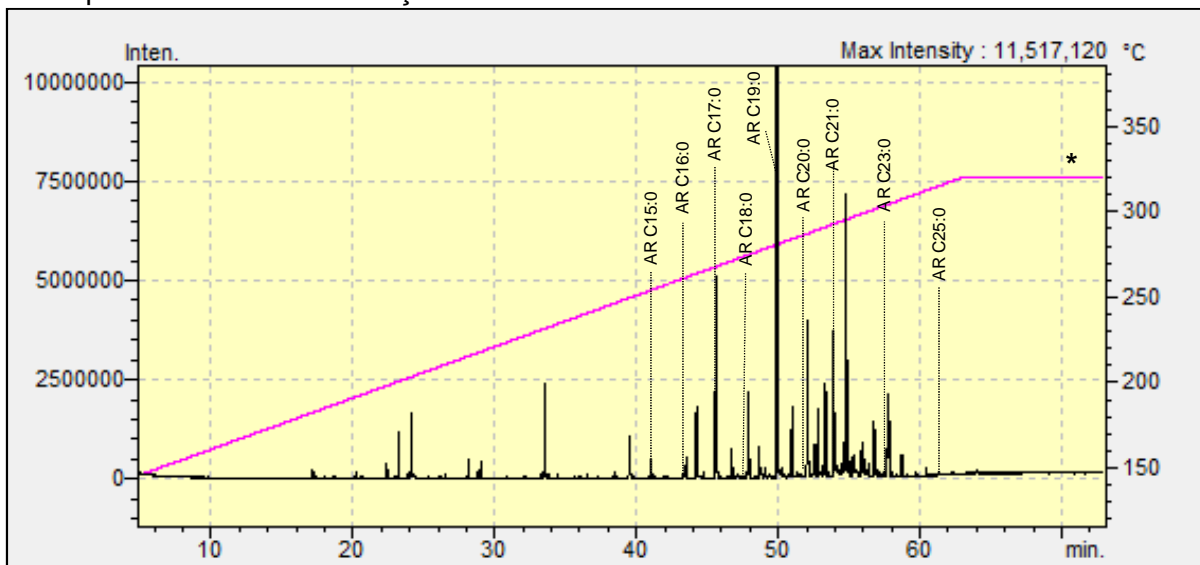


## Resultados

e 5-nonadecilresorcinol são aqueles presente em maior teor nas ceras estudadas (Figura 42).

Os alquilresorcinóis tem grande potencial como biomarcador para consumo de grãos, havendo muito interesse em sua composição para a dieta humana. Em análises de extratos de cereais foram encontradas série homólogas de alquilresorcinois de C15, C17, C19, C21, C23, C25. Sendo o alquilresorcinol C19:0 majoritários para o centeio e C20:0 para o trigo. (ROSS et al., 2003; KNÖDLER et al., 2008). Knödler et al., (2007), em outro estudo relataram que os alquilresorcinois desempenham papel importante na proteção contra fitopatógenos. Em outra pesquisa Knödler considerou os alquilresorcinóis isolados de casca da manga verde responsáveis pela resistência a *Alternaria alternata*, um fungo causador da doença de manchas preta concêntricas pequenas em frutos de manga (KNÖDLER et al., 2007; TAVARES, 2005).

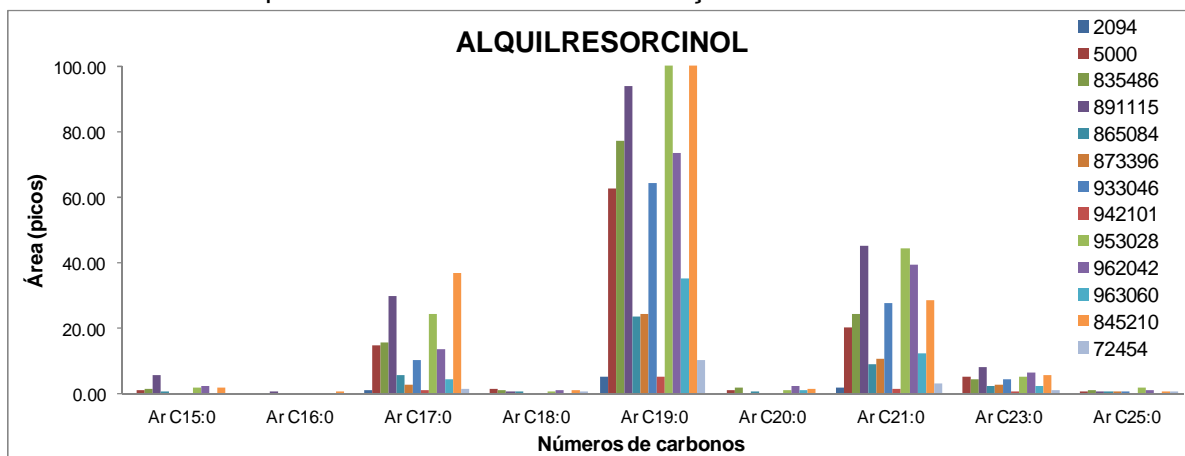
**Figura 41:** Indicação da série homóloga de alquilresorcinóis identificado em amostras de cera epicuticular de cana-de-açúcar.



**Legenda:** AR: Alquilresorcinol;  $C_{n+1}$ : número de átomos de carbono do Alquilresorcinol.  
\*: rampa de programação linear de temperatura.

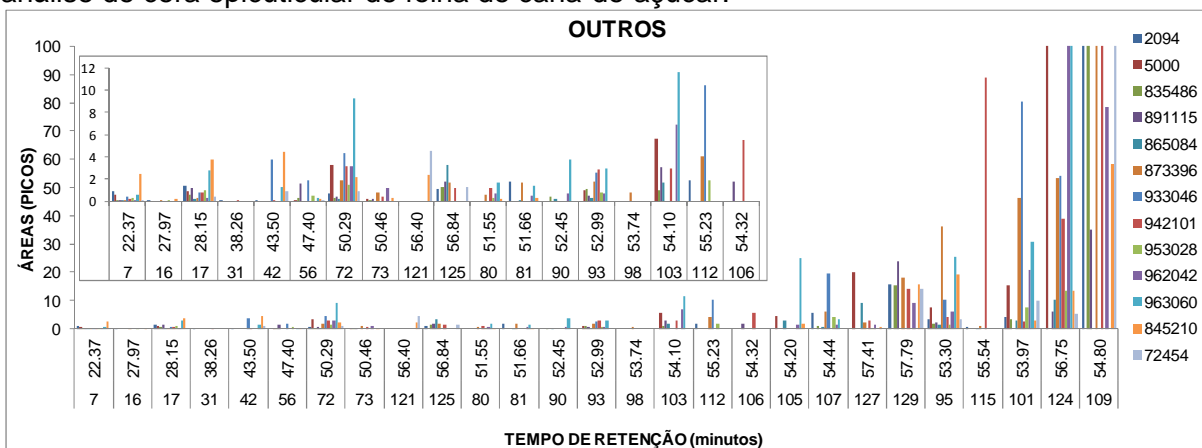
## Resultados

**Figura 42:** Comparação do teor relativo da série homóloga de alquilresorcinol identificados na análise de cera epicuticular de folha de cana-de-açúcar.



Outros constituintes de cera epicuticular de cana-de-açúcar tiveram proposta de identificação e incluem os ácidos graxos insaturados ácido palmítico C16:1, ácido linoléico C18:2, ácido oleico C18:1, o monoglicerídeo monopalmitina e o esqualeno. Adicionalmente foram identificados alguns esteróides (colesterol, campesterol, estigmasterol,  $\beta$ -sitosterol) e triterpenos ( $\beta$ -amirina e friedelina) (**Figura 43**). Estas substâncias já foram relatadas em torta de filtro e em cera de cana-de-açúcar (GOERGES et al., 2006; NUISSIER et al., 2002 e DESHMAN, 1971).

**Figura 43:** Comparação do teor relativo de compostos com proposta de identificação da análise de cera epicuticular de folha de cana-de-açúcar.

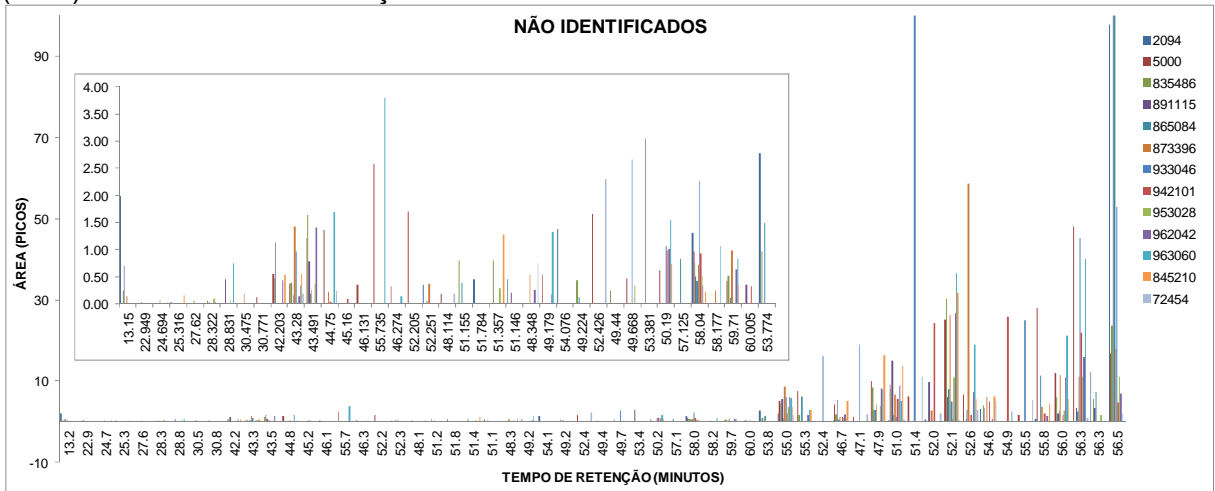


**Legenda:** 7: ácido palmítico (C16:1), 16: ácido linoléico (C18:2), 17: ácido oleico (C18:1), 31: monopalmitina, 42: esqualeno, 56, 95, 98, 101, 106, 107, 115, 121 e 129: possíveis triterpenóides, 72: colesterol, 73:  $\alpha$ -tocoferol, 90: campesterol, 93: estigmasterol, 105:  $\beta$ -sitosterol, 80, 81, 103, 109, 124 e 127: possíveis esteróides, 112:  $\beta$ -amirina e 125: friedelina.

## Resultados

Várias substâncias ainda não puderam ser identificadas embora algumas delas foram encontradas em grande quantidade nas amostras estudadas (**Figura 44**).

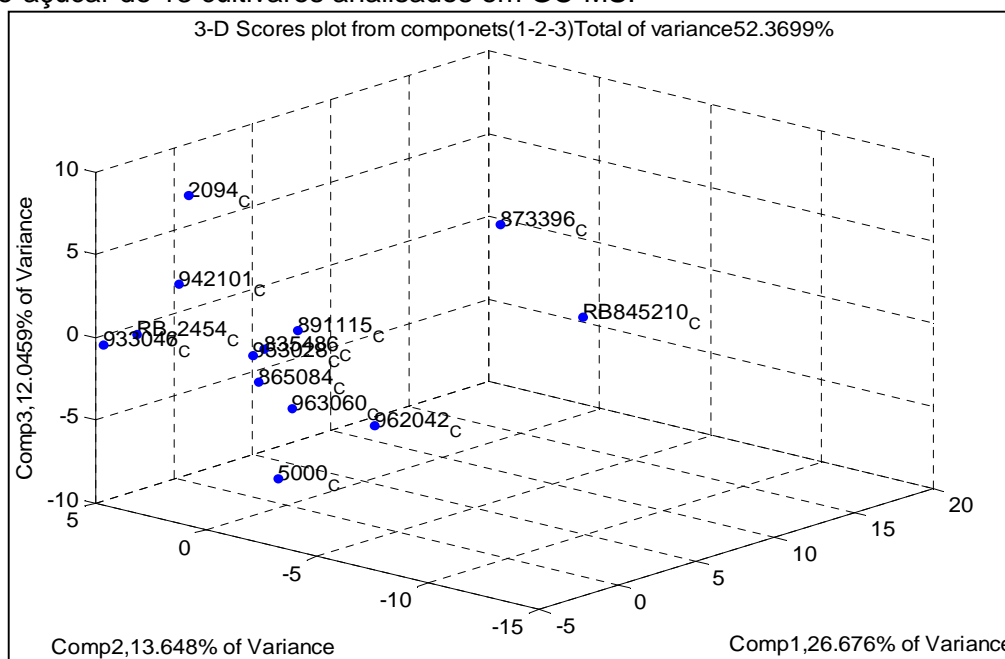
**Figura 44:** Comparação do teor relativo de compostos não identificados em cera epicuticular (TMS) de folha de cana-de-açúcar.



### 4.1.3.1 Classificação dos cultivares estudados por PCA em função da composição da cera epicuticular.

No gráfico de scores 3D PC1 x PC2 x PC3 (**Figura 45**), há dificuldade em visualizar e conseqüentemente propor agrupamentos de cultivares analisados em função da composição química da cera epicuticular.

**Figura 45:** Gráfico de 3D scores da PCA das análises da cera epicuticular de folhas de cana-de-açúcar de 13 cultivares analisados em GC-MS.

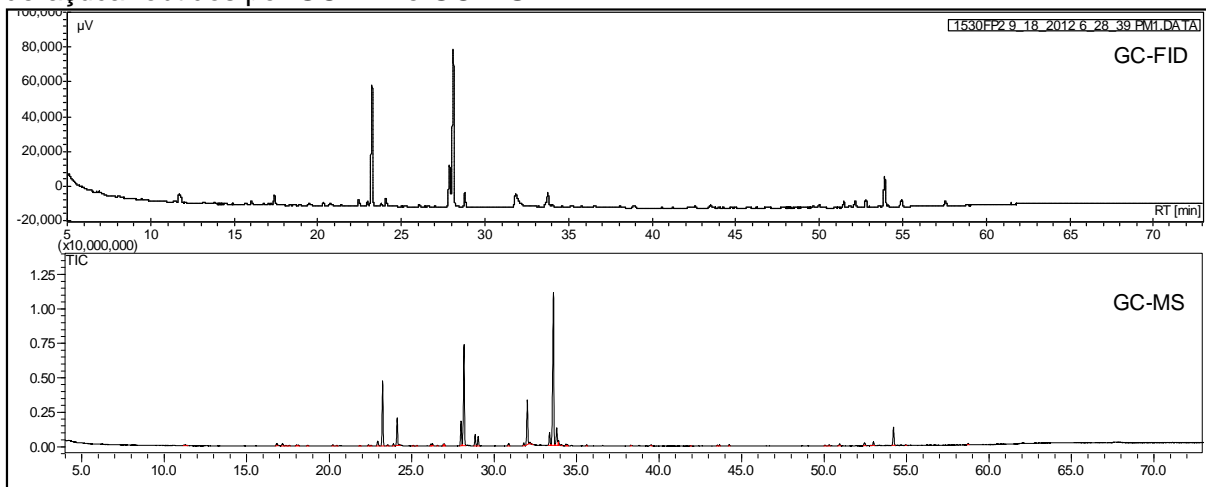


## 4.2 Análises qualitativas do extrato hexânico de folhas de cana-de-açúcar

A análise qualitativa de metabólitos apolares presentes nos extratos hexânicos de folhas de cana-de-açúcar foi feita para amostras de 16 cultivares (**Tabela 2**), analisados em duplicatas, tanto GC-FID como por GC-MS (**Figura 46**).

## Resultados

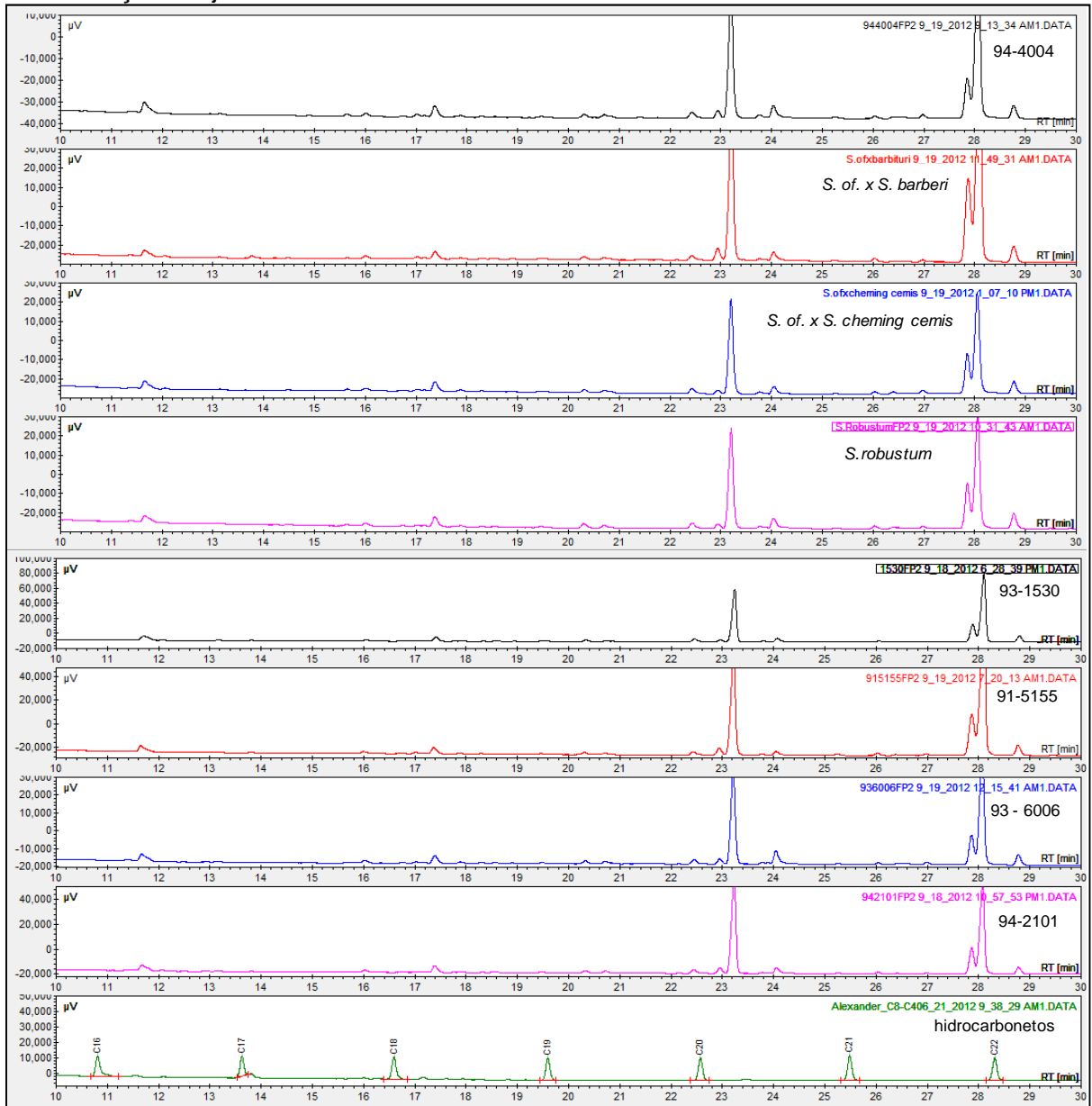
**Figura 46:** Exemplo de perfil cromatográfico de extrato hexânico (TMS) de folhas de cana-de-açúcar obtidos por GC-FID e GC-MS.



A comparação dos perfis cromatográficos obtidos para os 16 cultivares analisados revelaram diferenças significativas na constituição química. A fim de facilitar a visualização dessas diferenças, os cromatogramas foram ampliados em duas partes, isto é, de 10 a 30 minutos (**Figura 47 e 48**) e 30 a 65 minutos (**Figura 49 e 50**).

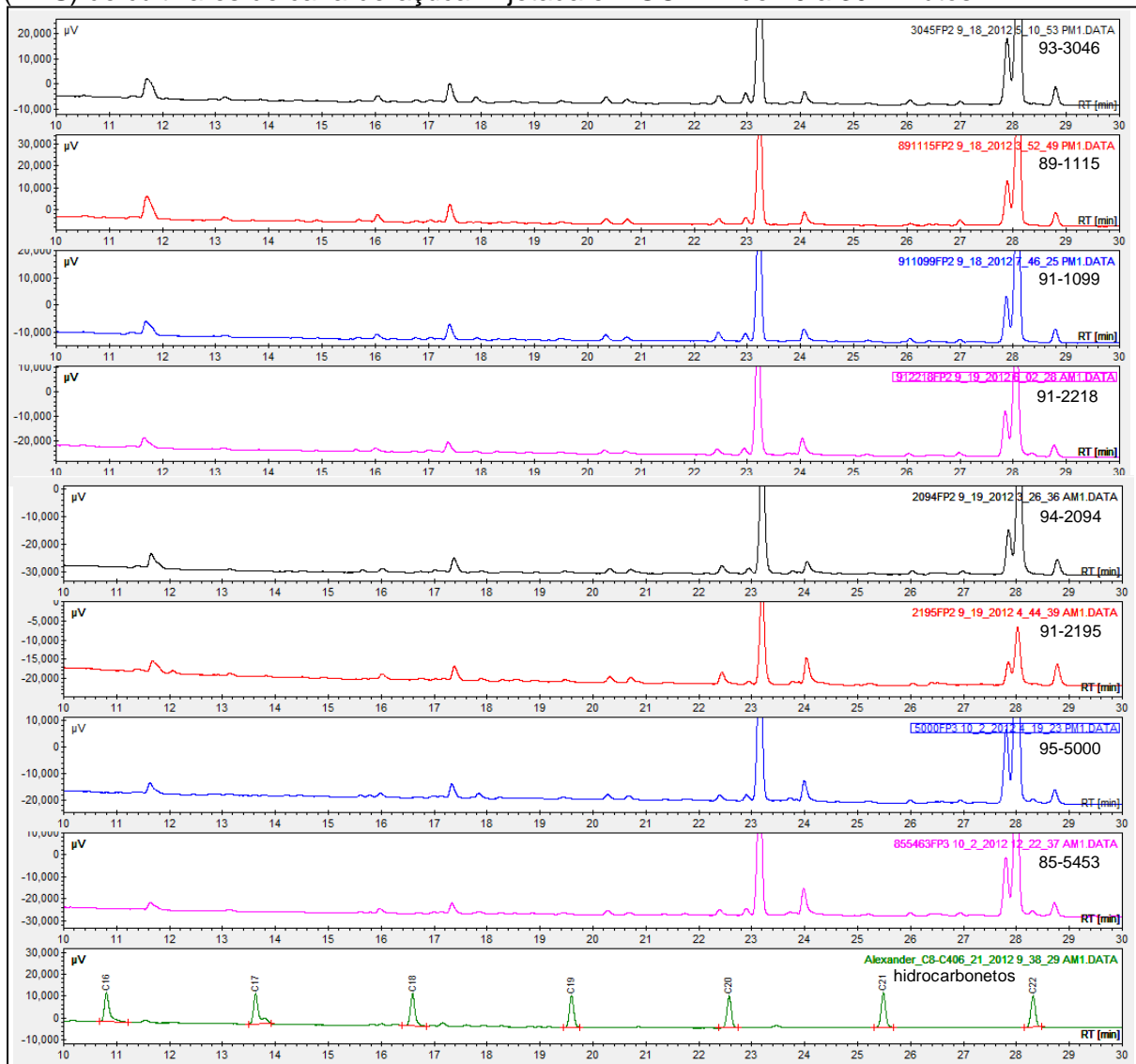
## Resultados

Figura 47: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 10 a 30 minutos.



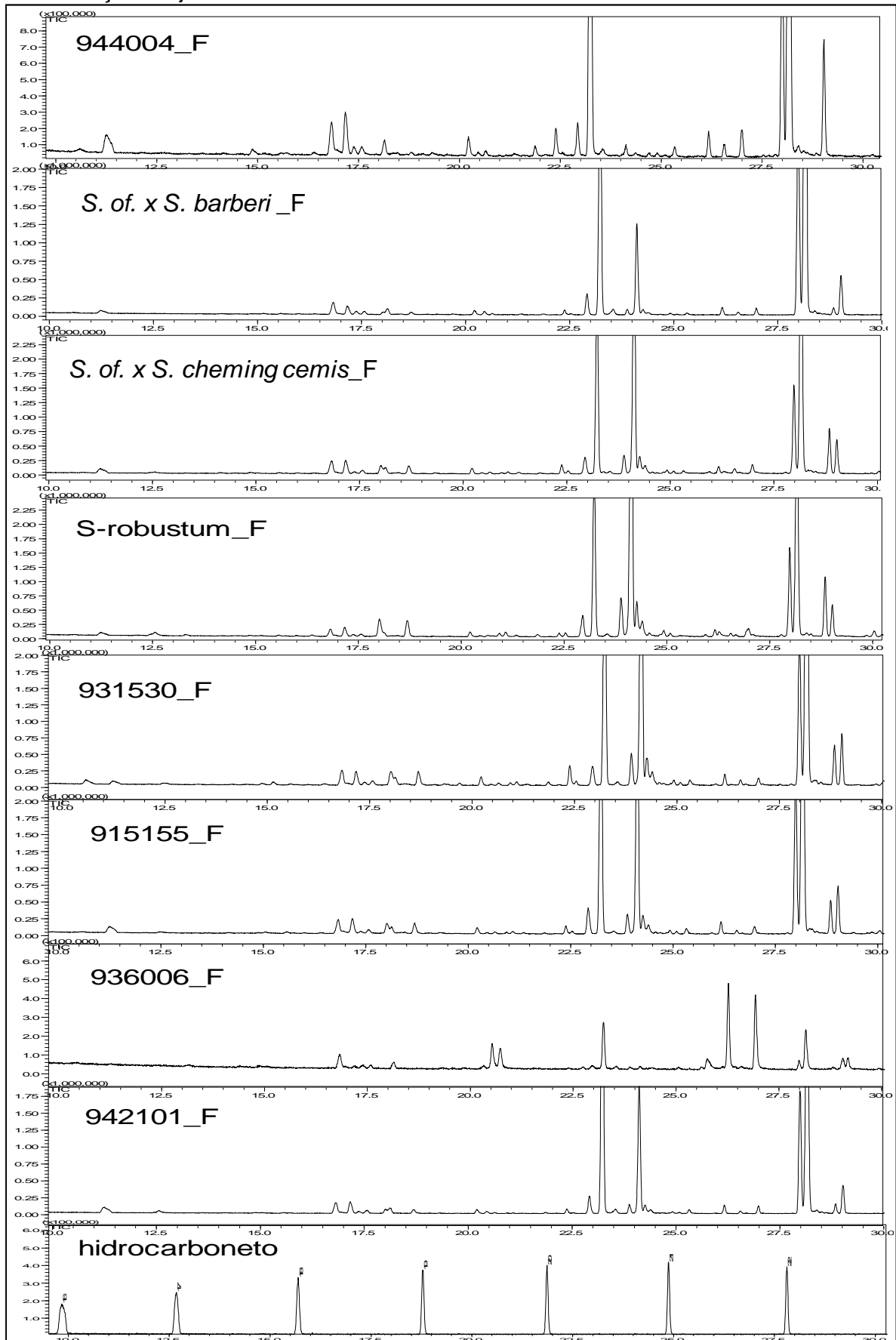
## Resultados

Continuação da Figura 47: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 10 a 30 minutos.



## Resultados

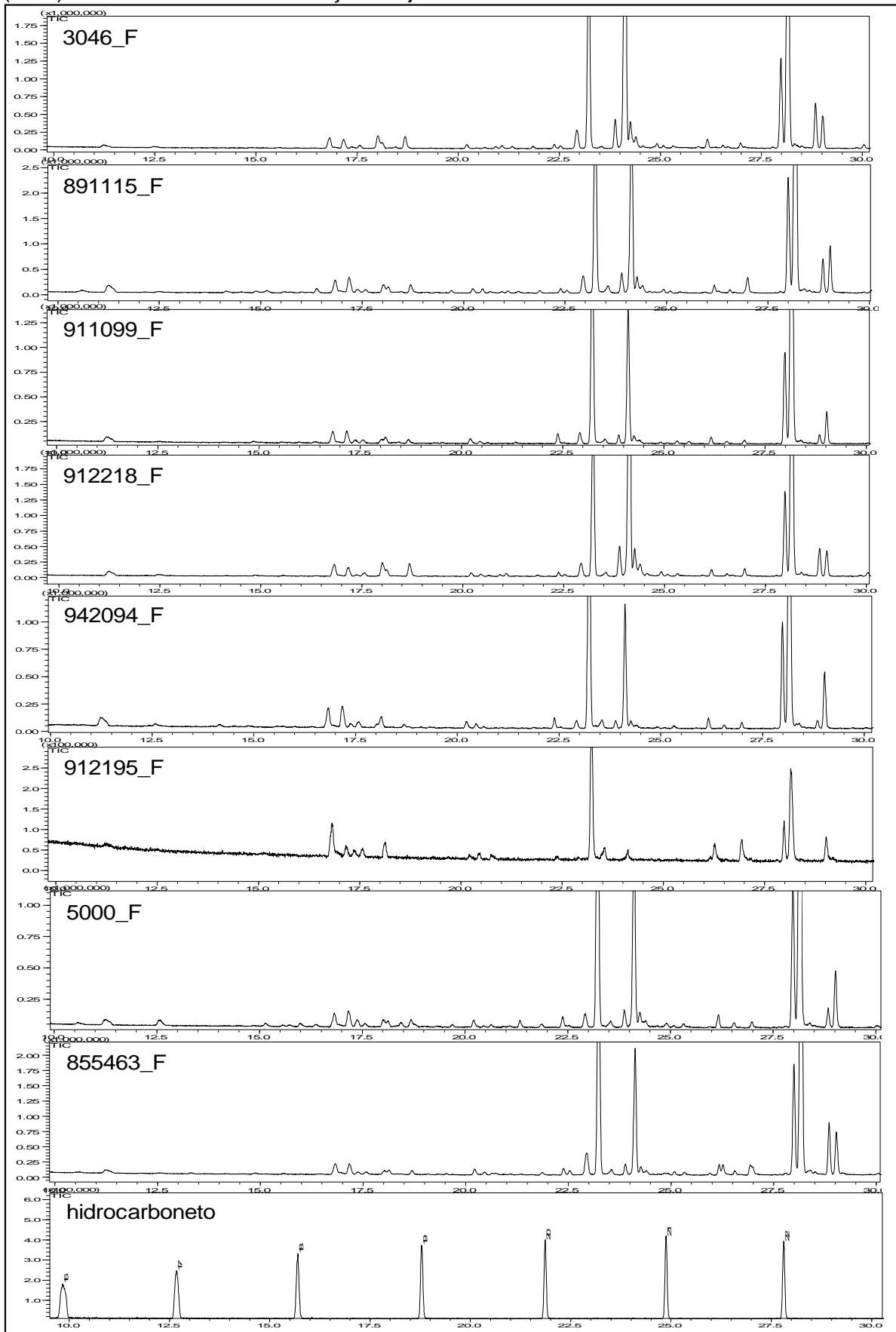
**Figura 48:** Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 10 a 30 minutos.





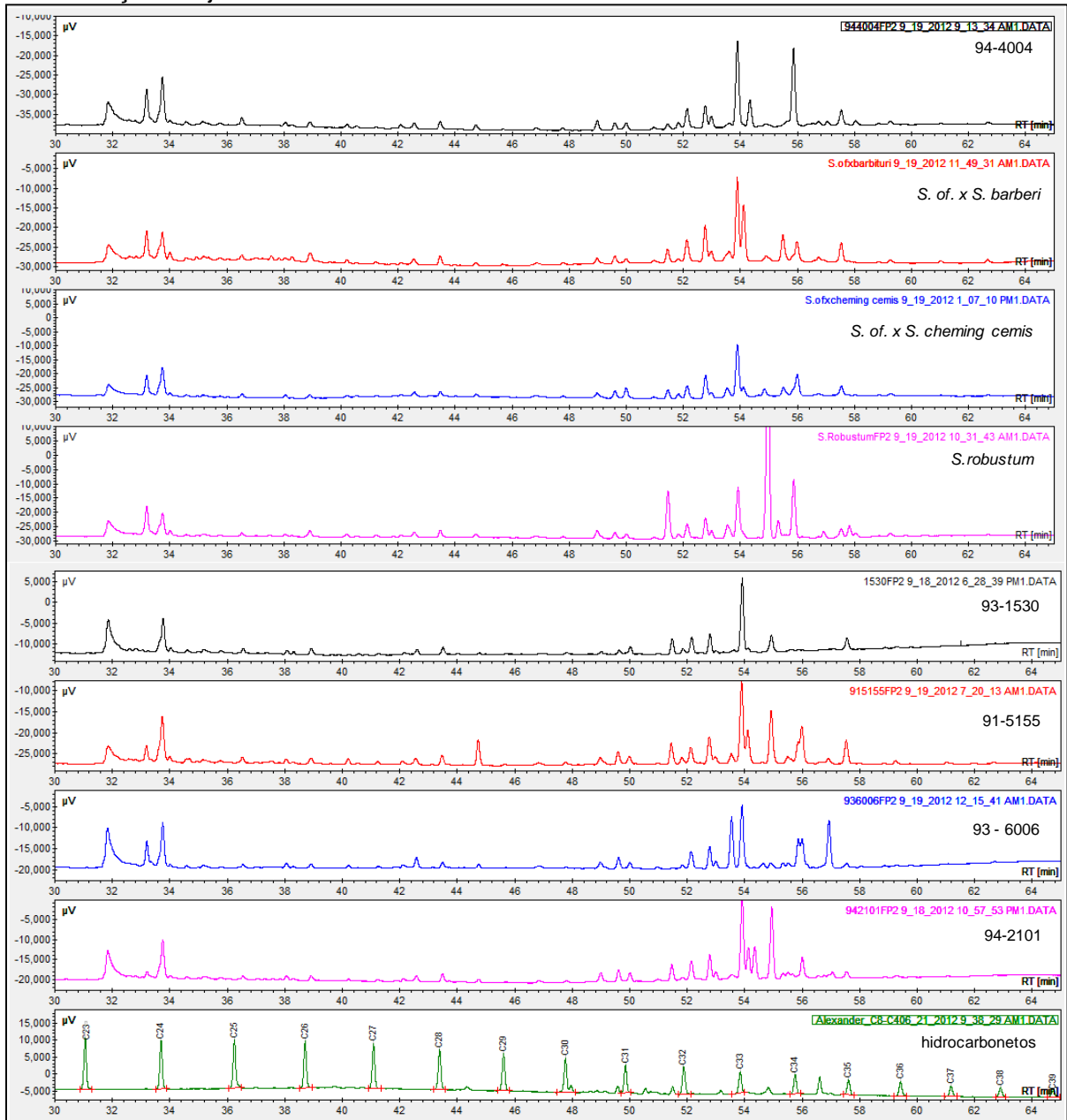
## Resultados

Continuação da Figura 48: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 10 a 30 minutos.



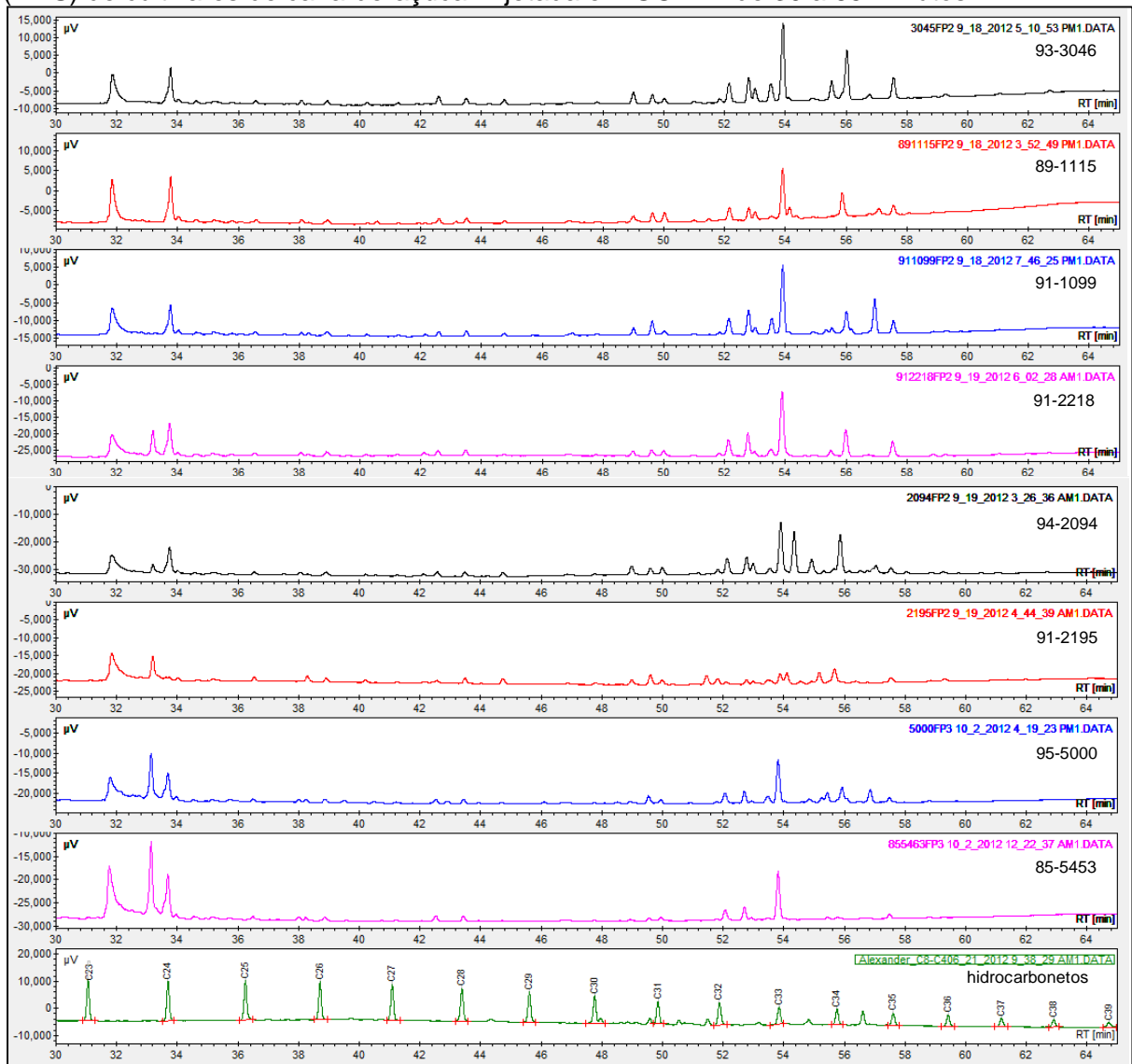
## Resultados

Figura 49: Cromatogramas ampliados da análise extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 30 a 65 minutos.



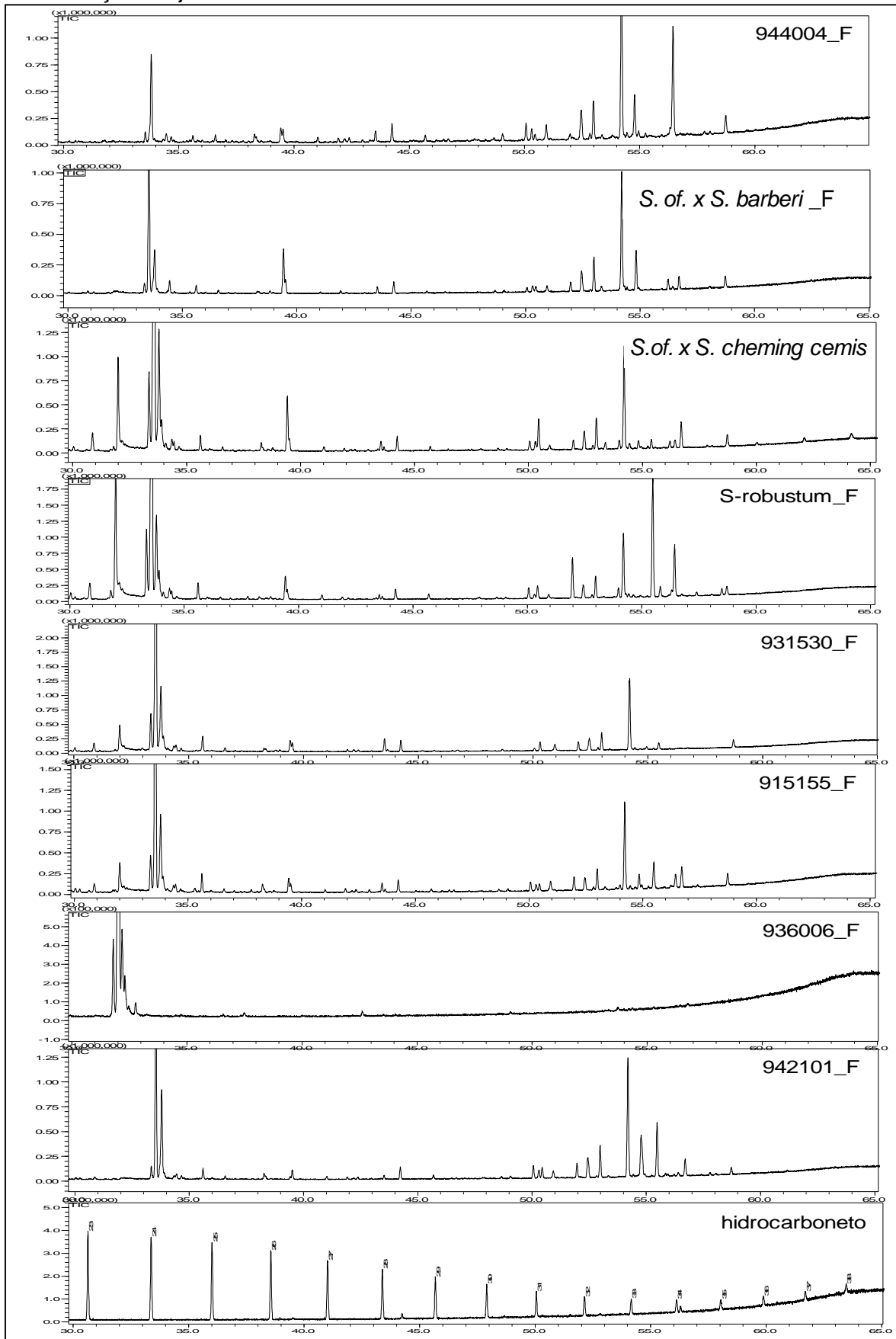
## Resultados

Continuação da Figura 49: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-FID de 30 a 65 minutos.



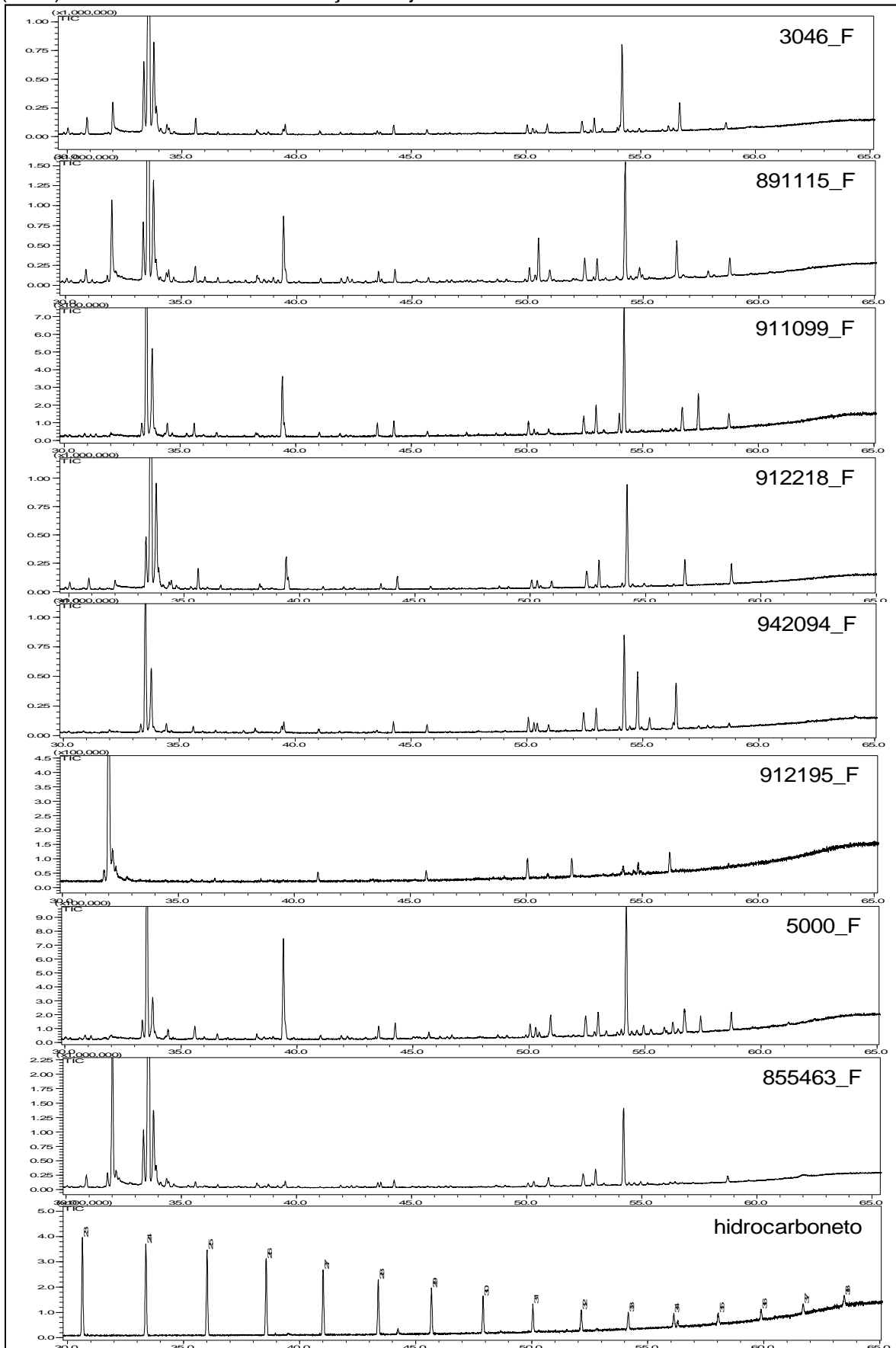
## Resultados

**Figura 50:** Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 30 a 65 minutos.



## Resultados

Continuação da Figura 50: Cromatogramas ampliados da análise do extrato hexânico (TMS) de cultivares de cana-de-açúcar injetada em GC-MS de 30 a 65 minutos.



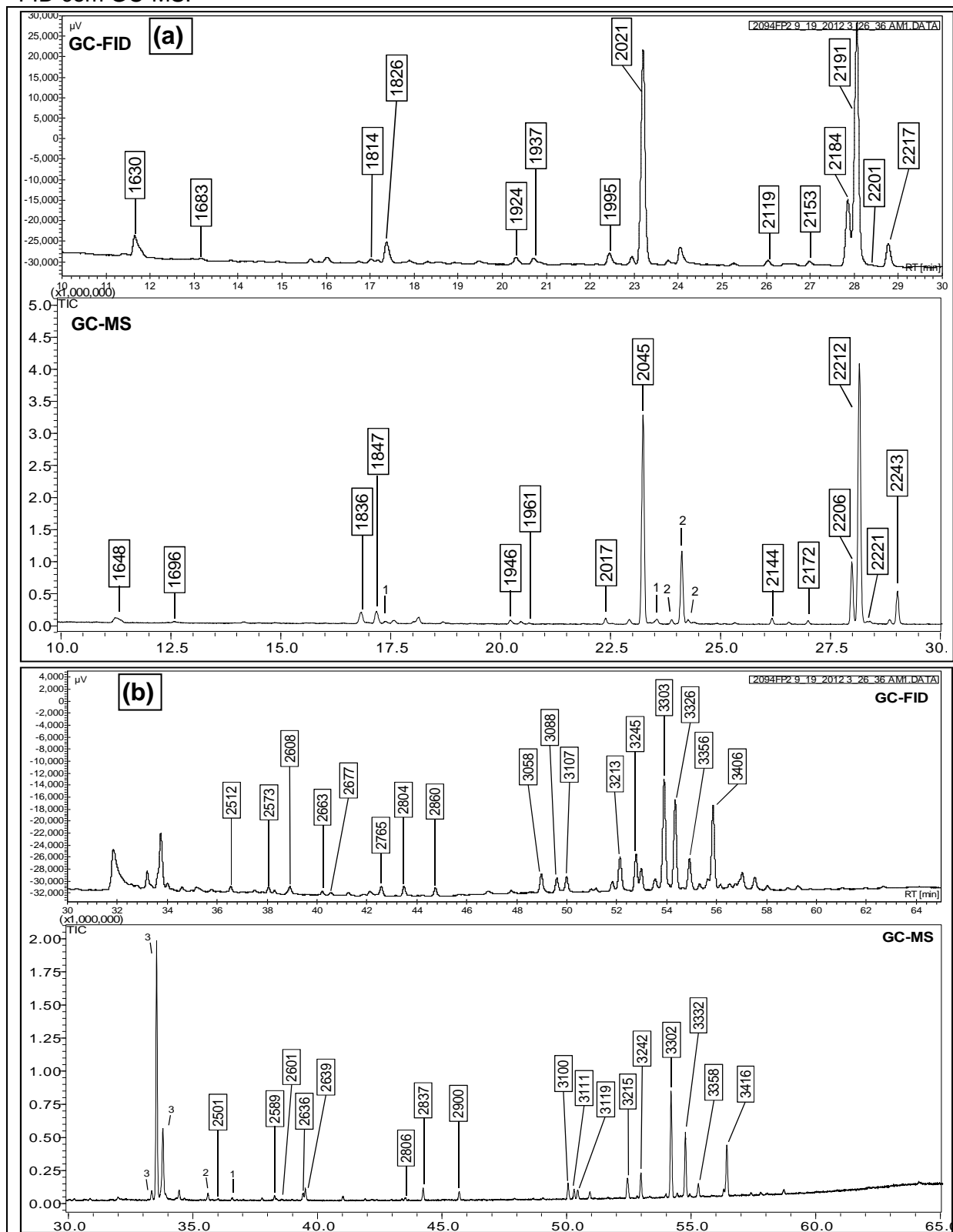
### 4.2.1 Identificação dos constituintes apolares do extrato hexânico por índice de retenção (IR) e espectrometria de massas (EM).

Para a identificação de constituintes do extrato hexânico de folhas de cultivares de cana-de-açúcar foi utilizado o IR de cada constituinte, calculado utilizando a **equação 1** e alcanos homólogos C8-C40 como referência, e os respectivos espectros de massas, ambos obtidos por GC-MS, seguindo a mesma estratégia relatada em detalhes no **item 4.1.1**.

A comparação dos dados de retenção e espectros de massas experimentais com os dados da literatura possibilitaram a identificação tentativa de 41 constituintes dos 65 detectados por GC-MS (**Figura 51**). Entre estes constituintes encontram-se vários homólogos de alcanos de cadeia linear, alcoóis e ácidos graxos, além de alguns esteroides e triterpenos (**Tabela 5**).

## Resultados

**Figura 51:** Comparação do perfil cromatográfico e do IR entre os tempos de retenção de 10 a 30 minutos (a) e de 30 a 65 minutos (b) das análises do extrato hexânico (TMS) de GC-FID com GC-MS.



**Legenda:** 1: fitalato; 2: alquil oleonitrila; 3: alquil oleamida

## Resultados

**Tabela 5:** Proposta de identificação dos constituintes do extrato hexânico (TMS) de folhas de cana-de-açúcar por comparação do IR das análises de GC-MS e GC-FID. Espectros de massas disponíveis no **anexo 4**, colocados em ordem crescente de retenção. Tabela contendo área de cada constituintes nos cultivares estudados esta disponível no **anexo 2**.

PICOS	GC-MS (coluna HP-5ms)			GC-FID (coluna SPB-5)			$\Delta$ IR	Identificação
	tR (min)	IR exp.	IR lit.	tR (min)	IR exp.	IR Lit.		
1	11.211	1648	1645	11.650	1630	<b>1649</b>	19	ácido láurico*
2	12.554	1696	1702	13.150	1683	<b>1702</b>	13	ácido subérico*
3	14.145	1749	1735	-	-	-	-	<i>cis</i> -ácido aconítico*
4	16.376	1822	1837	-	-	-	-	ácido isocitríco
5	16.82	1836	1840	17.020	1814	<b>1837</b>	22	neofitaadieno
6	17.166	1847	1843	17.380	1826	<b>1845</b>	21	ácido mirístico*
7	17.57	1861	-	-	-	-	-	-
8	18.095	1878	-	-	-	-	-	-
9	20.206	1946	1943	20.310	1924	<b>1945</b>	22	ácido pentadecanóico*
10	20.65	1961	1955	20.710	1937	-	23	hexadecanol*
11	22.382	2017	2023	22.430	1995	-	22	ácido palmitoleico*
12	22.933	2036	-	-	-	-	-	-
13	23.229	2045	2040	23.200	2021	<b>2047</b>	24	ácido palmítico*
14	25.329	2116	-	-	-	-	-	-
15	26.162	2144	2144	26.040	2119	<b>2144</b>	24	ácido margárico*
16	26.547	2157	2149	-	-	-	-	1-octadecanol*
17	26.981	2172	2181	26.980	2153	<b>2170</b>	19	fitol*
18	27.987	2206	2208	27.860	2184	<b>2210</b>	23	ácido linoléico*
19	28.158	2212	2218	28.060	2191	<b>2217</b>	22	<i>alfa</i> -ácido linolênico*
20	28.391	2221	2215	28.360	2201	<b>2221</b>	19	ácido oleico *
21	28.839	2236	-	-	-	-	-	-
22	29.014	2243	2248	28.780	2217	<b>2248</b>	26	ácido esteárico*
23	34.351	2437	-	-	-	-	-	-
24	34.433	2440	2447	-	-	-	-	ácido araquídico*
25	36.029	2501	2500	36.540	2512	<b>2500</b>	11	pentacosano
26	38.261	2589	2583/ 2606	38.050	2573	<b>2583/2606</b>	15	monopalmitin*
27	38.358	2592	-	-	-	-	-	-
28	38.581	2601	2600	-	-	-	-	hexacosano
29	39.424	2636	2610	40.210	2663	<b>2623</b>	28	sacarose*
30	39.505	2639	2632	40.540	2677	-	38	ácido behênico*
31	41.001	2700	2700	-	-	-	-	heptacosano
32	41.924	2739	2731	-	-	-	-	ácido tricosanoico*
33	42.974	2783	2773	-	-	-	-	monoestearina*
34	43.52	2806	2831	42.580	2765	<b>2824</b>	41	esqualeno
35	43.677	2813	-	-	-	-	-	-
36	44.239	2837	2834	43.480	2804	<b>2834</b>	33	ácido tetracosanóico*
37	45.676	2900	2900	44.730	2860	<b>2900</b>	40	nonacosano
38	48.665	3035	3035	48.980	3058	<b>3100</b>	22	ácido hexacosanóico*
39	49.887	3092	-	-	-	-	-	alquilresorcinol*
40	50.055	3100	3100	-	-	-	-	hentriacontano
41	50.288	3111	3155	49.610	3088	-	23	colesterol*
42	50.437	3119	3136	50.000	3107	<b>3149</b>	12	$\alpha$ -tocoferol*
43	50.94	3143	3136	-	-	-	-	octacosanol*
44	51.98	3193	-	-	-	-	-	-
45	52.44	3215	3204	52.140	3213	<b>3251</b>	2	campesterol*
46	52.81	3233	-	-	-	-	-	-
47	52.983	3242	3286	52.770	3245	<b>3286</b>	3	estigmasterol*
48	53.334	3259	-	-	-	-	-	-
49	53.978	3291	-	-	-	-	-	-
50	54.187	3302	3296	53.900	3303	<b>3348</b>	1	$\beta$ -sitosterol*
51	54.454	3315	-	-	-	-	-	-
52	54.78	3332	-	54.340	3326	-	6	-
53	54.831	3334	-	-	-	-	-	-



## Resultados

54	54.936	3340	3334	-	-	-	-	1-triacontanol*
55	55.294	3358	-	54.920	3356	-	2	-
56	55.48	3367	-	-	-	-	-	-
57	55.806	3384	-	-	-	-	-	-
58	56.206	3404	-	-	-	-	-	-
59	56.31	3410	-	-	-	-	-	-
60	56.429	3416	-	55.870	3406	-	10	-
61	56.696	3430	-	-	-	-	-	-
62	57.41	3467	-	-	-	-	-	-
63	57.805	3488	-	-	-	-	-	friedelina
64	58.501	3525	-	-	-	-	-	-
65	58.71	3536	3530	-	-	-	-	1-Dotriacontanol*

**Legenda:** **1:** índice de retenção usando coluna SPB-5; **2:** índice de retenção usando coluna ZB-5MS; \*: trimetilsil; **tR (min):** tempo de retenção em minutos; **IR cal:** índice de retenção calculado;  **$\Delta$ IR:** variação do índice calculado entre as duas colunas; **IR Lit.:** índice de retenção da literatura.

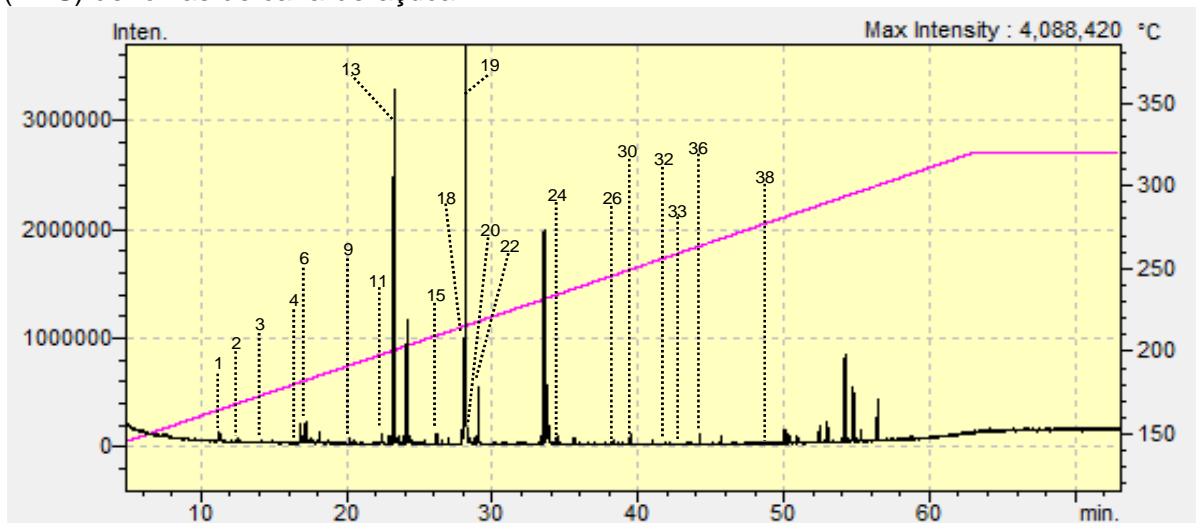
### 4.2.2 Comparação de alguns cultivares de cana-de-açúcar em relação composição do extrato hexânico de folhas.

A comparação de alguns cultivares de cana-de-açúcar em relação aos compostos obtidos a partir do extrato hexânico é discutida a seguir, iniciando-se pela análise da distribuição das classes de compostos homólogos identificados.

Diferentemente da cera epicuticular onde foram identificados praticamente apenas ácido graxos saturados homólogos, no extrato hexânico foram identificados ácidos graxos saturados e insaturados, como por exemplo, os ácidos: **15:** ácido margárico (C17:0) **18:** ácido linoleico (C18:2); **19:** ácido  $\alpha$ -linolênico (C18:1); **20:** ácido oleico (C18:0) (**Figura 52**).

## Resultados

**Figura 52:** Indicação dos ácidos graxos identificados em amostras dos extratos hexânicos (TMS) de folhas de cana-de-açúcar.



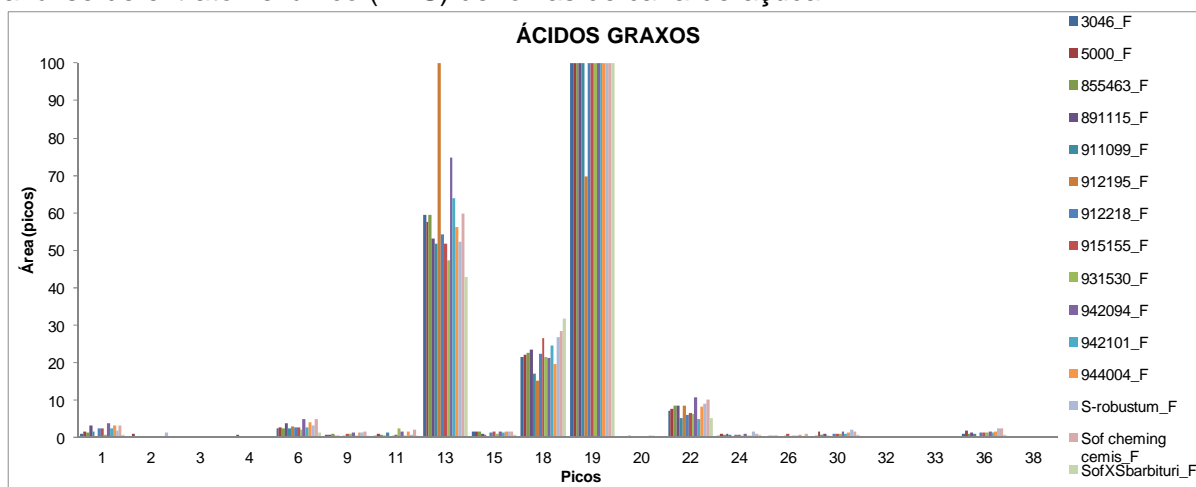
**Legenda:** 1: ácido láurico; 2: ácido subérico; 3: ácido *cis*-aconítico; 4: ácido isocítrico; 6: ácido mirístico; 9: ácido pentadecanóico; 11: ácido palmitoleico; 13: ácido palmítico; 15: ácido margárico; 18: ácido linoleico; 19: ácido  $\alpha$ -linolênico; 20: ácido oleico; 22: ácido esteárico; 24: ácido araquídico; 26: monopalmitina; 30: ácido behênico; 32: ácido tricosanóico; 33: monoestearina; 36: ácido tetracosanóico e 38: ácido hexacosanóico.

Os ácidos graxos presentes em maior teor foram, em ordem decrescente, ácido  $\alpha$ -linolênico (**19**), ácido palmítico (**13**), ácido linoleico (**18**), ácido esteárico (**22**) (**Figura 53**), sendo que a variação no teor dessas substâncias considerando os vários cultivares é visivelmente menor que a variação nos teores de ácidos graxos homólogos observada para cera epicuticular (**Figura 40**).

Os ácidos palmítico, ácido linoleico e ácido  $\alpha$ -linolênico são relatados como os principais ácidos extraídos de cera bruta de torta de filtro, apresentando atividade anti-inflamatória e analgésica em ensaios realizados em ratos (LEDÓN et al., 2007).

## Resultados

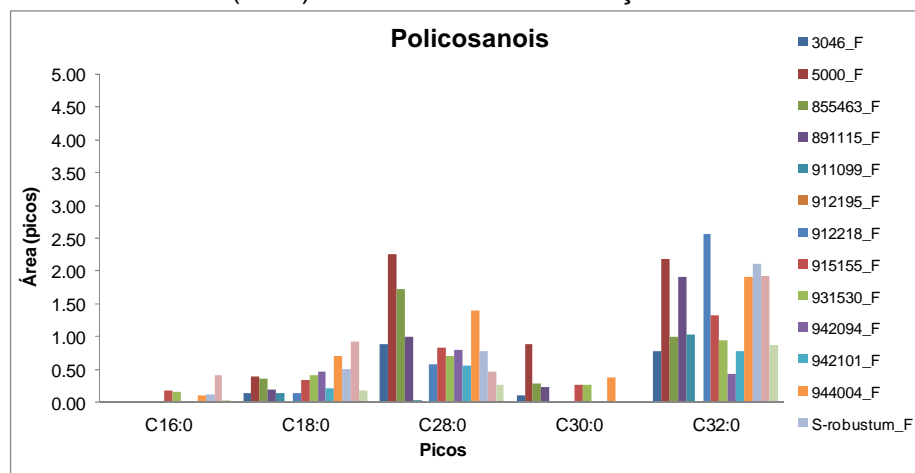
**Figura 53:** Comparação do teor relativo da série homóloga de ácidos graxos identificados na análise de extrato hexânico (TMS) de folhas de cana-de-açúcar.



**Legenda:** 1: ácido láurico; 2: ácido subérico; 3: ácido *cis*-aconítico; 4: ácido isocítrico; 6: ácido mirístico; 9: ácido pentadecanóico; 11: ácido palmitoleico; 13: ácido palmítico; 15: ácido margárico; 18: ácido linoleico; 19: ácido  $\alpha$ -linolênico; 20: ácido oleico; 22: ácido esteárico; 24: ácido araquídico; 26: ácido hexadecanóico, monopalmitina; 30: ácido behênico; 32: ácido tricosanóico; 33: Monoestearina; 36: ácido tetracosanóico e 38: ácido hexacosanóico.

Foram também identificados os policosanois C16, C18, C28, C30 e C32, Esses alcoóis de cadeia longa estão presentes no extrato hexânico como constituintes minoritários, sendo observadas grandes variações nos seus teores (**Figura 54**). Na cera epicuticular foi identificado praticamente só um policosanol, o dotriacontanol (C32), e em teor relativo significativamente maior do que em extrato hexânico (**Figura 38**).

**Figura 54:** Comparação do teor relativo da série homóloga de alcoóis identificados na análise de extrato hexânico (TMS) de folhas de cana-de-açúcar.

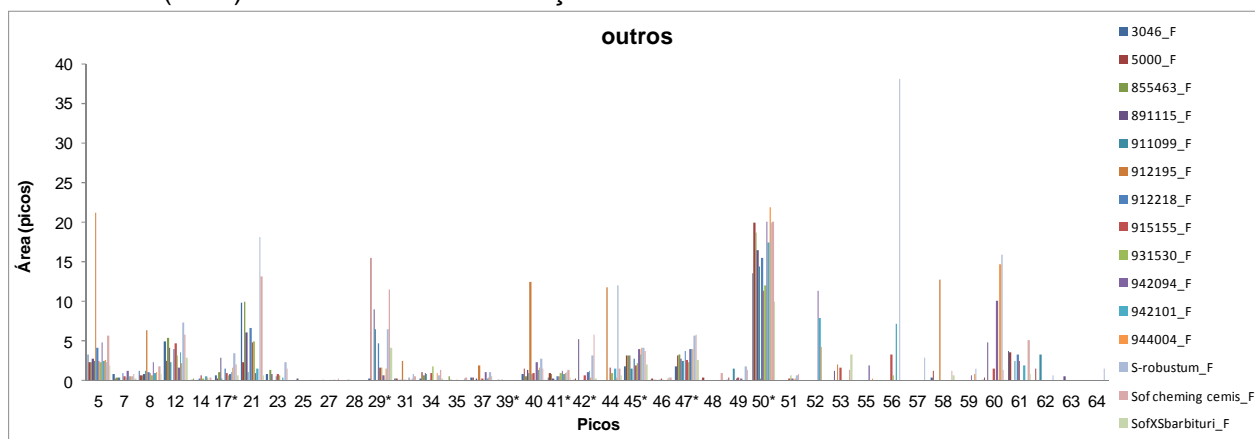


**Legenda:** 10: hexadecanol, 16: octadecanol, 43: octacosanol, 54: triacontanol, 65: dotriacontanol.

## Resultados

Outros constituintes como alcanos, triterpenóides e esteroides também foram detectados na análise de extrato hexânico de folhas de cana-de-açúcar, entre os quais é propostas a identificação de: neofitadieno (5), fitol (17), pentacosano (25), hexacosano (28), sacarose (29), heptacosano (31), esqualeno (34), nonacosano (37), alquilresorcinol C19:0 (39), hentriacontano(40), colesterol (41),  $\alpha$ -tocoferol (42), campesterol (45), estigmasterol (47),  $\beta$ -sitosterol (50), friedelina (63) (**Figura 55**). De acordo com Feng et al., (2014), os esteroides estigmasterol e  $\beta$ -sitosterol foram relatados como os principais esteroides e o campesterol e colesterol sendo os constituintes minoritários que foram identificados em uma avaliação de diferentes partes de cana-de-açúcar. No gráfico de barra das áreas normalizadas verifica-se que houve grande variação destes constituintes entre os cultivares, lembrando que essas amostras foram coletadas em campo, assim as variações desses constituintes podem estar relacionadas com a idade, clima ou local de cultivo. Outros constituintes prováveis triterpenóides, não foram identificados com os dados disponíveis, necessitando de informações adicionais para essa análise.

**Figura 55:** Comparação do teor relativo de outros constituintes identificados em extrato hexânicos (TMS) de folhas de cana-de-açúcar.



**Legenda:** 5: neofitadieno; 7: n.i; 8: n.i; 12: n.i; 14: n.i; 17: fitol; 21: n.i; 23: n.i; 25: Pentacosano; 27: n.i; 28: Hexacosano; 29: sacarose; 31: Heptacosano; 34: Esqualeno; 35: n.i; 37: Nonacosano; 39: alquilresorcinol; 40: Hentriacontano; 41: colesterol; 42: alfa-tocoferol; 44: n.i; 45: campesterol; 46: n.i; 47: estigmasterol; 48: n.i; 49: n.i; 50:  $\beta$  sitosterol; 51: n.i; 52: n.i; 53: n.i; 55: n.i; 56: n.i; 57: n.i; 58: n.i; 59: n.i; 60: n.i; 61: n.i; 62: n.i; 63: friedelina; 64: n.i; \* trimetilsilil.

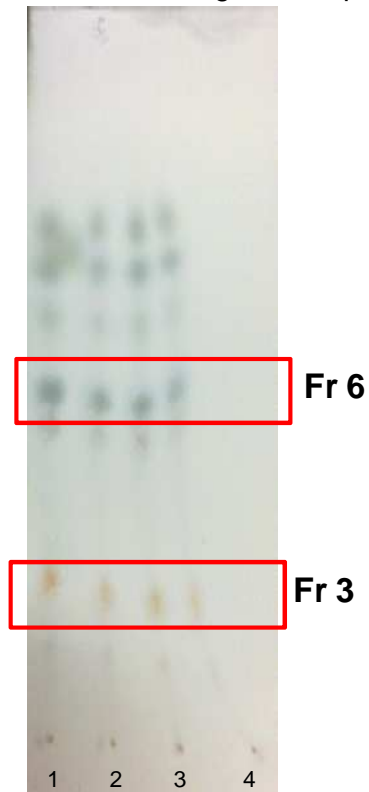


## Resultados

**Tabela 6:** Massas das frações de cera epicuticular analisadas por CCDP.

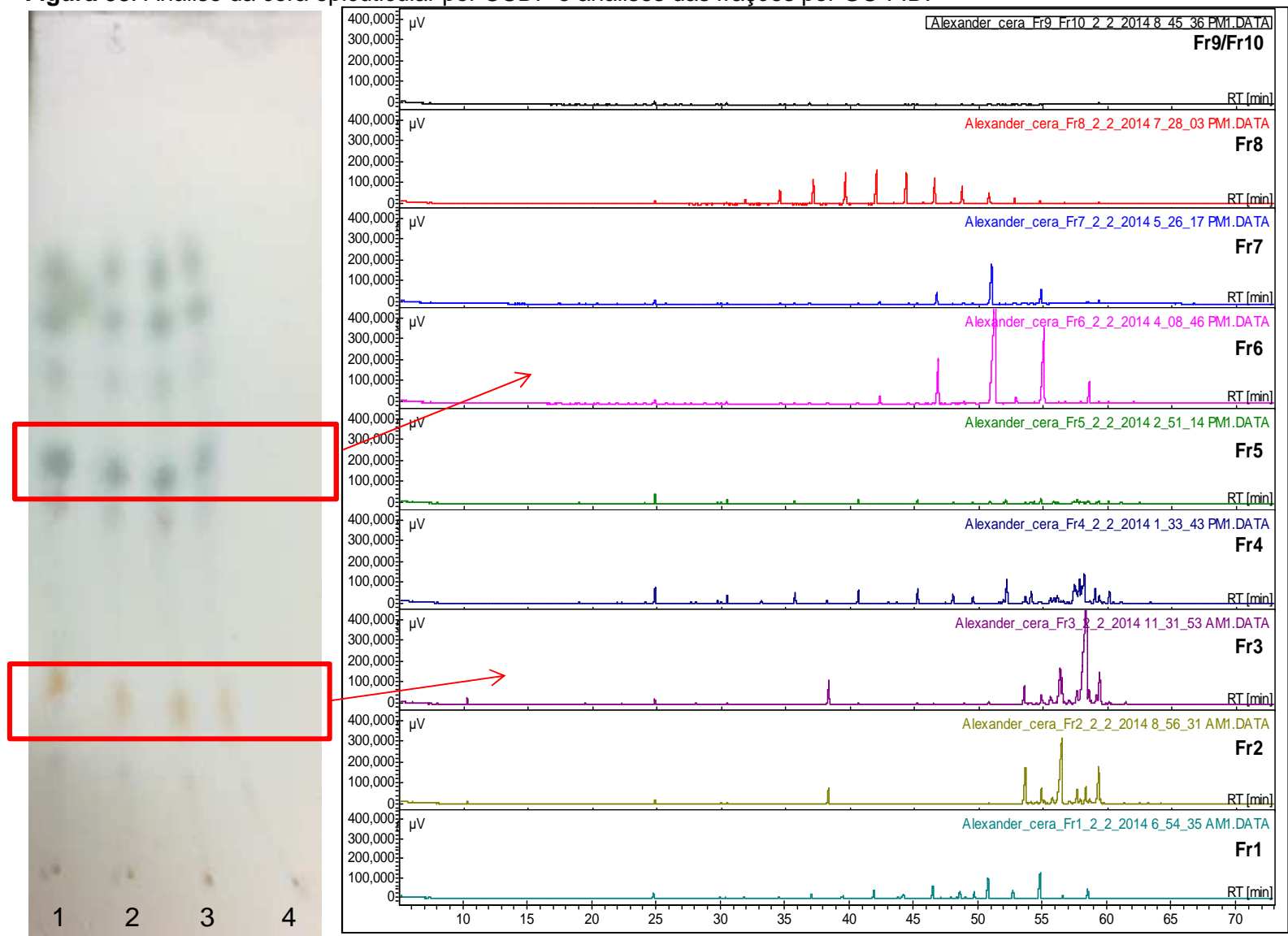
Frações	Massa (mg)
1	1
2	1.1
3	5
4	2.5
5	3
6	6
7	2
8	1
9	1
10	1

**Figura 57:** Cromatografia em camada delgada comparativa da cera epicuticular.



**Legenda:** 1, 2, 3 e 4: número de aplicações (replicatas)

Figura 58: Análise da cera epicuticular por CCDP e análises das frações por GC-FID.

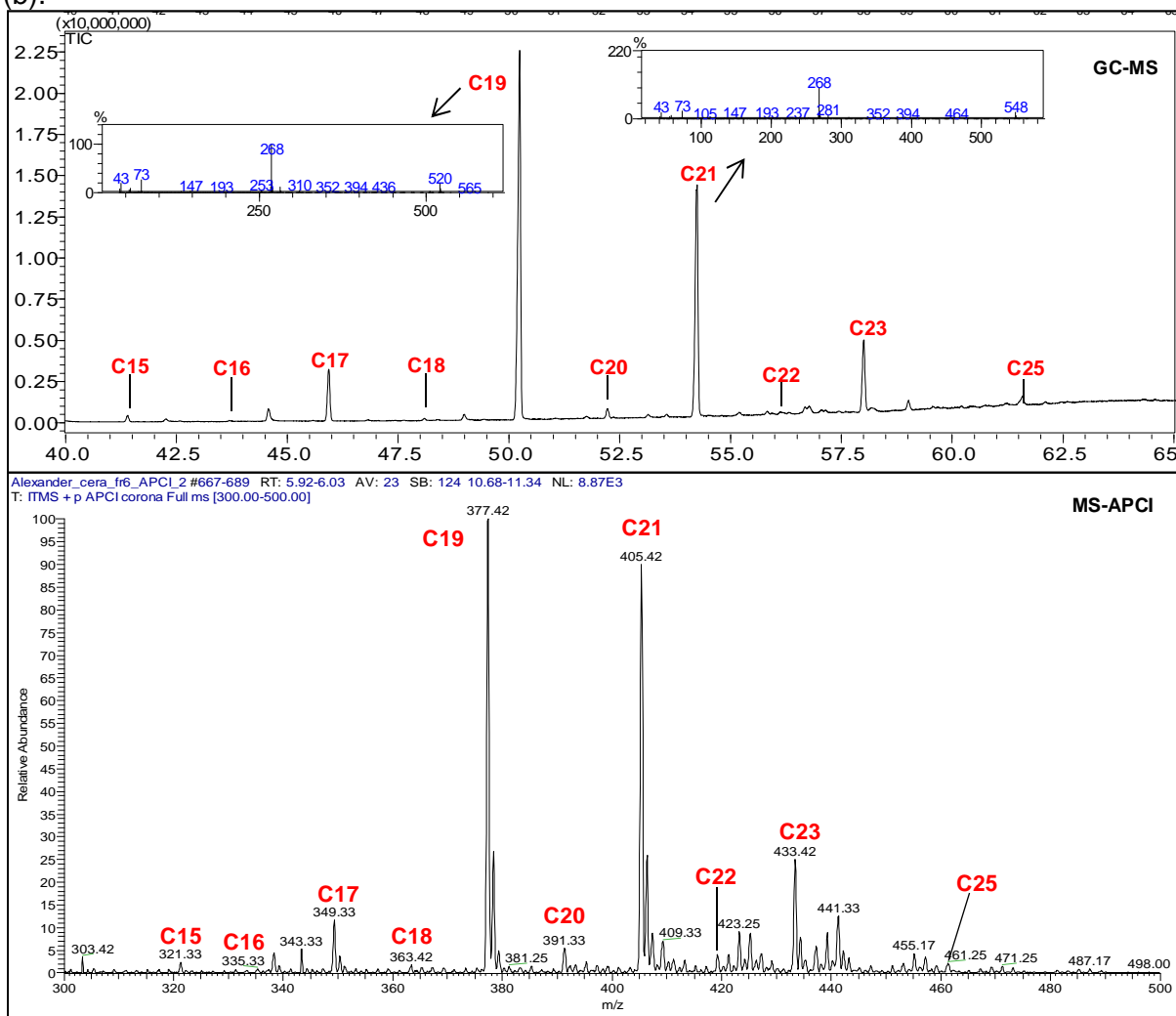


## Resultados

### 4.3.1.1 Análise estrutural de alquildiidrobenzenos

A análise da Fr6 por GC-MS e MS-APCI indicou a presença majoritária de nonadecildiidrobenzeno e heneicosildiidrobenzeno (**Figuras 59 e 60**), lembrando que previamente às análises por GC-MS, as amostras foram sililadas, enquanto que para análises por MS-APCI a amostra não sililada foi inserida diretamente no MS. O experimento de MS-APCI de baixa resolução da fração Fr 6 apresenta as moléculas protonadas  $[M+H]^+$  com  $m/z$  377 e 405, correspondentes aos dois compostos indicados acima.

**Figura 59:** Identificação de série homóloga de alquilresorcinol por GC-MS (a) e MS-APCI (b).

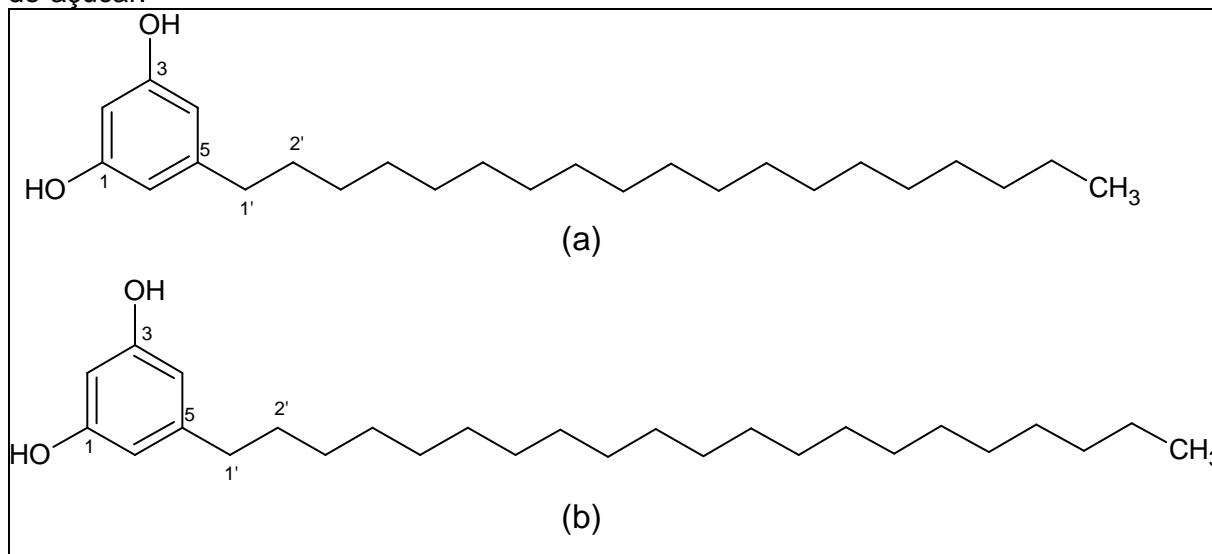


\* espectro de massas dos alquilresorcinóis (TMS) majoritários.



## Resultados

**Figura 60:** Estruturas de (a) nonadecilresorcinol (nonadecildiidroxi-benzeno) e (b) heneicosilresorcinol (heneicosildiidroxi-benzeno) identificados em cera epicuticular de cana-de-açúcar.



No espectro de RMN de  $^1\text{H}$  (**Figura 61**) observa-se um tripleto em  $\delta$  6,17 (1H, 2,1 Hz) e um duplete em  $\delta$  6,24 (2H, 2,1 Hz) característicos de um anel benzênico 1,3,5 trissubstituído e simétrico. No espectro de RMN de  $^{13}\text{C}$ , destaca-se ainda sinais de dois carbonos benzílicos oxigenado em  $\delta$  156,8 (2C), indicando se tratar de um 5-alkuil-1,3-diidroxi-benzeno. Adicionalmente observa-se um tripleto em  $\delta$  2,48 (7,7 Hz) atribuível ao metileno benzílico e outro em  $\delta$  0,88 (6,9 Hz) resultante da metila terminal da cadeia alquílica, além dos multipletos em  $\delta$  1,22-1,30 e  $\delta$  1,56 atribuíveis aos demais grupos metilênicos. Dessa forma concluímos que as substâncias homólogas presentes nesta fração são 5-alkuil-1,3-diidroxi-benzeno ou 5-alkuilresorcinois. Essa interpretação é corroborada pelos dados de RMN de  $^{13}\text{C}$  (**Figura 62**) e dados da literatura (**Tabela 7**).

## Resultados

Figura 61: Espectro de RMN de  $^1\text{H}$  do Alquilresorcinol ( $\text{CDCl}_3$ , 7,0 T).

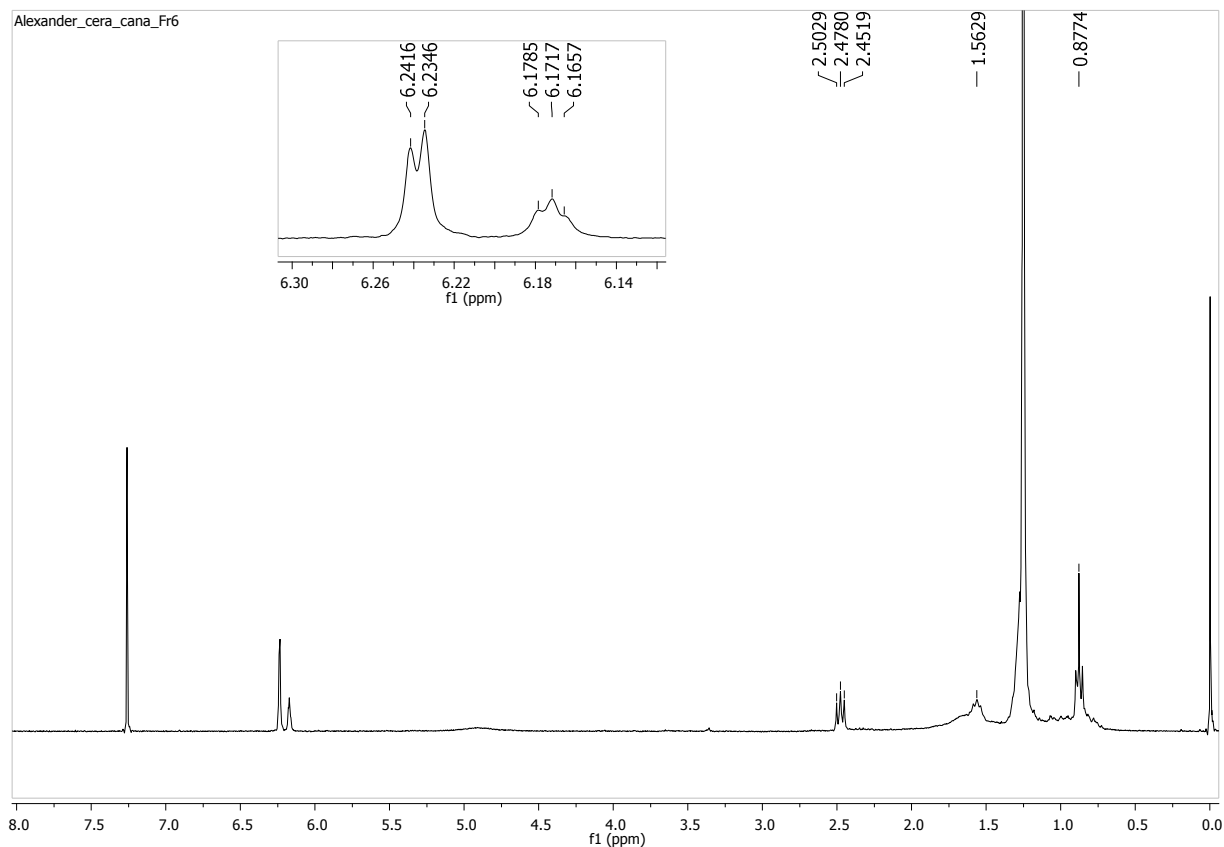
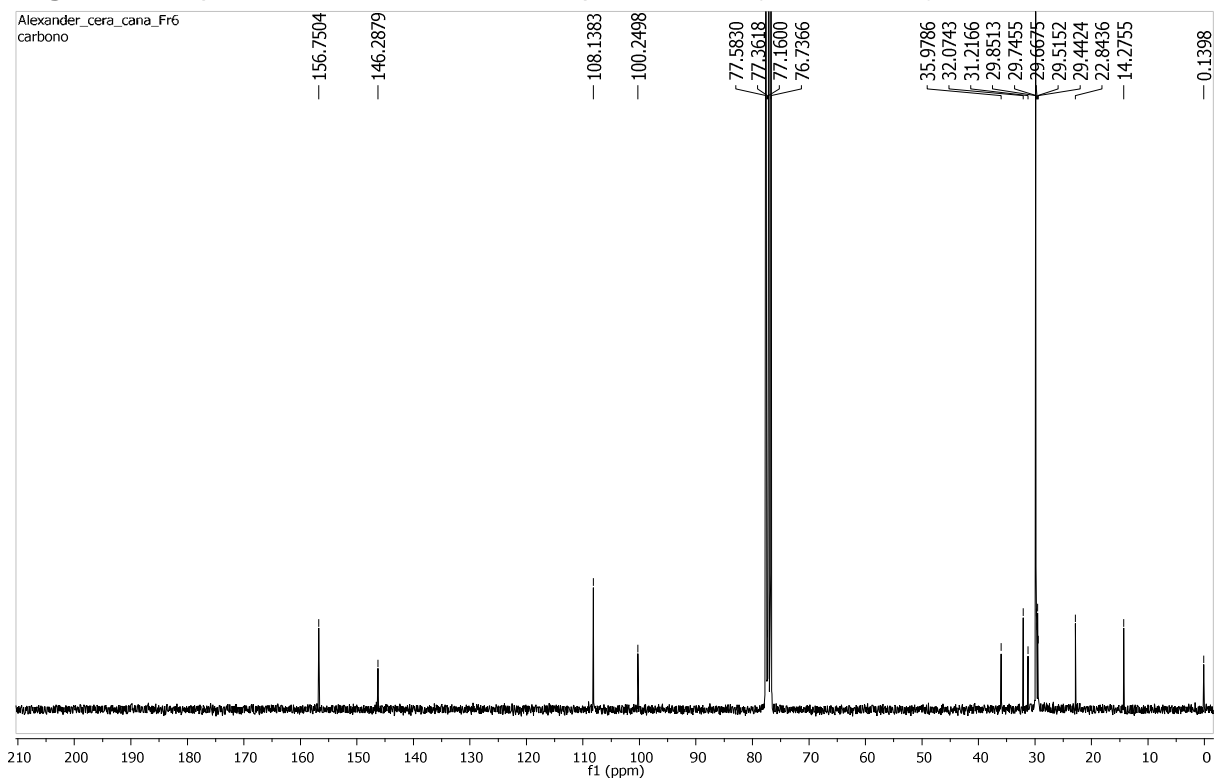


Figura 62: Espectro de RMN de  $^{13}\text{C}$  do Alquilresorcinol ( $\text{CDCl}_3$ , 7,0 T).



## Resultados

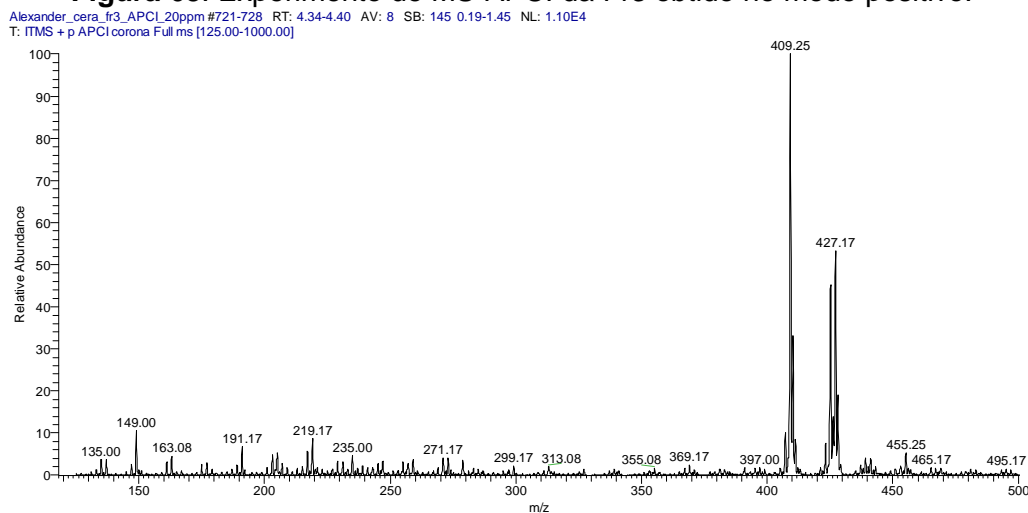
**Tabela 7:** Dados de RMN de  $^1\text{H}$  e  $^{13}\text{C}$  ( $\text{CDCl}_3$ , 7,0 T) de alquilresorcinol.

Posição	1		5-n-Heptadecylresorcinol (ZHU, 2012)	
	$\delta_{\text{H}}$ (J em Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (J em Hz)	$\delta_{\text{C}}$
1		156,8		157,2
2	6,17 <i>t</i> (2,1)	100,2	6,13 <i>t</i> (2,2)	99,9
3		156,8		157,2
4	6,24 <i>d</i> (2,1)	108,1	6,19 <i>d</i> (2,2)	107,3
5		146,3		145,7
6	6,24 <i>d</i> (2,1)	108,1	6,19 <i>d</i> (2,2)	107,3
1'	2,48 <i>t</i> (7,7)	36,0	2,43 <i>t</i> (7,7)	35,9
2'	1,56 <i>m</i>	31,2	1,52 <i>m</i>	31,1
3'	1,22-1,30 <i>m</i>	29,4	1,24-1,30 <i>m</i>	29,3
4'-14'	1,22-1,30 <i>m</i>	29,9-29,5	1,24-1,30 <i>m</i>	29,7-29,4
15'	1,22-1,30 <i>m</i>	29,9-29,5	1,24-1,30 <i>m</i>	31,9
16'	1,22-1,30 <i>m</i>	29,9-29,5	1,24-1,30 <i>m</i>	22,7
17'	1,22-1,30 <i>m</i>	32,0	0,86 <i>t</i> (6,7)	14,1
18'	1,22-1,30 <i>m</i>	22,8	-	-
19'	0,88 <i>t</i> (6,9)	14,3	-	-

### 4.3.1.2 Identificação do simiarenol

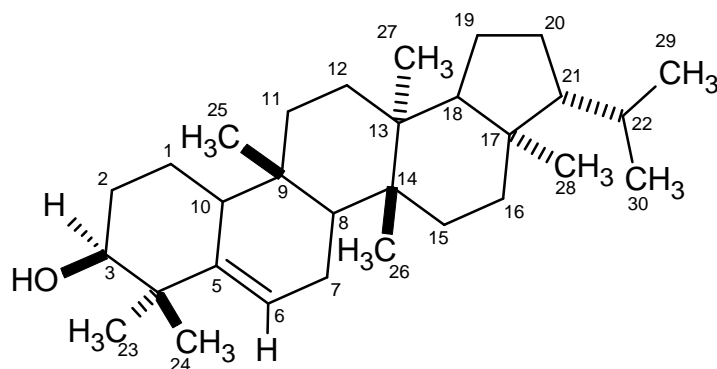
O constituinte principal da Fr3 corresponde ao composto com IR = 3431, cujo espectro de massas do derivado sililado obtido por EI tem características de triterpenos, isto é, íons com  $m/z$  134, 231, 259, 274, 408, 483 (VILEGAS et. al., 1997). O experimento MS-APCI, modo positivo apresenta molécula protonada em  $m/z$  427  $[\text{M}+\text{H}]^+$  e pico base  $m/z$  409  $[\text{M}+\text{H}-\text{H}_2\text{O}]^+$  característico da perda de uma molécula de água (**Figura 63**).

**Figura 63:** Experimento de MS-APCI da Fr3 obtido no modo positivo.



No espectro de RMN de  $^{13}\text{C}$  são observados sinais correspondentes a 30 carbonos, incluindo um grupo carbinólico em  $\delta_{\text{C}}$  76,5 ( $\delta_{\text{H}}$  3,47), dois carbonos olefínicos  $\delta_{\text{C}}$  142,1 e 122,1 ( $\delta_{\text{H}}$  5,62) e oito carbonos de grupos metílicos 15,1 ( $\delta_{\text{H}}$  0,93), 15,9 ( $\delta_{\text{H}}$  1,01), 16,2 ( $\delta_{\text{H}}$  0,79),  $\delta_{\text{C}}$  18,0 ( $\delta_{\text{H}}$  0,90), 22,1 ( $\delta_{\text{H}}$  0,87), 23,1 ( $\delta_{\text{H}}$  0,84), 29,3 ( $\delta_{\text{H}}$  1,05), 25,6 ( $\delta_{\text{H}}$  1,15), 29,3 ( $\delta_{\text{H}}$  1,05) (**Figura 65, 66, 67 e 68**), indicativos de um triterpeno pentacíclico com fórmula molecular  $\text{C}_{30}\text{H}_{50}\text{O}$ . Esses dados tem boa concordância com dados espectrais encontrados na literatura para o simiarenil (**Figura 64**) (Tabela 8).

**Figura 64:** Estrutura do simiarenil identificado em cera epicuticular.



## Resultados

**Tabela 8:** Dados de RMN de  $^1\text{H}$  e  $^{13}\text{C}$  ( $\text{CDCl}_3$ , 14,1 T) de simiarenol.

Posição	1		Simiarenol (JIN, 2013)	
	$\delta_{\text{H}}$ (J em Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (J em Hz)	$\delta_{\text{C}}$
1		18,2		18,0
2		27,9		27,7
3	3,47 brs	76,5	3,47 brs	76,3
4		41,0		40,8
5		142,1		141,9
6	5,62 brd (6,0)	122,1	5,62 dt, (2,0, 5,9)	122,0
7		24,2		24,0
8		44,4		44,2
9		35,0		34,8
10		50,4		50,2
11		34,3		34,1
12		29,2		28,9
13		38,8		38,6
14		39,5		39,3
15		29,3		29,0
16		35,6		35,4
17		42,9		42,8
18		51,9		51,7
19		20,1		19,9
20		28,5		28,3
21		60,2		60,0
22		30,9		30,8
23	1,05 s	29,3	1,05 s	29,0
24	1,15 s	25,6	1,14 s	25,5
25	0,90 s	18,0	0,89 s	17,8
26	1,01 s	15,9	1,00 s	15,7
27	0,93 s	15,1	0,92 s	15,0
28	0,79 s	16,2	0,78 s	16,1
29	0,87 brd (5,1)	22,1	0,88 d (6,5)	21,9
30	0,84 d (6,6)	23,1	0,83 d (6,5)	22,9

## Resultados

Figura 65: Espectro de RMN de  $^1\text{H}$  de simiarenil (CDCl<sub>3</sub>, 14,1 T).

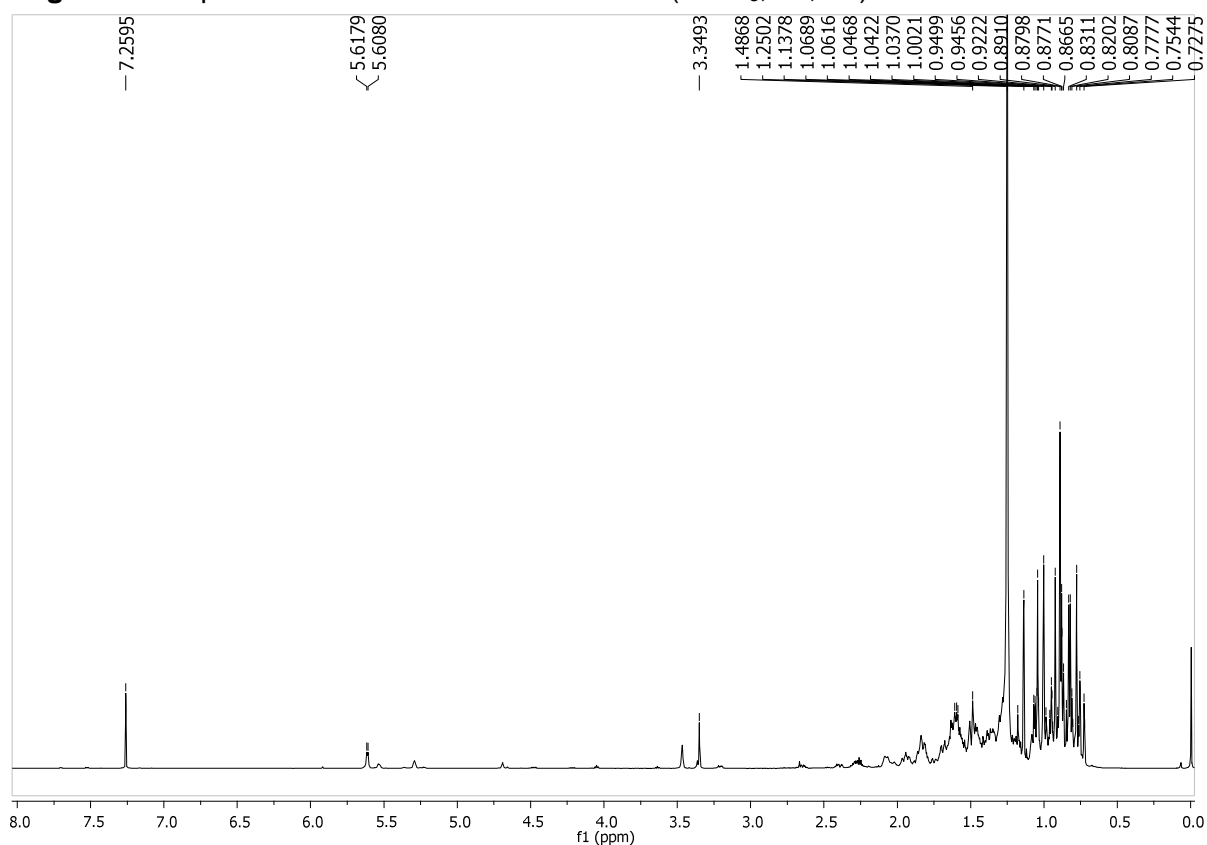
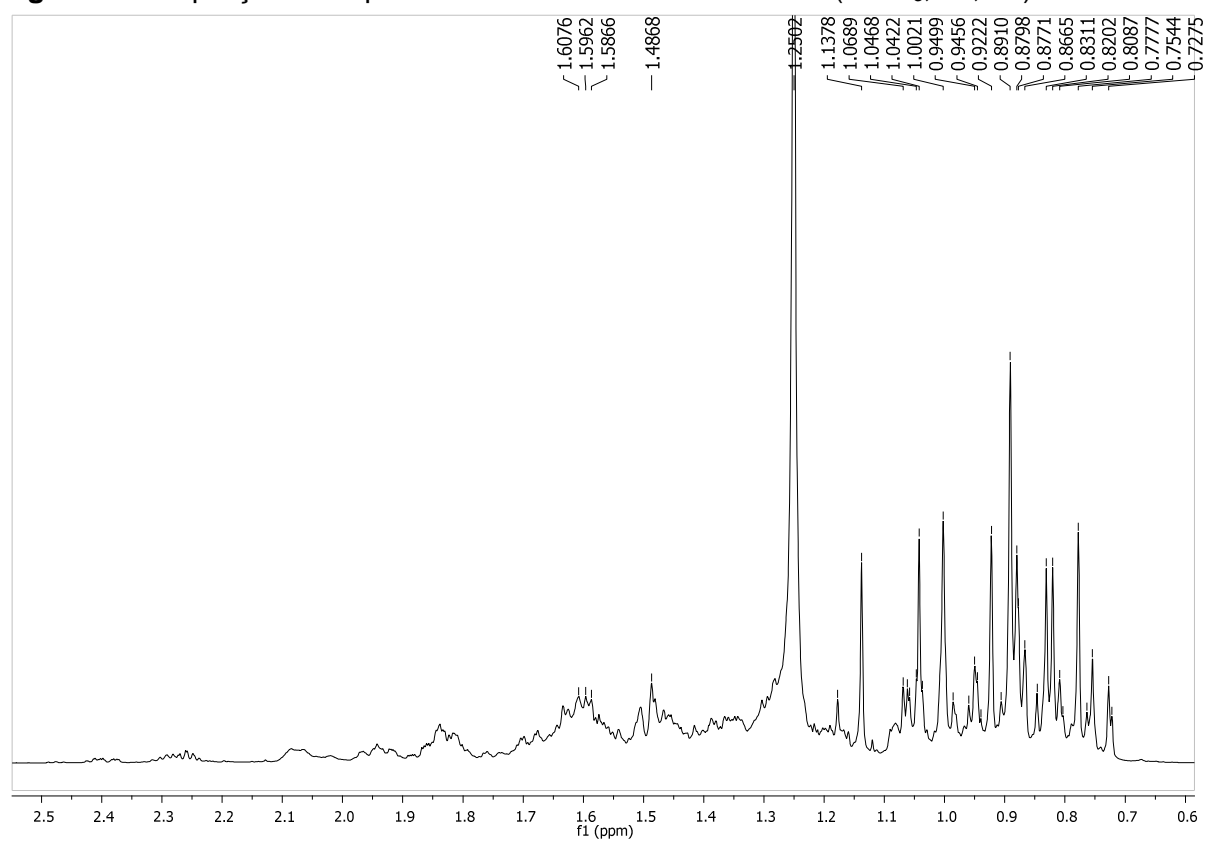
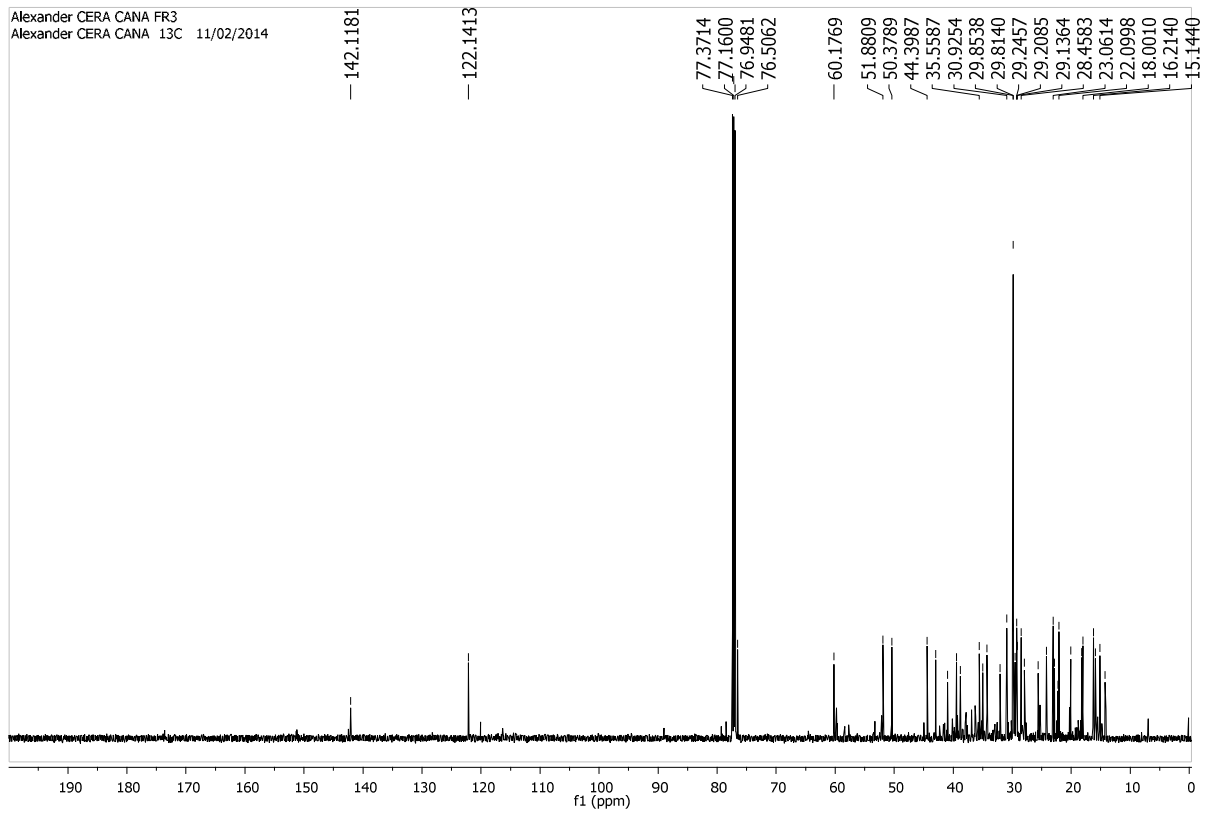


Figura 66: Ampliação do espectro de RMN de  $^1\text{H}$  de simiarenil (CDCl<sub>3</sub>, 14,1 T).

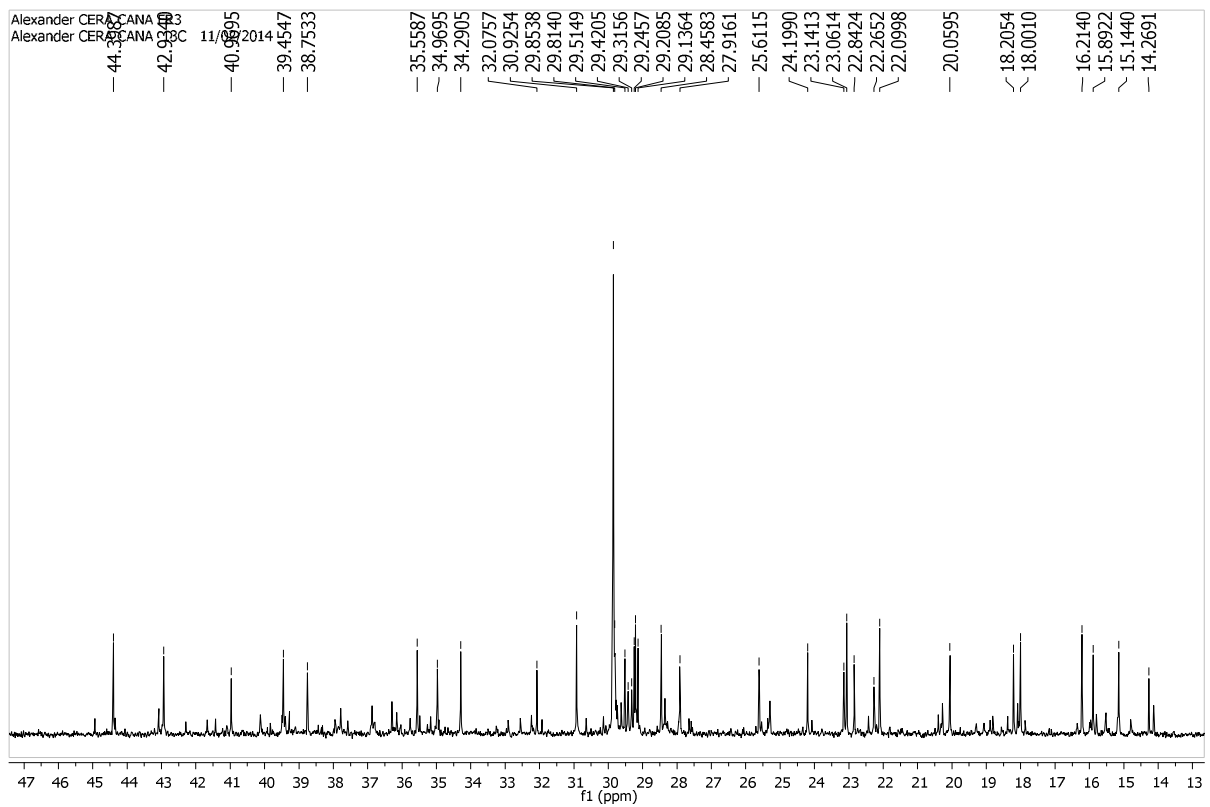


## Resultados

**Figura 67:** Espectro de RMN de  $^{13}\text{C}$  de simiarenol ( $\text{CHCl}_3$ , 14,1 T).



**Figura 68:** Ampliação do espectro de RMN de  $^{13}\text{C}$  de simiarenol ( $\text{CDCl}_3$ , 14,1 T).



### 4.4 Análises de metabolitos apolares em folhas de cana-de-açúcar inoculadas com ferrugem alaranjada

Na avaliação de metabolitos apolares em diferentes cultivares coletados em campo não foi possível propor uma separação/classificação dessas amostras em função da constituição química, provavelmente pela falta de controle como num experimento de cultivo, com os cultivares conhecidos (sem contaminação), temperatura e umidade controladas e inoculação de patógeno. Por isso foi realizado um experimento de cultivo com dois cultivares de cana-de-açúcar, um resistente (IAC95-5000) e outro susceptível (SP89-1115) à ferrugem alaranjada, para uma avaliação preliminar da viabilidade de aplicar as análises de compostos lipofílicos de folhas em estudos dessa natureza. As condições experimentais estão descritas no **item 3.2**. Foram analisadas amostra de folhas dos dois cultivares inoculados (I) e testemunho (T), obtidas após 0, 2, 5, 10, e 15 dias após a inoculação.

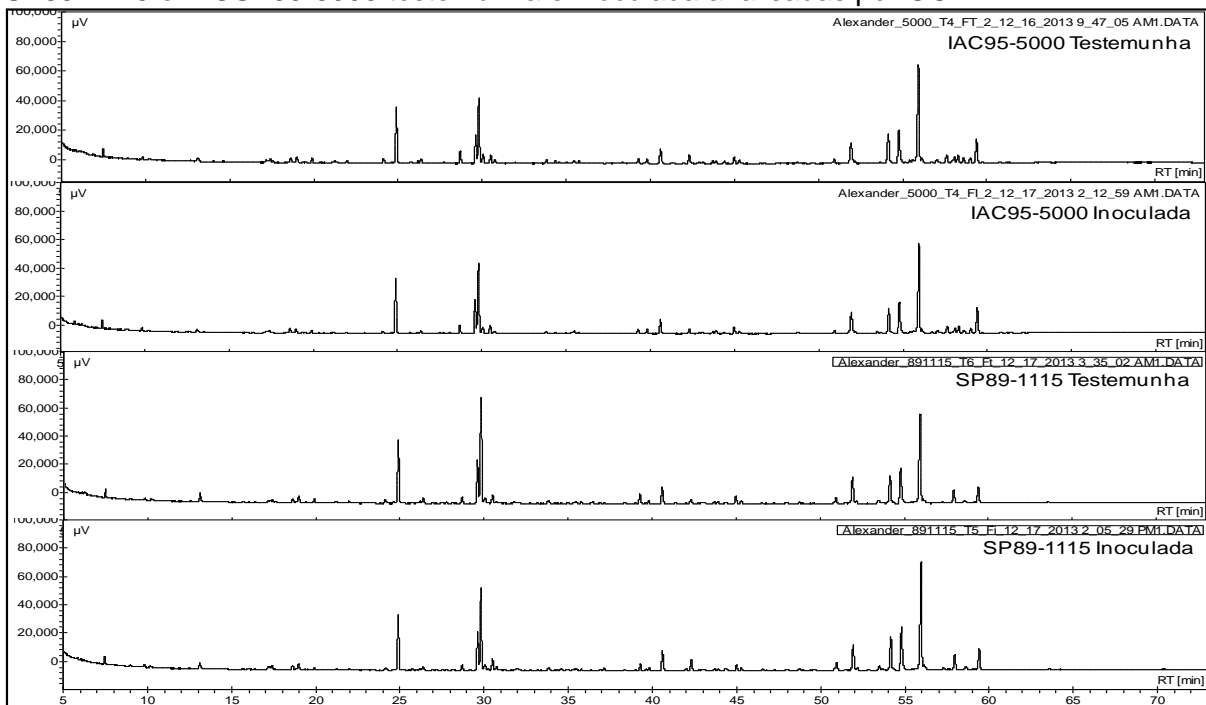
Nesse experimento não foi possível realizar todas as análises em quintuplicatas devido à falta de material, assim algumas amostras foram analisadas em duplicatas e em triplicatas nos sistemas cromatográficos GC-FID e apenas uma única injeção no GC-MS para proposta de identificação.

Comparando-se os cromatogramas dos cultivares IAC95-5000 (resistente) testemunha e inoculado na análise realizada em GC-FID, observa-se que não há diferença no perfil cromatográfico destas amostras, o mesmo acontecendo com o cultivar SP89-1115 (susceptível) (**Figura 69**).



## Resultados

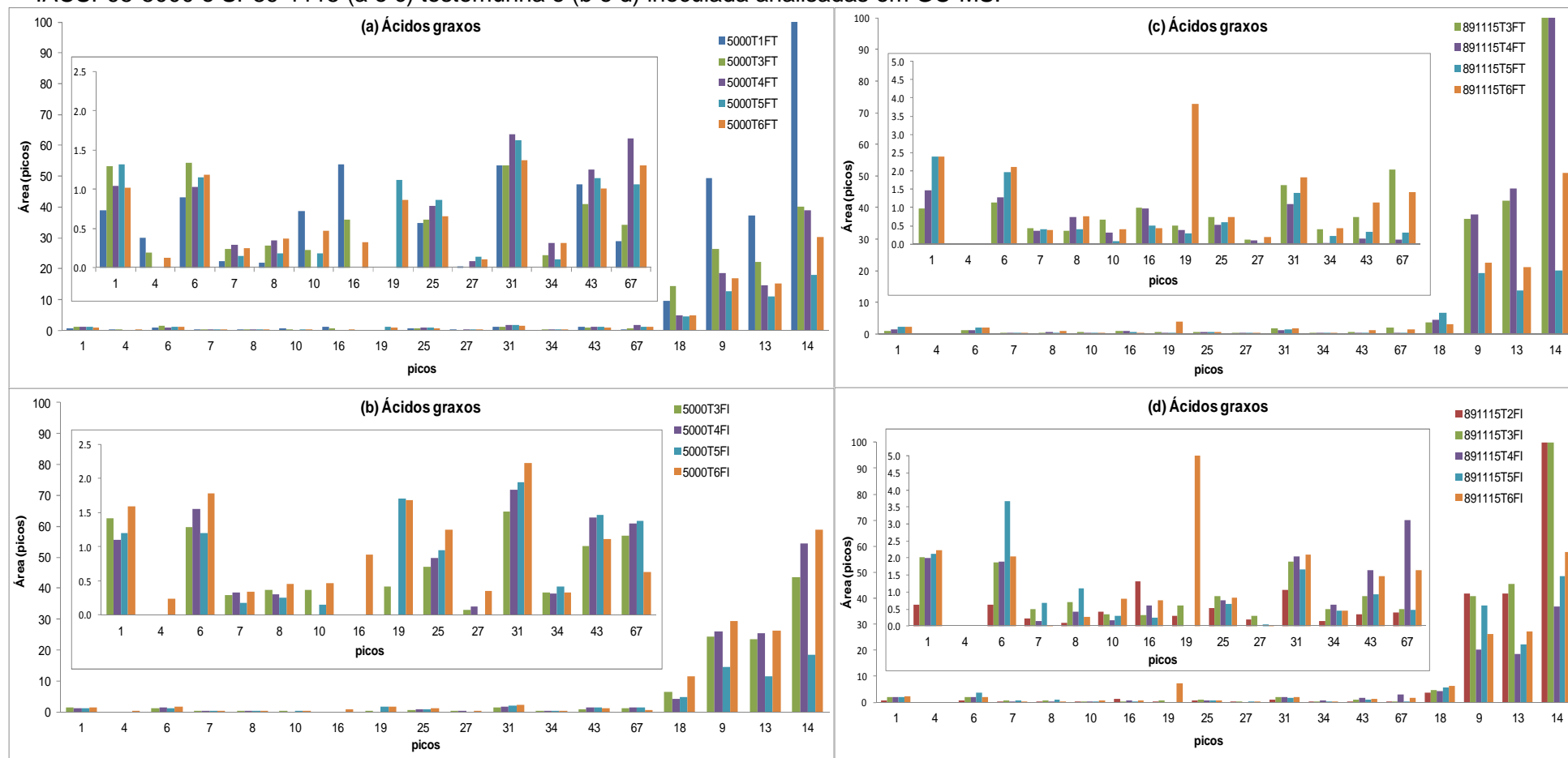
**Figura 69:** Análise de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares SP89-1115 e IACSP95-5000 testemunha e inoculada analisadas por GC-FID.



Análise comparativa detalhada do teor dos constituintes lipofílicos de folhas dos dois cultivares avaliados neste experimento de cultivo é apresentada nas **figuras 70-77**. Para os cultivares IACSP95-5000 e SP89-1115 analisados verifica-se variações das áreas entre os constituintes identificados, observa-se que os constituintes em maiores proporções são campesterol, colesterol, ácido linoleico, ácido palmítico, estigmasterol, dotriacontanol,  $\beta$ -sitosterol,  $\alpha$ -ácido linolênico, sendo o  $\beta$ -sitosterol o constituinte majoritário. As variações observadas podem ser inerentes a erros experimentais e a variações próprias do organismo estudado, não havendo indícios claros de mudanças qualitativas ou quantitativas na composição química induzidas pela inoculação do patógeno ou que possam indicar relação com a resistência da planta.

## Resultados

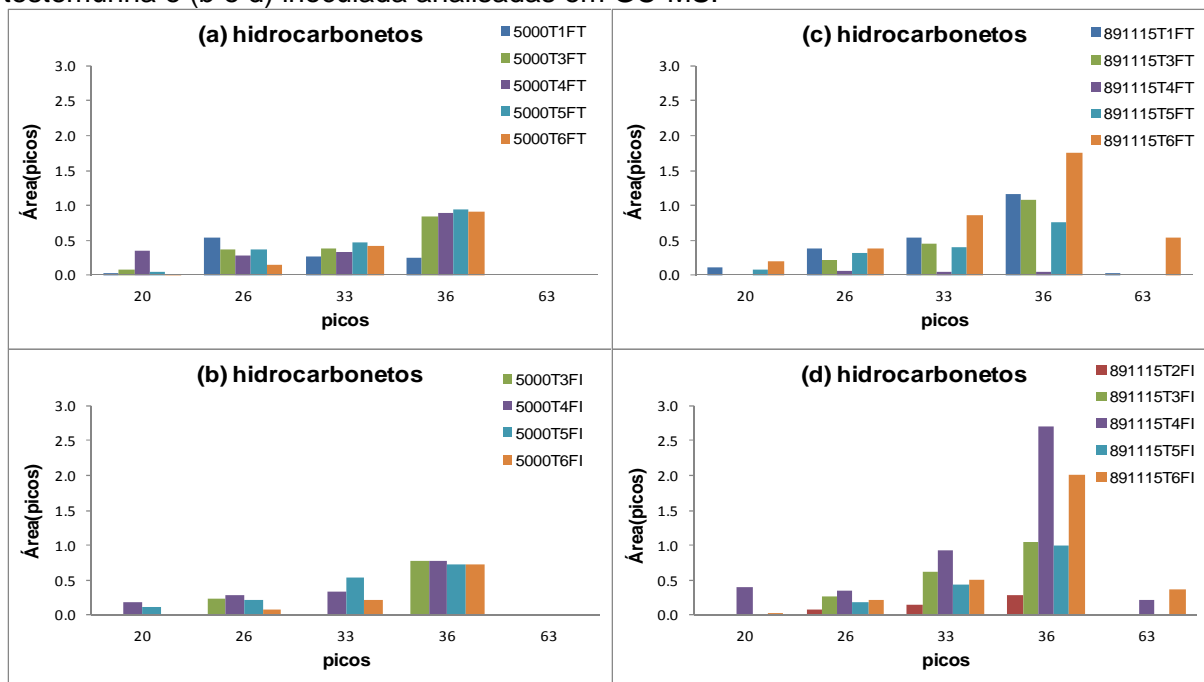
**Figura 70:** Gráfico de barra da área normalizada dos ácidos graxos de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS.



**Legenda:** 1: ácido láurico; 4: ácido azelaico; 6: ácido mirístico; 7: ácido pentadecanóico; 8: ácido palmitoleico; 9: ácido palmítico; 10: ácido margárico; 13: ácido linoleico; 14: alfa-ácido linolênico; 16: ácido oleico; 18: ácido esteárico; 19: ácido araquídico; 25: ácido Behênico; 27: ácido tricosanóico; 31: ácido tetracosanóico; 34: ácido hexacosanóico; 43: ácido octacosanoico; 67: ácido dotricontanoico.

## Resultados

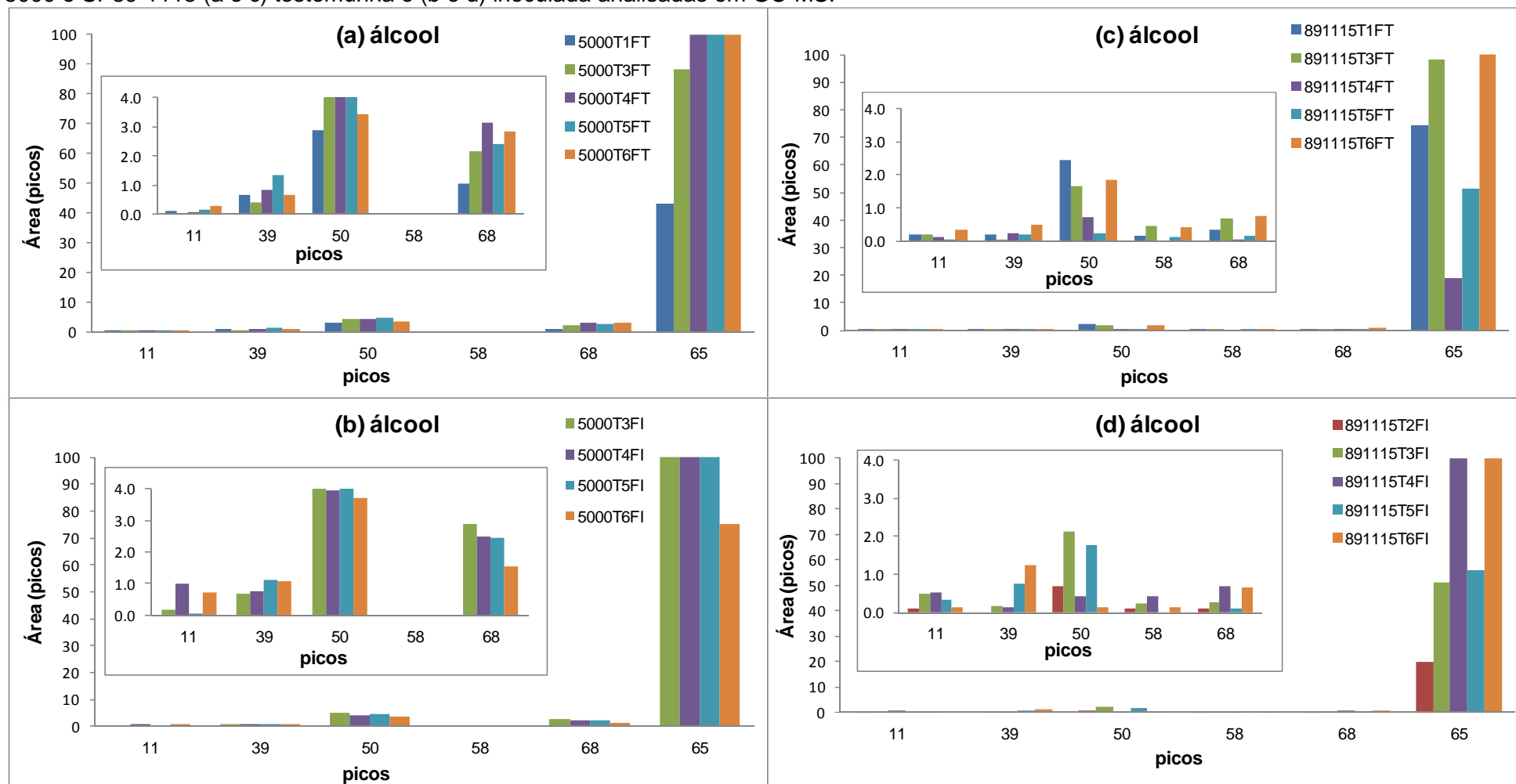
**Figura 71:** Gráfico de barra da área normalizada de hidrocarbonetos de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS.



**Legenda:** 20: pentacosano; 26: heptacosano; 33: nonacosano; 36: hentriacontano; 63: pentatriacontano.

## Resultados

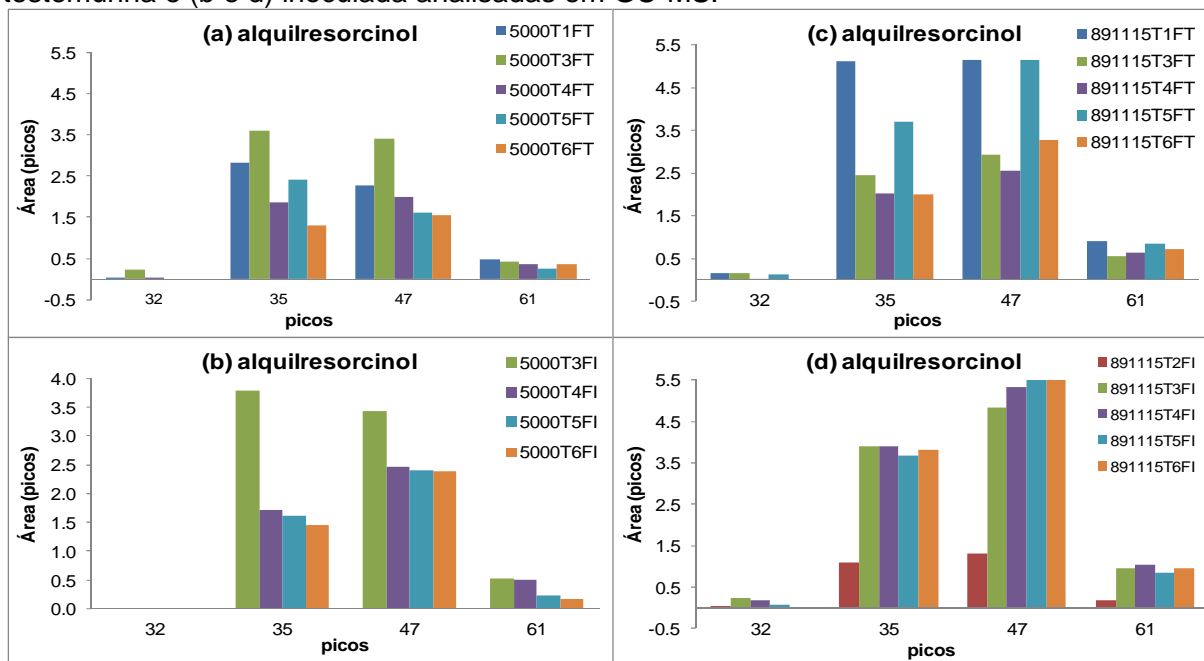
**Figura 72:** Gráfico de barra da área normalizada do álcool de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS.



**Legenda:** 11: octadecanol; 39: octacosanol; 50: triacontanol; 58: hentriacontanol; 68: tetratriacontanol; 65: dotriacontanol.

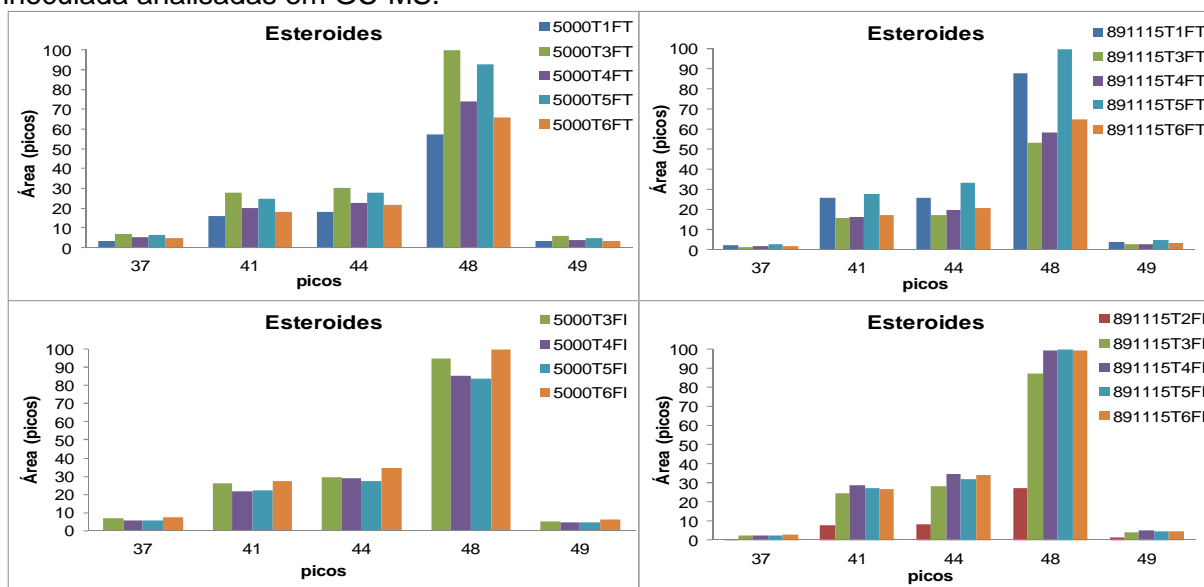
## Resultados

**Figura 73:** Gráfico de barra da área normalizada do alquilresorcinol de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS.



**Legenda:** 32: Ar C17:0; 35: Ar C19:0; 47: Ar C21:0; 61: Ar C23:0

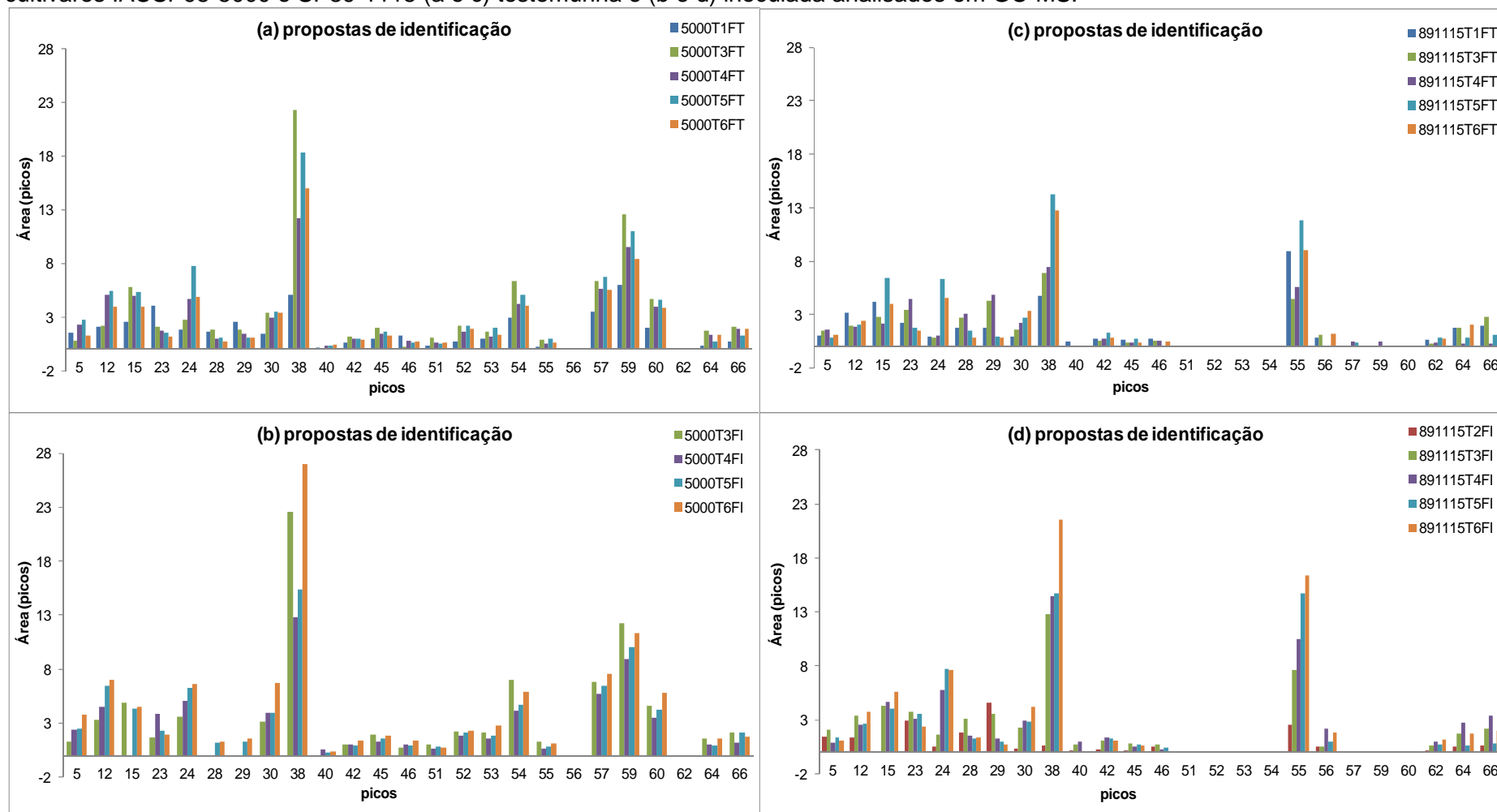
**Figura 74:** Gráfico de barra da área de esteroides de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisadas em GC-MS.



**Legenda:** 37: colesterol; 41: campesterol; 44: estigmasterol; 48:  $\beta$ -sitosterol; 49: estigmastanol.

## Resultados

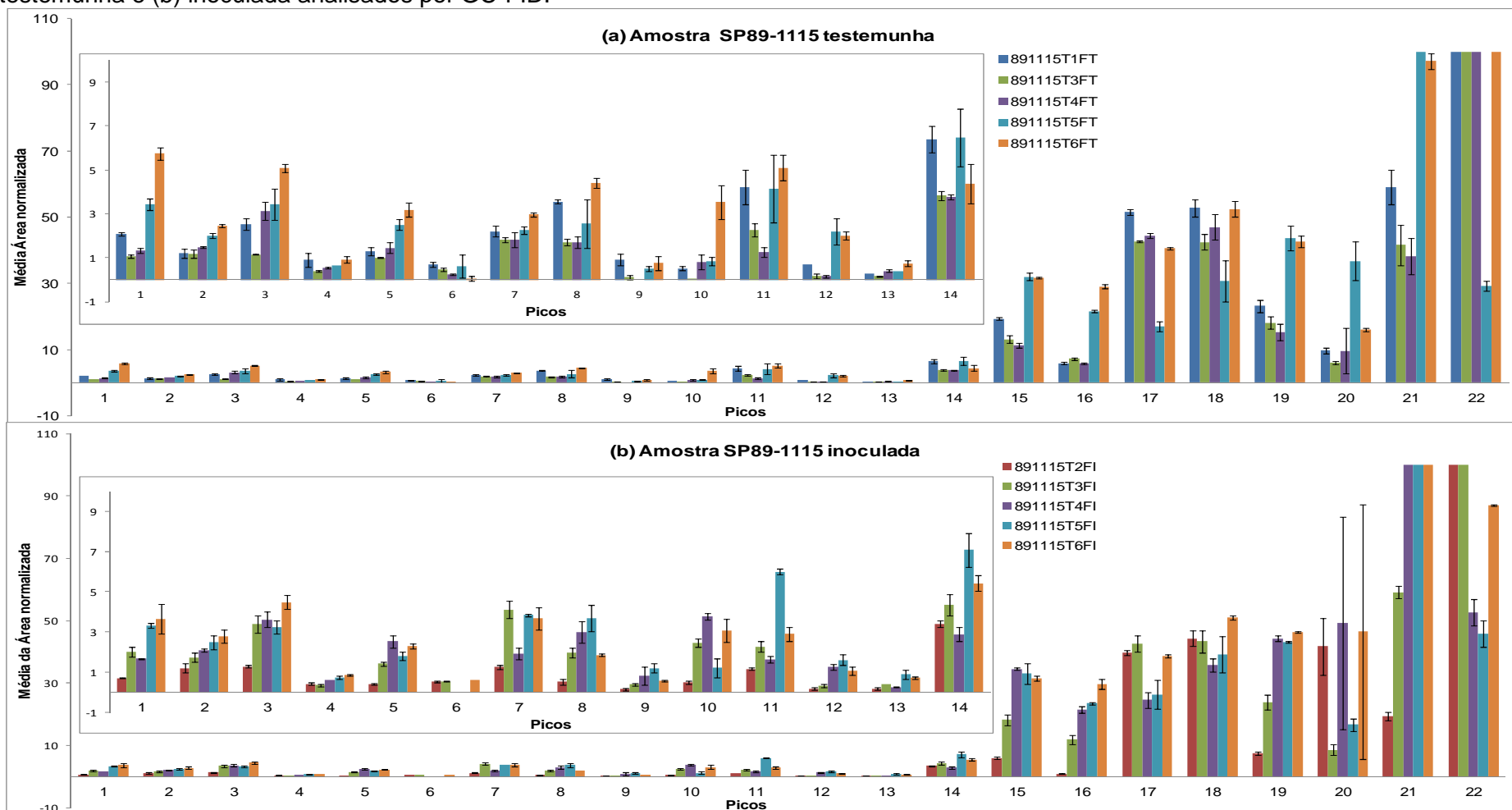
**Figura 75:** Gráfico de barra da área de compostos com propostas de identificação de extrato hexânico (TMS) de folhas de cana-de-açúcar dos cultivares IACSP95-5000 e SP89-1115 (a e c) testemunha e (b e d) inoculada analisados em GC-MS.



**Legenda:** 5: neofitadieno; 12: fitol; 15: n.i; 23: n.i; 24: n.i; 28: n.i; 29: n.i; 30: esqualeno; 38:  $\alpha$ -tocoferol; 40: n.i; 42: n.i; 45: n.i; 46:  $\alpha$ -tocoferolhidroquinona; 51: n.i; 52: n.i; 53: lanosterol; 54: n.i; 55: n.i; 56: n.i; 57: n.i; 59: n.i; 60: n.i; 62: friedelina; 64: n.i; 66: n.i.

## Resultados

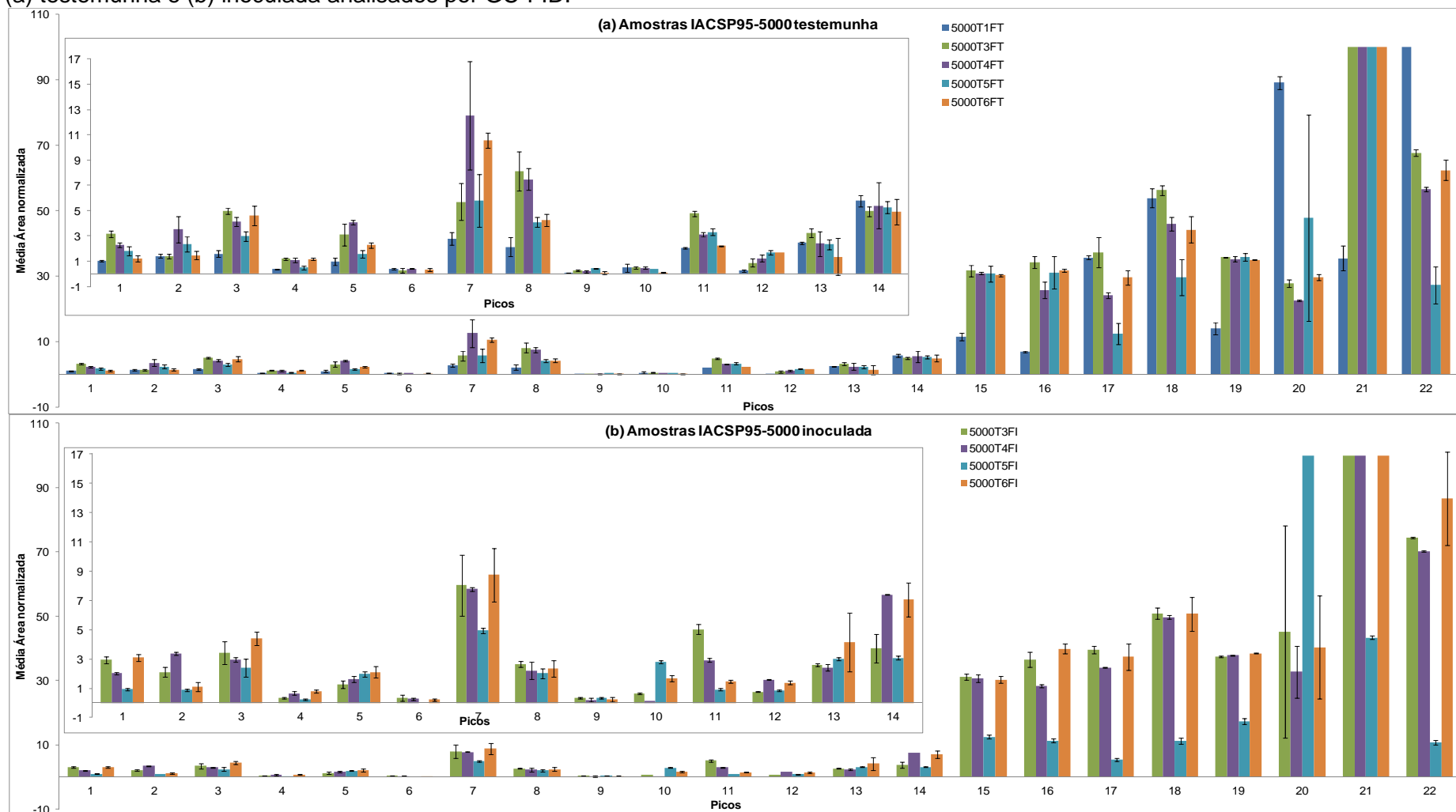
**Figura 76:** Gráfico de barra da média da área normalizada de extrato hexânico (TMS) de folhas de cana-de-açúcar do cultivar SP89-1115 (a) testemunha e (b) inoculada analisados por GC-FID.



**Legenda:** 1: ácido láurico; 2: neofitaadieno; 3: ácido mirístico; 4: ácido pentadecanóico; 5: ácido palmitoleico; 6: octadecanol; 7: fitol; 8: n.i; 9: nonacosano; 10: hentriacontano; 11: Ar C19:0; 12: alfa-tocoferol; 13: tetratriacontanol; 14: ácido esteárico; 15: campesterol; 16: colesterol; 17: ácido linoleico; 18: ácido palmítico; 19: estigmasterol; 20: dotriacontanol; 21:  $\beta$ -sitosterol; 22:  $\alpha$ -ácido linolênico.

## Resultados

**Figura 77:** Gráfico de barra da média da área normalizada de extrato hexânico (TMS) de folhas de cana-de-açúcar do cultivar IACSP95-5000 (a) testemunha e (b) inoculada analisados por GC-FID.



**Legenda:** 1: ácido láurico; 2: neofitaadieno; 3: ácido mirístico; 4: ácido pentadecanóico; 5: ácido palmitoleico; 6: octadecanol; 7: fitol; 8: n.i.; 9: nonacosano; 10: hentriacontano; 11: Ar C19:0; 12: alfa-tocoferol; 13: tetratriacontanol; 14: ácido esteárico; 15: campesterol; 16: colesterol; 17: ácido linoleico; 18: ácido palmítico; 19: estigmasterol; 20: dotriacontanol; 21:  $\beta$ -sitosterol; 22:  $\alpha$ -ácido linolênico.



### 5 Conclusão

Este estudo teve como principal objetivo caracterizar quimicamente a composição de cera epicuticular de folhas de cana-de-açúcar, além dos compostos lipofílicos de folhas obtidos pela extração com hexano. A comparação do perfil químico de ceras e do extrato hexânico de folhas entre várias cultivas de cana-de-açúcar também foi realizada.

As análises qualitativas resultaram na identificação de 58 compostos na cera epicuticular (138 observados) e 41 no extrato hexânico (65 observados) de folhas de cana-de-açúcar. Essas análises foram realizadas por GC-MS após sililação das amostras, e alicerçadas principalmente na comparação de índices de retenção e espectros de massas experimentais com dados da literatura e de biblioteca de espectros. Algumas propostas foram também reforçadas pela análise do padrão de fragmentação, entre as quais incluem-se séries homólogas de hidrocarbonetos, ácidos e alcoóis graxos e alquilresorcinóis, além de esteroides e triterpenos. A identificação de alquilresorcinóis e do triterpeno pentacíclico simiarenol foi confirmada por análise de frações de cera epicuticular por RMN de  $^1\text{H}$  e  $^{13}\text{C}$ . A julgar pelas massas de cada fração obtida no fracionamento da cera epicuticular de folhas, por CCD preparativa, e respectivos espectro de RMN  $^1\text{H}$ , conclui-se que os constituintes principais da cera são 5-nonadecil resorcinol, 5-heneicosil resorcinol e o triterpeno simiarenol.

Dentro da óptica do estudo metabolômico abordado nesse trabalho, as metodologias adotadas permitiram verificar a presença de elevada diversidade química/estrutural, tanto da cera epicuticular e do extrato hexânico de folhas de cana-de-açúcar. Portanto, estudos mais aprofundados da composição química dessas matrizes permitirão identificar ou elucidar os constituintes que não foram detectados. Além disso, a integração desses dados abre a possibilidade para compreender variações na composição química e correlaciona-las resistência da planta frente ao patógeno.

Na comparação dos perfis químicos de ceras epicuticulares e do extrato hexânico de folhas dos diversos cultivares de cana-de-açúcar acessados, observou-se variações qualitativas e quantitativas significativas mais aleatórias entre as amostras, inviabilizando o agrupamento de cultivares por similaridade química.

## CONCLUSÃO

---

No estudo preliminar realizado com cultivares susceptíveis e resistentes à ferrugem alaranjada (*Puccinia kuehni*), inoculados ou não com o patógeno, os perfis químicos de compostos lipofílicos (extrato hexânico) de folhas foram comparados após silição e análise por GC-MS. Os dados obtidos não indicaram diferenças nítidas entre os cultivares susceptível e resistente, nem entre as amostras testemunha e inoculadas, indicando que a resistência a este patógeno não deve estar associada a compostos lipofílicos. No entanto, experimentos adicionais ainda deverão ser realizados.

Adicionalmente, este trabalho resultou na implantação de uma metodologia de análise de compostos apolares de folhas de cana-de-açúcar e reforçou uma série de cuidados que devem ser tomados no uso de índices de retenção e espectrometria de massas para a identificação de compostos por GC-MS, bem como na atenção em relação à transferência de informações entre GC-MS e GC-FID, principalmente no que diz respeito a supostas similaridades entre colunas DB-5 e DB-5MS. Recomenda-se o uso de colunas iguais (FE e dimensões) e nas colunas similares. Acrescentamos a esses cuidados uma atenção especial a eventuais contaminantes oriundos de equipamentos, reagentes e acessórios utilizados na manipulação e preparação das amostras.

## REFERÊNCIAS

- AGILENT TECHNOLOGIES. **Elimine o ruído e pare de se preocupar com a distorção de picos de compostos ativos**. Santa Clara, 2010. Disponível em: <<http://www.chem.agilent.com/Library/brochures/5990-3758PTBR.pdf>>. Acesso em: 06 out. 2014.
- AGRIOS, G. N. **Plant pathology**. 5th ed. San Diego: Elsevier Academic Press, 2005.
- AMORIM, L.; PASCHOLATI, S. F. Ciclo de relações patógeno-hospedeiro. In: AMORIM, L. et al (Ed.). **Manual de fitopatologia: princípios e conceitos**. 4. ed. São Paulo: Ceres, 2011. v. 1, cap. 4, p. 59-98.
- ARCENEUX, G. Evaluation and timely utilization of sugarcane varieties. **Journal of the American Society of Sugar Cane Technologists**, v. 15, p. 83-97, 1968.
- BARBASSO, D. et al. First report of *Puccinia kuehnii*, causal agent of orange rust of sugarcane, in Brazil. **Plant Disease**, v. 94, n. 9, p. 1170-1170, 2010
- BARGEL, H. et al. Evans review no. 3: structure - function relationships of the plant cuticle and cuticular waxes - a smart material? **Functional Plant Biology**, v. 33, n. 10, p. 893-910, 2006.
- BEDENDO, I. P. Ferrugens. In: AMORIM, L. et al (Ed.). **Manual de fitopatologia: princípios e conceitos**. 4. ed. São Paulo: Ceres, 2011. v. 1, cap. 28, p. 479-485.
- BOU KHALIL, M. et al. Lipidomics era: accomplishments and challenges. **Mass Spectrometry Reviews**, v. 29, n. 6, p. 877-929, 2010.
- BRASIL. Ministério da Agricultura, Pecuária e Abastecimento. Assessoria de Gestão Estratégica. **Projeções do agronegócio Brasil 2008/09 a 2018/19**. Brasília, DF, 2009. Brasil. Disponível em: <[http://www.agricultura.gov.br/arq\\_editor/file/Ministerio/planos%20e%20programas/projecoes%20do%20agronegocio.pdf](http://www.agricultura.gov.br/arq_editor/file/Ministerio/planos%20e%20programas/projecoes%20do%20agronegocio.pdf)>. Acesso em: 27 set. 2013.
- BRASIL. Ministério da Agricultura, Pecuária e Abastecimento. Instrução normativa n 59, de 18 de dezembro de 2013. **Diário Oficial da União**, Brasília, DF, 19 dez. 2013. Seção 1, p. 91.
- BRERETON, R. G. Introduction to multivariate calibration in analytical chemistry. **Analyst**, v. 125, n. 11, p. 2125-2154, 2000.
- BURR, G. O. et al. The sugarcane plant. **Annual Review of Plant Physiology**, v. 8, p. 275-308, 1957.
- CARVALHO, S. A. D.; FURTADO, A. T. O melhoramento genético de cana-de-açúcar no Brasil e o desafio das mudanças climáticas globais. **Revista Gestão & Conexões**, v. 2, n. 1, p. 22-46, 2013.
- CASU, R. et al. Identification of differentially expressed transcripts from maturing stem of sugarcane by in silico analysis of stem expressed sequence tags and gene expression profiling. **Plant Molecular Biology**, v. 54, n. 4, p. 503-517, 2004.

- CAVALHEIRO, J. A. et al. Metabolômica de cana-de-açúcar e sua relação com a produção de biomassa vegetal para bioenergia. In: STRADIOTTO, N. R.; LEMOS, E. G. M. (Ed.). **Bioenergia: desenvolvimento, pesquisa e inovação**. Parte I: biomassa para bioenergia. São Paulo: Cultura Acadêmica, 2012. p. 13-34.
- CHAVES, A. et al. Presence of orange rust on sugarcane in the state of Pernambuco, Brazil. **Tropical Plant Pathology**, v. 38, n. 5, p. 443-446, 2013.
- D'AGOSTINI, S.; REBOUÇAS, M. M.; VITIELLO, N. Cana-de-açúcar: o início - pesquisa elaborada no Centro de Memória do Instituto Biológico. In: REUNIÃO ANUAL DO INSTITUTO BIOLÓGICO, 23., 2010, São Paulo. **Resumos...** [São Paulo]: [APTA], 2010. p. 161.
- DANIELS, J.; ROACH, B. T.; DON, J. H. Taxonomy and evolution. In: HEINZ, D. J. **Sugarcane improvement through breeding**. [S.l.]: Elsevier, 1987. Chap. 2, p. 7-84. (Developments in crop science, v.11).
- DESHMANE, S. S.; DEV, S. Higher isoprenoids-II: triterpenoids and steroids of *Saccharum officinarum* linn. **Tetrahedron**, v. 27, n. 6, p. 1109-1118, 1971.
- DROBY, S. et al. Presence of antifungal compounds in the peel of mango fruits and their relation to latent infections of *Alternaria alternata*. **Physiological and Molecular Plant Pathology**, v. 29, n. 2, p. 173-183, 1986.
- EGLINTON, G.; HAMILTON, R. J. Leaf epicuticular waxes. **Science**, v. 156, n. 3780, p. 1322-1335, 1967.
- FENG, S. et al. Phytochemical contents and antioxidant capacities of different parts of two sugarcane (*Saccharum officinarum* L.) cultivars. **Food Chemistry**, v. 151, p. 452-458, 2014.
- FERRARI, J. T. et al. Ferrugem alaranjada da cana-de-açúcar. **Documento Técnico/ Agência Paulista de Tecnologia dos Agronegócios**, n. 5, p. 1-8, 2010. Disponível em: <[http://www.biologico.sp.gov.br/docs/dt/ferrugem\\_cana.pdf](http://www.biologico.sp.gov.br/docs/dt/ferrugem_cana.pdf)>. Acesso em 21 nov. 2012.
- FERREIRA, M. M. C. et al. Chemometrics i: multivariate calibration, a tutorial. **Química Nova**, v. 22, n. 5, p. 724-731, 1999.
- FIGUEIREDO, P. Breve história da cana-de-açúcar e do papel do Instituto Agrônomo no seu estabelecimento no Brasil. In: DINARDO-MIRANDA, L. L. et al (Ed.). **Cana-de-açúcar**. Campinas: Instituto Agrônomo, 2008. Cap. 1, p. 31-44.
- FOOD AND AGRICULTURE ORGANIZATION OF THE UNITED NATIONS. **Food and agricultural commodities production**. Disponível em: <<http://faostat.fao.org/site/339/default.aspx>> Acesso em: 16 ago. 2013.
- GARCÍA, S. et al. Chemical basis of the resistance of barley seeds to pathogenic fungi. **Phytochemistry**, v. 44, n. 3, p. 415-418, 1997.
- GEORGES, P. et al. Ketosteroids and hydroxyketosteroids, minor metabolites of sugarcane wax. **Steroids**, v. 71, n. 8, p. 647-652, 2006.
- GOLM METABOLOME DATABASE. Disponível em: <<http://gmd.mpimp-golm.mpg.de/search.aspx>>. Acesso em: 05 set. 2013.

- HASSAN, M. K. et al. Concentrations of constitutive alk(en)ylresorcinols in peel of commercial mango varieties and resistance to postharvest anthracnose. **Physiological and Molecular Plant Pathology**, v. 71, n. 4/6, p. 158-165, 2007.
- HEREDIA, A. et al. La cutícula vegetal: estructura y funciones. **Ecología**, v. 12, n. 2, p. 293-305, 1998.
- HOARAU, J. Y. et al. Genetic dissection of a modern sugarcane cultivar (*Saccharum* spp.). I. Genome mapping with AFLP markers. **Theoretical and Applied Genetics**, v. 103, n. 1, p. 84-97, 2001.
- IRMAK, S.; DUNFORD, N. T.; MILLIGAN, J. Policosanol contents of beeswax, sugar cane and wheat extracts. **Food Chemistry**, v. 95, n. 2, p. 312-318, 2006.
- JETTER, R.; SCHÄFFER, S.; RIEDERER, M. Leaf cuticular waxes are arranged in chemically and mechanically distinct layers: evidence from *Prunus laurocerasus* L. **Plant, Cell & Environment**, v. 23, n. 6, p. 619-628, 2000.
- JIN, Q. et al. Chemical constituents from the aerial parts of *aster yomena*. **Natural Product Sciences**. v. 19, n. 3, p. 269-274, 2013.
- KITSON, F. G.; LARSEN, B.; MCEWEN, C. N. **Gas chromatography and mass spectrometry: a practical guide**. San Diego: Academic Press, 1996.
- KNÖDLER, M. et al. Characterization of major and minor alk(en)ylresorcinols from mango (*Mangifera indica* L.) peels by high-performance liquid chromatography/atmospheric pressure chemical ionization mass spectrometry. **Rapid Communications in Mass Spectrometry**, v. 21, n. 6, p. 945-951, 2007.
- KNÖDLER, M. et al. Anti-inflammatory 5-(11'Z-heptadecenyl)- and 5-(8'Z,11'Z-heptadecadienyl)-resorcinols from mango (*Mangifera indica* L.) peels. **Phytochemistry**, v. 69, n. 4, p. 988-993, 2008.
- KOZUBEK, A.; TYMAN, J. H. P. Resorcinolic lipids, the natural non-isoprenoid phenolic amphiphiles and their biological activity. **Chemical Reviews**, v. 99, n. 1, p. 1-26, 1998.
- LEDÓN, N. et al. Effects of a mixture of fatty acids from sugar cane (*Saccharum officinarum* L.) wax oil in two models of inflammation: zymosan-induced arthritis and mice tail test of psoriasis. **Phytomedicine: International Journal of Phytotherapy and Phytopharmacology**, v. 14, n. 10, p. 690-695, 2007.
- MACLEAN, D. J. Axenic culture and metabolism of rust fungi. In: SCOTT, K. J; CHAKRAVORTY, A. K. (Ed.). **The rust fungi**. London; New York: Academic Press, 1982. Chap. 2, p. 37-120.
- MADRIGAL, R. V. et al. Alkyl-and alkenylresorcinols in *Rapanea laetevirens* seed lipids. **Lipids**, v. 12, n. 4, p. 402-406, 1977.
- MAGAREY, R. C.; NIELSEN, W. A.; MAGNANINI, A. J. Environmental requirements for spore germination in three sugarcane leaf pathogens. **Proceedings of the Australian Society of Sugar Cane Technologists**, v. 26, p. 1-7, 2004.
- MASSOLA JUNIOR, N. S.; KRUGNER, T. L. Fungos fitopatogênicos. In: AMORIM, L. et al (Ed.). **Manual de fitopatologia: princípios e conceitos**. 4. ed. São Paulo: Ceres, 2011. v. 1, cap. 8, p.149-206.

MATHWORKS. **MATLAB**<sup>®</sup>: the language of technical computing. Version: R2010a, 2011. Disponível em: <<http://www.mathworks.com/products/matlab>>. Acesso em: 04 set. 2012.

McLafferty, F. W.; Turecek, F. **Interpretation of mass spectra**. 4th ed. Sausalito: University Science Books, 1993.

MOREIRA, A. S.; GONÇALVES, C. R.; RICCI, A. Reaction of thirteen sugarcane varieties to orange rust, caused by *puccinia kuehnii*. In: AMERICAN PHYTOPATHOLOGICAL SOCIETY ANNUAL MEETING, 2012, Providence. **Abstracts**. [S. l.] APS, 2012. Disponível em: <[http://www.apsnet.org/meetings/Documents/2012\\_Meeting\\_Abstracts/aps12abP255.htm](http://www.apsnet.org/meetings/Documents/2012_Meeting_Abstracts/aps12abP255.htm)>. Acesso em: 23 maio 2013.

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY. **NIST livro de química na web**: base de dados de referência padrão do NIST número 69. Disponível em: <<http://webbook.nist.gov/chemistry/>>. Acesso em: 11 ago. 2013.

NIELSEN, N.-P. V.; CARSTENSEN, J. M.; SMEDSGAARD, J. Aligning of single and multiple wavelength chromatographic profiles for chemometric data analysis using correlation optimised warping. **Journal of Chromatography A**, v. 805, n. 1/2, p. 17-35, 1998.

NUISSIER, G. et al. Composition of sugarcane waxes in rum factory wastes. **Phytochemistry**, v. 61, n. 6, p. 721-726, 2002.

OLIVEIRA, A. F. M.; MEIRELLES, S. T.; SALATINO, A. Epicuticular waxes from caatinga and cerrado species and their efficiency against water loss. **Anais da Academia Brasileira de Ciências**, v. 75, n. 4, p. 431-439, 2003.

PASCHOLATI, S. F. Fisiologia do parasitismo: como as plantas se defendem dos patógenos. In: AMORIM, L. et al (Ed.). **Manual de fitopatologia**: princípios e conceitos. 4. ed. São Paulo: Ceres, 2011. v. 1, cap. 35, p. 593-636.

PELLATI, F.; BENVENUTI, S. Chromatographic and electrophoretic methods for the analysis of phenethylamine alkaloids in *Citrus aurantium*. **Journal of Chromatography A**, v. 1161, n. 1/2, p. 71-88, 2007.

PURCELL, D. E. et al. A chemometrics investigation of sugarcane plant properties based on the molecular composition of epicuticular wax. **Chemometrics and Intelligent Laboratory Systems**, v. 76, n. 2, p. 135-147, 2005.

ROACH, B. T. Chromosome numbers in *Saccharum edule*. **CYTOLOGIA**, v. 37, n. 1, p. 155-161, 1972.

ROSS, A. B. et al. Alkylresorcinols in cereals and cereal products. **Journal of Agricultural and Food Chemistry**, v. 51, n. 14, p. 4111-4118, 2003.

ROSSETTO, R. Diagnose foliar. **Agência Embrapa de Informação Tecnológica**. Disponível em: <<http://www.agencia.cnptia.embrapa.br/gestor/cana-de-acucar/arvore/CONT000fkch7tf302wyiv80sq98yqk1vc13r.html>>. Acesso em: 23 jul. 2013.

SÃO PAULO (Estado). Secretaria de Agricultura e Abastecimento. Coordenadoria de Defesa Agropecuária. **Ferrugem alaranjada da cana-de-açúcar *Puccinia kuehnii***. Disponível em <<http://www.defesaagropecuaria.sp.gov.br/arquivos/ferrugem-alaranjada.pdf>>. Acesso em: 21 nov. 2012.

TAVARES, S. C. C. D. H.; COSTA, V. S. D. O.; LEITE, E. M. Manejo da mancha de alternária (*Alternaria alternata* e *A. solani*) na produção integrada de manga. **Instruções Técnicas da Embrapa Semi-Árido**, n. 64, out. 2005. Disponível em: <<http://www.agencia.cnptia.embrapa.br/recursos/INT64ID-At6sJExVMM.pdf>>. Acesso em: 17 fev. 2013.

TOMASI, G.; VAN DEN BERG, F.; ANDERSSON, C. Correlation optimized warping and dynamic time warping as preprocessing methods for chromatographic data. **Journal of Chemometrics**, v. 18, n. 5, p. 231-241, 2004.

UNIÃO DA INDÚSTRIA DE CANA-DE-AÇÚCAR. **Maior produtor mundial de cana-de-açúcar**. Disponível em: <<http://www.unica.com.br/faq/>>. Acesso em: 29 jun. 2013.

VAN DEN DOOL, H.; DEC. KRATZ, P. A generalization of the retention index system including linear temperature programmed gas-liquid partition chromatography. **Journal of Chromatography A**, v. 11, p. 463-471, 1963.

VILEGAS, J. H. Y. et al. Further triterpenes, steroids and furocoumarins from Brazilian medicinal plants of *Dorstenia* genus (*Moraceae*). **Journal of the Brazilian Chemical Society**, v. 8, n. 5, p. 529-535, 1997.

WENK, M. R. Lipidomics: new tools and applications. **Cell**, v. 143, n. 6, p. 888-895, 2010.

ZHU, Y.; SOROKA, D. N.; SANG, S. Synthesis and inhibitory activities against colon cancer cell growth and proteasome of alkylresorcinols. **Journal of Agricultural and Food Chemistry**, v. 60, n. 35, p. 8624-8631, 2012.

## ANEXOS

**Anexo 1:** Identificação de compostos da cera epicuticular (TMS) em variedades de cana-de-açúcar analisado por GC- MS.

ÁREA - GC-MS																	
PICOS	Tr(min)	IR cal.	IR lit. HP5ms	2094	5000	835486	891115	865084	873396	933046	942101	953028	962042	963060	845210	72454	COMPOSTOS
1	11.211	1648	1645	-	-	-	-	-	227141	-	-	-	-	-	-	-	Ácido láurico*
2	13.15	1716	-	1165439	-	124188	524518	-	147910	-	-	-	-	-	-	-	-
3	14.115	1748	1745	-	-	-	-	-	118914	-	-	-	-	-	-	-	Ácido tridecanoico*
4	17.155	1847	1843	560677	407579	116076	224668	204768	371814	82518	200154	252762	240981	272280	928888	111719	Ácido mirístico *
5	20.204	1946	1943	280221	230465	86676	120161	125035	231712	52961	139583	139823	134453	164222	595972	132755	Ácido pentadecanoico*
6	20.624	1960	1955	-	-	-	-	-	60941	-	49679	-	59713	93651	135881	-	Hexadecanol*
7	22.366	2017	2023	526335	318029	73244	170453	155972	91416	92342	150029	197936	140885	225272	1494928	133419	ácido palmitoleico*
8	22.949	2036	-	-	-	-	91143	-	-	-	-	-	-	-	-	-	-
9	23.215	2045	2040	4489751	2243679	1433109	1803216	1531130	1774920	566788	2731454	1848788	1403681	1903603	4543234	1346394	ácido palmítico*
10	24.694	2094	-	-	-	-	-	-	103191	-	-	-	-	-	57762	-	-
11	24.875	2100	2100	-	-	-	-	-	104863	-	-	-	-	-	-	-	heneicosano
12	25.316	2115	2126	43290	-	-	-	-	-	-	-	-	-	-	143261	-	cis - 10 - ácido heptadecanoico*
13	26.153	2144	2148	91687	103574	-	-	49963	186909	-	36437	32255	81055	81602	175482	41935	ácido margárico*
14	26.54	2157	2149/2165	90739	30963	80289	97434	90176	123701	-	119731	88091	121944	304617	469703	-	Octadecanol*
15	27.62	2194	-	-	-	-	-	-	82656	-	-	-	-	-	-	-	-
16	27.968	2206	2208	64434	-	-	-	-	77082	-	-	40055	-	-	146362	-	ácido linoleico*
17	28.153	2212	2215	803970	495691	267843	850322	314422	309899	133692	447719	611194	261305	893794	2217860	303301	ácido oléico*
18	28.322	2218	-	-	-	50645	-	81566	-	-	-	84370	70130	-	-	-	-
19	28.831	2236	-	-	-	-	368059	-	-	-	-	68155	-	279980	-	-	-
20	29.009	2243	2248	1761095	866860	789220	867896	648142	966590	151475	1573219	994239	731405	790716	1620441	595626	ácido esteárico*
21	30.475	2294	-	-	-	-	-	-	185669	-	-	-	-	-	-	-	-



## ANEXOS

22	30.625	<b>2300</b>	<b>2300</b>	37365	107716	44159	90879	-	183621	57450	-	-	61327	62225	88898	-	triacosano
23	30.771	<b>2342</b>	-	-	92961	-	-	-	-	-	-	-	-	-	-	-	-
24	31.783	<b>2342</b>	<b>2338</b>	-	138905	-	-	-	172199	-	-	-	74824	-	53743	-	ácido nonadecanóico*
25	32.107	<b>2354</b>	<b>2349</b>	-	-	-	-	-	39977	-	-	-	-	54975	-	-	eicosanol*
26	33.375	<b>2400</b>	<b>2400</b>	53187	60907	39140	-	-	155677	47687	-	-	79918	-	-	-	tetracosano
27	34.434	<b>2440</b>	<b>2447</b>	281467	380354	187082	198072	291860	690436	66041	146368	205489	388186	222596	385868	150993	ácido araquídico*
28	36.001	<b>2500</b>	<b>2500</b>	101529	154155	125445	115243	115426	442003	102370	87915	158263	272105	193732	219202	163037	pentacosano
29	36.995	<b>2539</b>	<b>2534</b>	90563	86611	-	-	83275	330378	-	-	-	92788	54537	53595	-	ácido Heneicosanóico*
30	37.3	<b>2551</b>	<b>2543</b>	-	-	24452	-	-	78219	-	-	-	67922	73478	92953	-	Docosanol*
31	38.255	<b>2589</b>	<b>2583/2006</b>	80578	-	-	-	-	-	-	88440	-	-	-	-	-	monopalmitin*
32	38.556	<b>2601</b>	<b>2600</b>	63641	150978	101422	92432	160789	352024	84800	65390	86126	291207	177645	137861	122028	hexacosano
33	39.509	<b>2639</b>	<b>2632</b>	4354246	1796429	2270003	2482843	3814101	9403528	703312	3044651	2579711	3693067	2167085	4599305	1398839	ácido Behênico*
34	41.011	<b>2700</b>	<b>2700</b>	422316	752741	831279	-	817765	3736838	665431	521700	1340229	-	1201396	1231012	433610	heptacosano
35	41.035	<b>2701</b>	-	-	516189	503068	3375876	484181	-	-	-	1056902	1422929	-	1144734	-	5-n-pentadecil resorcinol*
36	41.904	<b>2738</b>	<b>2731</b>	129600	78124	87418	-	132851	384241	-	85178	53459	176639	136206	129041	-	ácido tricosanóico*
37	42.203	<b>2750</b>	-	-	318904	228292	799464	-	-	-	-	-	338291	-	359318	-	-
38	43.28	<b>2796</b>	-	-	218625	188716	-	260655	1190031	157923	-	-	146185	157806	371905	177293	-
39	43.364	<b>2800</b>	-	-	-	-	139544	-	-	-	-	-	-	-	330385	-	5-n-hexadecil resorcinol*
40	43.374	<b>2800</b>	<b>2800</b>	98906	343610	211029	-	272700	179094	156832	78438	-	366754	238727	-	178011	octacosano
41	43.491	<b>2805</b>	-	-	655217	733193	578530	309645	249565	-	-	236109	965941	-	-	-	-
42	43.502	<b>2806</b>	<b>2812</b>	90268	-	-	-	-	-	475763	60361	-	-	454640	2630939	693431	esqualeno
43	44.229	<b>2837</b>	<b>2834</b>	6925032	2861059	4972716	4539584	6267178	14721943	979692	7119428	3565487	5514881	3462962	7710565	1789211	ácido tetracosanóico*
44	44.75	<b>2860</b>	-	-	737606	-	-	-	212567	-	59339	-	-	562598	-	215036	-

## ANEXOS

45	44.759	<b>2860</b>	-	-	-	181343	-	128428	-	-	-	-	231005	-	555905	-	-
46	45.16	<b>2877</b>	-	-	-	-	-	-	-	-	85294	-	-	-	-	-	-
47	45.582	<b>2897</b>	-	580856	7700907	6682931	18699792	7254346	2206703	1205508	513822	13437441	8592542	1279763	21290707	1041460	Ar:C17*
48	45.673	<b>2900</b>	<b>2900</b>	1941491	744104	480333	-	527369	2272716	542330	617342	568381	374207	809869	720653	332335	Nonacosano
49	46.131	<b>2920</b>	-	-	213625	-	-	-	-	-	-	-	-	-	-	-	-
50	46.274	<b>2927</b>	-	-	193234	-	-	-	-	-	-	-	-	94763	-	-	-
51	46.476	<b>2936</b>	<b>2937</b>	115917	-	138955	98933	246245	585478	-	127116	79422	160857	144372	246371	-	ácido pentacosanóico*
52	46.708	<b>2947</b>	-	111290	2281833	809807	3460786	644760	931160	-	693508	561799	1213795	336038	3091497	-	-
53	46.951	<b>2957</b>	-	-	-	373400	-	343524	-	-	-	-	-	-	196660	-	alquilresorcinol
54	47.071	<b>2963</b>	-	-	691284	-	-	-	-	2243475	-	-	-	-	-	1358851	-
55	47.161	<b>2967</b>	-	-	-	195054	-	-	-	-	-	-	-	-	407467	-	alquilresorcinol
56	47.395	<b>2977</b>	-	-	95321	145167	1062860	-	-	259404	-	288829	-	153788	193699	85448	esteroide
57	47.765	<b>2995</b>	-	-	595562	421781	452899	496189	-	-	-	341423	563350	-	634184	157362	Ar:C18*
58	47.826	<b>2996</b>	-	-	-	-	-	-	1010782	425537	-	-	-	328061	-	226612	-
59	47.902	<b>3000</b>	-	-	5235575	3737933	2000525	3960405	3410703	-	-	2139908	5308288	2372273	9492620	-	-
60	48.114	<b>3010</b>	-	-	130379	-	-	-	-	-	-	-	-	-	-	179357	-
61	48.348	<b>3021</b>	-	-	-	-	-	-	473801	-	-	-	226955	-	-	579296	triterpenoide
62	48.657	<b>3035</b>	<b>3035</b>	2486228	620116	2903809	1844597	3272194	9269508	337017	3157172	2182004	2253032	1549696	3862069	750749	ácido hexacosanóico*
63	48.838	<b>3044</b>	<b>3037</b>	-	-	-	-	298581	978844	-	-	-	-	376093	523702	-	Heptacosanol*
64	49.076	<b>3055</b>	-	-	-	231247	-	214138	-	-	-	243754	213013	177814	960834	-	alquilresorcinol
65	49.179	<b>3094</b>	-	-	307071	-	-	-	-	-	-	-	165768	450163	-	-	-
66	49.224	<b>3062</b>	-	-	-	210894	-	201875	-	-	-	-	-	-	-	-	-
67	49.44	<b>3072</b>	-	-	-	125401	-	-	-	-	-	-	-	-	-	-	-
68	49.668	<b>3082</b>	-	-	272579	-	-	-	-	353264	-	221813	-	-	-	-	-

## ANEXOS

69	49.856	<b>3091</b>	-	2786617	32397310	33523210	58877593	30971708	19545269	7448929	2720449	55598186	47556842	10592033	57884039	7077566	Ar:C19*
70	50.051	<b>3100</b>	<b>3100</b>	4283798	1365854	1411452	401313	839892	1877290	586904	2018314	1323043	1034470	1758948	1092805	436577	hentriacontano
71	50.19	<b>3108</b>	-	-	346547	-	-	-	-	169509	543871	-	716902	517073	478872	-	-
72	50.291	<b>3112</b>	-	431333	1738127	168037	370166	261564	1538602	546794	1649678	850577	2073519	2844259	1294624	711241	colesterol*
73	50.455	<b>3120</b>	<b>3136</b>	-	158354	73931	227723	-	695175	-	265284	-	817144	-	251044	-	$\alpha$ -tocoferol*
74	50.787	<b>3135</b>	<b>3120</b>	-	-	-	-	327217	953567	-	-	-	-	285413	264610	-	ácido heptacosanóico*
75	50.961	<b>3145</b>	-	238227	4724043	3489742	9486972	2155990	5490113	188637	2926204	2781739	5793279	1615145	8014154	380947	-
76	51.155	<b>3153</b>	-	-	-	368486	-	567347	-	-	-	-	-	-	-	-	alquilresorcinol
77	51.146	<b>3153</b>	-	297907	-	-	217475	-	-	-	-	-	-	-	-	-	-
78	51.357	<b>3163</b>	-	-	-	371314	-	-	-	-	-	188599	-	-	787473	-	alquilresorcinol
79	51.426	<b>3166</b>	-	-	3268714	-	-	-	-	11540323	-	-	-	-	-	7986156	-
80	51.545	<b>3171</b>	-	-	-	-	-	-	546198	-	628797	196087	488581	571384	176845	-	-
81	51.655	<b>3178</b>	-	1068923	-	-	-	163560	1420945	-	-	-	397349	465070	250586	-	-
82	51.784	<b>3183</b>	-	295735	-	-	-	-	-	-	-	-	-	-	-	-	-
83	51.91	<b>3190</b>	-	-	577160	722736	-	608486	-	-	-	575419	1507811	315107	710853	-	Ar C20:0*
84	51.971	<b>3192</b>	-	389058	-	-	6142744	-	2231319	-	12588884	-	-	-	-	1562642	-
85	52.087	<b>3198</b>	-	-	13074163	13151048	3859294	10585347	21161755	611236	457970	6015899	17334559	11077992	18444140	377000	-
86	52.205	<b>3203</b>	-	-	912391	-	-	-	-	-	-	-	-	-	-	-	-
87	52.251	<b>3206</b>	-	240356	-	-	128971	-	341915	-	-	-	-	-	-	-	-
88	52.38	<b>3212</b>	-	-	-	-	-	-	-	1899763	-	-	-	-	-	-	-
89	52.426	<b>3214</b>	-	-	890906	-	-	-	-	-	-	-	-	-	-	1675522	-
90	52.451	<b>3216</b>	<b>3204/3253</b>	-	-	199363	-	292576	-	-	-	-	509843	1173349	-	-	Campesterol*
91	52.588	<b>3223</b>	-	-	3504908	-	524602	4059709	47444565	-	844606	-	4732972	5730403	3240945	2163765	-
92	52.822	<b>3234</b>	-	4530308	811153	5328640	2379120	5720277	23062907	282973	2685677	3871597	2950985	4283954	7103380	558600	ácido octacosanóico*

## ANEXOS

93	52.993	<b>3292</b>	<b>3286</b>	-	520497	492652	410331	395607	1486258	344875	1529382	477978	510853	952580	-	-	estigmasterol*
94	53.18	<b>3251</b>	-	-	314574	553112	-	599727	3777224	-	-	-	918572	797017	1093197	-	alquilresorcinol
95	53.3	<b>3259</b>	-	1899358	3874706	758561	1493457	2077152	29161635	1250858	2224216	805890	3881966	7730577	11230750	2296077	-
96	53.381	<b>3262</b>	-	-	-	-	1990244	-	-	-	-	-	-	-	-	-	-
97	53.551	<b>3270</b>	-	-	-	199721	-	330445	-	-	-	-	404536	354898	-	-	alquilresocinol
98	53.74	<b>3279</b>	-	-	-	-	-	-	651664	-	-	-	-	-	-	-	-
99	53.774	<b>3281</b>	-	1614983	-	444555	-	2030293	-	-	-	-	-	-	-	-	-
100	53.896	<b>3288</b>	-	1082468	10392410	10582344	28402173	11542459	8413926	3223133	642090	24672776	25340902	3709959	16527398	2079452	Ar:C21*
101	53.968	<b>3291</b>	-	2320344	7930723	1410292	-	3698999	37436768	9272834	1349325	4211869	13426292	9290766	1861071	6992759	triterpenoide
102	54.076	<b>3296</b>	-	821447	-	-	-	-	-	-	-	-	-	-	-	-	esteroide
103	54.095	<b>3297</b>	-	-	2942560	474659	2023884	2265345	-	-	1580977	-	4533610	3534441	-	-	-
104	54.164	<b>3300</b>	<b>3300</b>	3672721	-	1431820	-	-	1680790	713483	1516771	384163	-	-	-	-	tritriacontano
105	54.2	<b>3302</b>	<b>3348/3296</b>	-	2434191	-	-	3779237	-	-	-	-	933999	7567232	1183344	-	$\beta$ -sitosterol*
106	54.321	<b>3308</b>	-	-	-	-	1208093	-	-	-	2880081	-	-	-	-	-	arundoina
107	54.443	<b>3315</b>	-	3146359	-	508124	-	841836	4791938	2320375	-	2333085	1031793	1032704	-	-	-
108	54.551	<b>3320</b>	-	1854233	-	1824020	2237533	-	4851194	-	2584152	-	506396	-	3626023	3676514	-
109	54.799	<b>3333</b>	-	56801778	-	43427254	22068295	-	80755476	-	51751634	-	50698308	-	33789289	71180202	-
110	54.861	<b>3336</b>	-	-	-	-	10397341	-	-	-	13439392	-	-	803514	-	-	-
111	54.969	<b>3341</b>	-	1190008	2681491	1929237	3618880	1370770	6957229	739383	1068689	2016808	3918692	1775022	2141761	1183539	-
112	55.228	<b>3355</b>	<b>3348</b>	1120596	-	-	-	-	3274963	1245840	-	1073107	-	-	-	-	$\beta$ -amirina*
113	55.312	<b>3359</b>	-	-	3910878	725951	-	8212239	-	-	-	-	1051596	953598	1779802	-	-
114	55.53	<b>3370</b>	-	-	865574	-	-	-	-	2909625	-	-	-	-	-	3846477	-
115	55.54	<b>3370</b>	-	448258	-	-	-	500579	839983	-	45999501	-	-	-	-	-	-
116	55.735	<b>3380</b>	-	-	1363747	-	-	-	-	-	-	-	-	1197485	-	-	-

## ANEXOS

117	55.835	<b>3385</b>	-	422589	14554457	-	-	15122856	2981116	-	1158402	-	979112	-	2620541	-	-
118	55.989	<b>3393</b>	-	-	6251234	2598766	1414024	3740689	9353855	-	912299	1530921	7134315	6401611	3322410	-	-
119	56.28	<b>3408</b>	-	-	24890085	-	2179197	3397204	9071372	5254323	11319036	6183442	10369742	12090220	285790	717341	-
120	56.315	<b>3410</b>	-	6933127	-	2464349	2268409	9770125	-	-	-	951371	-	-	-	-	-
121	56.404	<b>3415</b>	-	-	-	-	-	-	-	-	-	-	-	-	1407893	3238563	-
122	56.479	<b>3419</b>	-	55584620	8777625	10271522	62600714	132676687	14560188	6140354	2503181	6167374	4509114	686851	-	-	-
123	56.725	<b>3431</b>	<b>3432</b>	1490294	-	2839374	-	-	-	-	-	-	-	-	-	-	ácido triacontanoico*
124	56.747	<b>3433</b>	-	-	51775660	-	3851436	13617556	42914246	6281974	20121002	7445127	64600996	30070898	7781906	3742652	simiarenol
125	56.84	<b>3437</b>	-	630369	-	575841	1222585	4395616	1395803	-	675074	-	-	-	-	940705	-
126	57.125	<b>3452</b>	-	-	-	-	-	1160555	-	-	-	-	-	-	-	-	-
127	57.413	<b>3467</b>	-	-	10432255	-	-	12391187	1736491	-	1507586	198252	877358	-	311899	-	esteroide
128	57.688	<b>3482</b>	-	-	2630730	1869226	5080533	2720300	2183188	509942	176077	2930235	4110670	644811	3101699	735725	Ar C23:0*
129	57.793	<b>3487</b>	-	8887759	-	6698406	15116293	-	14689834	-	7464768	-	6027159	-	9102404	10020839	friedelina
130	58.04	<b>3500</b>	-	784229	533316	352734	407093	612177	618861	308416	520910	316677	277539	-	181569	-	-
131	58.177	<b>3507</b>	-	-	-	-	-	-	225978	-	-	-	-	-	373499	-	-
132	58.697	<b>3537</b>	<b>3530</b>	1219417	5279577	10083674	2363126	2260675	3761489	3493690	5621927	19488922	7569174	5783133	2218878	347645	dotriacontanol*
133	59.71	<b>3591</b>	-	-	244878	247378	-	183452	824943	-	-	-	472347	303598	257530	-	-
134	60.005	<b>3828</b>	-	-	-	-	315167	-	-	-	203541	-	-	-	-	-	-
135	60.434	<b>3630</b>	-	713405	245232	660245	266612	429310	2024828	-	937257	942232	550031	1021141	592751	-	ácido dotriacontanoico*
136	61.3	<b>3678</b>	-	-	217915	326010	435361	114477	141992	100500	-	884825	594855	-	286219	64956	Ar C25:0*
137	62.299	<b>3734</b>	-	-	162055	331840	-	-	-	-	-	250832	-	-	-	-	tetracontanol*
138	63.995	<b>3828</b>	-	315997	-	419111	-	261749	1073118	-	422454	342365	317942	641320	321053	-	ácido tetracontanoico*

Legenda: IR – índice de retenção.

# ANEXOS

## Anexo 2: Identificação de compostos das amostras do extrato hexânico (TMS) em variedades de cana-de-açúcar analisado por GC- MS.

ÁREA - GC-MS																			
	Tr (min)	IR cal HP5ms	IR lit. HP5ms	3046	5000	855463	891115	911099	912195	912218	915155	931530	942094	942101	944004	S-robustum	Sof cheming cemís	SofX Sbarbituri	Compostos
1	11.211	1648	1645	313722	406288	513134	1405649	405702		680498	925985	431921	729016	770026	1083173	459877	761235	339098	ácido láurico*
2	12.554	1696	1702	-	281097	-	-	-	-	-	-	-	-	142041	-	345913	-	-	ácido subérico*
3	14.145	1749	1735	-	-	-	145189	-	-	-	-	-	105742	-	-	-	-	-	cis-ácido aconítico*
4	16.376	1822	1837	-	-	-	409484	-	-	-	-	-	-	-	-	117860	-	-	ácido isocitrico
5	16.82	1836	1840	834832	525361	804182	1231456	581966	394049	1084185	967536	1118050	876600	817588	911075	582192	1272779	814507	neofitaadieno
6	17.166	1847	1843	638440	613117	875361	1585658	602066	122040	691998	1058042	1010551	909790	856651	1365803	759763	1140610	589979	ácido mirístico*
7	17.57	1861	-	240800	107056	191596	267413	143459	75140	287103	256888	241495	271566	210679	232815	181528	242070	185403	-
8	18.095	1878	-	340412	191174	278442	454895	317300	171889	337090	379821	396097	453515	343391	412742	-	447468	377733	-
9	20.206	1946	1943	225882	214265	366916	304444	191176	-	199833	386714	554353	269859	223025	462909	316229	406325	241854	ácido pentadecanóico*
10	20.65	1961	1955	55327	57631	-	107118	-	-	-	84686	149025	49389	-	103269	77766	136637	80369	hexadecanol*
11	22.382	2017	2023	150524	281102	362189	313066	356860	-	212915	368631	1189022	307806	217842	621923	237137	544037	239697	ácido palmitoleico*
12	22.933	2036	-	1223649	555600	1809090	1770836	552363	-	1032358	1845267	1486876	331239	1139293	778114	1678162	1298546	1183048	-
13	23.229	2045	2040	13848642	11795051	18989492	21366844	11062351	1582695	13330559	20224965	21130853	12894229	19077863	18024836	11636261	13065073	16314994	ácido palmítico*
14	25.329	2116	-	-	76872	141126	-	88403	-	112988	280773	230649	83445	204995	186054	-	136532	76087	-
15	26.162	2144	2144	435518	394475	580750	566875	225138	-	351768	657230	584067	323352	451518	552882	419867	382160	402007	Ácido margárico*
16	26.547	2157	2149	86645	137200	190842	186122	94495	-	94583	147748	259988	129168	121041	294590	162256	250093	133769	octadecanol*
17	26.981	2172	2181	205118	113918	417168	1281237	134071	-	421710	376819	360624	184707	402323	616344	830240	512090	316817	fitol*
18	27.987	2206	2208	5044484	4591079	7293824	9483457	3690211	303941	5552903	10333921	9687386	3696645	7385645	6299607	5959510	6213816	12050673	ácido linoléico*
19	28.158	2212	2218	23280197	20458487	31833284	40159499	21291749	1125364	24534858	39022686	44439807	17237740	29837535	32014829	22151991	21800054	37883865	alfa-ácido linolênico*
20	28.391	2221	2215	-	-	-	338781	63053	-	94443	-	201406	-	181418	183438	103994	-	135311	ácido oleico *

# ANEXOS

21	28.839	<b>2236</b>	-	2345799	533023	3228265	2561533	307658	-	1680389	1881001	2294423	211767	500336	-	4058905	2907369	301187	-
22	29.014	<b>2243</b>	<b>2248</b>	1746149	1655262	2740742	3566791	1183670	203053	1521660	2598373	2889055	1892782	1513164	2666736	2078832	2271560	2015537	ácido esteárico*
23	34.351	<b>2437</b>	-	243791	-	512643	461942	-	-	179337	345513	357275	-	172959	-	565862	379634	-	-
24	34.433	<b>2440</b>	<b>2447</b>	164820	253138	301692	526680	231057	-	258273	342220	355878	241404	192328	230707	375031	253582	350815	ácido araquídico*
25	36.029	<b>2501</b>	<b>2500</b>	-	-	-	220729	-	-	-	-	-	-	-	-	66194	-	-	Pentacosano
26	38.261	<b>2589</b>	<b>2583/2606</b>	96844	146956	236883	315068	-	-	169169	377712	200428	125344	195702	276180	120268	299440	-	monopalmitin*
27	38.358	<b>2592</b>	-	-	-	-	161146	-	-	-	-	136683	-	81829	124188	50725	98771	-	-
28	38.581	<b>2601</b>	<b>2600</b>	-	-	-	160410	-	-	-	-	-	-	-	-	-	-	-	Hexacosano
29	39.424	<b>2636</b>	<b>2610</b>	114278	3207132	-	3706378	1444145	-	1215947	642079	816190	168401	92944	565469	1495486	2546319	1613048	sacarose*
30	39.505	<b>2639</b>	<b>2632</b>	166428	363422	282542	482029	190565	-	320090	389780	544524	320832	351767	459812	498467	386266	358893	ácido behênico*
31	41.001	<b>2700</b>	<b>2700</b>	108346	99870	-	173870	80541	111843	82802	95272	-	113722	104400	156373	238738	169914	-	Heptacosano
32	41.924	<b>2739</b>	<b>2731</b>	57150	-	112780	196052	67080	-	82485	145224	113532	-	59750	146230	105720	108237	84830	ácido tricosanoico*
33	42.974	<b>2783</b>	<b>2773</b>	-	-	-	-	-	-	-	109184	-	-	-	67702	-	47718	-	Monoestearina*
34	43.52	<b>2806</b>	<b>2831</b>	115019	290463	282897	513194	240785	-	110801	382369	850442	-	114284	387190	202054	333343	190946	Esqualeno
35	43.677	<b>2813</b>	-	-	-	252900	122554	-	-	-	87462	78528	-	-	-	111803	123160	-	-
36	44.239	<b>2837</b>	<b>2834</b>	310157	433587	418448	633734	291348	-	397058	559754	719182	305682	463367	611979	570718	583115	373614	ácido tetracosanoico*
37	45.676	<b>2900</b>	<b>2900</b>	141611	131733	-	202080	68747	104631	80032	134651	96280	237158	137927	197920	293371	165774	66411	Nonacosano
38	48.665	<b>3035</b>	<b>3035</b>	-	-	-	-	-	-	60881	118311	99946	-	72797	-	85053	85168	-	ácido hexacosanoico*
39	49.887	<b>3092</b>	-	-	84306	-	122579	-	-	-	16721	-	-	-	-	-	-	-	alquilescinol*
40	50.055	<b>3100</b>	<b>3100</b>	245873	374039	249488	680559	272256	262770	279854	382522	132499	462123	482009	583234	647248	366530	142837	Hentriacontano
41	50.288	<b>3111</b>	<b>3155</b>	163848	245991	344154	239076	77134	-	212479	238597	518588	273936	302342	363551	290460	362112	204392	colesterol*
42	50.437	<b>3119</b>	<b>3136</b>	93180	112242	75945	2237198	-	-	73980	271863	-	239534	419660	177710	748690	1320899	171686	$\alpha$ -tocoferol*
43	50.94	<b>3143</b>	<b>3136</b>	260435	516626	624164	510426	68964	-	201058	342037	394431	187506	229172	514646	223861	150108	170501	octacosanol*

# ANEXOS

44	51.98	3193	-	-	-	-	-	-	251801	-	652211	515752	-	494971	197640	2720193	383372	310586	-
45	52.44	3215	3204	475522	716618	1078175	1403489	372969	-	748383	780216	1041603	743667	1066150	1378634	973985	872899	836555	campesterol*
46	52.81	3233	-	63601	116694	102102	161473	-	-	73335	118882	125500	-	-	168776	150089	137540	-	-
47	52.983	3242	3286	472376	699681	1152006	1190854	587089	-	982456	1027271	1148312	745943	1271478	1355716	1301202	1325394	1069961	estigmasterol*
48	53.334	3259	-	100251	132127	-	-	-	-	-	-	-	-	-	-	-	269405	126552	-
49	53.978	3291	-	87268	132908	-	-	392156	-	120849	159977	-	95144	-	-	462827	346967	-	-
50	54.187	3302	3296	3203871	4117036	6006525	6725292	3122193	78891	3848149	4458536	5432445	3496667	5254316	7073364	4455220	4407959	3819102	$\beta$ -sitosterol*
51	54.454	3315	-	-	-	-	-	-	-	-	113441	397203	104151	-	154505	199509	215215	-	-
52	54.78	3332	-	-	-	-	-	-	-	-	-	-	-	1990439	2414365	1436433	-	-	-
53	54.831	3334	-	-	-	-	620855	-	107016	-	639776	-	-	-	-	-	355364	1311039	-
54	54.936	3340	3334	81088	238588	166694	197012	-	-	-	123491	194939	-	-	188581	-	-	-	triacontanol*
55	55.294	3358	-	-	-	-	-	-	-	-	-	-	372448	-	151801	-	-	-	-
56	55.48	3367	-	-	-	-	-	-	-	-	1292062	397203	-	2220465	-	8461307	-	-	-
57	55.806	3384	-	-	-	-	-	-	-	-	-	-	-	-	-	680603	-	-	-
58	56.206	3404	-	159073	312186	-	-	-	266130	-	-	-	-	-	-	-	308799	350764	-
59	56.31	3410	-	-	-	-	-	-	-	-	-	-	174908	-	345544	382499	-	-	-
60	56.429	3416	-	75418	141086	-	2033106	-	-	-	622216	-	1783542	107080	4747863	3555324	340915	85543	-
61	56.696	3430	-	929467	794012	-	-	595169	-	869083	1000381	-	-	645395	-	-	1154312	399121	-
62	57.41	3467	-	-	380817	-	-	775464	-	-	-	-	-	-	-	212343	-	-	-
63	57.805	3488	-	-	-	-	309271	-	-	-	-	-	-	-	-	-	-	-	friedelina
64	58.501	3525	-	-	-	-	-	-	-	-	-	-	-	-	-	401150	-	-	-
65	58.71	3536	3530	238027	502061	395170	870139	282771	-	688470	535259	498909	123001	289974	675921	517208	468518	398171	Dotriacontanol*

Legenda: lk – índice de retenção.



**Anexo 3:** Identificação dos constituintes de cera epicuticular de folhas de cana-de-açúcar por comparação dos espectros de massas com dados das bibliotecas Wiley7 e Nist pelo software GCMS solutions Ver. 2.61

GC-MS	CERA EPICUTICULAR - FOLHAS DE CANA-DE-AÇÚCAR																																																																								
Tr	IR cal.	IR lit.																																																																							
11.211	1648	1645	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Resp</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>76</td><td>76</td><td>Dodecanoic acid, trimethylsilyl ester</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>NIST21.LIB</td></tr> <tr><td>2</td><td>76</td><td>76</td><td>Dodecanoic acid, trimethylsilyl ester (CAS) LA</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>76</td><td>76</td><td>Dodecanoic acid, trimethylsilyl ester \$\$ TriMet</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>NIST08.LIB</td></tr> <tr><td>4</td><td>76</td><td>76</td><td>Dodecanoic acid, trimethylsilyl ester \$\$ TriMet</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>NIST08.LIB</td></tr> <tr><td>5</td><td>76</td><td>76</td><td>Dodecanoic acid, trimethylsilyl ester</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>NIST21.LIB</td></tr> <tr><td>6</td><td>76</td><td>76</td><td>Dodecanoic acid, trimethylsilyl ester (CAS) LA</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>76</td><td>76</td><td>Dodecanoic acid, trimethylsilyl ester \$\$ TriMet</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>NIST08.LIB</td></tr> <tr><td>8</td><td>74</td><td>74</td><td>Dodecanoic acid, trimethylsilyl ester \$\$ TriMet</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>NIST107.LIB</td></tr> <tr><td>9</td><td>74</td><td>74</td><td>Dodecanoic acid, trimethylsilyl ester (CAS) LA</td><td>272</td><td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target: Dodecanoic acid, trimethylsilyl ester</p> <p>CAS#: 55520-95-1 Mol Wt: 272 Serial#: 16823            Cmpd Name: Dodecanoic acid, trimethylsilyl ester            Formula: C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>S Class Flag: No Class Flags</p>	Hit	Similar	Resp	Compound Name	Mol Wt	Formula	Library	1	76	76	Dodecanoic acid, trimethylsilyl ester	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST21.LIB	2	76	76	Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	WILEY229.LI	3	76	76	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST08.LIB	4	76	76	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST08.LIB	5	76	76	Dodecanoic acid, trimethylsilyl ester	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST21.LIB	6	76	76	Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	WILEY229.LI	7	76	76	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST08.LIB	8	74	74	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST107.LIB	9	74	74	Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	WILEY229.LI
Hit	Similar	Resp	Compound Name	Mol Wt	Formula	Library																																																																			
1	76	76	Dodecanoic acid, trimethylsilyl ester	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST21.LIB																																																																			
2	76	76	Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	WILEY229.LI																																																																			
3	76	76	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST08.LIB																																																																			
4	76	76	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST08.LIB																																																																			
5	76	76	Dodecanoic acid, trimethylsilyl ester	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST21.LIB																																																																			
6	76	76	Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	WILEY229.LI																																																																			
7	76	76	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST08.LIB																																																																			
8	74	74	Dodecanoic acid, trimethylsilyl ester \$\$ TriMet	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	NIST107.LIB																																																																			
9	74	74	Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub> S	WILEY229.LI																																																																			
13.165	1716	1710	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Resp</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>95</td><td>95</td><td>Xylitol, 5-O-(trimethylsilyloxy)-1,2,3,4,5-pentakis-O-(trimethylsilyl)-</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>2</td><td>90</td><td>90</td><td>Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>NIST21.LIB</td></tr> <tr><td>3</td><td>90</td><td>90</td><td>ARABITOL, 5TMS \$\$ Arabitol, pentakis-O-tri</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>90</td><td>90</td><td>ARABITOL, 5TMS \$\$ Arabitol, pentakis-O-tri</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>NIST107.LIB</td></tr> <tr><td>5</td><td>90</td><td>90</td><td>Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)- \$\$</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>89</td><td>89</td><td>Xylitol, 5TMS \$\$ Xylitol, 1,2,3,4,5-pentakis-</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>89</td><td>89</td><td>Xylitol, 5TMS \$\$ Xylitol, 1,2,3,4,5-pentakis-</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>88</td><td>88</td><td>RIBITOL, 1,2,3,4,5-PENTATMS \$\$ Ribitol, 1,2</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>88</td><td>88</td><td>RIBITOL, 1,2,3,4,5-PENTATMS \$\$ Ribitol, 1,2</td><td>512</td><td>C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target: Xylitol, 5-O-(trimethylsilyloxy)-1,2,3,4,5-pentakis-O-(trimethylsilyl)-</p> <p>CAS#: 14199-72-5 Mol Wt: 512 Serial#: 216400            Cmpd Name: Xylitol, 5TMS \$\$ Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)- (CAS) Trimethylsilyl ether of xylitol \$\$ XYLITOL-PENTATMS \$\$            Formula: C<sub>20</sub>H<sub>52</sub>O<sub>5</sub>S Class Flag: No Class Flags</p>	Hit	Similar	Resp	Compound Name	Mol Wt	Formula	Library	1	95	95	Xylitol, 5-O-(trimethylsilyloxy)-1,2,3,4,5-pentakis-O-(trimethylsilyl)-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI	2	90	90	Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	NIST21.LIB	3	90	90	ARABITOL, 5TMS \$\$ Arabitol, pentakis-O-tri	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI	4	90	90	ARABITOL, 5TMS \$\$ Arabitol, pentakis-O-tri	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	NIST107.LIB	5	90	90	Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)- \$\$	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	NIST08.LIB	6	89	89	Xylitol, 5TMS \$\$ Xylitol, 1,2,3,4,5-pentakis-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI	7	89	89	Xylitol, 5TMS \$\$ Xylitol, 1,2,3,4,5-pentakis-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI	8	88	88	RIBITOL, 1,2,3,4,5-PENTATMS \$\$ Ribitol, 1,2	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI	9	88	88	RIBITOL, 1,2,3,4,5-PENTATMS \$\$ Ribitol, 1,2	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI
Hit	Similar	Resp	Compound Name	Mol Wt	Formula	Library																																																																			
1	95	95	Xylitol, 5-O-(trimethylsilyloxy)-1,2,3,4,5-pentakis-O-(trimethylsilyl)-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI																																																																			
2	90	90	Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	NIST21.LIB																																																																			
3	90	90	ARABITOL, 5TMS \$\$ Arabitol, pentakis-O-tri	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI																																																																			
4	90	90	ARABITOL, 5TMS \$\$ Arabitol, pentakis-O-tri	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	NIST107.LIB																																																																			
5	90	90	Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)- \$\$	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	NIST08.LIB																																																																			
6	89	89	Xylitol, 5TMS \$\$ Xylitol, 1,2,3,4,5-pentakis-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI																																																																			
7	89	89	Xylitol, 5TMS \$\$ Xylitol, 1,2,3,4,5-pentakis-	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI																																																																			
8	88	88	RIBITOL, 1,2,3,4,5-PENTATMS \$\$ Ribitol, 1,2	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI																																																																			
9	88	88	RIBITOL, 1,2,3,4,5-PENTATMS \$\$ Ribitol, 1,2	512	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> S	WILEY229.LI																																																																			
14.115	1748	1745	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Resp</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>76</td><td>76</td><td>n-Tridecanoic acid, trimethylsilyl ester \$\$ Time</td><td>286</td><td>C<sub>16</sub>H<sub>34</sub>O<sub>2</sub>S</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>71</td><td>71</td><td>n-Tridecanoic acid, trimethylsilyl ester \$\$</td><td>286</td><td>C<sub>16</sub>H<sub>34</sub>O<sub>2</sub>S</td><td>NIST107.LIB</td></tr> <tr><td>3</td><td>71</td><td>71</td><td>n-Tridecanoic acid, trimethylsilyl ester \$\$ Time</td><td>286</td><td>C<sub>16</sub>H<sub>34</sub>O<sub>2</sub>S</td><td>NIST08.LIB</td></tr> <tr><td>4</td><td>68</td><td>68</td><td>TRIMETHYLSILYL ESTER OF 4-METHYLVA</td><td>188</td><td>C<sub>9</sub>H<sub>20</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>68</td><td>68</td><td>Octanoic acid, trimethylsilyl ester (CAS)</td><td>216</td><td>C<sub>11</sub>H<sub>24</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>68</td><td>68</td><td>Silane, trimethyl(trimethylsilyloxy)- (CAS) TRIDECAN</td><td>272</td><td>C<sub>16</sub>H<sub>36</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>68</td><td>68</td><td>NONANOIC ACID 1TMS \$\$ PELARGONIC A</td><td>230</td><td>C<sub>12</sub>H<sub>26</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>68</td><td>68</td><td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td><td>328</td><td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub>S</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target: n-Tridecanoic acid, trimethylsilyl ester</p> <p>CAS#: 169597-14-2 Mol Wt: 286 Serial#: 102104            Cmpd Name: n-Tridecanoic acid, trimethylsilyl ester \$\$ Trimethylsilyl tridecanoate # \$\$            Formula: C<sub>16</sub>H<sub>34</sub>O<sub>2</sub>S Class Flag: No Class Flags</p>	Hit	Similar	Resp	Compound Name	Mol Wt	Formula	Library	1	76	76	n-Tridecanoic acid, trimethylsilyl ester \$\$ Time	286	C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> S	NIST08.LIB	2	71	71	n-Tridecanoic acid, trimethylsilyl ester \$\$	286	C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> S	NIST107.LIB	3	71	71	n-Tridecanoic acid, trimethylsilyl ester \$\$ Time	286	C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> S	NIST08.LIB	4	68	68	TRIMETHYLSILYL ESTER OF 4-METHYLVA	188	C <sub>9</sub> H <sub>20</sub> O <sub>2</sub> S	WILEY229.LI	5	68	68	Octanoic acid, trimethylsilyl ester (CAS)	216	C <sub>11</sub> H <sub>24</sub> O <sub>2</sub> S	WILEY229.LI	6	68	68	Silane, trimethyl(trimethylsilyloxy)- (CAS) TRIDECAN	272	C <sub>16</sub> H <sub>36</sub> O <sub>2</sub> S	WILEY229.LI	7	68	68	NONANOIC ACID 1TMS \$\$ PELARGONIC A	230	C <sub>12</sub> H <sub>26</sub> O <sub>2</sub> S	WILEY229.LI	8	68	68	Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub> S	WILEY229.LI							
Hit	Similar	Resp	Compound Name	Mol Wt	Formula	Library																																																																			
1	76	76	n-Tridecanoic acid, trimethylsilyl ester \$\$ Time	286	C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> S	NIST08.LIB																																																																			
2	71	71	n-Tridecanoic acid, trimethylsilyl ester \$\$	286	C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> S	NIST107.LIB																																																																			
3	71	71	n-Tridecanoic acid, trimethylsilyl ester \$\$ Time	286	C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> S	NIST08.LIB																																																																			
4	68	68	TRIMETHYLSILYL ESTER OF 4-METHYLVA	188	C <sub>9</sub> H <sub>20</sub> O <sub>2</sub> S	WILEY229.LI																																																																			
5	68	68	Octanoic acid, trimethylsilyl ester (CAS)	216	C <sub>11</sub> H <sub>24</sub> O <sub>2</sub> S	WILEY229.LI																																																																			
6	68	68	Silane, trimethyl(trimethylsilyloxy)- (CAS) TRIDECAN	272	C <sub>16</sub> H <sub>36</sub> O <sub>2</sub> S	WILEY229.LI																																																																			
7	68	68	NONANOIC ACID 1TMS \$\$ PELARGONIC A	230	C <sub>12</sub> H <sub>26</sub> O <sub>2</sub> S	WILEY229.LI																																																																			
8	68	68	Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub> S	WILEY229.LI																																																																			

<p>17.152</p>	<p>1847</p>	<p>1843</p>	<p>Target</p> <p>1: 300: Tetradecanoic acid, trimethylsilyl ester (CAS) MYRISTIC ACID MONOTMS <math>\delta\delta</math> MONOTRIMETHYLSYLYL MYRISTIC ACID <math>\delta\delta</math> Trimethylsilyl ester of Tetradecanoic acid <math>\delta\delta</math></p> <p>Base Peak: 73/ 10,000</p> <p>Me(C17)12C(1)OSiMe3</p> <p>CAS# 18603-17-3 Mol Wt 300 Serial# 145447</p> <p>Cmpd Name: Tetradecanoic acid, trimethylsilyl ester (CAS) MYRISTIC ACID MONOTMS <math>\delta\delta</math> MONOTRIMETHYLSYLYL MYRISTIC ACID <math>\delta\delta</math> Trimethylsilyl ester of Tetradecanoic acid <math>\delta\delta</math></p> <p>Formula C17H36O2Si Class Flag No Class Flags</p>
<p>17.366</p>	<p>1854</p>	<p>1868</p>	<p>Target</p> <p>1: 278: Diisobutyl phthalate <math>\delta\delta</math></p> <p>Base Peak: 149/ 10,000</p> <p>Diisobutyl phthalate <math>\delta\delta</math></p> <p>CAS# 84-69-5 Mol Wt 278 Serial# 130111</p> <p>Cmpd Name: Diisobutyl phthalate <math>\delta\delta</math></p> <p>Formula C16H22O4 Class Flag No Class Flags</p>
<p>18.007</p>	<p>1875</p>	<p>-</p>	<p>Target</p> <p>10: 263: Oleanitole</p> <p>Base Peak: 55/ 10,000</p> <p>Oleanitole</p> <p>CAS# 0-00-0 Mol Wt 263 Serial# 85504</p> <p>Cmpd Name: Oleanitole</p> <p>Formula C18H32N Class Flag No Class Flags</p>
<p>18.009</p>	<p>1875</p>	<p>-</p>	<p>Target</p> <p>2: 263: Oleanitole</p> <p>Base Peak: 41/ 10,000</p> <p>Oleanitole</p> <p>CAS# 0-00-0 Mol Wt 263 Serial# 85504</p> <p>Cmpd Name: Oleanitole</p> <p>Formula C18H32N Class Flag No Class Flags</p>

<p>18.686</p>	<p>1897</p>	<p>-</p>	<p>Target</p> <p>1: 105: Tridecanenitrile \$S\$ Dodecyl cyanide \$S\$ n-Dodecyl cyanide \$S\$ 1-Cyanododecane \$S\$ Tridecanenitrile \$S\$ Tridecane nitrile \$S\$</p> <p>CAS#: 629-60-7 Mol Wt: 195 Serial#: 39973</p> <p>Comp Name: Tridecanenitrile \$S\$ Dodecyl cyanide \$S\$ n-Dodecyl cyanide \$S\$ 1-Cyanododecane \$S\$ Tridecanenitrile \$S\$ Tridecane nitrile \$S\$</p> <p>Formula: C13H25N Class Flag: No Class Flags</p>
<p>18.694</p>	<p>1897</p>	<p>-</p>	<p>Target</p> <p>1: 167: Undecanenitrile \$S\$ Undecanone nitrile \$S\$ n-Decyl cyanide \$S\$ Undecanoic acid nitrile \$S\$ 1-Cyanodecane \$S\$</p> <p>CAS#: 2244-07-7 Mol Wt: 167 Serial#: 23709</p> <p>Comp Name: Undecanenitrile \$S\$ Undecanone nitrile \$S\$ n-Decyl cyanide \$S\$ Undecanoic acid nitrile \$S\$ 1-Cyanodecane \$S\$</p> <p>Formula: C11H21N Class Flag: No Class Flags</p>
<p>20.210</p>	<p>1946</p>	<p>1942</p>	<p>Target</p> <p>1: 314: n-Pentadecanoic acid, trimethylsilyl ester \$S\$ n-Pentadecanoic acid, trimethylsilyl ester \$S\$ Trimethylsilyl pentadecanoate # \$S\$</p> <p>CAS#: 74367-22-9 Mol Wt: 314 Serial#: 121973</p> <p>Comp Name: n-Pentadecanoic acid, trimethylsilyl ester \$S\$ n-Pentadecanoic acid, trimethylsilyl ester \$S\$ Trimethylsilyl pentadecanoate # \$S\$</p> <p>Formula: C18H36O2Si Class Flag: No Class Flags</p>
<p>20.64</p>	<p>1960</p>	<p>1955</p>	<p>Target</p> <p>2: 314: Silane, hexadecyl(trimethyl)silyl \$S\$ 1-Trimethylsilyloxyhexadecane \$S\$ (Hexadecyl(trimethyl)silane # \$S\$</p> <p>CAS#: 6221-90-5 Mol Wt: 314 Serial#: 24993</p> <p>Comp Name: Silane, hexadecyl(trimethyl)silyl \$S\$ 1-Trimethylsilyloxyhexadecane \$S\$ (Hexadecyl(trimethyl)silane # \$S\$</p> <p>Formula: C19H42OSi Class Flag: No Class Flags</p>

<p>21.334</p>	<p>1983</p>	<p>1793</p>	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>87</td> <td>CP</td> <td>D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)</td> <td>540</td> <td>C21H52O6Si3</td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>87</td> <td>CP</td> <td>Peribenzylthyl(4)-ribose hydrate SS</td> <td>452</td> <td>C18H44O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>87</td> <td>CP</td> <td>alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)</td> <td>540</td> <td>C21H52O6Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>87</td> <td>CP</td> <td>alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)</td> <td>540</td> <td>C21H52O6Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>87</td> <td>CP</td> <td>alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)</td> <td>540</td> <td>C21H52O6Si3</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>87</td> <td>CP</td> <td>Glucose, pentakis-O-(trimethylsilyl) SS</td> <td>540</td> <td>C21H52O6Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>87</td> <td>CP</td> <td>Glucopyranose, pentakis-O-(trimethylsilyl)</td> <td>540</td> <td>C21H52O6Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>87</td> <td>CP</td> <td>beta-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)</td> <td>540</td> <td>C21H52O6Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>87</td> <td>CP</td> <td>beta-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)</td> <td>540</td> <td>C21H52O6Si3</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 540 D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl) (CAS) MANNULOSE-PENTATMS SS</p> <p>CAS# 99829-69-6 Mol Wt: 540 Serial# 219115</p> <p>Comp Name: D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl) (CAS) MANNULOSE-PENTATMS SS</p> <p>Formula: C21H52O6Si3 Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	87	CP	D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	WILEY229.LI	2	87	CP	Peribenzylthyl(4)-ribose hydrate SS	452	C18H44O5	WILEY229.LI	3	87	CP	alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB	4	87	CP	alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB	5	87	CP	alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	WILEY229.LI	6	87	CP	Glucose, pentakis-O-(trimethylsilyl) SS	540	C21H52O6Si3	NIST107.LIB	7	87	CP	Glucopyranose, pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB	8	87	CP	beta-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB	9	87	CP	beta-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																			
1	87	CP	D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	WILEY229.LI																																																																			
2	87	CP	Peribenzylthyl(4)-ribose hydrate SS	452	C18H44O5	WILEY229.LI																																																																			
3	87	CP	alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB																																																																			
4	87	CP	alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB																																																																			
5	87	CP	alpha-D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	WILEY229.LI																																																																			
6	87	CP	Glucose, pentakis-O-(trimethylsilyl) SS	540	C21H52O6Si3	NIST107.LIB																																																																			
7	87	CP	Glucopyranose, pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB																																																																			
8	87	CP	beta-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB																																																																			
9	87	CP	beta-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)	540	C21H52O6Si3	NIST107.LIB																																																																			
<p>22.375</p>	<p>2017</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>80</td> <td>CP</td> <td>PALMITOLEIC ACID TMS SS</td> <td>326</td> <td>C19H38O2Si</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>80</td> <td>CP</td> <td>Palmitoleic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>80</td> <td>CP</td> <td>Palmitoleic acid, trimethylsilyl ester SS Tms</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>80</td> <td>CP</td> <td>PALMITOLEIC ACID TMS SS</td> <td>326</td> <td>C19H38O2Si</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>2: 326 PALMITOLEIC ACID TMS SS</p> <p>CAS# 0-00-0 Mol Wt: 326 Serial# 161535</p> <p>Comp Name: PALMITOLEIC ACID TMS SS</p> <p>Formula: C19H38O2Si Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	NIST08.LIB	2	80	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI	3	80	CP	Palmitoleic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB	4	80	CP	Palmitoleic acid, trimethylsilyl ester SS Tms	326	C19H38O2Si	NIST08.LIB	5	80	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI	6	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB	7	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB	8	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB	9	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																			
1	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	NIST08.LIB																																																																			
2	80	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI																																																																			
3	80	CP	Palmitoleic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
4	80	CP	Palmitoleic acid, trimethylsilyl ester SS Tms	326	C19H38O2Si	NIST08.LIB																																																																			
5	80	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI																																																																			
6	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
7	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
8	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
9	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
<p>22.377</p>	<p>2017</p>	<p>2023</p>	<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester</td> <td>326</td> <td>C19H38O2Si</td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>80</td> <td>CP</td> <td>cis-9-Octadecenoic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>80</td> <td>CP</td> <td>PALMITOLEIC ACID TMS SS</td> <td>326</td> <td>C19H38O2Si</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>79</td> <td>CP</td> <td>TRANS-9-OCTADECENOIC ACID TMS SS</td> <td>326</td> <td>C19H38O2Si</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>79</td> <td>CP</td> <td>trans-9-Octadecenoic acid, trimethylsilyl ester</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>79</td> <td>CP</td> <td>trans-9-Octadecenoic acid, trimethylsilyl ester</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>79</td> <td>CP</td> <td>PALMITOLEIC ACID TMS SS</td> <td>326</td> <td>C19H38O2Si</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>79</td> <td>CP</td> <td>Palmitoleic acid, trimethylsilyl ester SS</td> <td>326</td> <td>C19H38O2Si</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>4: 326 PALMITOLEIC ACID TMS SS</p> <p>CAS# 0-00-0 Mol Wt: 326 Serial# 161535</p> <p>Comp Name: PALMITOLEIC ACID TMS SS</p> <p>Formula: C19H38O2Si Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	WILEY229.LI	2	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB	3	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB	4	80	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI	5	79	CP	TRANS-9-OCTADECENOIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI	6	79	CP	trans-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	NIST107.LIB	7	79	CP	trans-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	NIST107.LIB	8	79	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI	9	79	CP	Palmitoleic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																			
1	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	WILEY229.LI																																																																			
2	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
3	80	CP	cis-9-Octadecenoic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
4	80	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI																																																																			
5	79	CP	TRANS-9-OCTADECENOIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI																																																																			
6	79	CP	trans-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	NIST107.LIB																																																																			
7	79	CP	trans-9-Octadecenoic acid, trimethylsilyl ester	326	C19H38O2Si	NIST107.LIB																																																																			
8	79	CP	PALMITOLEIC ACID TMS SS	326	C19H38O2Si	WILEY229.LI																																																																			
9	79	CP	Palmitoleic acid, trimethylsilyl ester SS	326	C19H38O2Si	NIST107.LIB																																																																			
<p>22.949</p>	<p>2036</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>64</td> <td>CP</td> <td>7-OH-7-ME OCTANOIC ACID 2TMS SS</td> <td>318</td> <td>C15H34O4</td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>62</td> <td>CP</td> <td>2,3-DI(1-ETHYL)INDOL-2-YL(1-ETHYL)BIS-O(1-ETHYL)UREA</td> <td>262</td> <td>C12H20O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>61</td> <td>CP</td> <td>1,6-DI(2-ETHYL)INDOL-2-YL(1-ETHYL)UREA</td> <td>250</td> <td>C12H20O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>62</td> <td>CP</td> <td>Silene, 11-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-</td> <td>242</td> <td>C13H26O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>60</td> <td>CP</td> <td>D-Glucose, 2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-</td> <td>467</td> <td>C18H45N1O</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>60</td> <td>CP</td> <td>Silene, 11-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-</td> <td>242</td> <td>C13H26O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>59</td> <td>CP</td> <td>25-Triethylsilyloxy-4-cholesten-3-one SS</td> <td>472</td> <td>C30H52O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>59</td> <td>CP</td> <td>Galactose, 2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-</td> <td>467</td> <td>C18H45N1O</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>59</td> <td>CP</td> <td>Silene, 10-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-</td> <td>146</td> <td>C6H10S2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 318 7-OH-7-ME OCTANOIC ACID 2TMS SS</p> <p>CAS# 0-00-0 Mol Wt: 318 Serial# 156673</p> <p>Comp Name: 7-OH-7-ME OCTANOIC ACID 2TMS SS</p> <p>Formula: C15H34O4 Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	64	CP	7-OH-7-ME OCTANOIC ACID 2TMS SS	318	C15H34O4	WILEY229.LI	2	62	CP	2,3-DI(1-ETHYL)INDOL-2-YL(1-ETHYL)BIS-O(1-ETHYL)UREA	262	C12H20O2	WILEY229.LI	3	61	CP	1,6-DI(2-ETHYL)INDOL-2-YL(1-ETHYL)UREA	250	C12H20O2	WILEY229.LI	4	62	CP	Silene, 11-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	242	C13H26O2	WILEY229.LI	5	60	CP	D-Glucose, 2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	467	C18H45N1O	WILEY229.LI	6	60	CP	Silene, 11-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	242	C13H26O2	WILEY229.LI	7	59	CP	25-Triethylsilyloxy-4-cholesten-3-one SS	472	C30H52O2	WILEY229.LI	8	59	CP	Galactose, 2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	467	C18H45N1O	WILEY229.LI	9	59	CP	Silene, 10-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	146	C6H10S2	WILEY229.LI
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																			
1	64	CP	7-OH-7-ME OCTANOIC ACID 2TMS SS	318	C15H34O4	WILEY229.LI																																																																			
2	62	CP	2,3-DI(1-ETHYL)INDOL-2-YL(1-ETHYL)BIS-O(1-ETHYL)UREA	262	C12H20O2	WILEY229.LI																																																																			
3	61	CP	1,6-DI(2-ETHYL)INDOL-2-YL(1-ETHYL)UREA	250	C12H20O2	WILEY229.LI																																																																			
4	62	CP	Silene, 11-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	242	C13H26O2	WILEY229.LI																																																																			
5	60	CP	D-Glucose, 2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	467	C18H45N1O	WILEY229.LI																																																																			
6	60	CP	Silene, 11-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	242	C13H26O2	WILEY229.LI																																																																			
7	59	CP	25-Triethylsilyloxy-4-cholesten-3-one SS	472	C30H52O2	WILEY229.LI																																																																			
8	59	CP	Galactose, 2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	467	C18H45N1O	WILEY229.LI																																																																			
9	59	CP	Silene, 10-(5-ethyltetrahydro-5-methyl-2H-pyridin-2-ylidene)-2-amino-2-deoxy-, tetraakis(trimethylsilyloxy)-	146	C6H10S2	WILEY229.LI																																																																			



<p>22.955</p>	<p>2036</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Regio</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>71</td> <td>71</td> <td></td> <td>3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl-<math>\delta\delta</math></td> <td>262</td> <td>C<sub>12</sub>H<sub>20</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>71</td> <td>71</td> <td></td> <td>3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl-<math>\delta\delta</math></td> <td>262</td> <td>C<sub>12</sub>H<sub>20</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>70</td> <td>70</td> <td></td> <td>7-OH-7-ME-OCTANOIC ACID 2TMS <math>\delta\delta</math></td> <td>210</td> <td>C<sub>18</sub>H<sub>34</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>69</td> <td>69</td> <td></td> <td>2-METHYL-1,2-PROPANEDIOL 2TMS <math>\delta\delta</math> 1,2-</td> <td>234</td> <td>C<sub>10</sub>H<sub>26</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>68</td> <td>68</td> <td></td> <td>2-METHYL-1,2-PROPANEDIOL 2TMS <math>\delta\delta</math> 1,2-</td> <td>234</td> <td>C<sub>10</sub>H<sub>26</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>68</td> <td>68</td> <td></td> <td>Slane, [dimethyl(methyl)trimethyl- (CAS) 2</td> <td>146</td> <td>C<sub>8</sub>H<sub>18</sub>S<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>67</td> <td>67</td> <td></td> <td>Propanoic acid, 2-methyl-2-(trimethylsilyloxy)-</td> <td>248</td> <td>C<sub>10</sub>H<sub>24</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>66</td> <td>66</td> <td></td> <td>5-OH-5-ME-HEXANOIC ACID 2TMS <math>\delta\delta</math> 5-HY</td> <td>290</td> <td>C<sub>13</sub>H<sub>26</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 262: 3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl-<math>\delta\delta</math> 2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxo-2,7-disulfolactone <math>\delta\delta</math></p> <p>CAS#: 6730-56-7 Mol Wt: 262 Serial#: 84487</p> <p>Cmpd Name: 3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl-<math>\delta\delta</math> 2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxo-2,7-disulfolactone <math>\delta\delta</math></p> <p>Formula: C<sub>12</sub>H<sub>20</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library	71	71		3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl- $\delta\delta$	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	WILEY229.LI	71	71		3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl- $\delta\delta$	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	NIST107.LIB	70	70		7-OH-7-ME-OCTANOIC ACID 2TMS $\delta\delta$	210	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI	69	69		2-METHYL-1,2-PROPANEDIOL 2TMS $\delta\delta$ 1,2-	234	C <sub>10</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI	68	68		2-METHYL-1,2-PROPANEDIOL 2TMS $\delta\delta$ 1,2-	234	C <sub>10</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI	68	68		Slane, [dimethyl(methyl)trimethyl- (CAS) 2	146	C <sub>8</sub> H <sub>18</sub> S <sub>2</sub>	WILEY229.LI	67	67		Propanoic acid, 2-methyl-2-(trimethylsilyloxy)-	248	C <sub>10</sub> H <sub>24</sub> O <sub>3</sub>	WILEY229.LI	66	66		5-OH-5-ME-HEXANOIC ACID 2TMS $\delta\delta$ 5-HY	290	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI							
RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library																																																																			
71	71		3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl- $\delta\delta$	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	WILEY229.LI																																																																			
71	71		3,6-Dioxo-2,7-disulfolactone, 2,2,4,4,5,5,7,7-octamethyl- $\delta\delta$	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	NIST107.LIB																																																																			
70	70		7-OH-7-ME-OCTANOIC ACID 2TMS $\delta\delta$	210	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI																																																																			
69	69		2-METHYL-1,2-PROPANEDIOL 2TMS $\delta\delta$ 1,2-	234	C <sub>10</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI																																																																			
68	68		2-METHYL-1,2-PROPANEDIOL 2TMS $\delta\delta$ 1,2-	234	C <sub>10</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI																																																																			
68	68		Slane, [dimethyl(methyl)trimethyl- (CAS) 2	146	C <sub>8</sub> H <sub>18</sub> S <sub>2</sub>	WILEY229.LI																																																																			
67	67		Propanoic acid, 2-methyl-2-(trimethylsilyloxy)-	248	C <sub>10</sub> H <sub>24</sub> O <sub>3</sub>	WILEY229.LI																																																																			
66	66		5-OH-5-ME-HEXANOIC ACID 2TMS $\delta\delta$ 5-HY	290	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI																																																																			
<p>23.225</p>	<p>2045</p>	<p>2047</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Regio</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>95</td> <td>95</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST121.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST121.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>93</td> <td>93</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 328: Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palmitic acid, trimethylsilyl ester <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math></p> <p>CAS#: 55520-89-3 Mol Wt: 328 Serial#: 131372</p> <p>Cmpd Name: Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palmitic acid, trimethylsilyl ester <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math></p> <p>Formula: C<sub>19</sub>H<sub>40</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library	95	95		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI	94	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI	94	94		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	93	93		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST107.LIB
RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library																																																																			
95	95		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
93	93		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST107.LIB																																																																			
<p>23.226</p>	<p>2045</p>	<p>2040</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Regio</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>95</td> <td>95</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>95</td> <td>95</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST108.LIB</td> </tr> <tr> <td>95</td> <td>95</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST121.LIB</td> </tr> <tr> <td>95</td> <td>95</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST121.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palm</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 328: Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palmitic acid, trimethylsilyl ester <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math></p> <p>CAS#: 55520-89-3 Mol Wt: 328 Serial#: 131372</p> <p>Cmpd Name: Hexadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Palmitic acid, trimethylsilyl ester <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math> Trimethylsilyl palmitate <math>\delta\delta</math></p> <p>Formula: C<sub>19</sub>H<sub>40</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library	95	95		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	95	95		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST108.LIB	95	95		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB	95	95		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI	94	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI	94	94		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST107.LIB
RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library																																																																			
95	95		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
95	95		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST108.LIB																																																																			
95	95		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB																																																																			
95	95		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST121.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
94	94		Hexadecanoic acid, trimethylsilyl ester $\delta\delta$ Palm	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	NIST107.LIB																																																																			
<p>24.679</p>	<p>2094</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Regio</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>72</td> <td>72</td> <td></td> <td>Heptadecanoic acid, trimethylsilyl ester (CAS)</td> <td>342</td> <td>C<sub>20</sub>H<sub>42</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>70</td> <td>70</td> <td></td> <td>Heptadecanoic acid, trimethylsilyl ester <math>\delta\delta</math> Tr</td> <td>342</td> <td>C<sub>20</sub>H<sub>42</sub>O<sub>2</sub></td> <td>NIST108.LIB</td> </tr> <tr> <td>70</td> <td>70</td> <td></td> <td>Heptadecanoic acid, trimethylsilyl ester <math>\delta\delta</math></td> <td>342</td> <td>C<sub>20</sub>H<sub>42</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>70</td> <td>70</td> <td></td> <td>Heptadecanoic acid, trimethylsilyl ester (CAS)</td> <td>342</td> <td>C<sub>20</sub>H<sub>42</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>69</td> <td>69</td> <td></td> <td>Heptadecanoic acid, trimethylsilyl ester (CAS)</td> <td>342</td> <td>C<sub>20</sub>H<sub>42</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>66</td> <td>66</td> <td></td> <td>TRIMETHYLSILYL ESTER OF TETRAICOSA</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>66</td> <td>66</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester (CAS) S</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>65</td> <td>65</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>65</td> <td>65</td> <td></td> <td>Nonadecanoic acid, trimethylsilyl ester (CAS)</td> <td>370</td> <td>C<sub>22</sub>H<sub>46</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 342: Heptadecanoic acid, trimethylsilyl ester (CAS) HEPTADECANOIC ACID 1TMS <math>\delta\delta</math> HEPTADECANOIC ACID-MONO1TMS <math>\delta\delta</math></p> <p>CAS#: 55517-50-3 Mol Wt: 342 Serial#: 170157</p> <p>Cmpd Name: Heptadecanoic acid, trimethylsilyl ester (CAS) HEPTADECANOIC ACID 1TMS <math>\delta\delta</math> HEPTADECANOIC ACID-MONO1TMS <math>\delta\delta</math></p> <p>Formula: C<sub>20</sub>H<sub>42</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library	72	72		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI	70	70		Heptadecanoic acid, trimethylsilyl ester $\delta\delta$ Tr	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	NIST108.LIB	70	70		Heptadecanoic acid, trimethylsilyl ester $\delta\delta$	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	NIST107.LIB	70	70		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI	69	69		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI	66	66		TRIMETHYLSILYL ESTER OF TETRAICOSA	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	WILEY229.LI	66	66		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI	65	65		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI	65	65		Nonadecanoic acid, trimethylsilyl ester (CAS)	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI
RT	Similar	Regio	Compound Name	Mol Wt	Formula	Library																																																																			
72	72		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI																																																																			
70	70		Heptadecanoic acid, trimethylsilyl ester $\delta\delta$ Tr	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	NIST108.LIB																																																																			
70	70		Heptadecanoic acid, trimethylsilyl ester $\delta\delta$	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	NIST107.LIB																																																																			
70	70		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI																																																																			
69	69		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI																																																																			
66	66		TRIMETHYLSILYL ESTER OF TETRAICOSA	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	WILEY229.LI																																																																			
66	66		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI																																																																			
65	65		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI																																																																			
65	65		Nonadecanoic acid, trimethylsilyl ester (CAS)	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI																																																																			

<p>25.31</p>	<p>2115</p>	<p>2126</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>77</td> <td>81</td> <td></td> <td>6-(3-OCTADECENOIC ACID 11MS) \$S</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>81</td> <td></td> <td>11-Eicosenoic acid, trimethyl ester \$S</td> <td>382</td> <td>C29H50O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>81</td> <td></td> <td>11-Eicosenoic acid, trimethyl ester</td> <td>382</td> <td>C29H50O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>10</td> <td>81</td> <td></td> <td>Oleic acid, trimethyl ester \$S</td> <td>354</td> <td>C21H42O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>11</td> <td>81</td> <td></td> <td>Oleic acid, trimethyl ester (CAS) TRIMETH</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>12</td> <td>80</td> <td></td> <td>Oleic acid, trimethyl ester \$S</td> <td>354</td> <td>C21H42O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>13</td> <td>80</td> <td></td> <td>cis-13-Docosanoic acid, trimethyl ester</td> <td>410</td> <td>C29H50O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>14</td> <td>80</td> <td></td> <td>cis-13-Docosanoic acid, trimethyl ester</td> <td>410</td> <td>C29H50O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>15</td> <td>80</td> <td></td> <td>11-Oleic-10-TRIDECENOIC ACID 11MS \$S</td> <td>394</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>14 : 340 cis-10-Heptadecenoic acid, trimethyl ester</p> <p>CAS# 0-00-0 Mol Wt: 340 Smiles: 129156      Cpnd Name: cis-10-Heptadecenoic acid, trimethyl ester      Formula: C20H40O2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	77	81		6-(3-OCTADECENOIC ACID 11MS) \$S	354	C21H42O2	WILEY229.LI	8	81		11-Eicosenoic acid, trimethyl ester \$S	382	C29H50O2	NIST107.LIB	9	81		11-Eicosenoic acid, trimethyl ester	382	C29H50O2	NIST08.LIB	10	81		Oleic acid, trimethyl ester \$S	354	C21H42O2	NIST107.LIB	11	81		Oleic acid, trimethyl ester (CAS) TRIMETH	354	C21H42O2	WILEY229.LI	12	80		Oleic acid, trimethyl ester \$S	354	C21H42O2	NIST08.LIB	13	80		cis-13-Docosanoic acid, trimethyl ester	410	C29H50O2	NIST08.LIB	14	80		cis-13-Docosanoic acid, trimethyl ester	410	C29H50O2	NIST107.LIB	15	80		11-Oleic-10-TRIDECENOIC ACID 11MS \$S	394	C21H42O2	WILEY229.LI
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
77	81		6-(3-OCTADECENOIC ACID 11MS) \$S	354	C21H42O2	WILEY229.LI																																																																			
8	81		11-Eicosenoic acid, trimethyl ester \$S	382	C29H50O2	NIST107.LIB																																																																			
9	81		11-Eicosenoic acid, trimethyl ester	382	C29H50O2	NIST08.LIB																																																																			
10	81		Oleic acid, trimethyl ester \$S	354	C21H42O2	NIST107.LIB																																																																			
11	81		Oleic acid, trimethyl ester (CAS) TRIMETH	354	C21H42O2	WILEY229.LI																																																																			
12	80		Oleic acid, trimethyl ester \$S	354	C21H42O2	NIST08.LIB																																																																			
13	80		cis-13-Docosanoic acid, trimethyl ester	410	C29H50O2	NIST08.LIB																																																																			
14	80		cis-13-Docosanoic acid, trimethyl ester	410	C29H50O2	NIST107.LIB																																																																			
15	80		11-Oleic-10-TRIDECENOIC ACID 11MS \$S	394	C21H42O2	WILEY229.LI																																																																			
<p>26.156</p>	<p>2144</p>	<p>2148</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>11</td> <td>85</td> <td></td> <td>Heptadecanoic acid, trimethyl ester \$S</td> <td>342</td> <td>C20H40O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>85</td> <td></td> <td>Heptadecanoic acid, trimethyl ester \$S</td> <td>342</td> <td>C20H40O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>85</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>84</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>84</td> <td></td> <td>Heptadecanoic acid, trimethyl ester</td> <td>342</td> <td>C20H40O2</td> <td>NIST2.LIB</td> </tr> <tr> <td>6</td> <td>84</td> <td></td> <td>Heptadecanoic acid, trimethyl ester \$S</td> <td>342</td> <td>C20H40O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>81</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>81</td> <td></td> <td>Nonadecanoic acid, trimethyl ester \$S</td> <td>370</td> <td>C22H42O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>81</td> <td></td> <td>Octadecanoic acid, trimethyl ester \$S</td> <td>356</td> <td>C21H42O2</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1 : 242 Heptadecanoic acid, trimethyl ester \$S</p> <p>CAS# 55517-58-3 Mol Wt: 342 Smiles: 82574      Cpnd Name: Heptadecanoic acid, trimethyl ester \$S      Formula: C20H40O2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	11	85		Heptadecanoic acid, trimethyl ester \$S	342	C20H40O2	NIST107.LIB	2	85		Heptadecanoic acid, trimethyl ester \$S	342	C20H40O2	NIST08.LIB	3	85		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H40O2	WILEY229.LI	4	84		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H40O2	WILEY229.LI	5	84		Heptadecanoic acid, trimethyl ester	342	C20H40O2	NIST2.LIB	6	84		Heptadecanoic acid, trimethyl ester \$S	342	C20H40O2	NIST08.LIB	7	81		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H40O2	WILEY229.LI	8	81		Nonadecanoic acid, trimethyl ester \$S	370	C22H42O2	NIST08.LIB	9	81		Octadecanoic acid, trimethyl ester \$S	356	C21H42O2	NIST107.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
11	85		Heptadecanoic acid, trimethyl ester \$S	342	C20H40O2	NIST107.LIB																																																																			
2	85		Heptadecanoic acid, trimethyl ester \$S	342	C20H40O2	NIST08.LIB																																																																			
3	85		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H40O2	WILEY229.LI																																																																			
4	84		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H40O2	WILEY229.LI																																																																			
5	84		Heptadecanoic acid, trimethyl ester	342	C20H40O2	NIST2.LIB																																																																			
6	84		Heptadecanoic acid, trimethyl ester \$S	342	C20H40O2	NIST08.LIB																																																																			
7	81		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H40O2	WILEY229.LI																																																																			
8	81		Nonadecanoic acid, trimethyl ester \$S	370	C22H42O2	NIST08.LIB																																																																			
9	81		Octadecanoic acid, trimethyl ester \$S	356	C21H42O2	NIST107.LIB																																																																			
<p>26.54</p>	<p>2157</p>	<p>2149</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>91</td> <td></td> <td>1-Trimethylsilyloctadecane \$S</td> <td>342</td> <td>C21H46OSi</td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>81</td> <td></td> <td>Octadecanoic acid, trimethyl ester \$S</td> <td>356</td> <td>C21H42O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>81</td> <td></td> <td>1-Dimethylprop-2-enylsilyloctadecane \$S</td> <td>368</td> <td>C29H54OSi</td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>87</td> <td></td> <td>1-Dimethylprop-2-enylsilyloctadecane \$S</td> <td>368</td> <td>C29H54OSi</td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>86</td> <td></td> <td>1-Dimethylchloromethylsilyloctadecane \$S</td> <td>376</td> <td>C21H46OSi</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>86</td> <td></td> <td>1-Dimethylchloromethylsilyloctadecane \$S</td> <td>376</td> <td>C21H46OSi</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>85</td> <td></td> <td>1-Dimethylsilyloctadecane</td> <td>412</td> <td>C29H56OSi</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>84</td> <td></td> <td>1-Octadecanol, tert-butyl dimethylsilyl ether</td> <td>384</td> <td>C24H50OSi</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>83</td> <td></td> <td>1-Dimethylbutylsilyloctadecane</td> <td>364</td> <td>C24H52OSi</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>2 : 342 Silane, trimethyl(octadecyl)- \$S\$ Octadecyltrimethylsilane \$S\$ 1-Trimethylsilyloctadecane \$S\$ Octadecane, 1-trimethylsilyloxy- \$S\$ (Octadecylsilyloctadecane \$S\$ 1-Octadecanol, trimethylsilyl ether \$S\$ Octadecyl trimethylsilyl ether \$S\$</p> <p>CAS# 18748-08-6 Mol Wt: 342 Smiles: 26003      Cpnd Name: Silane, trimethyl(octadecyl)- \$S\$ Octadecyltrimethylsilane \$S\$ 1-Trimethylsilyloctadecane \$S\$ Octadecane, 1-trimethylsilyloxy- \$S\$ (Octadecylsilyloctadecane \$S\$ 1-Octadecanol, trimethylsilyl ether \$S\$ Octadecyl trimethylsilyl ether \$S\$      Formula: C21H46OSi Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	91		1-Trimethylsilyloctadecane \$S	342	C21H46OSi	NIST107.LIB	2	81		Octadecanoic acid, trimethyl ester \$S	356	C21H42O2	NIST107.LIB	3	81		1-Dimethylprop-2-enylsilyloctadecane \$S	368	C29H54OSi	NIST107.LIB	4	87		1-Dimethylprop-2-enylsilyloctadecane \$S	368	C29H54OSi	NIST107.LIB	5	86		1-Dimethylchloromethylsilyloctadecane \$S	376	C21H46OSi	NIST107.LIB	6	86		1-Dimethylchloromethylsilyloctadecane \$S	376	C21H46OSi	NIST08.LIB	7	85		1-Dimethylsilyloctadecane	412	C29H56OSi	NIST08.LIB	8	84		1-Octadecanol, tert-butyl dimethylsilyl ether	384	C24H50OSi	NIST08.LIB	9	83		1-Dimethylbutylsilyloctadecane	364	C24H52OSi	NIST08.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	91		1-Trimethylsilyloctadecane \$S	342	C21H46OSi	NIST107.LIB																																																																			
2	81		Octadecanoic acid, trimethyl ester \$S	356	C21H42O2	NIST107.LIB																																																																			
3	81		1-Dimethylprop-2-enylsilyloctadecane \$S	368	C29H54OSi	NIST107.LIB																																																																			
4	87		1-Dimethylprop-2-enylsilyloctadecane \$S	368	C29H54OSi	NIST107.LIB																																																																			
5	86		1-Dimethylchloromethylsilyloctadecane \$S	376	C21H46OSi	NIST107.LIB																																																																			
6	86		1-Dimethylchloromethylsilyloctadecane \$S	376	C21H46OSi	NIST08.LIB																																																																			
7	85		1-Dimethylsilyloctadecane	412	C29H56OSi	NIST08.LIB																																																																			
8	84		1-Octadecanol, tert-butyl dimethylsilyl ether	384	C24H50OSi	NIST08.LIB																																																																			
9	83		1-Dimethylbutylsilyloctadecane	364	C24H52OSi	NIST08.LIB																																																																			
<p>27.966</p>	<p>2206</p>	<p>2201</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>11</td> <td>83</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z), trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>83</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z), trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>83</td> <td></td> <td>11,14-Eicosadienoic acid, trimethyl ester</td> <td>380</td> <td>C29H50O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>14</td> <td>83</td> <td></td> <td>11,14-Eicosadienoic acid, trimethyl ester \$S</td> <td>380</td> <td>C29H50O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>83</td> <td></td> <td>11,14-EICOSADIENOIC ACID 11MS \$S</td> <td>380</td> <td>C29H50O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>81</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z), trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>81</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z), trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST21.LIB</td> </tr> <tr> <td>9</td> <td>81</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z), trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1 : 262 9,12-Octadecadienoic acid (Z,Z), trimethyl ester \$S\$ Linoleic acid trimethylsilyl ester \$S\$</p> <p>CAS# 56299-07-5 Mol Wt: 352 Smiles: 146189      Cpnd Name: 9,12-Octadecadienoic acid (Z,Z), trimethylsilyl ester \$S\$ Linoleic acid trimethylsilyl ester \$S\$      Formula: C21H40O2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	11	83		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	WILEY229.LI	3	83		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	NIST107.LIB	4	83		11,14-Eicosadienoic acid, trimethyl ester	380	C29H50O2	NIST08.LIB	14	83		11,14-Eicosadienoic acid, trimethyl ester \$S	380	C29H50O2	NIST107.LIB	5	83		11,14-EICOSADIENOIC ACID 11MS \$S	380	C29H50O2	WILEY229.LI	7	81		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	WILEY229.LI	8	81		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	NIST21.LIB	9	81		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	NIST08.LIB							
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
11	83		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	WILEY229.LI																																																																			
3	83		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	NIST107.LIB																																																																			
4	83		11,14-Eicosadienoic acid, trimethyl ester	380	C29H50O2	NIST08.LIB																																																																			
14	83		11,14-Eicosadienoic acid, trimethyl ester \$S	380	C29H50O2	NIST107.LIB																																																																			
5	83		11,14-EICOSADIENOIC ACID 11MS \$S	380	C29H50O2	WILEY229.LI																																																																			
7	81		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	WILEY229.LI																																																																			
8	81		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	NIST21.LIB																																																																			
9	81		9,12-Octadecadienoic acid (Z,Z), trimethyl ester	352	C21H40O2	NIST08.LIB																																																																			

<p>28.15</p>	<p>2212</p>	<p>2215</p>	<p>Target</p> <p>79: 354 : Oleic acid, trimethylsilyl ester (CAS) TRIMETHYLSILYL ESTER OF OLEIC ACID \$\$\$ MONOTRIMETHYLSILYL OLEIC ACID \$\$\$ OLEIC ACID MONOTMS \$\$\$</p> <p>Base Peak: 79/ 10.000</p> <p>Chemical Structure: <chem>Me(CH2)7CH(CH2)7C(O)OSiMe3</chem></p> <p>CAS#: 21556-26-3 Mol Wt: 354 Serial#: 175900</p> <p>Cepid Name: Oleic acid, trimethylsilyl ester (CAS) TRIMETHYLSILYL ESTER OF OLEIC ACID \$\$\$ MONOTRIMETHYLSILYL OLEIC ACID \$\$\$ OLEIC ACID MONOTMS \$\$\$</p> <p>Formula: C21 H42 O2 Si Class Flag: No Class Flags</p>
<p>28.324</p>	<p>2218</p>	<p>-</p>	<p>Target</p> <p>11: 405 : Androst-2-en-17-amine, 4,4-dimethyl-4(2-phenylethyl)-, hydrochloride, (5.alpha.) (CAS) 4,4-DIMETHYL-17-((2-(BETA-PHENYLETHYLAMINO)5ALPHA-ANDROST-2-ENE HYDROCHLORIDE \$\$\$</p> <p>Base Peak: 314/ 10.000</p> <p>Chemical Structure: <chem>C29H43N</chem></p> <p>CAS#: 53206-45-6 Mol Wt: 405 Serial#: 195640</p> <p>Cepid Name: Androst-2-en-17-amine, 4,4-dimethyl-4(2-phenylethyl)-, hydrochloride, (5.alpha.) (CAS) 4,4-DIMETHYL-17-((2-(BETA-PHENYLETHYLAMINO)5ALPHA-ANDROST-2-ENE HYDROCHLORIDE \$\$\$</p> <p>Formula: C29 H43 N Class Flag: No Class Flags</p>
<p>28.84</p>	<p>2236</p>	<p>-</p>	<p>Target</p> <p>1: 160 : Sterane, (1,1-dimethylpropoxy)trimethyl- \$\$\$ tet-Propyl trimethylsilyl ether # \$\$\$ 2-Methyl-3-pentanol, trimethylsilyl ether \$\$\$</p> <p>Base Peak: 131/ 10.000</p> <p>Chemical Structure: <chem>C29H50O</chem></p> <p>CAS#: 6693-16-3 Mol Wt: 160 Serial#: 20012</p> <p>Cepid Name: Sterane, (1,1-dimethylpropoxy)trimethyl- \$\$\$ tet-Propyl trimethylsilyl ether # \$\$\$ 2-Methyl-3-pentanol, trimethylsilyl ether \$\$\$</p> <p>Formula: C29 H50 O Class Flag: No Class Flags</p>
<p>29.013</p>	<p>2243</p>	<p>2239</p>	<p>Target</p> <p>1: 356 : Octadecanoic acid, trimethylsilyl ester (CAS) STEARIC ACID-MONOTMS \$\$\$ Trimethylsilyl ester of Octadecanoic acid \$\$\$ TMS ESTER OF STEARIC ACID \$\$\$ Stearic acid, trimethylsilyl ester \$\$\$ MONOTRIMETHYLSILYL STEARIC ACID \$\$\$</p> <p>Base Peak: 79/ 10.000</p> <p>Chemical Structure: <chem>Me(CH2)7C(O)OSiMe3</chem></p> <p>CAS#: 10749-01-9 Mol Wt: 356 Serial#: 170852</p> <p>Cepid Name: Octadecanoic acid, trimethylsilyl ester (CAS) STEARIC ACID-MONOTMS \$\$\$ Trimethylsilyl ester of Octadecanoic acid \$\$\$ TMS ESTER OF STEARIC ACID \$\$\$ Stearic acid, trimethylsilyl ester \$\$\$ MONOTRIMETHYLSILYL STEARIC ACID \$\$\$</p> <p>Formula: C21 H44 O2 Si Class Flag: No Class Flags</p>

<p>30.642</p>	<p>2300</p>	<p>2300</p>	<p>Target</p> <p>1: 2300: Docosane (CAS) n-Docosane 33 C22H46 STANDARD 33</p> <p>CAS# 629-97-0 Mol Wt: 310 Serial#: 152108</p> <p>Cmpd Name: Docosane (CAS) n-Docosane 33 C22H46 STANDARD 33</p> <p>Formula: C22H46 Class Flag: No Class Flags</p>
<p>30.856</p>	<p>2308</p>	<p>-</p>	<p>Target</p> <p>1: 262: 2,3-BUTANDIOL, 2,3-DIMETHYL-BIS-O-(TRIMETHYLSILYL)- 33</p> <p>CAS# 0-00-0 Mol Wt: 262 Serial#: 117961</p> <p>Cmpd Name: 2,3-BUTANDIOL, 2,3-DIMETHYL-BIS-O-(TRIMETHYLSILYL)- 33</p> <p>Formula: C12H30O2Si2 Class Flag: No Class Flags</p>
<p>36.02</p>	<p>2500</p>	<p>2500</p>	<p>Target</p> <p>3: 338: Tetracosane (CAS) n-Tetracosane 33</p> <p>CAS# 646-31-1 Mol Wt: 338 Serial#: 168330</p> <p>Cmpd Name: Tetracosane (CAS) n-Tetracosane 33</p> <p>Formula: C24H50 Class Flag: No Class Flags</p>
<p>38.564</p>	<p>2600</p>	<p>2600</p>	<p>Target</p> <p>11: 202: Eicosane (CAS) n-Eicosane 33</p> <p>CAS# 112-95-8 Mol Wt: 282 Serial#: 133325</p> <p>Cmpd Name: Eicosane (CAS) n-Eicosane 33</p> <p>Formula: C20H42 Class Flag: No Class Flags</p>



<p>39.509</p>	<p>2639</p>	<p>2632</p>	<p>Target</p> <p>1: 412 Docosanoic acid, trimethylsilyl ester #5</p> <p>CAS# 74367-36-5 Mol Wt 412 Serial# 171217</p> <p>Cmpd Name: Docosanoic acid, trimethylsilyl ester #5</p> <p>Formula: C25H50O2</p>
<p>41.04</p>	<p>2700</p>	<p>2700</p>	<p>Target</p> <p>11: 380 Heptacosane #5</p> <p>CAS# 593-45-7 Mol Wt 380 Serial# 26822</p> <p>Cmpd Name: Heptacosane #5</p> <p>Formula: C27H56</p>
<p>41.04</p>	<p>2701</p>	<p>-</p>	<p>Target</p> <p>1: 439 I-Valine, n-heptafluorobutyl-, nonyl ester</p> <p>CAS# 0-00-0 Mol Wt 439 Serial# 177098</p> <p>Cmpd Name: I-Valine, n-heptafluorobutyl-, nonyl ester</p> <p>Formula: C19H28F7NO3</p>
<p>44.234</p>	<p>2837</p>	<p>2848</p>	<p>Target</p> <p>2: 440 Tetraacosanoic acid, trimethylsilyl ester #5</p> <p>CAS# 74367-37-6 Mol Wt 440 Serial# 177349</p> <p>Cmpd Name: Tetraacosanoic acid, trimethylsilyl ester #5</p> <p>Formula: C27H56O2</p>

<p>45.596</p>	<p>2897</p>	<p>-</p>	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Reg</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>77</td> <td>C</td> <td>Olivetol, bis(trimethylsilyl) ether</td> <td>324</td> <td>C<sub>19</sub>H<sub>32</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>51</td> <td>C</td> <td>3-Hydroxyacetic acid, bis(trimethylsilyl) ester</td> <td>263</td> <td>C<sub>12</sub>H<sub>24</sub>N<sub>2</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>67</td> <td>F</td> <td>alpha-Phenyl-beta-trimethylsilyloxy styrene S5</td> <td>268</td> <td>C<sub>17</sub>H<sub>20</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>66</td> <td>F</td> <td>1,4-Bis(trimethylsilyloxy)-2-methylbenzene S5</td> <td>268</td> <td>C<sub>13</sub>H<sub>24</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>64</td> <td>F</td> <td>2-METHYLBIS(OH)CYCLO DITHIOL S5</td> <td>268</td> <td>C<sub>13</sub>H<sub>24</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>63</td> <td>F</td> <td>ibenzocyclo[1,2,3]hepta-2,6-diene S5</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>63</td> <td>F</td> <td>Spicy[1,4]oxone-9,9-dicyclo[3,2,1,0]hepta-3,1,0-dithione S5</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>61</td> <td>F</td> <td>4-METHYLBIS(OH)CYCLO DITHIOL S5</td> <td>268</td> <td>C<sub>13</sub>H<sub>24</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>61</td> <td>F</td> <td>3-Benzidien-3,8-dithiodicthioheptalidene S</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 324: Olivetol, bis(trimethylsilyl) ether</p> <p>CAS# 0-00-0 Mol Wt: 324 Serial# 129432</p> <p>Cmpd Name: Olivetol, bis(trimethylsilyl) ether</p> <p>Formula: C<sub>19</sub>H<sub>32</sub>O<sub>3</sub> Class Flag: No Class Flags</p>	HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library	1	77	C	Olivetol, bis(trimethylsilyl) ether	324	C <sub>19</sub> H <sub>32</sub> O <sub>3</sub>	WILEY229.LI	2	51	C	3-Hydroxyacetic acid, bis(trimethylsilyl) ester	263	C <sub>12</sub> H <sub>24</sub> N <sub>2</sub> O	WILEY229.LI	3	67	F	alpha-Phenyl-beta-trimethylsilyloxy styrene S5	268	C <sub>17</sub> H <sub>20</sub> O	WILEY229.LI	4	66	F	1,4-Bis(trimethylsilyloxy)-2-methylbenzene S5	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI	5	64	F	2-METHYLBIS(OH)CYCLO DITHIOL S5	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI	6	63	F	ibenzocyclo[1,2,3]hepta-2,6-diene S5	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI	7	63	F	Spicy[1,4]oxone-9,9-dicyclo[3,2,1,0]hepta-3,1,0-dithione S5	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI	8	61	F	4-METHYLBIS(OH)CYCLO DITHIOL S5	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI	9	61	F	3-Benzidien-3,8-dithiodicthioheptalidene S	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI
HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library																																																																			
1	77	C	Olivetol, bis(trimethylsilyl) ether	324	C <sub>19</sub> H <sub>32</sub> O <sub>3</sub>	WILEY229.LI																																																																			
2	51	C	3-Hydroxyacetic acid, bis(trimethylsilyl) ester	263	C <sub>12</sub> H <sub>24</sub> N <sub>2</sub> O	WILEY229.LI																																																																			
3	67	F	alpha-Phenyl-beta-trimethylsilyloxy styrene S5	268	C <sub>17</sub> H <sub>20</sub> O	WILEY229.LI																																																																			
4	66	F	1,4-Bis(trimethylsilyloxy)-2-methylbenzene S5	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	64	F	2-METHYLBIS(OH)CYCLO DITHIOL S5	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI																																																																			
6	63	F	ibenzocyclo[1,2,3]hepta-2,6-diene S5	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
7	63	F	Spicy[1,4]oxone-9,9-dicyclo[3,2,1,0]hepta-3,1,0-dithione S5	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
8	61	F	4-METHYLBIS(OH)CYCLO DITHIOL S5	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI																																																																			
9	61	F	3-Benzidien-3,8-dithiodicthioheptalidene S	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
<p>45.596</p>	<p>2900</p>	<p>2900</p>	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Reg</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>85</td> <td>F</td> <td>Tetradecane S5 n-Tetradecane S5</td> <td>476</td> <td>C<sub>34</sub>H<sub>70</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>87</td> <td>F</td> <td>Tetradecane S5 n-Tetradecane S5</td> <td>618</td> <td>C<sub>44</sub>H<sub>90</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>87</td> <td>F</td> <td>Tetradecane S5 n-Tetradecane S5</td> <td>618</td> <td>C<sub>44</sub>H<sub>90</sub></td> <td>NIST21.LIB</td> </tr> <tr> <td>4</td> <td>87</td> <td>F</td> <td>Tetradecane S5 n-Tetradecane S5</td> <td>476</td> <td>C<sub>34</sub>H<sub>70</sub></td> <td>NIST06.LIB</td> </tr> <tr> <td>5</td> <td>87</td> <td>F</td> <td>Nonacosane S5 n-Nonacosane S5</td> <td>408</td> <td>C<sub>29</sub>H<sub>60</sub></td> <td>NIST06.LIB</td> </tr> <tr> <td>6</td> <td>87</td> <td>F</td> <td>Nonacosane S5 n-Nonacosane S5</td> <td>296</td> <td>C<sub>21</sub>H<sub>44</sub></td> <td>NIST06.LIB</td> </tr> <tr> <td>7</td> <td>87</td> <td>F</td> <td>Nonacosane S5 n-Nonacosane S5</td> <td>296</td> <td>C<sub>21</sub>H<sub>44</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>87</td> <td>F</td> <td>Nonacosane S5 n-Nonacosane S5</td> <td>408</td> <td>C<sub>29</sub>H<sub>60</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>87</td> <td>F</td> <td>Nonacosane</td> <td>268</td> <td>C<sub>19</sub>H<sub>40</sub></td> <td>NIST121.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>0: 408: Nonacosane S5 n-Nonacosane S5</p> <p>CAS# 630-03-5 Mol Wt: 408 Serial# 94191</p> <p>Cmpd Name: Nonacosane S5 n-Nonacosane S5</p> <p>Formula: C<sub>29</sub>H<sub>60</sub> Class Flag: No Class Flags</p>	HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library	1	85	F	Tetradecane S5 n-Tetradecane S5	476	C <sub>34</sub> H <sub>70</sub>	NIST107.LIB	2	87	F	Tetradecane S5 n-Tetradecane S5	618	C <sub>44</sub> H <sub>90</sub>	NIST08.LIB	3	87	F	Tetradecane S5 n-Tetradecane S5	618	C <sub>44</sub> H <sub>90</sub>	NIST21.LIB	4	87	F	Tetradecane S5 n-Tetradecane S5	476	C <sub>34</sub> H <sub>70</sub>	NIST06.LIB	5	87	F	Nonacosane S5 n-Nonacosane S5	408	C <sub>29</sub> H <sub>60</sub>	NIST06.LIB	6	87	F	Nonacosane S5 n-Nonacosane S5	296	C <sub>21</sub> H <sub>44</sub>	NIST06.LIB	7	87	F	Nonacosane S5 n-Nonacosane S5	296	C <sub>21</sub> H <sub>44</sub>	NIST107.LIB	8	87	F	Nonacosane S5 n-Nonacosane S5	408	C <sub>29</sub> H <sub>60</sub>	NIST107.LIB	9	87	F	Nonacosane	268	C <sub>19</sub> H <sub>40</sub>	NIST121.LIB
HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library																																																																			
1	85	F	Tetradecane S5 n-Tetradecane S5	476	C <sub>34</sub> H <sub>70</sub>	NIST107.LIB																																																																			
2	87	F	Tetradecane S5 n-Tetradecane S5	618	C <sub>44</sub> H <sub>90</sub>	NIST08.LIB																																																																			
3	87	F	Tetradecane S5 n-Tetradecane S5	618	C <sub>44</sub> H <sub>90</sub>	NIST21.LIB																																																																			
4	87	F	Tetradecane S5 n-Tetradecane S5	476	C <sub>34</sub> H <sub>70</sub>	NIST06.LIB																																																																			
5	87	F	Nonacosane S5 n-Nonacosane S5	408	C <sub>29</sub> H <sub>60</sub>	NIST06.LIB																																																																			
6	87	F	Nonacosane S5 n-Nonacosane S5	296	C <sub>21</sub> H <sub>44</sub>	NIST06.LIB																																																																			
7	87	F	Nonacosane S5 n-Nonacosane S5	296	C <sub>21</sub> H <sub>44</sub>	NIST107.LIB																																																																			
8	87	F	Nonacosane S5 n-Nonacosane S5	408	C <sub>29</sub> H <sub>60</sub>	NIST107.LIB																																																																			
9	87	F	Nonacosane	268	C <sub>19</sub> H <sub>40</sub>	NIST121.LIB																																																																			
<p>46.479</p>	<p>2936</p>	<p>2922</p>	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Reg</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>73</td> <td>C</td> <td>Pentacosanoic acid, trimethylsilyl ester</td> <td>454</td> <td>C<sub>29</sub>H<sub>60</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>73</td> <td>F</td> <td>Nonacosanoic acid, trimethylsilyl ester</td> <td>468</td> <td>C<sub>29</sub>H<sub>60</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>73</td> <td>F</td> <td>TRIMETHYLSILYL ESTER OF TETRACOSA</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>73</td> <td>F</td> <td>Pentacosanoic acid, trimethylsilyl ester S5</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>73</td> <td>F</td> <td>Tetradecanoic acid, trimethylsilyl ester S5 Tam</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>71</td> <td>F</td> <td>Dodecanoic acid, trimethylsilyl ester (CAS) DO</td> <td>412</td> <td>C<sub>25</sub>H<sub>52</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>71</td> <td>F</td> <td>Dodecanoic acid, trimethylsilyl ester S5 Trimeth</td> <td>412</td> <td>C<sub>25</sub>H<sub>52</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>71</td> <td>F</td> <td>Dodecanoic acid, trimethylsilyl ester S5</td> <td>412</td> <td>C<sub>25</sub>H<sub>52</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>71</td> <td>F</td> <td>Octadecanoic acid, trimethylsilyl ester (CAS) S</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 454: Pentacosanoic acid, trimethylsilyl ester</p> <p>CAS# 0-00-0 Mol Wt: 454 Serial# 179617</p> <p>Cmpd Name: Pentacosanoic acid, trimethylsilyl ester</p> <p>Formula: C<sub>29</sub>H<sub>60</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library	1	73	C	Pentacosanoic acid, trimethylsilyl ester	454	C <sub>29</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB	2	73	F	Nonacosanoic acid, trimethylsilyl ester	468	C <sub>29</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB	3	73	F	TRIMETHYLSILYL ESTER OF TETRACOSA	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	WILEY229.LI	4	73	F	Pentacosanoic acid, trimethylsilyl ester S5	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB	5	73	F	Tetradecanoic acid, trimethylsilyl ester S5 Tam	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB	6	71	F	Dodecanoic acid, trimethylsilyl ester (CAS) DO	412	C <sub>25</sub> H <sub>52</sub> O <sub>2</sub>	WILEY229.LI	7	71	F	Dodecanoic acid, trimethylsilyl ester S5 Trimeth	412	C <sub>25</sub> H <sub>52</sub> O <sub>2</sub>	NIST08.LIB	8	71	F	Dodecanoic acid, trimethylsilyl ester S5	412	C <sub>25</sub> H <sub>52</sub> O <sub>2</sub>	NIST107.LIB	9	71	F	Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI
HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library																																																																			
1	73	C	Pentacosanoic acid, trimethylsilyl ester	454	C <sub>29</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB																																																																			
2	73	F	Nonacosanoic acid, trimethylsilyl ester	468	C <sub>29</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB																																																																			
3	73	F	TRIMETHYLSILYL ESTER OF TETRACOSA	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	WILEY229.LI																																																																			
4	73	F	Pentacosanoic acid, trimethylsilyl ester S5	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB																																																																			
5	73	F	Tetradecanoic acid, trimethylsilyl ester S5 Tam	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB																																																																			
6	71	F	Dodecanoic acid, trimethylsilyl ester (CAS) DO	412	C <sub>25</sub> H <sub>52</sub> O <sub>2</sub>	WILEY229.LI																																																																			
7	71	F	Dodecanoic acid, trimethylsilyl ester S5 Trimeth	412	C <sub>25</sub> H <sub>52</sub> O <sub>2</sub>	NIST08.LIB																																																																			
8	71	F	Dodecanoic acid, trimethylsilyl ester S5	412	C <sub>25</sub> H <sub>52</sub> O <sub>2</sub>	NIST107.LIB																																																																			
9	71	F	Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI																																																																			
<p>46.711</p>	<p>2946</p>	<p>-</p>	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Reg</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>64</td> <td>C</td> <td>10-acetoxy-9-anthrol, bis(trimethylsilyl) ether S5</td> <td>324</td> <td>C<sub>19</sub>H<sub>20</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>61</td> <td>F</td> <td>1,4-Bis(trimethylsilyloxy)-2,5-dimethylbenzene S5</td> <td>282</td> <td>C<sub>14</sub>H<sub>26</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>61</td> <td>F</td> <td>HEPTAMETHYL-CYCLOHEPTASILOXANE S5</td> <td>282</td> <td>C<sub>7</sub>H<sub>12</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>60</td> <td>F</td> <td>Stane, bicyclo[4.2.0]octa-3,7-diene-7,8-diylo</td> <td>282</td> <td>C<sub>14</sub>H<sub>26</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>59</td> <td>F</td> <td>1-Propanone, 1-(2,4,6-trimethylsilyloxy)phen</td> <td>310</td> <td>C<sub>15</sub>H<sub>28</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>58</td> <td>F</td> <td>10-bis(trimethylsilyloxy)-9,9-dicyclo[3,2,1,0]hepta-3,1,0-dithione S5</td> <td>324</td> <td>C<sub>19</sub>H<sub>20</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>58</td> <td>F</td> <td>1-bis(trimethylsilyloxy)-2-trimethylsilyloxypropane</td> <td>296</td> <td>C<sub>18</sub>H<sub>34</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>58</td> <td>F</td> <td>(1,5-dimethoxy-2-trimethylsilyloxy)benzyltrimethylsilyl</td> <td>296</td> <td>C<sub>15</sub>H<sub>28</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>57</td> <td>F</td> <td>TRIMETHYLSILYL ESTER OF 3-METHYL-2-</td> <td>296</td> <td>C<sub>14</sub>H<sub>24</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 324: 10-acetoxy-9-anthrol, bis(trimethylsilyl) ether S5</p> <p>CAS# 98540-96-6 Mol Wt: 324 Serial# 160375</p> <p>Cmpd Name: 10-acetoxy-9-anthrol, bis(trimethylsilyl) ether S5</p> <p>Formula: C<sub>19</sub>H<sub>20</sub>O<sub>3</sub> Class Flag: No Class Flags</p>	HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library	1	64	C	10-acetoxy-9-anthrol, bis(trimethylsilyl) ether S5	324	C <sub>19</sub> H <sub>20</sub> O <sub>3</sub>	WILEY229.LI	2	61	F	1,4-Bis(trimethylsilyloxy)-2,5-dimethylbenzene S5	282	C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI	3	61	F	HEPTAMETHYL-CYCLOHEPTASILOXANE S5	282	C <sub>7</sub> H <sub>12</sub> O <sub>4</sub>	WILEY229.LI	4	60	F	Stane, bicyclo[4.2.0]octa-3,7-diene-7,8-diylo	282	C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI	5	59	F	1-Propanone, 1-(2,4,6-trimethylsilyloxy)phen	310	C <sub>15</sub> H <sub>28</sub> O <sub>3</sub>	WILEY229.LI	6	58	F	10-bis(trimethylsilyloxy)-9,9-dicyclo[3,2,1,0]hepta-3,1,0-dithione S5	324	C <sub>19</sub> H <sub>20</sub> O <sub>3</sub>	WILEY229.LI	7	58	F	1-bis(trimethylsilyloxy)-2-trimethylsilyloxypropane	296	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI	8	58	F	(1,5-dimethoxy-2-trimethylsilyloxy)benzyltrimethylsilyl	296	C <sub>15</sub> H <sub>28</sub> O <sub>2</sub>	WILEY229.LI	9	57	F	TRIMETHYLSILYL ESTER OF 3-METHYL-2-	296	C <sub>14</sub> H <sub>24</sub> O <sub>3</sub>	WILEY229.LI
HM	Similar	Reg	Compound Name	Mol Wt	Formula	Library																																																																			
1	64	C	10-acetoxy-9-anthrol, bis(trimethylsilyl) ether S5	324	C <sub>19</sub> H <sub>20</sub> O <sub>3</sub>	WILEY229.LI																																																																			
2	61	F	1,4-Bis(trimethylsilyloxy)-2,5-dimethylbenzene S5	282	C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI																																																																			
3	61	F	HEPTAMETHYL-CYCLOHEPTASILOXANE S5	282	C <sub>7</sub> H <sub>12</sub> O <sub>4</sub>	WILEY229.LI																																																																			
4	60	F	Stane, bicyclo[4.2.0]octa-3,7-diene-7,8-diylo	282	C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	59	F	1-Propanone, 1-(2,4,6-trimethylsilyloxy)phen	310	C <sub>15</sub> H <sub>28</sub> O <sub>3</sub>	WILEY229.LI																																																																			
6	58	F	10-bis(trimethylsilyloxy)-9,9-dicyclo[3,2,1,0]hepta-3,1,0-dithione S5	324	C <sub>19</sub> H <sub>20</sub> O <sub>3</sub>	WILEY229.LI																																																																			
7	58	F	1-bis(trimethylsilyloxy)-2-trimethylsilyloxypropane	296	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI																																																																			
8	58	F	(1,5-dimethoxy-2-trimethylsilyloxy)benzyltrimethylsilyl	296	C <sub>15</sub> H <sub>28</sub> O <sub>2</sub>	WILEY229.LI																																																																			
9	57	F	TRIMETHYLSILYL ESTER OF 3-METHYL-2-	296	C <sub>14</sub> H <sub>24</sub> O <sub>3</sub>	WILEY229.LI																																																																			

# ANEXOS

<p>46.935</p>	<p>2956</p>	<p>-</p>	
<p>47.067</p>	<p>2963</p>	<p>-</p>	
<p>47.161</p>	<p>2967</p>	<p>-</p>	
<p>47.384</p>	<p>2977</p>	<p>-</p>	



<p>47.765</p>	<p>2994</p>	<p>-</p>	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>2.76</td> <td>92</td> <td>Q</td> <td>Dibutyl bis(bis(2-ethylhexyl) ether)</td> <td>628</td> <td>C<sub>48</sub>H<sub>100</sub>O<sub>4</sub></td> <td>NIST02.LIB</td> </tr> <tr> <td>2</td> <td>55</td> <td>F</td> <td>alpha-Phenyl-beta-methylstyrene \$S\$</td> <td>268</td> <td>C<sub>17</sub>H<sub>20</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>66</td> <td>F</td> <td>3-Pyridinacetic acid, 5-(2-methylallyl)oxy-</td> <td>263</td> <td>C<sub>12</sub>H<sub>11</sub>N</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>55</td> <td>F</td> <td>1,4-Bis(methylsilyloxy)-2-methylbenzene \$S\$</td> <td>268</td> <td>C<sub>13</sub>H<sub>24</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>64</td> <td>F</td> <td>Spino[9H]fluorene-9,9'-bicyclo[3.3.1]oct-8(9H)-one</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>63</td> <td>F</td> <td>2-METHYLRESORCINOL DITHIOL \$S\$</td> <td>268</td> <td>C<sub>13</sub>H<sub>14</sub>S<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>63</td> <td>F</td> <td>libenyl[1,1'-bicyclo[2,2]nona-2,6,8-triene \$S\$</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>62</td> <td>F</td> <td>9H-Fluorene, 9,9'-bicyclo[3.3.1]oct-8(9H)-one</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>61</td> <td>F</td> <td>2,5-Bis(4-hydroxyphenyl)thiophene \$S\$ Phenol</td> <td>268</td> <td>C<sub>16</sub>H<sub>12</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 324: Dibutyl bis(bis(2-ethylhexyl) ether)</p> <p>CAS# 0-00-0 Mol Wt: 628 Serial#: 120432</p> <p>Capd Name: Dibutyl bis(bis(2-ethylhexyl) ether)</p> <p>Formula: C<sub>48</sub>H<sub>100</sub>O<sub>4</sub> Class Flag: No Class Flag</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	2.76	92	Q	Dibutyl bis(bis(2-ethylhexyl) ether)	628	C <sub>48</sub> H <sub>100</sub> O <sub>4</sub>	NIST02.LIB	2	55	F	alpha-Phenyl-beta-methylstyrene \$S\$	268	C <sub>17</sub> H <sub>20</sub> O	WILEY229.LI	3	66	F	3-Pyridinacetic acid, 5-(2-methylallyl)oxy-	263	C <sub>12</sub> H <sub>11</sub> N	WILEY229.LI	4	55	F	1,4-Bis(methylsilyloxy)-2-methylbenzene \$S\$	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI	5	64	F	Spino[9H]fluorene-9,9'-bicyclo[3.3.1]oct-8(9H)-one	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI	6	63	F	2-METHYLRESORCINOL DITHIOL \$S\$	268	C <sub>13</sub> H <sub>14</sub> S <sub>2</sub>	WILEY229.LI	7	63	F	libenyl[1,1'-bicyclo[2,2]nona-2,6,8-triene \$S\$	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI	8	62	F	9H-Fluorene, 9,9'-bicyclo[3.3.1]oct-8(9H)-one	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI	9	61	F	2,5-Bis(4-hydroxyphenyl)thiophene \$S\$ Phenol	268	C <sub>16</sub> H <sub>12</sub> O <sub>2</sub>	WILEY229.LI
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
2.76	92	Q	Dibutyl bis(bis(2-ethylhexyl) ether)	628	C <sub>48</sub> H <sub>100</sub> O <sub>4</sub>	NIST02.LIB																																																																			
2	55	F	alpha-Phenyl-beta-methylstyrene \$S\$	268	C <sub>17</sub> H <sub>20</sub> O	WILEY229.LI																																																																			
3	66	F	3-Pyridinacetic acid, 5-(2-methylallyl)oxy-	263	C <sub>12</sub> H <sub>11</sub> N	WILEY229.LI																																																																			
4	55	F	1,4-Bis(methylsilyloxy)-2-methylbenzene \$S\$	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	64	F	Spino[9H]fluorene-9,9'-bicyclo[3.3.1]oct-8(9H)-one	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
6	63	F	2-METHYLRESORCINOL DITHIOL \$S\$	268	C <sub>13</sub> H <sub>14</sub> S <sub>2</sub>	WILEY229.LI																																																																			
7	63	F	libenyl[1,1'-bicyclo[2,2]nona-2,6,8-triene \$S\$	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
8	62	F	9H-Fluorene, 9,9'-bicyclo[3.3.1]oct-8(9H)-one	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
9	61	F	2,5-Bis(4-hydroxyphenyl)thiophene \$S\$ Phenol	268	C <sub>16</sub> H <sub>12</sub> O <sub>2</sub>	WILEY229.LI																																																																			
<p>47.912</p>	<p>3000</p>	<p>-</p>	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>57</td> <td>Q</td> <td>2,6-DIHYDROXYBENZOIDIC ACID 3TMS \$S\$ m</td> <td>370</td> <td>C<sub>16</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>55</td> <td>F</td> <td>Cyclopentasiloxane, decamethyl-, (CAS) Dimet</td> <td>370</td> <td>C<sub>10</sub>H<sub>30</sub>O<sub>5</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>55</td> <td>F</td> <td>Benzoic acid, 2,5-bis(methylsilyloxy)-, trimethyls</td> <td>370</td> <td>C<sub>16</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>55</td> <td>F</td> <td>Benzeneacetic acid, alpha-(4-methylphenyl)ethyl</td> <td>472</td> <td>C<sub>20</sub>H<sub>20</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>55</td> <td>F</td> <td>2,6-DIHYDROXYBENZOIDIC ACID 3TMS \$S\$ m</td> <td>370</td> <td>C<sub>16</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>54</td> <td>F</td> <td>TRIMETHYLSILYL ESTER OF 2,3-BIS(TRIM</td> <td>370</td> <td>C<sub>16</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>53</td> <td>F</td> <td>3,4-DIHYDROXYBENZYL ALCOHOL 3TMS \$</td> <td>366</td> <td>C<sub>16</sub>H<sub>32</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>53</td> <td>F</td> <td>Benzoic acid, 2,4-bis(methylsilyloxy)-, trimet</td> <td>370</td> <td>C<sub>16</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>53</td> <td>F</td> <td>Benzeneethanamine, N-(pentafluorophenyl)m</td> <td>563</td> <td>C<sub>24</sub>H<sub>34</sub>F<sub>5</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>2: 370: Cyclopentasiloxane, decamethyl-, (CAS) Dimethylsiloxane pentamer \$S\$ DECAMETHYL-CYCLOPENTASILOXANE \$S\$ Decamethylcyclopentasiloxane \$S\$ Union Carbide 7158 Silicone Fluid \$S\$ Dow Corning 345 \$S\$ NUC Silicone Y5 7158 \$S\$ Dow Corning 345 FN</p> <p>CAS# 541-02-6 Mol Wt: 370 Serial#: 182520</p> <p>Capd Name: Cyclopentasiloxane, decamethyl-, (CAS) Dimethylsiloxane pentamer \$S\$ DECAMETHYL-CYCLOPENTASILOXANE \$S\$ Decamethylcyclopentasiloxane \$S\$ Union Carbide 7158 Silicone Fluid \$S\$ Dow Corning 345 \$S\$ NUC Silicone Y5 7158 \$S\$ Dow Corning</p> <p>Formula: C<sub>10</sub>H<sub>30</sub>O<sub>5</sub> Class Flag: No Class Flag</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	57	Q	2,6-DIHYDROXYBENZOIDIC ACID 3TMS \$S\$ m	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	2	55	F	Cyclopentasiloxane, decamethyl-, (CAS) Dimet	370	C <sub>10</sub> H <sub>30</sub> O <sub>5</sub>	WILEY229.LI	3	55	F	Benzoic acid, 2,5-bis(methylsilyloxy)-, trimethyls	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	4	55	F	Benzeneacetic acid, alpha-(4-methylphenyl)ethyl	472	C <sub>20</sub> H <sub>20</sub> O <sub>2</sub>	WILEY229.LI	5	55	F	2,6-DIHYDROXYBENZOIDIC ACID 3TMS \$S\$ m	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	6	54	F	TRIMETHYLSILYL ESTER OF 2,3-BIS(TRIM	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	7	53	F	3,4-DIHYDROXYBENZYL ALCOHOL 3TMS \$	366	C <sub>16</sub> H <sub>32</sub> O <sub>3</sub>	WILEY229.LI	8	53	F	Benzoic acid, 2,4-bis(methylsilyloxy)-, trimet	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	9	53	F	Benzeneethanamine, N-(pentafluorophenyl)m	563	C <sub>24</sub> H <sub>34</sub> F <sub>5</sub>	WILEY229.LI
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	57	Q	2,6-DIHYDROXYBENZOIDIC ACID 3TMS \$S\$ m	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
2	55	F	Cyclopentasiloxane, decamethyl-, (CAS) Dimet	370	C <sub>10</sub> H <sub>30</sub> O <sub>5</sub>	WILEY229.LI																																																																			
3	55	F	Benzoic acid, 2,5-bis(methylsilyloxy)-, trimethyls	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
4	55	F	Benzeneacetic acid, alpha-(4-methylphenyl)ethyl	472	C <sub>20</sub> H <sub>20</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	55	F	2,6-DIHYDROXYBENZOIDIC ACID 3TMS \$S\$ m	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
6	54	F	TRIMETHYLSILYL ESTER OF 2,3-BIS(TRIM	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
7	53	F	3,4-DIHYDROXYBENZYL ALCOHOL 3TMS \$	366	C <sub>16</sub> H <sub>32</sub> O <sub>3</sub>	WILEY229.LI																																																																			
8	53	F	Benzoic acid, 2,4-bis(methylsilyloxy)-, trimet	370	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
9	53	F	Benzeneethanamine, N-(pentafluorophenyl)m	563	C <sub>24</sub> H <sub>34</sub> F <sub>5</sub>	WILEY229.LI																																																																			
<p>48.114</p>	<p>3010</p>	<p>-</p>	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>55</td> <td>Q</td> <td>octyl-diphenylamine \$S\$</td> <td>210</td> <td>C<sub>21</sub>H<sub>28</sub>N<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>58</td> <td>F</td> <td>4-amino-5-methylamino-1,8-dioxane \$S\$ 9H-Fluore</td> <td>210</td> <td>C<sub>18</sub>H<sub>14</sub>N<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>58</td> <td>F</td> <td>2-chloro-5-methyl-4-(2'-phenyl)pyrimidine \$S\$ Pyr</td> <td>210</td> <td>C<sub>13</sub>H<sub>7</sub>ClN<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>58</td> <td>F</td> <td>6-METHYL-2-ETHYLENEBIS(OXY)-3-OXABIC</td> <td>210</td> <td>C<sub>11</sub>H<sub>14</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>58</td> <td>F</td> <td>2-(ALPHA-DIETHYLPHOSPHORIC ACID) DIACRIDINE \$S\$ Acrid</td> <td>207</td> <td>C<sub>15</sub>H<sub>10</sub>D<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>58</td> <td>F</td> <td>DI-2,5-DIMETHYL-3-STYRYL-PYRAZINE \$S\$</td> <td>210</td> <td>C<sub>16</sub>H<sub>14</sub>N<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>57</td> <td>F</td> <td>1-(5-methylamino)methyl-5-methoxy-2H-benzotri</td> <td>254</td> <td>C<sub>16</sub>H<sub>18</sub>N<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>57</td> <td>F</td> <td>2,6-Dimethyl-4-methylsilyloxy-1,3-cyclohexa</td> <td>210</td> <td>C<sub>12</sub>H<sub>22</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>57</td> <td>F</td> <td>BETA-D-FRUCTOPYRANOSE, 1-N-DIBENZ</td> <td>647</td> <td>C<sub>32</sub>H<sub>57</sub>N<sub>2</sub>O</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 261: octyl-diphenylamine \$S\$</p> <p>CAS# 0-00-0 Mol Wt: 201 Serial#: 132293</p> <p>Capd Name: octyl-diphenylamine \$S\$</p> <p>Formula: C<sub>20</sub>H<sub>27</sub>N Class Flag: No Class Flag</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	55	Q	octyl-diphenylamine \$S\$	210	C <sub>21</sub> H <sub>28</sub> N <sub>2</sub>	WILEY229.LI	2	58	F	4-amino-5-methylamino-1,8-dioxane \$S\$ 9H-Fluore	210	C <sub>18</sub> H <sub>14</sub> N <sub>2</sub>	WILEY229.LI	3	58	F	2-chloro-5-methyl-4-(2'-phenyl)pyrimidine \$S\$ Pyr	210	C <sub>13</sub> H <sub>7</sub> ClN <sub>2</sub>	WILEY229.LI	4	58	F	6-METHYL-2-ETHYLENEBIS(OXY)-3-OXABIC	210	C <sub>11</sub> H <sub>14</sub> O <sub>4</sub>	WILEY229.LI	5	58	F	2-(ALPHA-DIETHYLPHOSPHORIC ACID) DIACRIDINE \$S\$ Acrid	207	C <sub>15</sub> H <sub>10</sub> D <sub>3</sub>	WILEY229.LI	6	58	F	DI-2,5-DIMETHYL-3-STYRYL-PYRAZINE \$S\$	210	C <sub>16</sub> H <sub>14</sub> N <sub>2</sub>	WILEY229.LI	7	57	F	1-(5-methylamino)methyl-5-methoxy-2H-benzotri	254	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub>	WILEY229.LI	8	57	F	2,6-Dimethyl-4-methylsilyloxy-1,3-cyclohexa	210	C <sub>12</sub> H <sub>22</sub> O	WILEY229.LI	9	57	F	BETA-D-FRUCTOPYRANOSE, 1-N-DIBENZ	647	C <sub>32</sub> H <sub>57</sub> N <sub>2</sub> O	WILEY229.LI
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	55	Q	octyl-diphenylamine \$S\$	210	C <sub>21</sub> H <sub>28</sub> N <sub>2</sub>	WILEY229.LI																																																																			
2	58	F	4-amino-5-methylamino-1,8-dioxane \$S\$ 9H-Fluore	210	C <sub>18</sub> H <sub>14</sub> N <sub>2</sub>	WILEY229.LI																																																																			
3	58	F	2-chloro-5-methyl-4-(2'-phenyl)pyrimidine \$S\$ Pyr	210	C <sub>13</sub> H <sub>7</sub> ClN <sub>2</sub>	WILEY229.LI																																																																			
4	58	F	6-METHYL-2-ETHYLENEBIS(OXY)-3-OXABIC	210	C <sub>11</sub> H <sub>14</sub> O <sub>4</sub>	WILEY229.LI																																																																			
5	58	F	2-(ALPHA-DIETHYLPHOSPHORIC ACID) DIACRIDINE \$S\$ Acrid	207	C <sub>15</sub> H <sub>10</sub> D <sub>3</sub>	WILEY229.LI																																																																			
6	58	F	DI-2,5-DIMETHYL-3-STYRYL-PYRAZINE \$S\$	210	C <sub>16</sub> H <sub>14</sub> N <sub>2</sub>	WILEY229.LI																																																																			
7	57	F	1-(5-methylamino)methyl-5-methoxy-2H-benzotri	254	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub>	WILEY229.LI																																																																			
8	57	F	2,6-Dimethyl-4-methylsilyloxy-1,3-cyclohexa	210	C <sub>12</sub> H <sub>22</sub> O	WILEY229.LI																																																																			
9	57	F	BETA-D-FRUCTOPYRANOSE, 1-N-DIBENZ	647	C <sub>32</sub> H <sub>57</sub> N <sub>2</sub> O	WILEY229.LI																																																																			
<p>48.348</p>	<p>3021</p>	<p>-</p>	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>78</td> <td>Q</td> <td>D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Frie</td> <td>428</td> <td>C<sub>30</sub>H<sub>52</sub>O</td> <td>NIST02.LIB</td> </tr> <tr> <td>2</td> <td>78</td> <td>F</td> <td>D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Frie</td> <td>428</td> <td>C<sub>30</sub>H<sub>52</sub>O</td> <td>NIST02.LIB</td> </tr> <tr> <td>3</td> <td>77</td> <td>F</td> <td>Acetic acid, 4,4a,8b,8a,11,11,12b,14a-octalim</td> <td>404</td> <td>C<sub>28</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>77</td> <td>F</td> <td>Acetic acid, 4,4a,8b,8a,11,11,12b,14a-octalim</td> <td>404</td> <td>C<sub>28</sub>H<sub>40</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>75</td> <td>F</td> <td>SCLAROLIDE \$S\$</td> <td>250</td> <td>C<sub>16</sub>H<sub>26</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>75</td> <td>F</td> <td>Friedelin \$S\$ D,A-Friedel-Craun-3-one \$S\$ Fried</td> <td>426</td> <td>C<sub>30</sub>H<sub>50</sub>O</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>75</td> <td>F</td> <td>Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel</td> <td>426</td> <td>C<sub>30</sub>H<sub>50</sub>O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>74</td> <td>F</td> <td>Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel</td> <td>426</td> <td>C<sub>30</sub>H<sub>50</sub>O</td> <td>NIST21.LIB</td> </tr> <tr> <td>9</td> <td>74</td> <td>F</td> <td>Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel</td> <td>426</td> <td>C<sub>30</sub>H<sub>50</sub>O</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 428: D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ Epibatadinol \$S\$ 4,4a,8b,8a,11,11,12b,14a-Octamethyldecahydro-6-piceneol \$S\$</p> <p>CAS# 10671-57-3 Mol Wt: 420 Serial#: 175100</p> <p>Capd Name: D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ Epibatadinol \$S\$ 4,4a,8b,8a,11,11,12b,14a-Octamethyldecahydro-6-piceneol \$S\$</p> <p>Formula: C<sub>30</sub>H<sub>52</sub>O Class Flag: No Class Flag</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	78	Q	D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Frie	428	C <sub>30</sub> H <sub>52</sub> O	NIST02.LIB	2	78	F	D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Frie	428	C <sub>30</sub> H <sub>52</sub> O	NIST02.LIB	3	77	F	Acetic acid, 4,4a,8b,8a,11,11,12b,14a-octalim	404	C <sub>28</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB	4	77	F	Acetic acid, 4,4a,8b,8a,11,11,12b,14a-octalim	404	C <sub>28</sub> H <sub>40</sub> O <sub>2</sub>	NIST107.LIB	5	75	F	SCLAROLIDE \$S\$	250	C <sub>16</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI	6	75	F	Friedelin \$S\$ D,A-Friedel-Craun-3-one \$S\$ Fried	426	C <sub>30</sub> H <sub>50</sub> O	NIST107.LIB	7	75	F	Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel	426	C <sub>30</sub> H <sub>50</sub> O	NIST08.LIB	8	74	F	Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel	426	C <sub>30</sub> H <sub>50</sub> O	NIST21.LIB	9	74	F	Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel	426	C <sub>30</sub> H <sub>50</sub> O	NIST08.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	78	Q	D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Frie	428	C <sub>30</sub> H <sub>52</sub> O	NIST02.LIB																																																																			
2	78	F	D,A-Friedel-Craun-7-ol (7 alpha) \$S\$ D,A-Frie	428	C <sub>30</sub> H <sub>52</sub> O	NIST02.LIB																																																																			
3	77	F	Acetic acid, 4,4a,8b,8a,11,11,12b,14a-octalim	404	C <sub>28</sub> H <sub>40</sub> O <sub>2</sub>	NIST08.LIB																																																																			
4	77	F	Acetic acid, 4,4a,8b,8a,11,11,12b,14a-octalim	404	C <sub>28</sub> H <sub>40</sub> O <sub>2</sub>	NIST107.LIB																																																																			
5	75	F	SCLAROLIDE \$S\$	250	C <sub>16</sub> H <sub>26</sub> O <sub>2</sub>	WILEY229.LI																																																																			
6	75	F	Friedelin \$S\$ D,A-Friedel-Craun-3-one \$S\$ Fried	426	C <sub>30</sub> H <sub>50</sub> O	NIST107.LIB																																																																			
7	75	F	Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel	426	C <sub>30</sub> H <sub>50</sub> O	NIST08.LIB																																																																			
8	74	F	Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel	426	C <sub>30</sub> H <sub>50</sub> O	NIST21.LIB																																																																			
9	74	F	Friedelin-3-one \$S\$ Friedelin \$S\$ D,A-Friedel	426	C <sub>30</sub> H <sub>50</sub> O	NIST08.LIB																																																																			

<p>48.649</p>	<p>3035</p>	<p>3045</p>	<p>Target</p> <p>1: 469: Hexacosanoic acid, trimethylsilyl ester</p> <p>CAS: 0:00:0 Mol Wt: 469 Serial: 181479</p> <p>Cmpd Name: Hexacosanoic acid, trimethylsilyl ester</p> <p>Formula: C29H60O2</p>
<p>48.838</p>	<p>3044</p>	<p>3037</p>	<p>Target</p> <p>1: 469: Silane, heptacosyloxytrimethyl-</p> <p>CAS: 0:00:0 Mol Wt: 469 Serial: 181497</p> <p>Cmpd Name: Silane, heptacosyloxytrimethyl-</p> <p>Formula: C38H84OSi</p>
<p>49.082</p>	<p>3054</p>	<p>-</p>	<p>Target</p> <p>1: 324: Olivetol, bis(trimethylsilyl) ether</p> <p>CAS: 0:00:0 Mol Wt: 324 Serial: 129432</p> <p>Cmpd Name: Olivetol, bis(trimethylsilyl) ether</p> <p>Formula: C17H32O2Si2</p>
<p>49.179</p>	<p>3059</p>	<p>-</p>	<p>Target</p> <p>2: 514: Lanost-9(11)en-18-oi acid, 23-(acetyloxy)-3,20-dihydroxy-, gamma-lactone, (3 beta, 20 alpha)- (CAS)</p> <p>CAS: 36872-76-1 Mol Wt: 514 Serial: 216746</p> <p>Cmpd Name: Lanost-9(11)en-18-oi acid, 23-(acetyloxy)-3,20-dihydroxy-, gamma-lactone, (3 beta, 20 alpha)- (CAS)</p> <p>Formula: C32H50O5</p>

<p>49.44</p>	<p>3072</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similarity</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>52</td><td>1</td><td>Benzeneacetic acid, 3-(4-methylphenyl)-</td><td>176</td><td>C10H12O2</td><td>WILEY229.LI</td></tr> <tr><td>2</td><td>52</td><td>2</td><td>2-(4-HYDROXYBENZYL)ACID 3TRMS SS</td><td>370</td><td>C16H30O4</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>51</td><td>3</td><td>1,3-Bis(4-propyl-5-ethyl-2-(1-hydroxyethyl)-2,5-bis(trimethylsilyloxy)-1-methyl-1H-imidazol-5-yl)benzene</td><td>594</td><td>C36H42N4</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>51</td><td>4</td><td>Benzeneacetic acid, 2,5-bis(trimethylsilyloxy)-1-methyl-</td><td>370</td><td>C16H30O4</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>50</td><td>5</td><td>TRIMETHYLSILYL ESTER OF 2,3-BIS(TRIMETHYLSILYLOXY)METHANEDIC ACID</td><td>370</td><td>C16H30O4</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>50</td><td>6</td><td>3,4-DIHYDROXYMANDELIC ACID-TETRAT</td><td>472</td><td>C10H14O5</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>49</td><td>7</td><td>Benzoic acid, 2-(4-methylphenyl)-, trimet</td><td>370</td><td>C16H30O4</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>49</td><td>8</td><td>Cyclopentadecane, dicosanoate, C-43, Diast</td><td>370</td><td>C10H14O5</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>48</td><td>9</td><td>1,5-BIS(TRIMETHYLSILYLOXY)-2-TRIMETH</td><td>573</td><td>C24H51N O</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target</p> <p>1: 472: Benzeneacetic acid, alpha, 3-(4-tol)trimethylsilyloxy-, trimethylsilyl ester (CAS) TETRAKIS(TRIMETHYLSILYL)-3,4-DIHYDROXYMANDELIC ACID SS 3,4-DIHYDROXYMANDELIC ACID 4TMS SS 1,2-BIS(TRIMETHYLSILYLOXY)-2-(2,4,6-TRIMETHYLSILYL)</p> <p>CAS# 27140-05-5 Mol Wt 472 Serial# 211002</p> <p>Capd Name: Benzeneacetic acid, alpha, 3-(4-tol)trimethylsilyloxy-, trimethylsilyl ester (CAS) TETRAKIS(TRIMETHYLSILYL)-3,4-DIHYDROXYMANDELIC ACID SS 3,4-DIHYDROXYMANDELIC ACID 4TMS SS 1,2-BIS(TRIMETHYLSILYLOXY)-2-(2,4,6-TRIMETHYLSILYL)</p> <p>Formula: C20H40O5SH Class Flag No Class Flags</p>	#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library	1	52	1	Benzeneacetic acid, 3-(4-methylphenyl)-	176	C10H12O2	WILEY229.LI	2	52	2	2-(4-HYDROXYBENZYL)ACID 3TRMS SS	370	C16H30O4	WILEY229.LI	3	51	3	1,3-Bis(4-propyl-5-ethyl-2-(1-hydroxyethyl)-2,5-bis(trimethylsilyloxy)-1-methyl-1H-imidazol-5-yl)benzene	594	C36H42N4	WILEY229.LI	4	51	4	Benzeneacetic acid, 2,5-bis(trimethylsilyloxy)-1-methyl-	370	C16H30O4	WILEY229.LI	5	50	5	TRIMETHYLSILYL ESTER OF 2,3-BIS(TRIMETHYLSILYLOXY)METHANEDIC ACID	370	C16H30O4	WILEY229.LI	6	50	6	3,4-DIHYDROXYMANDELIC ACID-TETRAT	472	C10H14O5	WILEY229.LI	7	49	7	Benzoic acid, 2-(4-methylphenyl)-, trimet	370	C16H30O4	WILEY229.LI	8	49	8	Cyclopentadecane, dicosanoate, C-43, Diast	370	C10H14O5	WILEY229.LI	9	48	9	1,5-BIS(TRIMETHYLSILYLOXY)-2-TRIMETH	573	C24H51N O	WILEY229.LI
#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	52	1	Benzeneacetic acid, 3-(4-methylphenyl)-	176	C10H12O2	WILEY229.LI																																																																			
2	52	2	2-(4-HYDROXYBENZYL)ACID 3TRMS SS	370	C16H30O4	WILEY229.LI																																																																			
3	51	3	1,3-Bis(4-propyl-5-ethyl-2-(1-hydroxyethyl)-2,5-bis(trimethylsilyloxy)-1-methyl-1H-imidazol-5-yl)benzene	594	C36H42N4	WILEY229.LI																																																																			
4	51	4	Benzeneacetic acid, 2,5-bis(trimethylsilyloxy)-1-methyl-	370	C16H30O4	WILEY229.LI																																																																			
5	50	5	TRIMETHYLSILYL ESTER OF 2,3-BIS(TRIMETHYLSILYLOXY)METHANEDIC ACID	370	C16H30O4	WILEY229.LI																																																																			
6	50	6	3,4-DIHYDROXYMANDELIC ACID-TETRAT	472	C10H14O5	WILEY229.LI																																																																			
7	49	7	Benzoic acid, 2-(4-methylphenyl)-, trimet	370	C16H30O4	WILEY229.LI																																																																			
8	49	8	Cyclopentadecane, dicosanoate, C-43, Diast	370	C10H14O5	WILEY229.LI																																																																			
9	48	9	1,5-BIS(TRIMETHYLSILYLOXY)-2-TRIMETH	573	C24H51N O	WILEY229.LI																																																																			
<p>49.617</p>	<p>3080</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similarity</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>51</td><td>1</td><td>3-(2-HYDROXYCYCLOHEXYL)PROPANOL 3TRM</td><td>353</td><td>C18H34O3</td><td>WILEY229.LI</td></tr> <tr><td>2</td><td>50</td><td>2</td><td>methyl 13-trimethylsilyloxyoctadecan-9(2L,11E)-diacetate SS</td><td>392</td><td>C22H42O4</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>50</td><td>3</td><td>Benzoic acid, alpha, 4-methyl-1-methylsilyl</td><td>384</td><td>C17H32O4</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>50</td><td>4</td><td>ACRYLSACURE, 2,3-BIS(TRIMETHYLSILYL)</td><td>320</td><td>C12H24O4</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>50</td><td>5</td><td>1-TRIMETHYLSILYLOXYCARBONYL-1-TRIM</td><td>436</td><td>C21H42O5</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>49</td><td>6</td><td>trimethylsilyl (3-ethoxy-4-methylsilyloxy)phenyl ac</td><td>428</td><td>C19H36O5</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>49</td><td>7</td><td>Benzoic acid, 2-(trimethylsilyloxy)-, trimethylsilyl</td><td>262</td><td>C13H22O3</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>48</td><td>8</td><td>Propionic acid, trimethylsilyl-, bis(trimethylsilyl)</td><td>320</td><td>C12H24O4</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>48</td><td>9</td><td>TRIMETHYLOCTADECYL-SILANE SS</td><td>326</td><td>C21H46Si</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target</p> <p>2: 302: methyl 13-trimethylsilyloxyoctadecan-9(2L,11E)-diacetate SS</p> <p>CAS# 0-00-0 Mol Wt 302 Serial# 107409</p> <p>Capd Name: methyl 13-trimethylsilyloxyoctadecan-9(2L,11E)-diacetate SS</p> <p>Formula: C22H42O3Si Class Flag No Class Flags</p>	#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library	1	51	1	3-(2-HYDROXYCYCLOHEXYL)PROPANOL 3TRM	353	C18H34O3	WILEY229.LI	2	50	2	methyl 13-trimethylsilyloxyoctadecan-9(2L,11E)-diacetate SS	392	C22H42O4	WILEY229.LI	3	50	3	Benzoic acid, alpha, 4-methyl-1-methylsilyl	384	C17H32O4	WILEY229.LI	4	50	4	ACRYLSACURE, 2,3-BIS(TRIMETHYLSILYL)	320	C12H24O4	WILEY229.LI	5	50	5	1-TRIMETHYLSILYLOXYCARBONYL-1-TRIM	436	C21H42O5	WILEY229.LI	6	49	6	trimethylsilyl (3-ethoxy-4-methylsilyloxy)phenyl ac	428	C19H36O5	WILEY229.LI	7	49	7	Benzoic acid, 2-(trimethylsilyloxy)-, trimethylsilyl	262	C13H22O3	WILEY229.LI	8	48	8	Propionic acid, trimethylsilyl-, bis(trimethylsilyl)	320	C12H24O4	WILEY229.LI	9	48	9	TRIMETHYLOCTADECYL-SILANE SS	326	C21H46Si	WILEY229.LI
#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	51	1	3-(2-HYDROXYCYCLOHEXYL)PROPANOL 3TRM	353	C18H34O3	WILEY229.LI																																																																			
2	50	2	methyl 13-trimethylsilyloxyoctadecan-9(2L,11E)-diacetate SS	392	C22H42O4	WILEY229.LI																																																																			
3	50	3	Benzoic acid, alpha, 4-methyl-1-methylsilyl	384	C17H32O4	WILEY229.LI																																																																			
4	50	4	ACRYLSACURE, 2,3-BIS(TRIMETHYLSILYL)	320	C12H24O4	WILEY229.LI																																																																			
5	50	5	1-TRIMETHYLSILYLOXYCARBONYL-1-TRIM	436	C21H42O5	WILEY229.LI																																																																			
6	49	6	trimethylsilyl (3-ethoxy-4-methylsilyloxy)phenyl ac	428	C19H36O5	WILEY229.LI																																																																			
7	49	7	Benzoic acid, 2-(trimethylsilyloxy)-, trimethylsilyl	262	C13H22O3	WILEY229.LI																																																																			
8	48	8	Propionic acid, trimethylsilyl-, bis(trimethylsilyl)	320	C12H24O4	WILEY229.LI																																																																			
9	48	9	TRIMETHYLOCTADECYL-SILANE SS	326	C21H46Si	WILEY229.LI																																																																			
<p>49.682</p>	<p>3083</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similarity</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>71</td><td>1</td><td>Stigmasterol SS Stigmasta-5,22-dien-3-ol, (3 beta)-</td><td>412</td><td>C29H50</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>70</td><td>2</td><td>Stigmat-5-en-3-ol, (3 beta, 24S)- (CAS) Clona</td><td>414</td><td>C29H50O</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>70</td><td>3</td><td>gamma-Stosterol SS Stigmat-5-en-3-ol, (3 beta)</td><td>414</td><td>C29H50O</td><td>NIST08.LIB</td></tr> <tr><td>4</td><td>69</td><td>4</td><td>Cyclopentadienyl Stigmastan-3-ene, 3', 7'-diethyl-</td><td>398</td><td>C28H46O</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>68</td><td>5</td><td>Androst-5-en-3-ol, 4,4-dimethyl-, (3 beta)- (CA)</td><td>302</td><td>C21H34O</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>68</td><td>6</td><td>Cyclohexanol SS 3,19-Cyclohexost-24(28)en</td><td>426</td><td>C30H50O</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>68</td><td>7</td><td>Cholest-5-ene, 2-methyl-, (3 beta)- (CAS) Ch</td><td>400</td><td>C28H48O</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>68</td><td>8</td><td>Stigmasta-5,22-dien-3-ol, (3 beta, 22E)- (CAS)</td><td>412</td><td>C29H48O</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>68</td><td>9</td><td>Ergosta-7,22-dien-3-ol, (3 beta, 22E)- (CAS) S</td><td>398</td><td>C28H46O</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target</p> <p>1: 412: Stigmasterol SS Stigmasta-5,22-dien-3-ol, (3 beta, 22E)- SS Stigmasta-5,22-dien-3 beta, -ol SS beta-Stigmastol SS (24S)-5,22-Stigmastadien-3 beta, -ol SS Stigmastin SS Phytosterol SS 5,22-Cholestadien-24-ethyl-3 beta-</p> <p>CAS# 83-48-7 Mol Wt 412 Serial# 171279</p> <p>Capd Name: Stigmasterol SS Stigmasta-5,22-dien-3-ol, (3 beta, 22E)- SS Stigmasta-5,22-dien-3 beta, -ol SS beta-Stigmastol SS (24S)-5,22-Stigmastadien-3 beta, -ol SS Stigmasta-5,22-dien-3-ol, (3 beta)- SS Stigmastin SS Phytosterol SS 5,22-Cholestadien-24-ethyl-</p> <p>Formula: C29H50 Class Flag No Class Flags</p>	#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library	1	71	1	Stigmasterol SS Stigmasta-5,22-dien-3-ol, (3 beta)-	412	C29H50	NIST08.LIB	2	70	2	Stigmat-5-en-3-ol, (3 beta, 24S)- (CAS) Clona	414	C29H50O	WILEY229.LI	3	70	3	gamma-Stosterol SS Stigmat-5-en-3-ol, (3 beta)	414	C29H50O	NIST08.LIB	4	69	4	Cyclopentadienyl Stigmastan-3-ene, 3', 7'-diethyl-	398	C28H46O	WILEY229.LI	5	68	5	Androst-5-en-3-ol, 4,4-dimethyl-, (3 beta)- (CA)	302	C21H34O	WILEY229.LI	6	68	6	Cyclohexanol SS 3,19-Cyclohexost-24(28)en	426	C30H50O	WILEY229.LI	7	68	7	Cholest-5-ene, 2-methyl-, (3 beta)- (CAS) Ch	400	C28H48O	WILEY229.LI	8	68	8	Stigmasta-5,22-dien-3-ol, (3 beta, 22E)- (CAS)	412	C29H48O	WILEY229.LI	9	68	9	Ergosta-7,22-dien-3-ol, (3 beta, 22E)- (CAS) S	398	C28H46O	WILEY229.LI
#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	71	1	Stigmasterol SS Stigmasta-5,22-dien-3-ol, (3 beta)-	412	C29H50	NIST08.LIB																																																																			
2	70	2	Stigmat-5-en-3-ol, (3 beta, 24S)- (CAS) Clona	414	C29H50O	WILEY229.LI																																																																			
3	70	3	gamma-Stosterol SS Stigmat-5-en-3-ol, (3 beta)	414	C29H50O	NIST08.LIB																																																																			
4	69	4	Cyclopentadienyl Stigmastan-3-ene, 3', 7'-diethyl-	398	C28H46O	WILEY229.LI																																																																			
5	68	5	Androst-5-en-3-ol, 4,4-dimethyl-, (3 beta)- (CA)	302	C21H34O	WILEY229.LI																																																																			
6	68	6	Cyclohexanol SS 3,19-Cyclohexost-24(28)en	426	C30H50O	WILEY229.LI																																																																			
7	68	7	Cholest-5-ene, 2-methyl-, (3 beta)- (CAS) Ch	400	C28H48O	WILEY229.LI																																																																			
8	68	8	Stigmasta-5,22-dien-3-ol, (3 beta, 22E)- (CAS)	412	C29H48O	WILEY229.LI																																																																			
9	68	9	Ergosta-7,22-dien-3-ol, (3 beta, 22E)- (CAS) S	398	C28H46O	WILEY229.LI																																																																			
<p>49.887</p>	<p>3092</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similarity</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>72</td><td>1</td><td>Olivetol, bis(trimethylsilyl) ether</td><td>324</td><td>C17H30O2Si2</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>66</td><td>2</td><td>1,4-Bis(trimethylsilyloxy)-2-methylbenzene SS</td><td>268</td><td>C13H24O2</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>66</td><td>3</td><td>3-Pyridinecarboxylic acid, 6-(trimethylsilyloxy)-</td><td>283</td><td>C12H21NO</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>65</td><td>4</td><td>alpha-Phenyl-beta-trimethylsilyloxypropene SS</td><td>269</td><td>C17H20O2</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>63</td><td>5</td><td>2-METHYLRISORNICOL DITMS SS</td><td>268</td><td>C13H24O2</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>62</td><td>6</td><td>ibenzof[3, f][benzof][2,2]pheno-2,6-diene SS</td><td>268</td><td>C21H16</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>62</td><td>7</td><td>Spino[4]fluorene-9,9-bisoxyl[3,3,1,0]triazole</td><td>268</td><td>C21H16</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>61</td><td>8</td><td>3-Benzofiden-3,6-dihydrocycloheptadiene S</td><td>268</td><td>C21H16</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>61</td><td>9</td><td>ORNICOLIS-METHYLRISORNICOLI DITMS</td><td>268</td><td>C13H24O2</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target</p> <p>1: 324: Olivetol, bis(trimethylsilyl) ether</p> <p>CAS# 0-00-0 Mol Wt 324 Serial# 128432</p> <p>Capd Name: Olivetol, bis(trimethylsilyl) ether</p> <p>Formula: C17H30O2Si2 Class Flag No Class Flags</p>	#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library	1	72	1	Olivetol, bis(trimethylsilyl) ether	324	C17H30O2Si2	NIST08.LIB	2	66	2	1,4-Bis(trimethylsilyloxy)-2-methylbenzene SS	268	C13H24O2	WILEY229.LI	3	66	3	3-Pyridinecarboxylic acid, 6-(trimethylsilyloxy)-	283	C12H21NO	WILEY229.LI	4	65	4	alpha-Phenyl-beta-trimethylsilyloxypropene SS	269	C17H20O2	WILEY229.LI	5	63	5	2-METHYLRISORNICOL DITMS SS	268	C13H24O2	WILEY229.LI	6	62	6	ibenzof[3, f][benzof][2,2]pheno-2,6-diene SS	268	C21H16	WILEY229.LI	7	62	7	Spino[4]fluorene-9,9-bisoxyl[3,3,1,0]triazole	268	C21H16	WILEY229.LI	8	61	8	3-Benzofiden-3,6-dihydrocycloheptadiene S	268	C21H16	WILEY229.LI	9	61	9	ORNICOLIS-METHYLRISORNICOLI DITMS	268	C13H24O2	WILEY229.LI
#	Similarity	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	72	1	Olivetol, bis(trimethylsilyl) ether	324	C17H30O2Si2	NIST08.LIB																																																																			
2	66	2	1,4-Bis(trimethylsilyloxy)-2-methylbenzene SS	268	C13H24O2	WILEY229.LI																																																																			
3	66	3	3-Pyridinecarboxylic acid, 6-(trimethylsilyloxy)-	283	C12H21NO	WILEY229.LI																																																																			
4	65	4	alpha-Phenyl-beta-trimethylsilyloxypropene SS	269	C17H20O2	WILEY229.LI																																																																			
5	63	5	2-METHYLRISORNICOL DITMS SS	268	C13H24O2	WILEY229.LI																																																																			
6	62	6	ibenzof[3, f][benzof][2,2]pheno-2,6-diene SS	268	C21H16	WILEY229.LI																																																																			
7	62	7	Spino[4]fluorene-9,9-bisoxyl[3,3,1,0]triazole	268	C21H16	WILEY229.LI																																																																			
8	61	8	3-Benzofiden-3,6-dihydrocycloheptadiene S	268	C21H16	WILEY229.LI																																																																			
9	61	9	ORNICOLIS-METHYLRISORNICOLI DITMS	268	C13H24O2	WILEY229.LI																																																																			



<p>50.051</p>	<p>3100</p>	<p>3100</p>	<table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Range</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>97</td><td>97</td><td>Tetrahydrocortane 5S n-Tetrahydrocortane 5S</td><td>618</td><td>C44H90</td><td>NIST01.LIB</td></tr> <tr><td>2</td><td>97</td><td>97</td><td>Tetrahydrocortane</td><td>618</td><td>C44H90</td><td>NIST21.LIB</td></tr> <tr><td>3</td><td>97</td><td>97</td><td>HEXACOSANE 5S</td><td>366</td><td>C26H54</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>97</td><td>97</td><td>Hexacosane</td><td>366</td><td>C26H54</td><td>NIST21.LIB</td></tr> <tr><td>5</td><td>96</td><td>96</td><td>Pentacosane 5S n-Pentacosane 5S</td><td>352</td><td>C25H52</td><td>NIST01.LIB</td></tr> <tr><td>6</td><td>96</td><td>96</td><td>Nonacosane (CAS) n-Nonacosane 5S Celdionol, decap-5S</td><td>408</td><td>C29H60</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>96</td><td>96</td><td>Nonacosane (CAS) n-Nonacosane 5S</td><td>392</td><td>C29H58</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>96</td><td>96</td><td>Nonacosane</td><td>408</td><td>C29H60</td><td>NIST21.LIB</td></tr> <tr><td>9</td><td>96</td><td>96</td><td>Pentacosane 5S n-Pentacosane 5S</td><td>352</td><td>C25H52</td><td>NIST107.LIB</td></tr> </tbody> </table> <p>Target</p> <p>6: 408: Nonacosane (CAS) n-Nonacosane 5S Celdionol, decap-5S</p> <p>CAS# 630-03-5 Mol Wt: 408 Serial#: 196628</p> <p>Comp Name: Nonacosane (CAS) n-Nonacosane 5S Celdionol, decap-5S</p> <p>Formula: C29H60 Class Flag: No Class Flags</p>	HM	Similar	Range	Compound Name	Mol Wt	Formula	Library	1	97	97	Tetrahydrocortane 5S n-Tetrahydrocortane 5S	618	C44H90	NIST01.LIB	2	97	97	Tetrahydrocortane	618	C44H90	NIST21.LIB	3	97	97	HEXACOSANE 5S	366	C26H54	WILEY229.LI	4	97	97	Hexacosane	366	C26H54	NIST21.LIB	5	96	96	Pentacosane 5S n-Pentacosane 5S	352	C25H52	NIST01.LIB	6	96	96	Nonacosane (CAS) n-Nonacosane 5S Celdionol, decap-5S	408	C29H60	WILEY229.LI	7	96	96	Nonacosane (CAS) n-Nonacosane 5S	392	C29H58	WILEY229.LI	8	96	96	Nonacosane	408	C29H60	NIST21.LIB	9	96	96	Pentacosane 5S n-Pentacosane 5S	352	C25H52	NIST107.LIB
HM	Similar	Range	Compound Name	Mol Wt	Formula	Library																																																																			
1	97	97	Tetrahydrocortane 5S n-Tetrahydrocortane 5S	618	C44H90	NIST01.LIB																																																																			
2	97	97	Tetrahydrocortane	618	C44H90	NIST21.LIB																																																																			
3	97	97	HEXACOSANE 5S	366	C26H54	WILEY229.LI																																																																			
4	97	97	Hexacosane	366	C26H54	NIST21.LIB																																																																			
5	96	96	Pentacosane 5S n-Pentacosane 5S	352	C25H52	NIST01.LIB																																																																			
6	96	96	Nonacosane (CAS) n-Nonacosane 5S Celdionol, decap-5S	408	C29H60	WILEY229.LI																																																																			
7	96	96	Nonacosane (CAS) n-Nonacosane 5S	392	C29H58	WILEY229.LI																																																																			
8	96	96	Nonacosane	408	C29H60	NIST21.LIB																																																																			
9	96	96	Pentacosane 5S n-Pentacosane 5S	352	C25H52	NIST107.LIB																																																																			
<p>50.19</p>	<p>3107</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Range</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>64</td><td>64</td><td>Stigmasterol (CAS) 24Z</td><td>410</td><td>C31H50O3</td><td>WILEY229.LI</td></tr> <tr><td>2</td><td>64</td><td>64</td><td>METHYL CHOLANATE 5S</td><td>410</td><td>C31H50O3</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>64</td><td>64</td><td>5,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)</td><td>440</td><td>C31H52O</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>63</td><td>63</td><td>5,19-Cyclo-9 beta lanostane-3 beta, 25-diol (C</td><td>444</td><td>C30H52O2</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>62</td><td>62</td><td>ANDROPHOLANOL 5S</td><td>390</td><td>C29H48O5</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>62</td><td>62</td><td>5,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)</td><td>440</td><td>C31H52O</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>62</td><td>62</td><td>5,19-Cyclolanost-25-en-3, 25-diol, (3 beta, 2</td><td>442</td><td>C30H50O2</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>51</td><td>51</td><td>Camphene 5S 1,3,6,10-Cyclooctadecatriene</td><td>272</td><td>C20H32</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>61</td><td>61</td><td>11-ALPHA-HYDROXYRESIBUROGININ 5S</td><td>400</td><td>C24H32O5</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target</p> <p>1: 484: Stigmasterol (4 alpha-methylgonane-7,24(28)-dien-3 beta-yl) (CAS) 4-ALPHA-METHYL-24-METHYLENE-DIHYDROXYMESTEROL TMS 5S</p> <p>CAS# 23649-45-5 Mol Wt: 484 Serial#: 213228</p> <p>Comp Name: Stigmasterol (4 alpha-methylgonane-7,24(28)-dien-3 beta-yl) (CAS) 4-ALPHA-METHYL-24-METHYLENE-DIHYDROXYMESTEROL TMS 5S</p> <p>Formula: C32H56O5I Class Flag: No Class Flags</p>	HM	Similar	Range	Compound Name	Mol Wt	Formula	Library	1	64	64	Stigmasterol (CAS) 24Z	410	C31H50O3	WILEY229.LI	2	64	64	METHYL CHOLANATE 5S	410	C31H50O3	WILEY229.LI	3	64	64	5,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.LI	4	63	63	5,19-Cyclo-9 beta lanostane-3 beta, 25-diol (C	444	C30H52O2	WILEY229.LI	5	62	62	ANDROPHOLANOL 5S	390	C29H48O5	WILEY229.LI	6	62	62	5,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.LI	7	62	62	5,19-Cyclolanost-25-en-3, 25-diol, (3 beta, 2	442	C30H50O2	WILEY229.LI	8	51	51	Camphene 5S 1,3,6,10-Cyclooctadecatriene	272	C20H32	WILEY229.LI	9	61	61	11-ALPHA-HYDROXYRESIBUROGININ 5S	400	C24H32O5	WILEY229.LI
HM	Similar	Range	Compound Name	Mol Wt	Formula	Library																																																																			
1	64	64	Stigmasterol (CAS) 24Z	410	C31H50O3	WILEY229.LI																																																																			
2	64	64	METHYL CHOLANATE 5S	410	C31H50O3	WILEY229.LI																																																																			
3	64	64	5,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.LI																																																																			
4	63	63	5,19-Cyclo-9 beta lanostane-3 beta, 25-diol (C	444	C30H52O2	WILEY229.LI																																																																			
5	62	62	ANDROPHOLANOL 5S	390	C29H48O5	WILEY229.LI																																																																			
6	62	62	5,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.LI																																																																			
7	62	62	5,19-Cyclolanost-25-en-3, 25-diol, (3 beta, 2	442	C30H50O2	WILEY229.LI																																																																			
8	51	51	Camphene 5S 1,3,6,10-Cyclooctadecatriene	272	C20H32	WILEY229.LI																																																																			
9	61	61	11-ALPHA-HYDROXYRESIBUROGININ 5S	400	C24H32O5	WILEY229.LI																																																																			
<p>50.313</p>	<p>3113</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Range</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>73</td><td>73</td><td>Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)</td><td>458</td><td>C30H54O5</td><td>NIST01.LIB</td></tr> <tr><td>2</td><td>73</td><td>73</td><td>Cholesterol (methyl) ether 5S</td><td>458</td><td>C30H54O5</td><td>NIST21.LIB</td></tr> <tr><td>3</td><td>73</td><td>73</td><td>Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)</td><td>498</td><td>C33H58O5</td><td>NIST107.LIB</td></tr> <tr><td>4</td><td>73</td><td>73</td><td>Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)</td><td>498</td><td>C33H58O5</td><td>NIST01.LIB</td></tr> <tr><td>5</td><td>73</td><td>73</td><td>Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)</td><td>458</td><td>C30H54O5</td><td>NIST01.LIB</td></tr> <tr><td>6</td><td>73</td><td>73</td><td>Cholesterol (methyl) ether 5S</td><td>458</td><td>C30H54O5</td><td>NIST21.LIB</td></tr> <tr><td>7</td><td>73</td><td>73</td><td>Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)</td><td>458</td><td>C30H54O5</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>72</td><td>72</td><td>Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)</td><td>498</td><td>C33H58O5</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>72</td><td>72</td><td>Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)</td><td>458</td><td>C30H54O5</td><td>NIST01.LIB</td></tr> </tbody> </table> <p>Target</p> <p>1: 458: Cholesterol (methyl) ether 5S Stigmasterol, (3 beta) cholesterol 5-ene-3-yl) (methyl) 5S Stigmasterol (cholesterol) (methyl) 5S 3 beta, (1-methyl) cholesterol 5-ene 5S Cholesterol 5-ene, 3 (methyl) (methyl), (3 beta) 5S Monomethyl) d</p> <p>CAS# 1856-05-9 Mol Wt: 458 Serial#: 27034</p> <p>Comp Name: Cholesterol (methyl) ether 5S Stigmasterol, (3 beta) cholesterol 5-ene-3-yl) (methyl) 5S Stigmasterol (cholesterol) (methyl) 5S 3 beta, (1-methyl) cholesterol 5-ene 5S Cholesterol 5-ene, 3 (methyl) (methyl), (3 beta) 5S Monomethyl) d</p> <p>Formula: C30H54O5I Class Flag: No Class Flags</p>	HM	Similar	Range	Compound Name	Mol Wt	Formula	Library	1	73	73	Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)	458	C30H54O5	NIST01.LIB	2	73	73	Cholesterol (methyl) ether 5S	458	C30H54O5	NIST21.LIB	3	73	73	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	498	C33H58O5	NIST107.LIB	4	73	73	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	498	C33H58O5	NIST01.LIB	5	73	73	Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)	458	C30H54O5	NIST01.LIB	6	73	73	Cholesterol (methyl) ether 5S	458	C30H54O5	NIST21.LIB	7	73	73	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	458	C30H54O5	WILEY229.LI	8	72	72	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	498	C33H58O5	WILEY229.LI	9	72	72	Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)	458	C30H54O5	NIST01.LIB
HM	Similar	Range	Compound Name	Mol Wt	Formula	Library																																																																			
1	73	73	Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)	458	C30H54O5	NIST01.LIB																																																																			
2	73	73	Cholesterol (methyl) ether 5S	458	C30H54O5	NIST21.LIB																																																																			
3	73	73	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	498	C33H58O5	NIST107.LIB																																																																			
4	73	73	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	498	C33H58O5	NIST01.LIB																																																																			
5	73	73	Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)	458	C30H54O5	NIST01.LIB																																																																			
6	73	73	Cholesterol (methyl) ether 5S	458	C30H54O5	NIST21.LIB																																																																			
7	73	73	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	458	C30H54O5	WILEY229.LI																																																																			
8	72	72	Stigmasterol (beta) lanosta-8,24-dien-3-yl) (methyl)	498	C33H58O5	WILEY229.LI																																																																			
9	72	72	Cholesterol (methyl) ether 5S Stigmasterol, (3 beta)	458	C30H54O5	NIST01.LIB																																																																			
<p>50.455</p>	<p>3119</p>	<p>3136 3156</p>	<table border="1"> <thead> <tr> <th>HM</th> <th>Similar</th> <th>Range</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>83</td><td>83</td><td>alpha-Tocopherol (vitamin E), (methyl) derivative</td><td>502</td><td>C30H58O2S</td><td>NIST01.LIB</td></tr> <tr><td>2</td><td>50</td><td>50</td><td>Nonsteroidal derivative of Tocopherol 5</td><td>252</td><td>C15H18O4</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>49</td><td>49</td><td>Stigmasterol (beta) lanosta-8,17 beta-yl) (methyl)</td><td>592</td><td>C30H56O4</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>48</td><td>48</td><td>carbamidic acid, methyl-, (methyl) (methyl)</td><td>236</td><td>C12H20N2</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>47</td><td>47</td><td>3a beta- (E)-ethyl-2-methyl-5-oxo-3a,4,5,6,7,7</td><td>236</td><td>C14H24O5</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>47</td><td>47</td><td>2,6-DIMETHYL-6-(1-TRIMETHYLHYDROXYMETHYL)</td><td>236</td><td>C14H24O4</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>47</td><td>47</td><td>6,6-dimethyl-2 (methyl) (methyl)-4-oxo-2,3,</td><td>252</td><td>C14H24O2</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>46</td><td>46</td><td>2-methyl-2-butyl isofenolate-TMS-derivative</td><td>304</td><td>C18H26O4</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>46</td><td>46</td><td>2,4-hydroxydiphenyl-5-(3,4-dimethyl) (methyl)</td><td>516</td><td>C25H40N2</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target</p> <p>1: 502: Alpha-Tocopherol (vitamin E), (methyl) derivative 5S alpha-Tocopherol, (methyl) ether 5S Tocopherol, alpha-toc-derivative (high mass adjustment-100.1) 5S Tocopherol (2,5,7,8-tetramethyl-2-(4,8,12-trimethyl)decyl)-3,4-dihydro-2H-chromen-6-yl) (methyl)</p> <p>CAS# 1733-26-8 Mol Wt: 502 Serial#: 184830</p> <p>Comp Name: alpha-Tocopherol (vitamin E), (methyl) derivative 5S alpha-Tocopherol, (methyl) ether 5S Tocopherol, alpha-toc-derivative (high mass adjustment-100.1) 5S Tocopherol (2,5,7,8-tetramethyl-2-(4,8,12-trimethyl)decyl)-3,4-dihydro-2H-chromen-6-yl) (methyl)</p> <p>Formula: C30H58O2S Class Flag: No Class Flags</p>	HM	Similar	Range	Compound Name	Mol Wt	Formula	Library	1	83	83	alpha-Tocopherol (vitamin E), (methyl) derivative	502	C30H58O2S	NIST01.LIB	2	50	50	Nonsteroidal derivative of Tocopherol 5	252	C15H18O4	WILEY229.LI	3	49	49	Stigmasterol (beta) lanosta-8,17 beta-yl) (methyl)	592	C30H56O4	WILEY229.LI	4	48	48	carbamidic acid, methyl-, (methyl) (methyl)	236	C12H20N2	WILEY229.LI	5	47	47	3a beta- (E)-ethyl-2-methyl-5-oxo-3a,4,5,6,7,7	236	C14H24O5	WILEY229.LI	6	47	47	2,6-DIMETHYL-6-(1-TRIMETHYLHYDROXYMETHYL)	236	C14H24O4	WILEY229.LI	7	47	47	6,6-dimethyl-2 (methyl) (methyl)-4-oxo-2,3,	252	C14H24O2	WILEY229.LI	8	46	46	2-methyl-2-butyl isofenolate-TMS-derivative	304	C18H26O4	WILEY229.LI	9	46	46	2,4-hydroxydiphenyl-5-(3,4-dimethyl) (methyl)	516	C25H40N2	WILEY229.LI
HM	Similar	Range	Compound Name	Mol Wt	Formula	Library																																																																			
1	83	83	alpha-Tocopherol (vitamin E), (methyl) derivative	502	C30H58O2S	NIST01.LIB																																																																			
2	50	50	Nonsteroidal derivative of Tocopherol 5	252	C15H18O4	WILEY229.LI																																																																			
3	49	49	Stigmasterol (beta) lanosta-8,17 beta-yl) (methyl)	592	C30H56O4	WILEY229.LI																																																																			
4	48	48	carbamidic acid, methyl-, (methyl) (methyl)	236	C12H20N2	WILEY229.LI																																																																			
5	47	47	3a beta- (E)-ethyl-2-methyl-5-oxo-3a,4,5,6,7,7	236	C14H24O5	WILEY229.LI																																																																			
6	47	47	2,6-DIMETHYL-6-(1-TRIMETHYLHYDROXYMETHYL)	236	C14H24O4	WILEY229.LI																																																																			
7	47	47	6,6-dimethyl-2 (methyl) (methyl)-4-oxo-2,3,	252	C14H24O2	WILEY229.LI																																																																			
8	46	46	2-methyl-2-butyl isofenolate-TMS-derivative	304	C18H26O4	WILEY229.LI																																																																			
9	46	46	2,4-hydroxydiphenyl-5-(3,4-dimethyl) (methyl)	516	C25H40N2	WILEY229.LI																																																																			

<p>50.792</p>	<p>3136</p>	<p>3120 GMD</p>	<p>Target</p> <p>1: 468: Hexanoic acid, trimethylsilyl ester</p> <p>CAS#: 0-00-0 Mol Wt: 468 Serial#: 181479</p> <p>Compound Name: Hexanoic acid, trimethylsilyl ester</p> <p>Mol Wt: 468 Formula: C15H30O2 Library: WILEY229.LI</p>
<p>50.983</p>	<p>3145</p>	<p>-</p>	<p>Target</p> <p>1: 278: ALPHA, 04-CYCLOHEXANONE, 2,4-DINITROPHENYLHYDRAZONE</p> <p>CAS#: 25117-40-2 Mol Wt: 278 Serial#: 129722</p> <p>Compound Name: ALPHA, 04-CYCLOHEXANONE, 2,4-DINITROPHENYLHYDRAZONE</p> <p>Mol Wt: 278 Formula: C12H18O4 N4 Library: WILEY229.LI</p>
<p>51.14</p>	<p>3152</p>	<p>-</p>	<p>Target</p> <p>1: 283: 5-alpha-Androst-16-ene-17-carbonitrile (CAS)</p> <p>CAS#: 7704-88-3 Mol Wt: 283 Serial#: 133638</p> <p>Compound Name: 5-alpha-Androst-16-ene-17-carbonitrile (CAS)</p> <p>Mol Wt: 283 Formula: C20H29N Library: WILEY229.LI</p>
<p>51.361</p>	<p>3163</p>	<p>-</p>	<p>Target</p> <p>1: 492: Butanamide, 2,2,3,3,4,4,4-heptafluoro-N,N-bis(trimethylsilyloxy)propan-2-yl-</p> <p>CAS#: 55471-01-7 Mol Wt: 493 Serial#: 214253</p> <p>Compound Name: Butanamide, 2,2,3,3,4,4,4-heptafluoro-N,N-bis(trimethylsilyloxy)propan-2-yl-</p> <p>Mol Wt: 493 Formula: C18H26F7N O3 Si2 Library: WILEY229.LI</p>



<p>51.426</p>	<p>3166</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>70</td><td>CF</td><td>2,2-Dibutylpropane-5,5-Diimine, 2,2-dibutyl</td><td>357</td><td>C31H52N2</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>68</td><td></td><td>D,TRIMETHYLSILYL,NITROBENZENE,5,5</td><td>211</td><td>C9H13N O3</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>63</td><td>CF</td><td><b>2,4-DIMETHYL-5H-PYRIDO[3,2-B]INDOLE</b></td><td>196</td><td>C13H12N2</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>61</td><td></td><td>4-(6-Propoxyphenyl)-2-methylimidazole,5,5-tetraol</td><td>438</td><td>C22H32O5</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>67</td><td></td><td>CAMPHORTRIMETHYLSILYL ENOL ETHER</td><td>224</td><td>C13H24O 5</td><td>WILEY229.U</td></tr> <tr><td>6</td><td>66</td><td></td><td>2,4-dimethyl-alpha-carboline,5,5</td><td>196</td><td>C13H12N2</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>65</td><td></td><td>2,2-dimethyl-4-ethyl-2H-pyridine,5,5</td><td>426</td><td>C20H28N2</td><td>WILEY229.U</td></tr> <tr><td>8</td><td>65</td><td></td><td>2,6,6,7-Tetrahydrochromeno[1,9-bc]luran,5,5</td><td>196</td><td>C14H12O 2</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>65</td><td></td><td>3-(1-methylpropyl-2-yl)indole,5,5,1H-indole,3-(1-</td><td>196</td><td>C13H12N2</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>3: 196: 2,4-DIMETHYL-5H-PYRIDO[3,2-B]INDOLE,5,5 5H-Pyrido[3,2-b]indole, 2,4-dimethyl (CAS) 2,4-Dimethyl-5H-pyrido[3,2-b]indole,5,5</p> <p>Base Peak: 196/10.000</p> <p>CAS# 62905-17-6 Mol Wt: 196 Serial#: 64229</p> <p>Comp Name: 2,4-DIMETHYL-5H-PYRIDO[3,2-B]INDOLE,5,5 5H-Pyrido[3,2-b]indole, 2,4-dimethyl (CAS) 2,4-Dimethyl-5H-pyrido[3,2-b]indole,5,5</p> <p>Formula: C13H12N2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	70	CF	2,2-Dibutylpropane-5,5-Diimine, 2,2-dibutyl	357	C31H52N2	WILEY229.U	2	68		D,TRIMETHYLSILYL,NITROBENZENE,5,5	211	C9H13N O3	WILEY229.U	3	63	CF	<b>2,4-DIMETHYL-5H-PYRIDO[3,2-B]INDOLE</b>	196	C13H12N2	WILEY229.U	4	61		4-(6-Propoxyphenyl)-2-methylimidazole,5,5-tetraol	438	C22H32O5	WILEY229.U	5	67		CAMPHORTRIMETHYLSILYL ENOL ETHER	224	C13H24O 5	WILEY229.U	6	66		2,4-dimethyl-alpha-carboline,5,5	196	C13H12N2	WILEY229.U	7	65		2,2-dimethyl-4-ethyl-2H-pyridine,5,5	426	C20H28N2	WILEY229.U	8	65		2,6,6,7-Tetrahydrochromeno[1,9-bc]luran,5,5	196	C14H12O 2	WILEY229.U	9	65		3-(1-methylpropyl-2-yl)indole,5,5,1H-indole,3-(1-	196	C13H12N2	WILEY229.U
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	70	CF	2,2-Dibutylpropane-5,5-Diimine, 2,2-dibutyl	357	C31H52N2	WILEY229.U																																																																			
2	68		D,TRIMETHYLSILYL,NITROBENZENE,5,5	211	C9H13N O3	WILEY229.U																																																																			
3	63	CF	<b>2,4-DIMETHYL-5H-PYRIDO[3,2-B]INDOLE</b>	196	C13H12N2	WILEY229.U																																																																			
4	61		4-(6-Propoxyphenyl)-2-methylimidazole,5,5-tetraol	438	C22H32O5	WILEY229.U																																																																			
5	67		CAMPHORTRIMETHYLSILYL ENOL ETHER	224	C13H24O 5	WILEY229.U																																																																			
6	66		2,4-dimethyl-alpha-carboline,5,5	196	C13H12N2	WILEY229.U																																																																			
7	65		2,2-dimethyl-4-ethyl-2H-pyridine,5,5	426	C20H28N2	WILEY229.U																																																																			
8	65		2,6,6,7-Tetrahydrochromeno[1,9-bc]luran,5,5	196	C14H12O 2	WILEY229.U																																																																			
9	65		3-(1-methylpropyl-2-yl)indole,5,5,1H-indole,3-(1-	196	C13H12N2	WILEY229.U																																																																			
<p>51.538</p>	<p>3171</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>71</td><td>CF</td><td><b>9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-</b></td><td>440</td><td>C31H50O</td><td>NIST107.LIB</td></tr> <tr><td>2</td><td>71</td><td></td><td>9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-</td><td>440</td><td>C31H50O</td><td>NIST107.LIB</td></tr> <tr><td>3</td><td>73</td><td></td><td>9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-</td><td>440</td><td>C31H50O</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>72</td><td></td><td>9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (</td><td>484</td><td>C32H52O3</td><td>NIST08.LIB</td></tr> <tr><td>5</td><td>72</td><td></td><td>9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (</td><td>484</td><td>C32H52O3</td><td>WILEY229.U</td></tr> <tr><td>6</td><td>72</td><td></td><td>9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (</td><td>484</td><td>C32H52O3</td><td>NIST107.LIB</td></tr> <tr><td>7</td><td>70</td><td></td><td>9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23</td><td>442</td><td>C30H50O2</td><td>NIST08.LIB</td></tr> <tr><td>8</td><td>70</td><td></td><td>9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23</td><td>442</td><td>C30H50O2</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>70</td><td></td><td>9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23</td><td>442</td><td>C30H50O2</td><td>NIST107.LIB</td></tr> </tbody> </table> <p>Target</p> <p>1: 440: 9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-,5,5 9,19-Cyclo-9-beta-lanostan-3-beta-,ol, 24-methylene-,5,5 24-Methylene-cyclolanostan-3-(4-1-oxopropyl-1-methyl-4-pentenyl)-3a,6,6,12a-tetramethylhexadecahydro-1H-cyclopenta[a]cyclopropa[e]phenanthren-7</p> <p>Base Peak: 389/10.000</p> <p>CAS# 1449-09-8 Mol Wt: 440 Serial#: 177403</p> <p>Comp Name: 9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-,5,5 9,19-Cyclo-9-beta-lanostan-3-beta-,ol, 24-methylene-,5,5 24-Methylene-cyclolanostan-3-(4-1-oxopropyl-1-methyl-4-pentenyl)-3a,6,6,12a-tetramethylhexadecahydro-1H-cyclopenta[a]cyclopropa[e]phenanthren-7</p> <p>Formula: C31H50O Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	71	CF	<b>9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-</b>	440	C31H50O	NIST107.LIB	2	71		9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-	440	C31H50O	NIST107.LIB	3	73		9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-	440	C31H50O	WILEY229.U	4	72		9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (	484	C32H52O3	NIST08.LIB	5	72		9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (	484	C32H52O3	WILEY229.U	6	72		9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (	484	C32H52O3	NIST107.LIB	7	70		9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23	442	C30H50O2	NIST08.LIB	8	70		9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23	442	C30H50O2	WILEY229.U	9	70		9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23	442	C30H50O2	NIST107.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	71	CF	<b>9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-</b>	440	C31H50O	NIST107.LIB																																																																			
2	71		9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-	440	C31H50O	NIST107.LIB																																																																			
3	73		9,19-Cyclolanostan-3-ol, 24-methylene-, (3-beta)-	440	C31H50O	WILEY229.U																																																																			
4	72		9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (	484	C32H52O3	NIST08.LIB																																																																			
5	72		9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (	484	C32H52O3	WILEY229.U																																																																			
6	72		9,19-Cyclolanost-23-ene-3,25-diol, 3-acetate, (	484	C32H52O3	NIST107.LIB																																																																			
7	70		9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23	442	C30H50O2	NIST08.LIB																																																																			
8	70		9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23	442	C30H50O2	WILEY229.U																																																																			
9	70		9,19-Cyclolanost-23-ene-3,25-diol, (3-beta), 23	442	C30H50O2	NIST107.LIB																																																																			
<p>51.655</p>	<p>3177</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>73</td><td>CF</td><td><b>Betulin,5,5-Lup-20(29)-ene-3,28-diol, (3-beta)-</b></td><td>442</td><td>C30H50O2</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>74</td><td></td><td>Lup-20(29)-ene-3-ol, acetate, (3-beta)-,5,5-Lup-</td><td>468</td><td>C32H52O2</td><td>NIST107.LIB</td></tr> <tr><td>3</td><td>74</td><td></td><td>Lup-20(29)-ene-3-ol, acetate, (3-beta)-,5,5-Lup-</td><td>468</td><td>C32H52O2</td><td>NIST107.LIB</td></tr> <tr><td>4</td><td>74</td><td></td><td>METHYL COMMATE B,5,5</td><td>470</td><td>C31H50O3</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>71</td><td></td><td>Acetic acid, 17-(1,5-dimethylhex-4-enyl)-4,4,8,8-</td><td>468</td><td>C26H52O2</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>71</td><td></td><td>IR,45,75,119,2,4,8-Tetramethylcyclop[5,3,</td><td>204</td><td>C15H24</td><td>NIST08.LIB</td></tr> <tr><td>7</td><td>71</td><td></td><td>Acetic acid, 17-(1,5-dimethylhex-4-enyl)-4,4,8,8-</td><td>468</td><td>C26H52O2</td><td>NIST107.LIB</td></tr> <tr><td>8</td><td>71</td><td></td><td>IR,4,3a,11R,2,2,4,8-Tetramethylcyclop[5,3,1</td><td>204</td><td>C15H24</td><td>NIST107.LIB</td></tr> <tr><td>9</td><td>69</td><td></td><td>Delta-18-ene (CAS), DELTA-18-OLEFANE</td><td>410</td><td>C30H50</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>1: 442: Betulin,5,5-Lup-20(29)-ene-3,28-diol, (3-beta)-,5,5-Lup-20(29)-ene-3-beta-,28-diol,5,5 Betuline,5,5 Betulinol,5,5 Betulinol,5,5 Lup-20(30)-ene-3-beta-,28-diol,5,5 Trochol,5,5 3aH-Cyclopenta[a]cyclopropane, lup-20(29)-ene-3,28-diol deriv.,5,5 Lup-20(29)-ene-3,28-diol,5,5</p> <p>Base Peak: 190/10.000</p> <p>CAS# 473-98-3 Mol Wt: 442 Serial#: 27739</p> <p>Comp Name: Betulin,5,5-Lup-20(29)-ene-3,28-diol, (3-beta)-,5,5-Lup-20(29)-ene-3-beta-,28-diol,5,5 Betuline,5,5 Betulinol,5,5 Betulinol,5,5 Lup-20(30)-ene-3-beta-,28-diol,5,5 Trochol,5,5 3aH-Cyclopenta[a]cyclopropane, lup-20(29)-ene-3,28-diol deriv.,5,5 Lup-20(29)-ene-3,28-diol,5,5</p> <p>Formula: C30H50O2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	73	CF	<b>Betulin,5,5-Lup-20(29)-ene-3,28-diol, (3-beta)-</b>	442	C30H50O2	NIST08.LIB	2	74		Lup-20(29)-ene-3-ol, acetate, (3-beta)-,5,5-Lup-	468	C32H52O2	NIST107.LIB	3	74		Lup-20(29)-ene-3-ol, acetate, (3-beta)-,5,5-Lup-	468	C32H52O2	NIST107.LIB	4	74		METHYL COMMATE B,5,5	470	C31H50O3	WILEY229.U	5	71		Acetic acid, 17-(1,5-dimethylhex-4-enyl)-4,4,8,8-	468	C26H52O2	NIST08.LIB	6	71		IR,45,75,119,2,4,8-Tetramethylcyclop[5,3,	204	C15H24	NIST08.LIB	7	71		Acetic acid, 17-(1,5-dimethylhex-4-enyl)-4,4,8,8-	468	C26H52O2	NIST107.LIB	8	71		IR,4,3a,11R,2,2,4,8-Tetramethylcyclop[5,3,1	204	C15H24	NIST107.LIB	9	69		Delta-18-ene (CAS), DELTA-18-OLEFANE	410	C30H50	WILEY229.U
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	73	CF	<b>Betulin,5,5-Lup-20(29)-ene-3,28-diol, (3-beta)-</b>	442	C30H50O2	NIST08.LIB																																																																			
2	74		Lup-20(29)-ene-3-ol, acetate, (3-beta)-,5,5-Lup-	468	C32H52O2	NIST107.LIB																																																																			
3	74		Lup-20(29)-ene-3-ol, acetate, (3-beta)-,5,5-Lup-	468	C32H52O2	NIST107.LIB																																																																			
4	74		METHYL COMMATE B,5,5	470	C31H50O3	WILEY229.U																																																																			
5	71		Acetic acid, 17-(1,5-dimethylhex-4-enyl)-4,4,8,8-	468	C26H52O2	NIST08.LIB																																																																			
6	71		IR,45,75,119,2,4,8-Tetramethylcyclop[5,3,	204	C15H24	NIST08.LIB																																																																			
7	71		Acetic acid, 17-(1,5-dimethylhex-4-enyl)-4,4,8,8-	468	C26H52O2	NIST107.LIB																																																																			
8	71		IR,4,3a,11R,2,2,4,8-Tetramethylcyclop[5,3,1	204	C15H24	NIST107.LIB																																																																			
9	69		Delta-18-ene (CAS), DELTA-18-OLEFANE	410	C30H50	WILEY229.U																																																																			
<p>51.784</p>	<p>3183</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>77</td><td>CF</td><td><b>METHYL COMMATE C,5,5</b></td><td>486</td><td>C31H50O4</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>77</td><td></td><td>METHYL COMMATE A,5,5</td><td>500</td><td>C32H52O4</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>75</td><td></td><td>beta-Aryln trimethylsilyl ether,5,5 Silane, trim</td><td>498</td><td>C33H50O 5</td><td>NIST107.LIB</td></tr> <tr><td>4</td><td>75</td><td></td><td>Silane, trimethyl[O-beta]-olean-12-en-3-yl[oxyl]</td><td>490</td><td>C33H58O 5</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>75</td><td></td><td>beta-Aryln trimethylsilyl ether,5,5 Silane, trim</td><td>498</td><td>C33H50O 5</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>74</td><td></td><td>NDROLINS-12-ENE,5,5</td><td>396</td><td>C29H48</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>73</td><td></td><td>NDROLIN-12-ENE,5,5</td><td>396</td><td>C29H48</td><td>WILEY229.U</td></tr> <tr><td>8</td><td>72</td><td></td><td>4,4,6a,9a,11,11,14a-Octamethyl-1,4,4a,5,6</td><td>424</td><td>C30H48O</td><td>NIST107.LIB</td></tr> <tr><td>9</td><td>72</td><td></td><td>4,4,6a,9a,11,11,14a-Octamethyl-1,4,4a,5,6</td><td>424</td><td>C30H48O</td><td>NIST08.LIB</td></tr> </tbody> </table> <p>Target</p> <p>1: 486: METHYL COMMATE C,5,5</p> <p>Base Peak: 219/10.000</p> <p>CAS# 0-00-0 Mol Wt: 486 Serial#: 213499</p> <p>Comp Name: METHYL COMMATE C,5,5</p> <p>Formula: C31H50O4 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	77	CF	<b>METHYL COMMATE C,5,5</b>	486	C31H50O4	WILEY229.U	2	77		METHYL COMMATE A,5,5	500	C32H52O4	WILEY229.U	3	75		beta-Aryln trimethylsilyl ether,5,5 Silane, trim	498	C33H50O 5	NIST107.LIB	4	75		Silane, trimethyl[O-beta]-olean-12-en-3-yl[oxyl]	490	C33H58O 5	WILEY229.U	5	75		beta-Aryln trimethylsilyl ether,5,5 Silane, trim	498	C33H50O 5	NIST08.LIB	6	74		NDROLINS-12-ENE,5,5	396	C29H48	WILEY229.U	7	73		NDROLIN-12-ENE,5,5	396	C29H48	WILEY229.U	8	72		4,4,6a,9a,11,11,14a-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST107.LIB	9	72		4,4,6a,9a,11,11,14a-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST08.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	77	CF	<b>METHYL COMMATE C,5,5</b>	486	C31H50O4	WILEY229.U																																																																			
2	77		METHYL COMMATE A,5,5	500	C32H52O4	WILEY229.U																																																																			
3	75		beta-Aryln trimethylsilyl ether,5,5 Silane, trim	498	C33H50O 5	NIST107.LIB																																																																			
4	75		Silane, trimethyl[O-beta]-olean-12-en-3-yl[oxyl]	490	C33H58O 5	WILEY229.U																																																																			
5	75		beta-Aryln trimethylsilyl ether,5,5 Silane, trim	498	C33H50O 5	NIST08.LIB																																																																			
6	74		NDROLINS-12-ENE,5,5	396	C29H48	WILEY229.U																																																																			
7	73		NDROLIN-12-ENE,5,5	396	C29H48	WILEY229.U																																																																			
8	72		4,4,6a,9a,11,11,14a-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST107.LIB																																																																			
9	72		4,4,6a,9a,11,11,14a-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST08.LIB																																																																			

<p>51.895</p>	<p>3188</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>75</td> <td>1</td> <td>Olivetol, bis(trimethylsilyl) ether</td> <td>324</td> <td>C<sub>21</sub>H<sub>30</sub>O<sub>2</sub></td> <td>NIST02.LI</td> </tr> <tr> <td>2</td> <td>65</td> <td>2</td> <td>3-Pyridinecarboxylic acid, 5-(trimethylsilyloxy)-</td> <td>203</td> <td>C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>65</td> <td>3</td> <td>alpha-Phenyl-beta-terphenylacetylene \$S\$</td> <td>268</td> <td>C<sub>17</sub>H<sub>10</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>64</td> <td>4</td> <td>1,4-Bis(trimethylsilyloxy)benzene \$S\$</td> <td>268</td> <td>C<sub>13</sub>H<sub>24</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>63</td> <td>5</td> <td>2-METHYLRESORCINOL DITMS \$S\$</td> <td>268</td> <td>C<sub>13</sub>H<sub>24</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>61</td> <td>6</td> <td>terbenzyl[1,3,5-triazolo[4,5-b]pyridin-2-ylidene-2,6-diene \$S\$</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>61</td> <td>7</td> <td>Spms[3H-fluorene-9-thiopyridinyl(3,1,1,0,2,8)triazol]</td> <td>268</td> <td>C<sub>21</sub>H<sub>16</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>60</td> <td>8</td> <td>ORONOL-5-METHYLRESORCINOL DITMS</td> <td>268</td> <td>C<sub>13</sub>H<sub>24</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>60</td> <td>9</td> <td>TMS-5-norpropyl-1,3-dihydrobenzene \$S\$ 1,3-</td> <td>296</td> <td>C<sub>15</sub>H<sub>28</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: Olivetol, bis(trimethylsilyl) ether</p> <p>CAS# B-00-0 Mol Wt: 324 Serial# 120432</p> <p>Captd Name: Olivetol, bis(trimethylsilyl) ether</p> <p>Formula: C<sub>21</sub>H<sub>30</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	#	Similar	Rank	Compound Name	Mol Wt	Formula	Library	1	75	1	Olivetol, bis(trimethylsilyl) ether	324	C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>	NIST02.LI	2	65	2	3-Pyridinecarboxylic acid, 5-(trimethylsilyloxy)-	203	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O	WILEY229.LI	3	65	3	alpha-Phenyl-beta-terphenylacetylene \$S\$	268	C <sub>17</sub> H <sub>10</sub> O	WILEY229.LI	4	64	4	1,4-Bis(trimethylsilyloxy)benzene \$S\$	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI	5	63	5	2-METHYLRESORCINOL DITMS \$S\$	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI	6	61	6	terbenzyl[1,3,5-triazolo[4,5-b]pyridin-2-ylidene-2,6-diene \$S\$	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI	7	61	7	Spms[3H-fluorene-9-thiopyridinyl(3,1,1,0,2,8)triazol]	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI	8	60	8	ORONOL-5-METHYLRESORCINOL DITMS	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI	9	60	9	TMS-5-norpropyl-1,3-dihydrobenzene \$S\$ 1,3-	296	C <sub>15</sub> H <sub>28</sub> O <sub>2</sub>	WILEY229.LI
#	Similar	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	75	1	Olivetol, bis(trimethylsilyl) ether	324	C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>	NIST02.LI																																																																			
2	65	2	3-Pyridinecarboxylic acid, 5-(trimethylsilyloxy)-	203	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O	WILEY229.LI																																																																			
3	65	3	alpha-Phenyl-beta-terphenylacetylene \$S\$	268	C <sub>17</sub> H <sub>10</sub> O	WILEY229.LI																																																																			
4	64	4	1,4-Bis(trimethylsilyloxy)benzene \$S\$	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	63	5	2-METHYLRESORCINOL DITMS \$S\$	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI																																																																			
6	61	6	terbenzyl[1,3,5-triazolo[4,5-b]pyridin-2-ylidene-2,6-diene \$S\$	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
7	61	7	Spms[3H-fluorene-9-thiopyridinyl(3,1,1,0,2,8)triazol]	268	C <sub>21</sub> H <sub>16</sub>	WILEY229.LI																																																																			
8	60	8	ORONOL-5-METHYLRESORCINOL DITMS	268	C <sub>13</sub> H <sub>24</sub> O <sub>2</sub>	WILEY229.LI																																																																			
9	60	9	TMS-5-norpropyl-1,3-dihydrobenzene \$S\$ 1,3-	296	C <sub>15</sub> H <sub>28</sub> O <sub>2</sub>	WILEY229.LI																																																																			
<p>51.989</p>	<p>51.989</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>75</td> <td>1</td> <td>METHYL COMMATTE B \$S\$</td> <td>470</td> <td>C<sub>31</sub>H<sub>50</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>75</td> <td>2</td> <td>Senarin \$S\$ (sen-20(20)ene-3,20-diol, (3 beta)-)</td> <td>442</td> <td>C<sub>30</sub>H<sub>50</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>75</td> <td>3</td> <td>Farnesyl bromide \$S\$</td> <td>284</td> <td>C<sub>15</sub>H<sub>26</sub>Br</td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>75</td> <td>4</td> <td>(1-Caryophyllene-11) \$S\$</td> <td>204</td> <td>C<sub>15</sub>H<sub>24</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>75</td> <td>5</td> <td>Farnesyl bromide \$S\$ (2E,6E)-1-bromo-3,7,11-tri</td> <td>284</td> <td>C<sub>15</sub>H<sub>26</sub>Br</td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>74</td> <td>6</td> <td>1R,4s,7s,11R,2,2,4,8-Tetramethylcyclo[5.3.1]</td> <td>204</td> <td>C<sub>15</sub>H<sub>24</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>74</td> <td>7</td> <td>1R,4S,7S,11R,2,2,4,8-Tetramethylcyclo[5.3.1]</td> <td>204</td> <td>C<sub>15</sub>H<sub>24</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>72</td> <td>8</td> <td>9,19-Cyclolanol-23-ene-3,25-diol, (3 beta, 23</td> <td>442</td> <td>C<sub>30</sub>H<sub>50</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>72</td> <td>9</td> <td>9,19-Cyclolanol-23-ene-3,25-diol, (3 beta, 23</td> <td>442</td> <td>C<sub>30</sub>H<sub>50</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 470: METHYL COMMATTE B \$S\$</p> <p>CAS# 0-00-0 Mol Wt: 470 Serial# 210915</p> <p>Captd Name: METHYL COMMATTE B \$S\$</p> <p>Formula: C<sub>31</sub>H<sub>50</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	#	Similar	Rank	Compound Name	Mol Wt	Formula	Library	1	75	1	METHYL COMMATTE B \$S\$	470	C <sub>31</sub> H <sub>50</sub> O <sub>2</sub>	WILEY229.LI	2	75	2	Senarin \$S\$ (sen-20(20)ene-3,20-diol, (3 beta)-)	442	C <sub>30</sub> H <sub>50</sub> O <sub>2</sub>	NIST08.LIB	3	75	3	Farnesyl bromide \$S\$	284	C <sub>15</sub> H <sub>26</sub> Br	NIST107.LIB	4	75	4	(1-Caryophyllene-11) \$S\$	204	C <sub>15</sub> H <sub>24</sub>	NIST107.LIB	5	75	5	Farnesyl bromide \$S\$ (2E,6E)-1-bromo-3,7,11-tri	284	C <sub>15</sub> H <sub>26</sub> Br	NIST08.LIB	6	74	6	1R,4s,7s,11R,2,2,4,8-Tetramethylcyclo[5.3.1]	204	C <sub>15</sub> H <sub>24</sub>	NIST107.LIB	7	74	7	1R,4S,7S,11R,2,2,4,8-Tetramethylcyclo[5.3.1]	204	C <sub>15</sub> H <sub>24</sub>	NIST08.LIB	8	72	8	9,19-Cyclolanol-23-ene-3,25-diol, (3 beta, 23	442	C <sub>30</sub> H <sub>50</sub> O <sub>2</sub>	NIST107.LIB	9	72	9	9,19-Cyclolanol-23-ene-3,25-diol, (3 beta, 23	442	C <sub>30</sub> H <sub>50</sub> O <sub>2</sub>	NIST08.LIB
#	Similar	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	75	1	METHYL COMMATTE B \$S\$	470	C <sub>31</sub> H <sub>50</sub> O <sub>2</sub>	WILEY229.LI																																																																			
2	75	2	Senarin \$S\$ (sen-20(20)ene-3,20-diol, (3 beta)-)	442	C <sub>30</sub> H <sub>50</sub> O <sub>2</sub>	NIST08.LIB																																																																			
3	75	3	Farnesyl bromide \$S\$	284	C <sub>15</sub> H <sub>26</sub> Br	NIST107.LIB																																																																			
4	75	4	(1-Caryophyllene-11) \$S\$	204	C <sub>15</sub> H <sub>24</sub>	NIST107.LIB																																																																			
5	75	5	Farnesyl bromide \$S\$ (2E,6E)-1-bromo-3,7,11-tri	284	C <sub>15</sub> H <sub>26</sub> Br	NIST08.LIB																																																																			
6	74	6	1R,4s,7s,11R,2,2,4,8-Tetramethylcyclo[5.3.1]	204	C <sub>15</sub> H <sub>24</sub>	NIST107.LIB																																																																			
7	74	7	1R,4S,7S,11R,2,2,4,8-Tetramethylcyclo[5.3.1]	204	C <sub>15</sub> H <sub>24</sub>	NIST08.LIB																																																																			
8	72	8	9,19-Cyclolanol-23-ene-3,25-diol, (3 beta, 23	442	C <sub>30</sub> H <sub>50</sub> O <sub>2</sub>	NIST107.LIB																																																																			
9	72	9	9,19-Cyclolanol-23-ene-3,25-diol, (3 beta, 23	442	C <sub>30</sub> H <sub>50</sub> O <sub>2</sub>	NIST08.LIB																																																																			
<p>52.071</p>	<p>3197</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>54</td> <td>1</td> <td>2,6-Dihydroxybenzoic acid, 3-TMS \$S\$ bis(trimethylsilyloxy) methanone \$S\$</td> <td>370</td> <td>C<sub>16</sub>H<sub>20</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>54</td> <td>2</td> <td>Benzoic acid, 2,6-bis(trimethylsilyloxy), trimethylsilyl ester</td> <td>370</td> <td>C<sub>16</sub>H<sub>20</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>54</td> <td>3</td> <td>4,4'-Bis(2,6-di-tert-butylperyl)benzene \$S\$ Benzene</td> <td>608</td> <td>C<sub>46</sub>H<sub>56</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>54</td> <td>4</td> <td>2,4-DIHYDROXYBENZYL ALCOHOL, 3-TMS \$S\$</td> <td>356</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>54</td> <td>5</td> <td>Cycloperilbenzene, decamethyl-, (CAS) (Stere)</td> <td>370</td> <td>C<sub>10</sub>H<sub>20</sub>O<sub>5</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>53</td> <td>6</td> <td>Benzenoacetic acid, alpha-(3,4-dimethylsilyl)</td> <td>472</td> <td>C<sub>20</sub>H<sub>40</sub>O<sub>5</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>53</td> <td>7</td> <td>2,6-DIHYDROXYBENZOIDIC ACID 3-TMS \$S\$ m</td> <td>370</td> <td>C<sub>16</sub>H<sub>20</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>52</td> <td>8</td> <td>Benzoic acid, 2,4-bis(trimethylsilyloxy), trimet</td> <td>370</td> <td>C<sub>16</sub>H<sub>20</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>52</td> <td>9</td> <td>TRIMETHYLSILYL ESTER OF 2,3,6-TRISTRIM</td> <td>370</td> <td>C<sub>16</sub>H<sub>20</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 2,6-DIHYDROXYBENZOIDIC ACID 3-TMS \$S\$ bis(trimethylsilyloxy) methanone \$S\$ Benzoic acid, 2,6-bis(trimethylsilyloxy), trimethylsilyl ester \$S\$ Benzoic acid, 2,6-bis(trimethylsilyloxy), trimethylsilyl ester \$S\$</p> <p>CAS# 3702-85-2 Mol Wt: 370 Serial# 183625</p> <p>Captd Name: 2,6-DIHYDROXYBENZOIDIC ACID 3-TMS \$S\$ bis(trimethylsilyloxy) methanone \$S\$ Benzoic acid, 2,6-bis(trimethylsilyloxy), trimethylsilyl ester \$S\$ Benzoic acid, 2,6-bis(trimethylsilyloxy), trimethylsilyl ester \$S\$</p> <p>Formula: C<sub>16</sub>H<sub>20</sub>O<sub>4</sub> Class Flag: No Class Flags</p>	#	Similar	Rank	Compound Name	Mol Wt	Formula	Library	1	54	1	2,6-Dihydroxybenzoic acid, 3-TMS \$S\$ bis(trimethylsilyloxy) methanone \$S\$	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI	2	54	2	Benzoic acid, 2,6-bis(trimethylsilyloxy), trimethylsilyl ester	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI	3	54	3	4,4'-Bis(2,6-di-tert-butylperyl)benzene \$S\$ Benzene	608	C <sub>46</sub> H <sub>56</sub>	WILEY229.LI	4	54	4	2,4-DIHYDROXYBENZYL ALCOHOL, 3-TMS \$S\$	356	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI	5	54	5	Cycloperilbenzene, decamethyl-, (CAS) (Stere)	370	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub>	WILEY229.LI	6	53	6	Benzenoacetic acid, alpha-(3,4-dimethylsilyl)	472	C <sub>20</sub> H <sub>40</sub> O <sub>5</sub>	WILEY229.LI	7	53	7	2,6-DIHYDROXYBENZOIDIC ACID 3-TMS \$S\$ m	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI	8	52	8	Benzoic acid, 2,4-bis(trimethylsilyloxy), trimet	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI	9	52	9	TRIMETHYLSILYL ESTER OF 2,3,6-TRISTRIM	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI
#	Similar	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	54	1	2,6-Dihydroxybenzoic acid, 3-TMS \$S\$ bis(trimethylsilyloxy) methanone \$S\$	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI																																																																			
2	54	2	Benzoic acid, 2,6-bis(trimethylsilyloxy), trimethylsilyl ester	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI																																																																			
3	54	3	4,4'-Bis(2,6-di-tert-butylperyl)benzene \$S\$ Benzene	608	C <sub>46</sub> H <sub>56</sub>	WILEY229.LI																																																																			
4	54	4	2,4-DIHYDROXYBENZYL ALCOHOL, 3-TMS \$S\$	356	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI																																																																			
5	54	5	Cycloperilbenzene, decamethyl-, (CAS) (Stere)	370	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub>	WILEY229.LI																																																																			
6	53	6	Benzenoacetic acid, alpha-(3,4-dimethylsilyl)	472	C <sub>20</sub> H <sub>40</sub> O <sub>5</sub>	WILEY229.LI																																																																			
7	53	7	2,6-DIHYDROXYBENZOIDIC ACID 3-TMS \$S\$ m	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI																																																																			
8	52	8	Benzoic acid, 2,4-bis(trimethylsilyloxy), trimet	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI																																																																			
9	52	9	TRIMETHYLSILYL ESTER OF 2,3,6-TRISTRIM	370	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	WILEY229.LI																																																																			
<p>52.205</p>	<p>3203</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Rank</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>56</td> <td>1</td> <td>Prog-4-ene-3,20-dione, 6,16-dimethyl-, (S)-beta-</td> <td>342</td> <td>C<sub>23</sub>H<sub>34</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>56</td> <td>2</td> <td>LEEDENOXIDE-01 \$S\$</td> <td>220</td> <td>C<sub>15</sub>H<sub>24</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>56</td> <td>3</td> <td>Prog-4-ene-3,20-dione, 6,16-dimethyl-, (CAS)</td> <td>342</td> <td>C<sub>23</sub>H<sub>34</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>56</td> <td>4</td> <td>VRIDIFLOROL \$S\$</td> <td>222</td> <td>C<sub>15</sub>H<sub>26</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>56</td> <td>5</td> <td>spathulanol \$S\$</td> <td>222</td> <td>C<sub>15</sub>H<sub>26</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>56</td> <td>6</td> <td>ARISTOLENEPOXIDE \$S\$</td> <td>220</td> <td>C<sub>15</sub>H<sub>24</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>55</td> <td>7</td> <td>Prog-4-ene-3,20-dione, 17-ethyl-, (CAS) 17-AL</td> <td>342</td> <td>C<sub>23</sub>H<sub>34</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>55</td> <td>8</td> <td>DIETYLALPHA-CEDRENEPOXIDE \$S\$</td> <td>220</td> <td>C<sub>15</sub>H<sub>24</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>54</td> <td>9</td> <td>CALANDRENEPOXIDE \$S\$</td> <td>220</td> <td>C<sub>15</sub>H<sub>24</sub>O</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 342: Prog-4-ene-3,20-dione, 6,16-dimethyl-, (S)-beta-, 16-ALPHA-DIMETHYL-PROGESTERONE \$S\$ Prog-4-ene-3,20-dione, 6,16-beta, 16-alpha-dimethyl-, \$S\$</p> <p>CAS# 1816-79-1 Mol Wt: 342 Serial# 170321</p> <p>Captd Name: Prog-4-ene-3,20-dione, 6,16-dimethyl-, (S)-beta-, 16-ALPHA-DIMETHYL-PROGESTERONE \$S\$ Prog-4-ene-3,20-dione, 6,16-beta, 16-alpha-dimethyl-, \$S\$</p> <p>Formula: C<sub>23</sub>H<sub>34</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	#	Similar	Rank	Compound Name	Mol Wt	Formula	Library	1	56	1	Prog-4-ene-3,20-dione, 6,16-dimethyl-, (S)-beta-	342	C <sub>23</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI	2	56	2	LEEDENOXIDE-01 \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI	3	56	3	Prog-4-ene-3,20-dione, 6,16-dimethyl-, (CAS)	342	C <sub>23</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI	4	56	4	VRIDIFLOROL \$S\$	222	C <sub>15</sub> H <sub>26</sub> O	WILEY229.LI	5	56	5	spathulanol \$S\$	222	C <sub>15</sub> H <sub>26</sub> O	WILEY229.LI	6	56	6	ARISTOLENEPOXIDE \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI	7	55	7	Prog-4-ene-3,20-dione, 17-ethyl-, (CAS) 17-AL	342	C <sub>23</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI	8	55	8	DIETYLALPHA-CEDRENEPOXIDE \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI	9	54	9	CALANDRENEPOXIDE \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI
#	Similar	Rank	Compound Name	Mol Wt	Formula	Library																																																																			
1	56	1	Prog-4-ene-3,20-dione, 6,16-dimethyl-, (S)-beta-	342	C <sub>23</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI																																																																			
2	56	2	LEEDENOXIDE-01 \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI																																																																			
3	56	3	Prog-4-ene-3,20-dione, 6,16-dimethyl-, (CAS)	342	C <sub>23</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI																																																																			
4	56	4	VRIDIFLOROL \$S\$	222	C <sub>15</sub> H <sub>26</sub> O	WILEY229.LI																																																																			
5	56	5	spathulanol \$S\$	222	C <sub>15</sub> H <sub>26</sub> O	WILEY229.LI																																																																			
6	56	6	ARISTOLENEPOXIDE \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI																																																																			
7	55	7	Prog-4-ene-3,20-dione, 17-ethyl-, (CAS) 17-AL	342	C <sub>23</sub> H <sub>34</sub> O <sub>2</sub>	WILEY229.LI																																																																			
8	55	8	DIETYLALPHA-CEDRENEPOXIDE \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI																																																																			
9	54	9	CALANDRENEPOXIDE \$S\$	220	C <sub>15</sub> H <sub>24</sub> O	WILEY229.LI																																																																			

<p>52.251</p>	<p>3206</p>	<p>-</p>	<p>Target: 1: 486: METHYL COMMATE D \$\$\$</p> <p>CAS# 0-00-0 Mol Wt: 486 Serial#: 213498</p> <p>Compound Name: METHYL COMMATE D \$\$\$</p> <p>Formula: C31H50O4 Class Flag: No Class Flags</p>
<p>52.451</p>	<p>3216</p>	<p>3253 3204</p>	<p>Target: 1: 472: Campesterol</p> <p>CAS# 0-00-0 Mol Wt: 472 Serial#: 181992</p> <p>Compound Name: Campesterol</p> <p>Formula: C31H50O5 Class Flag: No Class Flags</p>
<p>52.593</p>	<p>3223</p>	<p>-</p>	<p>Target: 15: 260: Androstane, (5 beta)- (CAS) 5 beta-Androstane</p> <p>CAS# 438-23-3 Mol Wt: 260 Serial#: 117142</p> <p>Compound Name: Androstane, (5 beta)- (CAS) 5 beta-Androstane</p> <p>Formula: C19H32 Class Flag: No Class Flags</p>
<p>52.822</p>	<p>3234</p>	<p>3232 GMD</p>	<p>Target: 1: 466: Hexanoic acid, trimethylsilyl ester</p> <p>CAS# 0-00-0 Mol Wt: 466 Serial#: 181479</p> <p>Compound Name: Hexanoic acid, trimethylsilyl ester</p> <p>Formula: C29H50O2S Class Flag: No Class Flags</p>



<p>52.98</p>	<p>3242</p>	<p>3286</p>	<p>Target</p> <p>1: 484: Stigmastrol trimethyl ether 5S Sllane, trimethyl(3 beta, 22E)-stigmasta-5,22-dien-3-yl(oy) 5S Sllane, trimethyl(stigmasta-5,22-dien-3 beta-yl(oy)) 5S 3 beta-(Trimethyl(ox)stigmasta-5,22-diene 5S (2E)-3(trimethyl(ox)stigmasta-5,22-diene 5S</p> <p>CAS#: 14030-29-6 Mol Wt: 484 Serial#: 183323</p> <p>Cmpd Name: Stigmastrol trimethyl ether 5S Sllane, trimethyl(3 beta, 22E)-stigmasta-5,22-dien-3-yl(oy) 5S Sllane, trimethyl(stigmasta-5,22-dien-3 beta-yl(oy)) 5S 3 beta-(Trimethyl(ox)stigmasta-5,22-diene 5S (2E)-3(trimethyl(ox)stigmasta-5,22-diene 5S</p> <p>Formula: C39H50O5 Class Flag: No Class Flags</p>
<p>53.181</p>	<p>3252</p>	<p>-</p>	<p>Target</p> <p>1: 263: 3-Pyridinecarboxylic acid, 6-((trimethyl(ox)yl), trimethyl(ox)yl ester (CAS)-2-TRIMETHYLSILOXY-5-TRIMETHYLSILOXY-CARBONYLPYRIDINE 5S</p> <p>CAS#: 86972-82-4 Mol Wt: 283 Serial#: 133470</p> <p>Cmpd Name: 3-Pyridinecarboxylic acid, 6-((trimethyl(ox)yl), trimethyl(ox)yl ester (CAS)-2-TRIMETHYLSILOXY-5-TRIMETHYLSILOXY-CARBONYLPYRIDINE 5S</p> <p>Formula: C12H21N O3 Si2 Class Flag: No Class Flags</p>
<p>53.360</p>	<p>3261</p>	<p>-</p>	<p>Target</p> <p>1: 424: D-Friedolean-14-en-3-one (CAS) Taraxerone 5S Taraxerone 5S Stigmastrol 5S Taraxen-14-en-3-one 5S DELTA,14-Taraxene-3-one 5S</p> <p>CAS#: 514-07-8 Mol Wt: 424 Serial#: 201286</p> <p>Cmpd Name: D-Friedolean-14-en-3-one (CAS) Taraxerone 5S Taraxerone 5S Stigmastrol 5S Taraxen-14-en-3-one 5S DELTA,14-Taraxene-3-one 5S</p> <p>Formula: C30H48O Class Flag: No Class Flags</p>
<p>53.569</p>	<p>3271</p>	<p>-</p>	<p>Target</p> <p>1: 269: Benzene, 1-methyl-3,5-bis(trimethyl(ox)yl) 5S</p> <p>CAS#: 83267-67-4 Mol Wt: 268 Serial#: 61039</p> <p>Cmpd Name: Benzene, 1-methyl-3,5-bis(trimethyl(ox)yl) 5S</p> <p>Formula: C13H20OSi2 Class Flag: No Class Flags</p>

<p>53.74</p>	<p>3279</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Peak</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>55</td> <td>74</td> <td>✓</td> <td>4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one</td> <td>424</td> <td>C30H48O</td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>85</td> <td>✓</td> <td>4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one</td> <td>424</td> <td>C30H48O</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>82</td> <td>✓</td> <td>NOROLEAN-12-ENE</td> <td>396</td> <td>C29H48</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>81</td> <td>✓</td> <td>4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one</td> <td>424</td> <td>C30H48O</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>81</td> <td>✓</td> <td>4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one</td> <td>424</td> <td>C30H48O</td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>80</td> <td>✓</td> <td>METHYL COMMATE A</td> <td>500</td> <td>C32H52O4</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>78</td> <td>✓</td> <td>METHYL COMMATE C</td> <td>486</td> <td>C31H50O4</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>78</td> <td>✓</td> <td>Olean-12-ene</td> <td>410</td> <td>C30H50</td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>78</td> <td>✓</td> <td>Olean-12-ene</td> <td>410</td> <td>C30H50</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 424: 4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one</p> <p>CAS# 0-00-0 Mol Wt: 424 Serial#: 96159      Copd Name: 4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one      Formula: C30H48O Class Flag: No Class Flags</p>	RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library	55	74	✓	4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST107.LIB	2	85	✓	4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST08.LIB	3	82	✓	NOROLEAN-12-ENE	396	C29H48	WILEY229.LI	4	81	✓	4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST08.LIB	5	81	✓	4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST08.LIB	6	80	✓	METHYL COMMATE A	500	C32H52O4	WILEY229.LI	7	78	✓	METHYL COMMATE C	486	C31H50O4	WILEY229.LI	8	78	✓	Olean-12-ene	410	C30H50	NIST107.LIB	9	78	✓	Olean-12-ene	410	C30H50	NIST08.LIB
RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library																																																																			
55	74	✓	4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST107.LIB																																																																			
2	85	✓	4,4,6a,8a,11,11,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST08.LIB																																																																			
3	82	✓	NOROLEAN-12-ENE	396	C29H48	WILEY229.LI																																																																			
4	81	✓	4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST08.LIB																																																																			
5	81	✓	4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	424	C30H48O	NIST08.LIB																																																																			
6	80	✓	METHYL COMMATE A	500	C32H52O4	WILEY229.LI																																																																			
7	78	✓	METHYL COMMATE C	486	C31H50O4	WILEY229.LI																																																																			
8	78	✓	Olean-12-ene	410	C30H50	NIST107.LIB																																																																			
9	78	✓	Olean-12-ene	410	C30H50	NIST08.LIB																																																																			
<p>53.774</p>	<p>3281</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Peak</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>15</td> <td>74</td> <td>✓</td> <td>D-B-Friedo-B'-A'-neogammax-5-en-3-ol, (3 beta)-</td> <td>426</td> <td>C30H50O</td> <td>NIST107.LIB</td> </tr> <tr> <td>16</td> <td>73</td> <td>✓</td> <td>(3S)-isotriethylol acetate</td> <td>264</td> <td>C17H28O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>17</td> <td>73</td> <td>✓</td> <td>Thujopene</td> <td>204</td> <td>C15H24</td> <td>NIST107.LIB</td> </tr> <tr> <td>18</td> <td>73</td> <td>✓</td> <td>Thujopene</td> <td>204</td> <td>C15H24</td> <td>NIST08.LIB</td> </tr> <tr> <td>19</td> <td>73</td> <td>✓</td> <td>25-Nor-9,19-cyclolanostan-24-one, 3-acetate</td> <td>518</td> <td>C38H60O3</td> <td>NIST08.LIB</td> </tr> <tr> <td>20</td> <td>73</td> <td>✓</td> <td>25-Nor-9,19-cyclolanostan-24-one, 3-acetate</td> <td>518</td> <td>C38H60O3</td> <td>NIST107.LIB</td> </tr> <tr> <td>21</td> <td>73</td> <td>✓</td> <td>Longivibene</td> <td>218</td> <td>C19H20O</td> <td>NIST107.LIB</td> </tr> <tr> <td>22</td> <td>73</td> <td>✓</td> <td>Longivibene</td> <td>218</td> <td>C19H20O</td> <td>NIST08.LIB</td> </tr> <tr> <td>23</td> <td>73</td> <td>✓</td> <td>beta-Gulonic 55 Azulene, 1,2,3,4,5,6,7,8-oc</td> <td>204</td> <td>C15H24</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>15: 426: D-B-Friedo-B'-A'-neogammax-5-en-3-ol, (3 beta)-</p> <p>CAS# 1615-34-7 Mol Wt: 426 Serial#: 96390      Copd Name: D-B-Friedo-B'-A'-neogammax-5-en-3-ol, (3 beta)-      Formula: C30H50O Class Flag: No Class Flags</p>	RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library	15	74	✓	D-B-Friedo-B'-A'-neogammax-5-en-3-ol, (3 beta)-	426	C30H50O	NIST107.LIB	16	73	✓	(3S)-isotriethylol acetate	264	C17H28O2	NIST08.LIB	17	73	✓	Thujopene	204	C15H24	NIST107.LIB	18	73	✓	Thujopene	204	C15H24	NIST08.LIB	19	73	✓	25-Nor-9,19-cyclolanostan-24-one, 3-acetate	518	C38H60O3	NIST08.LIB	20	73	✓	25-Nor-9,19-cyclolanostan-24-one, 3-acetate	518	C38H60O3	NIST107.LIB	21	73	✓	Longivibene	218	C19H20O	NIST107.LIB	22	73	✓	Longivibene	218	C19H20O	NIST08.LIB	23	73	✓	beta-Gulonic 55 Azulene, 1,2,3,4,5,6,7,8-oc	204	C15H24	WILEY229.LI
RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library																																																																			
15	74	✓	D-B-Friedo-B'-A'-neogammax-5-en-3-ol, (3 beta)-	426	C30H50O	NIST107.LIB																																																																			
16	73	✓	(3S)-isotriethylol acetate	264	C17H28O2	NIST08.LIB																																																																			
17	73	✓	Thujopene	204	C15H24	NIST107.LIB																																																																			
18	73	✓	Thujopene	204	C15H24	NIST08.LIB																																																																			
19	73	✓	25-Nor-9,19-cyclolanostan-24-one, 3-acetate	518	C38H60O3	NIST08.LIB																																																																			
20	73	✓	25-Nor-9,19-cyclolanostan-24-one, 3-acetate	518	C38H60O3	NIST107.LIB																																																																			
21	73	✓	Longivibene	218	C19H20O	NIST107.LIB																																																																			
22	73	✓	Longivibene	218	C19H20O	NIST08.LIB																																																																			
23	73	✓	beta-Gulonic 55 Azulene, 1,2,3,4,5,6,7,8-oc	204	C15H24	WILEY229.LI																																																																			
<p>53.909</p>	<p>3288</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Peak</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>74</td> <td>✓</td> <td>Olivetol, bis(benzyloxy) ether</td> <td>324</td> <td>C17H20O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>71</td> <td>✓</td> <td>1-Valine, n-heptafluorobutyl, isohexyl ester</td> <td>357</td> <td>C15H22F7NO</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>68</td> <td>✓</td> <td>alpha-Phenyl beta-phenethylisopropylene</td> <td>288</td> <td>C17H20O</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>65</td> <td>✓</td> <td>3-Pyridinecarboxylic acid, 6-(benzethoxy)oxy</td> <td>283</td> <td>C12H21NO</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>64</td> <td>✓</td> <td>1,4-Bis(benzyloxy)-2-methylbenzene</td> <td>268</td> <td>C13H24O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>63</td> <td>✓</td> <td>isobutyl 3-bicyclo[3.2.2]nonane-2,5-diene-5-yl</td> <td>255</td> <td>C21H36</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>63</td> <td>✓</td> <td>Spicythiolumene 9,9-isopropyl-3,1-dithiopyr</td> <td>288</td> <td>C21H36</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>62</td> <td>✓</td> <td>3-Benzyliden-3,8-dihydrocycloheptadiene</td> <td>268</td> <td>C21H36</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>60</td> <td>✓</td> <td>2-METHYLRESORCINOL, DIMMS</td> <td>268</td> <td>C13H24O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 324: Olivetol, bis(benzyloxy) ether</p> <p>CAS# 0-00-0 Mol Wt: 324 Serial#: 128432      Copd Name: Olivetol, bis(benzyloxy) ether      Formula: C17H20O2 Class Flag: No Class Flags</p>	RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library	1	74	✓	Olivetol, bis(benzyloxy) ether	324	C17H20O2	NIST08.LIB	2	71	✓	1-Valine, n-heptafluorobutyl, isohexyl ester	357	C15H22F7NO	NIST08.LIB	3	68	✓	alpha-Phenyl beta-phenethylisopropylene	288	C17H20O	WILEY229.LI	4	65	✓	3-Pyridinecarboxylic acid, 6-(benzethoxy)oxy	283	C12H21NO	WILEY229.LI	5	64	✓	1,4-Bis(benzyloxy)-2-methylbenzene	268	C13H24O2	WILEY229.LI	6	63	✓	isobutyl 3-bicyclo[3.2.2]nonane-2,5-diene-5-yl	255	C21H36	WILEY229.LI	7	63	✓	Spicythiolumene 9,9-isopropyl-3,1-dithiopyr	288	C21H36	WILEY229.LI	8	62	✓	3-Benzyliden-3,8-dihydrocycloheptadiene	268	C21H36	WILEY229.LI	9	60	✓	2-METHYLRESORCINOL, DIMMS	268	C13H24O2	WILEY229.LI
RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library																																																																			
1	74	✓	Olivetol, bis(benzyloxy) ether	324	C17H20O2	NIST08.LIB																																																																			
2	71	✓	1-Valine, n-heptafluorobutyl, isohexyl ester	357	C15H22F7NO	NIST08.LIB																																																																			
3	68	✓	alpha-Phenyl beta-phenethylisopropylene	288	C17H20O	WILEY229.LI																																																																			
4	65	✓	3-Pyridinecarboxylic acid, 6-(benzethoxy)oxy	283	C12H21NO	WILEY229.LI																																																																			
5	64	✓	1,4-Bis(benzyloxy)-2-methylbenzene	268	C13H24O2	WILEY229.LI																																																																			
6	63	✓	isobutyl 3-bicyclo[3.2.2]nonane-2,5-diene-5-yl	255	C21H36	WILEY229.LI																																																																			
7	63	✓	Spicythiolumene 9,9-isopropyl-3,1-dithiopyr	288	C21H36	WILEY229.LI																																																																			
8	62	✓	3-Benzyliden-3,8-dihydrocycloheptadiene	268	C21H36	WILEY229.LI																																																																			
9	60	✓	2-METHYLRESORCINOL, DIMMS	268	C13H24O2	WILEY229.LI																																																																			
<p>53.98</p>	<p>3291</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Peak</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>79</td> <td>✓</td> <td>METHYL COMMATE D</td> <td>486</td> <td>C31H50O4</td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>76</td> <td>✓</td> <td>Farnesyl bromide</td> <td>284</td> <td>C15H28Br</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>76</td> <td>✓</td> <td>Farnesyl bromide</td> <td>284</td> <td>C15H28Br</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>76</td> <td>✓</td> <td>METHYL COMMATE B</td> <td>470</td> <td>C31H50O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>75</td> <td>✓</td> <td>METHYL COMMATE C</td> <td>486</td> <td>C31H50O4</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>75</td> <td>✓</td> <td>14-Nor-Saccharosyl-12-ene, 14 alpha, 20 bet</td> <td>454</td> <td>C31H50O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>75</td> <td>✓</td> <td>14-Nor-Saccharosyl-12-ene, 14 alpha, 20 bet</td> <td>454</td> <td>C31H50O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>74</td> <td>✓</td> <td>Guai-3,9-diene</td> <td>204</td> <td>C15H24</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>74</td> <td>✓</td> <td>1R,4S,7S,11R,2,2,4,8-Tetramethylcyclo[5.3.1]</td> <td>204</td> <td>C15H24</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 486: METHYL COMMATE D</p> <p>CAS# 0-00-0 Mol Wt: 486 Serial#: 213498      Copd Name: METHYL COMMATE D      Formula: C31H50O4 Class Flag: No Class Flags</p>	RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library	1	79	✓	METHYL COMMATE D	486	C31H50O4	WILEY229.LI	2	76	✓	Farnesyl bromide	284	C15H28Br	NIST107.LIB	3	76	✓	Farnesyl bromide	284	C15H28Br	NIST08.LIB	4	76	✓	METHYL COMMATE B	470	C31H50O3	WILEY229.LI	5	75	✓	METHYL COMMATE C	486	C31H50O4	WILEY229.LI	6	75	✓	14-Nor-Saccharosyl-12-ene, 14 alpha, 20 bet	454	C31H50O2	NIST107.LIB	7	75	✓	14-Nor-Saccharosyl-12-ene, 14 alpha, 20 bet	454	C31H50O2	NIST08.LIB	8	74	✓	Guai-3,9-diene	204	C15H24	NIST08.LIB	9	74	✓	1R,4S,7S,11R,2,2,4,8-Tetramethylcyclo[5.3.1]	204	C15H24	NIST08.LIB
RT	Similar	Peak	Compound Name	Mol Wt	Formula	Library																																																																			
1	79	✓	METHYL COMMATE D	486	C31H50O4	WILEY229.LI																																																																			
2	76	✓	Farnesyl bromide	284	C15H28Br	NIST107.LIB																																																																			
3	76	✓	Farnesyl bromide	284	C15H28Br	NIST08.LIB																																																																			
4	76	✓	METHYL COMMATE B	470	C31H50O3	WILEY229.LI																																																																			
5	75	✓	METHYL COMMATE C	486	C31H50O4	WILEY229.LI																																																																			
6	75	✓	14-Nor-Saccharosyl-12-ene, 14 alpha, 20 bet	454	C31H50O2	NIST107.LIB																																																																			
7	75	✓	14-Nor-Saccharosyl-12-ene, 14 alpha, 20 bet	454	C31H50O2	NIST08.LIB																																																																			
8	74	✓	Guai-3,9-diene	204	C15H24	NIST08.LIB																																																																			
9	74	✓	1R,4S,7S,11R,2,2,4,8-Tetramethylcyclo[5.3.1]	204	C15H24	NIST08.LIB																																																																			

<p>54.089</p>	<p>3297</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Height</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>83</td> <td>75</td> <td>Silane, (3 beta) lanosta-8,24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>NIST07.LIB</td> </tr> <tr> <td>2</td> <td>83</td> <td>75</td> <td>Silane, (3 beta) lanosta-8,24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>82</td> <td>75</td> <td>Silane, (3 beta) lanosta-8,24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>WILEY229.LIB</td> </tr> <tr> <td>4</td> <td>76</td> <td>75</td> <td>Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>NIST07.LIB</td> </tr> <tr> <td>5</td> <td>76</td> <td>75</td> <td>Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>WILEY229.LIB</td> </tr> <tr> <td>6</td> <td>76</td> <td>75</td> <td>Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>71</td> <td>75</td> <td>Silane, (3 beta) lanosta-8,24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>71</td> <td>75</td> <td>Silane, (3 beta) lanosta-8,24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>71</td> <td>75</td> <td>Silane, (3 beta) lanosta-8,24-dien-3-ylacetate</td> <td>498</td> <td>C33H58O5</td> <td>WILEY229.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>3: 498: Silane, (3 beta) lanosta-8,24-dien-3-ylacetate (CAS) LANOSTEROL TRIMETHYLSILYL ETHER \$\$\$</p> <p>CAS#: 55433-04-0 Mol Wt: 498 Serial#: 214956</p> <p>Compound Name: Silane, (3 beta) lanosta-8,24-dien-3-ylacetate (CAS) LANOSTEROL TRIMETHYLSILYL ETHER \$\$\$</p> <p>Formula: C33H58O5</p>	RT	Similar	Height	Compound Name	Mol Wt	Formula	Library	1	83	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST07.LIB	2	83	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST08.LIB	3	82	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	WILEY229.LIB	4	76	75	Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate	498	C33H58O5	NIST07.LIB	5	76	75	Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate	498	C33H58O5	WILEY229.LIB	6	76	75	Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate	498	C33H58O5	NIST107.LIB	7	71	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST107.LIB	8	71	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST08.LIB	9	71	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	WILEY229.LIB
RT	Similar	Height	Compound Name	Mol Wt	Formula	Library																																																																			
1	83	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST07.LIB																																																																			
2	83	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST08.LIB																																																																			
3	82	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	WILEY229.LIB																																																																			
4	76	75	Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate	498	C33H58O5	NIST07.LIB																																																																			
5	76	75	Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate	498	C33H58O5	WILEY229.LIB																																																																			
6	76	75	Silane, (3 beta) lanosta-9(11),24-dien-3-ylacetate	498	C33H58O5	NIST107.LIB																																																																			
7	71	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST107.LIB																																																																			
8	71	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	NIST08.LIB																																																																			
9	71	75	Silane, (3 beta) lanosta-8,24-dien-3-ylacetate	498	C33H58O5	WILEY229.LIB																																																																			
<p>54.321</p>	<p>3308</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Height</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>74</td> <td>75</td> <td>D-C-Friedo-8'A-neogammacer-9(11)ene, 3m</td> <td>440</td> <td>C31H52O</td> <td>NIST07.LIB</td> </tr> <tr> <td>2</td> <td>74</td> <td>75</td> <td>D-C-Friedo-8'A-neogammacer-9(11)ene, 3m</td> <td>440</td> <td>C31H52O</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>74</td> <td>75</td> <td>D-C-Friedo-8'A-neogammacer-9(11)ene, 3m</td> <td>440</td> <td>C31H52O</td> <td>WILEY229.LIB</td> </tr> <tr> <td>4</td> <td>71</td> <td>75</td> <td>Lanost-8-en-3-ol, 24-methylene-, (3 beta)-5S</td> <td>440</td> <td>C31H52O</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>71</td> <td>75</td> <td>Lanost-8-en-3-ol, 24-methylene-, (3 beta)-5S</td> <td>440</td> <td>C31H52O</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>69</td> <td>75</td> <td>24-METHYLENE DIHYDROLANOSTEROL, 5</td> <td>440</td> <td>C31H52O</td> <td>WILEY229.LIB</td> </tr> <tr> <td>7</td> <td>67</td> <td>75</td> <td>Cholestan-24-ene, 3,17-dihydroxy-, (3 alpha)-5</td> <td>438</td> <td>C27H44O3</td> <td>WILEY229.LIB</td> </tr> <tr> <td>8</td> <td>67</td> <td>75</td> <td>9,19-Cyclolanost-24-en-3-ol, (3 beta)-, (CAS) C</td> <td>426</td> <td>C30H50O</td> <td>WILEY229.LIB</td> </tr> <tr> <td>9</td> <td>66</td> <td>75</td> <td>Pregnan-20-ene, 3,17-dihydroxy-, (3 alpha)-, (C</td> <td>334</td> <td>C21H34O3</td> <td>WILEY229.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 440: D-C-Friedo-8'A-neogammacer-9(11)ene, 3-methoxy-, (3 beta)-5S D-C-Friedo-8'A-neogammacer-9(11)ene, 3 beta-methoxy-5S Arundin 5S Ferrocenyl methyl ether \$\$\$</p> <p>CAS#: 4555-56-0 Mol Wt: 440 Serial#: 97915</p> <p>Compound Name: D-C-Friedo-8'A-neogammacer-9(11)ene, 3-methoxy-, (3 beta)-5S D-C-Friedo-8'A-neogammacer-9(11)ene, 3 beta-methoxy-5S Arundin 5S Ferrocenyl methyl ether \$\$\$</p> <p>Formula: C31H52O</p>	RT	Similar	Height	Compound Name	Mol Wt	Formula	Library	1	74	75	D-C-Friedo-8'A-neogammacer-9(11)ene, 3m	440	C31H52O	NIST07.LIB	2	74	75	D-C-Friedo-8'A-neogammacer-9(11)ene, 3m	440	C31H52O	NIST08.LIB	3	74	75	D-C-Friedo-8'A-neogammacer-9(11)ene, 3m	440	C31H52O	WILEY229.LIB	4	71	75	Lanost-8-en-3-ol, 24-methylene-, (3 beta)-5S	440	C31H52O	NIST08.LIB	5	71	75	Lanost-8-en-3-ol, 24-methylene-, (3 beta)-5S	440	C31H52O	NIST107.LIB	6	69	75	24-METHYLENE DIHYDROLANOSTEROL, 5	440	C31H52O	WILEY229.LIB	7	67	75	Cholestan-24-ene, 3,17-dihydroxy-, (3 alpha)-5	438	C27H44O3	WILEY229.LIB	8	67	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-, (CAS) C	426	C30H50O	WILEY229.LIB	9	66	75	Pregnan-20-ene, 3,17-dihydroxy-, (3 alpha)-, (C	334	C21H34O3	WILEY229.LIB
RT	Similar	Height	Compound Name	Mol Wt	Formula	Library																																																																			
1	74	75	D-C-Friedo-8'A-neogammacer-9(11)ene, 3m	440	C31H52O	NIST07.LIB																																																																			
2	74	75	D-C-Friedo-8'A-neogammacer-9(11)ene, 3m	440	C31H52O	NIST08.LIB																																																																			
3	74	75	D-C-Friedo-8'A-neogammacer-9(11)ene, 3m	440	C31H52O	WILEY229.LIB																																																																			
4	71	75	Lanost-8-en-3-ol, 24-methylene-, (3 beta)-5S	440	C31H52O	NIST08.LIB																																																																			
5	71	75	Lanost-8-en-3-ol, 24-methylene-, (3 beta)-5S	440	C31H52O	NIST107.LIB																																																																			
6	69	75	24-METHYLENE DIHYDROLANOSTEROL, 5	440	C31H52O	WILEY229.LIB																																																																			
7	67	75	Cholestan-24-ene, 3,17-dihydroxy-, (3 alpha)-5	438	C27H44O3	WILEY229.LIB																																																																			
8	67	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-, (CAS) C	426	C30H50O	WILEY229.LIB																																																																			
9	66	75	Pregnan-20-ene, 3,17-dihydroxy-, (3 alpha)-, (C	334	C21H34O3	WILEY229.LIB																																																																			
<p>54.432</p>	<p>3314</p>	<p>3348</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Height</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>86</td> <td>75</td> <td>NOROLEAN 12-ENE 5S</td> <td>396</td> <td>C29H48</td> <td>WILEY229.LIB</td> </tr> <tr> <td>2</td> <td>86</td> <td>75</td> <td>METHYL DIMMATE A 5S</td> <td>500</td> <td>C32H52O4</td> <td>WILEY229.LIB</td> </tr> <tr> <td>3</td> <td>84</td> <td>75</td> <td>4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6</td> <td>424</td> <td>C30H48O</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>84</td> <td>75</td> <td>4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6</td> <td>424</td> <td>C30H48O</td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>84</td> <td>75</td> <td>4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6</td> <td>424</td> <td>C30H48O</td> <td>NIST07.LIB</td> </tr> <tr> <td>6</td> <td>84</td> <td>75</td> <td>beta-Amyrin trimethylsilyl ether 5S Silane, trim</td> <td>498</td> <td>C33H58O5</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>84</td> <td>75</td> <td>beta-Amyrin trimethylsilyl ether 5S Silane, trim</td> <td>498</td> <td>C33H58O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>83</td> <td>75</td> <td>4,4,8a,8b,9a,11,12,14b-Octamethyl-1,4,4a,5,6</td> <td>424</td> <td>C30H48O</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>83</td> <td>75</td> <td>4,4,8a,8b,9a,11,12,14b-Octamethyl-1,4,4a,5,6</td> <td>424</td> <td>C30H48O</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>3: 498: Silane, trimethylsilyl ether (CAS) Silane, trimethylsilyl ether 5S Silane, trimethylsilyl ether (3 beta)-ylacetate 5S</p> <p>CAS#: 1721-67-1 Mol Wt: 498 Serial#: 214951</p> <p>Compound Name: Silane, trimethylsilyl ether (CAS) Silane, trimethylsilyl ether 5S Silane, trimethylsilyl ether (3 beta)-ylacetate 5S</p> <p>Formula: C33H58O5</p>	RT	Similar	Height	Compound Name	Mol Wt	Formula	Library	1	86	75	NOROLEAN 12-ENE 5S	396	C29H48	WILEY229.LIB	2	86	75	METHYL DIMMATE A 5S	500	C32H52O4	WILEY229.LIB	3	84	75	4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST08.LIB	4	84	75	4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST107.LIB	5	84	75	4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST07.LIB	6	84	75	beta-Amyrin trimethylsilyl ether 5S Silane, trim	498	C33H58O5	NIST107.LIB	7	84	75	beta-Amyrin trimethylsilyl ether 5S Silane, trim	498	C33H58O5	NIST08.LIB	8	83	75	4,4,8a,8b,9a,11,12,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST08.LIB	9	83	75	4,4,8a,8b,9a,11,12,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST107.LIB
RT	Similar	Height	Compound Name	Mol Wt	Formula	Library																																																																			
1	86	75	NOROLEAN 12-ENE 5S	396	C29H48	WILEY229.LIB																																																																			
2	86	75	METHYL DIMMATE A 5S	500	C32H52O4	WILEY229.LIB																																																																			
3	84	75	4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST08.LIB																																																																			
4	84	75	4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST107.LIB																																																																			
5	84	75	4,4,8a,8b,9a,11,11,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST07.LIB																																																																			
6	84	75	beta-Amyrin trimethylsilyl ether 5S Silane, trim	498	C33H58O5	NIST107.LIB																																																																			
7	84	75	beta-Amyrin trimethylsilyl ether 5S Silane, trim	498	C33H58O5	NIST08.LIB																																																																			
8	83	75	4,4,8a,8b,9a,11,12,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST08.LIB																																																																			
9	83	75	4,4,8a,8b,9a,11,12,14b-Octamethyl-1,4,4a,5,6	424	C30H48O	NIST107.LIB																																																																			
<p>54.56</p>	<p>3321</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Height</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>75</td> <td>75</td> <td>9,19-Cyclolanost-24-en-3-ol, 4,14-dimethyl-</td> <td>468</td> <td>C32H52O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>75</td> <td>75</td> <td>9,19-Cyclolanost-24-en-3-ol, acetate 5S</td> <td>468</td> <td>C32H52O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>75</td> <td>75</td> <td>9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23</td> <td>442</td> <td>C30H50O2</td> <td>WILEY229.LIB</td> </tr> <tr> <td>4</td> <td>75</td> <td>75</td> <td>9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23</td> <td>442</td> <td>C30H50O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>75</td> <td>75</td> <td>9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23</td> <td>442</td> <td>C30H50O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>74</td> <td>75</td> <td>9,19-Cyclolanost-24-en-3-ol, (3 beta)-5S 9,19-</td> <td>426</td> <td>C30H50O</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>74</td> <td>75</td> <td>9,19-Cyclolanost-24-en-3-ol, (3 beta)-5S 9,19-</td> <td>426</td> <td>C30H50O</td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>74</td> <td>75</td> <td>9,19-Cyclolanost-24-en-3-ol, (3 beta)-, (CAS) C</td> <td>426</td> <td>C30H50O</td> <td>WILEY229.LIB</td> </tr> <tr> <td>9</td> <td>74</td> <td>75</td> <td>9,19-Cyclolanost-3-ol, 24-methylene-, (3 bet</td> <td>440</td> <td>C31H52O</td> <td>WILEY229.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>2: 468: 9,19-Cyclolanost-24-en-3-ol, acetate 5S</p> <p>CAS#: 124094-10-6 Mol Wt: 468 Serial#: 100392</p> <p>Compound Name: 9,19-Cyclolanost-24-en-3-ol, acetate 5S</p> <p>Formula: C32H52O2</p>	RT	Similar	Height	Compound Name	Mol Wt	Formula	Library	1	75	75	9,19-Cyclolanost-24-en-3-ol, 4,14-dimethyl-	468	C32H52O2	NIST08.LIB	2	75	75	9,19-Cyclolanost-24-en-3-ol, acetate 5S	468	C32H52O2	NIST107.LIB	3	75	75	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23	442	C30H50O2	WILEY229.LIB	4	75	75	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23	442	C30H50O2	NIST08.LIB	5	75	75	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23	442	C30H50O2	NIST107.LIB	6	74	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-5S 9,19-	426	C30H50O	NIST08.LIB	7	74	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-5S 9,19-	426	C30H50O	NIST107.LIB	8	74	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-, (CAS) C	426	C30H50O	WILEY229.LIB	9	74	75	9,19-Cyclolanost-3-ol, 24-methylene-, (3 bet	440	C31H52O	WILEY229.LIB
RT	Similar	Height	Compound Name	Mol Wt	Formula	Library																																																																			
1	75	75	9,19-Cyclolanost-24-en-3-ol, 4,14-dimethyl-	468	C32H52O2	NIST08.LIB																																																																			
2	75	75	9,19-Cyclolanost-24-en-3-ol, acetate 5S	468	C32H52O2	NIST107.LIB																																																																			
3	75	75	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23	442	C30H50O2	WILEY229.LIB																																																																			
4	75	75	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23	442	C30H50O2	NIST08.LIB																																																																			
5	75	75	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta)-23	442	C30H50O2	NIST107.LIB																																																																			
6	74	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-5S 9,19-	426	C30H50O	NIST08.LIB																																																																			
7	74	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-5S 9,19-	426	C30H50O	NIST107.LIB																																																																			
8	74	75	9,19-Cyclolanost-24-en-3-ol, (3 beta)-, (CAS) C	426	C30H50O	WILEY229.LIB																																																																			
9	74	75	9,19-Cyclolanost-3-ol, 24-methylene-, (3 bet	440	C31H52O	WILEY229.LIB																																																																			



<p>54.832</p>	<p>3334</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>65</td><td>✓</td><td>Stilene, (S)-19-cyclo-9-beta-ferrocenyl-24-en-3-ol</td><td>436</td><td>C33H50O</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>65</td><td>✓</td><td>Stilene, (S)-beta-5,14-dimethylcholesterol</td><td>484</td><td>C32H56O</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>65</td><td>✓</td><td>1-Naphthalenepropanol, alpha-ethenylcyclohexylidene-</td><td>272</td><td>C20H28O</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>55</td><td>✓</td><td>Stilene, (S)-beta-ferrocenyl-5-ene-3-ylidene-1-methyl-</td><td>436</td><td>C33H54O</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>65</td><td>✓</td><td>Stilene, trimethyl(2)-beta-4, alpha-5, alpha-1,4-</td><td>470</td><td>C31H54O</td><td>WILEY229.U</td></tr> <tr><td>6</td><td>65</td><td>✓</td><td>5,19-Cyclolanost-24-en-3-ol, (3)-beta-)- (CAS) C</td><td>426</td><td>C30H50O</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>54</td><td>✓</td><td>Stilene, (S)-beta-ferrocenyl-5-ene-3-ylidene-</td><td>436</td><td>C33H50O</td><td>WILEY229.U</td></tr> <tr><td>8</td><td>63</td><td>✓</td><td>DIHYDROSELAENE 55</td><td>274</td><td>C20H34</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>63</td><td>✓</td><td>2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15</td><td>410</td><td>C30H50</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>3: 252: 1-Naphthalenepropanol, alpha-ethenylcyclohexylidene-, alpha-5,5,8a-tetramethyl-2-methylene-, dihydro deriv., [(1S)-[1-alpha-(5'-1,4a-beta,8a-alpha)]]- (CAS) DIHYDROMANDIOL 55</p> <p>CAS# 72300-94-2 Mol Wt: 292 Serial# 140305</p> <p>Copd Name: 1-Naphthalenepropanol, alpha-ethenylcyclohexylidene-, alpha-5,5,8a-tetramethyl-2-methylene-, dihydro deriv., [(1S)-[1-alpha-(5'-1,4a-beta,8a-alpha)]]- (CAS) DIHYDROMANDIOL 55</p> <p>Formula: C20H36O Class Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	65	✓	Stilene, (S)-19-cyclo-9-beta-ferrocenyl-24-en-3-ol	436	C33H50O	WILEY229.U	2	65	✓	Stilene, (S)-beta-5,14-dimethylcholesterol	484	C32H56O	WILEY229.U	3	65	✓	1-Naphthalenepropanol, alpha-ethenylcyclohexylidene-	272	C20H28O	WILEY229.U	4	55	✓	Stilene, (S)-beta-ferrocenyl-5-ene-3-ylidene-1-methyl-	436	C33H54O	WILEY229.U	5	65	✓	Stilene, trimethyl(2)-beta-4, alpha-5, alpha-1,4-	470	C31H54O	WILEY229.U	6	65	✓	5,19-Cyclolanost-24-en-3-ol, (3)-beta-)- (CAS) C	426	C30H50O	WILEY229.U	7	54	✓	Stilene, (S)-beta-ferrocenyl-5-ene-3-ylidene-	436	C33H50O	WILEY229.U	8	63	✓	DIHYDROSELAENE 55	274	C20H34	WILEY229.U	9	63	✓	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15	410	C30H50	WILEY229.U
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	65	✓	Stilene, (S)-19-cyclo-9-beta-ferrocenyl-24-en-3-ol	436	C33H50O	WILEY229.U																																																																			
2	65	✓	Stilene, (S)-beta-5,14-dimethylcholesterol	484	C32H56O	WILEY229.U																																																																			
3	65	✓	1-Naphthalenepropanol, alpha-ethenylcyclohexylidene-	272	C20H28O	WILEY229.U																																																																			
4	55	✓	Stilene, (S)-beta-ferrocenyl-5-ene-3-ylidene-1-methyl-	436	C33H54O	WILEY229.U																																																																			
5	65	✓	Stilene, trimethyl(2)-beta-4, alpha-5, alpha-1,4-	470	C31H54O	WILEY229.U																																																																			
6	65	✓	5,19-Cyclolanost-24-en-3-ol, (3)-beta-)- (CAS) C	426	C30H50O	WILEY229.U																																																																			
7	54	✓	Stilene, (S)-beta-ferrocenyl-5-ene-3-ylidene-	436	C33H50O	WILEY229.U																																																																			
8	63	✓	DIHYDROSELAENE 55	274	C20H34	WILEY229.U																																																																			
9	63	✓	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15	410	C30H50	WILEY229.U																																																																			
<p>54.88</p>	<p>3337</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>62</td><td>✓</td><td>34-METHYLOXIFEROL-3-OXO-ANDROSTEROID 4</td><td>440</td><td>C31H52O</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>62</td><td>✓</td><td>D-C-Fiedo-8'-A'-neogammacer-9(11)ene, 3-ene, 3-oxo-</td><td>440</td><td>C31H52O</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>58</td><td>✓</td><td>Lanosterol-3-beta-yl-11-beta-19-epoxy-19-oxo-</td><td>612</td><td>C32H53O3</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>54</td><td>✓</td><td>Cholestan-24-ene, 3,12-dihydroxy-, (2)-alpha-, 5-</td><td>418</td><td>C27H46O3</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>54</td><td>✓</td><td>Cholan-24-ic acid, 3,12-dihydroxy-, (2)-alpha-, 5-</td><td>392</td><td>C24H40O4</td><td>WILEY229.U</td></tr> <tr><td>6</td><td>54</td><td>✓</td><td>Ergostane-3,12-diol, (3)-alpha-, 5-beta-, 12-alpha-</td><td>418</td><td>C28H50O2</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>53</td><td>✓</td><td>Cholest-5-en-3-ol, 14-methyl-, acetate, (3)-beta-</td><td>442</td><td>C30H52O2</td><td>WILEY229.U</td></tr> <tr><td>8</td><td>53</td><td>✓</td><td>Stigmata-7,22-dien-3-ol, (3)-beta-, 5-alpha-, 22E</td><td>412</td><td>C29H48O</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>53</td><td>✓</td><td>Ergosta-7,22-dien-3-ol, (3)-beta-, 22E)- (CAS) 5-</td><td>398</td><td>C28H48O</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>2: 440: D-C-Fiedo-8'-A'-neogammacer-9(11)ene, 3-ene, 3-oxo-, (3)-beta-)- (CAS) Androstan 55 Ferrocenyl methyl ether 55 D-C-Fiedo-8'-A'-neogammacer-9(11)ene, 3-beta-oxo-</p> <p>CAS# 4555-55-0 Mol Wt: 440 Serial# 205132</p> <p>Copd Name: D-C-Fiedo-8'-A'-neogammacer-9(11)ene, 3-ene, 3-oxo-, (3)-beta-)- (CAS) Androstan 55 Ferrocenyl methyl ether 55 D-C-Fiedo-8'-A'-neogammacer-9(11)ene, 3-beta-oxo-</p> <p>Formula: C31H52O Class Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	62	✓	34-METHYLOXIFEROL-3-OXO-ANDROSTEROID 4	440	C31H52O	WILEY229.U	2	62	✓	D-C-Fiedo-8'-A'-neogammacer-9(11)ene, 3-ene, 3-oxo-	440	C31H52O	WILEY229.U	3	58	✓	Lanosterol-3-beta-yl-11-beta-19-epoxy-19-oxo-	612	C32H53O3	WILEY229.U	4	54	✓	Cholestan-24-ene, 3,12-dihydroxy-, (2)-alpha-, 5-	418	C27H46O3	WILEY229.U	5	54	✓	Cholan-24-ic acid, 3,12-dihydroxy-, (2)-alpha-, 5-	392	C24H40O4	WILEY229.U	6	54	✓	Ergostane-3,12-diol, (3)-alpha-, 5-beta-, 12-alpha-	418	C28H50O2	WILEY229.U	7	53	✓	Cholest-5-en-3-ol, 14-methyl-, acetate, (3)-beta-	442	C30H52O2	WILEY229.U	8	53	✓	Stigmata-7,22-dien-3-ol, (3)-beta-, 5-alpha-, 22E	412	C29H48O	WILEY229.U	9	53	✓	Ergosta-7,22-dien-3-ol, (3)-beta-, 22E)- (CAS) 5-	398	C28H48O	WILEY229.U
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	62	✓	34-METHYLOXIFEROL-3-OXO-ANDROSTEROID 4	440	C31H52O	WILEY229.U																																																																			
2	62	✓	D-C-Fiedo-8'-A'-neogammacer-9(11)ene, 3-ene, 3-oxo-	440	C31H52O	WILEY229.U																																																																			
3	58	✓	Lanosterol-3-beta-yl-11-beta-19-epoxy-19-oxo-	612	C32H53O3	WILEY229.U																																																																			
4	54	✓	Cholestan-24-ene, 3,12-dihydroxy-, (2)-alpha-, 5-	418	C27H46O3	WILEY229.U																																																																			
5	54	✓	Cholan-24-ic acid, 3,12-dihydroxy-, (2)-alpha-, 5-	392	C24H40O4	WILEY229.U																																																																			
6	54	✓	Ergostane-3,12-diol, (3)-alpha-, 5-beta-, 12-alpha-	418	C28H50O2	WILEY229.U																																																																			
7	53	✓	Cholest-5-en-3-ol, 14-methyl-, acetate, (3)-beta-	442	C30H52O2	WILEY229.U																																																																			
8	53	✓	Stigmata-7,22-dien-3-ol, (3)-beta-, 5-alpha-, 22E	412	C29H48O	WILEY229.U																																																																			
9	53	✓	Ergosta-7,22-dien-3-ol, (3)-beta-, 22E)- (CAS) 5-	398	C28H48O	WILEY229.U																																																																			
<p>54.971</p>	<p>3342</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>64</td><td>✓</td><td>10-acetoxyl-9-antihydroxymethyl ether 55</td><td>324</td><td>C19H28O3</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>60</td><td>✓</td><td>1,4-Bis(trimethylsilyloxy)-2,5-dimethylbenzene 55</td><td>292</td><td>C14H26O2</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>57</td><td>✓</td><td>10-hydroxy-10-acetylphenone trimethyl ether</td><td>324</td><td>C19H28O3</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>47</td><td>✓</td><td>isopropylmethylcyclohexyltriisobutylsiloxane 5</td><td>292</td><td>C17H32O4</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>56</td><td>✓</td><td>1-trimethylsilyloxy-5-trimethylsilyloxyphenol</td><td>296</td><td>C18H24Si2</td><td>WILEY229.U</td></tr> <tr><td>6</td><td>56</td><td>✓</td><td>2-ETHYL-4-O-4,6-TRIMETHYLPYRIDIN-3-YL</td><td>282</td><td>C17H18N2</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>56</td><td>✓</td><td>(4,5-dimethoxy-2-trimethylsilyloxy)trimethylsilyl</td><td>296</td><td>C19H28O3</td><td>WILEY229.U</td></tr> <tr><td>8</td><td>54</td><td>✓</td><td>Stilene, bicyclo[4.2.0]octa-3,7-diene-7,8-diol</td><td>282</td><td>C14H26O2</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>54</td><td>✓</td><td>1-Propanone, 1-(2,4-bis(trimethylsilyloxy)phenyl</td><td>310</td><td>C15H26O3</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>1: 324: 10-acetoxyl-9-antihydroxymethyl ether 55</p> <p>CAS# 90540-96-6 Mol Wt: 324 Serial# 160375</p> <p>Copd Name: 10-acetoxyl-9-antihydroxymethyl ether 55</p> <p>Formula: C19H28O3 SI Class Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	64	✓	10-acetoxyl-9-antihydroxymethyl ether 55	324	C19H28O3	WILEY229.U	2	60	✓	1,4-Bis(trimethylsilyloxy)-2,5-dimethylbenzene 55	292	C14H26O2	WILEY229.U	3	57	✓	10-hydroxy-10-acetylphenone trimethyl ether	324	C19H28O3	WILEY229.U	4	47	✓	isopropylmethylcyclohexyltriisobutylsiloxane 5	292	C17H32O4	WILEY229.U	5	56	✓	1-trimethylsilyloxy-5-trimethylsilyloxyphenol	296	C18H24Si2	WILEY229.U	6	56	✓	2-ETHYL-4-O-4,6-TRIMETHYLPYRIDIN-3-YL	282	C17H18N2	WILEY229.U	7	56	✓	(4,5-dimethoxy-2-trimethylsilyloxy)trimethylsilyl	296	C19H28O3	WILEY229.U	8	54	✓	Stilene, bicyclo[4.2.0]octa-3,7-diene-7,8-diol	282	C14H26O2	WILEY229.U	9	54	✓	1-Propanone, 1-(2,4-bis(trimethylsilyloxy)phenyl	310	C15H26O3	WILEY229.U
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	64	✓	10-acetoxyl-9-antihydroxymethyl ether 55	324	C19H28O3	WILEY229.U																																																																			
2	60	✓	1,4-Bis(trimethylsilyloxy)-2,5-dimethylbenzene 55	292	C14H26O2	WILEY229.U																																																																			
3	57	✓	10-hydroxy-10-acetylphenone trimethyl ether	324	C19H28O3	WILEY229.U																																																																			
4	47	✓	isopropylmethylcyclohexyltriisobutylsiloxane 5	292	C17H32O4	WILEY229.U																																																																			
5	56	✓	1-trimethylsilyloxy-5-trimethylsilyloxyphenol	296	C18H24Si2	WILEY229.U																																																																			
6	56	✓	2-ETHYL-4-O-4,6-TRIMETHYLPYRIDIN-3-YL	282	C17H18N2	WILEY229.U																																																																			
7	56	✓	(4,5-dimethoxy-2-trimethylsilyloxy)trimethylsilyl	296	C19H28O3	WILEY229.U																																																																			
8	54	✓	Stilene, bicyclo[4.2.0]octa-3,7-diene-7,8-diol	282	C14H26O2	WILEY229.U																																																																			
9	54	✓	1-Propanone, 1-(2,4-bis(trimethylsilyloxy)phenyl	310	C15H26O3	WILEY229.U																																																																			
<p>55.021</p>	<p>3344</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>69</td><td>✓</td><td>Stilene, (S)-beta-pregnan-3, alpha-, 6, alpha-ylidene-</td><td>464</td><td>C27H52O2</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>64</td><td>✓</td><td>METHYL COMMATTE B 55</td><td>470</td><td>C31H50O3</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>63</td><td>✓</td><td>A'-Nagammacer-22(22)ene (CAS) Hopane B</td><td>410</td><td>C30H50</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>62</td><td>✓</td><td>Stilene, (S)-19-cyclo-9-beta-ferrocenyl-24-en-3-ol</td><td>436</td><td>C33H50O</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>62</td><td>✓</td><td>METHYL COMMATTE D 55</td><td>486</td><td>C31H50O4</td><td>WILEY229.U</td></tr> <tr><td>6</td><td>62</td><td>✓</td><td>5B-PREGNANE-3A,6A-DIOL TMS 55</td><td>464</td><td>C27H52O2</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>62</td><td>✓</td><td>alpha-selinene 55</td><td>204</td><td>C15H24</td><td>WILEY229.U</td></tr> <tr><td>8</td><td>61</td><td>✓</td><td>Stilene, (S)-beta-5, alpha-(4,4-dimethylcholesterol</td><td>484</td><td>C32H56O</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>61</td><td>✓</td><td>5,19-Cyclolanost-24-en-3-ol, (3)-beta-)- (CAS) C</td><td>426</td><td>C30H50O</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>1: 464: Stilene, (S)-beta-pregnan-3, alpha-, 6, alpha-ylidene-)- (CAS) 5-BETA-PREGNANE-3,ALPHA,6,ALPHA-DIOL TMS 55 3,ALPHA,6,ALPHA-DIHYDROXY-5-BETA-PREGNANE-3,6-TMS 55</p> <p>CAS# 33203-07-7 Mol Wt: 464 Serial# 200699</p> <p>Copd Name: Stilene, (S)-beta-pregnan-3, alpha-, 6, alpha-ylidene-)- (CAS) 5-BETA-PREGNANE-3,ALPHA,6,ALPHA-DIOL TMS 55 3,ALPHA,6,ALPHA-DIHYDROXY-5-BETA-PREGNANE-3,6-TMS 55</p> <p>Formula: C27H52O2 SI2 Class Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	69	✓	Stilene, (S)-beta-pregnan-3, alpha-, 6, alpha-ylidene-	464	C27H52O2	WILEY229.U	2	64	✓	METHYL COMMATTE B 55	470	C31H50O3	WILEY229.U	3	63	✓	A'-Nagammacer-22(22)ene (CAS) Hopane B	410	C30H50	WILEY229.U	4	62	✓	Stilene, (S)-19-cyclo-9-beta-ferrocenyl-24-en-3-ol	436	C33H50O	WILEY229.U	5	62	✓	METHYL COMMATTE D 55	486	C31H50O4	WILEY229.U	6	62	✓	5B-PREGNANE-3A,6A-DIOL TMS 55	464	C27H52O2	WILEY229.U	7	62	✓	alpha-selinene 55	204	C15H24	WILEY229.U	8	61	✓	Stilene, (S)-beta-5, alpha-(4,4-dimethylcholesterol	484	C32H56O	WILEY229.U	9	61	✓	5,19-Cyclolanost-24-en-3-ol, (3)-beta-)- (CAS) C	426	C30H50O	WILEY229.U
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	69	✓	Stilene, (S)-beta-pregnan-3, alpha-, 6, alpha-ylidene-	464	C27H52O2	WILEY229.U																																																																			
2	64	✓	METHYL COMMATTE B 55	470	C31H50O3	WILEY229.U																																																																			
3	63	✓	A'-Nagammacer-22(22)ene (CAS) Hopane B	410	C30H50	WILEY229.U																																																																			
4	62	✓	Stilene, (S)-19-cyclo-9-beta-ferrocenyl-24-en-3-ol	436	C33H50O	WILEY229.U																																																																			
5	62	✓	METHYL COMMATTE D 55	486	C31H50O4	WILEY229.U																																																																			
6	62	✓	5B-PREGNANE-3A,6A-DIOL TMS 55	464	C27H52O2	WILEY229.U																																																																			
7	62	✓	alpha-selinene 55	204	C15H24	WILEY229.U																																																																			
8	61	✓	Stilene, (S)-beta-5, alpha-(4,4-dimethylcholesterol	484	C32H56O	WILEY229.U																																																																			
9	61	✓	5,19-Cyclolanost-24-en-3-ol, (3)-beta-)- (CAS) C	426	C30H50O	WILEY229.U																																																																			

<p>55.228</p>	<p>3355</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>87</td><td>PF</td><td>METHYL COMMATE 1-SS</td><td>353</td><td>C12H15O4</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>85</td><td></td><td>NORUNS-12-ENE SS</td><td>396</td><td>C29H48</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>83</td><td></td><td>METHYL COMMATE C-SS</td><td>405</td><td>C31H50O4</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>81</td><td></td><td>4,4,6a,8a,11,12,14a-Octamethyl-1,4,4a,5,6</td><td>424</td><td>C30H40O</td><td>NIST08.LIB</td></tr> <tr><td>5</td><td>81</td><td></td><td>4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6</td><td>424</td><td>C30H40O</td><td>NIST107.LIB</td></tr> <tr><td>6</td><td>80</td><td></td><td>Uns-12-en-3-ol, acetate, (3 beta) - SS Uns-12-e</td><td>468</td><td>C32H52O2</td><td>NIST107.LIB</td></tr> <tr><td>7</td><td>80</td><td></td><td>Uns-12-en-3-ol, acetate, (3 beta) - SS Uns-12-e</td><td>468</td><td>C32H52O2</td><td>NIST08.LIB</td></tr> <tr><td>8</td><td>79</td><td></td><td>3-METHYLNURS-12-ENE SS</td><td>424</td><td>C30H48O</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>79</td><td>PF</td><td>Silene, trimethyl(3 beta)olean-12-en-3-yl(ox)yl</td><td>490</td><td>C33H50O5</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>9: 490: Silene, trimethyl(3 beta)olean-12-en-3-yl(ox)yl (CAS) beta-Amyrin trimethyl ether SS Silene, trimethyl(olean-12-en-3 beta-yl)oxyl SS</p> <p>CAS# 1721-67-1 Mol Wt 490 Serial# 214951</p> <p>Comp Name: Silene, trimethyl(3 beta)olean-12-en-3-yl(ox)yl (CAS) beta-Amyrin trimethyl ether SS Silene, trimethyl(olean-12-en-3 beta-yl)oxyl SS</p> <p>Formula: C33H50O5 Clasi Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	87	PF	METHYL COMMATE 1-SS	353	C12H15O4	WILEY229.U	2	85		NORUNS-12-ENE SS	396	C29H48	WILEY229.U	3	83		METHYL COMMATE C-SS	405	C31H50O4	WILEY229.U	4	81		4,4,6a,8a,11,12,14a-Octamethyl-1,4,4a,5,6	424	C30H40O	NIST08.LIB	5	81		4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6	424	C30H40O	NIST107.LIB	6	80		Uns-12-en-3-ol, acetate, (3 beta) - SS Uns-12-e	468	C32H52O2	NIST107.LIB	7	80		Uns-12-en-3-ol, acetate, (3 beta) - SS Uns-12-e	468	C32H52O2	NIST08.LIB	8	79		3-METHYLNURS-12-ENE SS	424	C30H48O	WILEY229.U	9	79	PF	Silene, trimethyl(3 beta)olean-12-en-3-yl(ox)yl	490	C33H50O5	WILEY229.U
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	87	PF	METHYL COMMATE 1-SS	353	C12H15O4	WILEY229.U																																																																			
2	85		NORUNS-12-ENE SS	396	C29H48	WILEY229.U																																																																			
3	83		METHYL COMMATE C-SS	405	C31H50O4	WILEY229.U																																																																			
4	81		4,4,6a,8a,11,12,14a-Octamethyl-1,4,4a,5,6	424	C30H40O	NIST08.LIB																																																																			
5	81		4,4,6a,8a,11,12,14b-Octamethyl-1,4,4a,5,6	424	C30H40O	NIST107.LIB																																																																			
6	80		Uns-12-en-3-ol, acetate, (3 beta) - SS Uns-12-e	468	C32H52O2	NIST107.LIB																																																																			
7	80		Uns-12-en-3-ol, acetate, (3 beta) - SS Uns-12-e	468	C32H52O2	NIST08.LIB																																																																			
8	79		3-METHYLNURS-12-ENE SS	424	C30H48O	WILEY229.U																																																																			
9	79	PF	Silene, trimethyl(3 beta)olean-12-en-3-yl(ox)yl	490	C33H50O5	WILEY229.U																																																																			
<p>55.294</p>	<p>3358</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>81</td><td>PF</td><td>Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl</td><td>490</td><td>C33H50O5</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>81</td><td></td><td>Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl</td><td>490</td><td>C33H50O5</td><td>NIST107.LIB</td></tr> <tr><td>3</td><td>80</td><td></td><td>Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl</td><td>490</td><td>C33H50O5</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>74</td><td></td><td>Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl</td><td>490</td><td>C33H50O5</td><td>NIST107.LIB</td></tr> <tr><td>5</td><td>74</td><td></td><td>Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl</td><td>490</td><td>C33H50O5</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>74</td><td></td><td>Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl</td><td>490</td><td>C33H50O5</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>71</td><td></td><td>Lanosta-8,24-dien-3-ol, acetate, (3 beta) -</td><td>468</td><td>C32H52O2</td><td>NIST107.LIB</td></tr> <tr><td>8</td><td>71</td><td></td><td>Lanosta-8,24-dien-3-ol, acetate, (3 beta) -</td><td>468</td><td>C32H52O2</td><td>NIST08.LIB</td></tr> <tr><td>9</td><td>70</td><td></td><td>Silene, (3 beta)cyclo-lanosta-24-en-3 beta</td><td>490</td><td>C33H50O5</td><td>NIST08.LIB</td></tr> </tbody> </table> <p>Target</p> <p>1: 498: Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yltrimethyl SS 3(1)trimethyl(ox)yl(ox)lanosta-8,24-diene SS</p> <p>CAS# 55493-04-0 Mol Wt 490 Serial# 104519</p> <p>Comp Name: Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yltrimethyl SS 3(1)trimethyl(ox)yl(ox)lanosta-8,24-diene SS</p> <p>Formula: C33H50O5 Clasi Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	81	PF	Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl	490	C33H50O5	NIST08.LIB	2	81		Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl	490	C33H50O5	NIST107.LIB	3	80		Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl	490	C33H50O5	WILEY229.U	4	74		Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl	490	C33H50O5	NIST107.LIB	5	74		Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl	490	C33H50O5	NIST08.LIB	6	74		Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl	490	C33H50O5	WILEY229.U	7	71		Lanosta-8,24-dien-3-ol, acetate, (3 beta) -	468	C32H52O2	NIST107.LIB	8	71		Lanosta-8,24-dien-3-ol, acetate, (3 beta) -	468	C32H52O2	NIST08.LIB	9	70		Silene, (3 beta)cyclo-lanosta-24-en-3 beta	490	C33H50O5	NIST08.LIB
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	81	PF	Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl	490	C33H50O5	NIST08.LIB																																																																			
2	81		Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl	490	C33H50O5	NIST107.LIB																																																																			
3	80		Silene, (3 beta)lanosta-8,24-dien-3-yl(ox)yl	490	C33H50O5	WILEY229.U																																																																			
4	74		Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl	490	C33H50O5	NIST107.LIB																																																																			
5	74		Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl	490	C33H50O5	NIST08.LIB																																																																			
6	74		Silene, (3 beta)lanosta-9(11),24-dien-3-yl(ox)yl	490	C33H50O5	WILEY229.U																																																																			
7	71		Lanosta-8,24-dien-3-ol, acetate, (3 beta) -	468	C32H52O2	NIST107.LIB																																																																			
8	71		Lanosta-8,24-dien-3-ol, acetate, (3 beta) -	468	C32H52O2	NIST08.LIB																																																																			
9	70		Silene, (3 beta)cyclo-lanosta-24-en-3 beta	490	C33H50O5	NIST08.LIB																																																																			
<p>55.525</p>	<p>3370</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>63</td><td>PF</td><td>2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS</td><td>197</td><td>C13H27N</td><td>WILEY229.U</td></tr> <tr><td>2</td><td>63</td><td></td><td>2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS</td><td>197</td><td>C13H27N</td><td>WILEY229.U</td></tr> <tr><td>3</td><td>66</td><td></td><td>2,4-DIMETHYL-5H-PYRIDO(2,3-B)INDOLE S</td><td>196</td><td>C13H12N2</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>66</td><td></td><td>CAMPHORTRIMETHYLSILYLBIOMOL ETHER</td><td>224</td><td>C13H24O5</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>64</td><td></td><td>2,4-dimethyl-5-ethyl-2H-imidazole SS</td><td>196</td><td>C13H12N2</td><td>WILEY229.U</td></tr> <tr><td>6</td><td>64</td><td></td><td>2,2-dimethyl-5-ethyl-2H-imidazole SS</td><td>226</td><td>C15H20N2</td><td>WILEY229.U</td></tr> <tr><td>7</td><td>64</td><td></td><td>O-TRIMETHYLSILYL-NITROBENZENE SS S</td><td>211</td><td>C9H13N O3</td><td>WILEY229.U</td></tr> <tr><td>8</td><td>63</td><td></td><td>1-(O-CYANO-2-METHYL-4-P-METHYLPHEN</td><td>196</td><td>C13H12N2</td><td>WILEY229.U</td></tr> <tr><td>9</td><td>63</td><td></td><td>2,5,6,7-Tetrahydrobenzo[1,9-b]Luran SS</td><td>196</td><td>C14H12O</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>1: 197: 2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS</p> <p>CAS# 82144-98-6 Mol Wt 197 Serial# 64973</p> <p>Comp Name: 2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS</p> <p>Formula: C13H27N Clasi Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	63	PF	2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS	197	C13H27N	WILEY229.U	2	63		2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS	197	C13H27N	WILEY229.U	3	66		2,4-DIMETHYL-5H-PYRIDO(2,3-B)INDOLE S	196	C13H12N2	WILEY229.U	4	66		CAMPHORTRIMETHYLSILYLBIOMOL ETHER	224	C13H24O5	WILEY229.U	5	64		2,4-dimethyl-5-ethyl-2H-imidazole SS	196	C13H12N2	WILEY229.U	6	64		2,2-dimethyl-5-ethyl-2H-imidazole SS	226	C15H20N2	WILEY229.U	7	64		O-TRIMETHYLSILYL-NITROBENZENE SS S	211	C9H13N O3	WILEY229.U	8	63		1-(O-CYANO-2-METHYL-4-P-METHYLPHEN	196	C13H12N2	WILEY229.U	9	63		2,5,6,7-Tetrahydrobenzo[1,9-b]Luran SS	196	C14H12O	WILEY229.U
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	63	PF	2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS	197	C13H27N	WILEY229.U																																																																			
2	63		2,2-Dibutylpiperidine SS Piperidine, 2,2-dibutyl SS	197	C13H27N	WILEY229.U																																																																			
3	66		2,4-DIMETHYL-5H-PYRIDO(2,3-B)INDOLE S	196	C13H12N2	WILEY229.U																																																																			
4	66		CAMPHORTRIMETHYLSILYLBIOMOL ETHER	224	C13H24O5	WILEY229.U																																																																			
5	64		2,4-dimethyl-5-ethyl-2H-imidazole SS	196	C13H12N2	WILEY229.U																																																																			
6	64		2,2-dimethyl-5-ethyl-2H-imidazole SS	226	C15H20N2	WILEY229.U																																																																			
7	64		O-TRIMETHYLSILYL-NITROBENZENE SS S	211	C9H13N O3	WILEY229.U																																																																			
8	63		1-(O-CYANO-2-METHYL-4-P-METHYLPHEN	196	C13H12N2	WILEY229.U																																																																			
9	63		2,5,6,7-Tetrahydrobenzo[1,9-b]Luran SS	196	C14H12O	WILEY229.U																																																																			
<p>55.545</p>	<p>3371</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>72</td><td>PF</td><td>9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)</td><td>440</td><td>C31H52O</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>72</td><td></td><td>9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)</td><td>440</td><td>C31H52O</td><td>NIST107.LIB</td></tr> <tr><td>3</td><td>73</td><td></td><td>9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)</td><td>440</td><td>C31H52O</td><td>WILEY229.U</td></tr> <tr><td>4</td><td>72</td><td></td><td>9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)</td><td>440</td><td>C31H52O</td><td>WILEY229.U</td></tr> <tr><td>5</td><td>72</td><td></td><td>9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)</td><td>440</td><td>C31H52O</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>73</td><td></td><td>9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)</td><td>440</td><td>C31H52O</td><td>NIST107.LIB</td></tr> <tr><td>7</td><td>73</td><td></td><td>9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol S</td><td>444</td><td>C30H52O2</td><td>NIST08.LIB</td></tr> <tr><td>8</td><td>73</td><td></td><td>9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol S</td><td>444</td><td>C30H52O2</td><td>NIST107.LIB</td></tr> <tr><td>9</td><td>73</td><td></td><td>9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol C</td><td>444</td><td>C30H52O2</td><td>WILEY229.U</td></tr> </tbody> </table> <p>Target</p> <p>1: 440: 9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta) SS 9,19-Cyclo-9 beta-lanostan-3 beta-ol, 24-methylene SS 24-Methylene-cyclo-lanostan SS</p> <p>CAS# 1449-09-0 Mol Wt 440 Serial# 97920</p> <p>Comp Name: 9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta) SS 9,19-Cyclo-9 beta-lanostan-3 beta-ol, 24-methylene SS 24-Methylene-cyclo-lanostan SS</p> <p>Formula: C31H52O Clasi Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	72	PF	9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	NIST08.LIB	2	72		9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	NIST107.LIB	3	73		9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.U	4	72		9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.U	5	72		9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	NIST08.LIB	6	73		9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	NIST107.LIB	7	73		9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol S	444	C30H52O2	NIST08.LIB	8	73		9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol S	444	C30H52O2	NIST107.LIB	9	73		9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol C	444	C30H52O2	WILEY229.U
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	72	PF	9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	NIST08.LIB																																																																			
2	72		9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	NIST107.LIB																																																																			
3	73		9,19-Cyclolanostan-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.U																																																																			
4	72		9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.U																																																																			
5	72		9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	NIST08.LIB																																																																			
6	73		9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	NIST107.LIB																																																																			
7	73		9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol S	444	C30H52O2	NIST08.LIB																																																																			
8	73		9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol S	444	C30H52O2	NIST107.LIB																																																																			
9	73		9,19-Cyclo-9 beta-lanostane-3 beta, 25-diol C	444	C30H52O2	WILEY229.U																																																																			



<p>55.852</p>	<p>3386</p>	<p>-</p>	<p>Target</p> <p>2: 430: TETRAHYDRODAMMARADIENOL 55</p> <p>CAS# 0-00-0 Mol Wt: 430 Serial#: 202962              Cmpd Name: TETRAHYDRODAMMARADIENOL 55              Formula: C30H54O Class Flag: No Class Flags</p>
<p>55.988</p>	<p>3393</p>	<p>-</p>	<p>Target</p> <p>1: 724: Ergostane-5,25-diol, 3,6,12-tri[(trimethylsilyloxy), 25-acetate, (3 beta, 5 alpha, 6 beta, 12 beta)]- [CAS]</p> <p>CAS# 86053-01-1 Mol Wt: 724 Serial#: 229908              Cmpd Name: Ergostane-5,25-diol, 3,6,12-tri[(trimethylsilyloxy), 25-acetate, (3 beta, 5 alpha, 6 beta, 12 beta)]- [CAS]              Formula: C39H76O6Si3 Class Flag: No Class Flags</p>
<p>56.223</p>	<p>3405</p>	<p>-</p>	<p>Target</p> <p>1: 490: Sítane, [3 beta] Hancosta-8,24-dien-3-yl(ox)trimethyl- 55</p> <p>CAS# 55433-04-0 Mol Wt: 490 Serial#: 102202              Cmpd Name: Sítane, [3 beta] Hancosta-8,24-dien-3-yl(ox)trimethyl- 55              Formula: C33H58O5 Class Flag: No Class Flags</p>
<p>56.315</p>	<p>3410</p>	<p>-</p>	<p>Target</p> <p>1: 460: 5,19-Cyclolanost-24-en-3-ol, acetate 55</p> <p>CAS# 124094-10-6 Mol Wt: 460 Serial#: 100352              Cmpd Name: 5,19-Cyclolanost-24-en-3-ol, acetate 55              Formula: C32H52O2 Class Flag: No Class Flags</p>

<p>56.479</p>	<p>3419</p>	<p>-</p>	
<p>56.725</p>	<p>3431</p>	<p>3432 GDM</p>	
<p>56.758</p>	<p>3433</p>	<p>-</p>	
<p>56.835</p>	<p>3437</p>	<p>-</p>	

<p>57.418</p> <p>3467</p>	<p>-</p>	<p>1: 498: Silene, [E]-beta-hionoside-8,24-dien-3-yl(ox)imethyl-3-3-Timethylsilyloxy)hionoside-8,24-diene # 55</p> <p>CAS# 85433-04-0 Mol Wt: 498 Serial# 104519</p> <p>Cmpd Name: Silene, [E]-beta-hionoside-8,24-dien-3-yl(ox)imethyl-3-3-Timethylsilyloxy)hionoside-8,24-diene # 55</p> <p>Formula: C39H58O5</p> <p>Class Flag: No Class Flags.</p>
<p>57.688</p> <p>3482</p>	<p>-</p>	<p>1: 324: Olivetol, bis(trimethylsilyl) ether</p> <p>CAS# 0-00-0 Mol Wt: 324 Serial# 120432</p> <p>Cmpd Name: Olivetol, bis(trimethylsilyl) ether</p> <p>Formula: C17H32O2Si2</p> <p>Class Flag: No Class Flags.</p>
<p>57.814</p> <p>3488</p>	<p>-</p>	<p>3: 426: Friedelin-3-one # Friedelin # D-A-Friedelin-3-one # Friedelin # Friedelin # 4,4a,6b,8a,11,11,12b,14a-Octamethylcyclohexa-3,2H-pyrene # 5</p> <p>CAS# 559-74-0 Mol Wt: 426 Serial# 174629</p> <p>Cmpd Name: Friedelin-3-one # Friedelin # D-A-Friedelin-3-one # Friedelin # Friedelin # 4,4a,6b,8a,11,11,12b,14a-Octamethylcyclohexa-3,2H-pyrene # 5</p> <p>Formula: C30H50</p> <p>Class Flag: No Class Flags.</p>
<p>58.04</p> <p>3500</p>	<p>-</p>	<p>13: 354: Dodecane, 1,1'-oxybis-[(CAS)]DIDODECANE ETHER # D1N-DODECYL ETHER # Dodecyl ether # Dilauryl ether # Didodecyl ether # 5</p> <p>CAS# 4542-57-8 Mol Wt: 354 Serial# 176136</p> <p>Cmpd Name: Dodecane, 1,1'-oxybis-[(CAS)]DIDODECANE ETHER # D1N-DODECYL ETHER # Dodecyl ether # Dilauryl ether # Didodecyl ether # 5</p> <p>Formula: C24H50O</p> <p>Class Flag: No Class Flags.</p>



<p>58.697</p>	<p>3536</p>	<p>3529</p>	<p>Target</p> <p>1: 538: Slsane, (dibutacryloyloxy)dimethyl</p> <p>CAS: 0-00-0 Mol Wt: 538 Smiles: 188885              Cpnd Name: Slsane, (dibutacryloyloxy)dimethyl              Formula: C29H47O5 Class Flag: No Class Flags</p>
<p>60.434</p>	<p>3630</p>	<p>-</p>	<p>Target</p> <p>1: 468: Hexanoic acid, trimethyl ester</p> <p>CAS: 0-00-0 Mol Wt: 468 Smiles: 181479              Cpnd Name: Hexanoic acid, trimethyl ester              Formula: C28H50O5 Class Flag: No Class Flags</p>
<p>61.3</p>	<p>3678</p>	<p>-</p>	<p>Target</p> <p>1: 268: 2-METHYLBRESORCINOL, DITMS</p> <p>CAS: 0-00-0 Mol Wt: 268 Smiles: 122609              Cpnd Name: 2-METHYLBRESORCINOL, DITMS              Formula: C13H24O2Si2 Class Flag: No Class Flags</p>
<p>62.278</p>	<p>3733</p>	<p>3726</p>	<p>Target</p> <p>1: 566: Slsane, trimethyltetraacetyloxy</p> <p>CAS: 0-00-0 Mol Wt: 566 Smiles: 188057              Cpnd Name: Slsane, trimethyltetraacetyloxy              Formula: C37H70O5 Class Flag: No Class Flags</p>

<p>64.001</p>	<p>3827</p>	<p>-</p>	<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>75</td> <td>C</td> <td>Hexacosanoic acid, trimethylsilyl ester</td> <td>458</td> <td>C<sub>28</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>75</td> <td></td> <td>TRIMETHYLSILYL ESTER OF TETRACOSA</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>WILEY225.LI</td> </tr> <tr> <td>3</td> <td>75</td> <td></td> <td>Tetracosanoic acid, trimethylsilyl ester S5</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>75</td> <td></td> <td>Tetracosanoic acid, trimethylsilyl ester S5 Trim</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>74</td> <td></td> <td>Pentacosanoic acid, trimethylsilyl ester</td> <td>454</td> <td>C<sub>28</sub>H<sub>58</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>74</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester S5 Bear</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>74</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester S5 Bear</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>74</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>NIST121.LIB</td> </tr> <tr> <td>9</td> <td>74</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester (CAS) 5</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>WILEY225.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1 : 469 : Hexacosanoic acid, trimethylsilyl ester</p> <p>CAS# 0 00 0 Mol Wt 460 Sear# 101479          Capd Name: Hexacosanoic acid, trimethylsilyl ester          Formula: C<sub>28</sub>H<sub>56</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	#	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	75	C	Hexacosanoic acid, trimethylsilyl ester	458	C <sub>28</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB	2	75		TRIMETHYLSILYL ESTER OF TETRACOSA	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	WILEY225.LI	3	75		Tetracosanoic acid, trimethylsilyl ester S5	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB	4	75		Tetracosanoic acid, trimethylsilyl ester S5 Trim	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB	5	74		Pentacosanoic acid, trimethylsilyl ester	454	C <sub>28</sub> H <sub>58</sub> O <sub>2</sub>	NIST08.LIB	6	74		Octadecanoic acid, trimethylsilyl ester S5 Bear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST08.LIB	7	74		Octadecanoic acid, trimethylsilyl ester S5 Bear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST107.LIB	8	74		Octadecanoic acid, trimethylsilyl ester	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST121.LIB	9	74		Octadecanoic acid, trimethylsilyl ester (CAS) 5	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY225.LI
#	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	75	C	Hexacosanoic acid, trimethylsilyl ester	458	C <sub>28</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB																																																																			
2	75		TRIMETHYLSILYL ESTER OF TETRACOSA	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	WILEY225.LI																																																																			
3	75		Tetracosanoic acid, trimethylsilyl ester S5	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB																																																																			
4	75		Tetracosanoic acid, trimethylsilyl ester S5 Trim	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB																																																																			
5	74		Pentacosanoic acid, trimethylsilyl ester	454	C <sub>28</sub> H <sub>58</sub> O <sub>2</sub>	NIST08.LIB																																																																			
6	74		Octadecanoic acid, trimethylsilyl ester S5 Bear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST08.LIB																																																																			
7	74		Octadecanoic acid, trimethylsilyl ester S5 Bear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST107.LIB																																																																			
8	74		Octadecanoic acid, trimethylsilyl ester	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST121.LIB																																																																			
9	74		Octadecanoic acid, trimethylsilyl ester (CAS) 5	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY225.LI																																																																			

**Anexo 4:** Identificação dos constituintes do extrato hexânico derivado (TMS) de folhas de cana-de-açúcar por comparação dos espectros de massas com dados das bibliotecas Wiley7 e Nist pelo software GCMS solutions Ver. 2.61

GC-MS			Tabela de extrato hexânico - folhas de cana-de-açúcar																																																																						
Tr	IR Cal.	IR Lit.																																																																							
11.256	1650	1643	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>IR</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>91</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester \$S\$</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>NIST02.LIB</td> </tr> <tr> <td>2</td> <td>91</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester (CAS)</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>89</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>89</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester (CAS) LA</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>89</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>89</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>NIST171.LIB</td> </tr> <tr> <td>7</td> <td>87</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>87</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet</td> <td>272</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target: Base Peak: 73/ 10,000</p> <p>1: 272: Dodecanoic acid, trimethylsilyl ester \$S\$ Trimethylsilyl laurate \$S\$</p> <p>CAS#: 55520-95-1 Mol Wt: 272 Serial#: 22035          Cmpd Name: Dodecanoic acid, trimethylsilyl ester \$S\$ Trimethylsilyl laurate \$S\$          Formula: C<sub>15</sub>H<sub>30</sub>O<sub>2</sub> Class Flag: No Class Flags.</p>	IR	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	91		Dodecanoic acid, trimethylsilyl ester \$S\$	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST02.LIB	2	91		Dodecanoic acid, trimethylsilyl ester (CAS)	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	WILEY229.LI	3	89		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB	4	89		Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	WILEY229.LI	5	89		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB	6	89		Dodecanoic acid, trimethylsilyl ester	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST171.LIB	7	87		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB	8	87		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB							
IR	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																			
1	91		Dodecanoic acid, trimethylsilyl ester \$S\$	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST02.LIB																																																																			
2	91		Dodecanoic acid, trimethylsilyl ester (CAS)	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	WILEY229.LI																																																																			
3	89		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB																																																																			
4	89		Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	89		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB																																																																			
6	89		Dodecanoic acid, trimethylsilyl ester	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST171.LIB																																																																			
7	87		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB																																																																			
8	87		Dodecanoic acid, trimethylsilyl ester \$S\$ Trimet	272	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	NIST08.LIB																																																																			
12.569	1696		<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>IR</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>79</td> <td></td> <td>Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Su</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>79</td> <td></td> <td>Octanedioic acid, bis(trimethylsilyl) ester (CAS)</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>79</td> <td></td> <td>Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Su</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>79</td> <td></td> <td>Octanedioic acid, bis(trimethylsilyl) ester</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>NIST171.LIB</td> </tr> <tr> <td>5</td> <td>78</td> <td></td> <td>Octanedioic acid, bis(trimethylsilyl) ester (CAS)</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>78</td> <td></td> <td>Heptanedioic acid, 4-methyl-, bis(trimethylsilyl)</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>78</td> <td></td> <td>BIS(TRIMETHYLSILYL)ESTER OF 3-METHY</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>78</td> <td></td> <td>Heptanedioic acid, 3-methyl-, bis(trimethylsilyl)</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>78</td> <td></td> <td>BIS(TRIMETHYLSILYL)ESTER OF 4-METHY</td> <td>318</td> <td>C<sub>14</sub>H<sub>30</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target: Base Peak: 73/ 10,000</p> <p>1: 318: Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Suberic acid trimethylsilyl ester \$S\$ Suberic acid (Im) \$S\$ Suberic acid, di(trimethylsilyl) ester \$S\$ Bis(trimethylsilyl) suberate \$S\$</p> <p>CAS#: 83199-48-0 Mol Wt: 318 Serial#: 124342          Cmpd Name: Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Suberic acid trimethylsilyl ester \$S\$ Suberic acid (Im) \$S\$ Suberic acid, di(trimethylsilyl) ester \$S\$ Bis(trimethylsilyl) suberate \$S\$          Formula: C<sub>14</sub>H<sub>30</sub>O<sub>4</sub> Class Flag: No Class Flags.</p>	IR	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	79		Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Su	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST08.LIB	2	79		Octanedioic acid, bis(trimethylsilyl) ester (CAS)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	3	79		Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Su	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST08.LIB	4	79		Octanedioic acid, bis(trimethylsilyl) ester	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST171.LIB	5	78		Octanedioic acid, bis(trimethylsilyl) ester (CAS)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	6	78		Heptanedioic acid, 4-methyl-, bis(trimethylsilyl)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST08.LIB	7	78		BIS(TRIMETHYLSILYL)ESTER OF 3-METHY	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI	8	78		Heptanedioic acid, 3-methyl-, bis(trimethylsilyl)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST107.LIB	9	78		BIS(TRIMETHYLSILYL)ESTER OF 4-METHY	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI
IR	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																			
1	79		Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Su	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST08.LIB																																																																			
2	79		Octanedioic acid, bis(trimethylsilyl) ester (CAS)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
3	79		Octanedioic acid, bis(trimethylsilyl) ester \$S\$ Su	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST08.LIB																																																																			
4	79		Octanedioic acid, bis(trimethylsilyl) ester	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST171.LIB																																																																			
5	78		Octanedioic acid, bis(trimethylsilyl) ester (CAS)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
6	78		Heptanedioic acid, 4-methyl-, bis(trimethylsilyl)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST08.LIB																																																																			
7	78		BIS(TRIMETHYLSILYL)ESTER OF 3-METHY	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
8	78		Heptanedioic acid, 3-methyl-, bis(trimethylsilyl)	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	NIST107.LIB																																																																			
9	78		BIS(TRIMETHYLSILYL)ESTER OF 4-METHY	318	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub>	WILEY229.LI																																																																			
14.145	1749	1735	<p>Report View Compound Info Process Help</p> <table border="1"> <thead> <tr> <th>IR</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>82</td> <td>78</td> <td></td> <td>1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>82</td> <td>78</td> <td></td> <td>1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>NIST171.LIB</td> </tr> <tr> <td>82</td> <td>78</td> <td></td> <td>TRIS (TRIMETHYLSILYL) ESTER OF ACONI</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>NIST171.LIB</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>NIST171.LIB</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>CIS-ACONITIC ACID-TRITMS \$S\$ 1-Propene-1</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>TRIS (TRIMETHYLSILYL) ESTER OF ACONI</td> <td>390</td> <td>C<sub>15</sub>H<sub>30</sub>O<sub>6</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target: Base Peak: 73/ 10,000</p> <p>0: 1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester, (Z)- \$S\$ cis-Aconitic acid (Im) \$S\$ Tris(trimethylsilyl) (1E)-1-propene-1,2,3-tricarboxylate \$S\$</p> <p>Name: 1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester, (Z)- \$S\$ cis-Aconitic acid (Im) \$S\$ Tris(trimethylsilyl) (1E)-1-propene-1,2,3-tricarboxylate \$S\$          #: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub> Class Flag: No Class Flags.</p>	IR	Similar	Flags	Compound Name	Mol Wt	Formula	Library	82	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST08.LIB	82	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST171.LIB	82	78		TRIS (TRIMETHYLSILYL) ESTER OF ACONI	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	WILEY229.LI	78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST107.LIB	78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST08.LIB	78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST171.LIB	78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST171.LIB	78	78		CIS-ACONITIC ACID-TRITMS \$S\$ 1-Propene-1	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	WILEY229.LI	78	78		TRIS (TRIMETHYLSILYL) ESTER OF ACONI	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	WILEY229.LI
IR	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																			
82	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST08.LIB																																																																			
82	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST171.LIB																																																																			
82	78		TRIS (TRIMETHYLSILYL) ESTER OF ACONI	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	WILEY229.LI																																																																			
78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST107.LIB																																																																			
78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST08.LIB																																																																			
78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST171.LIB																																																																			
78	78		1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	NIST171.LIB																																																																			
78	78		CIS-ACONITIC ACID-TRITMS \$S\$ 1-Propene-1	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	WILEY229.LI																																																																			
78	78		TRIS (TRIMETHYLSILYL) ESTER OF ACONI	390	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub>	WILEY229.LI																																																																			

# ANEXOS

<p><b>16.376</b></p>	<p><b>1822</b></p>	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>84</td> <td>C</td> <td>Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-[[trimethylsilyloxy]oxy]-, bis(trimethylsilyloxy) ester</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>84</td> <td>C</td> <td>ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>84</td> <td>C</td> <td>Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>83</td> <td>C</td> <td>1,2,3-Propanetricarboxylic acid, 2(trimethylsilyloxy)-</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>83</td> <td>C</td> <td>ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>83</td> <td>C</td> <td>1,2,3-Propanetricarboxylic acid, 2(trimethylsilyloxy)-</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>82</td> <td>C</td> <td>ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>82</td> <td>C</td> <td>Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>82</td> <td>C</td> <td>Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-</td> <td>480</td> <td>C<sub>18</sub>H<sub>40</sub>O<sub>7</sub></td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target: Base Peak: 73/ 10,000</p> <p>1: 480: Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-[[trimethylsilyloxy]oxy]-, bis(trimethylsilyloxy) ester SS 1,2,3-Propanetricarboxylic acid, 1-[[trimethylsilyloxy]oxy]-, bis(trimethylsilyloxy) ester SS 1,5-Bis(trimethylsilyloxy)-2,3-dideoxy-4-O-(trimethylsilyl)-</p> <p>CAS# 000737-02-1 Mol Wt: 480 Serial#: 182714</p> <p>Comp Name: Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-[[trimethylsilyloxy]oxy]-, bis(trimethylsilyloxy) ester SS 1,2,3-Propanetricarboxylic acid, 1-[[trimethylsilyloxy]oxy]-, bis(trimethylsilyloxy) ester SS 1,5-Bis(trimethylsilyloxy)-2,3-dideoxy-4-O-(trimethylsilyl)-</p> <p>Formula: C<sub>18</sub>H<sub>40</sub>O<sub>7</sub> Class Flag: No Class Flag</p>	Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	84	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-[[trimethylsilyloxy]oxy]-, bis(trimethylsilyloxy) ester	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB	2	84	C	ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	WILEY229.LI	3	84	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB	4	83	C	1,2,3-Propanetricarboxylic acid, 2(trimethylsilyloxy)-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB	5	83	C	ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	WILEY229.LI	6	83	C	1,2,3-Propanetricarboxylic acid, 2(trimethylsilyloxy)-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB	7	82	C	ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	WILEY229.LI	8	82	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB	9	82	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB
Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																		
1	84	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-[[trimethylsilyloxy]oxy]-, bis(trimethylsilyloxy) ester	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB																																																																		
2	84	C	ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	WILEY229.LI																																																																		
3	84	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB																																																																		
4	83	C	1,2,3-Propanetricarboxylic acid, 2(trimethylsilyloxy)-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB																																																																		
5	83	C	ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	WILEY229.LI																																																																		
6	83	C	1,2,3-Propanetricarboxylic acid, 2(trimethylsilyloxy)-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB																																																																		
7	82	C	ISOCITRIC ACID-TETRAHYMS SS ISOCITRIC	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	WILEY229.LI																																																																		
8	82	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB																																																																		
9	82	C	Pentanoic acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-	480	C <sub>18</sub> H <sub>40</sub> O <sub>7</sub>	NIST08.LIB																																																																		
<p><b>16.820</b></p>	<p><b>1836</b></p>	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>87</td> <td>C</td> <td>NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS</td> <td>278</td> <td>C<sub>20</sub>H<sub>38</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>87</td> <td>C</td> <td>24-Hexadecene-1-ol, 3,7,11,15-tetramethyl-, [E]</td> <td>278</td> <td>C<sub>20</sub>H<sub>40</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>88</td> <td>C</td> <td>NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS</td> <td>278</td> <td>C<sub>20</sub>H<sub>38</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>88</td> <td>C</td> <td>3,7,11,15-Tetramethyl-2-hexadecene-1-ol SS</td> <td>296</td> <td>C<sub>20</sub>H<sub>40</sub>O</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>88</td> <td>C</td> <td>3,7,11,15-Tetramethyl-2-hexadecene-1-ol SS (2)</td> <td>296</td> <td>C<sub>20</sub>H<sub>40</sub>O</td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>87</td> <td>C</td> <td>Pentadecanal- SS</td> <td>226</td> <td>C<sub>15</sub>H<sub>30</sub>O</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>87</td> <td>C</td> <td>Pentadecanal- SS</td> <td>226</td> <td>C<sub>15</sub>H<sub>30</sub>O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>87</td> <td>C</td> <td>Oxane, tetradecyl- SS Hexadecane, 1,2-epoxi</td> <td>240</td> <td>C<sub>16</sub>H<sub>32</sub>O</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>87</td> <td>C</td> <td>Oxane, tetradecyl-</td> <td>240</td> <td>C<sub>16</sub>H<sub>32</sub>O</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target: Base Peak: 69/ 10,000</p> <p>1: 278: NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS</p> <p>CAS# 0-00-0 Mol Wt: 278 Serial#: 130563</p> <p>Comp Name: NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS</p> <p>Formula: C<sub>20</sub>H<sub>38</sub> Class Flag: No Class Flag</p>	Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	87	C	NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS	278	C <sub>20</sub> H <sub>38</sub>	WILEY229.LI	2	87	C	24-Hexadecene-1-ol, 3,7,11,15-tetramethyl-, [E]	278	C <sub>20</sub> H <sub>40</sub> O	WILEY229.LI	3	88	C	NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS	278	C <sub>20</sub> H <sub>38</sub>	WILEY229.LI	4	88	C	3,7,11,15-Tetramethyl-2-hexadecene-1-ol SS	296	C <sub>20</sub> H <sub>40</sub> O	NIST08.LIB	5	88	C	3,7,11,15-Tetramethyl-2-hexadecene-1-ol SS (2)	296	C <sub>20</sub> H <sub>40</sub> O	NIST08.LIB	6	87	C	Pentadecanal- SS	226	C <sub>15</sub> H <sub>30</sub> O	NIST08.LIB	7	87	C	Pentadecanal- SS	226	C <sub>15</sub> H <sub>30</sub> O	NIST08.LIB	8	87	C	Oxane, tetradecyl- SS Hexadecane, 1,2-epoxi	240	C <sub>16</sub> H <sub>32</sub> O	NIST08.LIB	9	87	C	Oxane, tetradecyl-	240	C <sub>16</sub> H <sub>32</sub> O	NIST08.LIB
Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																		
1	87	C	NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS	278	C <sub>20</sub> H <sub>38</sub>	WILEY229.LI																																																																		
2	87	C	24-Hexadecene-1-ol, 3,7,11,15-tetramethyl-, [E]	278	C <sub>20</sub> H <sub>40</sub> O	WILEY229.LI																																																																		
3	88	C	NEOPHYTADIENE SS 2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECENE SS	278	C <sub>20</sub> H <sub>38</sub>	WILEY229.LI																																																																		
4	88	C	3,7,11,15-Tetramethyl-2-hexadecene-1-ol SS	296	C <sub>20</sub> H <sub>40</sub> O	NIST08.LIB																																																																		
5	88	C	3,7,11,15-Tetramethyl-2-hexadecene-1-ol SS (2)	296	C <sub>20</sub> H <sub>40</sub> O	NIST08.LIB																																																																		
6	87	C	Pentadecanal- SS	226	C <sub>15</sub> H <sub>30</sub> O	NIST08.LIB																																																																		
7	87	C	Pentadecanal- SS	226	C <sub>15</sub> H <sub>30</sub> O	NIST08.LIB																																																																		
8	87	C	Oxane, tetradecyl- SS Hexadecane, 1,2-epoxi	240	C <sub>16</sub> H <sub>32</sub> O	NIST08.LIB																																																																		
9	87	C	Oxane, tetradecyl-	240	C <sub>16</sub> H <sub>32</sub> O	NIST08.LIB																																																																		
<p><b>17.166</b></p>	<p><b>1847</b></p>	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>92</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester (CAS)</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>92</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester (CAS)</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>92</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester SS Tm</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>92</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>88</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester SS Tm</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>88</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>88</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester SS Tm</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>88</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester SS Tm</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>88</td> <td>C</td> <td>Tetradecanoic acid, trimethylsilyl ester (CAS)</td> <td>300</td> <td>C<sub>17</sub>H<sub>36</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target: Base Peak: 73/ 10,000</p> <p>1: 300: Tetradecanoic acid, trimethylsilyl ester (CAS) MYRISTIC ACID MONOTMS SS MONOTRIMETHYLSILYL MYRISTIC ACID SS Trimethylsilyl ester of Tetradecanoic acid SS</p> <p>CAS# 19603-17-3 Mol Wt: 300 Serial#: 145447</p> <p>Comp Name: Tetradecanoic acid, trimethylsilyl ester (CAS) MYRISTIC ACID MONOTMS SS MONOTRIMETHYLSILYL MYRISTIC ACID SS Trimethylsilyl ester of Tetradecanoic acid SS</p> <p>Formula: C<sub>17</sub>H<sub>36</sub>O<sub>2</sub> Class Flag: No Class Flag</p>	Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	92	C	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	WILEY229.LI	2	92	C	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	WILEY229.LI	3	92	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB	4	92	C	Tetradecanoic acid, trimethylsilyl ester	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB	5	88	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB	6	88	C	Tetradecanoic acid, trimethylsilyl ester	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB	7	88	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB	8	88	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB	9	88	C	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	WILEY229.LI
Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																		
1	92	C	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	WILEY229.LI																																																																		
2	92	C	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	WILEY229.LI																																																																		
3	92	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB																																																																		
4	92	C	Tetradecanoic acid, trimethylsilyl ester	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB																																																																		
5	88	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB																																																																		
6	88	C	Tetradecanoic acid, trimethylsilyl ester	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB																																																																		
7	88	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB																																																																		
8	88	C	Tetradecanoic acid, trimethylsilyl ester SS Tm	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	NIST08.LIB																																																																		
9	88	C	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub>	WILEY229.LI																																																																		
<p><b>17.375</b></p>	<p><b>1854</b></p>	<p>Similarity Search Results</p> <table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>87</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>87</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>87</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>86</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>86</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>86</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>86</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>86</td> <td>C</td> <td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>86</td> <td>C</td> <td>Dicobutyl phthalate SS</td> <td>278</td> <td>C<sub>16</sub>H<sub>22</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target: Base Peak: 149/ 10,000</p> <p>1: 278: 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester SS Phthalic acid, diisobutyl ester SS Diisobutyl phthalate SS Hexapla: M/18 SS Isobutyl phthalate SS Palmitol IC SS Dlp SS Diisobutylester isopropyl thalove SS Kodaflex DBP SS Palmitol IC SS Uniglex 11</p> <p>CAS# 84-69-5 Mol Wt: 278 Serial#: 23197</p> <p>Comp Name: 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester SS Phthalic acid, diisobutyl ester SS Diisobutyl phthalate SS Hexapla: M/18 SS Isobutyl phthalate SS Palmitol IC SS Dlp SS Diisobutylester isopropyl thalove SS Kodaflex DBP SS Palmitol IC SS Uniglex 11</p> <p>Formula: C<sub>16</sub>H<sub>22</sub>O<sub>4</sub> Class Flag: No Class Flag</p>	Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	87	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB	2	87	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI	3	87	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB	4	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI	5	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB	6	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB	7	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI	8	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI	9	86	C	Dicobutyl phthalate SS	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI
Rank	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																		
1	87	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB																																																																		
2	87	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI																																																																		
3	87	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB																																																																		
4	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI																																																																		
5	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB																																																																		
6	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	NIST08.LIB																																																																		
7	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI																																																																		
8	86	C	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI																																																																		
9	86	C	Dicobutyl phthalate SS	278	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	WILEY229.LI																																																																		



# ANEXOS

<p><b>17.578</b></p>	<p><b>1861</b></p>		<p>Target: 1: 278: NEOPHYTADIENE \$S\$ 2,6,10-TRIMETHYL-1,4-ETHYLENE-14-PENTADECENE \$S\$</p> <p>CAS# 0-00-0 Mol Wt: 278 Serial#: 130563          Comp Name: NEOPHYTADIENE \$S\$ 2,6,10-TRIMETHYL-1,4-ETHYLENE-14-PENTADECENE \$S\$          Formula: C20H38 Class Flag: No Class Flags</p>
<p><b>18.011</b></p>	<p><b>1875</b></p>		<p>Target: 1: 263: Oleavite</p> <p>CAS# 0-00-0 Mol Wt: 263 Serial#: 85504          Comp Name: Oleavite          Formula: C18H36N Class Flag: No Class Flags</p>
<p><b>18.095</b></p>	<p><b>1878</b></p>		<p>Target: 1: 296: 3,7,11,15-Tetramethyl-2-hexadecan-1-ol \$S\$ (DE)-3,7,11,15-Tetramethyl-2-hexadecan-1-ol \$S\$</p> <p>CAS# 103009-53-7 Mol Wt: 296 Serial#: 100255          Comp Name: 3,7,11,15-Tetramethyl-2-hexadecan-1-ol \$S\$ (DE)-3,7,11,15-Tetramethyl-2-hexadecan-1-ol \$S\$          Formula: C28H58 Class Flag: No Class Flags</p>
<p><b>18.688</b></p>	<p><b>1897</b></p>		<p>Target: 1: 237: Hexadecanetriole \$S\$ Palmitole \$S\$ Palmitic acid, nile \$S\$ 1-Cyanoheptadecane \$S\$</p> <p>CAS# 628-79-8 Mol Wt: 237 Serial#: 20294          Comp Name: Hexadecanetriole \$S\$ Palmitole \$S\$ Palmitic acid, nile \$S\$ 1-Cyanoheptadecane \$S\$          Formula: C18H32N Class Flag: No Class Flags</p>



# ANEXOS

<p><b>20.225</b></p>	<p><b>1947</b></p>		<p>Similar Compounds:</p> <table border="1"> <thead> <tr> <th>Similar</th> <th>Regid</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>31</td><td>n-Pentadecanoic acid, trimethylsilyl ester 55 n-</td><td>314</td><td>C19H30O2S</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>82</td><td>n-Pentadecanoic acid, trimethylsilyl ester 55 n-</td><td>314</td><td>C19H30O2S</td><td>NIST08.LIB</td></tr> <tr><td>3</td><td>82</td><td>n-Tetradecanoic acid, trimethylsilyl ester 55 Tera</td><td>298</td><td>C18H34O2S</td><td>NIST08.LIB</td></tr> <tr><td>4</td><td>81</td><td>TRIMETHYLSILOXY ESTER OF TETRADECA</td><td>440</td><td>C21H46O2</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>81</td><td>Tetradecanoic acid, trimethylsilyl ester 55 Tet</td><td>440</td><td>C21H46O2S</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>81</td><td>Tetradecanoic acid, trimethylsilyl ester 55</td><td>440</td><td>C21H46O2S</td><td>NIST107.LIB</td></tr> <tr><td>7</td><td>80</td><td>Hexadecanoic acid, trimethylsilyl ester 55 Palm</td><td>328</td><td>C19H40O2S</td><td>NIST08.LIB</td></tr> <tr><td>8</td><td>80</td><td>Hexadecanoic acid, trimethylsilyl ester</td><td>328</td><td>C19H40O2S</td><td>NIST121.LIB</td></tr> <tr><td>9</td><td>80</td><td>Tetradecanoic acid, trimethylsilyl ester (CAS)</td><td>300</td><td>C17H36O2</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target: Base Peak: 117/10,000</p> <p>2: 314: n-Pentadecanoic acid, trimethylsilyl ester 55 n-Pentadecanoic acid, trimethylsilyl ester 55 Trimethylsilyl pentadecanoate # 55</p> <p>CAS# 74367-22-9 Mol Wt: 314 Serial#: 24901</p> <p>Comp Name: n-Pentadecanoic acid, trimethylsilyl ester 55 n-Pentadecanoic acid, trimethylsilyl ester 55 Trimethylsilyl pentadecanoate # 55</p> <p>Formula: C19H30O2S Class Flag: No Class Flags.</p>	Similar	Regid	Compound Name	Mol Wt	Formula	Library	1	31	n-Pentadecanoic acid, trimethylsilyl ester 55 n-	314	C19H30O2S	NIST08.LIB	2	82	n-Pentadecanoic acid, trimethylsilyl ester 55 n-	314	C19H30O2S	NIST08.LIB	3	82	n-Tetradecanoic acid, trimethylsilyl ester 55 Tera	298	C18H34O2S	NIST08.LIB	4	81	TRIMETHYLSILOXY ESTER OF TETRADECA	440	C21H46O2	WILEY229.LI	5	81	Tetradecanoic acid, trimethylsilyl ester 55 Tet	440	C21H46O2S	NIST08.LIB	6	81	Tetradecanoic acid, trimethylsilyl ester 55	440	C21H46O2S	NIST107.LIB	7	80	Hexadecanoic acid, trimethylsilyl ester 55 Palm	328	C19H40O2S	NIST08.LIB	8	80	Hexadecanoic acid, trimethylsilyl ester	328	C19H40O2S	NIST121.LIB	9	80	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C17H36O2	WILEY229.LI
Similar	Regid	Compound Name	Mol Wt	Formula	Library																																																										
1	31	n-Pentadecanoic acid, trimethylsilyl ester 55 n-	314	C19H30O2S	NIST08.LIB																																																										
2	82	n-Pentadecanoic acid, trimethylsilyl ester 55 n-	314	C19H30O2S	NIST08.LIB																																																										
3	82	n-Tetradecanoic acid, trimethylsilyl ester 55 Tera	298	C18H34O2S	NIST08.LIB																																																										
4	81	TRIMETHYLSILOXY ESTER OF TETRADECA	440	C21H46O2	WILEY229.LI																																																										
5	81	Tetradecanoic acid, trimethylsilyl ester 55 Tet	440	C21H46O2S	NIST08.LIB																																																										
6	81	Tetradecanoic acid, trimethylsilyl ester 55	440	C21H46O2S	NIST107.LIB																																																										
7	80	Hexadecanoic acid, trimethylsilyl ester 55 Palm	328	C19H40O2S	NIST08.LIB																																																										
8	80	Hexadecanoic acid, trimethylsilyl ester	328	C19H40O2S	NIST121.LIB																																																										
9	80	Tetradecanoic acid, trimethylsilyl ester (CAS)	300	C17H36O2	WILEY229.LI																																																										
<p><b>20.650</b></p>	<p><b>1961</b></p>	<p><b>1955</b></p>	<p>Similar Compounds:</p> <table border="1"> <thead> <tr> <th>Similar</th> <th>Regid</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>86</td><td>82</td><td>1-HEXADECANOL-MONOTMS 55</td><td>314</td><td>C19H42O S</td><td>WILEY229.LI</td></tr> <tr><td>82</td><td>82</td><td>Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl</td><td>314</td><td>C19H42OSi</td><td>NIST08.LIB</td></tr> <tr><td>80</td><td>80</td><td>Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl</td><td>314</td><td>C19H42OSi</td><td>NIST107.LIB</td></tr> <tr><td>80</td><td>80</td><td>Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl</td><td>314</td><td>C19H42OSi</td><td>NIST08.LIB</td></tr> <tr><td>80</td><td>80</td><td>Silane, (hexadecyloxy)trimethyl- (CAS) MONOT</td><td>314</td><td>C19H42O S</td><td>WILEY229.LI</td></tr> <tr><td>79</td><td>79</td><td>Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl</td><td>314</td><td>C19H42OSi</td><td>NIST107.LIB</td></tr> <tr><td>79</td><td>79</td><td>Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl</td><td>314</td><td>C19H42OSi</td><td>NIST08.LIB</td></tr> <tr><td>79</td><td>79</td><td>Silane, (hexadecyloxy)trimethyl- (CAS) MONOT</td><td>314</td><td>C19H42OSi</td><td>NIST121.LIB</td></tr> <tr><td>79</td><td>79</td><td>Silane, (hexadecyloxy)trimethyl- (CAS) MONOT</td><td>314</td><td>C19H42O S</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target: Base Peak: 299/10,000</p> <p>: Silane, (hexadecyloxy)trimethyl- 55 1-Trimethylsilyloxyhexadecane 55 (Hexadecyloxy)trimethylsilane # 55</p> <p>6221-90-5 Mol Wt: 314 Serial#: 24994</p> <p>Name: Silane, (hexadecyloxy)trimethyl- 55 1-Trimethylsilyloxyhexadecane 55 (Hexadecyloxy)trimethylsilane # 55</p> <p>Formula: C19H42OSi Class Flag: No Class Flags.</p>	Similar	Regid	Compound Name	Mol Wt	Formula	Library	86	82	1-HEXADECANOL-MONOTMS 55	314	C19H42O S	WILEY229.LI	82	82	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST08.LIB	80	80	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST107.LIB	80	80	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST08.LIB	80	80	Silane, (hexadecyloxy)trimethyl- (CAS) MONOT	314	C19H42O S	WILEY229.LI	79	79	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST107.LIB	79	79	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST08.LIB	79	79	Silane, (hexadecyloxy)trimethyl- (CAS) MONOT	314	C19H42OSi	NIST121.LIB	79	79	Silane, (hexadecyloxy)trimethyl- (CAS) MONOT	314	C19H42O S	WILEY229.LI
Similar	Regid	Compound Name	Mol Wt	Formula	Library																																																										
86	82	1-HEXADECANOL-MONOTMS 55	314	C19H42O S	WILEY229.LI																																																										
82	82	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST08.LIB																																																										
80	80	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST107.LIB																																																										
80	80	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST08.LIB																																																										
80	80	Silane, (hexadecyloxy)trimethyl- (CAS) MONOT	314	C19H42O S	WILEY229.LI																																																										
79	79	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST107.LIB																																																										
79	79	Silane, (hexadecyloxy)trimethyl- 55 1-Trimethyl	314	C19H42OSi	NIST08.LIB																																																										
79	79	Silane, (hexadecyloxy)trimethyl- (CAS) MONOT	314	C19H42OSi	NIST121.LIB																																																										
79	79	Silane, (hexadecyloxy)trimethyl- (CAS) MONOT	314	C19H42O S	WILEY229.LI																																																										
<p><b>22.389</b></p>	<p><b>2018</b></p>		<p>Similar Compounds:</p> <table border="1"> <thead> <tr> <th>Similar</th> <th>Regid</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>87</td><td>cap 9 Hexadecanoic acid, trimethylsilyl ester</td><td>328</td><td>C19H38O2S</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>86</td><td>PALMITOLEIC ACID TMS 55</td><td>591</td><td>C38H74O2</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>86</td><td>Palmitoleic acid, trimethylsilyl ester 55</td><td>328</td><td>C19H38O2S</td><td>NIST107.LIB</td></tr> <tr><td>4</td><td>86</td><td>Palmitoleic acid, trimethylsilyl ester 55 Trimet</td><td>328</td><td>C19H38O2S</td><td>NIST08.LIB</td></tr> <tr><td>5</td><td>85</td><td>ole 6-Octadecanoic acid, trimethylsilyl ester 55</td><td>384</td><td>C21H42O2S</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>85</td><td>PALMITOLEIC ACID TMS 55</td><td>328</td><td>C19H38O2</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>85</td><td>ole 6-Octadecanoic acid, trimethylsilyl ester 55</td><td>384</td><td>C21H42O2S</td><td>NIST08.LIB</td></tr> <tr><td>8</td><td>85</td><td>ole 6-Octadecanoic acid, trimethylsilyl ester 55</td><td>384</td><td>C21H42O2S</td><td>NIST107.LIB</td></tr> <tr><td>9</td><td>84</td><td>6-CIS-OCTADECENOIC ACID TMS 55</td><td>384</td><td>C21H42O2</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target: Base Peak: 117/10,000</p> <p>6: 328: PALMITOLEIC ACID TMS 55</p> <p>CAS# 0-00-0 Mol Wt: 328 Serial#: 161535</p> <p>Comp Name: PALMITOLEIC ACID TMS 55</p> <p>Formula: C19H38O2Si Class Flag: No Class Flags.</p>	Similar	Regid	Compound Name	Mol Wt	Formula	Library	1	87	cap 9 Hexadecanoic acid, trimethylsilyl ester	328	C19H38O2S	NIST08.LIB	2	86	PALMITOLEIC ACID TMS 55	591	C38H74O2	WILEY229.LI	3	86	Palmitoleic acid, trimethylsilyl ester 55	328	C19H38O2S	NIST107.LIB	4	86	Palmitoleic acid, trimethylsilyl ester 55 Trimet	328	C19H38O2S	NIST08.LIB	5	85	ole 6-Octadecanoic acid, trimethylsilyl ester 55	384	C21H42O2S	NIST08.LIB	6	85	PALMITOLEIC ACID TMS 55	328	C19H38O2	WILEY229.LI	7	85	ole 6-Octadecanoic acid, trimethylsilyl ester 55	384	C21H42O2S	NIST08.LIB	8	85	ole 6-Octadecanoic acid, trimethylsilyl ester 55	384	C21H42O2S	NIST107.LIB	9	84	6-CIS-OCTADECENOIC ACID TMS 55	384	C21H42O2	WILEY229.LI
Similar	Regid	Compound Name	Mol Wt	Formula	Library																																																										
1	87	cap 9 Hexadecanoic acid, trimethylsilyl ester	328	C19H38O2S	NIST08.LIB																																																										
2	86	PALMITOLEIC ACID TMS 55	591	C38H74O2	WILEY229.LI																																																										
3	86	Palmitoleic acid, trimethylsilyl ester 55	328	C19H38O2S	NIST107.LIB																																																										
4	86	Palmitoleic acid, trimethylsilyl ester 55 Trimet	328	C19H38O2S	NIST08.LIB																																																										
5	85	ole 6-Octadecanoic acid, trimethylsilyl ester 55	384	C21H42O2S	NIST08.LIB																																																										
6	85	PALMITOLEIC ACID TMS 55	328	C19H38O2	WILEY229.LI																																																										
7	85	ole 6-Octadecanoic acid, trimethylsilyl ester 55	384	C21H42O2S	NIST08.LIB																																																										
8	85	ole 6-Octadecanoic acid, trimethylsilyl ester 55	384	C21H42O2S	NIST107.LIB																																																										
9	84	6-CIS-OCTADECENOIC ACID TMS 55	384	C21H42O2	WILEY229.LI																																																										
<p><b>22.955</b></p>	<p><b>2036</b></p>		<p>Similar Compounds:</p> <table border="1"> <thead> <tr> <th>Similar</th> <th>Regid</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>77</td><td>82</td><td>7-OH-7-ME OCTANOIC ACID TMS 55</td><td>318</td><td>C15H34O3</td><td>WILEY229.LI</td></tr> <tr><td>77</td><td>77</td><td>7-Trimethylsilyloxy-7-methyloctanoic acid, time</td><td>318</td><td>C15H34O3S</td><td>NIST08.LIB</td></tr> <tr><td>77</td><td>77</td><td>7-Trimethylsilyloxy-7-methyloctanoic acid, time</td><td>318</td><td>C15H34O3S</td><td>NIST107.LIB</td></tr> <tr><td>77</td><td>77</td><td>2-Methyl-5-pentenoic acid, trimethylsilyl ether</td><td>174</td><td>C9H20O2S</td><td>NIST08.LIB</td></tr> <tr><td>76</td><td>76</td><td>Silane, (1,1-dimethylpropoxy)trimethyl- 55 ter-P</td><td>160</td><td>C8H20O3S</td><td>NIST08.LIB</td></tr> <tr><td>75</td><td>75</td><td>Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-</td><td>290</td><td>C14H34O2S</td><td>NIST08.LIB</td></tr> <tr><td>75</td><td>75</td><td>Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-</td><td>290</td><td>C14H34O2S</td><td>NIST107.LIB</td></tr> <tr><td>75</td><td>75</td><td>3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct</td><td>262</td><td>C12H20O2S</td><td>NIST107.LIB</td></tr> <tr><td>75</td><td>75</td><td>3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct</td><td>262</td><td>C12H20O2S</td><td>NIST08.LIB</td></tr> </tbody> </table> <p>Target: Base Peak: 131/10,000</p> <p>8: 7-OH-7-ME OCTANOIC ACID TMS 55</p> <p>0-00-0 Mol Wt: 318 Serial#: 156679</p> <p>Name: 7-OH-7-ME OCTANOIC ACID TMS 55</p> <p>Formula: C15H34O3Si2 Class Flag: No Class Flags.</p>	Similar	Regid	Compound Name	Mol Wt	Formula	Library	77	82	7-OH-7-ME OCTANOIC ACID TMS 55	318	C15H34O3	WILEY229.LI	77	77	7-Trimethylsilyloxy-7-methyloctanoic acid, time	318	C15H34O3S	NIST08.LIB	77	77	7-Trimethylsilyloxy-7-methyloctanoic acid, time	318	C15H34O3S	NIST107.LIB	77	77	2-Methyl-5-pentenoic acid, trimethylsilyl ether	174	C9H20O2S	NIST08.LIB	76	76	Silane, (1,1-dimethylpropoxy)trimethyl- 55 ter-P	160	C8H20O3S	NIST08.LIB	75	75	Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2S	NIST08.LIB	75	75	Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2S	NIST107.LIB	75	75	3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct	262	C12H20O2S	NIST107.LIB	75	75	3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct	262	C12H20O2S	NIST08.LIB
Similar	Regid	Compound Name	Mol Wt	Formula	Library																																																										
77	82	7-OH-7-ME OCTANOIC ACID TMS 55	318	C15H34O3	WILEY229.LI																																																										
77	77	7-Trimethylsilyloxy-7-methyloctanoic acid, time	318	C15H34O3S	NIST08.LIB																																																										
77	77	7-Trimethylsilyloxy-7-methyloctanoic acid, time	318	C15H34O3S	NIST107.LIB																																																										
77	77	2-Methyl-5-pentenoic acid, trimethylsilyl ether	174	C9H20O2S	NIST08.LIB																																																										
76	76	Silane, (1,1-dimethylpropoxy)trimethyl- 55 ter-P	160	C8H20O3S	NIST08.LIB																																																										
75	75	Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2S	NIST08.LIB																																																										
75	75	Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2S	NIST107.LIB																																																										
75	75	3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct	262	C12H20O2S	NIST107.LIB																																																										
75	75	3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct	262	C12H20O2S	NIST08.LIB																																																										

<p><b>23.229</b></p>	<p><b>2045</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>96</td> <td>✓</td> <td>Hexadecanoic acid, trimethylsilyl ester \$S Palm</td> <td>328</td> <td>C19H40O2Si</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>96</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester</td> <td>328</td> <td>C19H40O2Si</td> <td>NIST21.LIB</td> </tr> <tr> <td>3</td> <td>96</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester \$S Palm</td> <td>328</td> <td>C19H40O2Si</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>96</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C19H40O2</td> <td>WILEY229.LIB</td> </tr> <tr> <td>5</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester \$S Palm</td> <td>328</td> <td>C19H40O2Si</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester \$S Palm</td> <td>328</td> <td>C19H40O2Si</td> <td>NIST08a.LIB</td> </tr> <tr> <td>7</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C19H40O2</td> <td>WILEY229.LIB</td> </tr> <tr> <td>8</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester \$S Palm</td> <td>328</td> <td>C19H40O2Si</td> <td>NIST08a.LIB</td> </tr> <tr> <td>9</td> <td>94</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester</td> <td>328</td> <td>C19H40O2Si</td> <td>NIST21.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1 : 328: Hexadecanoic acid, trimethylsilyl ester \$S Palm; acid, trimethylsilyl ester \$S Trimethylsilyl palmitate # \$S Trimethylsilyl palmitate # \$S</p> <p>CAS#: 55520-89-3 Mol Wt: 328 Serial#: 131372      Cmpd Name: Hexadecanoic acid, trimethylsilyl ester \$S Palm; acid, trimethylsilyl ester \$S Trimethylsilyl palmitate # \$S Trimethylsilyl palmitate # \$S      Formula: C19H40O2Si Class Flag: No Class Flags      Ret Index: 1987</p>	RT	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	96	✓	Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08.LIB	2	96		Hexadecanoic acid, trimethylsilyl ester	328	C19H40O2Si	NIST21.LIB	3	96		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08.LIB	4	96		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C19H40O2	WILEY229.LIB	5	94		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST107.LIB	6	94		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08a.LIB	7	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C19H40O2	WILEY229.LIB	8	94		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08a.LIB	9	94		Hexadecanoic acid, trimethylsilyl ester	328	C19H40O2Si	NIST21.LIB
RT	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	96	✓	Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08.LIB																																																																		
2	96		Hexadecanoic acid, trimethylsilyl ester	328	C19H40O2Si	NIST21.LIB																																																																		
3	96		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08.LIB																																																																		
4	96		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C19H40O2	WILEY229.LIB																																																																		
5	94		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST107.LIB																																																																		
6	94		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08a.LIB																																																																		
7	94		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C19H40O2	WILEY229.LIB																																																																		
8	94		Hexadecanoic acid, trimethylsilyl ester \$S Palm	328	C19H40O2Si	NIST08a.LIB																																																																		
9	94		Hexadecanoic acid, trimethylsilyl ester	328	C19H40O2Si	NIST21.LIB																																																																		
<p><b>23.569</b></p>	<p><b>2057</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>33</td> <td>✓</td> <td>DHSOPENTYLPHTHALATE \$S</td> <td>306</td> <td>C18H26O4</td> <td>WILEY229.LIB</td> </tr> <tr> <td>2</td> <td>90</td> <td></td> <td>1,2-Benzenedicarboxylic acid, dipentyl ester \$</td> <td>306</td> <td>C18H26O4</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>87</td> <td></td> <td>1,2-Benzenedicarboxylic acid, dipentyl ester \$</td> <td>306</td> <td>C18H26O4</td> <td>NIST08a.LIB</td> </tr> <tr> <td>4</td> <td>87</td> <td></td> <td>1,2-Benzenedicarboxylic acid, dipentyl ester</td> <td>306</td> <td>C18H26O4</td> <td>NIST21.LIB</td> </tr> <tr> <td>5</td> <td>87</td> <td></td> <td>1,2-Benzenedicarboxylic acid, dipentyl ester (C</td> <td>306</td> <td>C18H26O4</td> <td>WILEY229.LIB</td> </tr> <tr> <td>6</td> <td>87</td> <td></td> <td>1,2-Benzenedicarboxylic acid, dipentyl ester \$</td> <td>306</td> <td>C18H26O4</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>86</td> <td></td> <td>1,2-Benzenedicarboxylic acid, dipentyl ester (C</td> <td>306</td> <td>C18H26O4</td> <td>WILEY229.LIB</td> </tr> <tr> <td>8</td> <td>85</td> <td></td> <td>Phthalic acid, di(2-methylbutyl) ester</td> <td>306</td> <td>C18H26O4</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>84</td> <td></td> <td>1,2-Benzenedicarboxylic acid, dipentyl ester (C</td> <td>306</td> <td>C18H26O4</td> <td>WILEY229.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1 : 306: DHSOPENTYLPHTHALATE \$S</p> <p>CAS#: 0-00-0 Mol Wt: 306 Serial#: 149301      Cmpd Name: DHSOPENTYLPHTHALATE \$S      Formula: C18H26O4 Class Flag: No Class Flags</p>	RT	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	33	✓	DHSOPENTYLPHTHALATE \$S	306	C18H26O4	WILEY229.LIB	2	90		1,2-Benzenedicarboxylic acid, dipentyl ester \$	306	C18H26O4	NIST107.LIB	3	87		1,2-Benzenedicarboxylic acid, dipentyl ester \$	306	C18H26O4	NIST08a.LIB	4	87		1,2-Benzenedicarboxylic acid, dipentyl ester	306	C18H26O4	NIST21.LIB	5	87		1,2-Benzenedicarboxylic acid, dipentyl ester (C	306	C18H26O4	WILEY229.LIB	6	87		1,2-Benzenedicarboxylic acid, dipentyl ester \$	306	C18H26O4	NIST08.LIB	7	86		1,2-Benzenedicarboxylic acid, dipentyl ester (C	306	C18H26O4	WILEY229.LIB	8	85		Phthalic acid, di(2-methylbutyl) ester	306	C18H26O4	NIST08.LIB	9	84		1,2-Benzenedicarboxylic acid, dipentyl ester (C	306	C18H26O4	WILEY229.LIB
RT	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	33	✓	DHSOPENTYLPHTHALATE \$S	306	C18H26O4	WILEY229.LIB																																																																		
2	90		1,2-Benzenedicarboxylic acid, dipentyl ester \$	306	C18H26O4	NIST107.LIB																																																																		
3	87		1,2-Benzenedicarboxylic acid, dipentyl ester \$	306	C18H26O4	NIST08a.LIB																																																																		
4	87		1,2-Benzenedicarboxylic acid, dipentyl ester	306	C18H26O4	NIST21.LIB																																																																		
5	87		1,2-Benzenedicarboxylic acid, dipentyl ester (C	306	C18H26O4	WILEY229.LIB																																																																		
6	87		1,2-Benzenedicarboxylic acid, dipentyl ester \$	306	C18H26O4	NIST08.LIB																																																																		
7	86		1,2-Benzenedicarboxylic acid, dipentyl ester (C	306	C18H26O4	WILEY229.LIB																																																																		
8	85		Phthalic acid, di(2-methylbutyl) ester	306	C18H26O4	NIST08.LIB																																																																		
9	84		1,2-Benzenedicarboxylic acid, dipentyl ester (C	306	C18H26O4	WILEY229.LIB																																																																		
<p><b>24.126</b></p>	<p><b>2075</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>83</td> <td>✓</td> <td>9-Octadecenal, (Z)- (CAS) CIS-OCTADEC-9-E</td> <td>266</td> <td>C18H34O</td> <td>WILEY229.LIB</td> </tr> <tr> <td>2</td> <td>83</td> <td></td> <td>9-Octadecenal, (Z)- \$S Oxadeflyde \$S cis-9-</td> <td>266</td> <td>C18H34O</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>83</td> <td></td> <td>9-Octadecenal, (Z)- \$S Oxadeflyde \$S cis-9-</td> <td>266</td> <td>C18H34O</td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>82</td> <td>✓</td> <td>Oleanole</td> <td>263</td> <td>C18H33N</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>82</td> <td></td> <td>13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$</td> <td>266</td> <td>C18H34O</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>82</td> <td></td> <td>13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$</td> <td>266</td> <td>C18H34O</td> <td>NIST08a.LIB</td> </tr> <tr> <td>7</td> <td>82</td> <td></td> <td>8-Hexadecenal, 14-methyl-, (Z)- \$S 14-Methyl-</td> <td>252</td> <td>C17H32O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>82</td> <td></td> <td>13-Oxabicyclo[10.1.0]tridecane \$S Cycloode</td> <td>182</td> <td>C12H22O</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>82</td> <td></td> <td>cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>4 : 263: Oleanole</p> <p>CAS#: 0-00-0 Mol Wt: 263 Serial#: 85504      Cmpd Name: Oleanole      Formula: C18H33N Class Flag: No Class Flags</p>	RT	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	83	✓	9-Octadecenal, (Z)- (CAS) CIS-OCTADEC-9-E	266	C18H34O	WILEY229.LIB	2	83		9-Octadecenal, (Z)- \$S Oxadeflyde \$S cis-9-	266	C18H34O	NIST08.LIB	3	83		9-Octadecenal, (Z)- \$S Oxadeflyde \$S cis-9-	266	C18H34O	NIST107.LIB	4	82	✓	Oleanole	263	C18H33N	NIST08.LIB	5	82		13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST107.LIB	6	82		13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST08a.LIB	7	82		8-Hexadecenal, 14-methyl-, (Z)- \$S 14-Methyl-	252	C17H32O	NIST08.LIB	8	82		13-Oxabicyclo[10.1.0]tridecane \$S Cycloode	182	C12H22O	NIST08.LIB	9	82		cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB
RT	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	83	✓	9-Octadecenal, (Z)- (CAS) CIS-OCTADEC-9-E	266	C18H34O	WILEY229.LIB																																																																		
2	83		9-Octadecenal, (Z)- \$S Oxadeflyde \$S cis-9-	266	C18H34O	NIST08.LIB																																																																		
3	83		9-Octadecenal, (Z)- \$S Oxadeflyde \$S cis-9-	266	C18H34O	NIST107.LIB																																																																		
4	82	✓	Oleanole	263	C18H33N	NIST08.LIB																																																																		
5	82		13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST107.LIB																																																																		
6	82		13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST08a.LIB																																																																		
7	82		8-Hexadecenal, 14-methyl-, (Z)- \$S 14-Methyl-	252	C17H32O	NIST08.LIB																																																																		
8	82		13-Oxabicyclo[10.1.0]tridecane \$S Cycloode	182	C12H22O	NIST08.LIB																																																																		
9	82		cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB																																																																		

<p>24.131</p> <p>2075</p>		<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>95</td> <td><input checked="" type="checkbox"/></td> <td>Oleantrile</td> <td>263</td> <td>C18H33N</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>85</td> <td><input type="checkbox"/></td> <td>Hexadecenitrile \$S</td> <td>235</td> <td>C16H29N</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>85</td> <td><input type="checkbox"/></td> <td>Hexadecenitrile \$S (3E)-3-Hexadecenitrile</td> <td>235</td> <td>C16H29N</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>85</td> <td><input type="checkbox"/></td> <td>cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-11-Hexadecenal</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-11-Hexadecenal \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>84</td> <td><input type="checkbox"/></td> <td>cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>83</td> <td><input type="checkbox"/></td> <td>13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$</td> <td>266</td> <td>C18H34O</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>83</td> <td><input type="checkbox"/></td> <td>13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$</td> <td>266</td> <td>C18H34O</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1: 263 : Oleantrile</p> <p>CAS#: 0-00-0 Mol Wt: 263 Serial#: 85504          Cmpd Name: Oleantrile          Formula: C18H33N Class Flag: No Class Flags.          Ret Index: 2064</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	95	<input checked="" type="checkbox"/>	Oleantrile	263	C18H33N	NIST08.LIB	2	85	<input type="checkbox"/>	Hexadecenitrile \$S	235	C16H29N	NIST107.LIB	3	85	<input type="checkbox"/>	Hexadecenitrile \$S (3E)-3-Hexadecenitrile	235	C16H29N	NIST08.LIB	4	85	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB	5	84	<input type="checkbox"/>	E-11-Hexadecenal	238	C16H30O	NIST08.LIB	6	84	<input type="checkbox"/>	E-11-Hexadecenal \$S	238	C16H30O	NIST107.LIB	7	84	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB	8	83	<input type="checkbox"/>	13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST08.LIB	9	83	<input type="checkbox"/>	13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST107.LIB
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	95	<input checked="" type="checkbox"/>	Oleantrile	263	C18H33N	NIST08.LIB																																																																		
2	85	<input type="checkbox"/>	Hexadecenitrile \$S	235	C16H29N	NIST107.LIB																																																																		
3	85	<input type="checkbox"/>	Hexadecenitrile \$S (3E)-3-Hexadecenitrile	235	C16H29N	NIST08.LIB																																																																		
4	85	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB																																																																		
5	84	<input type="checkbox"/>	E-11-Hexadecenal	238	C16H30O	NIST08.LIB																																																																		
6	84	<input type="checkbox"/>	E-11-Hexadecenal \$S	238	C16H30O	NIST107.LIB																																																																		
7	84	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB																																																																		
8	83	<input type="checkbox"/>	13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST08.LIB																																																																		
9	83	<input type="checkbox"/>	13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST107.LIB																																																																		
<p>24.26</p> <p>2080</p>		<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>93</td> <td><input checked="" type="checkbox"/></td> <td>Oleantrile</td> <td>263</td> <td>C18H33N</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>85</td> <td><input type="checkbox"/></td> <td>Hexadecenitrile \$S</td> <td>235</td> <td>C16H29N</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>85</td> <td><input type="checkbox"/></td> <td>Hexadecenitrile \$S (3E)-3-Hexadecenitrile</td> <td>235</td> <td>C16H29N</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-11-Hexadecenal</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-11-Hexadecenal \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>84</td> <td><input type="checkbox"/></td> <td>cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>84</td> <td><input type="checkbox"/></td> <td>13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$</td> <td>266</td> <td>C18H34O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-9-Heptadecenal \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-9-Hexadecenal</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1: 263 : Oleantrile</p> <p>CAS#: 0-00-0 Mol Wt: 263 Serial#: 85504          Cmpd Name: Oleantrile          Formula: C18H33N Class Flag: No Class Flags.          Ret Index: 2064</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	93	<input checked="" type="checkbox"/>	Oleantrile	263	C18H33N	NIST08.LIB	2	85	<input type="checkbox"/>	Hexadecenitrile \$S	235	C16H29N	NIST107.LIB	3	85	<input type="checkbox"/>	Hexadecenitrile \$S (3E)-3-Hexadecenitrile	235	C16H29N	NIST08.LIB	4	84	<input type="checkbox"/>	E-11-Hexadecenal	238	C16H30O	NIST08.LIB	5	84	<input type="checkbox"/>	E-11-Hexadecenal \$S	238	C16H30O	NIST107.LIB	6	84	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB	7	84	<input type="checkbox"/>	13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST08.LIB	8	84	<input type="checkbox"/>	E-9-Heptadecenal \$S	238	C16H30O	NIST107.LIB	9	84	<input type="checkbox"/>	E-9-Hexadecenal	238	C16H30O	NIST08.LIB
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	93	<input checked="" type="checkbox"/>	Oleantrile	263	C18H33N	NIST08.LIB																																																																		
2	85	<input type="checkbox"/>	Hexadecenitrile \$S	235	C16H29N	NIST107.LIB																																																																		
3	85	<input type="checkbox"/>	Hexadecenitrile \$S (3E)-3-Hexadecenitrile	235	C16H29N	NIST08.LIB																																																																		
4	84	<input type="checkbox"/>	E-11-Hexadecenal	238	C16H30O	NIST08.LIB																																																																		
5	84	<input type="checkbox"/>	E-11-Hexadecenal \$S	238	C16H30O	NIST107.LIB																																																																		
6	84	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB																																																																		
7	84	<input type="checkbox"/>	13-Octadecenal, (Z)- \$S cis-13-Octadecenal \$	266	C18H34O	NIST08.LIB																																																																		
8	84	<input type="checkbox"/>	E-9-Heptadecenal \$S	238	C16H30O	NIST107.LIB																																																																		
9	84	<input type="checkbox"/>	E-9-Hexadecenal	238	C16H30O	NIST08.LIB																																																																		
<p>24.389</p> <p>2084</p>		<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>92</td> <td><input checked="" type="checkbox"/></td> <td>Oleantrile</td> <td>263</td> <td>C18H33N</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>85</td> <td><input type="checkbox"/></td> <td>E-11-Hexadecenal</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>85</td> <td><input type="checkbox"/></td> <td>cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>85</td> <td><input type="checkbox"/></td> <td>E-11-Hexadecenal \$S</td> <td>238</td> <td>C16H30O</td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-9-Tetradecenal \$S</td> <td>210</td> <td>C14H26O</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>84</td> <td><input type="checkbox"/></td> <td>E-9-Tetradecenal</td> <td>210</td> <td>C14H26O</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>84</td> <td><input type="checkbox"/></td> <td>7-Tetradecenal, (Z)- \$S 7-Tetradecenal \$S (</td> <td>210</td> <td>C14H26O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>84</td> <td><input type="checkbox"/></td> <td>9-Octadecenal, (Z)- \$S (CAS) CIS-OCTADEC-9-E</td> <td>266</td> <td>C18H34O</td> <td>WILEY225.LI</td> </tr> <tr> <td>9</td> <td>84</td> <td><input type="checkbox"/></td> <td>9-Octadecenal, (Z)- \$S Octadecenal \$S cis-9-</td> <td>266</td> <td>C18H34O</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1: 263 : Oleantrile</p> <p>CAS#: 0-00-0 Mol Wt: 263 Serial#: 85504          Cmpd Name: Oleantrile          Formula: C18H33N Class Flag: No Class Flags.</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	92	<input checked="" type="checkbox"/>	Oleantrile	263	C18H33N	NIST08.LIB	2	85	<input type="checkbox"/>	E-11-Hexadecenal	238	C16H30O	NIST08.LIB	3	85	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB	4	85	<input type="checkbox"/>	E-11-Hexadecenal \$S	238	C16H30O	NIST107.LIB	5	84	<input type="checkbox"/>	E-9-Tetradecenal \$S	210	C14H26O	NIST107.LIB	6	84	<input type="checkbox"/>	E-9-Tetradecenal	210	C14H26O	NIST08.LIB	7	84	<input type="checkbox"/>	7-Tetradecenal, (Z)- \$S 7-Tetradecenal \$S (	210	C14H26O	NIST08.LIB	8	84	<input type="checkbox"/>	9-Octadecenal, (Z)- \$S (CAS) CIS-OCTADEC-9-E	266	C18H34O	WILEY225.LI	9	84	<input type="checkbox"/>	9-Octadecenal, (Z)- \$S Octadecenal \$S cis-9-	266	C18H34O	NIST107.LIB
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	92	<input checked="" type="checkbox"/>	Oleantrile	263	C18H33N	NIST08.LIB																																																																		
2	85	<input type="checkbox"/>	E-11-Hexadecenal	238	C16H30O	NIST08.LIB																																																																		
3	85	<input type="checkbox"/>	cis-9-Hexadecenal \$S 9-Hexadecenal, (Z)- \$S	238	C16H30O	NIST08.LIB																																																																		
4	85	<input type="checkbox"/>	E-11-Hexadecenal \$S	238	C16H30O	NIST107.LIB																																																																		
5	84	<input type="checkbox"/>	E-9-Tetradecenal \$S	210	C14H26O	NIST107.LIB																																																																		
6	84	<input type="checkbox"/>	E-9-Tetradecenal	210	C14H26O	NIST08.LIB																																																																		
7	84	<input type="checkbox"/>	7-Tetradecenal, (Z)- \$S 7-Tetradecenal \$S (	210	C14H26O	NIST08.LIB																																																																		
8	84	<input type="checkbox"/>	9-Octadecenal, (Z)- \$S (CAS) CIS-OCTADEC-9-E	266	C18H34O	WILEY225.LI																																																																		
9	84	<input type="checkbox"/>	9-Octadecenal, (Z)- \$S Octadecenal \$S cis-9-	266	C18H34O	NIST107.LIB																																																																		

# ANEXOS

<p><b>25.090</b></p>	<p><b>2107</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>74</td> <td>74</td> <td>CP</td> <td>7-Timethylhept-7-methyloctanoic acid Tms</td> <td>318</td> <td>C19H34O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>74</td> <td>74</td> <td></td> <td>7-OH-7-ME-OCTANOIC ACID 2TMS SS</td> <td>318</td> <td>C15H34O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>71</td> <td>71</td> <td></td> <td>Stane, (1,1-dimethylpropyl)imethyl- SS Int-P</td> <td>160</td> <td>C8H20O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>71</td> <td>71</td> <td></td> <td>2-Methyl-3-pentanol, trimethyl ester</td> <td>174</td> <td>C9H20O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>71</td> <td>71</td> <td></td> <td>Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-</td> <td>290</td> <td>C14H34O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>71</td> <td>71</td> <td></td> <td>Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-</td> <td>290</td> <td>C14H34O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>69</td> <td>69</td> <td></td> <td>ETHYL 7-OH-7-ME-OCTANOATE 1TMS SS</td> <td>274</td> <td>C14H30O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>69</td> <td>69</td> <td></td> <td>Tetradecanoic acid, trimethyl ester CAS</td> <td>300</td> <td>C17H36O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target: 7-Timethylhept-7-methyloctanoic acid, trimethyl ester</p> <p>CAS# 0-00-0 Mol Wt. 318 Serial# 124428</p> <p>Comp Name: 7-Timethylhept-7-methyloctanoic acid, trimethyl ester</p> <p>Formula: C19H34O2</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	74	74	CP	7-Timethylhept-7-methyloctanoic acid Tms	318	C19H34O2	NIST08.LIB	74	74		7-OH-7-ME-OCTANOIC ACID 2TMS SS	318	C15H34O3	WILEY229.LI	71	71		Stane, (1,1-dimethylpropyl)imethyl- SS Int-P	160	C8H20O2	NIST08.LIB	71	71		2-Methyl-3-pentanol, trimethyl ester	174	C9H20O5	NIST08.LIB	71	71		Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2	NIST107.LIB	71	71		Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2	NIST08.LIB	69	69		ETHYL 7-OH-7-ME-OCTANOATE 1TMS SS	274	C14H30O3	WILEY229.LI	69	69		Tetradecanoic acid, trimethyl ester CAS	300	C17H36O2	WILEY229.LI							
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
74	74	CP	7-Timethylhept-7-methyloctanoic acid Tms	318	C19H34O2	NIST08.LIB																																																																		
74	74		7-OH-7-ME-OCTANOIC ACID 2TMS SS	318	C15H34O3	WILEY229.LI																																																																		
71	71		Stane, (1,1-dimethylpropyl)imethyl- SS Int-P	160	C8H20O2	NIST08.LIB																																																																		
71	71		2-Methyl-3-pentanol, trimethyl ester	174	C9H20O5	NIST08.LIB																																																																		
71	71		Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2	NIST107.LIB																																																																		
71	71		Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	290	C14H34O2	NIST08.LIB																																																																		
69	69		ETHYL 7-OH-7-ME-OCTANOATE 1TMS SS	274	C14H30O3	WILEY229.LI																																																																		
69	69		Tetradecanoic acid, trimethyl ester CAS	300	C17H36O2	WILEY229.LI																																																																		
<p><b>25.337</b></p>	<p><b>2116</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>80</td> <td>80</td> <td>CP</td> <td>Heptadecanoic acid, trimethyl ester SS T1</td> <td>342</td> <td>C20H42O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester SS</td> <td>342</td> <td>C20H42O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester SS T1</td> <td>342</td> <td>C20H42O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>TRIMETHYLSILYL ESTER OF TETRADECANOIC ACID</td> <td>440</td> <td>C27H56O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>Tetradecanoic acid, trimethyl ester SS</td> <td>440</td> <td>C27H56O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>Tetradecanoic acid, trimethyl ester SS Tms</td> <td>440</td> <td>C27H56O2</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target: Heptadecanoic acid, trimethyl ester SS Trimethylsilyl heptadecanoate # SS</p> <p>CAS# 59517-58-3 Mol Wt. 342 Serial# 140433</p> <p>Comp Name: Heptadecanoic acid, trimethyl ester SS Trimethylsilyl heptadecanoate # SS</p> <p>Formula: C20H42O2</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	80	80	CP	Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB	80	80		Heptadecanoic acid, trimethyl ester SS	342	C20H42O2	NIST107.LIB	80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI	80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI	80	80		Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB	78	78		TRIMETHYLSILYL ESTER OF TETRADECANOIC ACID	440	C27H56O2	WILEY229.LI	78	78		Tetradecanoic acid, trimethyl ester SS	440	C27H56O2	NIST107.LIB	78	78		Tetradecanoic acid, trimethyl ester SS Tms	440	C27H56O2	NIST08.LIB							
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
80	80	CP	Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB																																																																		
80	80		Heptadecanoic acid, trimethyl ester SS	342	C20H42O2	NIST107.LIB																																																																		
80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI																																																																		
80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI																																																																		
80	80		Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB																																																																		
78	78		TRIMETHYLSILYL ESTER OF TETRADECANOIC ACID	440	C27H56O2	WILEY229.LI																																																																		
78	78		Tetradecanoic acid, trimethyl ester SS	440	C27H56O2	NIST107.LIB																																																																		
78	78		Tetradecanoic acid, trimethyl ester SS Tms	440	C27H56O2	NIST08.LIB																																																																		
<p><b>26.176</b></p>	<p><b>2144</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>80</td> <td>80</td> <td>CP</td> <td>Heptadecanoic acid, trimethyl ester SS</td> <td>342</td> <td>C20H42O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester SS T1</td> <td>342</td> <td>C20H42O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester SS T1</td> <td>342</td> <td>C20H42O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>80</td> <td>80</td> <td></td> <td>Heptadecanoic acid, trimethyl ester</td> <td>342</td> <td>C20H42O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>85</td> <td>85</td> <td></td> <td>Nonadecanoic acid, trimethyl ester SS Tms</td> <td>370</td> <td>C22H46O2</td> <td>NIST08.LIB</td> </tr> <tr> <td>84</td> <td>84</td> <td></td> <td>Octadecanoic acid, trimethyl ester (CAS) S</td> <td>356</td> <td>C21H44O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>84</td> <td>84</td> <td></td> <td>Octadecanoic acid, trimethyl ester SS Stear</td> <td>356</td> <td>C21H44O2</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target: Heptadecanoic acid, trimethyl ester SS</p> <p>CAS# 59517-58-3 Mol Wt. 342 Serial# 82574</p> <p>Comp Name: Heptadecanoic acid, trimethyl ester SS</p> <p>Formula: C20H42O2</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	80	80	CP	Heptadecanoic acid, trimethyl ester SS	342	C20H42O2	NIST107.LIB	80	80		Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB	80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI	80	80		Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB	80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI	80	80		Heptadecanoic acid, trimethyl ester	342	C20H42O2	NIST107.LIB	85	85		Nonadecanoic acid, trimethyl ester SS Tms	370	C22H46O2	NIST08.LIB	84	84		Octadecanoic acid, trimethyl ester (CAS) S	356	C21H44O2	WILEY229.LI	84	84		Octadecanoic acid, trimethyl ester SS Stear	356	C21H44O2	NIST107.LIB
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
80	80	CP	Heptadecanoic acid, trimethyl ester SS	342	C20H42O2	NIST107.LIB																																																																		
80	80		Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB																																																																		
80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI																																																																		
80	80		Heptadecanoic acid, trimethyl ester SS T1	342	C20H42O2	NIST08.LIB																																																																		
80	80		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI																																																																		
80	80		Heptadecanoic acid, trimethyl ester	342	C20H42O2	NIST107.LIB																																																																		
85	85		Nonadecanoic acid, trimethyl ester SS Tms	370	C22H46O2	NIST08.LIB																																																																		
84	84		Octadecanoic acid, trimethyl ester (CAS) S	356	C21H44O2	WILEY229.LI																																																																		
84	84		Octadecanoic acid, trimethyl ester SS Stear	356	C21H44O2	NIST107.LIB																																																																		
<p><b>26.564</b></p>	<p><b>2158</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>84</td> <td>84</td> <td>CP</td> <td>Stane, trimethyl(octadecyloxy) SS Octadecyloxy</td> <td>342</td> <td>C21H46O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>84</td> <td>84</td> <td></td> <td>Octadecanoic acid, trimethyl ester SS Tms</td> <td>342</td> <td>C21H46O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>84</td> <td>84</td> <td></td> <td>Stane, trimethyl(octadecyloxy) SS Octadecyloxy</td> <td>342</td> <td>C21H46O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>84</td> <td>84</td> <td></td> <td>1-Trimethylsilyloctadecane SS</td> <td>342</td> <td>C21H46O5</td> <td>NIST107.LIB</td> </tr> <tr> <td>83</td> <td>83</td> <td></td> <td>Stane, dimethyl(octadecyloxy)propyl- SS</td> <td>370</td> <td>C23H50O5</td> <td>NIST107.LIB</td> </tr> <tr> <td>83</td> <td>83</td> <td></td> <td>Stane, dimethyl(octadecyloxy)propyl- SS Dimet</td> <td>370</td> <td>C23H50O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>83</td> <td>83</td> <td></td> <td>1-Octadecanol, tetraethyltrimethylsilyl ether</td> <td>384</td> <td>C24H52O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>Stane, (1,1-dimethylpropyl)dimethyl(octadecyloxy)-</td> <td>384</td> <td>C24H52O5</td> <td>NIST08.LIB</td> </tr> <tr> <td>81</td> <td>81</td> <td></td> <td>1-Dimethylpropan-2-ylmethyloctadecane SS</td> <td>368</td> <td>C23H48O5</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target: Stane, trimethyl(octadecyloxy) SS Octadecyloxy trimethylsilyl SS 1-Octadecanol, trimethylsilyl ether SS Octadecyl trimethylsilyl ether SS</p> <p>CAS# 10740-98-6 Mol Wt. 342 Serial# 140506</p> <p>Comp Name: Stane, trimethyl(octadecyloxy) SS Octadecyloxy trimethylsilyl SS 1-Octadecanol, trimethylsilyl ether SS Octadecyl trimethylsilyl ether SS</p> <p>Formula: C21H46O5</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	84	84	CP	Stane, trimethyl(octadecyloxy) SS Octadecyloxy	342	C21H46O5	NIST08.LIB	84	84		Octadecanoic acid, trimethyl ester SS Tms	342	C21H46O5	WILEY229.LI	84	84		Stane, trimethyl(octadecyloxy) SS Octadecyloxy	342	C21H46O5	NIST08.LIB	84	84		1-Trimethylsilyloctadecane SS	342	C21H46O5	NIST107.LIB	83	83		Stane, dimethyl(octadecyloxy)propyl- SS	370	C23H50O5	NIST107.LIB	83	83		Stane, dimethyl(octadecyloxy)propyl- SS Dimet	370	C23H50O5	NIST08.LIB	83	83		1-Octadecanol, tetraethyltrimethylsilyl ether	384	C24H52O5	NIST08.LIB	82	82		Stane, (1,1-dimethylpropyl)dimethyl(octadecyloxy)-	384	C24H52O5	NIST08.LIB	81	81		1-Dimethylpropan-2-ylmethyloctadecane SS	368	C23H48O5	NIST107.LIB
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
84	84	CP	Stane, trimethyl(octadecyloxy) SS Octadecyloxy	342	C21H46O5	NIST08.LIB																																																																		
84	84		Octadecanoic acid, trimethyl ester SS Tms	342	C21H46O5	WILEY229.LI																																																																		
84	84		Stane, trimethyl(octadecyloxy) SS Octadecyloxy	342	C21H46O5	NIST08.LIB																																																																		
84	84		1-Trimethylsilyloctadecane SS	342	C21H46O5	NIST107.LIB																																																																		
83	83		Stane, dimethyl(octadecyloxy)propyl- SS	370	C23H50O5	NIST107.LIB																																																																		
83	83		Stane, dimethyl(octadecyloxy)propyl- SS Dimet	370	C23H50O5	NIST08.LIB																																																																		
83	83		1-Octadecanol, tetraethyltrimethylsilyl ether	384	C24H52O5	NIST08.LIB																																																																		
82	82		Stane, (1,1-dimethylpropyl)dimethyl(octadecyloxy)-	384	C24H52O5	NIST08.LIB																																																																		
81	81		1-Dimethylpropan-2-ylmethyloctadecane SS	368	C23H48O5	NIST107.LIB																																																																		

# ANEXOS

<p><b>26.999</b></p>	<p><b>2172</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>72</td> <td>99</td> <td>CP</td> <td>Phytol, trimethyl ether</td> <td>350</td> <td>C23H48O5</td> <td>NIST07.LIB</td> </tr> <tr> <td>91</td> <td>91</td> <td></td> <td>Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]</td> <td>368</td> <td>C23H48O5</td> <td>NIST07.LIB</td> </tr> <tr> <td>91</td> <td>91</td> <td></td> <td>Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]</td> <td>368</td> <td>C23H48O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>91</td> <td>91</td> <td></td> <td>Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]</td> <td>368</td> <td>C23H48O5</td> <td>NIST08a.LIB</td> </tr> <tr> <td>95</td> <td>95</td> <td></td> <td>Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]</td> <td>368</td> <td>C23H48O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]</td> <td>368</td> <td>C23H48O5</td> <td>NIST21.LIB</td> </tr> <tr> <td>84</td> <td>84</td> <td></td> <td>Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]</td> <td>368</td> <td>C23H48O5</td> <td>NIST08a.LIB</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>MENTHOL TMS S8</td> <td>228</td> <td>C13H26O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>78</td> <td>78</td> <td></td> <td>Stane, trimethyl(5-methyl-2-ethylhexyl)octyl</td> <td>228</td> <td>C13H26O5</td> <td>NIST08a.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 350: Phytol, trimethyl ether</p> <p>CAS# 0-00-0 Mol Wt: 350 Serial: 15404</p> <p>Comp Name: Phytol, trimethyl ether</p> <p>Formula: C23H48O5 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	72	99	CP	Phytol, trimethyl ether	350	C23H48O5	NIST07.LIB	91	91		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST07.LIB	91	91		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	WILEY229.LI	91	91		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST08a.LIB	95	95		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	WILEY229.LI	94	94		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST21.LIB	84	84		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST08a.LIB	78	78		MENTHOL TMS S8	228	C13H26O5	WILEY229.LI	78	78		Stane, trimethyl(5-methyl-2-ethylhexyl)octyl	228	C13H26O5	NIST08a.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
72	99	CP	Phytol, trimethyl ether	350	C23H48O5	NIST07.LIB																																																																			
91	91		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST07.LIB																																																																			
91	91		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	WILEY229.LI																																																																			
91	91		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST08a.LIB																																																																			
95	95		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	WILEY229.LI																																																																			
94	94		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST21.LIB																																																																			
84	84		Stane, [3,7,11,15-tetramethyl-2-hexadecanyl]	368	C23H48O5	NIST08a.LIB																																																																			
78	78		MENTHOL TMS S8	228	C13H26O5	WILEY229.LI																																																																			
78	78		Stane, trimethyl(5-methyl-2-ethylhexyl)octyl	228	C13H26O5	NIST08a.LIB																																																																			
<p><b>27.979</b></p>	<p><b>2206</b></p>	<p><b>2208</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>95</td> <td>95</td> <td>CP</td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST07.LIB</td> </tr> <tr> <td>95</td> <td>95</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>95</td> <td>95</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>94</td> <td>94</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST21.LIB</td> </tr> <tr> <td>93</td> <td>93</td> <td></td> <td>Linoleic acid TMS S8</td> <td>352</td> <td>C21H40O2</td> <td>NIST07.LIB</td> </tr> <tr> <td>92</td> <td>92</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 352: 9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester S8</p> <p>CAS# 56259-07-5 Mol Wt: 352 Serial: 84722</p> <p>Comp Name: 9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester S8</p> <p>Formula: C21H40O2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	95	95	CP	9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST07.LIB	95	95		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	WILEY229.LI	95	95		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST08a.LIB	94	94		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST08a.LIB	94	94		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	WILEY229.LI	94	94		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST21.LIB	93	93		Linoleic acid TMS S8	352	C21H40O2	NIST07.LIB	92	92		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	WILEY229.LI							
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
95	95	CP	9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST07.LIB																																																																			
95	95		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	WILEY229.LI																																																																			
95	95		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST08a.LIB																																																																			
94	94		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST08a.LIB																																																																			
94	94		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	WILEY229.LI																																																																			
94	94		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST21.LIB																																																																			
93	93		Linoleic acid TMS S8	352	C21H40O2	NIST07.LIB																																																																			
92	92		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	WILEY229.LI																																																																			
<p><b>28.158</b></p>	<p><b>2212</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>95</td> <td>95</td> <td>CP</td> <td>ALPHA-LINOLENIC ACID TMS S8</td> <td>350</td> <td>C21H38O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>95</td> <td>95</td> <td></td> <td>alpha-Linolenic acid, trimethyl ester S8 Tr</td> <td>350</td> <td>C21H38O2</td> <td>NIST07.LIB</td> </tr> <tr> <td>92</td> <td>92</td> <td></td> <td>alpha-Linolenic acid, trimethyl ester S8 Tr</td> <td>350</td> <td>C21H38O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>92</td> <td>92</td> <td></td> <td>Linolenic acid TMS S8</td> <td>350</td> <td>C21H38O2</td> <td>NIST07.LIB</td> </tr> <tr> <td>91</td> <td>91</td> <td></td> <td>alpha-Linolenic acid, trimethyl ester S8 Tr</td> <td>350</td> <td>C21H38O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>85</td> <td>85</td> <td></td> <td>Linolenic acid, trimethyl ester</td> <td>350</td> <td>C21H38O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>83</td> <td>83</td> <td></td> <td>alpha-9,11-Eicosadienoic acid, trimethyl ester</td> <td>378</td> <td>C23H42O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester</td> <td>352</td> <td>C21H40O2</td> <td>NIST21.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 350: ALPHA-LINOLENIC ACID TMS S8</p> <p>CAS# 97844-13-8 Mol Wt: 350 Serial: 174950</p> <p>Comp Name: ALPHA-LINOLENIC ACID TMS S8</p> <p>Formula: C21H38O2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	95	95	CP	ALPHA-LINOLENIC ACID TMS S8	350	C21H38O2	WILEY229.LI	95	95		alpha-Linolenic acid, trimethyl ester S8 Tr	350	C21H38O2	NIST07.LIB	92	92		alpha-Linolenic acid, trimethyl ester S8 Tr	350	C21H38O2	NIST08a.LIB	92	92		Linolenic acid TMS S8	350	C21H38O2	NIST07.LIB	91	91		alpha-Linolenic acid, trimethyl ester S8 Tr	350	C21H38O2	NIST08a.LIB	85	85		Linolenic acid, trimethyl ester	350	C21H38O2	NIST08a.LIB	83	83		alpha-9,11-Eicosadienoic acid, trimethyl ester	378	C23H42O2	NIST08a.LIB	82	82		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST21.LIB							
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
95	95	CP	ALPHA-LINOLENIC ACID TMS S8	350	C21H38O2	WILEY229.LI																																																																			
95	95		alpha-Linolenic acid, trimethyl ester S8 Tr	350	C21H38O2	NIST07.LIB																																																																			
92	92		alpha-Linolenic acid, trimethyl ester S8 Tr	350	C21H38O2	NIST08a.LIB																																																																			
92	92		Linolenic acid TMS S8	350	C21H38O2	NIST07.LIB																																																																			
91	91		alpha-Linolenic acid, trimethyl ester S8 Tr	350	C21H38O2	NIST08a.LIB																																																																			
85	85		Linolenic acid, trimethyl ester	350	C21H38O2	NIST08a.LIB																																																																			
83	83		alpha-9,11-Eicosadienoic acid, trimethyl ester	378	C23H42O2	NIST08a.LIB																																																																			
82	82		9,12-Octadecadienoic acid (Z,Z)-, trimethyl ester	352	C21H40O2	NIST21.LIB																																																																			
<p><b>28.396</b></p>	<p><b>2221</b></p>	<p><b>2215</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>82</td> <td>82</td> <td>CP</td> <td>trans-9-Octadecenoic acid, trimethyl ester</td> <td>354</td> <td>C21H40O2</td> <td>NIST07.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>trans-9-Octadecenoic acid, trimethyl ester</td> <td>354</td> <td>C21H40O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>trans-9-OCTADECENOIC ACID TMS S8</td> <td>354</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>Oleic acid, trimethyl ester (CAS) TRIMETHYL</td> <td>354</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>Oleic acid, trimethyl ester S8</td> <td>354</td> <td>C21H40O2</td> <td>NIST07.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>11-ene-Octadecenoic acid, trimethyl ester S</td> <td>354</td> <td>C21H40O2</td> <td>NIST07.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>Oleic acid, trimethyl ester S8 Trimethyl (</td> <td>354</td> <td>C21H40O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>Oleic acid, trimethyl ester</td> <td>354</td> <td>C21H40O2</td> <td>NIST21.LIB</td> </tr> <tr> <td>82</td> <td>82</td> <td></td> <td>Oleic acid, trimethyl ester S8 Trimethyl (</td> <td>354</td> <td>C21H40O2</td> <td>NIST08a.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>4: 354: Oleic acid, trimethyl ester (CAS) TRIMETHYLSYL ESTER OF OLEIC ACID S8 MONOTRIMETHYLSYL OLEIC ACID S8 OLEIC ACID-MONOTMS S8</p> <p>CAS# 21596-26-3 Mol Wt: 354 Serial: 175988</p> <p>Comp Name: Oleic acid, trimethyl ester (CAS) TRIMETHYLSYL ESTER OF OLEIC ACID S8 MONOTRIMETHYLSYL OLEIC ACID S8 OLEIC ACID-MONOTMS S8</p> <p>Formula: C21H40O2 Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	82	82	CP	trans-9-Octadecenoic acid, trimethyl ester	354	C21H40O2	NIST07.LIB	82	82		trans-9-Octadecenoic acid, trimethyl ester	354	C21H40O2	NIST08a.LIB	82	82		trans-9-OCTADECENOIC ACID TMS S8	354	C21H40O2	WILEY229.LI	82	82		Oleic acid, trimethyl ester (CAS) TRIMETHYL	354	C21H40O2	WILEY229.LI	82	82		Oleic acid, trimethyl ester S8	354	C21H40O2	NIST07.LIB	82	82		11-ene-Octadecenoic acid, trimethyl ester S	354	C21H40O2	NIST07.LIB	82	82		Oleic acid, trimethyl ester S8 Trimethyl (	354	C21H40O2	NIST08a.LIB	82	82		Oleic acid, trimethyl ester	354	C21H40O2	NIST21.LIB	82	82		Oleic acid, trimethyl ester S8 Trimethyl (	354	C21H40O2	NIST08a.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
82	82	CP	trans-9-Octadecenoic acid, trimethyl ester	354	C21H40O2	NIST07.LIB																																																																			
82	82		trans-9-Octadecenoic acid, trimethyl ester	354	C21H40O2	NIST08a.LIB																																																																			
82	82		trans-9-OCTADECENOIC ACID TMS S8	354	C21H40O2	WILEY229.LI																																																																			
82	82		Oleic acid, trimethyl ester (CAS) TRIMETHYL	354	C21H40O2	WILEY229.LI																																																																			
82	82		Oleic acid, trimethyl ester S8	354	C21H40O2	NIST07.LIB																																																																			
82	82		11-ene-Octadecenoic acid, trimethyl ester S	354	C21H40O2	NIST07.LIB																																																																			
82	82		Oleic acid, trimethyl ester S8 Trimethyl (	354	C21H40O2	NIST08a.LIB																																																																			
82	82		Oleic acid, trimethyl ester	354	C21H40O2	NIST21.LIB																																																																			
82	82		Oleic acid, trimethyl ester S8 Trimethyl (	354	C21H40O2	NIST08a.LIB																																																																			



# ANEXOS

<p><b>28.849</b></p>	<p><b>2237</b></p>	<table border="1"> <thead> <tr> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>72</td> <td>C</td> <td>7-Trimethylsilyloxy-7-methyloctanoic acid trimethyl ester</td> <td>318</td> <td>C15H34O5Si3</td> <td>NIST07.LIB</td> </tr> <tr> <td>75</td> <td></td> <td>7-OH-7-ME-OCTANOIC ACID 2TMS SS</td> <td>318</td> <td>C15H34O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>75</td> <td></td> <td>2-Methyl-3-pentanol, trimethylsilyl ether</td> <td>174</td> <td>C9H20OSi3</td> <td>NIST08.LIB</td> </tr> <tr> <td>75</td> <td></td> <td>Linalol oxide, trimethylsilyl ether</td> <td>242</td> <td>C13H26O2Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>74</td> <td></td> <td>Slane, (1,1-dimethylpropoxy)trimethyl-SS tert-P</td> <td>160</td> <td>C8H20O3Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>72</td> <td></td> <td>Propanoic acid, t-butyl(dimethylsilyl) ester SS tert</td> <td>188</td> <td>C9H20O3Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>72</td> <td></td> <td>3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct</td> <td>262</td> <td>C12H20O10</td> <td>NIST107.LIB</td> </tr> <tr> <td>72</td> <td></td> <td>2,3-BUTANDIOL, 2,3-DIMETHYL-BIS-O-TTRI</td> <td>262</td> <td>C12H20O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Base Peak: 131/10.000</p> <p>9: 7-Trimethylsilyloxy-7-methyloctanoic acid, trimethylsilyl ester SS</p> <p>Base Peak: 131/10.000</p> <p>0: 0:0:0 Mol Wt: 318 Serial#: 76655</p> <p>Comp Name: 7-Trimethylsilyloxy-7-methyloctanoic acid, trimethylsilyl ester SS</p> <p>Formula: C15H34O5Si3 Class Flag: No Class Flags</p>	Similar	Flag	Compound Name	Mol Wt	Formula	Library	72	C	7-Trimethylsilyloxy-7-methyloctanoic acid trimethyl ester	318	C15H34O5Si3	NIST07.LIB	75		7-OH-7-ME-OCTANOIC ACID 2TMS SS	318	C15H34O3	WILEY229.LI	75		2-Methyl-3-pentanol, trimethylsilyl ether	174	C9H20OSi3	NIST08.LIB	75		Linalol oxide, trimethylsilyl ether	242	C13H26O2Si3	NIST08.LIB	74		Slane, (1,1-dimethylpropoxy)trimethyl-SS tert-P	160	C8H20O3Si3	NIST08.LIB	72		Propanoic acid, t-butyl(dimethylsilyl) ester SS tert	188	C9H20O3Si3	NIST08.LIB	72		3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct	262	C12H20O10	NIST107.LIB	72		2,3-BUTANDIOL, 2,3-DIMETHYL-BIS-O-TTRI	262	C12H20O2	WILEY229.LI						
Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																									
72	C	7-Trimethylsilyloxy-7-methyloctanoic acid trimethyl ester	318	C15H34O5Si3	NIST07.LIB																																																									
75		7-OH-7-ME-OCTANOIC ACID 2TMS SS	318	C15H34O3	WILEY229.LI																																																									
75		2-Methyl-3-pentanol, trimethylsilyl ether	174	C9H20OSi3	NIST08.LIB																																																									
75		Linalol oxide, trimethylsilyl ether	242	C13H26O2Si3	NIST08.LIB																																																									
74		Slane, (1,1-dimethylpropoxy)trimethyl-SS tert-P	160	C8H20O3Si3	NIST08.LIB																																																									
72		Propanoic acid, t-butyl(dimethylsilyl) ester SS tert	188	C9H20O3Si3	NIST08.LIB																																																									
72		3,6-Dioxo-2,7-dialdoctane, 2,2,4,4,5,5,7,7-oct	262	C12H20O10	NIST107.LIB																																																									
72		2,3-BUTANDIOL, 2,3-DIMETHYL-BIS-O-TTRI	262	C12H20O2	WILEY229.LI																																																									
<p><b>29.033</b></p>	<p><b>2243</b></p>	<table border="1"> <thead> <tr> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester SS Stear</td> <td>356</td> <td>C21H44O5Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester SS Stear</td> <td>356</td> <td>C21H44O5Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester SS Stear</td> <td>356</td> <td>C21H44O5Si3</td> <td>NIST11.LIB</td> </tr> <tr> <td>5</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester SS Stear</td> <td>356</td> <td>C21H44O5Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester (CAS) S</td> <td>356</td> <td>C21H44O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester (CAS) S</td> <td>356</td> <td>C21H44O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester SS Stear</td> <td>356</td> <td>C21H44O5Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester (CAS) S</td> <td>356</td> <td>C21H44O5</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Base Peak: 117/10.000</p> <p>1: 356: Octadecanoic acid, trimethylsilyl ester SS Stearic acid, trimethylsilyl ester SS Trimethylsilyl ester of Octadecanoic acid SS Trimethylsilyl stearate # SS Trimethylsilyl stearate # SS</p> <p>Base Peak: 117/10.000</p> <p>CAS# 18748-91-9 Mol Wt: 356 Serial#: 148420</p> <p>Comp Name: Octadecanoic acid, trimethylsilyl ester SS Stearic acid, trimethylsilyl ester SS Trimethylsilyl ester of Octadecanoic acid SS Trimethylsilyl stearate # SS</p> <p>Formula: C21H44O5Si3 Class Flag: No Class Flags</p>	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST107.LIB	3		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST08.LIB	4		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST11.LIB	5		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST08.LIB	6		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C21H44O5	WILEY229.LI	7		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C21H44O5	WILEY229.LI	8		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST107.LIB	9		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C21H44O5	WILEY229.LI						
Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																									
1		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST107.LIB																																																									
3		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST08.LIB																																																									
4		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST11.LIB																																																									
5		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST08.LIB																																																									
6		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C21H44O5	WILEY229.LI																																																									
7		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C21H44O5	WILEY229.LI																																																									
8		Octadecanoic acid, trimethylsilyl ester SS Stear	356	C21H44O5Si3	NIST107.LIB																																																									
9		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C21H44O5	WILEY229.LI																																																									
<p><b>30.042</b></p>	<p><b>2277</b></p>	<table border="1"> <thead> <tr> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> <td>Oleanthene</td> <td>263</td> <td>C18H31</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td></td> <td>9-Octadecenal, (Z)- (CAS) C15-OC1AUCD-9-E</td> <td>258</td> <td>C18H34O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td></td> <td>9-Octadecenal, (Z)- 9-Octadecyl SS cis-9-</td> <td>258</td> <td>C18H34O</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td></td> <td>9-Octadecenal, (Z)- 9-Octadecyl SS cis-9-</td> <td>258</td> <td>C18H34O</td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td></td> <td>as 9-Hexadecenal SS 9-Hexadecenal, (Z)- SS</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td></td> <td>7-Hexadecenal, (Z)- SS (Z)-7-Hexadecenal SS</td> <td>238</td> <td>C16H30O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td></td> <td>2-7-Hexadecenal SS</td> <td>238</td> <td>C16H30O</td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td></td> <td>8-Hexadecenal, 14-methyl-, (Z)- SS 14-Methyl-</td> <td>252</td> <td>C17H32O</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td></td> <td>13-Tetradecenal SS</td> <td>210</td> <td>C14H26O</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Base Peak: 55/10.000</p> <p>1: 263: Oleanthene</p> <p>Base Peak: 41/10.000</p> <p>CAS# 0:0:0:0 Mol Wt: 263 Serial#: 89504</p> <p>Comp Name: Oleanthene</p> <p>Formula: C18H31 Class Flag: No Class Flags</p>	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1		Oleanthene	263	C18H31	NIST08.LIB	2		9-Octadecenal, (Z)- (CAS) C15-OC1AUCD-9-E	258	C18H34O	WILEY229.LI	3		9-Octadecenal, (Z)- 9-Octadecyl SS cis-9-	258	C18H34O	NIST08.LIB	4		9-Octadecenal, (Z)- 9-Octadecyl SS cis-9-	258	C18H34O	NIST107.LIB	5		as 9-Hexadecenal SS 9-Hexadecenal, (Z)- SS	238	C16H30O	NIST08.LIB	6		7-Hexadecenal, (Z)- SS (Z)-7-Hexadecenal SS	238	C16H30O	NIST08.LIB	8		2-7-Hexadecenal SS	238	C16H30O	NIST107.LIB	8		8-Hexadecenal, 14-methyl-, (Z)- SS 14-Methyl-	252	C17H32O	NIST08.LIB	9		13-Tetradecenal SS	210	C14H26O	NIST107.LIB
Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																									
1		Oleanthene	263	C18H31	NIST08.LIB																																																									
2		9-Octadecenal, (Z)- (CAS) C15-OC1AUCD-9-E	258	C18H34O	WILEY229.LI																																																									
3		9-Octadecenal, (Z)- 9-Octadecyl SS cis-9-	258	C18H34O	NIST08.LIB																																																									
4		9-Octadecenal, (Z)- 9-Octadecyl SS cis-9-	258	C18H34O	NIST107.LIB																																																									
5		as 9-Hexadecenal SS 9-Hexadecenal, (Z)- SS	238	C16H30O	NIST08.LIB																																																									
6		7-Hexadecenal, (Z)- SS (Z)-7-Hexadecenal SS	238	C16H30O	NIST08.LIB																																																									
8		2-7-Hexadecenal SS	238	C16H30O	NIST107.LIB																																																									
8		8-Hexadecenal, 14-methyl-, (Z)- SS 14-Methyl-	252	C17H32O	NIST08.LIB																																																									
9		13-Tetradecenal SS	210	C14H26O	NIST107.LIB																																																									
<p><b>30.866</b></p>	<p><b>2308</b></p>	<table border="1"> <thead> <tr> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> <td>Oleanthene, N-trimethylsilyl</td> <td>253</td> <td>C19H41O3Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td></td> <td>Slane, [1-ethoxydecyl]trimethyl-SS</td> <td>258</td> <td>C19H40O3Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td></td> <td>Slane, [1-ethoxydecyl]trimethyl- (CAS) 3-DO</td> <td>258</td> <td>C19H40O3Si3</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td></td> <td>Slane, [1-ethoxydecyl]trimethyl-SS [1-Ethyl]</td> <td>258</td> <td>C19H40O3Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td></td> <td>3-Ethyl-3-trimethylsilyloxydecane</td> <td>230</td> <td>C19H40O3Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td></td> <td>3-Ethyl-3-trimethylsilyloxydecane SS</td> <td>230</td> <td>C19H40O3Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td></td> <td>6-Ethyl-3-trimethylsilyloxydecane SS</td> <td>258</td> <td>C19H40O3Si3</td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td></td> <td>6-Ethyl-3-trimethylsilyloxydecane</td> <td>258</td> <td>C19H40O3Si3</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td></td> <td>7-OH-7-ME-OCTANOIC ACID 2TMS SS</td> <td>318</td> <td>C15H34O3Si3</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Base Peak: 131/10.000</p> <p>1: 353: Oleanthene, N-trimethylsilyl</p> <p>Base Peak: 79/10.000</p> <p>CAS# 0:0:0:0 Mol Wt: 253 Serial#: 146609</p> <p>Comp Name: Oleanthene, N-trimethylsilyl</p> <p>Formula: C19H41O3Si3 Class Flag: No Class Flags</p>	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1		Oleanthene, N-trimethylsilyl	253	C19H41O3Si3	NIST08.LIB	2		Slane, [1-ethoxydecyl]trimethyl-SS	258	C19H40O3Si3	NIST107.LIB	3		Slane, [1-ethoxydecyl]trimethyl- (CAS) 3-DO	258	C19H40O3Si3	WILEY229.LI	4		Slane, [1-ethoxydecyl]trimethyl-SS [1-Ethyl]	258	C19H40O3Si3	NIST08.LIB	5		3-Ethyl-3-trimethylsilyloxydecane	230	C19H40O3Si3	NIST08.LIB	6		3-Ethyl-3-trimethylsilyloxydecane SS	230	C19H40O3Si3	NIST107.LIB	7		6-Ethyl-3-trimethylsilyloxydecane SS	258	C19H40O3Si3	NIST107.LIB	8		6-Ethyl-3-trimethylsilyloxydecane	258	C19H40O3Si3	NIST08.LIB	9		7-OH-7-ME-OCTANOIC ACID 2TMS SS	318	C15H34O3Si3	WILEY229.LI
Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																									
1		Oleanthene, N-trimethylsilyl	253	C19H41O3Si3	NIST08.LIB																																																									
2		Slane, [1-ethoxydecyl]trimethyl-SS	258	C19H40O3Si3	NIST107.LIB																																																									
3		Slane, [1-ethoxydecyl]trimethyl- (CAS) 3-DO	258	C19H40O3Si3	WILEY229.LI																																																									
4		Slane, [1-ethoxydecyl]trimethyl-SS [1-Ethyl]	258	C19H40O3Si3	NIST08.LIB																																																									
5		3-Ethyl-3-trimethylsilyloxydecane	230	C19H40O3Si3	NIST08.LIB																																																									
6		3-Ethyl-3-trimethylsilyloxydecane SS	230	C19H40O3Si3	NIST107.LIB																																																									
7		6-Ethyl-3-trimethylsilyloxydecane SS	258	C19H40O3Si3	NIST107.LIB																																																									
8		6-Ethyl-3-trimethylsilyloxydecane	258	C19H40O3Si3	NIST08.LIB																																																									
9		7-OH-7-ME-OCTANOIC ACID 2TMS SS	318	C15H34O3Si3	WILEY229.LI																																																									

# ANEXOS

<p><b>31.992</b></p>	<p><b>2350</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>72</td> <td>CP</td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST198.LIB</td> </tr> <tr> <td>2</td> <td>51</td> <td></td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>93</td> <td></td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST171.LIB</td> </tr> <tr> <td>4</td> <td>90</td> <td></td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>90</td> <td></td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST171.LIB</td> </tr> <tr> <td>6</td> <td>90</td> <td></td> <td>12-Docosanoic acid (Z)-delta-9</td> <td>327</td> <td>C22H42O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>7</td> <td>90</td> <td></td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>8</td> <td>89</td> <td></td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST08a.LIB</td> </tr> <tr> <td>9</td> <td>89</td> <td></td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1: 281.9-Octadecenoic acid (Z)-delta-9</p> <p>CAS# 301-02-0 Mol Wt: 281 Serial#: 23344</p> <p>Comp Name: 9-Octadecenoic acid (Z)-delta-9</p> <p>Formula: C18H34O2 Class Flag: No Class Flags</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB	2	51		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	WILEY229.LI	3	93		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST171.LIB	4	90		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	WILEY229.LI	5	90		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST171.LIB	6	90		12-Docosanoic acid (Z)-delta-9	327	C22H42O2	NIST08a.LIB	7	90		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST08a.LIB	8	89		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST08a.LIB	9	89		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST107.LIB
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
1	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB																																																																		
2	51		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	WILEY229.LI																																																																		
3	93		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST171.LIB																																																																		
4	90		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	WILEY229.LI																																																																		
5	90		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST171.LIB																																																																		
6	90		12-Docosanoic acid (Z)-delta-9	327	C22H42O2	NIST08a.LIB																																																																		
7	90		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST08a.LIB																																																																		
8	89		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST08a.LIB																																																																		
9	89		9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST107.LIB																																																																		
<p><b>33.345</b></p>	<p><b>2399</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>72</td> <td>CP</td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST198.LIB</td> </tr> <tr> <td>2</td> <td>72</td> <td>CP</td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>66</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-dimethyl</td> <td>352</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>67</td> <td></td> <td>MYRISTOLEIC ACID TMS SS</td> <td>298</td> <td>C17H34O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>66</td> <td></td> <td>PALMITOLEIC ACID TMS SS</td> <td>326</td> <td>C19H38O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>66</td> <td></td> <td>UNDECENOIC ACID TMS SS</td> <td>256</td> <td>C14H28O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>66</td> <td></td> <td>9,12-Octadecadienoic acid (Z,Z)-dimethyl</td> <td>352</td> <td>C21H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>65</td> <td></td> <td>11,14-EICOSADIENOIC ACID TMS SS</td> <td>380</td> <td>C23H44O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>65</td> <td></td> <td>11-EICOSAENOIC ACID TMS SS</td> <td>382</td> <td>C23H46O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>2: 353. Oleamide, N-henethyl</p> <p>CAS# 0-00-0 Mol Wt: 353 Serial#: 146689</p> <p>Comp Name: Oleamide, N-henethyl</p> <p>Formula: C21H43NO2 Class Flag: No Class Flags</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB	2	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST107.LIB	3	66		9,12-Octadecadienoic acid (Z,Z)-dimethyl	352	C21H40O2	WILEY229.LI	4	67		MYRISTOLEIC ACID TMS SS	298	C17H34O2	WILEY229.LI	5	66		PALMITOLEIC ACID TMS SS	326	C19H38O2	WILEY229.LI	6	66		UNDECENOIC ACID TMS SS	256	C14H28O2	WILEY229.LI	7	66		9,12-Octadecadienoic acid (Z,Z)-dimethyl	352	C21H40O2	WILEY229.LI	8	65		11,14-EICOSADIENOIC ACID TMS SS	380	C23H44O2	WILEY229.LI	9	65		11-EICOSAENOIC ACID TMS SS	382	C23H46O2	WILEY229.LI
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
1	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB																																																																		
2	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST107.LIB																																																																		
3	66		9,12-Octadecadienoic acid (Z,Z)-dimethyl	352	C21H40O2	WILEY229.LI																																																																		
4	67		MYRISTOLEIC ACID TMS SS	298	C17H34O2	WILEY229.LI																																																																		
5	66		PALMITOLEIC ACID TMS SS	326	C19H38O2	WILEY229.LI																																																																		
6	66		UNDECENOIC ACID TMS SS	256	C14H28O2	WILEY229.LI																																																																		
7	66		9,12-Octadecadienoic acid (Z,Z)-dimethyl	352	C21H40O2	WILEY229.LI																																																																		
8	65		11,14-EICOSADIENOIC ACID TMS SS	380	C23H44O2	WILEY229.LI																																																																		
9	65		11-EICOSAENOIC ACID TMS SS	382	C23H46O2	WILEY229.LI																																																																		
<p><b>33.545</b></p>	<p><b>2407</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>72</td> <td>CP</td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST198.LIB</td> </tr> <tr> <td>2</td> <td>50</td> <td></td> <td>TRANS-9-OCTADECENOIC ACID TMS SS</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>65</td> <td></td> <td>TRANS-9-OCTADECENOIC ACID TMS SS</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>65</td> <td></td> <td>Oleic acid, trimethyl ester (CAS) TRIMETH</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>64</td> <td></td> <td>Oleic acid, trimethyl ester (CAS) TRIMETH</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>64</td> <td></td> <td>11-EICOSAENOIC ACID TMS SS</td> <td>382</td> <td>C23H46O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>64</td> <td></td> <td>PALMITOLEIC ACID TMS SS</td> <td>326</td> <td>C19H38O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>63</td> <td></td> <td>TRIMETHYL SULTON ESTER OF 7-OXO-NONAN</td> <td>244</td> <td>C12H24O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>63</td> <td></td> <td>MYRISTOLEIC ACID TMS SS</td> <td>298</td> <td>C17H34O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 353. Oleamide, N-henethyl</p> <p>CAS# 0-00-0 Mol Wt: 353 Serial#: 146689</p> <p>Comp Name: Oleamide, N-henethyl</p> <p>Formula: C21H43NO2 Class Flag: No Class Flags</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB	2	50		TRANS-9-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI	3	65		TRANS-9-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI	4	65		Oleic acid, trimethyl ester (CAS) TRIMETH	354	C21H42O2	WILEY229.LI	5	64		Oleic acid, trimethyl ester (CAS) TRIMETH	354	C21H42O2	WILEY229.LI	6	64		11-EICOSAENOIC ACID TMS SS	382	C23H46O2	WILEY229.LI	7	64		PALMITOLEIC ACID TMS SS	326	C19H38O2	WILEY229.LI	8	63		TRIMETHYL SULTON ESTER OF 7-OXO-NONAN	244	C12H24O3	WILEY229.LI	9	63		MYRISTOLEIC ACID TMS SS	298	C17H34O2	WILEY229.LI
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
1	72	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB																																																																		
2	50		TRANS-9-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI																																																																		
3	65		TRANS-9-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI																																																																		
4	65		Oleic acid, trimethyl ester (CAS) TRIMETH	354	C21H42O2	WILEY229.LI																																																																		
5	64		Oleic acid, trimethyl ester (CAS) TRIMETH	354	C21H42O2	WILEY229.LI																																																																		
6	64		11-EICOSAENOIC ACID TMS SS	382	C23H46O2	WILEY229.LI																																																																		
7	64		PALMITOLEIC ACID TMS SS	326	C19H38O2	WILEY229.LI																																																																		
8	63		TRIMETHYL SULTON ESTER OF 7-OXO-NONAN	244	C12H24O3	WILEY229.LI																																																																		
9	63		MYRISTOLEIC ACID TMS SS	298	C17H34O2	WILEY229.LI																																																																		
<p><b>33.573</b></p>	<p><b>2408</b></p>	<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>65</td> <td>CP</td> <td>9-Octadecenoic acid (Z)-delta-9</td> <td>281</td> <td>C18H34O2</td> <td>NIST198.LIB</td> </tr> <tr> <td>2</td> <td>65</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS)</td> <td>342</td> <td>C20H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>65</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS) P</td> <td>328</td> <td>C19H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>65</td> <td></td> <td>11-OCTADECENOIC ACID TMS SS</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>64</td> <td></td> <td>Heptadecanoic acid, trimethyl ester (CAS) P</td> <td>328</td> <td>C19H40O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>64</td> <td></td> <td>5-OH-5-ME-HEXANOIC ACID TMS SS 5-HY</td> <td>290</td> <td>C13H30O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>64</td> <td></td> <td>PALMITOLEIC ACID TMS SS</td> <td>326</td> <td>C19H38O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>64</td> <td></td> <td>TRANS-9-OCTADECENOIC ACID TMS SS</td> <td>354</td> <td>C21H42O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>63</td> <td></td> <td>UNDECENOIC ACID TMS SS</td> <td>256</td> <td>C14H28O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1: 353. Oleamide, N-henethyl</p> <p>CAS# 0-00-0 Mol Wt: 353 Serial#: 146689</p> <p>Comp Name: Oleamide, N-henethyl</p> <p>Formula: C21H43NO2 Class Flag: No Class Flags</p>	RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	65	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB	2	65		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI	3	65		Heptadecanoic acid, trimethyl ester (CAS) P	328	C19H40O2	WILEY229.LI	4	65		11-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI	5	64		Heptadecanoic acid, trimethyl ester (CAS) P	328	C19H40O2	WILEY229.LI	6	64		5-OH-5-ME-HEXANOIC ACID TMS SS 5-HY	290	C13H30O3	WILEY229.LI	7	64		PALMITOLEIC ACID TMS SS	326	C19H38O2	WILEY229.LI	8	64		TRANS-9-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI	9	63		UNDECENOIC ACID TMS SS	256	C14H28O2	WILEY229.LI
RT	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																		
1	65	CP	9-Octadecenoic acid (Z)-delta-9	281	C18H34O2	NIST198.LIB																																																																		
2	65		Heptadecanoic acid, trimethyl ester (CAS)	342	C20H42O2	WILEY229.LI																																																																		
3	65		Heptadecanoic acid, trimethyl ester (CAS) P	328	C19H40O2	WILEY229.LI																																																																		
4	65		11-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI																																																																		
5	64		Heptadecanoic acid, trimethyl ester (CAS) P	328	C19H40O2	WILEY229.LI																																																																		
6	64		5-OH-5-ME-HEXANOIC ACID TMS SS 5-HY	290	C13H30O3	WILEY229.LI																																																																		
7	64		PALMITOLEIC ACID TMS SS	326	C19H38O2	WILEY229.LI																																																																		
8	64		TRANS-9-OCTADECENOIC ACID TMS SS	354	C21H42O2	WILEY229.LI																																																																		
9	63		UNDECENOIC ACID TMS SS	256	C14H28O2	WILEY229.LI																																																																		

# ANEXOS

<p><b>33.779</b></p>	<p><b>2415</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>57</td> <td>CP</td> <td><b>Octanoic acid, trimethylsilyl ester</b></td> <td>254</td> <td>C<sub>11</sub>H<sub>24</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>57</td> <td>CP</td> <td>Octanoic acid, trimethylsilyl ester (CAS) MON</td> <td>354</td> <td>C<sub>23</sub>H<sub>48</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>66</td> <td></td> <td>Stane, [1-ethyldecyl]oxy]trimethyl (CAS) 3-DO</td> <td>258</td> <td>C<sub>15</sub>H<sub>34</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>66</td> <td></td> <td>Nonadecanoic acid, trimethylsilyl ester (CAS)</td> <td>370</td> <td>C<sub>22</sub>H<sub>46</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>65</td> <td></td> <td>Dodecanoic acid, trimethylsilyl ester (CAS) LA</td> <td>272</td> <td>C<sub>15</sub>H<sub>32</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>65</td> <td></td> <td>UNDECANOIC ACID ITMS S5</td> <td>256</td> <td>C<sub>14</sub>H<sub>28</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>65</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>65</td> <td></td> <td>Heptadecanoic acid, trimethylsilyl ester (CAS)</td> <td>342</td> <td>C<sub>20</sub>H<sub>42</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>65</td> <td></td> <td>5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY</td> <td>290</td> <td>C<sub>13</sub>H<sub>30</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target:</p> <p>1 : 353: Oleamide, N-trimethylsilyl-</p> <p>CAS# : 0-00-0 Mol Wt: 353 Serial#: 146689</p> <p>Compound Name: Oleamide, N-trimethylsilyl-</p> <p>Formula: C<sub>21</sub>H<sub>42</sub>NOSi Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	57	CP	<b>Octanoic acid, trimethylsilyl ester</b>	254	C <sub>11</sub> H <sub>24</sub> O <sub>2</sub>	NIST107.LIB	2	57	CP	Octanoic acid, trimethylsilyl ester (CAS) MON	354	C <sub>23</sub> H <sub>48</sub> O <sub>2</sub>	WILEY229.LI	3	66		Stane, [1-ethyldecyl]oxy]trimethyl (CAS) 3-DO	258	C <sub>15</sub> H <sub>34</sub> O	WILEY229.LI	4	66		Nonadecanoic acid, trimethylsilyl ester (CAS)	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI	5	65		Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub>	WILEY229.LI	6	65		UNDECANOIC ACID ITMS S5	256	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	WILEY229.LI	7	65		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI	8	65		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI	9	65		5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	57	CP	<b>Octanoic acid, trimethylsilyl ester</b>	254	C <sub>11</sub> H <sub>24</sub> O <sub>2</sub>	NIST107.LIB																																																																			
2	57	CP	Octanoic acid, trimethylsilyl ester (CAS) MON	354	C <sub>23</sub> H <sub>48</sub> O <sub>2</sub>	WILEY229.LI																																																																			
3	66		Stane, [1-ethyldecyl]oxy]trimethyl (CAS) 3-DO	258	C <sub>15</sub> H <sub>34</sub> O	WILEY229.LI																																																																			
4	66		Nonadecanoic acid, trimethylsilyl ester (CAS)	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	65		Dodecanoic acid, trimethylsilyl ester (CAS) LA	272	C <sub>15</sub> H <sub>32</sub> O <sub>2</sub>	WILEY229.LI																																																																			
6	65		UNDECANOIC ACID ITMS S5	256	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	WILEY229.LI																																																																			
7	65		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI																																																																			
8	65		Heptadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI																																																																			
9	65		5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI																																																																			
<p><b>33.894</b></p>	<p><b>2420</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>64</td> <td>CP</td> <td><b>5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY</b></td> <td>290</td> <td>C<sub>13</sub>H<sub>30</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>64</td> <td>CP</td> <td>5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY</td> <td>290</td> <td>C<sub>13</sub>H<sub>30</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>63</td> <td></td> <td>Stane, [1-ethyldecyl]oxy]trimethyl (CAS) 3-DO</td> <td>258</td> <td>C<sub>15</sub>H<sub>34</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>62</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS) P</td> <td>328</td> <td>C<sub>19</sub>H<sub>40</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>61</td> <td></td> <td>METHYL 5OH-5METHYLHEXANOATE ITM</td> <td>232</td> <td>C<sub>11</sub>H<sub>24</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>61</td> <td></td> <td>ETHYL 5OH-5ME HEXANOATE ITMS S5</td> <td>246</td> <td>C<sub>12</sub>H<sub>26</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>61</td> <td></td> <td>Hexadecanoic acid, trimethylsilyl ester (CAS)</td> <td>342</td> <td>C<sub>20</sub>H<sub>42</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>61</td> <td></td> <td>7OH-7ME-OCTANOIC ACID 2TMS S5</td> <td>318</td> <td>C<sub>15</sub>H<sub>34</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>60</td> <td></td> <td>5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY</td> <td>290</td> <td>C<sub>13</sub>H<sub>30</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target:</p> <p>1 : 353: Oleamide, N-trimethylsilyl-</p> <p>CAS# : 0-00-0 Mol Wt: 353 Serial#: 146689</p> <p>Compound Name: Oleamide, N-trimethylsilyl-</p> <p>Formula: C<sub>21</sub>H<sub>42</sub>NOSi Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	64	CP	<b>5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY</b>	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI	2	64	CP	5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI	3	63		Stane, [1-ethyldecyl]oxy]trimethyl (CAS) 3-DO	258	C <sub>15</sub> H <sub>34</sub> O	WILEY229.LI	4	62		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI	5	61		METHYL 5OH-5METHYLHEXANOATE ITM	232	C <sub>11</sub> H <sub>24</sub> O <sub>3</sub>	WILEY229.LI	6	61		ETHYL 5OH-5ME HEXANOATE ITMS S5	246	C <sub>12</sub> H <sub>26</sub> O <sub>3</sub>	WILEY229.LI	7	61		Hexadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI	8	61		7OH-7ME-OCTANOIC ACID 2TMS S5	318	C <sub>15</sub> H <sub>34</sub> O <sub>3</sub>	WILEY229.LI	9	60		5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	64	CP	<b>5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY</b>	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI																																																																			
2	64	CP	5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI																																																																			
3	63		Stane, [1-ethyldecyl]oxy]trimethyl (CAS) 3-DO	258	C <sub>15</sub> H <sub>34</sub> O	WILEY229.LI																																																																			
4	62		Hexadecanoic acid, trimethylsilyl ester (CAS) P	328	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	61		METHYL 5OH-5METHYLHEXANOATE ITM	232	C <sub>11</sub> H <sub>24</sub> O <sub>3</sub>	WILEY229.LI																																																																			
6	61		ETHYL 5OH-5ME HEXANOATE ITMS S5	246	C <sub>12</sub> H <sub>26</sub> O <sub>3</sub>	WILEY229.LI																																																																			
7	61		Hexadecanoic acid, trimethylsilyl ester (CAS)	342	C <sub>20</sub> H <sub>42</sub> O <sub>2</sub>	WILEY229.LI																																																																			
8	61		7OH-7ME-OCTANOIC ACID 2TMS S5	318	C <sub>15</sub> H <sub>34</sub> O <sub>3</sub>	WILEY229.LI																																																																			
9	60		5-OH-5-ME-HEXANOIC ACID 2TMS S5 5-HY	290	C <sub>13</sub> H <sub>30</sub> O <sub>3</sub>	WILEY229.LI																																																																			
<p><b>34.354</b></p>	<p><b>2437</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>73</td> <td>CP</td> <td><b>7OH-7ME-OCTANOIC ACID 2TMS S5</b></td> <td>318</td> <td>C<sub>15</sub>H<sub>34</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>72</td> <td></td> <td>7-Trimethylsilyloxy-7-methyloctanoic acid tmsa</td> <td>318</td> <td>C<sub>15</sub>H<sub>34</sub>O<sub>3</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>72</td> <td></td> <td>Stane, [dimethylsilyloxy]trimethyl-</td> <td>146</td> <td>CH<sub>18</sub>SiO<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>72</td> <td></td> <td>Stane, [dimethylsilyloxy]trimethyl-</td> <td>146</td> <td>CH<sub>18</sub>SiO<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>5</td> <td>72</td> <td></td> <td>2,3-BUTANEDIOL, 2,3-DIMETHYL-BIS-O-(TRI</td> <td>262</td> <td>C<sub>12</sub>H<sub>20</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>72</td> <td></td> <td>3,6-Dioxo-2,7-dioxolane, 2,2,4,4,5,5,7,7-oct</td> <td>262</td> <td>C<sub>12</sub>H<sub>20</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>71</td> <td></td> <td>3-Trimethylsilyloxy-5-nonanoic S5</td> <td>212</td> <td>C<sub>12</sub>H<sub>24</sub>O<sub>3</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>71</td> <td></td> <td>Stane, [dimethylsilyloxy]trimethyl- S5 2,4-D</td> <td>146</td> <td>CH<sub>18</sub>SiO<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>9</td> <td>71</td> <td></td> <td>Stane, [dimethylsilyloxy]trimethyl- S5 2,4-D</td> <td>146</td> <td>CH<sub>18</sub>SiO<sub>2</sub></td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1 : 318: 7OH-7ME-OCTANOIC ACID 2TMS S5</p> <p>CAS# : 0-00-0 Mol Wt: 318 Serial#: 156679</p> <p>Compound Name: 7OH-7ME-OCTANOIC ACID 2TMS S5</p> <p>Formula: C<sub>15</sub>H<sub>34</sub>O<sub>3</sub> Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	73	CP	<b>7OH-7ME-OCTANOIC ACID 2TMS S5</b>	318	C <sub>15</sub> H <sub>34</sub> O <sub>3</sub>	WILEY229.LI	2	72		7-Trimethylsilyloxy-7-methyloctanoic acid tmsa	318	C <sub>15</sub> H <sub>34</sub> O <sub>3</sub>	NIST107.LIB	3	72		Stane, [dimethylsilyloxy]trimethyl-	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB	4	72		Stane, [dimethylsilyloxy]trimethyl-	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB	5	72		2,3-BUTANEDIOL, 2,3-DIMETHYL-BIS-O-(TRI	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	WILEY229.LI	6	72		3,6-Dioxo-2,7-dioxolane, 2,2,4,4,5,5,7,7-oct	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	NIST107.LIB	7	71		3-Trimethylsilyloxy-5-nonanoic S5	212	C <sub>12</sub> H <sub>24</sub> O <sub>3</sub>	NIST107.LIB	8	71		Stane, [dimethylsilyloxy]trimethyl- S5 2,4-D	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB	9	71		Stane, [dimethylsilyloxy]trimethyl- S5 2,4-D	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	73	CP	<b>7OH-7ME-OCTANOIC ACID 2TMS S5</b>	318	C <sub>15</sub> H <sub>34</sub> O <sub>3</sub>	WILEY229.LI																																																																			
2	72		7-Trimethylsilyloxy-7-methyloctanoic acid tmsa	318	C <sub>15</sub> H <sub>34</sub> O <sub>3</sub>	NIST107.LIB																																																																			
3	72		Stane, [dimethylsilyloxy]trimethyl-	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB																																																																			
4	72		Stane, [dimethylsilyloxy]trimethyl-	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB																																																																			
5	72		2,3-BUTANEDIOL, 2,3-DIMETHYL-BIS-O-(TRI	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	WILEY229.LI																																																																			
6	72		3,6-Dioxo-2,7-dioxolane, 2,2,4,4,5,5,7,7-oct	262	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	NIST107.LIB																																																																			
7	71		3-Trimethylsilyloxy-5-nonanoic S5	212	C <sub>12</sub> H <sub>24</sub> O <sub>3</sub>	NIST107.LIB																																																																			
8	71		Stane, [dimethylsilyloxy]trimethyl- S5 2,4-D	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB																																																																			
9	71		Stane, [dimethylsilyloxy]trimethyl- S5 2,4-D	146	CH <sub>18</sub> SiO <sub>2</sub>	NIST107.LIB																																																																			
<p><b>34.446</b></p>	<p><b>2441</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Flag</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>84</td> <td>CP</td> <td><b>Ecicosanoic acid, trimethylsilyl ester</b></td> <td>384</td> <td>C<sub>23</sub>H<sub>46</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>84</td> <td>CP</td> <td>Ecicosanoic acid, trimethylsilyl ester</td> <td>384</td> <td>C<sub>23</sub>H<sub>46</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>84</td> <td></td> <td>Ecicosanoic acid, trimethylsilyl ester (CAS) MON</td> <td>384</td> <td>C<sub>23</sub>H<sub>46</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>78</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester (CAS) S</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>78</td> <td></td> <td>Octadecanoic acid, trimethylsilyl ester S5 Dear</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>78</td> <td></td> <td>Nonadecanoic acid, trimethylsilyl ester S5</td> <td>370</td> <td>C<sub>22</sub>H<sub>46</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>78</td> <td></td> <td>Nonadecanoic acid, trimethylsilyl ester S5 Tm</td> <td>370</td> <td>C<sub>22</sub>H<sub>46</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>78</td> <td></td> <td>Nonadecanoic acid, trimethylsilyl ester (CAS)</td> <td>370</td> <td>C<sub>22</sub>H<sub>46</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>77</td> <td></td> <td>Tetacosanoic acid, trimethylsilyl ester S5</td> <td>440</td> <td>C<sub>27</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1 : 384: Ecicosanoic acid, trimethylsilyl ester</p> <p>CAS# : 55530-70-6 Mol Wt: 384 Serial#: 20023</p> <p>Compound Name: Ecicosanoic acid, trimethylsilyl ester</p> <p>Formula: C<sub>23</sub>H<sub>46</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library	1	84	CP	<b>Ecicosanoic acid, trimethylsilyl ester</b>	384	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB	2	84	CP	Ecicosanoic acid, trimethylsilyl ester	384	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB	3	84		Ecicosanoic acid, trimethylsilyl ester (CAS) MON	384	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI	4	78		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI	5	78		Octadecanoic acid, trimethylsilyl ester S5 Dear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST107.LIB	6	78		Nonadecanoic acid, trimethylsilyl ester S5	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB	7	78		Nonadecanoic acid, trimethylsilyl ester S5 Tm	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB	8	78		Nonadecanoic acid, trimethylsilyl ester (CAS)	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI	9	77		Tetacosanoic acid, trimethylsilyl ester S5	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB
RT	Similar	Flag	Compound Name	Mol Wt	Formula	Library																																																																			
1	84	CP	<b>Ecicosanoic acid, trimethylsilyl ester</b>	384	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB																																																																			
2	84	CP	Ecicosanoic acid, trimethylsilyl ester	384	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB																																																																			
3	84		Ecicosanoic acid, trimethylsilyl ester (CAS) MON	384	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI																																																																			
4	78		Octadecanoic acid, trimethylsilyl ester (CAS) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI																																																																			
5	78		Octadecanoic acid, trimethylsilyl ester S5 Dear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST107.LIB																																																																			
6	78		Nonadecanoic acid, trimethylsilyl ester S5	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB																																																																			
7	78		Nonadecanoic acid, trimethylsilyl ester S5 Tm	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	NIST107.LIB																																																																			
8	78		Nonadecanoic acid, trimethylsilyl ester (CAS)	370	C <sub>22</sub> H <sub>46</sub> O <sub>2</sub>	WILEY229.LI																																																																			
9	77		Tetacosanoic acid, trimethylsilyl ester S5	440	C <sub>27</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB																																																																			



# ANEXOS

<p><b>35.599</b></p>	<p><b>2484</b></p>		<p>Target</p> <p>1. 263 Olefinlike</p> <p>CAS# 0-00-0 Mol Wt. 263 Serial# 89504</p> <p>Comp Name: Olefinlike</p> <p>Formula: C18H32N Class Flag: No Class Flags</p>
<p><b>36.029</b></p>	<p><b>2501</b></p>		<p>Target</p> <p>6. 310. Docosane (CAS) n-Docosane \$S C22H46 STANDARD \$S</p> <p>CAS# 629-97-0 Mol Wt. 310 Serial# 152104</p> <p>Comp Name: Docosane (CAS) n-Docosane \$S C22H46 STANDARD \$S</p> <p>Formula: C22H46 Class Flag: No Class Flags</p>
<p><b>36.583</b></p>	<p><b>2522</b></p>		<p>Target</p> <p>1. 390. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester (CAS) Bis(2-ethylhexyl) phthalate \$S DOP \$S DEHP \$S DOF \$S ONOP \$S Octal \$S Flourel \$S Sical 150 \$S E-vplast 01 \$S Stalox DOP \$S E-vplast 00 \$S VestralAH \$S Trulox DOP \$S Bioflex01 \$S Waco</p> <p>CAS# 117-01-7 Mol Wt. 390 Serial# 150638</p> <p>Comp Name: 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester (CAS) Bis(2-ethylhexyl) phthalate \$S DOP \$S DEHP \$S DOF \$S ONOP \$S Octal \$S Flourel \$S Sical 150 \$S E-vplast 01 \$S Stalox DOP \$S E-vplast 00 \$S VestralAH \$S Trulox DOP \$S Bioflex01 \$S Waco</p> <p>Formula: C24H38O4 Class Flag: No Class Flags</p>
<p><b>38.27</b></p>	<p><b>2589</b></p>		<p>Target</p> <p>1. 474. Heptadecanoic acid, 2,3-bis(trimethylsilyloxy) ester (CAS) 1-MONOPALMITIN-DITHMS \$S Monopalmitin trimethylsilyl ether \$S 1-Monopalmitoylglycerol trimethylsilyl ether \$S</p> <p>CAS# 1160-74-6 Mol Wt. 474 Serial# 211507</p> <p>Comp Name: Heptadecanoic acid, 2,3-bis(trimethylsilyloxy) ester (CAS) 1-MONOPALMITIN-DITHMS \$S Monopalmitin trimethylsilyl ether \$S 1-Monopalmitoylglycerol trimethylsilyl ether \$S</p> <p>Formula: C25H54O4 Si2 Class Flag: No Class Flags</p>

<p>38.358</p>	<p>2592</p>		
<p>38.581</p>	<p>2601</p>		
<p>39.433</p>	<p>2636</p>		
<p>39.522</p>	<p>2640</p>		

# ANEXOS

<p><b>41.001</b></p>	<p><b>2700</b></p>	<p><b>2700</b></p>	<table border="1"> <thead> <tr> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>89</td><td></td><td>Docosane (CAS) n-Docosane \$S C22H46 ST</td><td>310</td><td>C22H46</td><td>WILEY225 LI</td></tr> <tr><td>89</td><td></td><td>Docosane \$S n-Docosane \$S Normal-docosane</td><td>310</td><td>C22H46</td><td>NIST107 LIB</td></tr> <tr><td>89</td><td></td><td>Heptadecane \$S n-Heptadecane \$S NormalH</td><td>240</td><td>C17H36</td><td>NIST107 LIB</td></tr> <tr><td>89</td><td></td><td><b>Octacosane</b></td><td><b>394</b></td><td><b>C28H58</b></td><td><b>NIST107 LIB</b></td></tr> <tr><td>89</td><td></td><td>OCTACOSANE \$S</td><td>394</td><td>C28H58</td><td>WILEY225 LI</td></tr> <tr><td>88</td><td></td><td>Tetracosane</td><td>338</td><td>C24H50</td><td>NIST21 LIB</td></tr> <tr><td>88</td><td></td><td>Tetracosane \$S n-Tetracosane \$S</td><td>338</td><td>C24H50</td><td>NIST08 LIB</td></tr> <tr><td>88</td><td></td><td>HEXACOSANE \$S</td><td>366</td><td>C26H54</td><td>WILEY225 LI</td></tr> <tr><td>88</td><td></td><td>Octadecane (CAS) n-Octadecane \$S</td><td>254</td><td>C18H38</td><td>WILEY225 LI</td></tr> </tbody> </table> <p>94: Octacosane</p> <p>630.02 - 4 Mol Wt: 394 Serial#: 20217</p> <p>Name: Octacosane</p> <p>Id: C28H58 Class Flag: No Class Flags.</p>	Similar	Regi	Compound Name	Mol Wt	Formula	Library	89		Docosane (CAS) n-Docosane \$S C22H46 ST	310	C22H46	WILEY225 LI	89		Docosane \$S n-Docosane \$S Normal-docosane	310	C22H46	NIST107 LIB	89		Heptadecane \$S n-Heptadecane \$S NormalH	240	C17H36	NIST107 LIB	89		<b>Octacosane</b>	<b>394</b>	<b>C28H58</b>	<b>NIST107 LIB</b>	89		OCTACOSANE \$S	394	C28H58	WILEY225 LI	88		Tetracosane	338	C24H50	NIST21 LIB	88		Tetracosane \$S n-Tetracosane \$S	338	C24H50	NIST08 LIB	88		HEXACOSANE \$S	366	C26H54	WILEY225 LI	88		Octadecane (CAS) n-Octadecane \$S	254	C18H38	WILEY225 LI										
Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																				
89		Docosane (CAS) n-Docosane \$S C22H46 ST	310	C22H46	WILEY225 LI																																																																				
89		Docosane \$S n-Docosane \$S Normal-docosane	310	C22H46	NIST107 LIB																																																																				
89		Heptadecane \$S n-Heptadecane \$S NormalH	240	C17H36	NIST107 LIB																																																																				
89		<b>Octacosane</b>	<b>394</b>	<b>C28H58</b>	<b>NIST107 LIB</b>																																																																				
89		OCTACOSANE \$S	394	C28H58	WILEY225 LI																																																																				
88		Tetracosane	338	C24H50	NIST21 LIB																																																																				
88		Tetracosane \$S n-Tetracosane \$S	338	C24H50	NIST08 LIB																																																																				
88		HEXACOSANE \$S	366	C26H54	WILEY225 LI																																																																				
88		Octadecane (CAS) n-Octadecane \$S	254	C18H38	WILEY225 LI																																																																				
<p><b>41.924</b></p>	<p><b>2739</b></p>	<p><b>2731</b></p>	<table border="1"> <thead> <tr> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>78</td><td></td><td>TRIMETHYLSILYL ESTER OF TETRACOSA</td><td>440</td><td>C27H56O2</td><td>WILEY225 LI</td></tr> <tr><td>78</td><td></td><td>Tetracosanoic acid, trimethylsilyl ester \$S Trim</td><td>440</td><td>C27H56O2S</td><td>NIST08 LIB</td></tr> <tr><td>78</td><td></td><td>Tetracosanoic acid, trimethylsilyl ester \$S</td><td>440</td><td>C27H56O2S</td><td>NIST107 LIB</td></tr> <tr><td>78</td><td></td><td><b>Docosanoic acid, trimethylsilyl ester \$S Trimeth</b></td><td><b>412</b></td><td><b>C25H50O2S</b></td><td><b>NIST08 LIB</b></td></tr> <tr><td>78</td><td></td><td>Hexacosanoic acid, trimethylsilyl ester</td><td>468</td><td>C29H60O2S</td><td>NIST08 LIB</td></tr> <tr><td>77</td><td></td><td>Pentacosanoic acid, trimethylsilyl ester</td><td>454</td><td>C28H50O2S</td><td>NIST08 LIB</td></tr> <tr><td>77</td><td></td><td>Docosanoic acid, trimethylsilyl ester (CAS) DO</td><td>412</td><td>C25H50O2</td><td>WILEY225 LI</td></tr> <tr><td>77</td><td></td><td>Docosanoic acid, trimethylsilyl ester \$S</td><td>412</td><td>C25H50O2S</td><td>NIST107 LIB</td></tr> <tr><td>77</td><td></td><td>Docosanoic acid, trimethylsilyl ester \$S Trimeth</td><td>412</td><td>C25H50O2S</td><td>NIST08 LIB</td></tr> </tbody> </table> <p>2: Docosanoic acid, trimethylsilyl ester \$S Trimethylsilyl docosanoate # \$S</p> <p>74367 - 36 - 5 Mol Wt: 412 Serial#: 171217</p> <p>Name: Docosanoic acid, trimethylsilyl ester \$S Trimethylsilyl docosanoate # \$S</p> <p>Id: C25H50O2Si Class Flag: No Class Flags.</p>	Similar	Regi	Compound Name	Mol Wt	Formula	Library	78		TRIMETHYLSILYL ESTER OF TETRACOSA	440	C27H56O2	WILEY225 LI	78		Tetracosanoic acid, trimethylsilyl ester \$S Trim	440	C27H56O2S	NIST08 LIB	78		Tetracosanoic acid, trimethylsilyl ester \$S	440	C27H56O2S	NIST107 LIB	78		<b>Docosanoic acid, trimethylsilyl ester \$S Trimeth</b>	<b>412</b>	<b>C25H50O2S</b>	<b>NIST08 LIB</b>	78		Hexacosanoic acid, trimethylsilyl ester	468	C29H60O2S	NIST08 LIB	77		Pentacosanoic acid, trimethylsilyl ester	454	C28H50O2S	NIST08 LIB	77		Docosanoic acid, trimethylsilyl ester (CAS) DO	412	C25H50O2	WILEY225 LI	77		Docosanoic acid, trimethylsilyl ester \$S	412	C25H50O2S	NIST107 LIB	77		Docosanoic acid, trimethylsilyl ester \$S Trimeth	412	C25H50O2S	NIST08 LIB										
Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																				
78		TRIMETHYLSILYL ESTER OF TETRACOSA	440	C27H56O2	WILEY225 LI																																																																				
78		Tetracosanoic acid, trimethylsilyl ester \$S Trim	440	C27H56O2S	NIST08 LIB																																																																				
78		Tetracosanoic acid, trimethylsilyl ester \$S	440	C27H56O2S	NIST107 LIB																																																																				
78		<b>Docosanoic acid, trimethylsilyl ester \$S Trimeth</b>	<b>412</b>	<b>C25H50O2S</b>	<b>NIST08 LIB</b>																																																																				
78		Hexacosanoic acid, trimethylsilyl ester	468	C29H60O2S	NIST08 LIB																																																																				
77		Pentacosanoic acid, trimethylsilyl ester	454	C28H50O2S	NIST08 LIB																																																																				
77		Docosanoic acid, trimethylsilyl ester (CAS) DO	412	C25H50O2	WILEY225 LI																																																																				
77		Docosanoic acid, trimethylsilyl ester \$S	412	C25H50O2S	NIST107 LIB																																																																				
77		Docosanoic acid, trimethylsilyl ester \$S Trimeth	412	C25H50O2S	NIST08 LIB																																																																				
<p><b>42.974</b></p>	<p><b>2783</b></p>		<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>76</td><td></td><td>Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr</td><td>502</td><td>C27H50O4S</td><td>NIST08 LIB</td></tr> <tr><td>2</td><td>76</td><td></td><td>Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr</td><td>502</td><td>C27H50O4</td><td>WILEY225 LI</td></tr> <tr><td>3</td><td>76</td><td></td><td>Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr</td><td>502</td><td>C27H50O4S</td><td>NIST21 LIB</td></tr> <tr><td>4</td><td>73</td><td></td><td>BIS-O-TRIMETHYLSILYL STEARIC ACID</td><td>502</td><td>C27H50O4</td><td>WILEY225 LI</td></tr> <tr><td>5</td><td>73</td><td></td><td>Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr</td><td>502</td><td>C27H50O4S</td><td>NIST08 LIB</td></tr> <tr><td>6</td><td>73</td><td></td><td>Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr</td><td>502</td><td>C27H50O4S</td><td>NIST21 LIB</td></tr> <tr><td>7</td><td>69</td><td></td><td>Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr</td><td>502</td><td>C27H50O4</td><td>WILEY225 LI</td></tr> <tr><td>8</td><td>68</td><td></td><td>Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr</td><td>502</td><td>C27H50O4</td><td>WILEY225 LI</td></tr> <tr><td>9</td><td>62</td><td></td><td>1,3-DISTEARIN TRIMETHYLSILYLETHERS</td><td>697</td><td>C42H84O5</td><td>WILEY225 LI</td></tr> </tbody> </table> <p>1: 502: Octadecanoic acid, 2,3-bis(trimethylsilyloxy)propyl ester \$S Stearic acid, 2,3-bis(trimethylsilyloxy)propyl ester # \$S 2,3-Bis(trimethylsilyloxy)propyl stearate # \$S</p> <p>CAS# 1168 - 75 - 6 Mol Wt: 502 Serial: 28929</p> <p>Cmpd Name: Octadecanoic acid, 2,3-bis(trimethylsilyloxy)propyl ester \$S Stearic acid, 2,3-bis(trimethylsilyloxy)propyl ester # \$S</p> <p>Formula: C27H50O4Si2 Class Flag: No Class Flags.</p>	#	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	76		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST08 LIB	2	76		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4	WILEY225 LI	3	76		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST21 LIB	4	73		BIS-O-TRIMETHYLSILYL STEARIC ACID	502	C27H50O4	WILEY225 LI	5	73		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST08 LIB	6	73		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST21 LIB	7	69		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4	WILEY225 LI	8	68		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4	WILEY225 LI	9	62		1,3-DISTEARIN TRIMETHYLSILYLETHERS	697	C42H84O5	WILEY225 LI
#	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																			
1	76		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST08 LIB																																																																			
2	76		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4	WILEY225 LI																																																																			
3	76		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST21 LIB																																																																			
4	73		BIS-O-TRIMETHYLSILYL STEARIC ACID	502	C27H50O4	WILEY225 LI																																																																			
5	73		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST08 LIB																																																																			
6	73		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4S	NIST21 LIB																																																																			
7	69		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4	WILEY225 LI																																																																			
8	68		Octadecanoic acid, 2,3-bis(trimethylsilyloxy)pr	502	C27H50O4	WILEY225 LI																																																																			
9	62		1,3-DISTEARIN TRIMETHYLSILYLETHERS	697	C42H84O5	WILEY225 LI																																																																			
<p><b>43.538</b></p>	<p><b>2807</b></p>		<table border="1"> <thead> <tr> <th>#</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>93</td><td></td><td>Squalene \$S 2,6,10,14,18,22-Tetracosahexene</td><td>410</td><td>C30H50</td><td>NIST08 LIB</td></tr> <tr><td>2</td><td>92</td><td></td><td>2,6,10,14,18,22-Tetracosahexene, 2,6,10,15</td><td>410</td><td>C30H50</td><td>NIST08 LIB</td></tr> <tr><td>3</td><td>91</td><td></td><td>Squalene \$S 2,6,10,14,18,22-Tetracosahexene</td><td>410</td><td>C30H50</td><td>NIST08 LIB</td></tr> <tr><td>4</td><td>91</td><td></td><td>2,6,10,14,18,22-Tetracosahexene, 2,6,10,15</td><td>410</td><td>C30H50</td><td>NIST08 LIB</td></tr> <tr><td>5</td><td>90</td><td></td><td>Squalene \$S 2,6,10,14,18,22-Tetracosahexene</td><td>410</td><td>C30H50</td><td>NIST08 LIB</td></tr> <tr><td>6</td><td>89</td><td></td><td>2,6,10,14,18,22-Tetracosahexene, 2,6,10,15</td><td>410</td><td>C30H50</td><td>WILEY225 LI</td></tr> <tr><td>7</td><td>93</td><td></td><td><b>Squalene</b></td><td><b>410</b></td><td><b>C30H50</b></td><td><b>NIST21 LIB</b></td></tr> <tr><td>8</td><td>89</td><td></td><td>2,6,10,14,18,22-Tetracosahexene, 2,6,10,15</td><td>410</td><td>C30H50</td><td>WILEY225 LI</td></tr> <tr><td>9</td><td>89</td><td></td><td>2,6,10,14,18-Pentamethyl-2,6,10,14,18-hexosa</td><td>342</td><td>C29H42</td><td>NIST107 LIB</td></tr> </tbody> </table> <p>7: 410: Squalene</p> <p>CAS# 7003 - 64 - 9 Mol Wt: 410 Serial: 20413</p> <p>Cmpd Name: Squalene</p> <p>Formula: C30H50 Class Flag: No Class Flags.</p>	#	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	93		Squalene \$S 2,6,10,14,18,22-Tetracosahexene	410	C30H50	NIST08 LIB	2	92		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	NIST08 LIB	3	91		Squalene \$S 2,6,10,14,18,22-Tetracosahexene	410	C30H50	NIST08 LIB	4	91		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	NIST08 LIB	5	90		Squalene \$S 2,6,10,14,18,22-Tetracosahexene	410	C30H50	NIST08 LIB	6	89		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	WILEY225 LI	7	93		<b>Squalene</b>	<b>410</b>	<b>C30H50</b>	<b>NIST21 LIB</b>	8	89		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	WILEY225 LI	9	89		2,6,10,14,18-Pentamethyl-2,6,10,14,18-hexosa	342	C29H42	NIST107 LIB
#	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																			
1	93		Squalene \$S 2,6,10,14,18,22-Tetracosahexene	410	C30H50	NIST08 LIB																																																																			
2	92		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	NIST08 LIB																																																																			
3	91		Squalene \$S 2,6,10,14,18,22-Tetracosahexene	410	C30H50	NIST08 LIB																																																																			
4	91		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	NIST08 LIB																																																																			
5	90		Squalene \$S 2,6,10,14,18,22-Tetracosahexene	410	C30H50	NIST08 LIB																																																																			
6	89		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	WILEY225 LI																																																																			
7	93		<b>Squalene</b>	<b>410</b>	<b>C30H50</b>	<b>NIST21 LIB</b>																																																																			
8	89		2,6,10,14,18,22-Tetracosahexene, 2,6,10,15	410	C30H50	WILEY225 LI																																																																			
9	89		2,6,10,14,18-Pentamethyl-2,6,10,14,18-hexosa	342	C29H42	NIST107 LIB																																																																			

# ANEXOS

<p><b>43.664</b></p>	<p><b>2812</b></p>		
<p><b>44.252</b></p>	<p><b>2838</b></p>		
<p><b>45.695</b></p>	<p><b>2901</b></p>		
<p><b>48.665</b></p>	<p><b>3035</b></p>	<p><b>3036</b></p>	



<p>49.857</p> <p>3091</p>		<table border="1"> <thead> <tr> <th>Index</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>53</td> <td>77</td> <td>C</td> <td>alpha-Phenyl-beta-timethylstyrene SS</td> <td>268</td> <td>C17H20</td> <td>WILEY229.LI</td> </tr> <tr> <td>57</td> <td>77</td> <td>C</td> <td>1-Methyl-5-methyl-2-phenylisobenzazole SS</td> <td>267</td> <td>C10H9N3O</td> <td>WILEY229.LI</td> </tr> <tr> <td>57</td> <td>77</td> <td>C</td> <td>9H-Fluorene, 9-(2,4,6-cycloheptatrien-1-yl)meth</td> <td>268</td> <td>C21H16</td> <td>WILEY229.LI</td> </tr> <tr> <td>57</td> <td>77</td> <td>C</td> <td>3-Indinecarboxylic acid, 6-(trimethylsilyloxy)-</td> <td>283</td> <td>C12H21NO</td> <td>WILEY229.LI</td> </tr> <tr> <td>56</td> <td>77</td> <td>C</td> <td>6-Hydroxycytosine SS Cinnar-6, 11-diol, 1,2-d</td> <td>317</td> <td>C17H19NO</td> <td>WILEY229.LI</td> </tr> <tr> <td>56</td> <td>77</td> <td>C</td> <td>tribenzo[f,j]bicyclo[3,2,2]nona-2,6,8-triene SS</td> <td>268</td> <td>C21H16</td> <td>WILEY229.LI</td> </tr> <tr> <td>56</td> <td>77</td> <td>C</td> <td>1-(1,1,2,3,3,3-hexafluoro-propyl)perimidin SS</td> <td>318</td> <td>C14H8F6N</td> <td>WILEY229.LI</td> </tr> <tr> <td>56</td> <td>77</td> <td>C</td> <td>Pentadecane, 2,6,10,14-tetramethyl- (CAS) Pn</td> <td>268</td> <td>C19H40</td> <td>WILEY229.LI</td> </tr> <tr> <td>55</td> <td>77</td> <td>C</td> <td>Soro[9H]fluorene-9-yl[endo]3,3,1,0E-dihonal</td> <td>268</td> <td>C21H16</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target: alpha-Phenyl-beta-timethylstyrene SS</p> <p>Base Peak: 268/10,000</p> <p>Mol Wt: 268    Serial#: 123049</p> <p>Class Flag: No Class Flags</p>	Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library	53	77	C	alpha-Phenyl-beta-timethylstyrene SS	268	C17H20	WILEY229.LI	57	77	C	1-Methyl-5-methyl-2-phenylisobenzazole SS	267	C10H9N3O	WILEY229.LI	57	77	C	9H-Fluorene, 9-(2,4,6-cycloheptatrien-1-yl)meth	268	C21H16	WILEY229.LI	57	77	C	3-Indinecarboxylic acid, 6-(trimethylsilyloxy)-	283	C12H21NO	WILEY229.LI	56	77	C	6-Hydroxycytosine SS Cinnar-6, 11-diol, 1,2-d	317	C17H19NO	WILEY229.LI	56	77	C	tribenzo[f,j]bicyclo[3,2,2]nona-2,6,8-triene SS	268	C21H16	WILEY229.LI	56	77	C	1-(1,1,2,3,3,3-hexafluoro-propyl)perimidin SS	318	C14H8F6N	WILEY229.LI	56	77	C	Pentadecane, 2,6,10,14-tetramethyl- (CAS) Pn	268	C19H40	WILEY229.LI	55	77	C	Soro[9H]fluorene-9-yl[endo]3,3,1,0E-dihonal	268	C21H16	WILEY229.LI
Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
53	77	C	alpha-Phenyl-beta-timethylstyrene SS	268	C17H20	WILEY229.LI																																																																		
57	77	C	1-Methyl-5-methyl-2-phenylisobenzazole SS	267	C10H9N3O	WILEY229.LI																																																																		
57	77	C	9H-Fluorene, 9-(2,4,6-cycloheptatrien-1-yl)meth	268	C21H16	WILEY229.LI																																																																		
57	77	C	3-Indinecarboxylic acid, 6-(trimethylsilyloxy)-	283	C12H21NO	WILEY229.LI																																																																		
56	77	C	6-Hydroxycytosine SS Cinnar-6, 11-diol, 1,2-d	317	C17H19NO	WILEY229.LI																																																																		
56	77	C	tribenzo[f,j]bicyclo[3,2,2]nona-2,6,8-triene SS	268	C21H16	WILEY229.LI																																																																		
56	77	C	1-(1,1,2,3,3,3-hexafluoro-propyl)perimidin SS	318	C14H8F6N	WILEY229.LI																																																																		
56	77	C	Pentadecane, 2,6,10,14-tetramethyl- (CAS) Pn	268	C19H40	WILEY229.LI																																																																		
55	77	C	Soro[9H]fluorene-9-yl[endo]3,3,1,0E-dihonal	268	C21H16	WILEY229.LI																																																																		
<p>50.051</p> <p>3100</p>		<table border="1"> <thead> <tr> <th>Index</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>87</td> <td>C</td> <td>Tetracontane SS n-Tetracontane SS</td> <td>476</td> <td>C34H70</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>87</td> <td>C</td> <td>Hexadecane, 2,6,10,14-tetramethyl- SS 2,6,1</td> <td>296</td> <td>C24H50</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>87</td> <td>C</td> <td>Hexadecane, 2,6,10,14-tetramethyl- (CAS) 2,</td> <td>296</td> <td>C24H50</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>87</td> <td>C</td> <td>Hexadecane, 2,6,10,14-tetramethyl- SS</td> <td>296</td> <td>C24H50</td> <td>NIST07.LIB</td> </tr> <tr> <td>5</td> <td>87</td> <td>C</td> <td>Tetracontane (CAS) n-Tetracontane SS</td> <td>338</td> <td>C34H70</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>87</td> <td>C</td> <td>Tridecanol, 2-methyl- SS</td> <td>242</td> <td>C16H34O</td> <td>NIST07.LIB</td> </tr> <tr> <td>7</td> <td>87</td> <td>C</td> <td>Tridecanol, 2-methyl- SS</td> <td>242</td> <td>C16H34O</td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>96</td> <td>C</td> <td>Tetracontane SS n-Tetracontane SS</td> <td>476</td> <td>C34H70</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>96</td> <td>C</td> <td>2-Bromotetradecane</td> <td>276</td> <td>C14H29Br</td> <td>NIST08.LIB</td> </tr> </tbody> </table> <p>Target: Tetracontane SS n-Tetracontane SS</p> <p>Base Peak: 57/10,000</p> <p>Mol Wt: 476    Serial#: 101047</p> <p>Class Flag: No Class Flags</p>	Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	87	C	Tetracontane SS n-Tetracontane SS	476	C34H70	NIST08.LIB	2	87	C	Hexadecane, 2,6,10,14-tetramethyl- SS 2,6,1	296	C24H50	NIST08.LIB	3	87	C	Hexadecane, 2,6,10,14-tetramethyl- (CAS) 2,	296	C24H50	WILEY229.LI	4	87	C	Hexadecane, 2,6,10,14-tetramethyl- SS	296	C24H50	NIST07.LIB	5	87	C	Tetracontane (CAS) n-Tetracontane SS	338	C34H70	WILEY229.LI	6	87	C	Tridecanol, 2-methyl- SS	242	C16H34O	NIST07.LIB	7	87	C	Tridecanol, 2-methyl- SS	242	C16H34O	NIST08.LIB	8	96	C	Tetracontane SS n-Tetracontane SS	476	C34H70	NIST08.LIB	9	96	C	2-Bromotetradecane	276	C14H29Br	NIST08.LIB
Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	87	C	Tetracontane SS n-Tetracontane SS	476	C34H70	NIST08.LIB																																																																		
2	87	C	Hexadecane, 2,6,10,14-tetramethyl- SS 2,6,1	296	C24H50	NIST08.LIB																																																																		
3	87	C	Hexadecane, 2,6,10,14-tetramethyl- (CAS) 2,	296	C24H50	WILEY229.LI																																																																		
4	87	C	Hexadecane, 2,6,10,14-tetramethyl- SS	296	C24H50	NIST07.LIB																																																																		
5	87	C	Tetracontane (CAS) n-Tetracontane SS	338	C34H70	WILEY229.LI																																																																		
6	87	C	Tridecanol, 2-methyl- SS	242	C16H34O	NIST07.LIB																																																																		
7	87	C	Tridecanol, 2-methyl- SS	242	C16H34O	NIST08.LIB																																																																		
8	96	C	Tetracontane SS n-Tetracontane SS	476	C34H70	NIST08.LIB																																																																		
9	96	C	2-Bromotetradecane	276	C14H29Br	NIST08.LIB																																																																		
<p>50.315</p> <p>3113</p>		<table border="1"> <thead> <tr> <th>Index</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>91</td> <td>C</td> <td>Cholesterol trimethyl ether SS Silane, [3]be</td> <td>458</td> <td>C30H54OSi</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>91</td> <td>C</td> <td>Cholesterol trimethyl ether SS Silane, [3]be</td> <td>458</td> <td>C30H54OSi</td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>89</td> <td>C</td> <td>Cholesterol trimethyl ether SS Silane, [3]be</td> <td>458</td> <td>C30H54OSi</td> <td>NIST08.LIB</td> </tr> <tr> <td>4</td> <td>89</td> <td>C</td> <td>Silane, [3]beta-cholest-5-en-3-yl(trimethyl)</td> <td>458</td> <td>C30H54OSi</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>89</td> <td>C</td> <td>Silane, [3]beta-cholest-5-en-3-yl(trimethyl)</td> <td>548</td> <td>C33H54O2Si</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>89</td> <td>C</td> <td>3-beta, 5-Bis(trimethylsilyloxy)-5-alpha-cholestan</td> <td>548</td> <td>C33H54O2Si</td> <td>NIST07.LIB</td> </tr> <tr> <td>7</td> <td>88</td> <td>C</td> <td>Silane, [3]beta-cholest-5-en-3-yl(trimethyl)</td> <td>458</td> <td>C30H54OSi</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>88</td> <td>C</td> <td>Cholesterol trimethyl ether SS Silane, [3]be</td> <td>458</td> <td>C30H54OSi</td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>88</td> <td>C</td> <td>Cholesterol trimethyl ether SS Silane, [3]be</td> <td>458</td> <td>C30H54OSi</td> <td>NIST07.LIB</td> </tr> </tbody> </table> <p>Target: Cholesterol trimethyl ether SS Silane, [3]be</p> <p>Base Peak: 129/10,000</p> <p>Mol Wt: 458    Serial#: 20778</p> <p>Class Flag: No Class Flags</p>	Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	91	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB	2	91	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB	3	89	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB	4	89	C	Silane, [3]beta-cholest-5-en-3-yl(trimethyl)	458	C30H54OSi	WILEY229.LI	5	89	C	Silane, [3]beta-cholest-5-en-3-yl(trimethyl)	548	C33H54O2Si	WILEY229.LI	6	89	C	3-beta, 5-Bis(trimethylsilyloxy)-5-alpha-cholestan	548	C33H54O2Si	NIST07.LIB	7	88	C	Silane, [3]beta-cholest-5-en-3-yl(trimethyl)	458	C30H54OSi	WILEY229.LI	8	88	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB	9	88	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST07.LIB
Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	91	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB																																																																		
2	91	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB																																																																		
3	89	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB																																																																		
4	89	C	Silane, [3]beta-cholest-5-en-3-yl(trimethyl)	458	C30H54OSi	WILEY229.LI																																																																		
5	89	C	Silane, [3]beta-cholest-5-en-3-yl(trimethyl)	548	C33H54O2Si	WILEY229.LI																																																																		
6	89	C	3-beta, 5-Bis(trimethylsilyloxy)-5-alpha-cholestan	548	C33H54O2Si	NIST07.LIB																																																																		
7	88	C	Silane, [3]beta-cholest-5-en-3-yl(trimethyl)	458	C30H54OSi	WILEY229.LI																																																																		
8	88	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST08.LIB																																																																		
9	88	C	Cholesterol trimethyl ether SS Silane, [3]be	458	C30H54OSi	NIST07.LIB																																																																		
<p>50.463</p> <p>3120</p>		<table border="1"> <thead> <tr> <th>Index</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>64</td> <td>C</td> <td>alpha-Tocopherol (vitamin E) trimethyl ether</td> <td>502</td> <td>C32H50O2Si</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>48</td> <td>C</td> <td>2,3,4,5-tetraphenylbutylphenylcyclopenta-2</td> <td>502</td> <td>C39H34</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>47</td> <td>C</td> <td>Mandelamethyl derivative of Thiophene 9</td> <td>252</td> <td>C10H16N4</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>47</td> <td>C</td> <td>3,6-bis(17-trimethylsilyloxy)androst-1,3,</td> <td>518</td> <td>C28H50O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>47</td> <td>C</td> <td>3a,beta-Ethynyl-2-trimethylsilyloxy-3a,4,5,6,7,7</td> <td>236</td> <td>C14H24O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>46</td> <td>C</td> <td>2,3,5,6-tetra-methylbenzene SS 1,1',2',2'-Te</td> <td>502</td> <td>C34H30O4</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>46</td> <td>C</td> <td>2,4-Dihydroxylindole, 5-(3,4-dimethylsilyloxy)</td> <td>516</td> <td>C25H40N2</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>46</td> <td>C</td> <td>Silane, [5]alpha-16.alpha.-17.beta.-tetra-1,3</td> <td>592</td> <td>C30H56O4</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>46</td> <td>C</td> <td>1-Ovanomethyl-6-methylbenzothioether SS 1</td> <td>227</td> <td>C15H11N5</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target: alpha-Tocopherol (vitamin E) trimethyl ether</p> <p>Base Peak: 502/10,000</p> <p>Mol Wt: 502    Serial#: 194830</p> <p>Class Flag: No Class Flags</p>	Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	64	C	alpha-Tocopherol (vitamin E) trimethyl ether	502	C32H50O2Si	NIST08.LIB	2	48	C	2,3,4,5-tetraphenylbutylphenylcyclopenta-2	502	C39H34	WILEY229.LI	3	47	C	Mandelamethyl derivative of Thiophene 9	252	C10H16N4	WILEY229.LI	4	47	C	3,6-bis(17-trimethylsilyloxy)androst-1,3,	518	C28H50O3	WILEY229.LI	5	47	C	3a,beta-Ethynyl-2-trimethylsilyloxy-3a,4,5,6,7,7	236	C14H24O3	WILEY229.LI	6	46	C	2,3,5,6-tetra-methylbenzene SS 1,1',2',2'-Te	502	C34H30O4	WILEY229.LI	7	46	C	2,4-Dihydroxylindole, 5-(3,4-dimethylsilyloxy)	516	C25H40N2	WILEY229.LI	8	46	C	Silane, [5]alpha-16.alpha.-17.beta.-tetra-1,3	592	C30H56O4	WILEY229.LI	9	46	C	1-Ovanomethyl-6-methylbenzothioether SS 1	227	C15H11N5	WILEY229.LI
Index	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	64	C	alpha-Tocopherol (vitamin E) trimethyl ether	502	C32H50O2Si	NIST08.LIB																																																																		
2	48	C	2,3,4,5-tetraphenylbutylphenylcyclopenta-2	502	C39H34	WILEY229.LI																																																																		
3	47	C	Mandelamethyl derivative of Thiophene 9	252	C10H16N4	WILEY229.LI																																																																		
4	47	C	3,6-bis(17-trimethylsilyloxy)androst-1,3,	518	C28H50O3	WILEY229.LI																																																																		
5	47	C	3a,beta-Ethynyl-2-trimethylsilyloxy-3a,4,5,6,7,7	236	C14H24O3	WILEY229.LI																																																																		
6	46	C	2,3,5,6-tetra-methylbenzene SS 1,1',2',2'-Te	502	C34H30O4	WILEY229.LI																																																																		
7	46	C	2,4-Dihydroxylindole, 5-(3,4-dimethylsilyloxy)	516	C25H40N2	WILEY229.LI																																																																		
8	46	C	Silane, [5]alpha-16.alpha.-17.beta.-tetra-1,3	592	C30H56O4	WILEY229.LI																																																																		
9	46	C	1-Ovanomethyl-6-methylbenzothioether SS 1	227	C15H11N5	WILEY229.LI																																																																		

# ANEXOS

<p><b>50.950</b></p>	<p><b>3143</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Ring</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>77</td> <td>6</td> <td>Stane, trimethyl(octacosyl)</td> <td>482</td> <td>C<sub>31</sub>H<sub>60</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>87</td> <td>6</td> <td>Stane, (1,1-dimethyl)dimethyl(octacosyl)</td> <td>524</td> <td>C<sub>34</sub>H<sub>62</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>81</td> <td>6</td> <td>Octacosanol trimethyl ether SS</td> <td>482</td> <td>C<sub>31</sub>H<sub>60</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>4</td> <td>81</td> <td>6</td> <td>Octacosanol trimethyl ether</td> <td>482</td> <td>C<sub>31</sub>H<sub>60</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>73</td> <td>6</td> <td>Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)</td> <td>751</td> <td>C<sub>43</sub>H<sub>88</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>73</td> <td>6</td> <td>Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)</td> <td>750</td> <td>C<sub>43</sub>H<sub>88</sub>O<sub>4</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>73</td> <td>6</td> <td>Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)</td> <td>750</td> <td>C<sub>43</sub>H<sub>88</sub>O<sub>4</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>65</td> <td>6</td> <td>Pentacosanoic acid, 2-trimethyl(oxy)-me</td> <td>482</td> <td>C<sub>29</sub>H<sub>58</sub>O<sub>3</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>65</td> <td>6</td> <td>Stane, 1(11-chloroundecyl)oxymethyl- CASI</td> <td>278</td> <td>C<sub>14</sub>H<sub>31</sub>Cl</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1 : 402: Stane, trimethyl(octacosyl)-</p> <p>CAS# 0 : 00 : 0 Mol Wt: 482 Serial: 183073</p> <p>Comp Name: Stane, trimethyl(octacosyl)</p> <p>Formula: C<sub>31</sub>H<sub>60</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library	1	77	6	Stane, trimethyl(octacosyl)	482	C <sub>31</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB	2	87	6	Stane, (1,1-dimethyl)dimethyl(octacosyl)	524	C <sub>34</sub> H <sub>62</sub> O <sub>2</sub>	NIST08.LIB	3	81	6	Octacosanol trimethyl ether SS	482	C <sub>31</sub> H <sub>60</sub> O <sub>2</sub>	NIST107.LIB	4	81	6	Octacosanol trimethyl ether	482	C <sub>31</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB	5	73	6	Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)	751	C <sub>43</sub> H <sub>88</sub> O <sub>4</sub>	WILEY229.LI	6	73	6	Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)	750	C <sub>43</sub> H <sub>88</sub> O <sub>4</sub>	NIST107.LIB	7	73	6	Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)	750	C <sub>43</sub> H <sub>88</sub> O <sub>4</sub>	NIST08.LIB	8	65	6	Pentacosanoic acid, 2-trimethyl(oxy)-me	482	C <sub>29</sub> H <sub>58</sub> O <sub>3</sub>	WILEY229.LI	9	65	6	Stane, 1(11-chloroundecyl)oxymethyl- CASI	278	C <sub>14</sub> H <sub>31</sub> Cl	WILEY229.LI
RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library																																																																			
1	77	6	Stane, trimethyl(octacosyl)	482	C <sub>31</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB																																																																			
2	87	6	Stane, (1,1-dimethyl)dimethyl(octacosyl)	524	C <sub>34</sub> H <sub>62</sub> O <sub>2</sub>	NIST08.LIB																																																																			
3	81	6	Octacosanol trimethyl ether SS	482	C <sub>31</sub> H <sub>60</sub> O <sub>2</sub>	NIST107.LIB																																																																			
4	81	6	Octacosanol trimethyl ether	482	C <sub>31</sub> H <sub>60</sub> O <sub>2</sub>	NIST08.LIB																																																																			
5	73	6	Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)	751	C <sub>43</sub> H <sub>88</sub> O <sub>4</sub>	WILEY229.LI																																																																			
6	73	6	Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)	750	C <sub>43</sub> H <sub>88</sub> O <sub>4</sub>	NIST107.LIB																																																																			
7	73	6	Lauroic acid, 2-(heptadecyloxy)-3-(octadecyloxy)	750	C <sub>43</sub> H <sub>88</sub> O <sub>4</sub>	NIST08.LIB																																																																			
8	65	6	Pentacosanoic acid, 2-trimethyl(oxy)-me	482	C <sub>29</sub> H <sub>58</sub> O <sub>3</sub>	WILEY229.LI																																																																			
9	65	6	Stane, 1(11-chloroundecyl)oxymethyl- CASI	278	C <sub>14</sub> H <sub>31</sub> Cl	WILEY229.LI																																																																			
<p><b>51.975</b></p>	<p><b>3192</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Ring</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>2</td> <td>77</td> <td>6</td> <td>Lup-20(29)en-3-yl acetate, (3beta)- SS</td> <td>468</td> <td>C<sub>29</sub>H<sub>50</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>76</td> <td>6</td> <td>METHYL COMMATE D SS</td> <td>486</td> <td>C<sub>31</sub>H<sub>60</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>75</td> <td>6</td> <td>METHYL COMMATE C SS</td> <td>486</td> <td>C<sub>31</sub>H<sub>60</sub>O<sub>4</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>76</td> <td>6</td> <td>Farnesyl bromide SS</td> <td>284</td> <td>C<sub>15</sub>H<sub>26</sub>Br</td> <td>NIST107.LIB</td> </tr> <tr> <td>6</td> <td>75</td> <td>6</td> <td>Farnesyl bromide SS (E,E)-1,6-Diisopropyl-3,7,11-he</td> <td>284</td> <td>C<sub>15</sub>H<sub>26</sub>Br</td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>75</td> <td>6</td> <td>10a,11a-Himachala-3(12),4-diene SS</td> <td>204</td> <td>C<sub>15</sub>H<sub>24</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>8</td> <td>75</td> <td>6</td> <td>10a,11a-Himachala-3(12),4-diene SS 5,5,9-Tri</td> <td>204</td> <td>C<sub>15</sub>H<sub>24</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>9</td> <td>74</td> <td>6</td> <td>Taraxerol methyl ether SS D-Friedolan-14-ene</td> <td>440</td> <td>C<sub>31</sub>H<sub>52</sub>O</td> <td>WILEY229.LI</td> </tr> <tr> <td>10</td> <td>74</td> <td>6</td> <td>alpha-selinene SS</td> <td>204</td> <td>C<sub>15</sub>H<sub>24</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>9 : 440: Taraxerol methyl ether SS D-Friedolan-14-ene, 3-methoxy-, (3beta)- (CASI)METHYL 2,4-DIHYDROXY-5-(2-METHOXY-6-METHOXY-CARBONYL-2'-5'-DIMETHYLPHENYL)BETA-METHOXY-DELTA,14-TARAXERENE SS Curogallin SS Curogallin SS</p> <p>CAS# 14021-23-9 Mol Wt: 440 Serial: 205131</p> <p>Comp Name: Taraxerol methyl ether SS D-Friedolan-14-ene, 3-methoxy-, (3beta)- (CASI)METHYL 2,4-DIHYDROXY-5-(2-METHOXY-6-METHOXY-CARBONYL-2'-5'-DIMETHYLPHENYL)BETA-METHOXY-DELTA,14-TARAXERENE SS Curogallin SS Curogallin SS</p> <p>Formula: C<sub>29</sub>H<sub>52</sub>O Class Flag: No Class Flags</p>	RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library	2	77	6	Lup-20(29)en-3-yl acetate, (3beta)- SS	468	C <sub>29</sub> H <sub>50</sub> O <sub>2</sub>	NIST107.LIB	3	76	6	METHYL COMMATE D SS	486	C <sub>31</sub> H <sub>60</sub> O <sub>4</sub>	WILEY229.LI	4	75	6	METHYL COMMATE C SS	486	C <sub>31</sub> H <sub>60</sub> O <sub>4</sub>	WILEY229.LI	5	76	6	Farnesyl bromide SS	284	C <sub>15</sub> H <sub>26</sub> Br	NIST107.LIB	6	75	6	Farnesyl bromide SS (E,E)-1,6-Diisopropyl-3,7,11-he	284	C <sub>15</sub> H <sub>26</sub> Br	NIST08.LIB	7	75	6	10a,11a-Himachala-3(12),4-diene SS	204	C <sub>15</sub> H <sub>24</sub>	NIST107.LIB	8	75	6	10a,11a-Himachala-3(12),4-diene SS 5,5,9-Tri	204	C <sub>15</sub> H <sub>24</sub>	NIST08.LIB	9	74	6	Taraxerol methyl ether SS D-Friedolan-14-ene	440	C <sub>31</sub> H <sub>52</sub> O	WILEY229.LI	10	74	6	alpha-selinene SS	204	C <sub>15</sub> H <sub>24</sub>	WILEY229.LI
RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library																																																																			
2	77	6	Lup-20(29)en-3-yl acetate, (3beta)- SS	468	C <sub>29</sub> H <sub>50</sub> O <sub>2</sub>	NIST107.LIB																																																																			
3	76	6	METHYL COMMATE D SS	486	C <sub>31</sub> H <sub>60</sub> O <sub>4</sub>	WILEY229.LI																																																																			
4	75	6	METHYL COMMATE C SS	486	C <sub>31</sub> H <sub>60</sub> O <sub>4</sub>	WILEY229.LI																																																																			
5	76	6	Farnesyl bromide SS	284	C <sub>15</sub> H <sub>26</sub> Br	NIST107.LIB																																																																			
6	75	6	Farnesyl bromide SS (E,E)-1,6-Diisopropyl-3,7,11-he	284	C <sub>15</sub> H <sub>26</sub> Br	NIST08.LIB																																																																			
7	75	6	10a,11a-Himachala-3(12),4-diene SS	204	C <sub>15</sub> H <sub>24</sub>	NIST107.LIB																																																																			
8	75	6	10a,11a-Himachala-3(12),4-diene SS 5,5,9-Tri	204	C <sub>15</sub> H <sub>24</sub>	NIST08.LIB																																																																			
9	74	6	Taraxerol methyl ether SS D-Friedolan-14-ene	440	C <sub>31</sub> H <sub>52</sub> O	WILEY229.LI																																																																			
10	74	6	alpha-selinene SS	204	C <sub>15</sub> H <sub>24</sub>	WILEY229.LI																																																																			
<p><b>52.46</b></p>	<p><b>3216</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Ring</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>77</td> <td>6</td> <td>Cholesterol</td> <td>386</td> <td>C<sub>28</sub>H<sub>48</sub>O</td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>77</td> <td>6</td> <td>Cholesterol trimethyl ether SS Stane, (3beta)</td> <td>458</td> <td>C<sub>30</sub>H<sub>54</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>3</td> <td>76</td> <td>6</td> <td>Stane, (3beta)-cholest-5-en-3-yl(trimethyl)</td> <td>458</td> <td>C<sub>30</sub>H<sub>54</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>76</td> <td>6</td> <td>Cholesterol trimethyl ether</td> <td>458</td> <td>C<sub>30</sub>H<sub>54</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>76</td> <td>6</td> <td>Cholesterol trimethyl ether SS Stane, (3beta)</td> <td>458</td> <td>C<sub>30</sub>H<sub>54</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>6</td> <td>76</td> <td>6</td> <td>Cholesterol trimethyl ether SS Stane, (3beta)</td> <td>458</td> <td>C<sub>30</sub>H<sub>54</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>7</td> <td>76</td> <td>6</td> <td>Cholesterol trimethyl ether</td> <td>458</td> <td>C<sub>30</sub>H<sub>54</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>76</td> <td>6</td> <td>Stane, trimethyl(3beta,20E)stigmasta-5,22-</td> <td>484</td> <td>C<sub>32</sub>H<sub>56</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>75</td> <td>6</td> <td>Stane, trimethyl(4beta, methylcholesterol)</td> <td>472</td> <td>C<sub>31</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target</p> <p>1 : 472: Campesterol</p> <p>CAS# 0 : 00 : 0 Mol Wt: 472 Serial: 181992</p> <p>Comp Name: Campesterol</p> <p>Formula: C<sub>31</sub>H<sub>56</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library	1	77	6	Cholesterol	386	C <sub>28</sub> H <sub>48</sub> O	NIST08.LIB	2	77	6	Cholesterol trimethyl ether SS Stane, (3beta)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB	3	76	6	Stane, (3beta)-cholest-5-en-3-yl(trimethyl)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	WILEY229.LI	4	76	6	Cholesterol trimethyl ether	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB	5	76	6	Cholesterol trimethyl ether SS Stane, (3beta)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB	6	76	6	Cholesterol trimethyl ether SS Stane, (3beta)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB	7	76	6	Cholesterol trimethyl ether	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB	8	76	6	Stane, trimethyl(3beta,20E)stigmasta-5,22-	484	C <sub>32</sub> H <sub>56</sub> O <sub>2</sub>	WILEY229.LI	9	75	6	Stane, trimethyl(4beta, methylcholesterol)	472	C <sub>31</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB
RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library																																																																			
1	77	6	Cholesterol	386	C <sub>28</sub> H <sub>48</sub> O	NIST08.LIB																																																																			
2	77	6	Cholesterol trimethyl ether SS Stane, (3beta)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB																																																																			
3	76	6	Stane, (3beta)-cholest-5-en-3-yl(trimethyl)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	WILEY229.LI																																																																			
4	76	6	Cholesterol trimethyl ether	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB																																																																			
5	76	6	Cholesterol trimethyl ether SS Stane, (3beta)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB																																																																			
6	76	6	Cholesterol trimethyl ether SS Stane, (3beta)	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB																																																																			
7	76	6	Cholesterol trimethyl ether	458	C <sub>30</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB																																																																			
8	76	6	Stane, trimethyl(3beta,20E)stigmasta-5,22-	484	C <sub>32</sub> H <sub>56</sub> O <sub>2</sub>	WILEY229.LI																																																																			
9	75	6	Stane, trimethyl(4beta, methylcholesterol)	472	C <sub>31</sub> H <sub>56</sub> O <sub>2</sub>	NIST107.LIB																																																																			
<p><b>52.835</b></p>	<p><b>3234</b></p>		<table border="1"> <thead> <tr> <th>RT</th> <th>Similar</th> <th>Ring</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>71</td> <td>6</td> <td>Hexacosanoic acid, trimethyl(alkyl) ester</td> <td>468</td> <td>C<sub>28</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>2</td> <td>71</td> <td>6</td> <td>Tetracosanoic acid, trimethyl(alkyl) ester SS</td> <td>440</td> <td>C<sub>27</sub>H<sub>54</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>71</td> <td>6</td> <td>TRIMETHYLSYL ESTER OF TETRACOSA</td> <td>440</td> <td>C<sub>27</sub>H<sub>54</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>71</td> <td>6</td> <td>Tetracosanoic acid, trimethyl(alkyl) ester SS Tam</td> <td>440</td> <td>C<sub>27</sub>H<sub>54</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>5</td> <td>71</td> <td>6</td> <td>Octadecanoic acid, trimethyl(alkyl) ester (CASI) S</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>71</td> <td>6</td> <td>Octadecanoic acid, trimethyl(alkyl) ester SS Stear</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>NIST107.LIB</td> </tr> <tr> <td>7</td> <td>70</td> <td>6</td> <td>Pentacosanoic acid, trimethyl(alkyl) ester</td> <td>454</td> <td>C<sub>28</sub>H<sub>56</sub>O<sub>2</sub></td> <td>NIST08.LIB</td> </tr> <tr> <td>8</td> <td>70</td> <td>6</td> <td>Docosanoic acid, trimethyl(alkyl) ester (CASI) DO</td> <td>412</td> <td>C<sub>25</sub>H<sub>50</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>69</td> <td>6</td> <td>Octadecanoic acid, trimethyl(alkyl) ester (CASI) S</td> <td>356</td> <td>C<sub>21</sub>H<sub>44</sub>O<sub>2</sub></td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target</p> <p>1 : 468: Hexacosanoic acid, trimethyl(alkyl) ester</p> <p>CAS# 0 : 00 : 0 Mol Wt: 468 Serial: 181479</p> <p>Comp Name: Hexacosanoic acid, trimethyl(alkyl) ester</p> <p>Formula: C<sub>28</sub>H<sub>56</sub>O<sub>2</sub> Class Flag: No Class Flags</p>	RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library	1	71	6	Hexacosanoic acid, trimethyl(alkyl) ester	468	C <sub>28</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB	2	71	6	Tetracosanoic acid, trimethyl(alkyl) ester SS	440	C <sub>27</sub> H <sub>54</sub> O <sub>2</sub>	NIST107.LIB	3	71	6	TRIMETHYLSYL ESTER OF TETRACOSA	440	C <sub>27</sub> H <sub>54</sub> O <sub>2</sub>	WILEY229.LI	4	71	6	Tetracosanoic acid, trimethyl(alkyl) ester SS Tam	440	C <sub>27</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB	5	71	6	Octadecanoic acid, trimethyl(alkyl) ester (CASI) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI	6	71	6	Octadecanoic acid, trimethyl(alkyl) ester SS Stear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST107.LIB	7	70	6	Pentacosanoic acid, trimethyl(alkyl) ester	454	C <sub>28</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB	8	70	6	Docosanoic acid, trimethyl(alkyl) ester (CASI) DO	412	C <sub>25</sub> H <sub>50</sub> O <sub>2</sub>	WILEY229.LI	9	69	6	Octadecanoic acid, trimethyl(alkyl) ester (CASI) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI
RT	Similar	Ring	Compound Name	Mol Wt	Formula	Library																																																																			
1	71	6	Hexacosanoic acid, trimethyl(alkyl) ester	468	C <sub>28</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB																																																																			
2	71	6	Tetracosanoic acid, trimethyl(alkyl) ester SS	440	C <sub>27</sub> H <sub>54</sub> O <sub>2</sub>	NIST107.LIB																																																																			
3	71	6	TRIMETHYLSYL ESTER OF TETRACOSA	440	C <sub>27</sub> H <sub>54</sub> O <sub>2</sub>	WILEY229.LI																																																																			
4	71	6	Tetracosanoic acid, trimethyl(alkyl) ester SS Tam	440	C <sub>27</sub> H <sub>54</sub> O <sub>2</sub>	NIST08.LIB																																																																			
5	71	6	Octadecanoic acid, trimethyl(alkyl) ester (CASI) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI																																																																			
6	71	6	Octadecanoic acid, trimethyl(alkyl) ester SS Stear	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	NIST107.LIB																																																																			
7	70	6	Pentacosanoic acid, trimethyl(alkyl) ester	454	C <sub>28</sub> H <sub>56</sub> O <sub>2</sub>	NIST08.LIB																																																																			
8	70	6	Docosanoic acid, trimethyl(alkyl) ester (CASI) DO	412	C <sub>25</sub> H <sub>50</sub> O <sub>2</sub>	WILEY229.LI																																																																			
9	69	6	Octadecanoic acid, trimethyl(alkyl) ester (CASI) S	356	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub>	WILEY229.LI																																																																			

<p><b>52.994</b></p>	<p><b>3243</b></p>		<table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>91</td><td>CP</td><td>Stigmasteryl dimethyl ether \$S\$ Slane, trimet</td><td>484</td><td>C32H50O2</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>91</td><td></td><td>Stigmasteryl dimethyl ether \$S\$ Slane, trimet</td><td>484</td><td>C32H50O2</td><td>NIST08.LIB</td></tr> <tr><td>3</td><td>93</td><td></td><td>Stigmasteryl dimethyl ether \$S\$ Slane, trimet</td><td>484</td><td>C32H50O2</td><td>NIST08.LIB</td></tr> <tr><td>4</td><td>83</td><td></td><td>Slane, trimethyl(3 beta)-stigmasta-5-en-3-yl-ox</td><td>486</td><td>C32H50O3</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>79</td><td></td><td>Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z</td><td>454</td><td>C31H50O2</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>79</td><td></td><td>Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z</td><td>454</td><td>C31H50O2</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>79</td><td></td><td>Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z</td><td>454</td><td>C31H50O2</td><td>NIST171.LIB</td></tr> <tr><td>8</td><td>78</td><td></td><td>Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z</td><td>454</td><td>C31H50O2</td><td>NIST171.LIB</td></tr> <tr><td>9</td><td>78</td><td></td><td>Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z</td><td>454</td><td>C31H50O2</td><td>NIST08.LIB</td></tr> </tbody> </table> <p>Target</p> <p>1: 484: Stigmasteryl dimethyl ether \$S\$ Slane, trimethyl(3 beta), 2Z)-stigmasta-5,22-dien-3-yl-ox) \$S\$ Slane, trimethyl(stigmasta-5,22-dien-3 beta-yl-ox) \$S\$ 3 beta-(1-trimethyl(3 beta)-stigmasta-5,22-diene # \$S\$</p> <p>CAS# 14030-29-6 Mol Wt: 484 Smiles: C32H50O2</p> <p>Comp Name: Stigmasteryl dimethyl ether \$S\$ Slane, trimethyl(3 beta), 2Z)-stigmasta-5,22-dien-3-yl-ox) \$S\$ Slane, trimethyl(stigmasta-5,22-dien-3 beta-yl-ox) \$S\$ 3 beta-(1-trimethyl(3 beta)-stigmasta-5,22-diene # \$S\$ (2E)-3(1-trimethyl(3 beta)-stigmasta-5,22-diene # \$S\$</p> <p>Formula: C32H50O2 Class Flag: No Class Flags</p>	Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	91	CP	Stigmasteryl dimethyl ether \$S\$ Slane, trimet	484	C32H50O2	NIST08.LIB	2	91		Stigmasteryl dimethyl ether \$S\$ Slane, trimet	484	C32H50O2	NIST08.LIB	3	93		Stigmasteryl dimethyl ether \$S\$ Slane, trimet	484	C32H50O2	NIST08.LIB	4	83		Slane, trimethyl(3 beta)-stigmasta-5-en-3-yl-ox	486	C32H50O3	WILEY229.LI	5	79		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST08.LIB	6	79		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	WILEY229.LI	7	79		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST171.LIB	8	78		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST171.LIB	9	78		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST08.LIB
Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																			
1	91	CP	Stigmasteryl dimethyl ether \$S\$ Slane, trimet	484	C32H50O2	NIST08.LIB																																																																			
2	91		Stigmasteryl dimethyl ether \$S\$ Slane, trimet	484	C32H50O2	NIST08.LIB																																																																			
3	93		Stigmasteryl dimethyl ether \$S\$ Slane, trimet	484	C32H50O2	NIST08.LIB																																																																			
4	83		Slane, trimethyl(3 beta)-stigmasta-5-en-3-yl-ox	486	C32H50O3	WILEY229.LI																																																																			
5	79		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST08.LIB																																																																			
6	79		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	WILEY229.LI																																																																			
7	79		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST171.LIB																																																																			
8	78		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST171.LIB																																																																			
9	78		Stigmasta-5,22-dien-3-ol, acetate, (3 beta), 2Z	454	C31H50O2	NIST08.LIB																																																																			
<p><b>53.377</b></p>	<p><b>3261</b></p>		<table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>81</td><td>CP</td><td>Lupenol \$S\$ Lup-20(29)-en-3-ol, (3 beta)-\$S\$ Lu</td><td>426</td><td>C39H50O</td><td>NIST107.LIB</td></tr> <tr><td>2</td><td>81</td><td></td><td>Lup-20(29)-en-3-ol, acetate, (3 beta) \$S\$ Lup</td><td>468</td><td>C39H50O2</td><td>NIST107.LIB</td></tr> <tr><td>3</td><td>77</td><td></td><td>Betulin \$S\$ Lup-20(29)-ene-3,23-diol, (3 beta)-</td><td>442</td><td>C39H50O2</td><td>NIST08.LIB</td></tr> <tr><td>4</td><td>76</td><td></td><td>4,4,6a,8a,11,12,14b-Octamethyl-dodecyl</td><td>444</td><td>C30H50O2</td><td>NIST107.LIB</td></tr> <tr><td>5</td><td>76</td><td></td><td>2,2,3,7-TETRAMETHYLTRIC(1,0,5)2,0,0 (</td><td>204</td><td>C15H24</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>76</td><td></td><td>TETRAHYDROQUINAMARIDENOL \$S\$</td><td>430</td><td>C30H54O</td><td>WILEY229.LI</td></tr> <tr><td>7</td><td>76</td><td></td><td>Scianol \$S\$ 1-Naphthalenepropanol, alpha-ve</td><td>308</td><td>C20H36O2</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>76</td><td></td><td>1-Naphthalenepropanol, alpha-ethyledecyl</td><td>308</td><td>C20H36O2</td><td>NIST107.LIB</td></tr> <tr><td>9</td><td>76</td><td></td><td>METHYL COMMATE B \$S\$</td><td>470</td><td>C31H50O3</td><td>WILEY229.LI</td></tr> </tbody> </table> <p>Target</p> <p>1: 426: Lupenol \$S\$ Lup-20(29)-en-3-ol, (3 beta)-\$S\$ Lup-20(29)-en-3 beta-ol \$S\$ beta-Vicool \$S\$ Cedrol \$S\$ Fagasterol \$S\$ Fagasterol \$S\$ Lupenol \$S\$ Monogonol \$S\$ Triterpene lupenol \$S\$ 1H-Cyclopent(a)phymene, lup-20(29)-en-3-ol deriv. \$S\$</p> <p>CAS# 545-47-1 Mol Wt: 426 Smiles: C39H50O</p> <p>Comp Name: Lupenol \$S\$ Lup-20(29)-en-3-ol, (3 beta)-\$S\$ Lup-20(29)-en-3 beta-ol \$S\$ beta-Vicool \$S\$ Cedrol \$S\$ Fagasterol \$S\$ Fagasterol \$S\$ Lupenol \$S\$ Monogonol \$S\$ Triterpene lupenol \$S\$ 1H-Cyclopent(a)phymene, lup-20(29)-en-3-ol deriv. \$S\$</p> <p>Formula: C39H50O Class Flag: No Class Flags</p>	Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	81	CP	Lupenol \$S\$ Lup-20(29)-en-3-ol, (3 beta)-\$S\$ Lu	426	C39H50O	NIST107.LIB	2	81		Lup-20(29)-en-3-ol, acetate, (3 beta) \$S\$ Lup	468	C39H50O2	NIST107.LIB	3	77		Betulin \$S\$ Lup-20(29)-ene-3,23-diol, (3 beta)-	442	C39H50O2	NIST08.LIB	4	76		4,4,6a,8a,11,12,14b-Octamethyl-dodecyl	444	C30H50O2	NIST107.LIB	5	76		2,2,3,7-TETRAMETHYLTRIC(1,0,5)2,0,0 (	204	C15H24	WILEY229.LI	6	76		TETRAHYDROQUINAMARIDENOL \$S\$	430	C30H54O	WILEY229.LI	7	76		Scianol \$S\$ 1-Naphthalenepropanol, alpha-ve	308	C20H36O2	WILEY229.LI	8	76		1-Naphthalenepropanol, alpha-ethyledecyl	308	C20H36O2	NIST107.LIB	9	76		METHYL COMMATE B \$S\$	470	C31H50O3	WILEY229.LI
Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																			
1	81	CP	Lupenol \$S\$ Lup-20(29)-en-3-ol, (3 beta)-\$S\$ Lu	426	C39H50O	NIST107.LIB																																																																			
2	81		Lup-20(29)-en-3-ol, acetate, (3 beta) \$S\$ Lup	468	C39H50O2	NIST107.LIB																																																																			
3	77		Betulin \$S\$ Lup-20(29)-ene-3,23-diol, (3 beta)-	442	C39H50O2	NIST08.LIB																																																																			
4	76		4,4,6a,8a,11,12,14b-Octamethyl-dodecyl	444	C30H50O2	NIST107.LIB																																																																			
5	76		2,2,3,7-TETRAMETHYLTRIC(1,0,5)2,0,0 (	204	C15H24	WILEY229.LI																																																																			
6	76		TETRAHYDROQUINAMARIDENOL \$S\$	430	C30H54O	WILEY229.LI																																																																			
7	76		Scianol \$S\$ 1-Naphthalenepropanol, alpha-ve	308	C20H36O2	WILEY229.LI																																																																			
8	76		1-Naphthalenepropanol, alpha-ethyledecyl	308	C20H36O2	NIST107.LIB																																																																			
9	76		METHYL COMMATE B \$S\$	470	C31H50O3	WILEY229.LI																																																																			
<p><b>53.989</b></p>	<p><b>3292</b></p>		<table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>73</td><td>CP</td><td>alpha-selinene \$S\$</td><td>234</td><td>C15H24</td><td>WILEY229.LI</td></tr> <tr><td>2</td><td>73</td><td></td><td>Slane, (3 alpha,5 beta,6 alpha)pregnan-3</td><td>464</td><td>C27H50O2</td><td>NIST107.LIB</td></tr> <tr><td>3</td><td>73</td><td></td><td>Slane, (5 beta, pregnan-3 alpha, 6 alpha, ylen</td><td>464</td><td>C27H50O2</td><td>WILEY229.LI</td></tr> <tr><td>4</td><td>72</td><td></td><td>Farnesyl bromide \$S\$</td><td>284</td><td>C15H26Br</td><td>NIST107.LIB</td></tr> <tr><td>5</td><td>71</td><td></td><td>Olean-18-ene (CAS) DELTA 18 OLEANENE</td><td>410</td><td>C30H50</td><td>WILEY229.LI</td></tr> <tr><td>6</td><td>71</td><td></td><td>Olean-18-ene \$S\$ Germanen \$S\$ Germanen</td><td>410</td><td>C30H50</td><td>NIST107.LIB</td></tr> <tr><td>7</td><td>71</td><td></td><td>gamma-Selinene \$S\$ Naphthalene, decahydro</td><td>204</td><td>C15H24</td><td>WILEY229.LI</td></tr> <tr><td>8</td><td>71</td><td></td><td>Naphthalene, decahydro-1,4-dimethyl-1-methyl</td><td>204</td><td>C15H24</td><td>NIST107.LIB</td></tr> <tr><td>9</td><td>71</td><td></td><td>Azulene, 1,2,3,3a,4,5,6,7octahydro-1,4-dimet</td><td>204</td><td>C15H24</td><td>NIST171.LIB</td></tr> </tbody> </table> <p>Target</p> <p>2: 464: Slane, (3 alpha,5 beta,6 alpha)pregnan-3,6-diol(biotinyl)bi(trimethyl)-\$S\$ Slane, (5 beta, pregnan-3 alpha, 6 alpha, ylenedicyclo)bi(trimethyl)-\$S\$ Slane, (5 beta, pregnan-3 alpha, 6 alpha, ylenedicyclo)bi(trimethyl)-\$S\$</p> <p>CAS# 33293-07-7 Mol Wt: 464 Smiles: C27H50O2</p> <p>Comp Name: Slane, (3 alpha,5 beta,6 alpha)pregnan-3,6-diol(biotinyl)bi(trimethyl)-\$S\$ Slane, (5 beta, pregnan-3 alpha, 6 alpha, ylenedicyclo)bi(trimethyl)-\$S\$ Slane, (5 beta, pregnan-3 alpha, 6 alpha, ylenedicyclo)bi(trimethyl)-\$S\$</p> <p>Formula: C27H50O2 Class Flag: No Class Flags</p>	Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	73	CP	alpha-selinene \$S\$	234	C15H24	WILEY229.LI	2	73		Slane, (3 alpha,5 beta,6 alpha)pregnan-3	464	C27H50O2	NIST107.LIB	3	73		Slane, (5 beta, pregnan-3 alpha, 6 alpha, ylen	464	C27H50O2	WILEY229.LI	4	72		Farnesyl bromide \$S\$	284	C15H26Br	NIST107.LIB	5	71		Olean-18-ene (CAS) DELTA 18 OLEANENE	410	C30H50	WILEY229.LI	6	71		Olean-18-ene \$S\$ Germanen \$S\$ Germanen	410	C30H50	NIST107.LIB	7	71		gamma-Selinene \$S\$ Naphthalene, decahydro	204	C15H24	WILEY229.LI	8	71		Naphthalene, decahydro-1,4-dimethyl-1-methyl	204	C15H24	NIST107.LIB	9	71		Azulene, 1,2,3,3a,4,5,6,7octahydro-1,4-dimet	204	C15H24	NIST171.LIB
Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																			
1	73	CP	alpha-selinene \$S\$	234	C15H24	WILEY229.LI																																																																			
2	73		Slane, (3 alpha,5 beta,6 alpha)pregnan-3	464	C27H50O2	NIST107.LIB																																																																			
3	73		Slane, (5 beta, pregnan-3 alpha, 6 alpha, ylen	464	C27H50O2	WILEY229.LI																																																																			
4	72		Farnesyl bromide \$S\$	284	C15H26Br	NIST107.LIB																																																																			
5	71		Olean-18-ene (CAS) DELTA 18 OLEANENE	410	C30H50	WILEY229.LI																																																																			
6	71		Olean-18-ene \$S\$ Germanen \$S\$ Germanen	410	C30H50	NIST107.LIB																																																																			
7	71		gamma-Selinene \$S\$ Naphthalene, decahydro	204	C15H24	WILEY229.LI																																																																			
8	71		Naphthalene, decahydro-1,4-dimethyl-1-methyl	204	C15H24	NIST107.LIB																																																																			
9	71		Azulene, 1,2,3,3a,4,5,6,7octahydro-1,4-dimet	204	C15H24	NIST171.LIB																																																																			
<p><b>54.214</b></p>	<p><b>3303</b></p>		<table border="1"> <thead> <tr> <th>Rank</th> <th>Similar</th> <th>Flags</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr><td>1</td><td>91</td><td>CP</td><td>beta-Sitosterol dimethyl ether \$S\$ Slane, tri</td><td>486</td><td>C32H50O2</td><td>NIST08.LIB</td></tr> <tr><td>2</td><td>87</td><td></td><td>Slane, trimethyl(3 beta, 2Z)-stigmasta-5,22</td><td>484</td><td>C32H50O3</td><td>WILEY229.LI</td></tr> <tr><td>3</td><td>86</td><td></td><td>beta-Sitosterol dimethyl ether \$S\$ Slane, tri</td><td>486</td><td>C32H50O2</td><td>NIST08.LIB</td></tr> <tr><td>4</td><td>80</td><td></td><td>Slane, trimethyl(3 beta)-stigmast-5-en-3-yl-ox</td><td>486</td><td>C32H50O3</td><td>WILEY229.LI</td></tr> <tr><td>5</td><td>80</td><td></td><td>beta-Sitosterol dimethyl ether \$S\$ Slane, tri</td><td>486</td><td>C32H50O2</td><td>NIST08.LIB</td></tr> <tr><td>6</td><td>80</td><td></td><td>beta-Sitosterol dimethyl ether \$S\$ Slane, tri</td><td>486</td><td>C32H50O2</td><td>NIST107.LIB</td></tr> <tr><td>7</td><td>78</td><td></td><td>Campesterol</td><td>472</td><td>C31H50O2</td><td>NIST08.LIB</td></tr> <tr><td>8</td><td>77</td><td></td><td>Slane, (3 beta)-cholest-5-en-3-yl-ox)trimethy</td><td>488</td><td>C33H54O3</td><td>WILEY229.LI</td></tr> <tr><td>9</td><td>77</td><td></td><td>Cholesterol dimethyl ether</td><td>458</td><td>C30H54O2</td><td>NIST171.LIB</td></tr> </tbody> </table> <p>Target</p> <p>1: 486: beta-Sitosterol dimethyl ether \$S\$ Slane, trimethyl(3 beta)-stigmast-5-en-3-yl-ox) \$S\$ Slane, trimethyl(stigmast-5-en-3 beta-yl-ox) \$S\$ 3(1-trimethyl(3 beta)-stigmast-5-ene # \$S\$</p> <p>CAS# 2625-40-9 Mol Wt: 486 Smiles: C32H50O2</p> <p>Comp Name: beta-Sitosterol dimethyl ether \$S\$ Slane, trimethyl(3 beta)-stigmast-5-en-3-yl-ox) \$S\$ Slane, trimethyl(stigmast-5-en-3 beta-yl-ox) \$S\$ 3(1-trimethyl(3 beta)-stigmast-5-ene # \$S\$</p> <p>Formula: C32H50O2 Class Flag: No Class Flags</p>	Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library	1	91	CP	beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST08.LIB	2	87		Slane, trimethyl(3 beta, 2Z)-stigmasta-5,22	484	C32H50O3	WILEY229.LI	3	86		beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST08.LIB	4	80		Slane, trimethyl(3 beta)-stigmast-5-en-3-yl-ox	486	C32H50O3	WILEY229.LI	5	80		beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST08.LIB	6	80		beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST107.LIB	7	78		Campesterol	472	C31H50O2	NIST08.LIB	8	77		Slane, (3 beta)-cholest-5-en-3-yl-ox)trimethy	488	C33H54O3	WILEY229.LI	9	77		Cholesterol dimethyl ether	458	C30H54O2	NIST171.LIB
Rank	Similar	Flags	Compound Name	Mol Wt	Formula	Library																																																																			
1	91	CP	beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST08.LIB																																																																			
2	87		Slane, trimethyl(3 beta, 2Z)-stigmasta-5,22	484	C32H50O3	WILEY229.LI																																																																			
3	86		beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST08.LIB																																																																			
4	80		Slane, trimethyl(3 beta)-stigmast-5-en-3-yl-ox	486	C32H50O3	WILEY229.LI																																																																			
5	80		beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST08.LIB																																																																			
6	80		beta-Sitosterol dimethyl ether \$S\$ Slane, tri	486	C32H50O2	NIST107.LIB																																																																			
7	78		Campesterol	472	C31H50O2	NIST08.LIB																																																																			
8	77		Slane, (3 beta)-cholest-5-en-3-yl-ox)trimethy	488	C33H54O3	WILEY229.LI																																																																			
9	77		Cholesterol dimethyl ether	458	C30H54O2	NIST171.LIB																																																																			





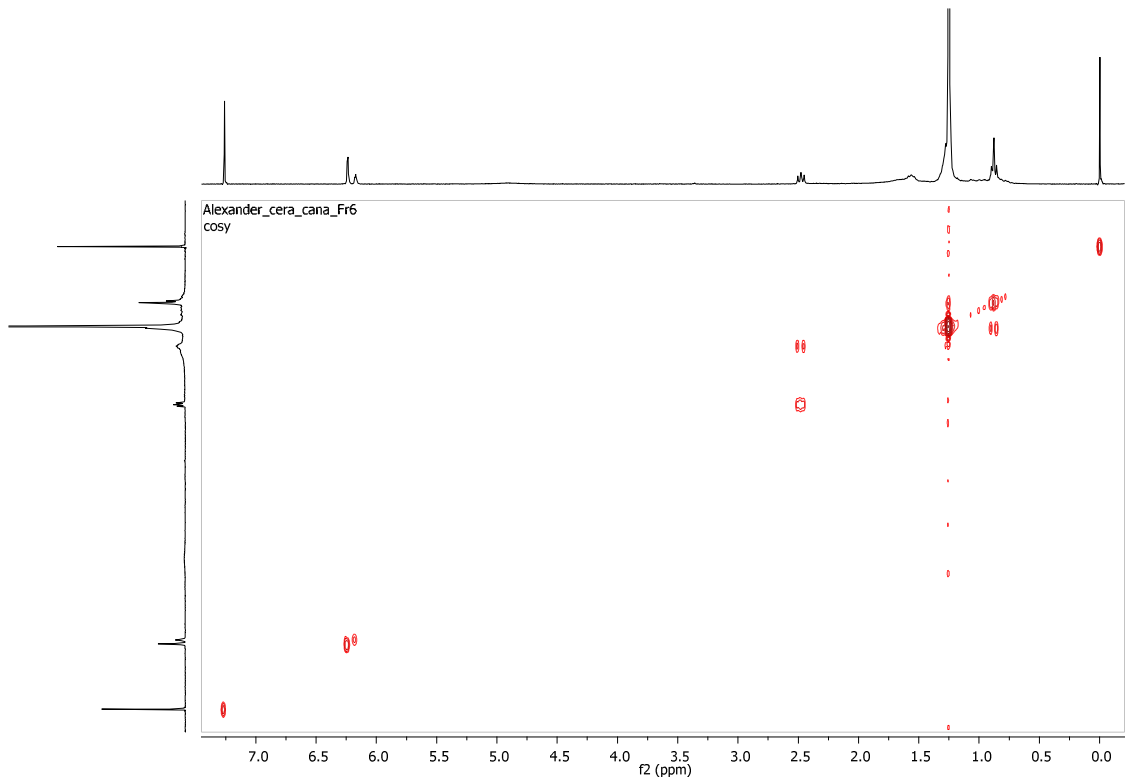


# ANEXOS

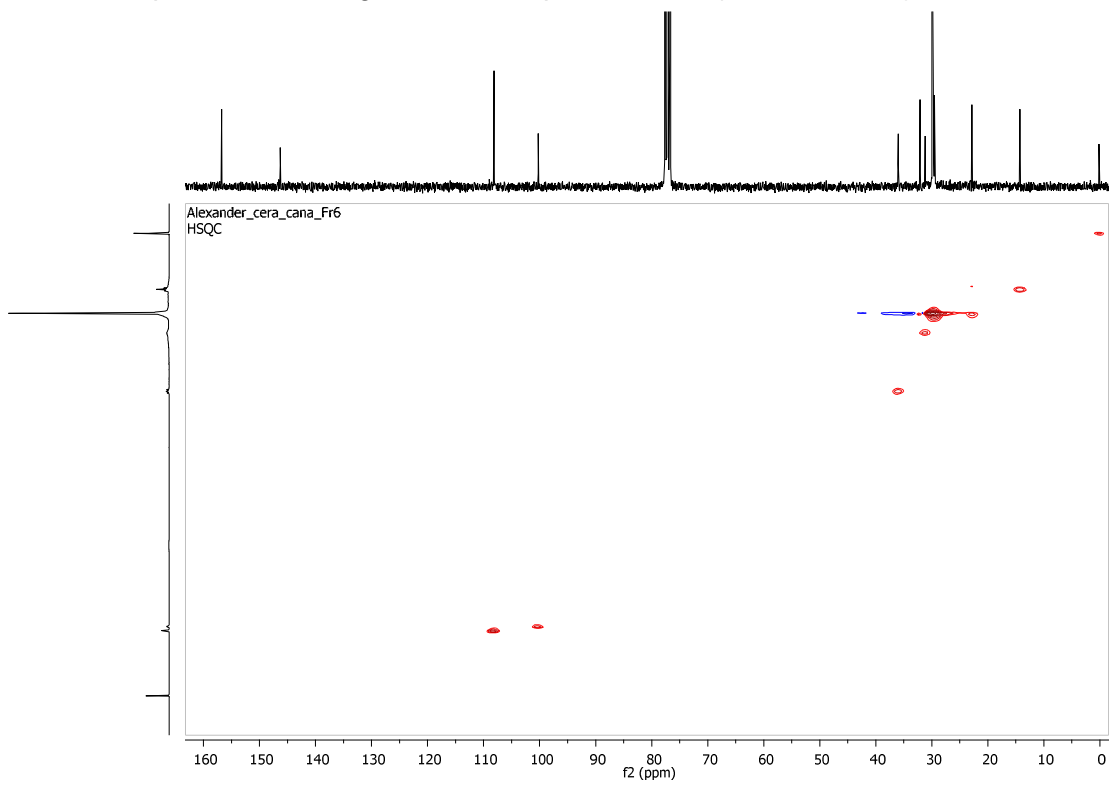
<p><b>56.309</b></p>	<p><b>3410</b></p>	<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>65</td> <td>✓</td> <td>9,19-Cyclolanost-24-en-3-ol (3 beta) CASIC</td> <td>426</td> <td>C30H50O</td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>63</td> <td>✓</td> <td>Cyclooctatriene 9,19-Cycloergost-24,25-dien</td> <td>426</td> <td>C30H50O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>62</td> <td>✓</td> <td>9,19-Cyclolanost-3-ol, 24-methylene-, (3 beta)</td> <td>440</td> <td>C31H52O</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>61</td> <td>✓</td> <td>9,19-Cyclo-9 beta-farnesane-3 beta, 25-diol (C)</td> <td>444</td> <td>C30H52O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>61</td> <td>✓</td> <td>Stilane, (9,19-cyclo-9 beta-farnesol-24-en-3 beta)</td> <td>438</td> <td>C30H50O</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>61</td> <td>✓</td> <td>9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)</td> <td>440</td> <td>C31H52O</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>60</td> <td>✓</td> <td>ANTI-1,3,7,11,15,19,23,27,31,35,39,43,12,12-OCTAHEPT</td> <td>272</td> <td>C20H32</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>60</td> <td>✓</td> <td>cyclooctyl acetate 5,5-9,19-Cycloergost-25</td> <td>468</td> <td>C32H52O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>59</td> <td>✓</td> <td>12 EPISILON, 17 EPISILON DIHYDROXYAN</td> <td>302</td> <td>C19H26O3</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target:</p> <p>1: 426: 9,19-Cyclolanost-24-en-3-ol, (3 beta) CASIC Cyclooctatriene 9,19-Cyclo-9 beta-farnesol-24-en-3 beta-ol</p> <p>CAS# 469-38-5 Mol Wt 426 Serial# 201750</p> <p>Comp Name: 9,19-Cyclolanost-24-en-3-ol, (3 beta) CASIC Cyclooctatriene 9,19-Cyclo-9 beta-farnesol-24-en-3 beta-ol</p> <p>Formula: C30H50O Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	65	✓	9,19-Cyclolanost-24-en-3-ol (3 beta) CASIC	426	C30H50O	WILEY229.LI	2	63	✓	Cyclooctatriene 9,19-Cycloergost-24,25-dien	426	C30H50O	WILEY229.LI	3	62	✓	9,19-Cyclolanost-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.LI	4	61	✓	9,19-Cyclo-9 beta-farnesane-3 beta, 25-diol (C)	444	C30H52O2	WILEY229.LI	5	61	✓	Stilane, (9,19-cyclo-9 beta-farnesol-24-en-3 beta)	438	C30H50O	WILEY229.LI	6	61	✓	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.LI	7	60	✓	ANTI-1,3,7,11,15,19,23,27,31,35,39,43,12,12-OCTAHEPT	272	C20H32	WILEY229.LI	8	60	✓	cyclooctyl acetate 5,5-9,19-Cycloergost-25	468	C32H52O2	WILEY229.LI	9	59	✓	12 EPISILON, 17 EPISILON DIHYDROXYAN	302	C19H26O3	WILEY229.LI
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	65	✓	9,19-Cyclolanost-24-en-3-ol (3 beta) CASIC	426	C30H50O	WILEY229.LI																																																																		
2	63	✓	Cyclooctatriene 9,19-Cycloergost-24,25-dien	426	C30H50O	WILEY229.LI																																																																		
3	62	✓	9,19-Cyclolanost-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.LI																																																																		
4	61	✓	9,19-Cyclo-9 beta-farnesane-3 beta, 25-diol (C)	444	C30H52O2	WILEY229.LI																																																																		
5	61	✓	Stilane, (9,19-cyclo-9 beta-farnesol-24-en-3 beta)	438	C30H50O	WILEY229.LI																																																																		
6	61	✓	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.LI																																																																		
7	60	✓	ANTI-1,3,7,11,15,19,23,27,31,35,39,43,12,12-OCTAHEPT	272	C20H32	WILEY229.LI																																																																		
8	60	✓	cyclooctyl acetate 5,5-9,19-Cycloergost-25	468	C32H52O2	WILEY229.LI																																																																		
9	59	✓	12 EPISILON, 17 EPISILON DIHYDROXYAN	302	C19H26O3	WILEY229.LI																																																																		
<p><b>56.446</b></p>	<p><b>3417</b></p>	<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>64</td> <td>✓</td> <td>D, B-Friedo-B' A' neogammasol-5-en-3-ol, (3 beta)</td> <td>426</td> <td>C30H50O</td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>63</td> <td>✓</td> <td>SOLANESOL 5,5</td> <td>631</td> <td>C45H74O</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>62</td> <td>✓</td> <td>alpha-Cedrol 5,5-14,3a,7-Methanocyclo-5-ol</td> <td>222</td> <td>C15H26O</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>62</td> <td>✓</td> <td>9,19-Cyclolanost-24-en-3-ol, (3 beta) CASIC</td> <td>426</td> <td>C30H50O</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>62</td> <td>✓</td> <td>Stilane, (3 beta)-alpha,14-dimethylacet</td> <td>464</td> <td>C32H56O</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>62</td> <td>✓</td> <td>Cholest-4-en-26-ol, 3-oxo-, cyclo-2E-ethylene</td> <td>442</td> <td>C29H46O3</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>62</td> <td>✓</td> <td>(12Z)-ABIENOL 5,5</td> <td>290</td> <td>C20H34O</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>62</td> <td>✓</td> <td>2,6,10,14,18,22-Tetracosahexane, 2,6,10,15</td> <td>410</td> <td>C30H50</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target:</p> <p>1: 426: D, B-Friedo-B' A' neogammasol-5-en-3-ol, (3 beta) Sesaranol 5,5 D, B-Friedo-B' A' neogammasol-5-en-3 beta-ol 5,5 E, B-Friedo-B' A' neogammasol-5-en-3 beta-ol 5,5 1H-Cyclopenta[1,2]chylene, D, B-Friedo-B' A' neogammasol-5-en-3-ol deriv. 5,5 beta-Sesaranol 5,5</p> <p>CAS# 10536-41-9 Mol Wt 426 Serial# 201768</p> <p>Comp Name: D, B-Friedo-B' A' neogammasol-5-en-3-ol, (3 beta) Sesaranol 5,5 D, B-Friedo-B' A' neogammasol-5-en-3 beta-ol 5,5 E, B-Friedo-B' A' neogammasol-5-en-3 beta-ol 5,5 1H-Cyclopenta[1,2]chylene, D, B-Friedo-B' A' neogammasol-5-en-3-ol deriv. 5,5 beta-Sesaranol 5,5</p> <p>Formula: C30H50O Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	64	✓	D, B-Friedo-B' A' neogammasol-5-en-3-ol, (3 beta)	426	C30H50O	WILEY229.LI	2	63	✓	SOLANESOL 5,5	631	C45H74O	WILEY229.LI	3	62	✓	alpha-Cedrol 5,5-14,3a,7-Methanocyclo-5-ol	222	C15H26O	WILEY229.LI	4	62	✓	9,19-Cyclolanost-24-en-3-ol, (3 beta) CASIC	426	C30H50O	WILEY229.LI	5	62	✓	Stilane, (3 beta)-alpha,14-dimethylacet	464	C32H56O	WILEY229.LI	6	62	✓	Cholest-4-en-26-ol, 3-oxo-, cyclo-2E-ethylene	442	C29H46O3	WILEY229.LI	7	62	✓	(12Z)-ABIENOL 5,5	290	C20H34O	WILEY229.LI	8	62	✓	2,6,10,14,18,22-Tetracosahexane, 2,6,10,15	410	C30H50	WILEY229.LI							
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	64	✓	D, B-Friedo-B' A' neogammasol-5-en-3-ol, (3 beta)	426	C30H50O	WILEY229.LI																																																																		
2	63	✓	SOLANESOL 5,5	631	C45H74O	WILEY229.LI																																																																		
3	62	✓	alpha-Cedrol 5,5-14,3a,7-Methanocyclo-5-ol	222	C15H26O	WILEY229.LI																																																																		
4	62	✓	9,19-Cyclolanost-24-en-3-ol, (3 beta) CASIC	426	C30H50O	WILEY229.LI																																																																		
5	62	✓	Stilane, (3 beta)-alpha,14-dimethylacet	464	C32H56O	WILEY229.LI																																																																		
6	62	✓	Cholest-4-en-26-ol, 3-oxo-, cyclo-2E-ethylene	442	C29H46O3	WILEY229.LI																																																																		
7	62	✓	(12Z)-ABIENOL 5,5	290	C20H34O	WILEY229.LI																																																																		
8	62	✓	2,6,10,14,18,22-Tetracosahexane, 2,6,10,15	410	C30H50	WILEY229.LI																																																																		
<p><b>56.696</b></p>	<p><b>3430</b></p>	<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>72</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>2</td> <td>71</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>3</td> <td>74</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>73</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>NIST107.LIB</td> </tr> </tbody> </table> <p>Target:</p> <p>1: 498: Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5</p> <p>CAS# 95493-84-0 Mol Wt 498 Serial# 102282</p> <p>Comp Name: Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5</p> <p>Formula: C32H50O5 Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	72	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI	2	71	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI	3	74	✓	Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI	4	73	✓	Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5	498	C32H50O5	NIST107.LIB																																			
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	72	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI																																																																		
2	71	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI																																																																		
3	74	✓	Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI																																																																		
4	73	✓	Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5	498	C32H50O5	NIST107.LIB																																																																		
<p><b>57.395</b></p>	<p><b>3466</b></p>	<table border="1"> <thead> <tr> <th>Hit</th> <th>Similar</th> <th>Regi</th> <th>Compound Name</th> <th>Mol Wt</th> <th>Formula</th> <th>Library</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>70</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>NIST107.LIB</td> </tr> <tr> <td>2</td> <td>70</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>NIST107.LIB</td> </tr> <tr> <td>3</td> <td>69</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>4</td> <td>68</td> <td>✓</td> <td>Stilane, trimethyl(alpha-methylergosta-7,24-dien-3-yl)</td> <td>484</td> <td>C32H56O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>5</td> <td>66</td> <td>✓</td> <td>9,19-Cyclo-9 beta-farnesane-3 beta, 25-diol (C)</td> <td>444</td> <td>C30H52O2</td> <td>WILEY229.LI</td> </tr> <tr> <td>6</td> <td>65</td> <td>✓</td> <td>9,19-Cyclolanost-3-ol, 24-methylene-, (3 beta)</td> <td>440</td> <td>C31H52O</td> <td>WILEY229.LI</td> </tr> <tr> <td>7</td> <td>64</td> <td>✓</td> <td>Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5</td> <td>498</td> <td>C32H50O5</td> <td>WILEY229.LI</td> </tr> <tr> <td>8</td> <td>64</td> <td>✓</td> <td>9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)</td> <td>440</td> <td>C31H52O</td> <td>WILEY229.LI</td> </tr> <tr> <td>9</td> <td>64</td> <td>✓</td> <td>9,19-Cyclolanost-23-ene-3,25-diol, (3 beta), 23</td> <td>442</td> <td>C30H50O2</td> <td>WILEY229.LI</td> </tr> </tbody> </table> <p>Target:</p> <p>1: 498: Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5 3-[(Trimethyl(alpha-methylergosta-8,24-dien-3-yl)]</p> <p>CAS# 95493-84-0 Mol Wt 498 Serial# 184519</p> <p>Comp Name: Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5 3-[(Trimethyl(alpha-methylergosta-8,24-dien-3-yl)]</p> <p>Formula: C32H50O5 Class Flag: No Class Flags</p>	Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library	1	70	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	NIST107.LIB	2	70	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	NIST107.LIB	3	69	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI	4	68	✓	Stilane, trimethyl(alpha-methylergosta-7,24-dien-3-yl)	484	C32H56O5	WILEY229.LI	5	66	✓	9,19-Cyclo-9 beta-farnesane-3 beta, 25-diol (C)	444	C30H52O2	WILEY229.LI	6	65	✓	9,19-Cyclolanost-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.LI	7	64	✓	Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI	8	64	✓	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.LI	9	64	✓	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta), 23	442	C30H50O2	WILEY229.LI
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library																																																																		
1	70	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	NIST107.LIB																																																																		
2	70	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	NIST107.LIB																																																																		
3	69	✓	Stilane, (3 beta)-Narosta-8,24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI																																																																		
4	68	✓	Stilane, trimethyl(alpha-methylergosta-7,24-dien-3-yl)	484	C32H56O5	WILEY229.LI																																																																		
5	66	✓	9,19-Cyclo-9 beta-farnesane-3 beta, 25-diol (C)	444	C30H52O2	WILEY229.LI																																																																		
6	65	✓	9,19-Cyclolanost-3-ol, 24-methylene-, (3 beta)	440	C31H52O	WILEY229.LI																																																																		
7	64	✓	Stilane, (3 beta)-Narosta-9(11),24-dien-3-yl(iso) 5,5	498	C32H50O5	WILEY229.LI																																																																		
8	64	✓	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3 beta)	440	C31H52O	WILEY229.LI																																																																		
9	64	✓	9,19-Cyclolanost-23-ene-3,25-diol, (3 beta), 23	442	C30H50O2	WILEY229.LI																																																																		

<p>57.805</p>	<p>3488</p>	<p>Target: Friedelin</p> <p>1: 426 Friedelin-3-one S1 Friedelin S1 D-A-Friedolan-3-one S1 Friedelin S1 Friedelin S1 4,4a,8b,8a,11,11,12b,14a-Octamethylcyclohexa-3(2H)picenone S1 S1</p> <p>CAS# 559-74-0 Mol Wt: 426 Serial# 174829              Comp Name: Friedelin-3-one S1 Friedelin S1 D-A-Friedolan-3-one S1 Friedelin S1 Friedelin S1 4,4a,8b,8a,11,11,12b,14a-Octamethylcyclohexa-3(2H)picenone S1 S1              Formula: C30H50O Class Flag: No Class Flags</p>
<p>58.739</p>	<p>3538</p>	<p>Target: Slane, [dotriacontyl]trimethyl</p> <p>1: 530 Slane, [dotriacontyl]trimethyl</p> <p>CAS# 0-00-0 Mol Wt: 538 Serial# 186885              Comp Name: Slane, [dotriacontyl]trimethyl              Formula: C52H104Si Class Flag: No Class Flags</p>

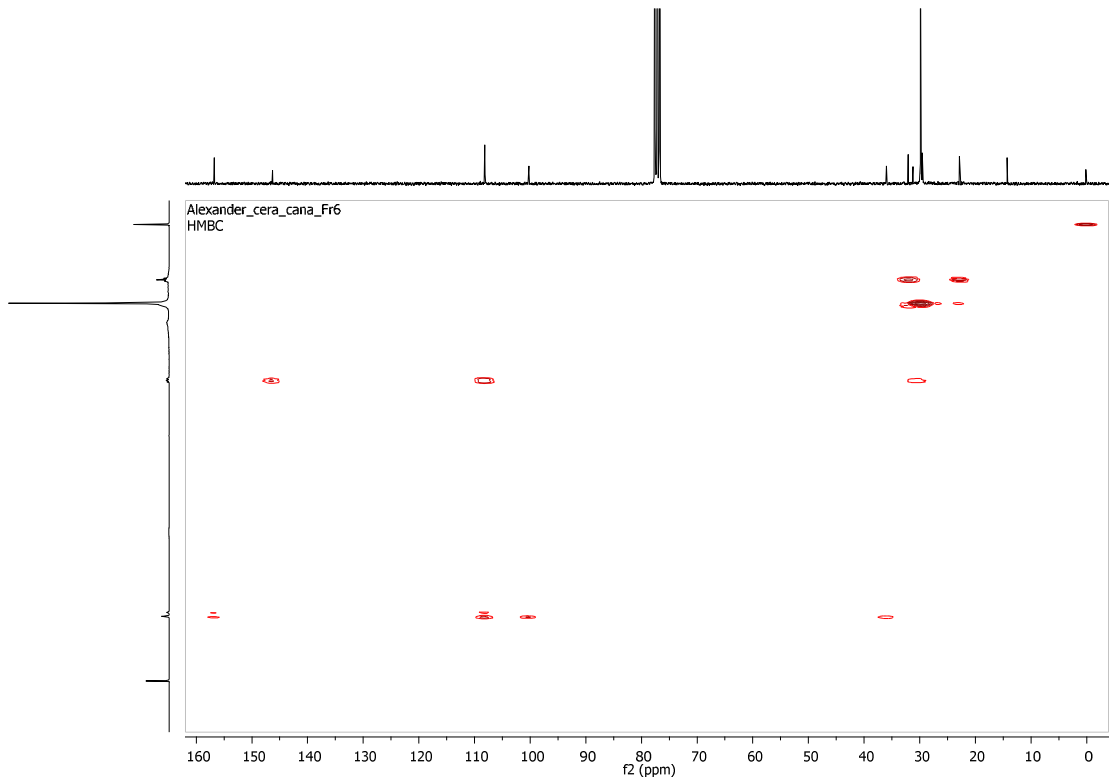
Anexo 5: Espectro de COSY do Alquilresorcinol ( $\text{CDCl}_3$ , 14,1 T)



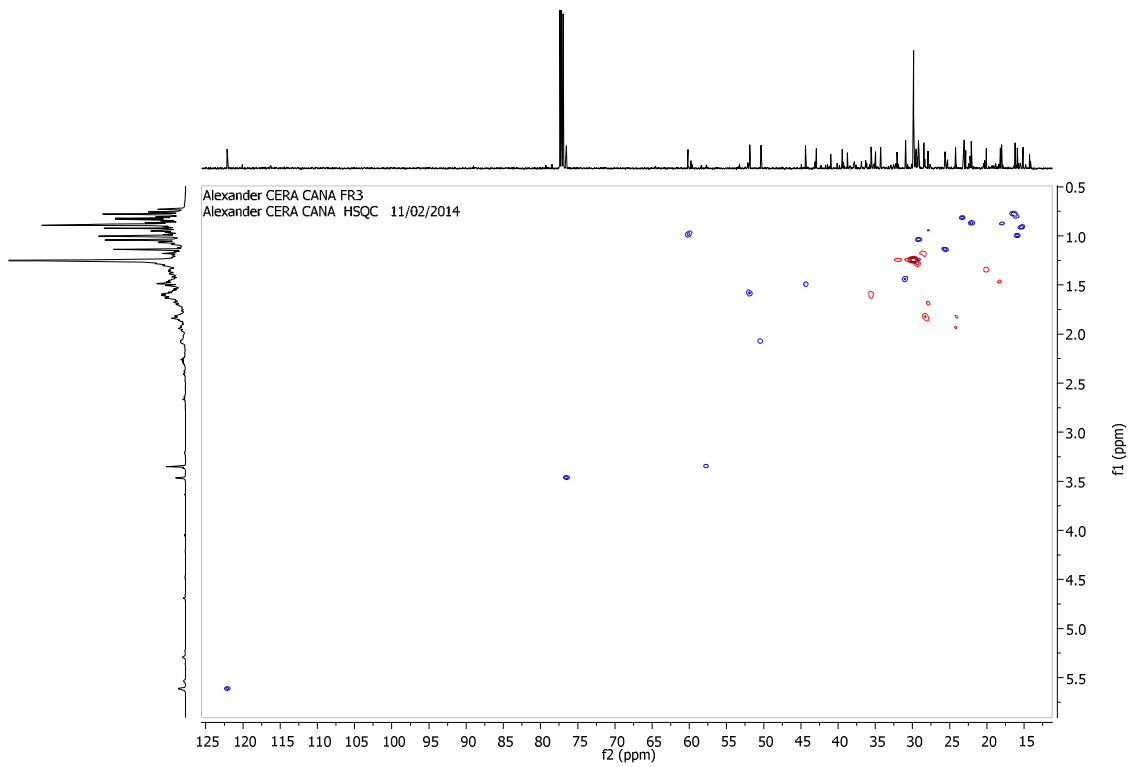
Anexo 6: Mapa de contorno gHSQC do Alquilresorcinol ( $\text{CDCl}_3$ , 14,1 T)



**Anexo 7:** Mapa de contorno gHMBC do Alquilresorcinol ( $\text{CDCl}_3$ , 14,1 T)

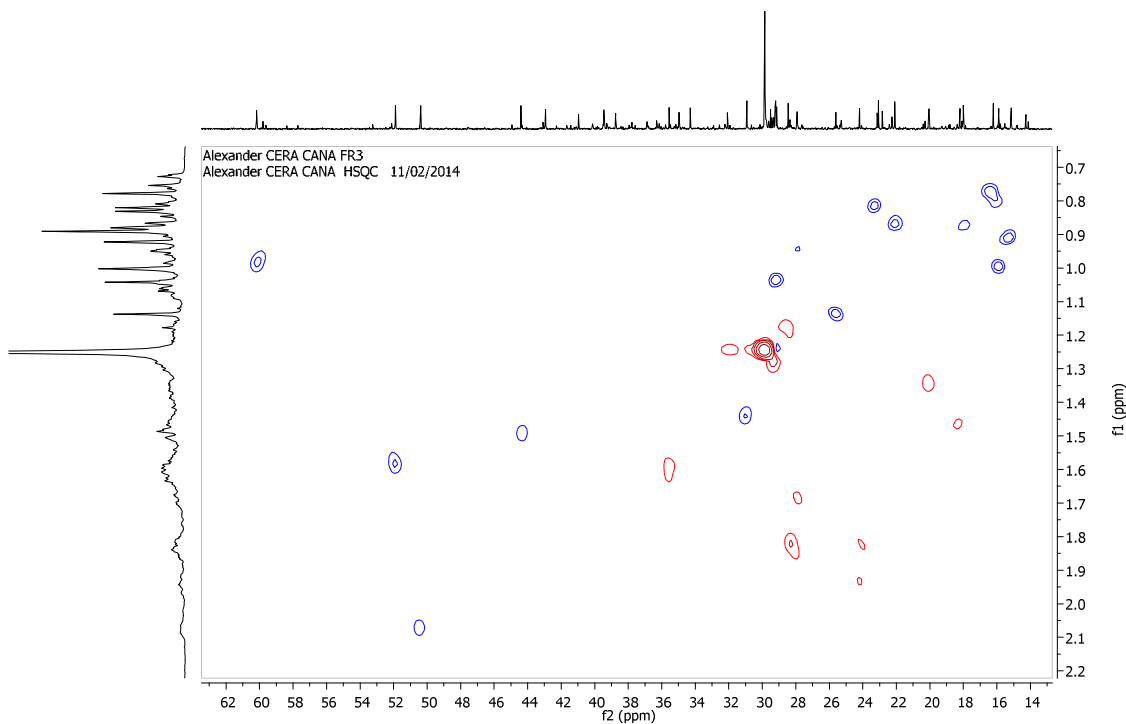


**Anexo 8:** Mapa de contorno gHMQC de simiarenol ( $\text{CDCl}_3$ , 14,1 T)

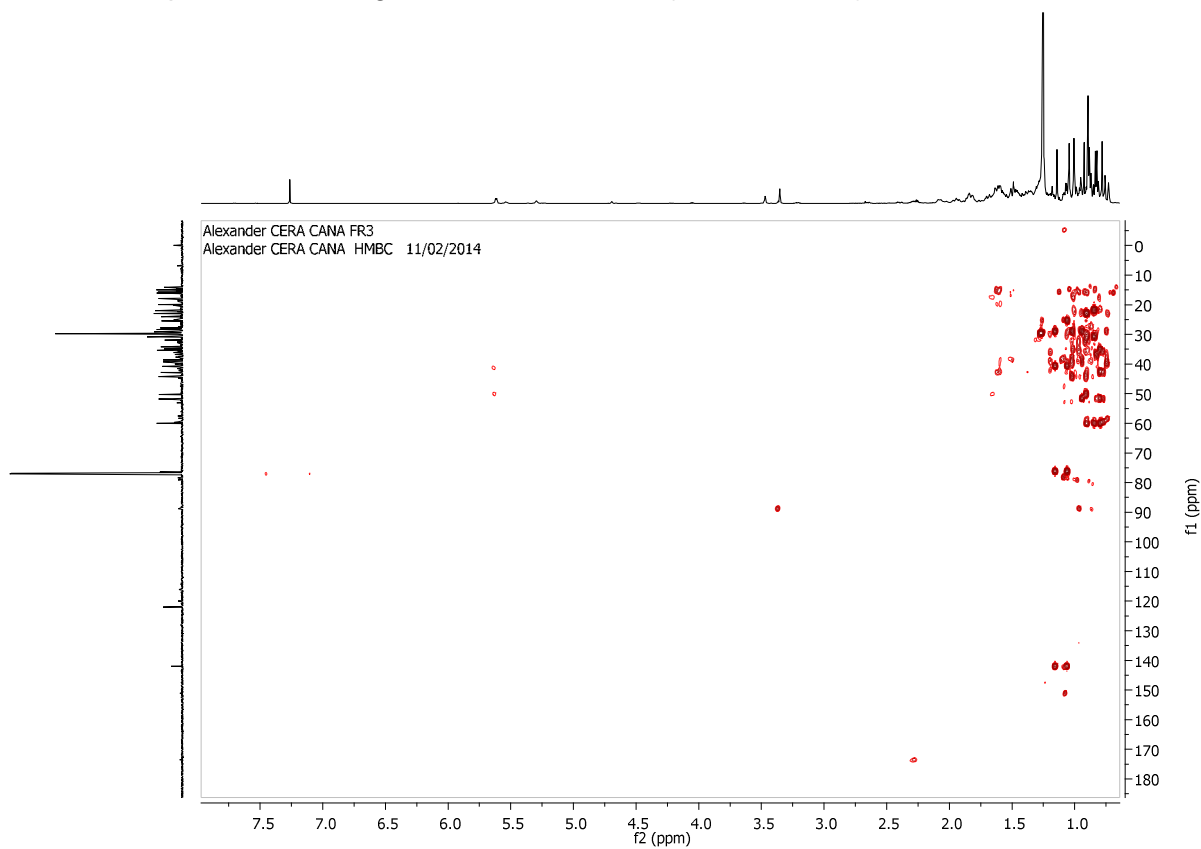




Anexo 9: Ampliação do mapa de contorno gHSQC de simiarenol (CDCl<sub>3</sub>, 14,1 T)

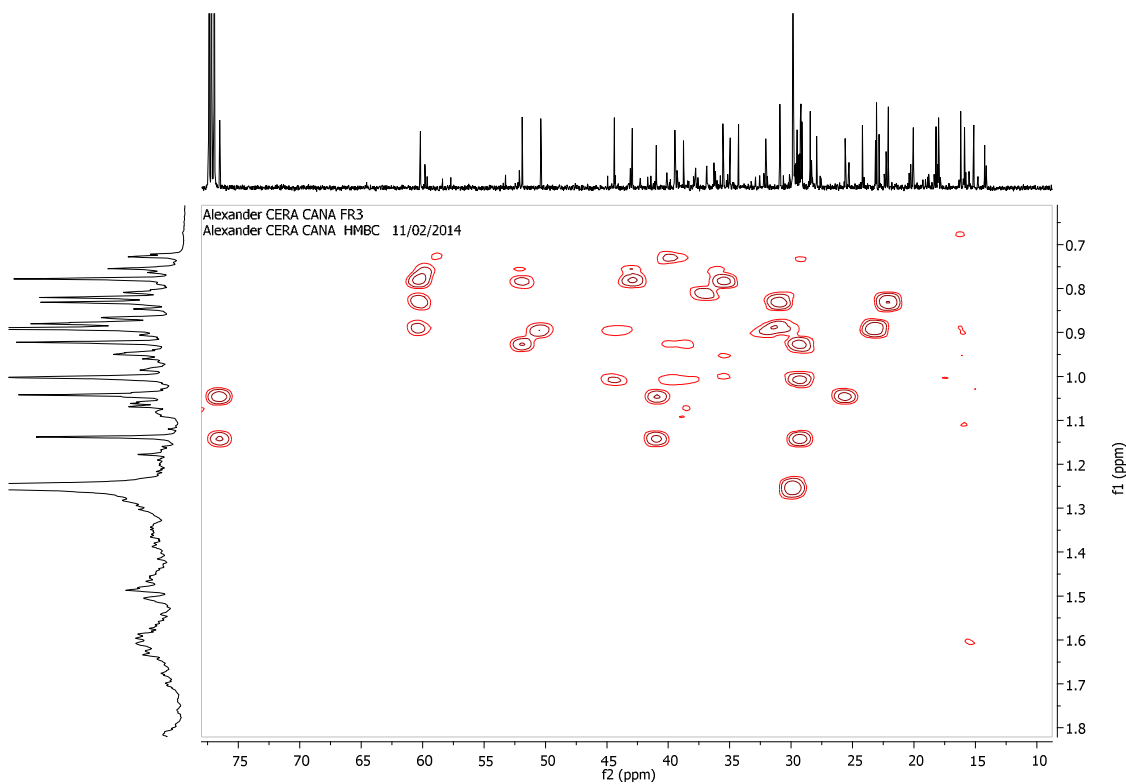


Anexo 10: Mapa de contorno gHMBC de simiarenol (CDCl<sub>3</sub>, 14,1 T)

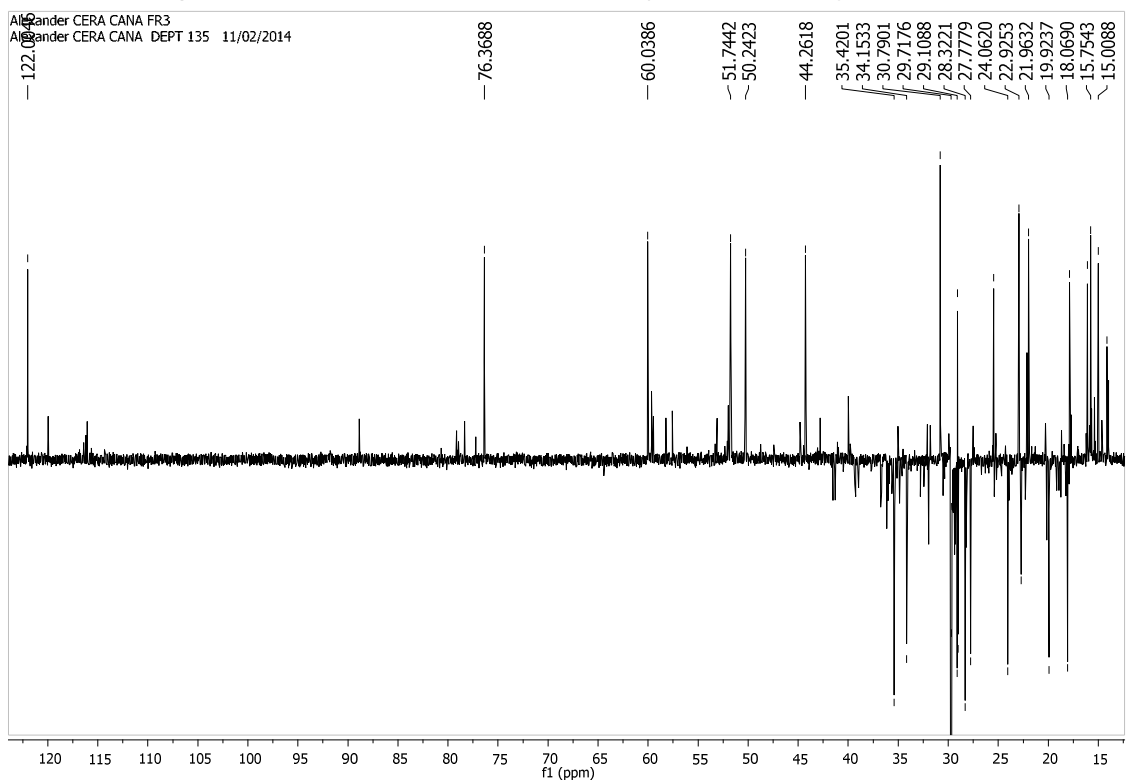




**Anexo 11:** Ampliação do mapa de contorno gHMBC de simiarenol (CDCl<sub>3</sub>, 14,1 T)



**Anexo 12:** Espectro de DEPT 135° de simiarenol (CDCl<sub>3</sub>, 14,1 T)



**Anexo 13: Ampliação do espectro de DEPT 135° de simiarenoil (CDCl<sub>3</sub>, 14,1 T)**

