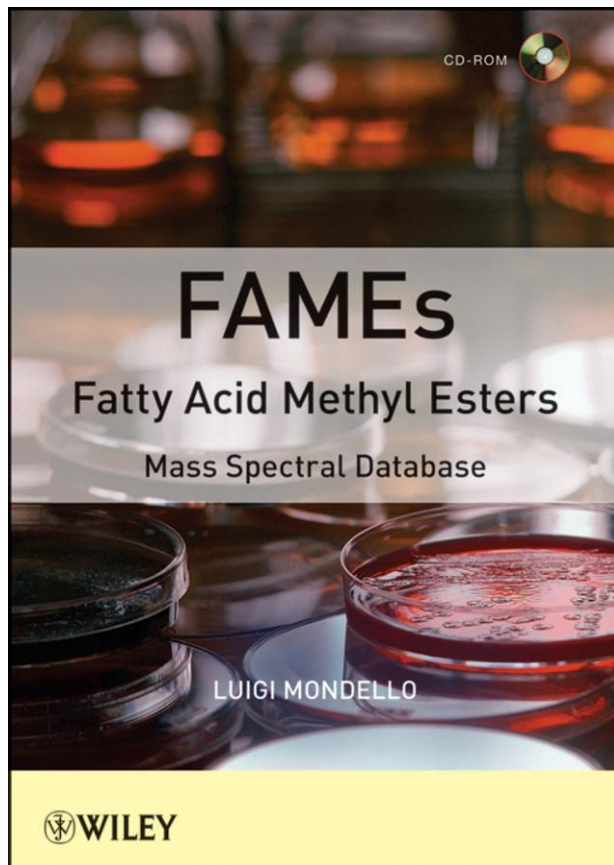


**INSTALLATION MANUAL****VERSION 1.0**

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FAMEs Fatty Acid Methyl Esters: Mass Spectral Database Copyright © 2011 John Wiley & Sons, Hoboken, New Jersey. All Rights Reserved

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## FOREWORD

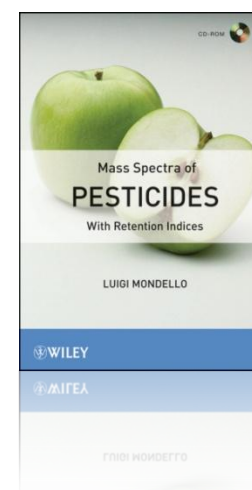
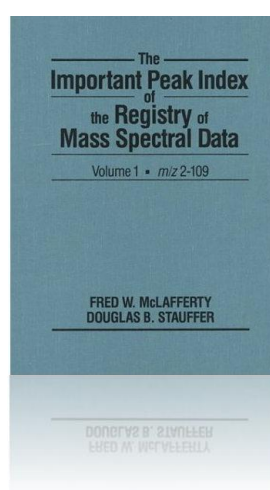
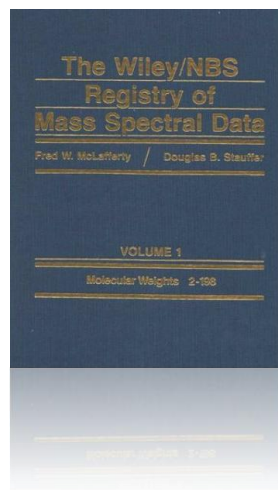
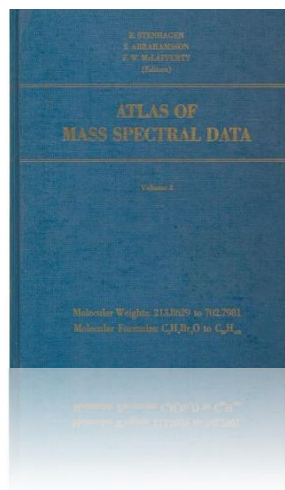
For over 40 years, John Wiley and Sons has worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry. Dr. Luigi Mondello continues this tradition with a highly controlled measurement of fatty acid methyl esters on a variety of columns, with a variety of linear retention index times.

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- 256 Spectra of Fatty Acid Methyl Esters
- 256 Searchable Structures
- Multiple LRI measurements per compound

## ACKNOWLEDGEMENTS

Edited and compiled by Dr. Luigi Mondello.



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Data submissions, editorial notes, corrections, should be addressed to the Wiley Registry at the address, below.

**Wiley Scientific, Technical and Medical Databases**

c/o John Wiley & Sons, Inc.

111 River Street

Hoboken, NJ 07030-5774

USA

Telephone: +1-201-748-6000

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e-mail: [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com)

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10475 Crosspoint Blvd.

Indianapolis, IN 46256

USA

<http://support.wiley.com>

## GETTING STARTED

### HARDWARE AND SOFTWARE RECOMMENDATIONS

- Operating System: Microsoft Windows (XP SP3, Vista SP2 or later, or Windows 7).
- CPU: AMD or Intel processor, preferably multiple core
- Memory: 2GB
- Disk Space: At least 2GB free disc space
- Software: 32-bit or 64-bit software

The library is provided in multiple native manufacturer formats, **but is not supplied with manufacturer software**. Mass spectrometry software should be installed prior to installing the mass spectrometry library, in any format.

If you have purchased the wrong format of the database, please contact Wiley customer care at <http://support.wiley.com> to order a replacement disc in the appropriate format. Shimadzu format for this database is available exclusively through Shimadzu Instruments.

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A license key accompanies the packaging provided with the CD. Only one manufacturer format plus the NIST MS Search format may be installed on any one machine.

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Wiley has provided you with a broad selection of native manufacturer formats to aid you in your installation. Please consult your software manufacturer's documentation and customer support before contacting Wiley customer support. This CD contains the following manufacturer formats:

<b>Format<sup>1</sup></b>	<b>Compatible Software (Manufacturer)</b>
<b>Chemstation.L</b>	Chemstation, MassHunter (Agilent)
<b>MassLynx</b>	MassLynx (Waters)
<b>MS Search<sup>2</sup></b>	MS Search (NIST)
<b>ND9</b>	MS Manager (ACD/Labs)
<b>Spectral ID</b>	Spectral ID (ThermoFisher, formerly Galactic)
<b>TurboMass</b>	TurboMass (PerkinElmer)

---

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<sup>2</sup> MS Search is compatible with most manufacturer software systems. Consult your software manufacturer's manual to determine compatibility.

## DIRECTORY STRUCTURE

The table below lists the formats, installation files, and their default target directories. If two directories are listed, the first directory is for the spectral data files, the second directory is for the structure files. If one directory is listed, all spectra and structure files are installed into that directory. All installations allow a manual override of the default directory path.

Format	Installation file	Default Directory
<b>Chemstation</b>	FAMES2011 - Chemstation.exe	C:\DATABASE\FAMES2011\ C:\DATABASE\FAMES2011\FAMES2011ST\
<b>MassHunter<sup>1</sup></b>	FAMES2011 - Chemstation.exe	C:\MassHunter\Libraries\ C:\MassHunter\Libraries\FAMES2011\FAMES2011ST\
<b>MassLynx</b>	FAMES2011 - MassLynx.exe	C:\MassLynx\IdentDB\ C:\MassLynx\StructDB\FAMES2011\
<b>MS Manager</b>	FAMES2011 – ND9.exe	c:\Program Files\ACD12\DATABASE\FAMES2011\
<b>MS Search</b>	FAMES2011 - MSSearch.exe	C:\NIST11\MSSEARCH\FAMES2011\
<b>SpectralID</b>	FAMES2011 - SpectralID.exe	C:\Program Files\Galactic\Data\
<b>TurboMass</b>	FAMES2011 - Turbomass.exe	C:\TurboMass\Identdb\ C:\TurboMass\Structdb\FAMES2011\

Additional Information: If you have any question, please do not hesitate to contact technical support. <http://support.wiley.com>

<sup>1</sup> MassHunter should be manually installed in these directories.

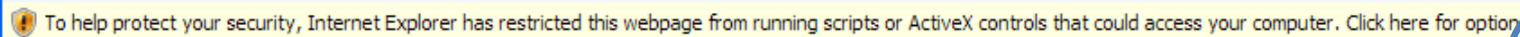


**STEP-BY-STEP INSTALLATION**

**Step 1.** Carefully read the End User License Agreement contained on the CD or the accompanying packaging before using and/or installing this product.

**Step 2.** If you plan on installing mass spectrometry software – install the software now, first.

**Step 3.** Installation.htm is included on the disc to simplify installation. Manual installation instructions are available elsewhere in this manual. Please note that the web page contains embedded links or ActiveX that may create warnings such as the following (1) and (2):

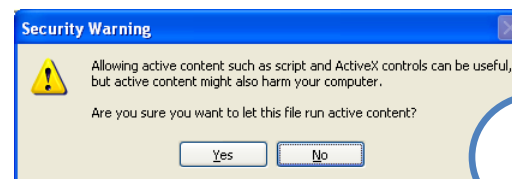


To help protect your security, Internet Explorer has restricted this webpage from running scripts or ActiveX controls that could access your computer. Click here for options

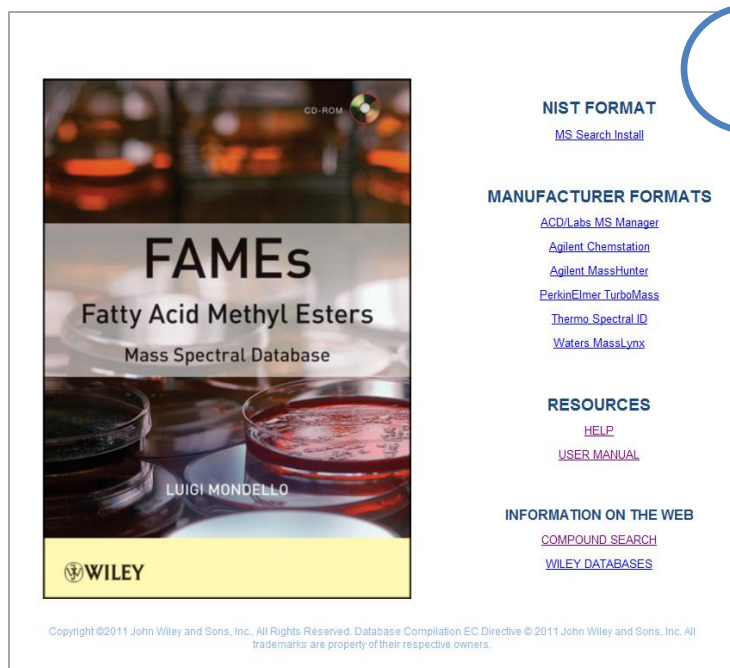
1

Installation screen (3) on your Web browser:

Choose one of the manufacturer formats and/or the MS Search Format. Your license entitles you to install the library on one machine. Please note that the installation files are unsigned – so the following warning will be displayed in Windows XP (4) or similarly in Windows 7:



2



CD-ROM

**FAMEs**  
Fatty Acid Methyl Esters  
Mass Spectral Database

LUIGI MONDELLO

**WILEY**

**NIST FORMAT**  
[MS Search Install](#)

**MANUFACTURER FORMATS**  
[ACDLabs MS Manager](#)  
[Agilent Chemstation](#)  
[Agilent MassHunter](#)  
[PerkinElmer TurboMass](#)  
[Thermo Spectral ID](#)  
[Waters MassLynx](#)

**RESOURCES**  
[HELP](#)  
[USER MANUAL](#)

**INFORMATION ON THE WEB**  
[COMPOUND SEARCH](#)  
[WILEY DATABASES](#)

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3



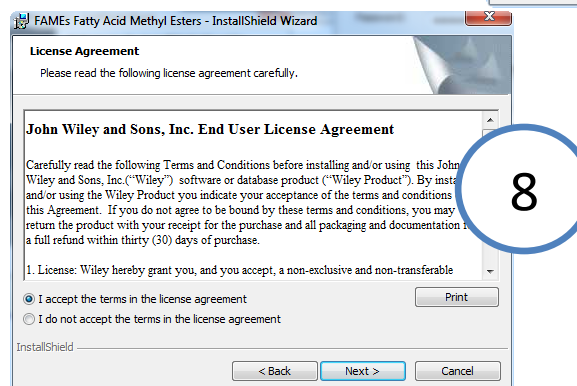
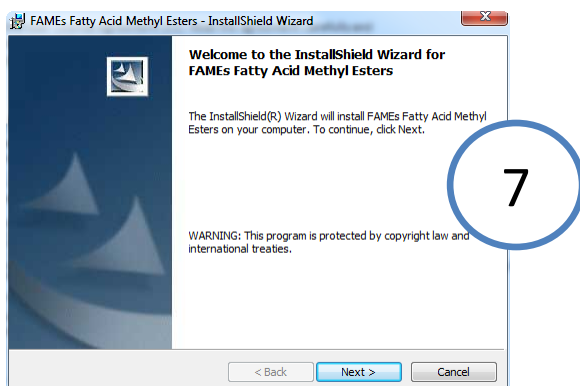
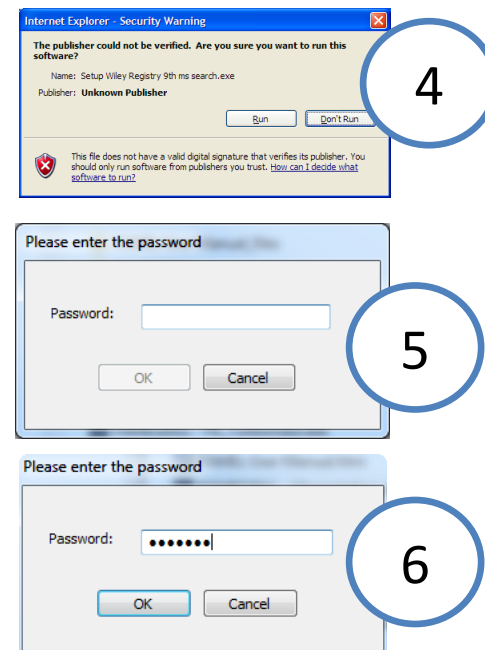
#### Step 4. Password and Install

Choose a format to install. Many users prefer to use native manufacturer format and MS Search format. You may choose to install one manufacturer format as well as the MS Search format. When you choose to install, you may get a series of warnings about publisher certificates (4). Choosing to run the installer will bring you to a password screen (5). Your password appears on the back of the CD packaging. It is case sensitive. Enter the password to begin the installation and press “OK” (6). If the password is incorrect, the “OK” button will not activate. If you have trouble at this stage, consult “Help” on the installation screen in your browser.

The InstallShield wizard will display the following screens, indicating that it is checking the computer for installation (checking available disk space, installer version, etc.). Once it is ready for installation, press “NEXT” to begin the installation, at which point it will begin uncompressing the library. The library is quite large, so this may take a considerable amount of time on some older systems:

#### Step 5. Welcome Screen, End User License Agreement

Once the installation is decompressed, a screen with “Welcome to the InstallShield Wizard . . .” Press “NEXT” to continue (7). The next screen contains the End User License Agreement (10). Read the agreement carefully and select the radio button labeled “I accept the terms in the license agreement” to proceed to install the library. Press “NEXT” to proceed to the next step.

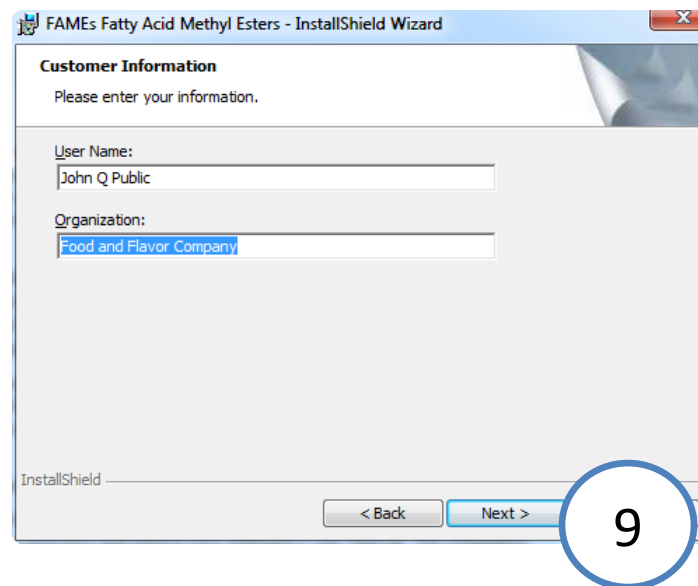
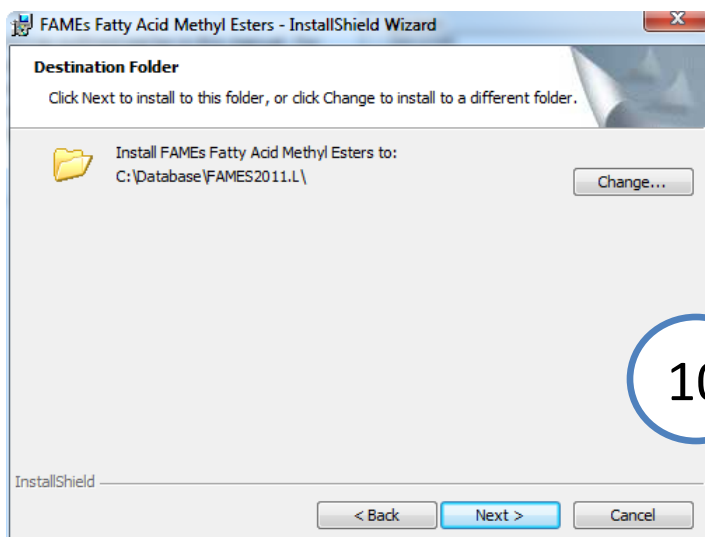


**Step 6. User Information**

Entering customer information is recommended for your records and support (9). This information is not collected by Wiley.

**Step 7. Directory Confirmation**

Each format installs in a directory as outlined earlier in this manual. For your installation to be successful, it must install in the directory specified in your software's user manual. The installation allows you to manually change the target directory yourself by pressing "Change" (10). If you are satisfied with the target directory, press "NEXT" to proceed with the installation.



### Step 8. Confirmation Screen (11)

Before starting the installation, the installer provides a summary of the destination folder and user information. Review this to ensure that it is correct. Press “BACK” to correct the user information or target directory (Steps 5 through 7).

If it is acceptable, choose to install it for “Anyone who uses this computer (all users)”. The installation screen will show you the progress of the installation. Press “CANCEL” at any time to cancel the installation.

### Step 9. Finish, Connect Library

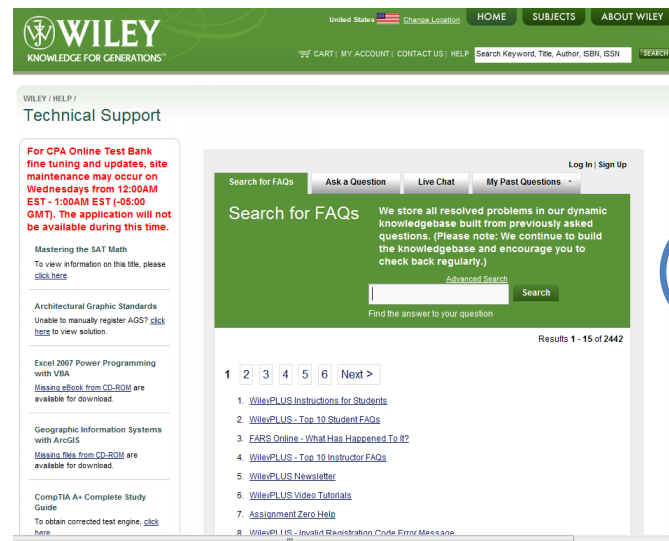
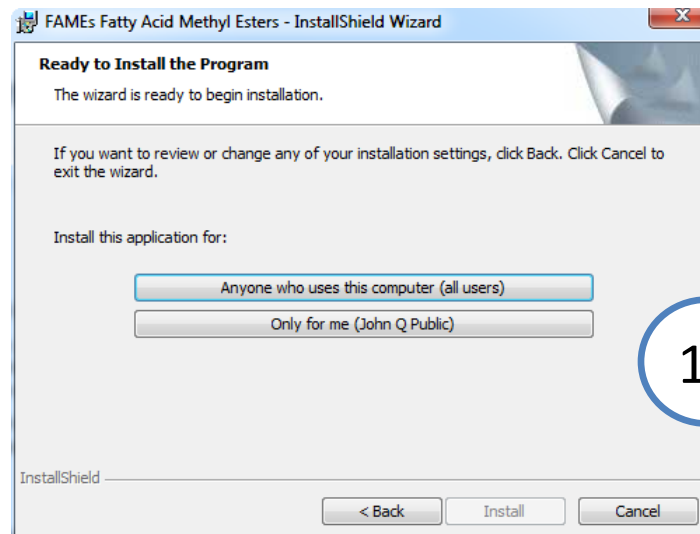
Once the installation is complete, press “Finish” to complete the installation. Be sure to consult your mass spectrometry software’s instructions for connecting to new libraries – some are automatic, but some require manual connection within the software.

### Repairing or Uninstalling

Repairing or uninstalling the library should be managed using the “Add/Remove Programs” utility in Windows. If the library is manually moved or removed, the Windows utility may not work.

### GETTING HELP

Getting Help go to <http://support.wiley.com> (12).



## DATABASE CONTENT

Wiley mass spectrometry libraries have a wide variety of uses. Practitioners and researchers are encouraged to evaluate their own needs and decide what libraries are appropriate for them.

Wiley Registry 9th Edition – A complete, general purpose high quality library for analytical laboratories. Often used as the foundation library for research, quality control, deformation, and for forensic, toxicology, and homeland defense applications.

Wiley Registry 9th/NIST 2011 – A more comprehensive library for mission-critical tasks, including quality control, deformation, forensics, toxicology, and homeland defense applications. This library forms the basis for toxicology screening, steroid screening, and related applications.

See [www.wiley.com/go/databases](http://www.wiley.com/go/databases) for other mass spectrometry, NMR, IR, and enterprise spectroscopy software from John Wiley and Sons, Inc.

## BASIC FUNCTIONS

The enclosed library can be used as the primary search library or can be searched along with other libraries. We recommend, for mission-critical tasks, that users consult both a general library such as Wiley Registry 9e/NIST 2011 Mass Spectral Library and a specialized library such as FAMEs.

## SEARCH TIPS

When using parametric searching, many text search programs provide better results when names are begun and ended with wild cards (e.g., “\*”). However, in NIST MSSearch, this approach will not work.

### ADDITIONAL FIELDS IN NIST MS SEARCH

The additional retention times are captured in the library in the comments field. To display the different measures times, go to "View"/"Comment fields Options"/ which will display the "Display comments field options" dialog. Indicate WileyID, RI1, RI2, RI3, and RI4 as the desired fields. This will then display them in the MS Search. MS Search will display literature retention times, as well.

**Display comment field options**

To show tag=value from Comments as separate line in spectrum text, enter tag as a separate line.

RI1  
 RI2  
 RI3  
 RI4

For example, if RI=132.1 is embedded in Comments, it can be displayed as a separate line in the text by entering the line:

RI

in the above field. Multiple lines will display multiple tag=value pairs in the order entered.

Show tag=value on plot

OK Cancel Help

**Name:** Et.C14:0  
**Formula:** C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>  
**MW:** 256 **Exact Mass:** 256.24023 **CAS#:** 124-06-1 **ID#:** 101 **DB:** fames2011  
**Other DBs:** None  
**Contributor:** Prof. L. Mondello (Chromaleont s.r.l./Univ. Messina, Italy)  
**WileyID:** LM\_FAMES2011\_101  
**RI1:** 2026 (Supelcowax-10 Alkanes; T: 0.25 um, D: 0.25mm, L: 30m)  
**RI2:** 1441 (Supelcowax-10 FAMES; T: 0.25 um, D: 0.25mm, L: 30m)  
**RI3:** 1400 (Supelcowax-10 FAEES; T: 0.25 um, D: 0.25mm, L: 30m)  
**RI4:** 1792 (SLB-5ms Alkanes; T: 0.25 um, D: 0.25mm, L: 30m)  
**Comment:** |RI:2026|  
**10 largest peaks:**  
 88 999 | 101 507 | 43 307 | 41 243 | 55 239 |  
 70 219 | 73 203 | 57 167 | 157 163 | 89 135 |  
**Synonyms:**  
 1. Tetradecanoic acid, ethyl ester  
 2. Myristate <ethyl->  
**Estimated non-polar retention index (n-alkane scale):**  
 Value: 1779 iu  
 Confidence interval (Esters): 47(50%) 201(95%) iu  
**Retention index:**  
 1. Value: 1778 iu  
 Column Type: Capillary  
 Column Class: Standard non-polar  
 Active Phase: BP-1  
 Column Length: 30 m  
 Carrier Gas: N2  
 Column Diameter: 0.32 mm  
 Phase Thickness: 0.25 um  
 Data Type: Linear RI  
 Program Type: Ramp  
 Start T: 60 C  
 End T: 220 C  
 Heat Rate: 5 K/min  
 End Time: 13 min  
 Source: Raina, V.K.; Kumar, A.; Srivastava, S.K.; Syamsundar, K.V.; Kahol, A.  
 2. Value: 1782 iu  
 Column Type: Capillary  
 Column Class: Standard non-polar  
 Active Phase: CP Sil 5 CB  
 Column Length: 60 m  
 Carrier Gas: He  
 Column Diameter: 0.32 mm  
 Phase Thickness: 0.25 um  
 Data Type: Linear RI  
 Program Type: Ramp  
 Start T: 60 C  
 End T: 280 C  
 Heat Rate: 3 K/min

### CAS RNS

Some mass spectrometry software programs rely on a field labeled "CAS-RN" to link spectral records with their corresponding structure record. As many of the compounds found within the Wiley Registry, NIST/EPA/NIH, and other mass spectral libraries are not in the CAS Registry or do not have an assigned CAS-RN, this engineering decision would result in those spectra not being linked to their unique structure. To solve this problem, Wiley has created unique identifiers for the sole purpose of linking the spectrum and its structure using this field. To differentiate these numbers from actual CAS-RNs, each number is prefixed with the number 999.

Please note that IDs prefixed with the number 999 do not in any way represent CAS Registry Numbers, nor are they used for anything other than referring to the structure record in the separate structure database as a workaround to accommodate engineering decisions made by other software publishers.

FAMEs contains 6 such non-CAS RN identifiers ("CAS RN" = 999.000.000 + recordid):

- 999000-13-0
- 999000-13-7
- 999000-17-2
- 999000-17-3
- 999000-22-7
- 999000-23-2

To read more about more modern methods of compound identification, please go to <http://www.inchitrust.org/>

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- Disease profiles, clinical applications and diagnostics

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