

Fatty Acid Methyl Ester (FAME) RTL Databases for GC and GC/MS

User contributed by:

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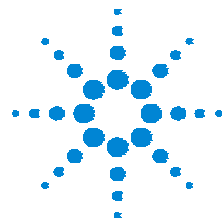
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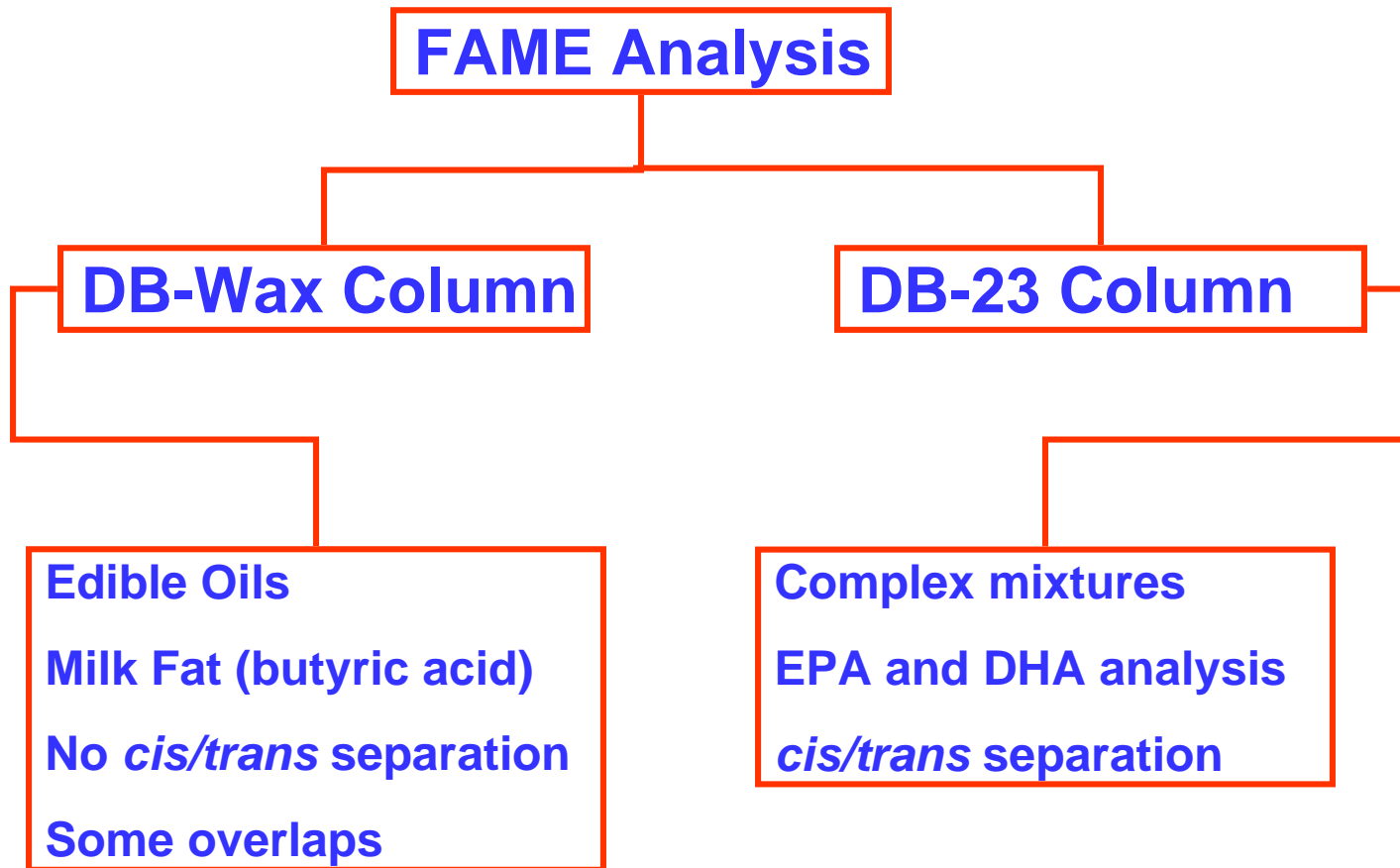
Agilent Technologies

Innovating the HP Way

Database Development

- **Developed at the:
Research Institute for Chromatography,
Pres. Kennedypark 20, B-8500 Kortrijk, Belgium**
- **Four different retention-time locked (RTL) methods were developed:**
 - **One GC and one GC/MS method using an Agilent J&W 30-m X 0.25-mm i.d. X 0.25- μ m DB-Wax column (part no. 122-7032)**
 - **One GC and one GC/MS method using an Agilent J&W 60-m X 0.25-mm i.d. X 0.15- μ m DB-23 column (part no. 122-2361)**
- **All methods were developed using methyl stearate (18:0) as the locking compound**
- **In all four methods, the retention time of methyl stearate was locked to 14.000 min**
- **All data were collected on Agilent GC/MS equipment**

Which Column Should I Use?



FAME RTL Databases Available for GC Analysis with Standard Detectors (e.g., FID)

- **Database for use with an Agilent J&W 30-m X 0.25-mm i.d. X 0.25- μ m DB-Wax column (part no. 122-7032) on an Agilent 6890 GC**
 - **Famdbwax.rtt**
- **Database for use with an Agilent J&W 60-m X 0.25-mm i.d. X 0.15- μ m DB-23 column (part no. 122-2361) on an Agilent 6890 GC**
 - **Famedb23.rtt**

These databases contain the locked retention times for 37 common FAMEs (You can add compounds to it.)

FAME RTL Databases Available for GC/MS

- **Databases for use with an Agilent J&W 30-m X 0.25-mm i.d. X 0.25- μ m DB-Wax column (part no. 122-7032) on an Agilent GC/MSD**
 - **Famdbwax.L** (spectral library folder containing 6 files)
 - **Famdbwax.scd** (screener database)
- **Database for use with an Agilent J&W 60-m X 0.25-mm i.d. X 0.15- μ m DB-23 column (part no. 122-2361) on an Agilent GC/MSD**
 - **Famedb23.L** (spectral library folder containing 6 files)
 - **Famedb23.scd** (screener database)

These databases contain the locked retention times and mass spectra for 37 common FAMEs (You can add compounds to it.)

Using the GC RTL FAME Databases for GC with Conventional Detectors

- **Download the two databases called:**
 - **Famdbwax.rtt**
 - **Famdb23.rtt**
- **Be sure that GC RTL software (Part No. G2080AA) is loaded on your GC ChemStation**
- **Copy these databases to the RTL file under HPChem (Usually C:\HPChem\RTL\)**
- **Download the Agilent application note entitled: “Improving the Analysis of Fatty Acid Methyl esters Using Retention Time Locked Methods and Retention Time Databases” (Publication No. 5988-5871EN) that is included with the FAME RTL databases**

Using the GC RTL FAME Databases for GC with Conventional Detectors (cont.)

- For basic RTL help and instruction:
 - Use the ChemStation “Help” under the drop down menu item RTLock/RTL Help Contents in the ChemStation Data Analysis view
 - Read the application notes listed at the end of this presentation. Instructions for downloading application notes are at the end of this presentation
- Install the DB-23 or DB-Wax column and set up the appropriate GC conditions listed in the application note (publication number 5988-5871EN) for the column you are using
- Run the five RTL calibration runs using methyl stearate as the calibration compound and lock its retention time to 14.000 minutes (same for both columns)

Using the GC RTL FAME Databases for GC with Conventional Detectors (cont.)

- Run FAME samples under locked conditions
- Confirm peak identities by using the “Click on plot” (or “Type in time”) features under the RTSearch drop down menu item
- Be sure to load the appropriate RTL Database into the search form that appears

Load the RTL database that matches your method

Search by Retention Time Table

Load Table... FAMDBWAX.RTT

2.35 Search RT, minutes

0.2 Search Window, minutes

Compound contains these elements: Br Cl F N O P S

Does not contain these elements: Br Cl F N O P S

Compound detected with:

Not detected with:

Search Cancel Help

To Make it Easier to Set up GC Locking Methods and to Search GC Databases...

...Download the following user-contributed macros from the Agilent web site at

(<http://www.chem.agilent.com/cag/servsup/usersoft/main.html#RTL>):

RTL Autolocker for GC

Automates GC retention time locking calibration and (re)locking of methods

RTL Autosearcher for GC

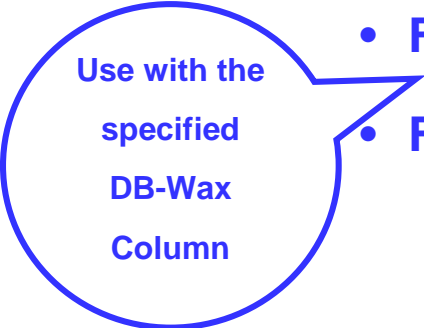
Automates RTL library searching for GC

Using the FAME RTL Databases Designed for GC/MS

- **Advantages of GC/MS RTL Fame Analysis:**
 - **Never have to update RT windows for quant databases**
 - **Use mass-spectral library searching AND locked retention times for more accurate peak identifications**
 - **Identify unknown peaks**
 - **Better identification of FAMES with similar spectra**

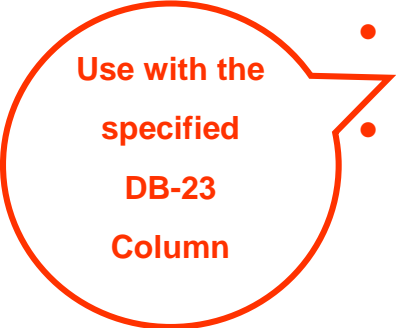
Using the FAME RTL Databases Designed for GC/MS

- Download the following databases (available at the end of this presentation)



Use with the
specified
DB-Wax
Column

- Famdbwax.L (folder with 6 mass spectral library files)
- Famewax.scd (file containing the RTL screener database)



Use with the
specified
DB-23
Column

- Famedb23.L (folder with 6 mass spectral library files)
- Famedb23.scd (file containing the RTL screener database)

Using the FAMEs RTL Databases Designed for GC/MS

- Copy all four databases to the Database folder - usually C:\Database
- Install one of the two columns specified - either the DB-Wax or DB-23
- Set up the nominal method using the GC/MS parameters specified in the application note (publication number 5988-5871EN) for the column you are using
- Use the GC/MS RTL software to make the 5 calibration runs automatically and lock the method
- Run samples using the RTL method
- Screen the chromatograms using the **Famewax.scd** or **Famedb23.scd** database according to the column and method in use
- Generate a screen report and review the data using the Results Screener (under “View/Results screener”)

Screeners Variables

- **The number of probable and possible “hits” can be globally changed by changing the following variables:**
 - **Retention time extraction window**
 - **Qualifier mode - relative or absolute**
 - **Ratio of qualifier ions to the target ion**
 - **Zero qualifiers - include or exclude**
 - **Subtraction Mode**
- **Integration parameters define peak detection**

Benefits of Using RTL Databases for GC/MS

- **Fastest identification of compounds**
 - **Screen FAMES in seconds**
- **Fastest confirmation of compounds**
 - **Eliminate “hits” with wrong RT**
- **Precise and reproducible RT on GC and GC/MS**
 - **Match GC RT to GC/MS RT**
 - **No need to update calibration table RTs**
- **Compounds identified by both RT and spectral library searching**
- **Make your own RTL database or add compounds to existing ones**
- **No additional cost for user-contributed databases**

Agilent Instruments and Software Required for GC RTL Methods

- **Gas Chromatograph**
 - 6890N with 7683 autosampler (tray & injector) and split/splitless inlet
 - Flame ionization detector (FID) - or other universal GC detector
- **Software**
 - G2070AA GC ChemStation software (or higher)
 - G2080AA GC RTL Software (or higher)
- **Column choices**
 - Agilent J&W 30-m X 0.25-mm i.d. X 0.25- μ m DB-Wax column (part no. 122-7032)
 - Agilent J&W 60-m X 0.25-mm i.d. X 0.15- μ m DB-23 column (part no. 122-2361)

Agilent Instruments and Software Required for GC/MS RTL Methods

- **Gas Chromatograph**
 - 6890N with 7683 autosampler (tray & injector) and split/splitless inlet
- **Mass Spectrometer**
 - 5973N MSD
- **Software**
 - G1701DA GC/MS ChemStation software (or higher)
- **Column choices**
 - Agilent J&W 30-m X 0.25-mm i.d. X 0.25- μ m DB-Wax column (part no. 122-7032)
 - Agilent J&W 60-m X 0.25-mm i.d. X 0.15- μ m DB-23 column (part no. 122-2361)

Files Included in the Download

GC RTL Databases

- Famdbwax.rtt - FAME retention time database for GC (DB-Wax column)
- Famedb23.rtt - FAME retention time database for GC (DB-23 column)
- **Application Note - Publication number 5988-5871EN**

GC/MS RTL Databases

- Famdbwax.L - Mass spectral library for 37 FAMEs (DB-Wax column)
- Famewax.scd - FAME GC/MS RTL screener database (DB-Wax column)
- Famedb23.L - Mass spectral library for 37 FAMEs (DB-23 column)
- Famedb23.scd - FAME GC/MS RTL screener database (DB-23 column)
- **Application Note - Publication number 5988-5871EN**

Recommended Reading to Learn More About RTL

- **Fast Screening of PCB Congeners Using the Agilent 6890/5973N GC/MSD System Application, [5980-1472E](#)**
- **Fast Screening of Pesticides and Endocrine Disrupters Using the Agilent 6890/5973N GC/MSD System, Part 1, [5968-9220E](#)**
- **Fast Screening of Pesticide and Endocrine Disrupters Using the Agilent 6890/5973N GC/MSD System, Part II, [5980-1057E](#)**
- **Retention Time Locking with the G1701BA MSD Productivity ChemStation, [5968-3433E](#)**
- **A Method Used to Screen for 567 Pesticides and Suspected Endocrine Disrupters, [5967-5860E](#)**

How To Download Application Notes from the Agilent Web Site

- Direct your browser to: www.agilent.com/chem
- Click on [Library](#)
- Click on [Online Literature](#)
- In the [Keyword](#) field, type the publication number (e.g., [5967-5860E](#)) for the application note you would like to view
- or, In the [Keyword](#) field, type RTL and search to find all Agilent literature on RTL