

# RTL GC/MS Databases for Organotin Derivatives

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# Database Development

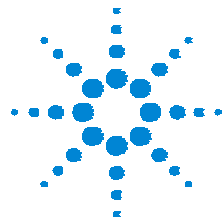
- **Developed at the:  
Research Institute for Chromatography,  
Pres. Kennedypark 20, B-8500 Kortrijk, Belgium**
- **Three different Retention Time Locked (RTL) Organotin databases were developed:**
  - **Methyl derivatives (using methylmagnesium bromide)**
  - **Ethyl derivatives (using sodium tetraethylborate)**
  - **Pentyl derivatives (using pentylmagnesium bromide)**
- **All methods were developed using tetrabutyltin as the locking compound (locked to a retention time of 16.000 min)**
- **All data were collected on Agilent GC/MS equipment**

## Compounds Included in the Databases with Key Mass Spectral Ions for the Three Types of Derivatives

Organotin solute	Abbreviation	Derivatisation 1	Derivatisation 2	Derivatisation 3
Reagent		Methyl-magnesium bromide	Pentyl-magnesiumbromide	Sodium tetraethylborate
Derivatives		Methyl-	Pentyl-	Ethyl-
triethyltin	TET	193, 191, 165, 163	179, 177, 249, 247	207, 205, 179, 177
tetraethyltin	TeET	207, 205, 179, 177	207, 205, 179, 177	207, 205, 179, 177
tripropyltin	TPT	179, 177, 221, 219	277, 275, 165, 163	235, 233, 249, 247
tetrapropyltin	TePT	249, 247, 207, 205	249, 247, 207, 205	249, 247, 207, 205
monobutyltin	MBT	165, 163, 151, 149	319, 317, 193, 191	235, 233, 179, 177
dibutyltin	DBT	151, 149, 207, 205	319, 317, 179, 177	263, 261, 207, 205
tributyltin	TBT	193, 191, 249, 247	305, 303, 179, 177	291, 289, 207, 205
tetrabutyltin	TeBT	291, 289, 179, 177	291, 289, 179, 177	291, 289, 179, 177
monophenyltin	MPhT	227, 225, 223, 197	339, 337, 197, 195	255, 253, 197, 195
diphenyltin	DPhT	289, 287, 285, 197	345, 343, 197, 195	303, 301, 197, 195
triphenyltin	TPhT	351, 349, 347, 197	351, 349, 347, 197	351, 349, 347, 197
tetraphenyltin	TePhT	351, 349, 347, 197	351, 349, 347, 197	351, 349, 347, 197
tricyclohexyltin (cyhexatin)	TCT	301, 299, 219, 217	357, 355, 205, 203	315, 313, 233, 231
monoocetyl tin	MOT	165, 163, 263, 261	375, 373, 193, 191	291, 289, 179, 177
dioctyltin	DOT	263, 261, 151, 149	417, 415, 375, 373	375, 373, 263, 261

# A Brief Introduction to Retention Time Locking (RTL)

You can download much more information here, at Agilent's web site. Simply type '**RTL**' into the search box to find helpful information such as application notes.

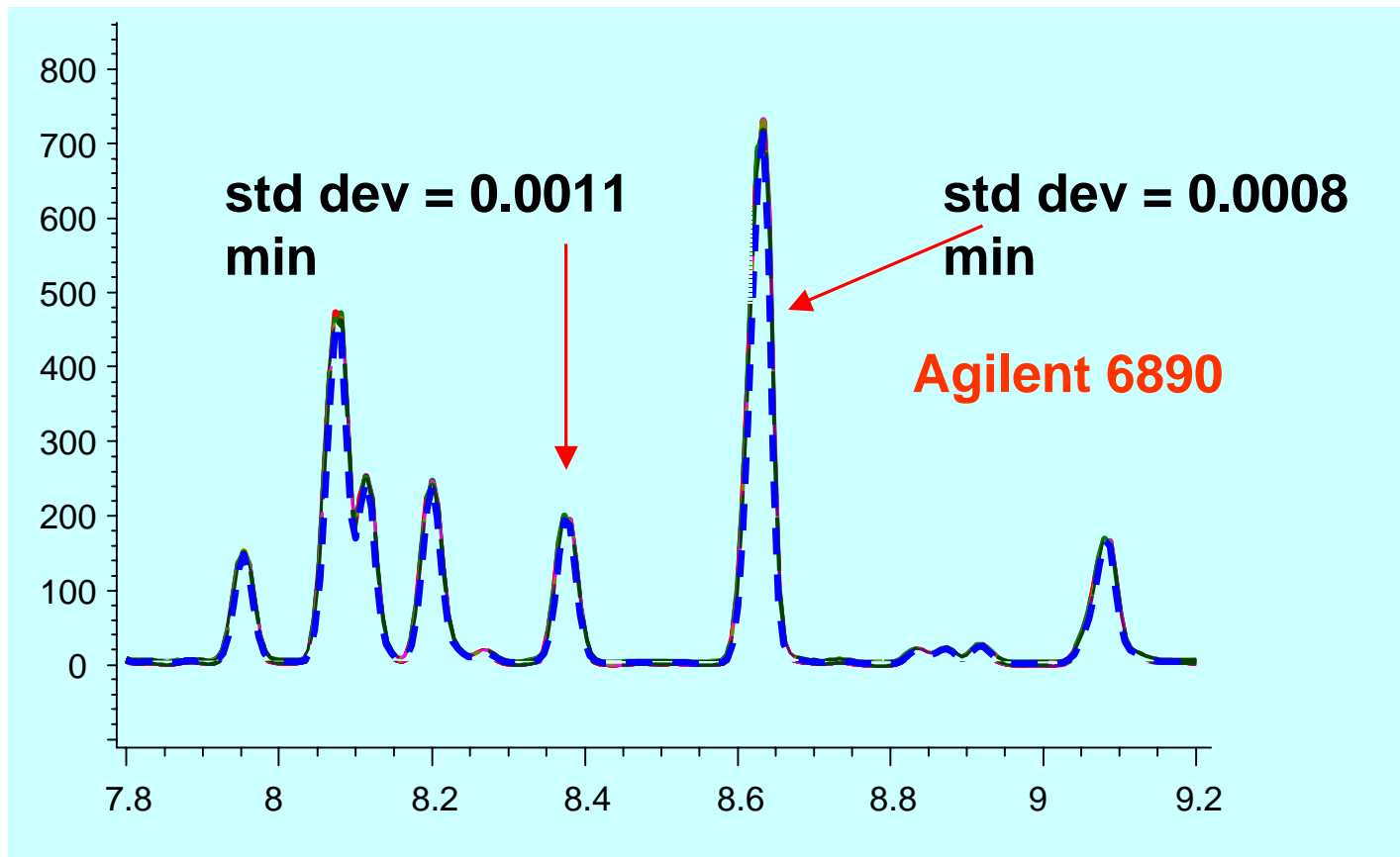


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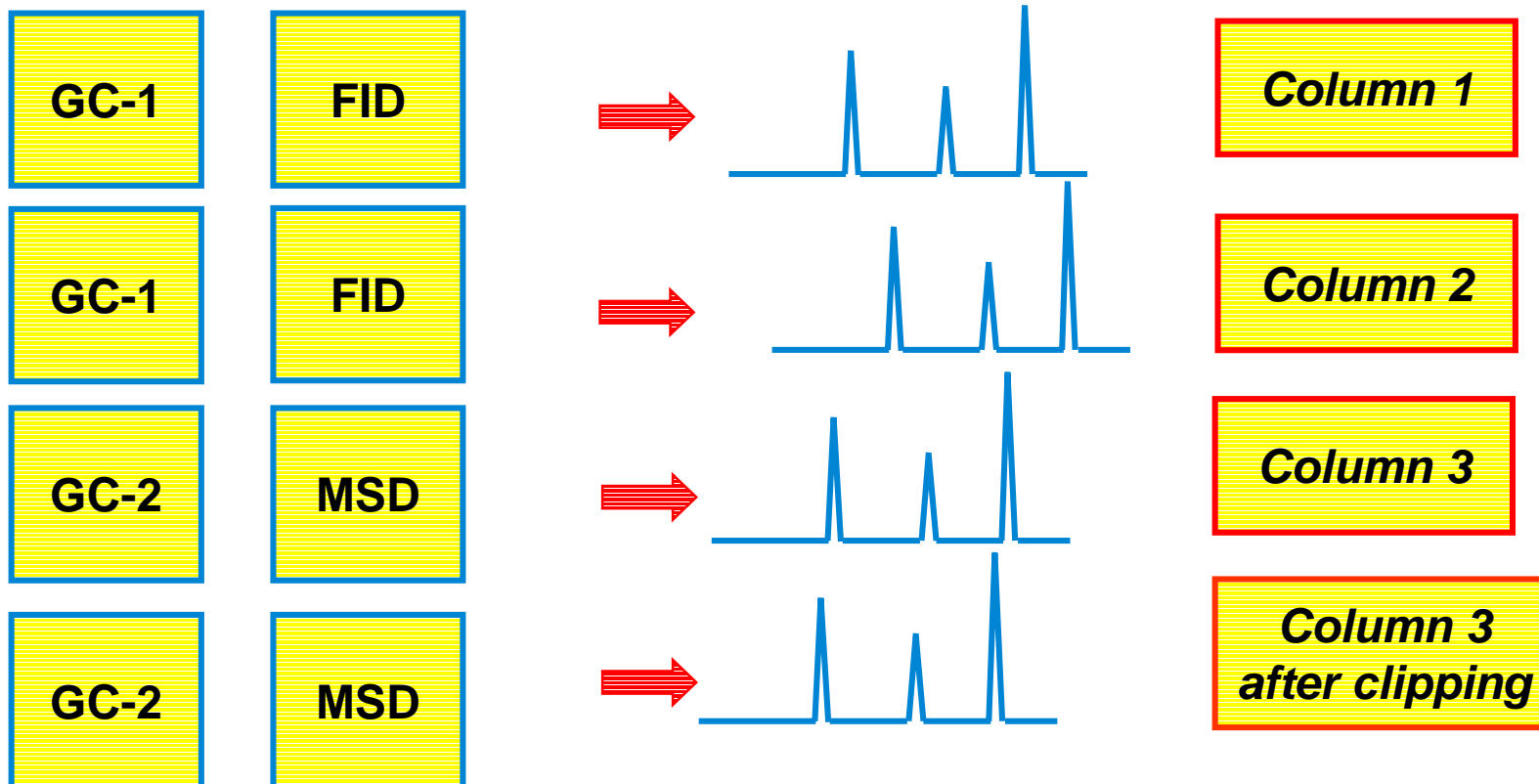
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# Using Agilent GCs, Retention Times are Extremely Repeatable from Run to Run

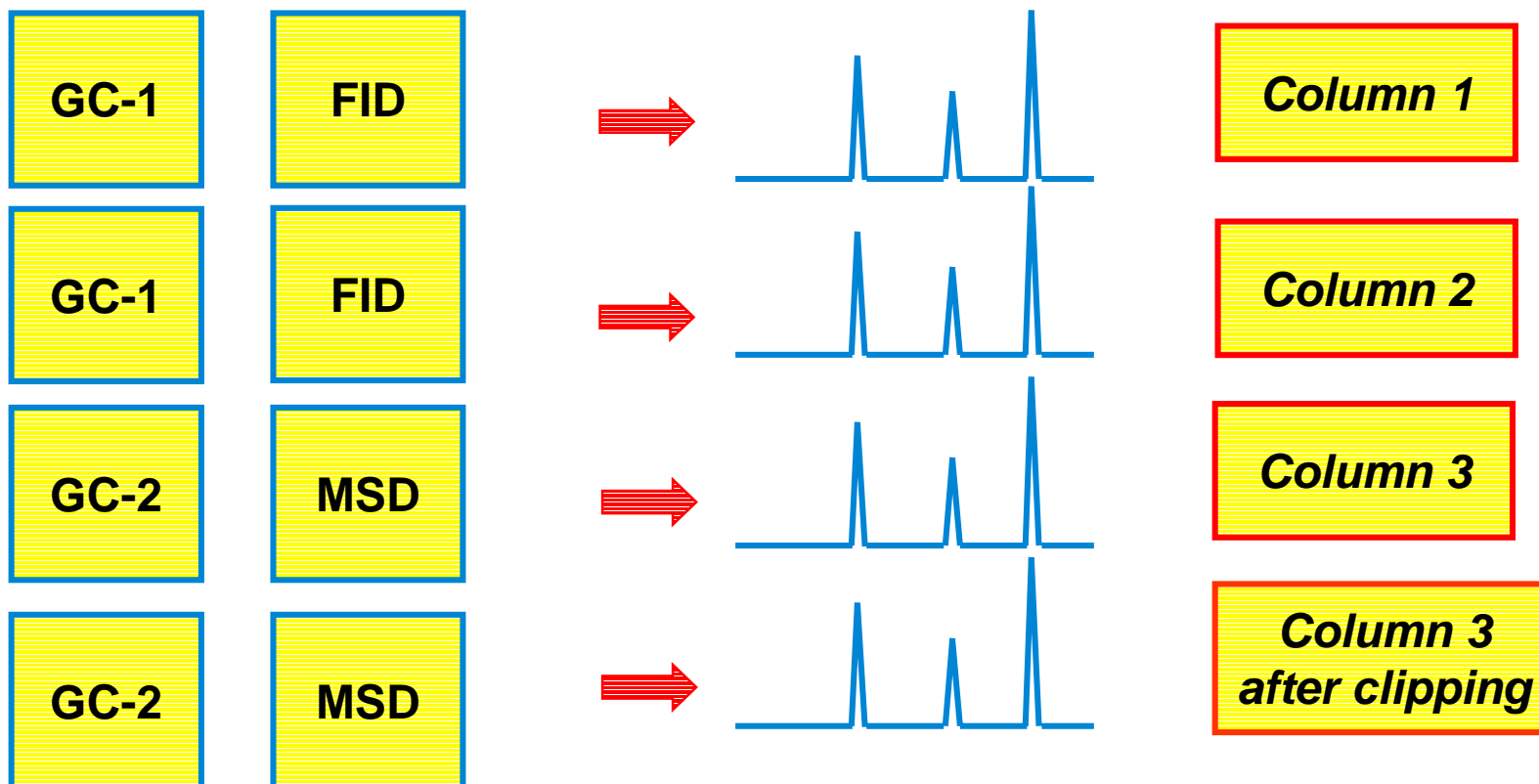
## Gasoline, 15 Runs Over 5 Days



# Retention Times Shift with Column Changes, Column Maintenance, or by Changing to MSD Detector



# After Locking, Retention Times are All the Same



# Retention Time Locking

## What is Retention Time Locking (RTL)?

The ability to precisely match chromatographic retention times in any systems to those in another chromatographic system with the same nominal method and column.

## How is Retention Time Locking Done?

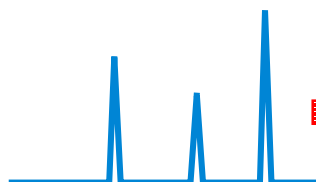
By adjusting column head pressure via EPC using interactive HP ChemStation software.

# With RTL, One can use Retention Time and Spectral Searching to Identify Compounds

**Step 1 - Record retention times and mass spectra under RT Locked conditions.**

**GC1**

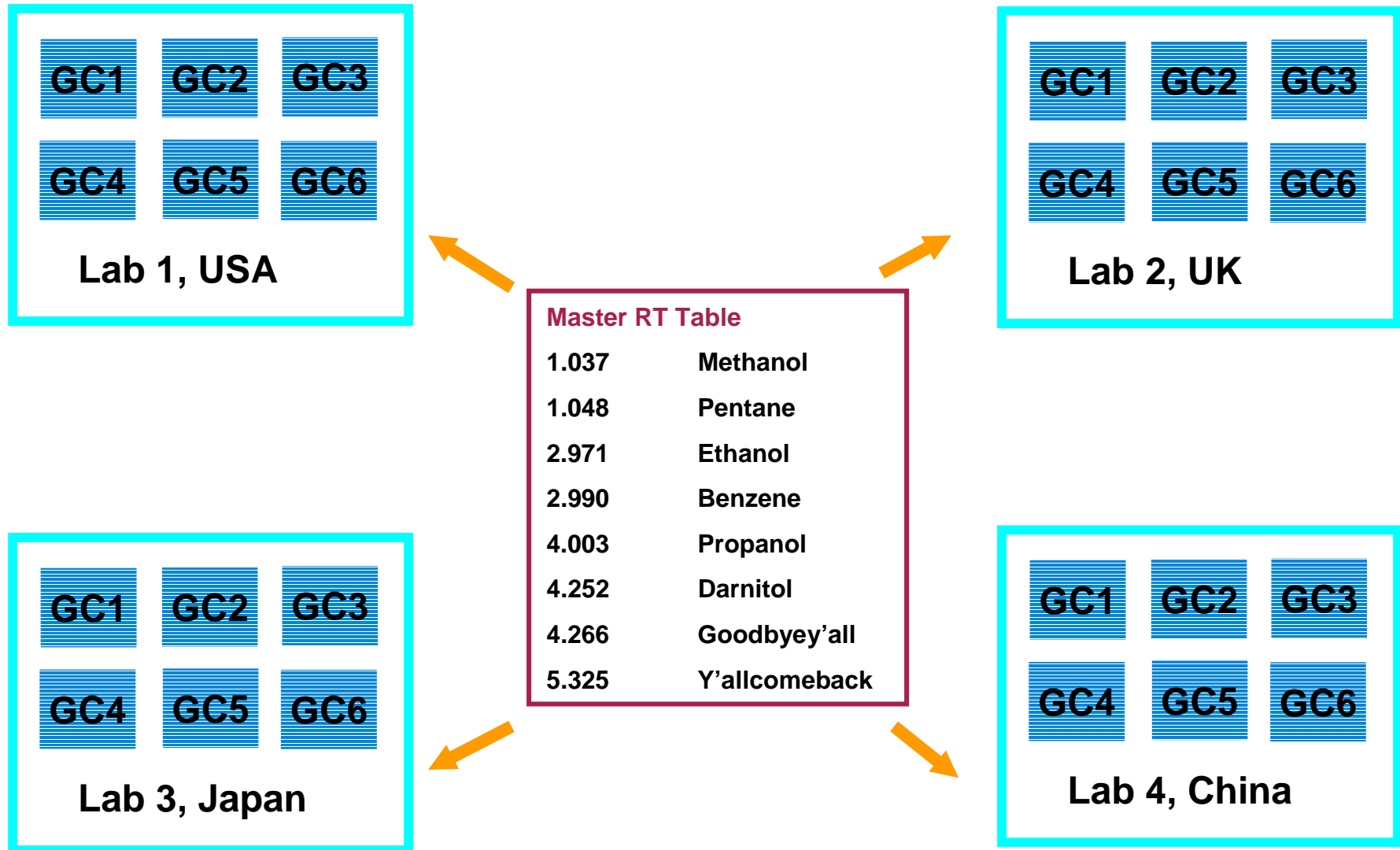
*MSD*



## Master RT Table

1.037	Methanol
1.048	Pentane
2.971	Ethanol
2.990	Benzene
4.003	Propanol
4.252	Darnitol
4.266	Goodbye y'all
5.325	Y'all comeback

# Use Locked RT Table Worldwide



# Using the Organotin RTL Databases for GC/MS

- **Advantages of GC/MS RTL Organotin Analysis:**
  - **Never have to update RT windows for quant databases**
  - **Never have to update SIM ion group timing**
  - **With Agilent's MS Screener Software, use mass spectral library searching AND locked retention times for more accurate peak identifications**
  - **Identify unknown peaks**
  - **Better identification of Organotins with similar spectra**

# Using the Organotin RTL Databases for GC/MS

- Download the following databases (available at the end of this presentation)
- If you want to analyze methyl derivatives, then download:
  - Tin\_Me.L (folder with 6 mass spectral library files)
  - Tin\_Me.scd (file containing the RTL screener database)
- If you want to analyze ethyl derivatives, then download:
  - Tin\_Et.L (folder with 6 mass spectral library files)
  - Tin\_Et.scd (file containing the RTL screener database)
- If you want to analyze pentyl derivatives, then download:
  - Tin\_Pent.L (folder with 6 mass spectral library files)
  - Tin\_Pent.scd (file containing the RTL screener database)

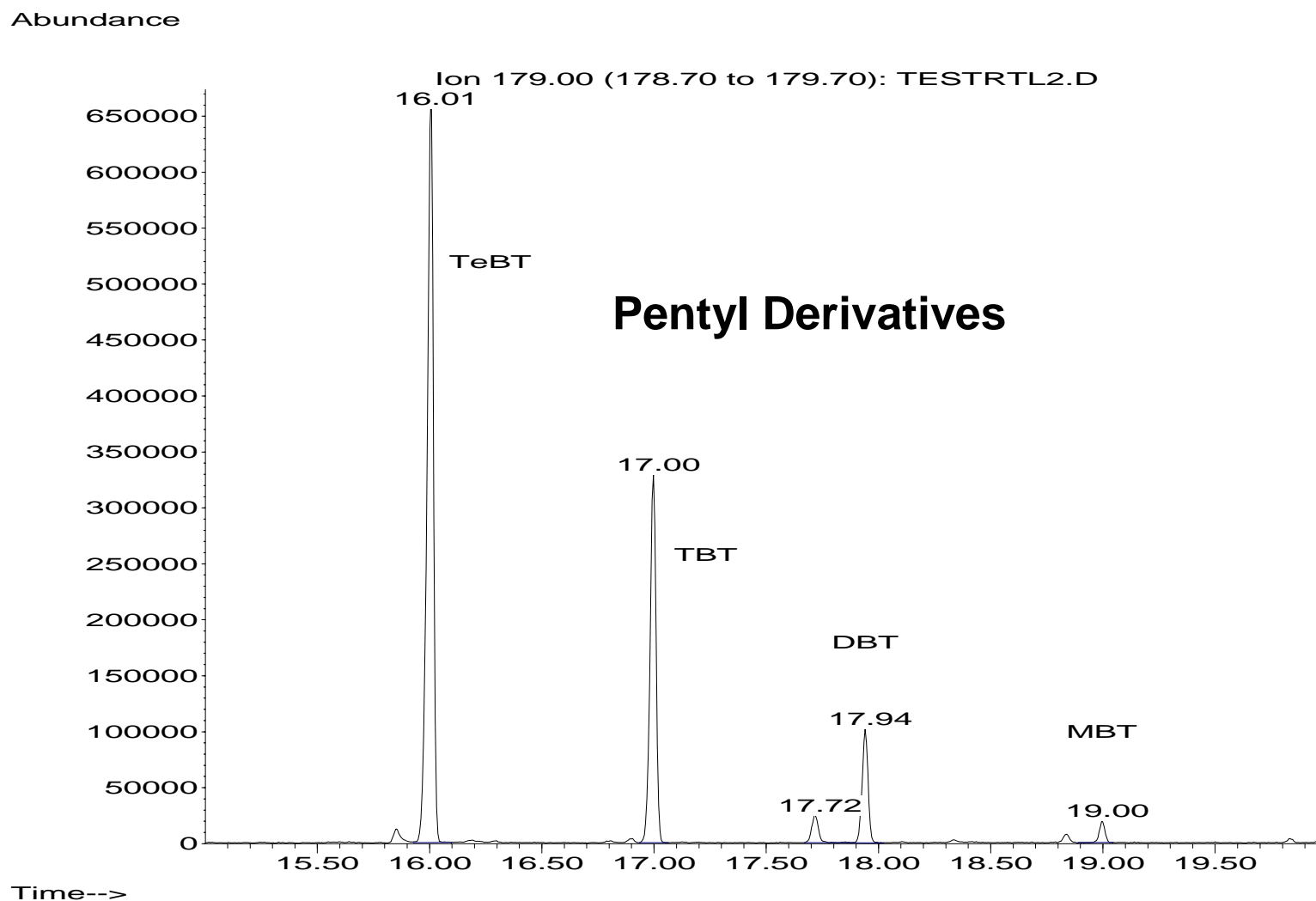
## Using the Organotin RTL Databases for GC/MS

- Copy the databases to the Database folder - usually C:\Database
- Install a 30 m X 0.25 mm X 0.25  $\mu$ m HP-5MS column (Agilent part No. 19091S-433)
- Set up the nominal method using the GC/MS parameters specified in the application note (Publication No. 5988-9256EN)
- 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 [Tin\\_Me.scd](#), [Tin\\_Et.scd](#), or [Tin\\_Pent.scd](#) database depending upon which derivative you made.
- Generate a screen report and review the data using the Results Screener (under “View/Results screener”)

# Screenener Variables

- **The number of probable and possible “hits” can be changed globally by adjusting the following variables in Agilent’s RTL software:**
  - **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**

# Extracted Ion Chromatogram Showing Butyltin Compounds Found in a Coastal Sediment Sample



# Benefits of Using RTL Databases for GC/MS

- **Fastest identification of compounds**
  - **Screen Organotins in seconds**
- **Fastest confirmation of compounds**
  - **Eliminate “hits” with wrong RT**
- **Precise and reproducible RT on any Agilent 6890/5973 GC/MS**
  - **No need to update calibration or SIM table RTs**
- **Compounds identified by both RT and spectral library searching**
  - **Fewer false positives and false negatives**
- **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/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**
  - Agilent J&W 30-m X 0.25-mm i.d. X 0.25- $\mu$ m HP-5MS (Part No. 19091S-433)

## Decide which Derivatives you will Make - then Download the Corresponding Databases

- Tin\_Me.L - Mass spectral library for 15 organotin compounds (Methyl derivatives)
- Tin\_Me.scd - Organotin GC/MS RTL screener database (Methyl derivatives)

or

- Tin\_Et.L - Mass spectral library for 15 organotin compounds (Ethyl derivatives)
- Tin\_Et.scd - Organotin GC/MS RTL screener database (Ethyl derivatives)

or

- Tin\_Pent.L - Mass spectral library for 15 organotin compounds (Pentyl derivatives)
- Tin\_Pent.scd - Organotin GC/MS RTL screener database (Pentyl derivatives)

**The following Application Note is included with each download:**

**Improving the Analysis of Organotin Compounds Using Retention Time Locked Methods and Retention Time Databases - Publication No. 5988-9256EN**

## Recommended Reading to Learn More About RTL

- **Improving the Analysis of Organotin Compounds Using Retention Time Locked Methods and Retention Time Databases, [5988-9256EN](#)**
- **Fast Screening of PCB Congeners Using the Agilent 6890/5973N GC/MSD System, [5980-1472E](#)**
- **Fast Screening of Pesticides and Endocrine Disrupters Using the Agilent 6890/5973N GC/MSD System, Part I, [5968-9220E](#)**
- **Fast Screening of Pesticide and Endocrine Disrupters Using the Agilent 6890/5973N GC/MSD System, Part II, [5980-1057E](#)**
- **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.chem.agilent.com](http://www.chem.agilent.com)
- Click on [Library](#)
- Click on [Online Literature](#)
- In the [Keyword](#) field, type the publication number (e.g., [5988-9256EN](#)) 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