

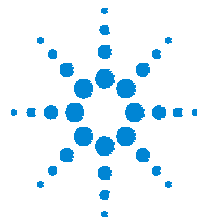
PCB Congener GC/MS RTL Database

User Contributed by

Mike Szelewski and C. Kai Meng

Agilent Technologies

Wilmington, Delaware, USA



Agilent Technologies

Innovating the HP Way

Database Development

- Developed at Agilent Technologies
- RTLocked to IUPAC Congener # 104 at 18.728 min
 - **2,2',4,6,6'-Pentachlorobiphenyl**
- 9 mixtures of PCB congeners obtained from Accustandard, New Haven, CT, USA
- All retention time and spectral data collected on Agilent GC/MSD systems
- Agilent HP-5MS column used, 30m x 250 μ m x 0.25 μ m part # 19091S-433

There are 3 Related Databases

- **2 Retention Time Locked Screener Databases**

- **rtl-pcb.scd, sorted by retention time**
- **cngr-srt.scd, sorted by IUPAC congener #**
- **209 PCB congeners**
- **precise retention times**
- **target ion and up to 3 qualifier ions**

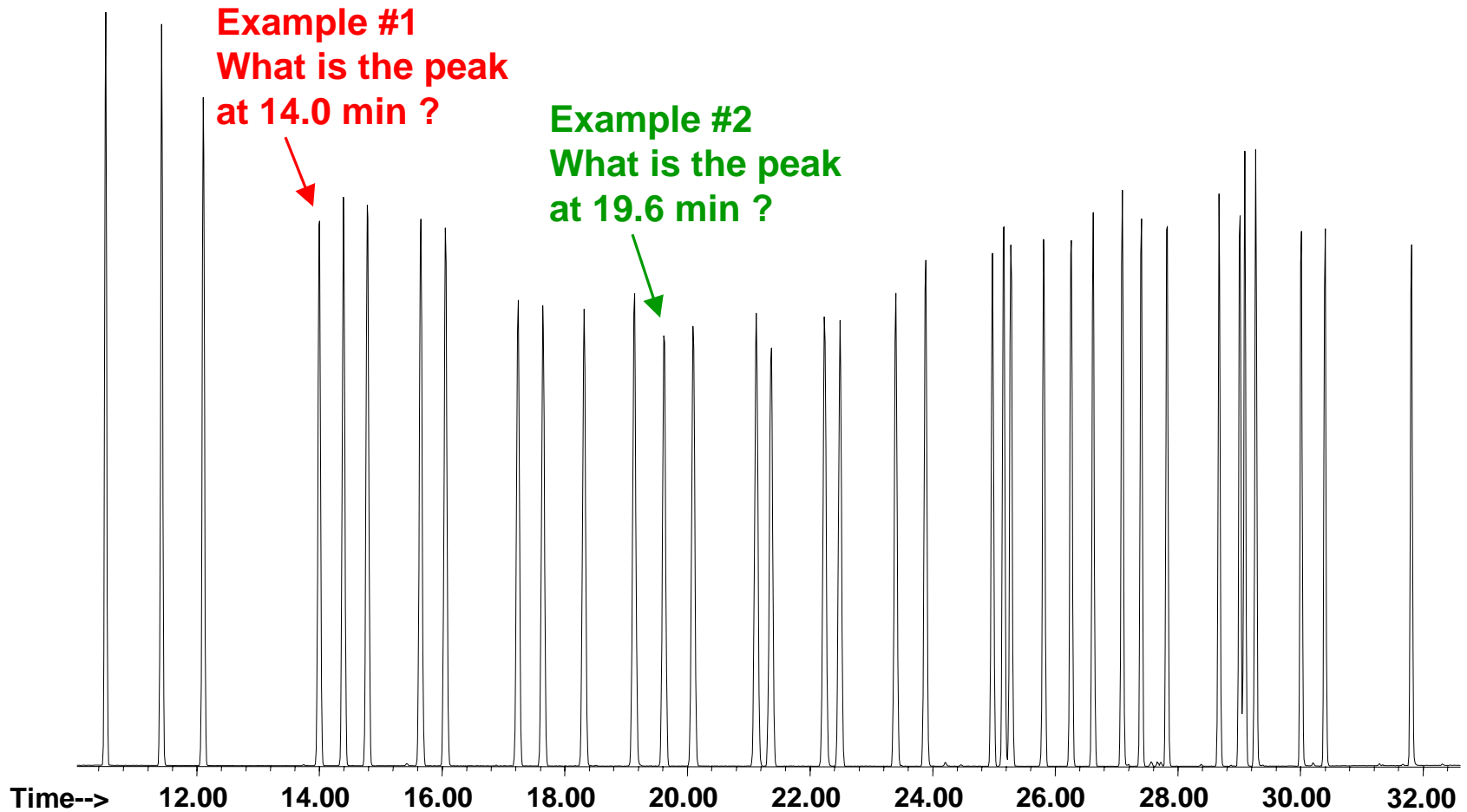
- **Mass Spectral Library**

- **rtl-pcb.L** (folder containing 6 files)
- **GC/MS Spectra for the 209 PCB congeners**

Using the PCB RTL Databases

- rtl-pcb.scd, cngr-srt.scd and rtl-pcb.L are copied to the Database folder, usually C:\Database
- The GC/MS system is retention time locked and an RTL method is established
- Samples are run using the RTL method
- Sample datafile is Screened using either rtl-pcb.scd or cngr-srt.scd
 - **Screeener report is generated**
- **Screeener Results are reviewed/modified**
- **Peak spectra can be searched/compared using rtl-pcb.L**

Test Sample TIC run RTLocked



Example #1 Partial Screener Report

Screen File: rtl-pcb.RES
Screen Database: rtl-pcb.SCD

Extraction Window: +/- 0.150 min
Qualifier Mode : Absolute
Qualifier % : 20
Zero qualifiers : Excluded
Subtraction Mode : Sub Lower Start/Stop

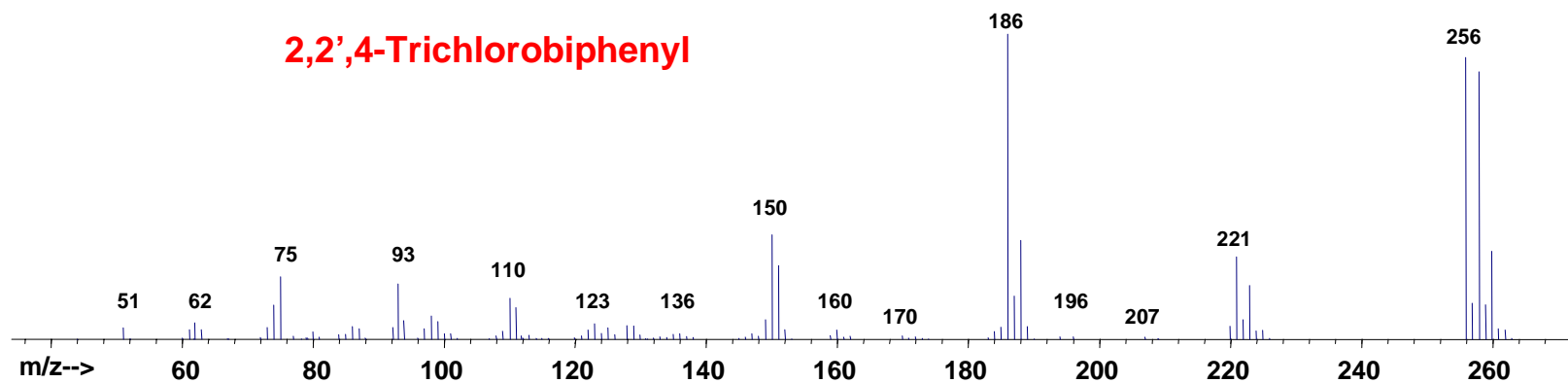
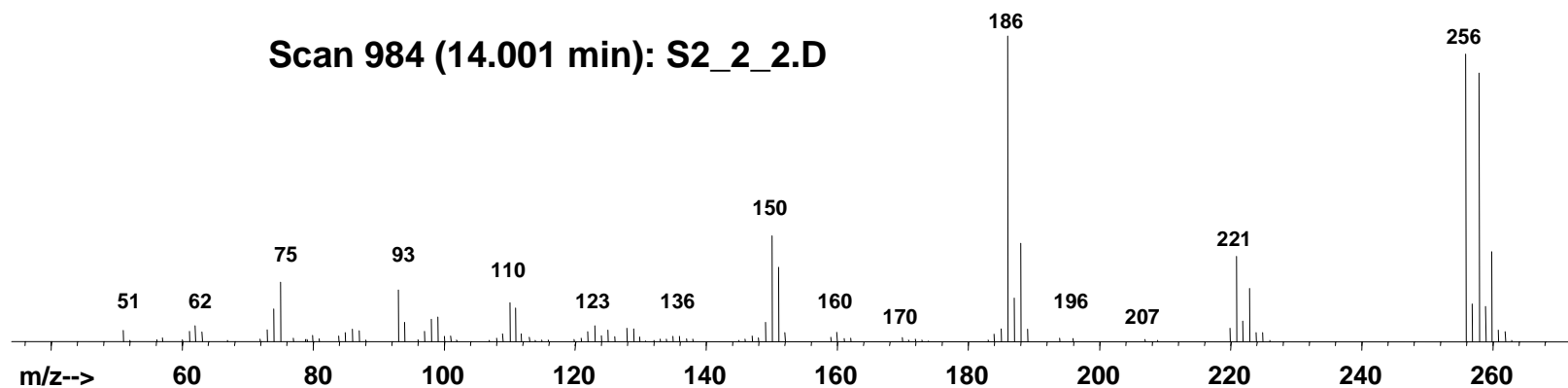
Compound	Status	ExpRT	Delta	Target m/z	Resp.	Qualifiers Out of Range	XCR
4 2,2'-Dichlorobiphenyl	?	10.511	+0.007	152	2876104	222,224,187	0.90
5 2,6-Dichlorobiphenyl	x	10.518	+0.002	222	3646177		0.98
6 2,5-Dichlorobiphenyl	x	11.413	+0.019	222	4069249		0.99
7 2,4-Dichlorobiphenyl	x	11.430	+0.002	222	4069801		0.99
9 2,4'-Dichlorobiphenyl	x	12.071	+0.041	222	3862544		0.99
10 2,3-Dichlorobiphenyl	x	12.111	+0.001	222	3879015		0.99
17 2,2',5-Trichlorobiphenyl	x	13.909	+0.092	186	2315545		0.97
18 4,4'-Dichlorobiphenyl	?	13.997	+0.004	222	148829	224,152,151	0.09
19 2,2',4-Trichlorobiphenyl	x	14.001	-0.000	186	2317519		0.97
20 2,3',6-Trichlorobiphenyl	x	14.391	+0.007	256	2776621		0.98
21 2,3,6-Trichlorobiphenyl	x	14.396	+0.002	256	2776621		0.98
22 2,2',3-Trichlorobiphenyl	?	14.777	+0.010	186	2115315	256,258,221	0.87
23 2,4',6-Trichlorobiphenyl	x	14.787	+0.001	256	3019433		0.98
27 2,2',6,6'-Tetrachlorobiph	x	15.429	+0.005	292	17719		0.94

Screener Report - User Analysis #1

- 3 entries in the Screener database, rtl-pcb.scd, have similar retention times
- 2 of these have very good cross-correlations (XCR) with their respective library entries (17, 19)
- 2 of these have very good r.t. agreement with their expected retention times (18, 19)
- Only 1 (19) has all qualifiers within expected ranges and very good r.t. agreement, its Status is marked “x” as a probable hit - 2,2',4-Trichlorobiphenyl
- ? Denotes a possible hit

Library Search #1 of rtl-pcb.L

Peak identification confirmed



Example #2 Partial Screener Report

Screen File: rtl-pcb.RES
Screen Database: rtl-pcb.SCD

Extraction Window: +/- 0.150 min
Qualifier Mode : Absolute
Qualifier % : 20
Zero qualifiers : Excluded
Subtraction Mode : Sub Lower Start/Stop

Compound	Status	ExpRT	Delta	Target m/z	Resp.	Qualifiers Out of Range	XCR
39 2,2',3,6-Tetrachlorobiphe	x	17.243	+0.002	292	1738771		0.72
40 3,3',5-Trichlorobiphenyl	?	17.261	-0.019	256	132121	186	0.08
41 2,2',3,6'-Tetrachlorobiph	x	17.649	+0.000	220	1683134		0.96
42 3,4',5-Trichlorobiphenyl	?	17.707	-0.058	256	141566	186	0.08
49 2,2',4,4'-Tetrachlorobiph	x	18.266	+0.057	292	1668779		0.96
50 2,4,4',6-Tetrachlorobiphe	?	18.287	+0.036	292	1992975	220	0.94
51 2,2',4,5-Tetrachlorobiphe	x	18.321	+0.003	292	2027302		0.97
58 3,4,4'-Trichlorobiphenyl	x	19.140	+0.002	256	3132819		0.99
61 2,3',4',6-Tetrachlorobiph	?	19.568	+0.060	292	1182179	220	0.92
62 2,2',3,4-Tetrachlorobiphe	x	19.625	+0.004	292	1736099		0.96
63 2,3,4',6-Tetrachlorobiphe	?	19.627	+0.002	292	1736099	220	0.92
64 2,3',4,5'-Tetrachlorobiph	?	19.701	-0.073	292	1522361	220	0.92
66 2,2',3,3'-Tetrachlorobiph	?	20.060	+0.040	220	125912	292,222	0.05
67 2,2',4,5',6-Pentachlorobi	x	20.101	+0.003	326	1881293		0.94
68 2,3,3',5-Tetrachlorobiphe	?	20.153	-0.051	292	70896	290,220	0.04

Screener Report - User Analysis #2

- 4 entries in the Screener database, rtl-pcb.scd, have the same target ion and similar retention times
- 2 of these have very good r.t. agreement with their expected retention times (62, 63)
- All 4 of these have very good cross correlations (XCR) with their respective library entries
- Only 1 (62) has all qualifiers within expected ranges and very good r.t. agreement, its Status is marked “x” as a probable hit - 2,2',3,4-Tetrachlorobiphenyl
- ? Denotes a possible hit

Screenener Variables

- **The number of probable and possible Hits can be globally changed through these variables**
 - **Extraction Window for retention time**
 - **Qualifier Mode, relative or absolute**
 - **Qualifier ratio to the target ion**
 - **Zero qualifiers, included or excluded**
 - **Subtraction Mode**
- **Integration parameters define peak detection**

Benefits of Using RTL Databases

- **Fastest Identification of Compounds**
 - Screen for 209 congeners in < 15 seconds
- **Fastest Confirmation of compounds**
 - Eliminate hits with wrong r.t.
- **Precise reproducible r.t. on GC and GC/MS**
 - Match GC r.t. to GC/MS r.t.
 - No need to update calibration tables
- **Compounds identified by both retention time and spectral information**
- **No Additional cost for User Contributed Databases**

Agilent Instrumentation Required

- **Gas Chromatograph**

- **6890N with Autosampler (tray & injector) and split/splitless inlet**

- **Mass Spectrometer**

- **5973N with EI source**

- **Software**

- **GC/MSD ChemStation G1701 CA version C.00.01 or higher (includes RTL and Screener)**

- **Column**

- **HP-5MS 30m x 250 μ m x 0.25 μ m part # 19091S-433**

Fast GC/MSD Analyses

- **2 More Retention Time Locked Screener Databases**

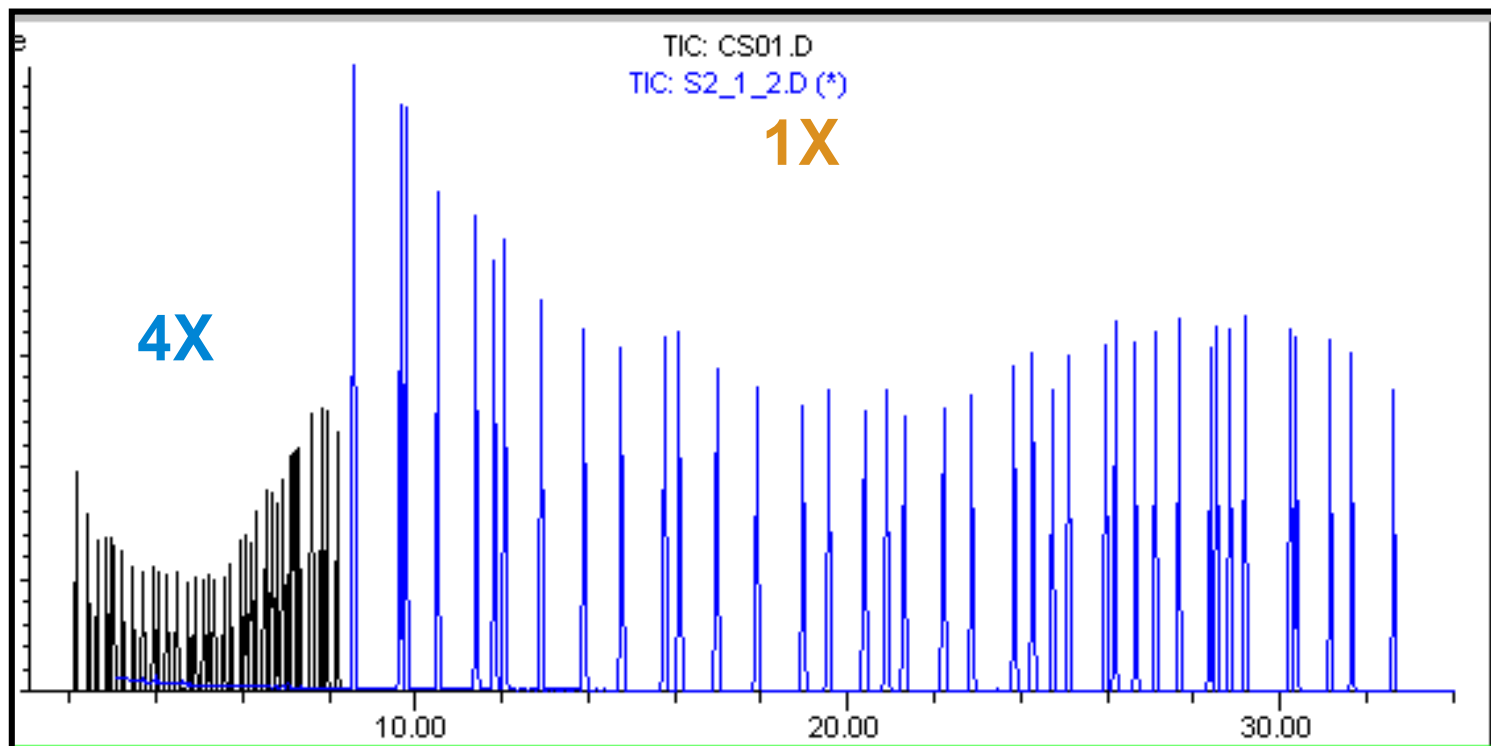
- **rtlpcb4x.scd, sorted by retention time**
- **cngr-4x.scd, sorted by IUPAC congener #**
- **209 PCB congeners**
- **precise retention times, each 4x faster than in the standard databases**
- **target ion and up to 3 qualifier ions**

Fast GC/MSD Requirements

- Agilent HP-5MS column, 15m x 250 μ m x 0.25 μ m part # 19091S-431
- MSD pumping capacity to handle a 3.8 mL/min column flow
- 6890 fast oven option (220/240V in USA)
- **These requirements are in addition to those previously given**

Total Ion Chromatogram of 39 PCB Congeners

Overlay of 1X and 4X analyses



Method Parameters

Method Parameters for normal and for fast PCB congener analyses are in the Application Note

“Fast Screening of PCB Congeners Using the Agilent 6890/5973N GC/MSD System”, 5980-1472E

This Application Note is included with the Databases download

Files Included in the Download

- rtl-pcb.scd - 1x speed, sorted by retention time
- cngr-srt.scd - 1x speed, sorted by IUPAC congener #
- rtlpcb4x.scd - 4x speed, sorted by retention time
- cngr-4x.scd - 4x speed, sorted by IUPAC congener #
- rtl-pcb.L - GC/MS spectra for 209 congeners
- rtl-pcb.txt - text listing of 209 congeners sorted by r.t.
- cngr-srt.txt - text listing of 209 congeners sorted by IUPAC#
- 5980-1472E - Application note

Additional Recommended Reading

- Retention Time Locking with the HP G1701BA MSD Productivity ChemStation, 5968-3433
- Efficient Screening for Pesticides and Endocrine Disrupters Using the HP 6890/5973 GC/MSD System, 5968-4884 (**very large file!**)
- Fast Screening of Pesticides and Endocrine Disrupters Using the Agilent 6890/5973N GC/MSD System Part I, 5968-9220
- Fast Screening of Pesticides and Endocrine Disrupters Using the Agilent 6890/5973N GC/MSD System Part II, 5980-1057
- Direct your web browser to www.chem.agilent.com
- Click on **Library**, then **Online Literature**
- In the **keyword** field type in the 8 digit number as it is listed above for the publication you would like to view