Pro ezGC® Chromatography Modeling Software

Analytical Innovations introduced the ezGC series of chromatography modeling programs four years ago. With our latest release, Pro ezGC for Windows Version 2, we are continuing our commitment to develop innovative and powerful tools for capillary gas chromatography.

Pro ezGC can answer questions like these.

- Will the column currently in my GC separate the components in my sample?
- Can I get greater resolution between the compounds?
- Am I using the best carrier gas linear velocity or pressure program?
- Can I shorten the analysis time?
- What stationary phase and column dimensions should I use?
- Should I use pressure programming or coupled columns?

The following sections explain how Pro ezGC works and how you can step up to enhanced chromatography.

Pro ezGC for Windows Features

Pro ezGC Thermodynamic Retention Index Database

Who Uses Pro ezGC

Pro ezGC and Electronic Pressure Control

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Pro ezGC Chromatography Modeling Software

You can save time and money when you use Pro ezGC to optimize your gas chromatographic analyses. This easy-to-use computer program implements the latest theoretical models to predict retention times and peak widths on capillary columns.

Services

Our experienced staff can help with your analytical method development, data validation and hazardous waste treatment studies.

Contact us

Company address, Pro ezGC technical support and e-mail addresses

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GC Optimization Software

AII created the ezGC® series of chromatography modeling programs so you can optimize your separations and save time and money. The easy-to-use software implements recently developed theoretical models for predicting component retention times and peak widths on capillary gas chromatography columns.

The computer programmers of AII have also written GC/MS data calculation and quantification software. We can provide custom programming and documentation for your special applications.

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Pro ezGC® for Windows Features

Pro ezGC for Windows Version 2:

Simultaneously optimizes the following parameters on single, dual and serially coupled columns:

- Single ramp, multi-ramp and isothermal temperature programs
- Carrier gas flow including single and multi-ramp pressure programs
- Column length, diameter and stationary phase film thickness

Uses thermodynamic retention indices (TRIs) to accurately predict retention times. An extensive database of TRIs is included with Pro ezGC. You can add your own compounds to the TRI database using measured or published retention times.

Calculates TRIs for your compounds using just two experimental runs

Predicts retention times to an accuracy of 0.1%

Models peak widths for accurate resolution predictions

Calculates the following indices:

- Kov^G
- Linear Temperature Program
- Equivalent Chain Lengths
- Relative Retention Times

Imports retention time data from AIA (Analytical Instrument Association) and ASCII files

Adjusts the model for your GC and for variation in the column length, diameter and film thickness

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Pro ezGC® Thermodynamic Retention Index Database

Pro ezGC includes an extensive database of thermodynamic retention indices that you can use to quickly optimize your separations. If your compounds are not in the database, you can use your experimental data or published retention times to expand the database.

The database includes compounds in the following six categories.

- Environmental
- Food and Flavors
- Drugs and Pharmaceuticals
- Petroleum
- Solvents and Chemicals
- FAMEs
- Abbreviations used in the Database

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Who Uses Pro ezGC®

Pro ezGC has become an indispensable tool for GC analyses, meeting the needs of many industries. These industries include:

Chemical, Auto and Pharmaceuticals Industries

GC analyses may be optimized and standardized for individual plants by having all necessary compounds in proprietary and commercial libraries. This will help facilitate the quick identification of contaminants in production and waste products, decreasing potential liabilities and loss of product.

Petroleum and Food Industries

By modeling with very high accuracy, reliable identifications are possible with any changes in the GC analysis. This allows for optimized targeted analyses for specific compounds without sacrificing the identification of other known compounds. Useful commercial libraries of compounds include Solvents & Chemicals, Volatiles, FAMEs, Fragrance & Flavors.

Environmental Laboratories

Increase laboratory competitiveness by decreasing analysis time. Many routine and non-routine analyses can be optimized using available commercial libraries. The commercial libraries include EPA Methods 502.2, 524.2, 551, 8240A, 8250, 8260, 505, 507, 508, 604, 608, 617, 1618, 515, 615, 8150B, and more. In-house GC method development is also now economically feasible.

Hospitals, Forensics Labs and Health Services Labs

Compounds and their metabolites may either be found in available libraries or may be experimentally determined and entered into custom libraries. This helps in the precise identification of compounds.

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Government

Optimization of various methods will result in significant saving for both government and industry in required analyses. This is true for any new methods developed as well as any existing methods.

Educational

Students may learn chromatography in a GC lab by modeling specific compounds and observing the actual experimental results. Students will also benefit by being able to investigate and corroborate the results of any changes in GC analysis conditions.

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Pro ezGC® and Electronic Pressure Control

Using Electronic Pressure Control to Improve GC Analyses

Electronic Pressure Control (EPC) gives you precise control of the GC column inlet pressure. The following discussion briefly answers these questions about EPC.

- What are the advantages of EPC?
- How does EPC accomplish this?
- When should you use EPC?
- What are the most important method development considerations when you use EPC?

Faster run times for an analysis

The most common application of EPC is to shorten the analysis time by increasing the column head pressure during a temperature-programmed run. Combining a pressure program with a lower final temperature can also shorten the equilibration time for the GC oven. If the most important consideration is the resolution of critical compounds at the end of an analysis, you may need to decrease the flow through the column and increase the oven temperature.

Improved column life

When the gas flow through the column increases during an analysis, compounds are eluted at lower temperatures. The lower operating temperatures will reduce the thermal stress on the column and decrease the column bleed.

Improved separations of compounds

EPC can help you resolve the critical compounds in your samples. You can carefully match the temperature program and pressure program so the compounds elute at the optimum elution column temperature. In many cases, the most efficient way to resolve multiple compounds in a single analysis is by

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combining multiple-ramp pressure and temperature programs.

Improved peak shapes

You can use EPC to increase the pressure in the injector during the time the sample is transferred to the column. This will improve the peak shape because the sample starts in a narrower band at the head of the column. After the sample is transferred to the column, you can rapidly lower the inlet pressure to give a normal linear velocity through the column. This technique works best when the starting temperature of the GC is much lower than the boiling point of the first eluting compound.

EPC will always give you higher productivity and better resolution, but finding the optimum combination of column parameters, temperature program and pressure program may be complicated and time consuming.

Pro ezGC for Windows, a chromatography modeling software tool, can quickly evaluate thousands of pressure and temperature programs and help you select the best conditions for your analysis.

Guidelines for Using Pro ezGC to Model EPC

1. When you begin optimizing a separation, try pressure and temperature programs that have one or two ramps. Programs that exceed two ramps for either the pressure or temperature program are generally only required when the compounds in the sample have a very wide range of volatilities.

2. If you change columns, you may need to apply an offset to each level of the pressure program. This offset compensates for variances in the column diameter. Try to use very slow ramps in the temperature program instead of isothermal holds because the retention times are more consistent when you change GCs or columns. You may include isothermal holds at the beginning and the end of the temperature program.

3. Do not exceed the minimum or maximum carrier gas flow

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rate for the detector or mass spectrometer. You can use the built-in Pro ezGC carrier gas flow calculator to calculate the gas flow at the highest and lowest temperature and pressure.

4. If you use a high inlet pressure immediately after injection followed by a rapid decrease in pressure to improve the peak shape, then include an isothermal hold at the beginning of the temperature program. The isothermal hold should last for the duration of the decreasing pressure ramp. The dead time of the column is very difficult to determine during a rapid pressure drop so the isothermal hold decreases the error in the predicted compound retention times. This is the only time you should rapidly lower the pressure on a column.

5. An oscillating pressure or temperature program may lead to greater errors in the predicted retention times and may result in deformed peaks. Try modeling oscillating programs only if you are unable to separate your compounds using simpler programs.

6. When you use Pro ezGC to optimize separations, you select the ranges of values you want to examine for each column parameter, pressure program and temperature program variable. This insures you will find the best method for your sample, column, and gas chromatograph.

7. When you model separations, including separations that use EPC, the average difference between the measured and predicted retention times is 1% and the average difference between the measured and predicted peak widths is 10%. When you enter measured retention times and peak widths for a few components in the chromatogram, Pro ezGC can adjust the model and reduce the average differences between the measured and predicted values to less than 0.1% for retention times and less than 5% for peak widths.

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Pro ezGC® Thermodynamic Retention Index Database - Environmental

The following groups of components are available in the environmental portion of the database.

PCDD/Fs, PCBs and PCNs

Volatiles and Semi-Volatiles

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Pro ezGC® and "Fast GC" Techniques

If you want to investigate "Fast GC" techniques, Pro ezGC can help you determine the columns and hardware you will need to reach your goals. Without changing your column or GC, Pro ezGC can normally reduce your analysis times by 15% to 50%.

All presented the following poster at PITTCON'97.

Practical Fast GC Analyses

John Garrett, Joseph Solch, Daniel Wagel,Garrett VanNess and Thomas O. Tiernan

Analytical Innovations, Inc.,

Abstract

Significant reductions in analysis times (>90%), can be achieved for a wide variety of analyses using Fast GC. The modeling program, Pro ezGC, can be used to predict practical solutions for a specific analysis. The program calculates temperature programs, flow rates and column dimensions for resolving critical analytes and meeting peak width and analysis time requirements. For more complex analyses, the program can model dual columns and coupled columns.

The maximum temperature programming rates for some newer GCs have increased to 300 C/sec while reset times have decreased. This allows for fast analyses of mixtures that contain a wide boiling point range. When using very fast programming rates, the injection technique and detector volume are the main constraints for good results as they directly affect the peak width of the target analytes. With good injection techniques and well designed detectors, most GCs can achieve a 50% reduction in analysis time for complex mixtures on 15m or longer columns.

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Raising the column temperature to shorten the retention time of late eluting components increases the column bleed. Pressure programming provides options for decreasing the analysis time without increasing the column bleed. Modeling both the pressure program and temperature program together often yields the best solution.

Short columns (<5m) or coupled columns are often the answer when there is a small targeted set of analytes. Fast programming rates in these instances are beneficial if there is a wide boiling point range of targeted compounds. Fast programming rapidly raises the column to its maximum temperature so strongly retained compounds are quickly eluted. In practice, a more conventional 10m or 15m column operated at a higher linear velocity can give results that are similar to the results obtained with a 5m column. When separations are optimized using a modeling program, conventional columns, short columns, and coupled columns are easily compared. Modeling is especially useful when evaluating the column length, diameter and film thickness with different temperature and pressure programs.

Modeling can help you take full advantage of your existing GC and columns. This often yields an acceptable result for a specific analysis without any additional expenditure of time and money. Modeling is also a practical way to explore Fast GC techniques and can aid in justifying the purchase of new GC hardware or columns.

Introduction

Significant reductions in analysis times (>90%) can be accurately predicted by a computer modeling program (Pro ezGC®). Using thermodynamic properties from a database, the program calculates the best combination of temperature program, carrier gas flow rate and column dimensions to resolve the critical analytes in the least amount of time.

The program can model a single column, dual columns or serially coupled columns in conjunction with uncoated precolumns and postcolumns. Additionally, the program supports the use of six levels of temperature and pressure programming.

First Example

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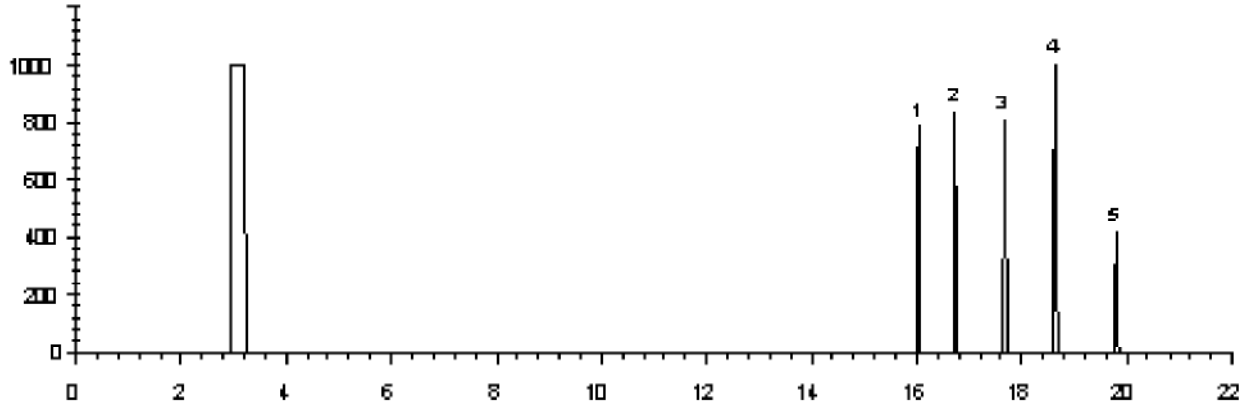
Fast GC often works best for a small number of compounds or for a larger number of compounds that are very similar in nature. This example will focus on the analysis of five barbiturates.

The first chromatogram shows an unoptimized separation. This chromatogram is similar to Alltech Associates, Inc. Chromatogram #1044 on an EC-5 column.

Barbiturates

5% phenyl / 95% methyl, 30 m x 0.25 mm x 0.25 µm
100°C (3) @ 10°C/min to 260°C (3), Inlet Pressure : 60.2 kPa



Run Time : 19.79 min	Min Rs Pair : 7.45
Carrier : Helium	Regulation : Constant Pressure
Flow : 0.650 ml/min	Temperature : 50°C
Dead Time : 2.685 min	Linear Velocity : 18.62 cm/sec

#	Component Name	Retention Time (min)	Peak Width (min)	Resolution
1.	Butabarbital	16.026	0.0701	7.45
2.	Amobarbital	16.726	0.0696	7.45
3.	Secobarbital	17.677	0.0704	11.57
4.	Hexobarbital	18.633	0.0723	11.57
5.	Phenobarbital	19.792	0.0769	13.00

The second chromatogram shows the same column optimized for the shortest run times while maintaining resolution of all the analytes. This optimized Normal-GC separation represents an 85% reduction in the run time compared to the original barbiturates separation.

Barbiturates - Optimized Normal-GC Separation

5% phenyl / 95% methy, 30 m x 0.25 mm x 0.25 µm
234°C (1) @ 30°C/min to 260°C (2), Inlet Pressure : 141.5 kPa

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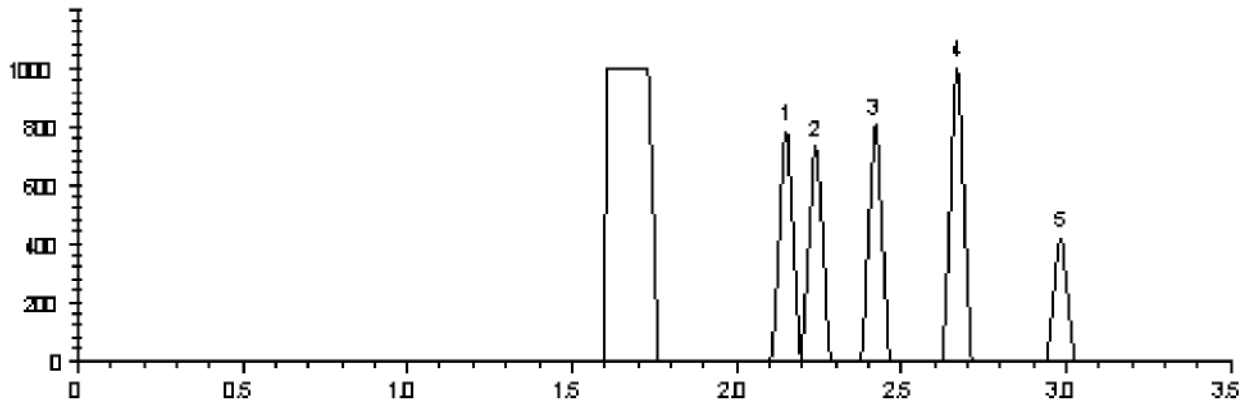

Run Time : 2.98 min	Min Rs Pair : 1.04
Carrier : Helium	Regulation : Constant Pressure
Flow : 0.943 ml/min	Temperature : 234°C
Dead Time : 1.603 min	Linear Velocity : 31.20 cm/sec

# Component Name	Retention Time (min)	Peak Width (min)	Resolution
1. Butabarbital	2.149	0.0874	1.04
2. Amobarbital	2.239	0.0865	1.04
3. Secobarbital	2.420	0.0857	2.10
4. Hexobarbital	2.669	0.0856	2.90
5. Phenobarbital	2.983	0.0853	3.68

The third chromatogram shows an optimized run that uses a short column, high linear velocities and fast ramp temperature program. This Fast GC separation represents a 90% reduction in run time from the Optimized Normal-GC separation.

Barbiturates - Fast GC Separation

5% phenyl / 95% methy, 3 m x 0.25 mm x 0.25 µm
180°C @120°C/min to 300°C Inlet Pressure : 49.7 kPa

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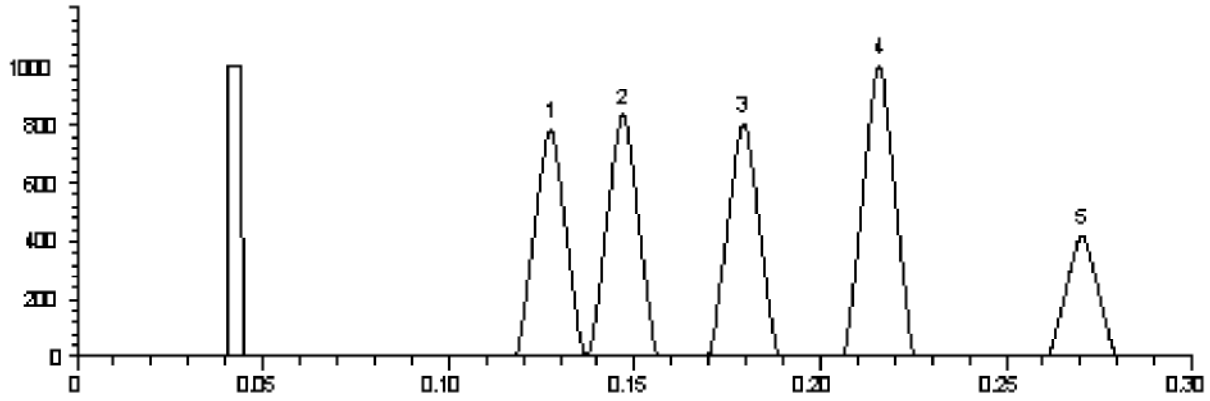

Run Time : 0.27 min	Min Rs Pair : 1.09
Carrier : Helium	Regulation : Constant Pressure
Flow : 2.93 ml/min	Temperature : 180°C
Dead Time : 0.0406 min	Linear Velocity : 123.11 cm/sec

# Component Name	Retention Time (sec)	Peak Width (sec)	Resolution
1. Butabarbital	7.63	1.080	1.09
2. Amobarbital	8.81	1.087	1.09
3. Secobarbital	10.76	1.094	1.79
4. Hexobarbital	12.95	1.104	1.99
5. Phenobarbital	16.23	1.092	2.97

Second Example

Often the first step in optimizing a GC analysis is to obtain adequate resolution of the target analytes. Once that is achieved, then further optimization of the analysis may proceed.

This Food and Flavors (F&F) example uses 32 compounds that were analyzed on two separate bonded phase columns from Restek Corporation, Stabilwax® (Crossbond® Carbowax®) and Rtx®-1 (crossbonded polydimethylsiloxane). The following two chromatograms show the fastest run times that resolved the most components on each column.

F&F - Stabilwax

Stabilwax, 30 m x 0.25 mm x 0.25 µm

80°C @ 12°C/min to 100°C @ 14°C/min to 200°C, Inlet Pressure : 128.8 kPa

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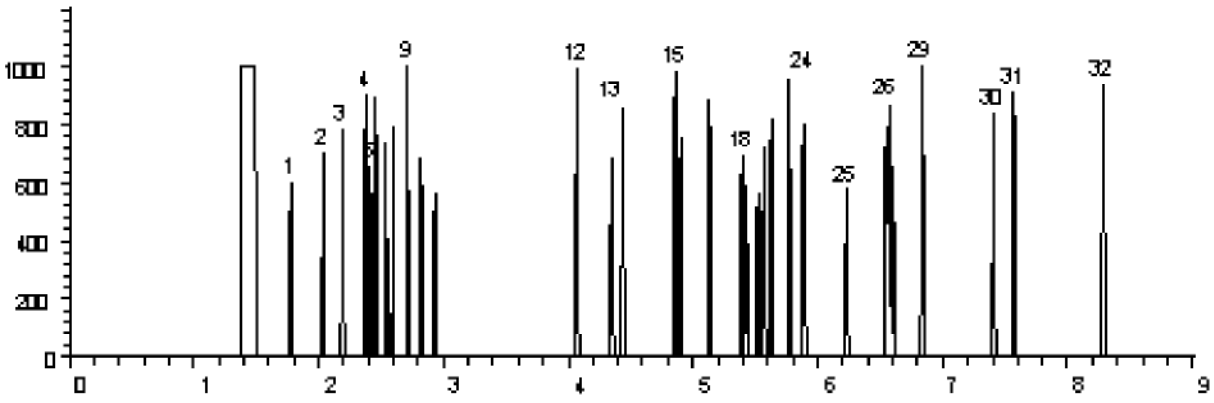
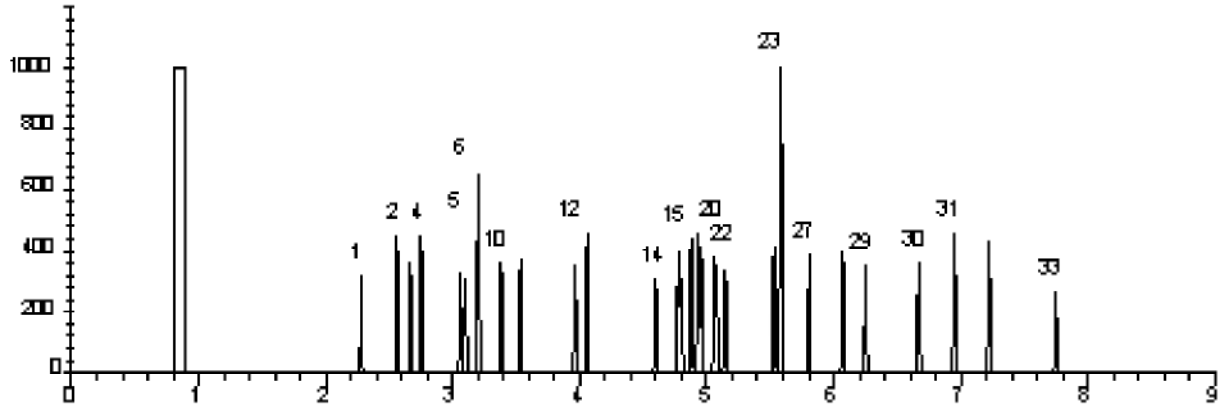


Run Time : 8.28 min	Min Rs Pair : 1.01
Separations : 28 of 32 resolved	
Carrier : Helium	Regulation : Constant Pressure
Flow : 1.51 ml/min	Temperature : 80°C
Dead Time : 1.375 min	Linear Velocity : 36.35 cm/sec

F&F - Rtx-1

Rtx-1 30 m x 0.25 mm x 0.25 µm

70°C @ 9°C/min to 100°C @ 14°C/min to 200°C, Inlet Pressure : 261.8 kPa



Run Time : 7.75 min	Min Rs Pair : 1.23
Separations : 21 of 33 resolved	
Carrier : Helium	Regulation : Constant Pressure
Flow : 2.85 ml/min	Temperature : 70°C
Dead Time : 0.838 min	Linear Velocity : 59.66 cm/sec

Neither the Rtx-1 nor the Stabilwax column was able to resolve all the components. The following chromatogram shows that a serially coupled column composed of the Rtx-1 and the Stabilwax resolved all the components.

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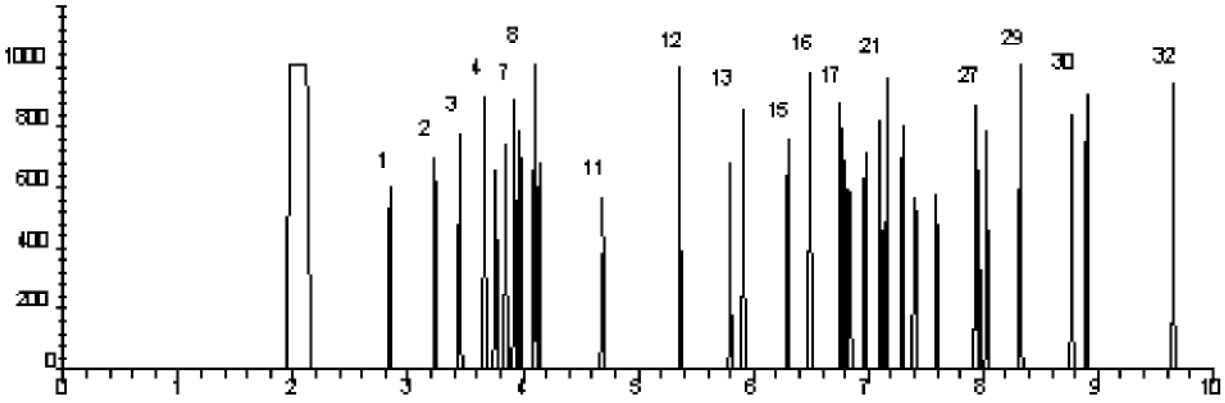
F&F - Serially Coupled Column

Stabilwax, 27m x 0.25 mm x 0.25 µm and Rtx-1, 12 m x 0.25 mm x 0.25 µm
55℃ @ 14℃/min to 200℃ (1), Inlet Pressure : 170.5 kPa

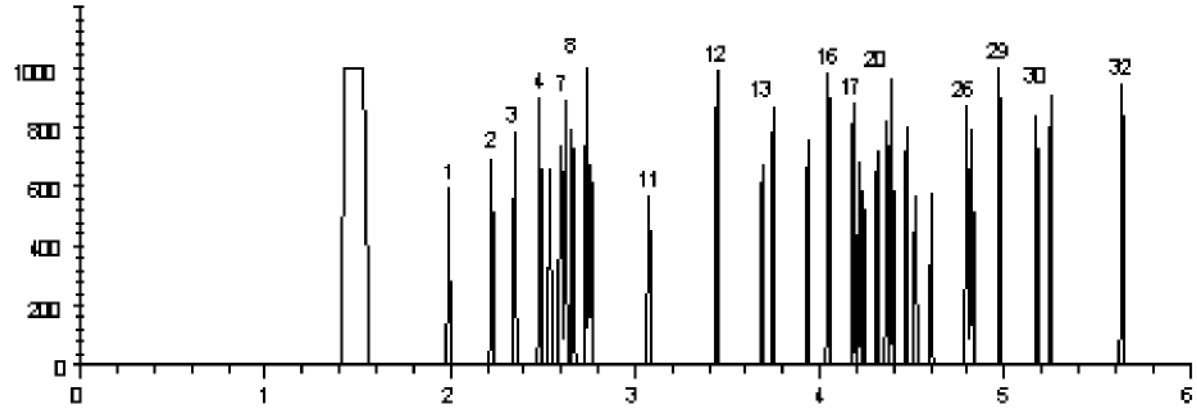


Run Time : 9.65 min	Min Rs Pair : 1.01
Separations : 32 of 32 resolved	
Precolumn : 5 m x 0.53 mm	
Carrier : Helium	Regulation : Constant Pressure
Flow : 1.86 ml/min	Temperature : 65℃
Dead Time : 1.736 min	Linear Velocity : 37.44 cm/sec

The previous chromatogram shows the fastest run time that resolved all of the components. The run time was reduced by 40% on the serially coupled column when a non-critical pair of components was left unresolved.

F&F - Serially Coupled Column

StabilWax, 19 m x 0.25 mm x 0.25 µm and Rtx-1, 8.50 m x 0.25 mm x 0.25 µm
60℃ @ 18℃/min to 85℃ @ 30℃/min to 200℃, Inlet Pressure : 160.3 kPa



Run Time : 5.63 min	Min Rs Pair : 1.00

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Separations : 30 of 32 resolved

Precolumn : 5 m x 0.53 mm

Carrier : Helium	Regulation : Constant Pressure
Flow : 2.45 ml/min	Temperature : 60℃
Dead Time : 1.393 min	Linear Velocity : 38.90 cm/sec

Third Example

In this example, the unique thermodynamic properties of compounds on a specific phase are used to model widely different column lengths, column diameter and column film thickness.

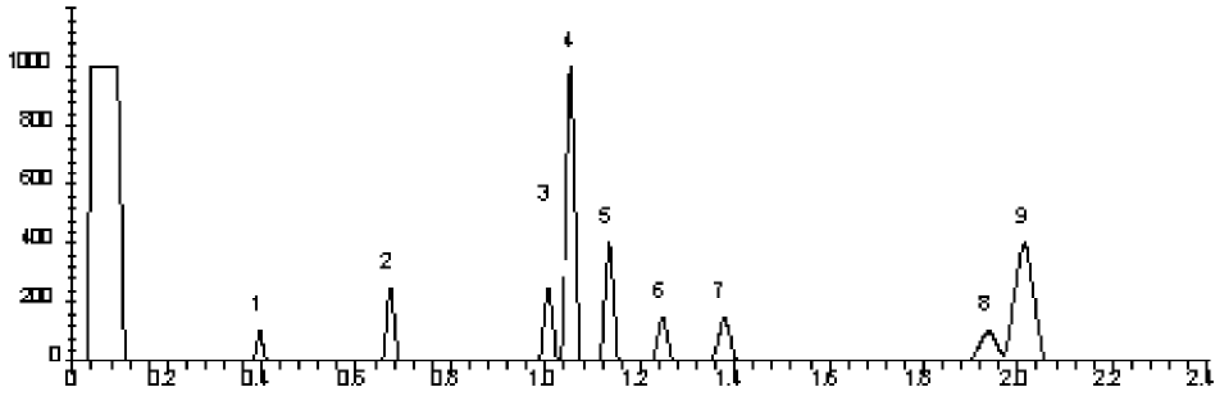
The FAMEs data for this example was originally collected using a 60 meter, 0.25 mm, 0.25 µ Stabilwax column. The thermodynamic properties calculated from this data were used to model a multicapillary column consisting of more than 900 separate 1 m x 0.04 mm x 0.02µm columns.

The following chromatogram shows the predicted elution profile for the multicapillary column that was calculated from the original data. This predicted chromatogram is in very close agreement with Alltech Chromatogram #2140 on MC-WAX.

FAMEs

Carbowax, 1 m x 0.040 mm x 0.200 µm

180℃ (0.20) @ 40℃/min to 210℃, Pressure Program : 260kPa(0.4) @ 75kPa/min to 360kPa



Run Time : 2.01 min	Min Rs Pair : 0.87
Carrier : Helium	Regulation : Pressure Program

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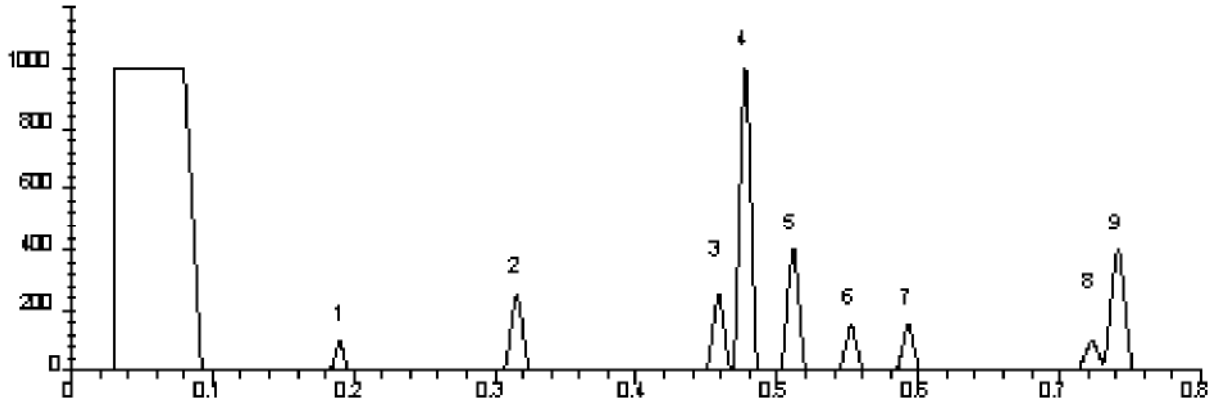
# Component Name	Retention Time (min)	Peak Width (min)	Resolution
1. me myristate	0.395	0.0289	9.37
2. me palmitate	0.672	0.0352	9.37
3. me stearate	1.005	0.0382	1.23
4. me oleate	1.052	0.0384	1.23
5. me linoleate	1.135	0.0389	2.14
6. me linolenate	1.247	0.0433	2.76
7. me arachidate	1.378	0.0515	2.84
8. me behenate	1.936	0.0816	0.87
9. me erucate	2.012	0.0868	0.87

A further reduction in run time could be achieved by using faster temperature and pressure programs.

FAMEs

Carbowax, 1 m x 0.040 mm x 0.200 µm

200℃ (0.20) @130℃/min to 250℃, Pressure Program : 320kPa @ 140kPa/min to 380kPa



Run Time : 0.74 min

Min Rs Pair : 0.90

Carrier : Helium

Regulation : Pressure Program

# Component Name	Retention Time (sec)	Peak Width (sec)	Resolution
1. me myristate	11.40	0.741	9.92
2. me palmitate	18.91	1.053	8.17
3. me stearate	27.49	1.001	1.13
4. me oleate	28.62	0.994	1.13

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5. me linoleate	30.66	0.989	2.06
6. me linolenate	33.13	0.980	2.49
7. me arachidate	35.56	0.959	2.49
8. me behenate	43.37	1.174	0.90
9. me erucate	44.46	1.246	0.90

Conclusion

Modeling and optimizing your present GC and capillary columns can provide improved run times without any additional expenditure of time and money.

In addition, modeling provides a practical way to explore the following features of Fast GC .

- Pressure programming
- Extremely fast temperature ramps (300 °C/sec)
- Microbore detector systems
- New capillary columns
- Short columns and narrow bore columns

You can use modeling to aid in justifying the purchase of new GC hardware or columns.

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Pro ezGC® Thermodynamic Retention Index Database - Environmental PCDD/ Fs, PCBs and PCNs

Library : All-5 PCDD/Fs(210)
Phase : 5%Phenyl-95%Methyl
Copyright : All

1 MCDD
2 MCDD
1 MCDF
2 MCDF
3 MCDF
4 MCDF
1,3 DICDD
1,4 DICDD
1,6 DICDD
1,7 DICDD
1,8 DICDD
2,7 DICDD
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2,3 DICDD
1,2 DICDD
1,3 DICDF
1,7 DICDF
2,4 DICDF
1,4 DICDF
1,8 DICDF
1,6 DICDF
3,7 DICDF
2,7 DICDF
1,2 DICDF
2,8 DICDF
2,3 DICDF
3,6 DICDF
2,6 DICDF
4,6 DICDF
3,4 DICDF
1,9 DICDF

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1,3,6 TRCDD
1,3,7 TRCDD
1,3,8 TRCDD
1,3,9 TRCDD
1,2,4 TRCDD
1,4,8 TRCDD
1,4,9 TRCDD
1,7,8 TRCDD
2,3,7 TRCDD
1,2,3 TRCDD
1,2,6 TRCDD
1,2,7 TRCDD
1,2,8 TRCDD
1,2,9 TRCDD
1,3,7 TRCDF
1,3,8 TRCDF
1,3,6 TRCDF
2,4,9 TRCDF
1,2,4 TRCDF
1,4,7 TRCDF
1,3,4 TRCDF
1,4,6 TRCDF
2,4,8 TRCDF
2,4,7 TRCDF
1,4,8 TRCDF
2,4,6 TRCDF
1,2,7 TRCDF
2,3,9 TRCDF
1,2,3 TRCDF
1,3,9 TRCDF
3,4,9 TRCDF
1,2,6 TRICDF
1,2,8 TRICDF
2,3,8 TRICDF
2,3,7 TRICDF
2,3,6 TRICDF
2,3,4 TRICDF
3,4,7 TRICDF
3,4,8 TRICDF
1,4,9 TRICDF
3,4,6 TRICDF
1,2,9 TRICDF
1,3,6,8 TCDD
1,3,7,9 TCDD
1,3,6,9 TCDD
1,4,6,9 TCDD
1,2,4,7 TCDD

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1,2,4,8 TCDD
1,3,7,8 TCDD
1,2,4,9 TCDD
1,2,4,6 TCDD
1,2,6,8 TCDD
1,4,7,8 TCDD
1,2,7,9 TCDD
1,2,6,9 TCDD
1,2,3,6 TCDD
1,2,3,4 TCDD
1,2,3,7 TCDD
1,2,3,8 TCDD
2,3,7,8 TCDD
1,2,3,9 TCDD
1,2,7,8 TCDD
1,2,6,7 TCDD
1,2,8,9 TCDD
1,3,6,8 TCDF
1,4,6,8 TCDF
2,4,6,8 TCDF
1,3,4,7 TCDF
1,3,7,8 TCDF
1,2,4,7 TCDF
1,3,4,6 TCDF
1,2,4,6 TCDF
1,3,6,7 TCDF
1,3,7,9 TCDF
1,3,4,8 TCDF
1,2,4,8 TCDF
1,2,6,8 TCDF
1,4,7,8 TCDF
1,4,6,7 TCDF
1,3,6,9 TCDF
1,2,3,7 TCDF
2,3,6,8 TCDF
2,4,6,7 TCDF
1,2,3,6 TCDF
1,4,6,9 TCDF
2,3,4,9 TCDF
1,2,3,4 TCDF
1,2,3,8 TCDF
1,2,7,8 TCDF
1,3,4,9 TCDF
1,2,6,7 TCDF
1,2,4,9 TCDF
2,3,7,8 TCDF
1,2,7,9 TCDF

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2,3,4,7 TCDF
2,3,4,6 TCDF
2,3,4,8 TCDF
3,4,6,7 TCDF
1,2,6,9 TCDF
2,3,6,7 TCDF
1,2,3,9 TCDF
1,2,8,9 TCDF
1,2,4,7,9 PeCDD
1,2,4,6,8 PeCDD
1,2,4,6,9 PeCDD
1,2,3,6,8 PeCDD
1,2,4,7,8 PeCDD
1,2,3,7,9 PeCDD
1,2,3,6,9 PeCDD
1,2,4,6,7 PeCDD
1,2,4,8,9 PeCDD
1,2,3,4,7 PeCDD
1,2,3,4,6 PeCDD
1,2,3,7,8 PeCDD
1,2,3,6,7 PeCDD
1,2,3,8,9 PeCDD
1,3,4,6,8 PeCDF
1,2,4,6,8 PeCDF
1,2,4,6,7 PeCDF
1,3,6,7,8 PeCDF
1,3,4,7,8 PeCDF
1,3,4,6,7 PeCDF
1,2,3,6,8 PeCDF
1,2,4,7,8 PeCDF
1,3,4,7,9 PeCDF
1,4,6,7,8 PeCDF
1,2,4,7,9 PeCDF
2,3,4,6,8 PeCDF
1,2,3,4,7 PeCDF
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1,2,4,6,9 PeCDF
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1,2,3,4,8 PeCDF
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1,2,3,7,9 PeCDF
1,2,3,6,7 PeCDF
1,2,6,7,9 PeCDF
1,2,3,6,9 PeCDF
2,3,4,7,8 PeCDF
2,3,4,6,7 PeCDF

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1,2,4,8,9 PeCDF
1,2,3,4,9 PeCDF
1,2,3,8,9 PeCDF
1,2,4,6,8,9 HxCDD
1,2,4,6,7,9 HxCDD
1,2,3,4,6,8 HxCDD
1,2,3,6,8,9 HxCDD
1,2,3,6,7,9 HxCDD
1,2,3,4,6,9 HxCDD
1,2,3,4,7,8 HxCDD
1,2,3,6,7,8 HxCDD
1,2,3,7,8,9 HxCDD
1,2,3,4,6,7 HxCDD
1,2,3,4,6,8 HxCDF
1,3,4,6,7,8 HxCDF
1,2,4,6,7,8 HxCDF
1,3,4,6,7,9 HxCDF
1,2,4,6,7,9 HxCDF
1,2,4,6,8,9 HxCDF
1,2,3,4,6,7 HxCDF
1,2,3,4,7,8 HxCDF
1,2,3,6,7,8 HxCDF
1,2,3,4,7,9 HxCDF
1,2,3,6,7,9 HxCDF
1,2,3,6,8,9 HxCDF
1,2,3,4,6,9 HxCDF
2,3,4,6,7,8 HxCDF
1,2,3,7,8,9 HxCDF
1,2,3,4,8,9 HxCDF
1,2,3,4,6,7,9 HpCDD
1,2,3,4,6,7,8 HpCDD
1,2,3,4,6,7,8 HpCDF
1,2,3,4,6,7,9 HpCDF
1,2,3,4,6,8,9 HpCDF
1,2,3,4,7,8,9 HpCDF
OCDD
OCDF

C14
C15
C16
C17
C18
C19
C20
C21
C22

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C23
C24
C25
C26
C28
C30
C32

References:
Jr. Chrom. 392 87 51-63
Donnelly et al
Jr. Chrom. 541 131-183
Ryan et al

Methods :
2378 Resolution Check
17 Substituted 2378s
Window Definers

Library : PCBs(209)
Phases : Rtx-35, Rtx-50, Rtx-502.2
Copyright : Restek Corp.

2-fluorobiphenyl
1 2
2 3
3 4
4 2,2'
5 2,3
6 2,3'
7 2,4
8 2,4'
9 2,5
10 2,6
11 3,3'
12 3,4
13 3,4'
14 3,5
15 4,4'
16 2,2',3
17 2,2',4
18 2,2',5
19 2,2',6
20 2,3,3'
21 2,3,4
22 2,3,4'

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23 2,3,5
24 2,3,6
25 2,3',4
26 2,3',5
27 2,3',6
28 2,4,4'
29 2,4,5
30 2,4,6
31 2,4',5
32 2,4',6
33 2',3,4
34 2',3,5
35 3,3',4
36 3,3',5
37 3,4,4'
38 3,4,5
39 3,4',5
40 2,2',3,3'
41 2,2',3,4
42 2,2',3,4'
43 2,2',3,5
44 2,2',3,5'
45 2,2',3,6
46 2,2',3,6'
47 2,2',4,4'
48 2,2',4,5
49 2,2',4,5'
50 2,2',4,6
51 2,2',4,6'
52 2,2',5,5'
53 2,2',5,6'
54 2,2',6,6'
55 2,3,3',4
56 2,3,3',4'
57 2,3,3',5
58 2,3,3',5'
59 2,3,3',6
60 2,3,4,4'
61 2,3,4,5
62 2,3,4,6
63 2,3,4',5
64 2,3,4',6
65 2,3,5,6
66 2,3',4,4'
67 2,3',4,5
68 2,3',4,5'
69 2,3',4,6

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70 2,3',4',5
71 2,3',4',6
72 2,3',5,5'
73 2,3',5',6
74 2,4,4',5
75 2,4,4',6
76 2',3,4,5
77 3,3',4,4'
78 3,3',4,5
79 3,3',4,5'
80 3,3',5,5'
81 3,4,4',5
82 2,2',3,3',4
83 2,2',3,3',5
84 2,2',3,3',6
85 2,2',3,4,4'
86 2,2',3,4,5
87 2,2',3,4,5'
88 2,2',3,4,6
89 2,2',3,4,6'
90 2,2',3,4',5
91 2,2',3,4',6
92 2,2',3,5,5'
93 2,2',3,5,6
94 2,2',3,5,6'
95 2,2',3,5',6
96 2,2',3,6,6'
97 2,2',3',4,5
98 2,2',3',4,6
99 2,2',4,4',5
100 2,2',4,4',6
101 2,2',4,5,5'
102 2,2',4,5,6'
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107 2,3,3',4',5
108 2,3,3',4,5'
109 2,3,3',4,6
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111 2,3,3',5,5'
112 2,3,3',5,6
113 2,3,3',5',6
114 2,3,4,4',5
115 2,3,4,4',6
116 2,3,4,5,6

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117 2,3,4',5,6
118 2,3',4,4',5
119 2,3',4,4',6
120 2,3',4,5,5'
121 2,3',4,5',6
122 2',3,3',4,5
123 2',3,4,4',5
124 2',3,4,5,5'
125 2',3,4,5,6'
126 3,3',4,4',5
127 3,3',4,5,5'
128 2,2',3,3',4,4'
129 2,2',3,3',4,5
130 2,2',3,3',4,5'
131 2,2',3,3',4,6
132 2,2',3,3',4,6'
133 2,2',3,3',5,5'
134 2,2',3,3',5,6
135 2,2',3,3',5,6'
136 2,2',3,3',6,6'
137 2,2',3,4,4',5
138 2,2',3,4,4',5'
139 2,2',3,4,4',6
140 2,2',3,4,4',6'
141 2,2',3,4,5,5'
142 2,2',3,4,5,6
143 2,2',3,4,5,6'
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145 2,2',3,4,6,6'
146 2,2',3,4',5,5'
147 2,2',3,4',5,6
148 2,2',3,4',5,6'
149 2,2',3,4',5',6
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152 2,2',3,5,6,6'
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154 2,2',4,4',5,6'
155 2,2',4,4',6,6'
156 2,3,3',4,4',5
157 2,3,3',4,4',5'
158 2,3,3',4,4',6
159 2,3,3',4,5,5'
160 2,3,3',4,5,6
161 2,3,3',4,5',6
162 2,3,3',4',5,5'
163 2,3,3',4',5,6

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164 2,3,3',4',5',6
165 2,3,3',5,5',6
166 2,3,4,4',5,6
167 2,3',4,4',5,5'
168 2,3',4,4',5',6
169 3,3',4,4',5,5'
170 2,2',3,3',4,4',5
171 2,2',3,3',4,4',6
172 2,2',3,3',4,5,5'
173 2,2',3,3',4,5,6
174 2,2',3,3',4,5,6'
175 2,2',3,3',4,5',6
176 2,2',3,3',4,6,6'
177 2,2',3,3',4',5,6
178 2,2',3,3',5,5',6
179 2,2',3,3',5,6,6'
180 2,2',3,4,4',5,5'
181 2,2',3,4,4',5,6
182 2,2',3,4,4',5,6'
183 2,2',3,4,4',5',6
184 2,2',3,4,4',6,6'
185 2,2',3,4,5,5',6
186 2,2',3,4,5,6,6'
187 2,2',3,4',5,5',6
188 2,2',3,4',5,6,6'
189 2,3,3',4,4',5,5'
190 2,3,3',4,4',5,6
191 2,3,3',4,4',5',6
192 2,3,3',4,5,5',6
193 2,3,3',4',5,5',6
194 2,2',3,3',4,4',5,5'
195 2,2',3,3',4,4',5,6
196 2,2',3,3',4,4',5,6'
197 2,2',3,3',4,4',6,6'
198 2,2',3,3',4,5,5',6
199 2,2',3,3',4,5,5',6'
200 2,2',3,3',4,5,6,6'
201 2,2',3,3',4,5',6,6'
202 2,2',3,3',5,5',6,6'
203 2,2',3,4,4',5,5',6
204 2,2',3,4,4',5,6,6'
205 2,3,3',4,4',5,5',6
206 2,2',3,3',4,4',5,5',6
207 2,2',3,3',4,4',5,6,6'
208 2,2',3,3',4,5,5',6,6'
209 Decachlorobiphenyl

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Methods :
Arochlor 1016
Arochlor 1221
Arochlor 1232
Arochlor 1242
Arochlor 1248
Arochlor 1254
Arochlor 1260

Library : All-5 PCBs(209) PCNs(75)
Phase : 5%Phenyl 95%Methyl
Copyright : All

Group 1 - PCBs
Biphenyl
1 2 MCB
2 3 MCB
3 4 MCB
4 2,2' DICB
5 2,3 DICB
6 2,3' DICB
7 2,4 DICB
8 2,4' DICB
9 2,5 DICB
10 2,6 DICB
11 3,3' DICB
12 3,4 DICB
13 3,4' DICB
14 3,5 DICB
15 4,4' DICB
16 2,2',3 TRCB
17 2,2',4 TRCB
18 2,2',5 TRCB
19 2,2',6 TRCB
20 2,3,3' TRCB
21 2,3,4 TRCB
22 2,3,4' TRCB
23 2,3,5 TRCB
24 2,3,6 TRCB
25 2,3',4 TRCB
26 2,3',5 TRCB
27 2,3',6 TRCB
28 2,4,4' TRCB
29 2,4,5 TRCB
30 2,4,6 TRCB
31 2,4',5 TRCB

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32 2,4',6 TRCB
33 2',3,4 TRCB
34 2',3,5 TRCB
35 3,3',4 TRCB
36 3,3',5 TRCB
37 3,4,4' TRCB
38 3,4,5 TRCB
39 3,4',5 TRCB
40 2,2',3,3' TCB
41 2,2',3,4 TCB
42 2,2',3,4' TCB
43 2,2',3,5 TCB
44 2,2',3,5' TCB
45 2,2',3,6 TCB
46 2,2',3,6' TCB
47 2,2',4,4' TCB
48 2,2',4,5 TCB
49 2,3',4,5' TCB
50 2,2',4,6 TCB
51 2,2',4,6' TCB
52 2,2',5,5' TCB
53 2,2',5,6' TCB
54 2,2',6,6' TCB
55 2,3,3',4 TCB
56 2,3,3',4' TCB
57 2,3,3',5 TCB
58 2,3,3',5' TCB
59 2,3,3',6 TCB
60 2,3,4,4' TCB
61 2,3,4,5 TCB
62 2,3,4,6 TCB
63 2,3,4',5 TCB
64 2,3,4',6 TCB
65 2,3,5,6 TCB
66 2,3',4,4' TCB
67 2,3',4,5 TCB
68 2,3',4,5' TCB
69 2,3',4,6 TCB
70 2,3',4',5 TCB
71 2,3',4',6 TCB
72 2,2',5,5' TCB
73 2,3',5',6 TCB
74 2,4,4',5 TCB
75 2,3,4',6 TCB
76 2',3,4,5 TCB
77 3,3',4,4' TCB
78 3,3',4,5 TCB

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79 3,3',5,5' TCB
80 3,3',5,5' TCB
81 3,4,4',5 TCB
82 2,2',3,3',4 PeCB
83 2,2',3,3',5 PeCB
84 2,2',3,3',6 PeCB
85 2,2',3,4,4' PeCB
86 2,3',3,4,5 PeCB
87 2,2',3,4,5' PeCB
88 2,2',3,4,6 PeCB
89 2,2',3,4,6' PeCB
90 2,2',3,4',5 PeCB
91 2,2',3,4',6 PeCB
92 2,2',3,5,5' PeCB
93 2,2',3,5,6 PeCB
94 2,2',3,5,6' PeCB
95 2,2',3,5',6 PeCB
96 2,2',3,6,6' PeCB
97 2,2',3',4,5 PeCB
98 2,2',3',4,6 PeCB
99 2,2',4,4',6 PeCB
100 2,2',4,4',6 PeCB
101 2,2',4,5,5' PeCB
102 2,2',4,5,6' PeCB
103 2,2',4,5',6 PeCB
104 2,2',4,6,6' PeCB
105 2,3,3',4,4' PeCB
106 2,3,3',4,4' PeCB
107 2,3,3',4',5 PeCB
108 2,3,3',4,5' PeCB
109 2,3,3',4,6 PeCB
110 2,3,3',4',6 PeCB
111 2,3,3',5,5' PeCB
112 2,3,3',5,6 PeCB
113 2,3,3',5',6 PeCB
114 2,3,4,4',5 PeCB
115 2,3,4,4',6 PeCB
116 2,3,4,5,6 PeCB
117 2,3,4',5,6 PeCB
118 2,3',4,4',5 PeCB
119 2,3',4,4',6 PeCB
120 2,3',4,5,5' PeCB
121 2,3',4,5',6 PeCB
122 2',3,3',4,5 PeCB
123 2',3,4,4',5 PeCB
124 2',3,4,5,5' PeCB
125 2',3,4,5,6' PeCB

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126 3,3',4,4',5 PeCB
127 3,3',4,5,5' PeCB
128 2,2',3,3',4,4' HxCB
129 2,2',3,3',4,5 HxCB
130 2,2',3,3',4,5' HxCB
131 2,2',3,3',4,6 HxCB
132 2,2',3,3',4,6' HxCB
133 2,2',3,3',5,5' HxCB
134 2,2',3,3',5,6 HxCB
135 2,2',3,3',5,6' HxCB
136 2,2',3,3',6,6' HxCB
137 2,2',3,4,4',5 HxCB
138 2,2',3,4,4',5' HxCB
139 2,2',3,4,4',6 HxCB
140 2,2',3,4,4',6' HxCB
141 2,2',3,4,5,5' HxCB
142 2,2',3,4,5,6 HxCB
143 2,2',3,4,5,6' HxCB
144 2,2',3,4,5',6 HxCB
145 2,2',3,4,6,6' HxCB
146 2,2',3,4',5,5' HxCB
147 2,2',3,4',5,6 HxCB
148 2,2',3,4',5,6' HxCB
149 2,2',3,4',5',6 HxCB
150 2,2',3,4',6,6' HxCB
151 2,2',3,5,5',6 HxCB
152 2,2',3,5,6,6' HxCB
153 2,2',4,4',5,5' HxCB
154 2,2',4,4',5,6' HxCB
155 2,2',4,4',6,6' HxCB
156 2,3,3',4,4',5 HxCB
157 2,3,3',4,4',5' HxCB
158 2,3,3',4,4',6 HxCB
159 2,3,3',4,5,5' HxCB
160 2,3,3',4,5,6 HxCB
161 2,3,3',4,5',6 HxCB
162 2,3,3',4',5,5' HxCB
163 2,3,3',4',5,6 HxCB
164 2,3,3',4,5',6 HxCB
165 2,3,3',5,5',6 HxCB
166 2,3,4,4',5,6 HxCB
167 2,3',4,4',5,5' HxCB
168 2,3',4,4',5',6 HxCB
169 3,3',4,4',5,5' HxCB
170 2,2',3,3',4,4',5
171 2,2',3,3',4,4',6
172 2,2',3,3',4,5,5'

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173 2,2',3,3',4,5,6
174 2,2',3,3',4,5,6'
175 2,2',3,3',4,5',6
176 2,2',3,3',4,6,6'
177 2,2',3,3',4',5,6
178 2,2',3,3',5,5',6
179 2,2',3,3',5,6,6'
180 2,2',3,4,4',5,5'
181 2,2',3,4,4',5,6
182 2,2',3,4,4',5,6'
183 2,2',3,4,4',5',6
184 2,2',3,4,4',6,6'
185 2,2',3,4,5,5',6
186 2,2',3,4,5,6,6'
187 2,2',3,4',5,5',6
188 2,2',3,4',5,6,6'
189 2,3,3',4,4',5,5'
190 2,3,3',4,4',5,6
191 2,3,3',4,4',5',6
192 2,3,3',4,5,5',6
193 2,3,3',4',5,5',6
194 2,2',3,3',4,4',5,5'
195 2,2',3,3',4,4',5,6
196 2,2',3,3',4,4',5',6
197 2,2',3,3',4,4',6,6'
198 2,2',3,3',4,5,5',6
199 2,2',3,3',4,5,6,6'
200 2,2',3,3',4,5',6,6'
201 2,2',3,3',4,5,5',6'
202 2,2',3,3',5,5',6,6'
203 2,2',3,4,4',5,5',6
204 2,2',3,4,4',5,6,6'
205 2,3,3',4,4',5,5',6
206 2,2',3,3',4,4',5,5',6
207 2,2',3,3',4,4',5,6,6'
208 2,2',3,3',4,5,5',6,6
209 DecaChloroBiphenyl

C13
C14
C15
C16
C17
C18
C19
C20
C21

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C22
C23
C24
C25
C26
C28
C30
C32

Reference:
Environ. Sci. Technol.
Vol 18 No 6 1984
Mullin et al

Group 2 - PCNs
1 1 MCN
2 2 MCN
3 1,2 DiCN
4 1,3 DiCN
5 1,4 DiCN
6 1,5 DiCN
7 1,6 DiCN
8 1,7 DiCN
9 1,8 DiCN
10 2,3 DiCN
11 2,6 DiCN
12 2,7 DiCN
13 1,2,3 TrCN
14 1,2,4 TrCN
15 1,2,5 TrCN
16 1,2,6 TrCN
17 1,2,7 TrCN
18 1,2,8 TrCN
19 1,3,5 TrCN
20 1,3,6 TrCN
21 1,3,7 TrCN
22 1,3,8 TrCN
23 1,4,5 TrCN
24 1,4,6 TrCN
25 1,6,7 TrCN
26 2,3,6 TrCN
27 1,2,3,4 TCN
28 1,2,3,5 TCN
29 1,2,3,6 TCN
30 1,2,3,7 TCN
31 1,2,3,8 TCN

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32 1,2,4,5 TCN
33 1,2,4,6 TCN
34 1,2,4,7 TCN
35 1,2,4,8 TCN
36 1,2,5,6 TCN
37 1,2,5,7 TCN
38 1,2,5,8 TCN
39 1,2,6,7 TCN
40 1,2,6,8 TCN
41 1,2,7,8 TCN
42 1,3,5,7 TCN
43 1,3,5,8 TCN
44 1,3,6,7 TCN
45 1,3,6,8 TCN
46 1,4,5,8 TCN
47 1,4,6,7 TCN
48 2,3,6,7 TCN
49 1,2,3,4,5 PeCN
50 1,2,3,4,6 PeCN
51 1,2,3,5,6 PeCN
52 1,2,3,5,7 PeCN
53 1,2,3,5,8 PeCN
54 1,2,3,6,7 PeCN
55 1,2,3,6,8 PeCN
56 1,2,3,7,8 PeCN
57 1,2,4,5,6 PeCN
58 1,2,4,5,7 PeCN
59 1,2,4,5,8 PeCN
60 1,2,4,6,7 PeCN
61 1,2,4,6,8 PeCN
62 1,2,4,7,8 PeCN
63 1,2,3,4,5,6 HxCN
64 1,2,3,4,5,7 HxCN
65 1,2,3,4,5,8 HxCN
66 1,2,3,4,6,7 HxCN
67 1,2,3,5,6,7 HxCN
68 1,2,3,5,6,8 HxCN
69 1,2,3,5,7,8 HxCN
70 1,2,3,6,7,8 HxCN
71 1,2,4,5,6,8 HxCN
72 1,2,4,5,7,8 HxCN
73 1,2,3,4,5,6,7 HpCN
74 1,2,3,4,5,6,8 HpCN
75 1,2,3,4,5,6,7,8 OCN

Reference:

J. Chrom. A 683 385-396

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Jarnberg et al.

Methods :
Arochlor 1016
Arochlor 1221
Arochlor 1232
Arochlor 1242
Arochlor 1248
Arochlor 1254
Arochlor 1260

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Pro ezGC® Thermodynamic Retention Index Database - Environmental Volatiles and Semi-Volatiles

Library : All-5 Pyridines & NPAHs
Phase : 5%Phenyl 95%Methyl
Copyright : All

1-(3-pyridyl)-2-(4-pyridy
1,2-dimethylcarbazole
1,2-dimethylindole
1,3-dimethylcarbazole
1,3-dinitropyrene
1,3-nitronaphthalene
1,4-dimethylcarbazole
1,4-dinitronaphthalene
1,5-dinitronaphthalene
1,6-dinitropyrene
1,8-dinitronaphthalene
1,8-dinitropyrene
1>3,6>8-hexahydropyrene
1>4-tetrahydrocarbazole
10-azabenzo[a]pyrene
10-methyl-5,6benzacridine
1368-tetranitronaphthalen
1-aminoanthracene
1-aminofluorene
1-aminoindan
1-aminonaphthalene
1-aminophenanthrene
1-aminopyrene
1-azabenz[a]anthracene
1-azachrysene
1-azafluoranthene
1-azapyrene
1-cyanonaphthalene
1-ME-9-nitroanphenanthren
1-methylcarbazole
1-methylindole
1-methylisoquinoline

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1-methylpyrene
1-nitro-2-methylquinoline
1-nitroanthraquinone
1-nitrofluoranthene
1-nitronaphthalene
1-nitropyrene
2-(2-aminoethyl)pyridine
2-(aminomethyl)pyridine
2,2':6',2'-terpyridine
2,2'-bipyridyl
2,2'-biquinoline
2,2'diME4,4'dinitrobibenz
2,2'-dinitrobibenzyl
2,2'-dinitrobiphenyl
2,2'-dipyridyl
2,2'-dipyridylamine
2,3,5-trimethylindole
2,3,5-trinitronaphthalene
2,3,6-trimethylpyridine
2,3-dimethylindole
2,3'-dipyridyl
2,4,6-trimethylpyridine
2,4-dimethylpyridine
2,4-dimethylquinoline
2,4'-dipyridyl
2,5-dimethylindole
2,5-dinitrofluorene
2,6-dimethylpyridine
2,6-dimethylquinoline
2,6-dinitro-9-fluorenone
2,7-dimethylpyrene
2,7-dimethylquinoline
2,7-dinitro-9-fluorenone
2,7-dinitrofluorene
2457tetranitro9fluorenone
2-amino-3-methylpyridine
2-amino-4-methylpyridine
2-amino-5-methylpyridine
2-amino-6-methylpyridine
2-aminoanthracene
2-aminobenzo[c]phenanthre
2-aminobiphenyl
2-aminofluorene
2-aminonaphthalene
2-aminophenanthrene
2-aminopyrene
2-aminopyridine

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2-azachrysene
2-azafluoranthene
2-azapyrene
2-cyanonaphthalene
2-cyanopyridine
2-dimethylaminopyridine
2-hydroxy4methylquinoline
2-hydroxyquinoline
2-methoxyquinoline
2-methyl-1,4-naphthoquino
2-methyl-2-quinoline
2-methylacridine
2-methylbenzo[f]quinoline
2-methylindole
2-methylpyrene
2-methylpyridine
2-methylquinoline
2-nitro-9-fluorenone
2-nitroaniline
2-nitroanthracene
2-nitrobiphenyl
2-nitrofluoranthene
2-nitrofluorene
2-nitronaphthalene
2-nitropyrene
2-phenylindole
2-phenylpyridine
2-picolinamide
2-pyridylacetonitrile
3-(aminomethyl)pyridine
3,3'-dipyridyl
3,4-dimethylpyridine
3,5-dimethylpyridine
3,5-diphenylpyridine
3-aminofluoranthene
3-aminofluorene
3-aminophenanthrene
3-aminopyridine
3-cyanopyridine
3-ethylpyridine
3-methyl-2-aminonaphthale
3-methyl-2-phenylpyridine
3-methylbenzo[f]quinoline
3-methylcarbazole
3-methylindole
3-methylpyridine
3-methylquinoline

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3-nitro-9-fluorenone
3-nitrobiphenyl
3-nitrodibenzofuran
3-nitrofluoranthene
3-nitrofluorene
3-phenylpyridine
4(aminomethyl)pyridine
4,4'-dinitrobibenzyl
4,4'-dipyridyl hydrate
4,5,9,10-tetrahydorpyrene
4,5-dihydropyrene
4-aminobenzo[c]phenanthre
4-aminobiphenyl
4-aminofluorene
4-aminophenanthrene
4-aminopyrene
4-aminopyridine
4-azabiphenyl
4-azachrysene
4-azafluorene
4-azapyrene
4-cyanopyridine
4-ethylpyridine
4H-benzo[def]carbazole
4-hydroxyquinoline
4-methylcarbazole
4-methylpyrene
4-methylpyridine
4-methylquinoline
4-nitroaniline
4-nitrobiphenyl
4-nitrophenyl phenylether
4-nitro-p-terphenyl
4-nitropyrene
4-nitroquinoline-n-oxide
5,7-diMEbenz[a]acridine
5-amino-2-methoxypyridine
5-aminochrysene
5-aminoindan
5H-indeno[1,2b]pyridine
5-nitro-1234tetrahydroNAP
5-nitro-6-methylquinoline
5-nitro-8-methylquinoline
5-nitroacenaphthene
5-nitroindan
5-nitroquinoline
6-aminobenzo[a]pyrene

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6-aminochrysene
6-methylquinoline
6-nitrobenzo[a]pyrene
6-nitrocoumarin
6-nitroquinoline
6-phenylquinoline
7,10-diMEbenz[a]acridine
7,9-diMEbenz[c]acridine
7-aminobenzo[a]pyrene
7-azafluoranthene
7-azaindole
7-methylindole
7-methylquinoline
7-nitro-1-tetralone
7-nitro-3,4benzocourmarin
7-nitrofluoranthene
8-hydroxyquinoline
8-methoxyquinoline
8-methylquinoline
8-nitro-7-methylquinoline
8-nitrofluoranthene
8-nitroquinaldine
8-nitroquinoline
9,10,12-triMEbenz[a]acrid
9-aminoanthracene
9-aminophenanthrene
9-cyanoanthracene
9-cyanophenanthrene
9-ethylcarbazole
9-ME-10-nitroanthracene
9-methylacridine
9-nitroanthracene
9-phenylcarbazole
acridan(9,10diydroacridi)
acridine
a-n-butylpyrene
benz[a]acridine
benz[c]acridine
benzo(a)pyrene
benzo[a]carbazole
benzo[b]carbazole
benzo[c]carbazole
benzo[c]cinnoline
benzo[def]carbazole
benzo[e]pyrene
benzo[f]quinoline
benzo[h]quinoline

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bis-(2-picolyl)amine
carbazole
chrysene
cyclopenta[cd]pyrene
D5-nitrobenzene (S)
dibenz[a,c]phenazine
dibenz[a,h]acridine
dibenz[a,j]acridine
dibenzo[a,g]carbazole
dibenzo[a,i]carbazole
dibenzo[c,g]carbazole
ethyl 2-picolinate
ethyl isonicotinate
ethyl nicotinate
indeno(1,2,3-cd)pyrene
indeno[1,2,3-cd]pyrene
indeno[123ij]isoquinoline
indole
isonicotinamide
isoquinoline
methyl isonicotinate
methyl nicotinate
methyl picolinate
methyl picolinimidate
naphthalene
nicotinamide
nitrobenzene
N-nitrosodi-n-propylamine
N-nitrosodiphenylamine
n-picolyl-2-picolinamidin
phenanthridine
phenantrhene
phenazine
picene
pyrene
pyridine
quinoline

C6
C7
C8
C9
C10
C11
C12
C13
C14

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C15
C16
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C26
C28
C30
C32
C34

References:
Jr Chrom 1982
Lee etal
Jr Chrom 388 1987 23-25
Ford etal

Library : All-5 Semivolatiles&PAHs
Phase : 5%Phenyl 95%Methyl
Copyright : All

0-terphenyl
1,12-dimethylbenz[a]antrh
1,1'-binaphthyl
1,2,4-trichlorobenzene
1,2,4trimethylnaphthalene
1,2'-binaphthyl
1,2-dichlorobenzene
1,2-dihydronaphthalene
1,2-dimethylnaphthalene
1,3,6,11-tetramethyltriph
1,3-dichlorobenzene
1,3-dimethylnaphthalene
1,3-dimethyltriphenylene
1,3-indanedione
1,4-dichlorobenzene
1,4-dihydronaphthalene
1,4-dimethylnaphthalene
1,4-naphthoquinone
1,4-napthoquinone

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1,5-dimethylnaphthalene
1,6,11-trimethyltriphenyl
1,6-dimethylnaphthalene
1,7-dimethylnaphthalene
1,8-dimethylnaphthalene
1,8-dimethylphenanthrene
1>12dodecahydrotriphenyle
1>3,10b-tetrahydrofluoran
1>3,6>8-hexahydropyrene
1>4-tetrahydrocarbazole
1>4-tetrahydrodibenzothio
1>4-tetrahydrophenanthren
1>8-octahydroanthracene
1>8-octahydrophenanthrene
11-benzo[a]fluorenone
11-methylbenz[a]anththrac
11-methylbenzo[a]fluorene
122a345-hexahydroacenapht
1234-tetrahydronaphthalen
1234-tetrahydroquinoline
1245-tetrachlorobenzene
12-methylbenz[a]anthracen
1367-tetramethylnaphthale
1-ethylnaphthalene
1-ethylpyrene
1-mehylanthracene
1methyl7isopropylphenanth
1-methylacenaphthylene
1-methylbenz[a]anthracene
1-methylchrysene
1-methylfluorene
1-methylnaphthalene
1-methylphenanthrene
1-methylpyrene
1-methyltriphenylene
1-phenylnaphthalene
1-phenylphenanthrene
2(2'naphthyl)benzo[b]thio
2,2'-binaphthyl
2,2'-bipyridyl
2,2'-biquinoline
2,2'-dimethylbiphenyl
2,3,5-trimethylindole
2,3dihydiben[def,mno]chry
2,3-dimethylindole
2,3-dimethylnaphthalene
2,4,6-tribromophenol (S)

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2,4-dinitrotoluene
2,6-dimethylnaphthalene
2,6-dimethylquinoline
2,6-dinitrotoluene
2,7-dimethylnaphthalene
2,7-dimethylphenanthrene
2,7-dimethylpyrene
2,-ethylbiphenyl
235-trimethylnaphthalene
236,trimethylnaphthalene
2367-tetramethylnaphthale
2-chloronaphthalene
2dimethyldibenzothiophene
2-ethylnaphthalene
2-ethylphenanthrene
2-fluorbiphenyl (S)
2-methyl-1,4-naphthoquino
2-methylacridine
2-methylanthracene
2-methylbenz[a]anthracene
2-methylbenzo[b]thiophene
2-methylbiphenyl
2-methylchrysene
2-methylfluorene
2-methylindole
2-methylnaphthalene
2-methylphenanthrene
2-methylpyrene
2-naphthylamine
2-nitroaniline
2-phenylindole
2-phenylnaphthalene
3,3'-dichlorobenzidine
3,3'-dimethylbiphenyl
3,5-dimethylnaphthalene
3,5-diphenylpyridine
3,6-dimethylphenanthrene
3-methylbenz[a]anthracene
3-methylbenzo[b]thiophene
3-methylbenzo[f]quinoline
3-methylbiphenyl
3-methylcholanthrene
3-methylchrysene
3-methylindole
3-methylphenanthrene
3-nitroaniline
4,4'-dimethylbiphenyl

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4,5,9,10-tetrahydorpyrene
4,5-dihydropyrene
456-trihydrobenz[de]anthr
46dimethyldibenzothiophen
4-bromophenyl phenyl ethe
4-chloroaniline
4-chlorophenyl phenyl eth
4H-benzo[def]carbazole
4H-cyclopenta[def]phenant
4-methldibenzothiophene
4-methylbiphenyl
4-methylchrysene
4-methylphenanthrene
4-methylpyrene
4-nitroaniline
5,12-dihydronaphthacene
5-ethylbenzo[b]-thiopene
5H-indeno[1,2b]pyridine
5-methylbenz[a]anthracene
5-methylchrysene
6-methylbenz[a]anthracene
6-methylchrysene
6-methylquinoline
6-phenylquinoline
7,12-dimethylbenz[a]anthr
7-benz[de]anthrene
7-methylbenz[a]anthracene
8-methylbenz[a]anthracene
8-methylquinoline
9,10-diethylphenanthrene
9,10-dihydoanthracene
9,10-dihydroacridine
9,10-dihydrophenanthrene
9,10dime3ethylphenanthren
9,10-dimethylanthracene
9-ethylcarbazole
9-ethylfluorene
9-ethylphenanthrene
9-fluorenone
9-isopropylphenanthrene
9-methyl-10-ethylphenanth
9methyl10phenylphenanthre
9-methylanthracene
9-methylbenz[a]anthracene
9-methylflurene
9-methylphenanthrene
9-n-butylfluorene

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9-n-hexylfluorene
9-n-propylfluorene
9-n-propylphenanthrene
9-phenylanthracene
9-phenylcarbazole
9-phenylphenanthrene
acenaphthene
acenaphthylene
acridine
a-n-butylpyrene
aniline
anthracene
anthrone
azulene
benz[a]acridine
benz[a]anthracene
benz[c]acridine
benzo(a)anthracene
benzo(a)pyrene
benzo(b)fluoranthene
benzo(g,h,i)perylene
benzo(k)fluoranthene
benzo[a]carbazole
benzo[a]fluorene
benzo[b]carbazole
benzo[b]chrysene
benzo[b]fluoranthene
benzo[b]fluorene
benzo[b]naphtho[2,1d]thio
benzo[b]thiophene
benzo[c]phenanthrene
benzo[e]pyrene
benzo[f]quinoline
benzo[ghi]fluoranthene
benzo[ghi]perylene
benzo[h]quinoline
benzo[j][fluoranthene
benzo[j]fluoranthene
benzo[k]fluoranthene
benzo[kl]xanthene
benzo[lmn]phenathridiene
benzoic acid
benzyl alcohol
biphenyl
bis(2-chloroethoxy)methan
bis(2-chloroethyl) ether
bis(2-chloroisopropyl)eth

bis(2-ethylhexyl) phthala
bis(2-ethylhexyl)phthalat
butyl benzyl phthalate
carbazole
chrysene
cis-x-hexahycrodibenzoTHI
cyclopenta[cd]pyrene
D10-acenaphthene (I)
D10-phenanthrene (I)
D12-chrysene (I)
D12-perylene
D12-perylene (I)
D14-p-terphenyl
D14-terphenyl (S)
D4-1,4-dichlorobenzene(I)
D5-nitrobenzene (S)
D6-phenol (S)
D8-naphthalene (I)
decahydronaphthalene
dibenz(a,h)anthracene
dibenz[a,c]anthracene
dibenz[a,h]anthracene
dibenzo(a,h)anthracene
dibenzo[c,kl]xanthene
dibenzo[def,mno]chrysene
dibenzofuran
dibenzo-p-dioxin
dibenzothiophene
diethyl phthalate
dimethyl phthalate
dinaphtho[1,2b;1',2'd]fur
di-n-butyl phthalate
di-n-octyl phthalate
diphenylethane
diphenylmethane
ethyldibenzothiophene
fluoranthene
fluorene
hexachlorobenzene
hexachlorobutadiene
hexachlorocyclopentadiene
hexachloroethane
indane
indene
indeno(1,2,3-cd)pyrene
indeno[1,2,3-cd]pyrene
indeno[123ij]isoquinoline

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indole
indoline
isophorone
isoquinoline
m-quaterphenyl
m-terphenyl
naphthacene
naphthalene
nitrobenzene
N-nitrosodi-n-propylamine
N-nitrosodiphenylamine
o-quaterphenyl
o-toluidine
pentacene
pentachlorobenzene
perylene
phenanthrene
phenanthridine
picene
p-quaterphenyl
p-terphenyl
pyrene
quinoline
quinoxaline
tetrachloroethane
tetralin
thianthrene
trans-x-hexahydrodibenzoT
triphenylene
xanthene

C12
C13
C14
C15
C16
C17
C18
C19
C20
C21
C22
C23
C24
C25
C28
C32

HROMalytic RESEARCH '07
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References:
Anal Chem Vol 51 No. 6
1979
Milton Lee & Curt White
HRCC Vol 9 1986
Rostad & Pereira

Library : All-5 SPAHs
Phase : 5%Phenyl 95%Methyl
Copyright : All

1,7-eimethyldibenzothioph
1>4-tetrahydrodibenzothio
10MEbenzo[b]NAP[1,2-d]Thi
10MEbenzo[b]NAP[2,1-d]Thi
10MEbenzo[b]NAP[2,3-d]Thi
10-MEphenanthro[2,1-b]Thi
11MEbenzo[b]NAP[1,2-d]Thi
11MEbenzo[b]naptho[23d]Th
122a345-hexahydroacenapht
13MEbenzo[]phenantrh[32]T
1-MEantrha[2,1-b]thiopene
1-MEbenzo[b]NAP[1,2-d]Thi
1-MEbenzo[b]NAP[2,1-d]Thi
1-MEbenzo[b]NAP[2,3-d]Thi
1-methyldibenzothiophene
1-methylnaphtho[2,1-b]Thi
2-(2'Naphthyl)benzo[b]Thi
2(2'naphthyl)benzo[b]thio
2,6-dimethyldibenzothioph
2,8-dimethyldibenzothioph
2dimethyldibenzothiophene
2-MEbenzo[b]NAP[1,2-d]Thi
2-MEbenzo[b]NAP[2,1-d]Thi
2-MEbenzo[b]NAP[2,3-d]Thi
2-methylbenzo[b]thiophene
2-methyldibenzothiophene
2-methylnaphtho[2,1-b]Thi
3,5-dimethylbenzo[b]Thi
3,6-dimethyldibenzothioph
3,7-dimethyldibenzothioph
3,8-dimethyldibenzothioph
3-ethyldibenzothiophene
3-MEbenzo[b]NAP[1,2-d]Thi
3-MEbenzo[b]NAP[2,1-d]Thi

3-MEbenzo[b]NAP[2,3-d]Thi
3-MEbenzo[b]NAP[9,10b]Thi
3-MEpheanthro[2,1-d]Thi
3-methylbenzo[b]thiophene
3-methyldibenzothiophene
4,6-dimethyldibenzothioph
46dimethyldibenzothiophen
4-MEbenzo[b]NAP[1,2-d]Thi
4-MEbenzo[b]NAP[2,1-d]Thi
4-MEbenzo[b]NAP[2,3-d]Thi
4-methylbenzo[b]thiophene
4-methyldibenzothiophene
4-methylnaphtho[1,2-b]Thi
4-methylnaphtho[2,1-b]Thi
5-ethylbenzo[b]-thiopene
5-ethylbenzo[b]thiophene
5-MEbenzo[b]NAP[2,1-d]Thi
5-methylbenzo[b]thiophene
5-methylnaphtho[2,1-b]Thi
6-MEbenzo[b]NAP[1,2-d]Thi
6-MEbenzo[b]NAP[2,1-d]Thi
6-MEbenzo[b]NAP[2,3-d]Thi
6-methylbenzo[b]thiophene
6-methylnaphtho[1,2-b]Thi
6-methylnaphtho[2,1-b]Thi
7-MEbenzo[b]NAP[2,1-d]Thi
7-MEbenzo[b]NAP[2,3-d]Thi
7-methylbenzo[b]thiophene
7-methylnaphtho[2,1-b]Thi
8-MEbenzo[b]NAP[1,2-d]Thi
8-MEbenzo[b]NAP[2,1-d]Thi
8-MEbenzo[b]NAP[2,3-d]Thi
8-methylnaphtho[1,2-b]Thi
8-methylnaphtho[2,1-b]Thi
9,13-H-triphenyleno[23b]T
9-MEbenzo[b]NAP[1,2-d]Thi
9-MEbenzo[b]NAP[2,1-d]Thi
9-MEbenzo[b]NAP[2,3-d]Thi
9-methyl-10-ethylphenanth
9-methylnaphtho[2,1-b]Thi
anthra[1,2-b]benzo[d]Thi
anthra[1,2-b]thiophene
anthra[2,1-b]thiophene
anthro[2,3-b]thiophene
benzo[1,2]phenaleno[43b]T
benzo[12]phenaleno[34be]T
benzo[23]PHanthro[45bed]T

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benzo[45]phenaleno[19bc]T
benzo[45]phenaleno[91bc]T
benzo[b]naphtho[1,2-d]Thi
benzo[b]naphtho[2,1-d]Thi
benzo[b]naphtho[2,3-d]Thi
benzo[b]phenanthro[1,2d]T
benzo[b]phenanthro[2,1d]T
benzo[b]phenanthro[2,3d]T
benzo[b]phenanthro[3,2d]T
benzo[b]phenanthro[3,4d]T
benzo[b]phenanthro[4,3d]T
benzo[b]phenanthro[910d]T
benzo[b]thiophene
benzothiazole
chrysene
chryseno[4,5-bed]thiophen
cis-x-hexahycrodibenzoTHI
dibenzothiophene
dinaphtho[1,2-b:1',2'-d]T
dinaphtho[1,2-b:2',1'-d]T
dinaphtho[1,db:2',3'd]Thi
dinaphtho[2,1-b:1',2'-d]T
dinaphto[2,3b:2',3'd]Thi
ethyldibenzothiophene
hexahydrodibenzoThi
naphthalene
naphtho[1,2-b]thiophene
naphtho[2,1-b]thiophene
naphtho[2,3-b]thiophene
phenaleno[6,7-be]thiophen
phenanthro[1,2-b]thiophen
phenanthro[2,1-b]thiophen
phenanthro[2,3-b]thiophen
phenanthro[3,2-b]thiophen
phenanthro[3,4-b]thiophen
phenanthro[4,3-b]thiophen
phenanthro[4,5-bed]thioph
phenanthro[9,10-b]thiophe
phenantrhene
picene
pyreno[1,2-b]thiophene
pyreno[2,3-b]thiophene
pyreno[4,5-b]thiophene
trans-x-hexahydrodibenzoT
triphenyleno[1,2b]thiophe
triphenyleno[2,1b]thiophe
triphenyleno[2,3b]thiophe

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triphenyleno[4,5-bed]Thi

C11
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C20
C21
C22
C23
C24
C25
C26
C28
C30
C32

References:
Jr Chrom 1982
Lee etal
HRCC 1986 Vol 9 328-334
Rostad & Pereira

Library : All-5 Volatiles
Phase : 5%Phenyl-95%Methyl
Copyright : All

1,1,1,2-tetrachloroehtane
1,1,1-trichloroethane
1,1,2,2-tetrachloroethane
1,1,2-trichloroethane
1,1-dichloroethane
1,1-dichloroethene
1,1-dichloropropene
1,2,3-trichlorobenzene
1,2,3-trichloropropane
1,2,4-trichlorobenzene
1,2,4-trimethylbenzene
1,2-chloroethane
1,2dibromo3chloropropane
1,2-dibromoethane

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1,2-dibromopropane
1,2-dichlorobenzene
1,2-dichloroethane
1,2-dichloropropane
1,3,5-trimethylbenzene
1,3-dibromopropane
1,3-dichlorobenzene
1,3-dichloropropane
1,3-xylene
1,4-dibromobutane
1,4-dichlorobenzene
1,4-dichlorobutane
1,4-xylene
1,5-dichloropentane
1-bromo-2-chloroethane
1-bromo-3-chloropropane
1-bromo-3-me-butane
1-bromobutnae
1-bromohexane
1-bromopentane
1-chlorobutane
1-chlorohexane
1-chloropentane
1-iodopropane
1-propanol
2- methyl-3-buten-2-ol
2,2,2-trifluoroethanol
2,2-dichloropropane
2,2-dimethyl-1-pentanol
2,3-dichloro-1-propylene
2,4-dimethyl-2-pentanol
2,4-dimethyl-3-pentanone
2-bromo-2-me-propane
2-butanol
2-buten-1-ol
2-chlor-2-me-butane
2-chloro-2-me-propane
2-chloro-2-methyl-butane
2-chlorobutane
2-chloropropane
2-chlorotoluene
2-ethyl-1-butanol
2-furanmethanol
2-heptanol
2-heptanone
2-hexanol
2-iodopropane

2-methoxyethanol
2-methyl-1-pentanol
2-methyl-3-pentanol
2-nitropropane
3-buten-1-ol
3-chloro-2-me-propylene
3-ethyl-3-pentanol
3-heptanone
3-hexanol
3-methyl-3-pentanol
3-pentanol
4-chlorotoluene
acetamide
allyl alcohol
allyl chloride
benzene
bromobenzene
bromochloromethane
bromocyclohexane
bromodichloromethane
bromoform
bromomethane
butyl acetate
butyl ether
carbon tetrachloride
chloroacentonitrile
chlorobenzene
chloroethane
chloroform
chloromethane
cis 1,2-dichloroethene
cis-1,2-dichloroethene
cis-1,2-dichloropropene
cyclohexane
cyclohexanol
cyclopentane
cyclopentanol
cyclopentanone
dibromochloromethane
dibromomethane
dichlorofluoromethane
dichloromethane
dimethyl sulfoxide
dimethylacetamide
dimethylformamide
ethyl acetate
ethyl chloroacetate

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ethyl propionate
ethylbenzene
ethylene glycol
formamide
hexachlorobutadiene
hexachloroethane
hexanol
iodoehtane
isoamyl alcohol
isopropylacetate
isopropylbenzene
methycyclohexane
methylene chloride
methylisomylketone
m-xylene
naphthalene
n-butylbenzene
nitroethane
n-propylbenzene
o-xylene
pentanal
p-isopropyltoluene
p-xylene
pyridine
sec-butylbenzene
styrene
tert-butylbenzene
tetrachloroethene
tetrachloroethylene
toluene
trans-1,2-dichloroethene
trans-1,2-dichloropropene
trans-1,4-dichloro2butene
trichlorethene
trichloroethene
trichlorofluoromethane
trichlorotrifluorethane
vinyl chloride

C3
C4
C5
C6
C7
C8
C9
C10

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C11
C12
C13

Reference:
HRCC Vol 9 1986 446-451
Vituki

Library : Volatiles
Phases : Rtx-1, Rtx-502.2, Rtx-624
Copyright : Restek Corp.

acetone
acetonitrile
acrolein
acrylonitrile
allyl alcohol
allyl chloride
benzene
benzene-d6
benzyl chloride
bis(2chloroethoxy)methan
bis(2chloroisopropyl)eth
bromobenzene
bromochloroacetonitrile
2-bromochlorobenzene
3-bromochlorobenzene
4-bromochlorobenzene
bromochloromethane
bromodichloromethane
4-bromofluorobenzene
bromoform
bromomethane
2-bromo-1-chloropropane
2-butanone
t-butyl alcohol
n-butylbenzene
sec-butylbenzene
tert-butylbenzene
carbon disulfide
carbon tetrachloride
chloroacetonitrile
chlorobenzene
chlorobenzene-d5
1-chlorobutane
chloroethane

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2-chloroethanol
2-chloroethylvinylether
chloroform
1-chlorohexane
chloromethane
3-chloropropionitrile
2-chlorotoluene
4-chlorotoluene
1-chloro-2-fluorobenzene
cyclohexane
dibromoacetonitrile
dibromochloromethane
1,2-dibromoethane (EDB)
dibromofluoromethane
dibromomethane
1,2-dibromo3chloropropane
dichloroacetonitrile
1,2-dichlorobenzene
1,3-dichlorobenzene
1,4-dichlorobenzene
1,2-dichlorobenzene-d4
1,4-dichlorobenzene-d4
1,4-dichlorobutane
dichlorodifluoromethane
1,1-dichloroethane
1,2-dichloroethane
1,2-dichloroethane-d4
1,1-dichloroethene
cis-1,2-dichloroethene
trans-1,2-dichloroethene
dichloromethane
1,2-dichloropropane
1,3-dichloropropane
2,2-dichloropropane
1,1-dichloropropanone
1,1-dichloropropene
cis-1,3-dichloropropene
trans-1,3dichloropropene
cis-1,4dichloro-2-butene
trans-1,4dichloro2butene
1,3-dichloro-2-propanol
diethyl ether
1,4-difluorobenzene
1,4-dioxane
epichlorohydrin
ethanol
ethyl methacrylate

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ethylbenzene
ethylbenzene-d5
ethylbenzene-d10
ethylene oxide
fluorobenzene
hexachlorobutadiene
hexachloroethane
2-hexanone
iodomethane
isobutyl alcohol
di-isopropyl ether
isopropylbenzene
p-isopropyltoluene
malononitrile
methacrylonitrile
methyl ethyl ketone
methyl iodide
methyl methacrylate
4methyl2pentanone (MIBK)
MTBE
methylacrylate
methylene chloride
naphthalene
nitrobenzene
2-nitropropane
pentachloroethane
pentafluorobenzene
2-picoline
propargyl alcohol
propionitrile
n-propylamine
n-propylbenzene
pyridine
styrene
1,1,1,2tetrachloroethane
1,1,2,2tetrachloroethane
tetrachloroethene
THF
thiophenol
toluene
toluene-d8
trichloroacetonitrile
1,2,3-trichlorobenzene
1,2,4-trichlorobenzene
1,1,1-trichloroethane
1,1,2-trichloroethane
trichloroethene

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trichlorofluoromethane
1,2,3-trichloropropane
1,1,1-trichloro2propane
112trichloro122trifluoro
trifluorotoluene
1,2,4-trimethylbenzene
1,3,5-trimethylbenzene
vinyl acetate
vinyl chloride
m-xylene
o-xylene
p-xylene

C3
C4
C5
C6
C7
C8
C9
C10
C11
C12
C13
C14

Methods:
EPA method 502.2
EPA method 524.2 rev 3.0
EPA method 524.2 rev 4.0
EPA method 551
EPA method 8240A
EPA method 8260

Library : Rtx-5 Semi-Volatiles
Phase : Rtx-5
Copyright : Restek Corp.

acenaphthene
acenaphthene-d10
acenaphthylene
Aldrin
anthracene
benzidine
benzoic acid
benzo(b)fluoranthene

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benzo(k)fluoranthene
benzo(g,h,i)perylene
benzo(a)anthracene
benzo(a)pyrene
benzyl alcohol
Alpha-BHC
Beta-BHC
Delta-BHC
Gamma-BHC
bis(2-chloroethoxy)methan
bis(2-chloroethyl)ether
bis(2-chloroisopropyl)eth
bis(2-ethylhexyl)phthalat
4-bromophenyl phenyl ethe
butyl benzyl phthalate
carbazole
4-chloroaniline
2-chloronaphthalene
4-chloro-3-methylphenol
2-chlorophenol
2-chlorophenol-d4
4-chlorophenyl phenyl eth
m-cresol
chrysene
chrysene-d12
4,4'-DDD
4,4'-DDE
4,4'-DDT
decane
decafluorotriphenylphosph
dibenzo(a,h)anthracene
dibenzofuran
di-n-butyl phthalate
1,3-dichlorobenzene
1,4-dichlorobenzene
1,4-dichlorobenzene-d4
1,2-dichlorobenzene
1,2-dichlorobenzene-d4
3,3'-dichlorobenzidine
2,4-dichlorophenol
Dieldrin
diethyl phthalate
2,4-dimethylphenol
dimethyl phthalate
2-methyl4,6-dinitrophenol
2,4-dinitrophenol
2,4-dinitrotoluene

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2,6-dinitrotoluene
di-n-octyl phthalate
docosane
dodecane
eicosane
Endosulfan I
Endosulfan II
Endosulfan Sulfate
Endrin
Endrin Aldehyde
Endrin Ketone
fluoranthene
fluorene
2-fluorobipohenyl
2-fluorophenol
Heptachlor
Heptachlor Epoxide
hexachlorobenzene
hexachlorobutadiene
hexachlorocyclopentadiene
hexachloroethane
hexacosane
hexadecane
indeno(1,2,3-cd)pyrene
isophorone
Lindane
Methoxychlor
2-methylnaphthalene
2-methylphenol
4-methylphenol
naphthalene
naphthalene-d8
2-nitroaniline
3-nitroaniline
4-nitroaniline
nitrobenzene
nitrobenzene-d5
2-nitrophenol
4-nitrophenol
N-nitrosodimethylamine
N-nitroso-di-n-propylamin
N-nitrosodiphenylamine
octacosane
octadecane
pentachlorophenol
perylene-d12
phenanthrene

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phenanthrene-d10
phenol
phenol-d6
pyrene
pyridine
p-terphenyl-d14
tetracosane
tetradecane
2,4,6-tribromophenol
1,2,4-trichlorobenzene
2,4,5-trichlorophenol
2,4,6-trichlorophenol

Methods:
EPA Method 8270

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Pro ezGC® Thermodynamic Retention Index Database - Environmental Pesticides

Library : All-1 Pesticides
Phase : 100%Methylsilicone
Copyright : All

acephate
alachlor
aldrin
ametryn
anilazine
azinphos, ethyl
azinphos, methyl
azodrin
barban
baytex
benefin
BHC, alpha
BHC, beta
BHC, delta
BHC, gamma (LINDANE)
BHC-beta
bifenox
biphenyl
biphenyl, D10
BOLSTAR
BOTRAN
bromophos
bulan
butachlor
captafol
captan
carbaryl (SEVIN)
carbophenothion
carboxin
chlordane, trans
chlordane, trans
chlordene, alpha

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chlordene, beta
chlordene, gamma
chlorfenvinphos
chlorobenzilate
chloropropylate
chlorothalonil
chloroxuron
chlorpropham
chlorpyrifos(DURSBAN)
chlorpyrifos, methyl
chlorthal, dimethyl
chlorthal-dimethyl
chrysene
chrysene, D12
CIODRIN
coumaphos
crotoxphos
crufomate
cupromid
cyanazine (BLADEX)
cygon
cygon OA
DASANIT
DCPA
DDD, o,p'
DDD, p,p'
DDE, o,p'
DDE, p,p'
DDT, o,p'
DDT, p,p'
DEF
DEMETON-S
diazinon
dichlobenil
dichlofluanid
dichlone
dichloran
dichlorofenthion
dicofol, o,p'
dicofol, p,p'
dicrotophos
dieldrin
dimethoate(CYGON)
dioxathion
diphenamid
diphenyl disulfide
disulfoton

disyston sulfoxide
endosulfan I
endosulfan II
endosulfan sulfate
endrin
endrin aldehyde
endrin ketone
EPN
ethalflualin
ethion
ethofumesate
ethoprop
ethyl parathion (DNTP)
ethylan
famphur
fenamaphos
fenitrothion
fenthion
folpet
fonophos
gardona
genite
guthion
heptachlor
heptachlor expoxcide
imazalil
imidan
iprodione
isobenzan
isodrin
isopropalin
KELTHANE
leptophos
malathion
metalaxyl
methidathion
methiocarb
methoxychlor
methoxychlor, o,p'
metroromuron
mevinphos (PHOSDRIN)
MGK 264
mirex
mobam
monitor
naled (DIBROM)
napropamide

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nemacur
nitrofen
nonachlor, cis
octachlor expoxide
octachlorostyrene
orthene
oxadiazon
OXAMYL
oxychlordane
oxyfluorfen
parathion
parathion, methyl
PCNB
pendimethalin
pentachloroanisole
permethyrin, cis
permethyrin, trans
perthane
phenanthrene
phenothiazine
phorate (THIMET)
phosalone
phosdrin, alpha
phosdrin, beta
picloram
pirimiphos-ethyl
profluralin
prometon
prometryn
pronamide
propazine
propetamphos
ronnel
safrotin
simazine
simetryn
sulfotep
sulphenone
sulprofos
supona
supracide
systox I
systox II
terbacil
terbufos
terbutryn
tetrachlorvinphos

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tetradifon
tetradimefon
thiabendazole
thimet
tolyfluanid
triadimefon
triflualin
triphenyl phosphate
trithion
vinclozolin
zolone
zytron

C13
C14
C15
C16
C17
C18
C19
C20
C21
C22
C23
C24
C25
C28

References:
Jr. Chrom. 393 (1987)
175-194
Saxton

Library : Rtx-5 Phenoxy-Acids
Phase : Rtx-5
Copyright : Restek Corp.

2,4-D
2,4-DB
2,4,5-T
2,4,5-TP
3,5-Dichlorobenzoic Acid
4-Nitrophenol
Acifluorfen
Amiben
Banvel

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Basagran
Bentazon
Blazer
Chloramben
Dalapon
DBOB
DCAA
Dicamba
Dichlorprop
Dinoseb
Docosane
DPA
Eicosane
Hexacosane
Hexadecane
MCPA
MCPP
Octadecane
PCP
Pentachlorophenol
Picloram
Premerg
Silvex
Tetracosane
Tetradecane
Tordon

Methods:
EPA Method 515.1
EPA Method 615
EPA Method 8150B

Library : Rtx-5 Pesticides
Phase : Rtx-5
Copyright : Restek Corp.

Group 1 - Chlorinated

Alachlor
Aldrin
Atrazine
Bayleton
BHC-alpha
BHC-beta
BHC-delta
BHC-gamma

Captafol
Captan
Carbophenothion
Chlordane-alpha
Chlordane-gamma
Chlorneb
Chlorobenzilate(a)
Chloropropylate
Chlorothalonil
Chlorpropham
Dacthal
DBCP
DCPA
4,4'-DDD
4,4'-DDE
4,4'-DDT
Decachlorobiphenyl
Cis-Di-allate
Trans-Di-allate
Dibutylchlorendate
Dichlone
Dichloran
Dicofol
Dieldrin
Docosane
Eicosane
Endosulfan I
Endosulfan II
Endosulfan Sulfate
Endrin
Endrin Aldehyde
Endrin Ketone
Ethylan
Etridiazole
Fenarimol
Heptachlor
Heptachlor Epoxide
Hexachlorobenzene
Hexachlorocyclopentadiene
Hexacosane
Hexadecane
Isodrin
Kelthane
Kepone
Lindane
Methoxychlor
Metolachlor

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Metribuzin
Mirex
Nitrofen
Cis-Nonachlor
Trans-Nonachlor
Octadecane
PCNB
Cis-Permethrin
Trans-Permethrin
Perthane
Pronamide
Propachlor
Rubigan
Simazine
Terbacil
Tetrachloro-m-xylene
Tetracosane
Tetradecane
TOK
Triadimefon
Trifluralin
1,3-dimethyl-2-nitrobenze

Group 2 - Nitrogen

Ametryn
Atraton
Benefin
Bromacil
Butachlor
Butylate
Carboxin
Cycloate
Diazinon
Dichlorvos
Diphenamid
Disulfoton
Dodecane
EPTC
Ethoprop
Fenamiphos
Fluridone
Hexazinone
Isopropalin
Merphos
Mevinphos

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MGK 264A
MGK 264B
Molinate
Napropamide
Norflurazon
Octacosane
Oxadiazon
Oxyfluorfen
Pebulate
Pendamethalin
Profluralin
Prometon
Prometryn
Propazine
Simetryn
Stirofos
Tebuthiuron
Terbufos
Terbutryn
Tricyclozole
Triphenyl phosphate
Vernolate

Group 3 - Organophos.

Azinphos methyl
Chlorfenvinphos
Chlorpyrifos
Coumaphos
Crotoxyphos
Demeton O
Demeton S
Dicrotophos
Dimethoate
Dioxathion
EPN
Ethion
Famphur
Fensulfothion
Fenthion
Malathion
Methyl Parathion
Mevinphos, alpha
Monocrotophos
Naled
Parathion

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Phorate
Phosmet
Phosphamidon
Ronnel
Sulfotep
Sulprofos
TEPP
Tetrachlorvinphos
Tokuthion
Trichloronate

Methods:
EPA Method 505
EPA Method 507
EPA Method 508
EPA Method 608
EPA Method 608.1
EPA Method 608.2
EPA Method 617
EPA Method 1618
CLP Pesticides
EPA Method 8141A

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Pro ezGC® Thermodynamic Retention Index Database - Food and Flavors

Library : F&Fs
Phases : Rtx-1, Stabilwax
Copyright : Restek Corp.

acetone
allyl acetate
allyl alcohol
4-allylanisole
amyl acetate
tert-amyl alcohol
amyl cinnamaldehyde
trans-anethole
alpha-angelicalactone
p-anisaldehyde
anisole
benzaldehyde
benzyl acetate
benzyl acetone
benzyl alcohol
borneol
bornyl acetate
1-butanol
2-butanol
2-butenal
cis-2-buten-1-ol
3-buten-1-ol
3-buten-2-ol
butryolactone
butyl acetate
tert-butyl acetate
tert-butyl alcohol
sec-butylbenzene
tert-butylbenzene
butyl butyrate
butyl propionate
camphene
camphor

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3-carene
carvacrol
carveol
r-carvone
s-carvone
carvone acetate
carvone hydrate
cis-carvyl acetate
trans-carvyl acetate
cis-carvyl propionate
trans-carvyl propionate
alpha-caryophyllene
beta-caryophyllene
caryophyllene oxide
1,8-cineole
trans-cinnamyl acid
trans-cinnamyl alcohol
trans-cinnamaldehyde
cinnamide
trans-cinnamyl acetate
citral a
citral b
citronellal
beta-citronellol
citronellyl acetate
citronellyl formate
coumarin
p-cresol
cumene
cumic acid
cumin alcohol
cuminaldehyde
cyclohexanone
cyclopentanol
cyclopentanone
para-cymene
decanal
1-decanol
2-decanone
dihydrocarveol
cis-dihydrocarvone
trans-dihydrocarvone
dihydrocoumarin
dihydrojasmone
2,3-dimethylanisole
2,4-dimethylanisole
2,5-dimethylanisole

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2,6-dimethylanisole
2,3-dimethylanisaldehyde
2,5-dimethylanisaldehyde
2,5-dimethylfuran
2,6-dimethyl-4-heptanone
2,2-dimethyl-3-pentanol
2,4-dimethyl-2-pentanol
2,4-dimethyl-3-pentanol
2,4-dimethyl-3-pentanone
2-dodecanone
estragole
ethyl acetate
ethyl acrylate
ethyl amyl ketone
ethyl benzoate
ethyl butanoate
2-ethyl-1-butanol
ethyl butyrate
ethyl decanoate
ethyl formate
2-ethylfuran
2-ethyl-1-hexanol
ethyl isobutyrate
ethyl laurate
ethyl-2-methyl butanoate
ethyl pentanoate
3-ethyl-3-pentanol
ethyl valerate
ethyl vanillin
eucalyptol
eugenol
cis-trans-farnesol
trans-trans-farnesol
fenchone
furfural
furfuryl acetate
furfuryl alcohol
geranial
geraniol
geranyl acetate
guaiazulene
heptanal
1-heptanol
2-heptanol
4-heptanol
2-heptanone
3-heptanone

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4-heptanone
hexanal
trans-2-hexenal
1-hexanol
2-hexanol
trans-2-hexenol
3-hexanol
2-hexanone
3-hexanone
cis-3-hexen-1-ol
trans-2-hexen-1-ol
4-hexen-3-one
hexyl acetate
alpha-humulene
indole
alpha-ionone
beta-ionone
isoamyl acetate
isoamyl alcohol
isoborneol
isobutyl acetate
isobutyl alcohol
isobutyl isobutyrate
isobutyraldehyde
isoeugenol
isomenthone
isopropyl acetate
isopropyl alcohol
isopropyl butyrate
cis-jasmone
limonene
linalool
linalool oxide
linalyl acetate
maltol
menthofuran
menthol
menthone
cis-menthyl acetate
trans-menthyl acetate
methyl acetate
3-methyl-p-anisaldehyde
2-methylanisole
3-methylanisole
4-methylanisole
alpha-methylbenzylalcohol
methyl benzoate

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methyl butanoate
2-methyl-1-butanol
2-methyl-2-butanol
3-methyl-1-butanol
3-methyl-2-butanol
3-methyl-2-butanone
2-methyl-3-buten-2-ol
3-methyl-2-buten-1-ol
methyl butyrate
2-methylcinnamaldehyde
alpha-methylcinnamic acid
6-methylcoumarin
7-methylcoumarin
methyl decanoate
methyl ethyl ketone (MEK)
2-methylfuran
5-methylfurfural
5-methyl-3-heptanone
methyl hexanoate
5-methyl-2-hexanone
methylisobutylketone/MIBK
methyl isobutyrate
methyl octanoate
methyl pentanoate
2-methyl-1-pentanol
2-methyl-3-pentanol
3-methyl-3-pentanol
2-methyl-3-pentanone
4-methyl-3-penten-2-one
2-methylpropanal
2-methyl-1-propanol
2-methyl-2-propanol
methyl propanoate
methyl valerate
myrcene
neomenthol
neopentanol
neral
cis-nerol
neryl acetate
nonanal
1-nonanol
2-nonanol
2-nonanone
3-nonanone
5-nonanone
nootketone

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cis-ocimene
trans-ocimene
octanal
1-octanol
2-octanol
2-octanone
3-octanone
1-octen-3-ol
pentanal
1-pentanol
2-pentanol
2-pentanone
3-pentanone
cis-2-penten-1-ol
3-penten-2-one
perillaldehyde
perillyl alcohol
alpha-phellandrene
pinacol
pinacol alcohol
pinacolone
alpha-pinene
beta-pinene
1-propanol
2-propanol
2-propanone
2-propen-1-ol
propyl acetate
propyl benzoate
propyl butyrate
propyl formate
propyl propanoate
propyn-1-ol
pulegone
pyridine
trabs-sabinene hydrate
salicaldehyde
alpha-terpinene
gamma-terpinene
alpha-terpineol
terpinen-4-ol
alpha-terpinolene
terpinyl acetate
tetrahydro-2-fufanmethano
tetrahydrofurfuryl acetat
thiazole
thiophene

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alpha-thujone
beta-thujone
thymol
triacetin
tricyclene
2-undecanone
valencene
valeraldehyde
delta-valerolactone
gamma-valerolactone
vanillin
vanillin acetate
verbenone
1,2-xylene
1,3-xylene
1,4-xylene

nonane
decane
undecane
dodecane
tridecane
tetradecane
pentadecane
hexadecane
heptadecane
octadecane
nonadecane
eicosane
heneicosane
docosane
tricosane
tetracosane
hexacosane

Methods:
pepmt\spearmt\mt\eucalpt
lemon\lime\orange\mandar
thyme\rosemary\sage oils
pine needle\dwarf pine
cinnamon\bois de rose oil
caraway\dill seed oils
star anise\ fennel oils

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Pro ezGC® Thermodynamic Retention Index Database - Drugs and Pharmaceuticals

Library : All-1 Drugs
Phase : 100% Methylsilicone
Copyright : All

6-monoacetylmorphine
7-aminoflunitrazepam
7-hydroxyamoxapine
8-hydroxyamoxapine
8-methyoxyloxapine
acepromazine
acetylcodeine
alimemazine
amantidine
aminophenazone metab.
amitriptyline
amitriptyline metab.
amoxapine
amphetamine
anileridine
aprindine
atropine
benactyzine
benzocaine
benzoylecgonine
benztropine
benzydamine
biperiden
bromazepam
bromodiphenhydramine
buclizine
bupivacaine
butacaine
butaperazine
cadaverine
carbamazepine
carbamazepine metab.
carbetaphentane

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carbinoxamine
chlordiazepoxide
chlorimipramine
chloroprocaine
chloroquine
chloroquine metab.
chlorothiazide
chlorpentermine
chlorpheniramine metab.
cholesterol
cinchocaine
cinnamoylcocaine
clemastine
clonazepam
clonidine
clotermine
clothiapine
clozapine
cotarmine
cotarmine decomp.
cyclobenzaprine
cyclomethylcaine
cyclopentamine
cycrimine
cyproheptadine
darvinoxamine
dextropropoxifene
dextropropoxyphene metab.
diacetylmorphine
diamorphine
dibenzepin
dicyclomine
diethylpropion
diethyltryptamine
dihydrocodeine
dimethindene
dimethyltryptamine
diphenhydramine metabolit
diphenylpyralamine
dipyrone
dipyrone metab.
dipyrone metab.
disopyramide
disopyramide met. decomp.
dispramide met. decomp.
doxylamine metabolite
dyphylline

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ecgonine methyl ester
ephedrine
ethlmorfine
ethoheptazine
ethylbenzoylecgonine
ethylmorphine
fentanyl
flurazepam metab.
heptabarbital
hydroxyamitryptyline
hydroxy-ethyl flurazepam
hydroxynortriptyline
hydroxyzine
hydroxyzine metab.
hyocyamine
hyoscine
isophedrine
isopropamide
levallorphan
lidocaine metabolite
lindane
lorazepam
loxepine
lupimine
MDA
meclizine
melitracene
mepazine
mephenesin
mephentermine
mepivicaine
mequitazine
mescaline
mesoridazine
methadone metab.
methamphetamine
methaqualone metab.
methdilazine
methenamine
methotrimeprazine
methotrimeprazine metab.
methotrmeprazine metab.
methoxamine
methylphenidate
metoclopramide
mianserin
morphine(BSTFA deriv.)

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naloxone
naphazoline
n-desmethyl diazepam
n-disalkylflurazepam
niflumic acid
nitrazepam
nomifensine
nordiazepam
nordoxepin
norephedrine
normeperidine
norpropoxyphene #1
norpropoxyphene #2
norpropoxyphene amide
norpropoxypheneamide
nortriptyline
orphenadrine
oxazepam
oxycodone
oxymetazoline
oxymorphone
oxyphenbutazone
papaverine
phenazopyridine
phendimetrazine
phenelezine
phenethylamine
phenindiamine
phenmetrazine
phenoxybenzamine
phentermine
phentoate
phenylpropanolamine
phenyramidol
phenytoin
pinazepam
piperidolate
pipradrol
pizotifen
pramoxine
prilocaine
procaine
promethazine
promzine
propoxycaine
propoxyphene decomp.
propranolol

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propylhexdrine
propyphenazone metab.
protriptyline
quinidine
quinine
thenyldiamine
thiethylperzine
thioridazine
thioridazine metab.
thonzylamine
trifluroperizine
trihexyphenidyl
trimethoprim
trimipramine
tripelennamine
triprolidine
zolamine

C9
C10
C11
C12
C13
C14
C15
C16
C17
C18
C19
C20
C21
C22
C23
C24
C25
C26
C28
C30
C32
C34

References:

HRC&CC 1990 Vol 13
754-758 Phillips etal
Jr. Chrom. 374(1986)
73-85 Lora-Tamayo etal

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HRC&CC Vol 6 (1983)
247-254 Anderson etal

Library : Drugs
Phases : Rtx-1, Rtx-5, Rtx-50, Rtx-200, Rtx-35
Copyright : Restek Corp.

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Acetophenetidin
Acetopromazine
Alphaprodine
Alprazolam
Amitriptyline
Amobarbital
Aprobarbital
Atropine
Barbital
Benzocaine
Benzphetamine
Bromazepam
Brompheniramine
Bupivacaine
Butabarbital
Butalbital
Butethal
Caffeine
Carisoprodal
Chlorpheniramine
Chlorpromazine
Chlorprothixene
Clobazam
Clomipramine
Clonazepam
Cocaine
Codeine
Cotinine
Desipramine
Desmethyldiazepam
Dextromethorphan
Diazepam
Dibucaine
Dimenhydrinate
Diphenhydramine
Diphenylhydantoin
Doxepin
Doxylamine
Ethosuximide

Flunitrazepam
Flurazepam
Glutethimide
Haloperidol
Hexobarbital
Hydrocodone
Hydromorphone
Imipramine
Ketamine
Levorphanol
Lidocaine
Lorazepam
Maprotyline
Medazepam
Meperidine
Mephobarbital
Meprobamate
Methadone
Methapyriline
Methaqualone
Methyprylon
Morphine
Nalorphine
Nicotine
Norcodeine
Nortriptyline
Papaverine
Pentazocine
Pentobarbital
Phencyclidine
Pheniramine
Phenobarbital
Phenothiazine
Phenylbutazone
Phenyltoloxamine
Prazepam
Primidone
Procainamide
Prochlorperazine
Promazine
Promethazine
Propoxyphene
Pyrilamine
Scopolamine
Secobarbital
Strychnine
Temazepam

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Tetracaine
Thiamylal
Thiopental
Thioridazine
Trazodone
Triazolam
Trifluoperazine
Trimeprazine
Trimipramine
Tripelennamine
Triprolidine
Valproic Acid
Verapamil

C10
C12
C14
C16
C18
C20
C22
C24
C26
C28
C30
C32
C34
C36
C40

Methods:
Benzodiazepines
Barbiturates
Phenothiazines
Opiates
Antidepressants
Anesthetics
Antihistamines

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Pro ezGC® Thermodynamic Retention Index Database - Petroleum

Library : All-1 Petroleum C1-C9
Phase : 100% MethylSilicone
Copyright : All

(1,2-diMEpropyl)cyclopent
(1MEbutyl)cyclopropane
(1-MEethyl)cyclopentane
(2-MEpropyl)cyclopentane
1,1,1,2-tetrachloroethane
1,1,1-trichloroethane
1,1,2,2-tetrachloroethane
1,1,2,2-tetraMEcycloprop
1,1,2-trichloroethane
1,1,2-triMEcyclohexane
1,1,2-triMEcyclopentane
1,1,3,3-tetraMEcyclopenta
1,1,3-trichloropropene
1,1,3-triMEcyclopentane
1,1,3trimethylcyclohexane
1,1,4-triMEcyclohexane
1,12trimethylcyclopentane
1,1-dichloro3,3diMEbutane
1,1-dichlorobutane
1,1-dichloroethane
1,1-diethylcyclopropane
1,1-dimethylcyclohexane
1,1-dimethylcyclopentane
1,2,2-triMEcyclopropane
1,2,3-trichloropropane
1,2,3-triMEcyclohexane
1,2-dichloro-2-MEpropane
1,2-dichloroethane
1,2-dichloropropane
1,2-dimethyl1cyclopentene
1,2-dimethylbenzene
1,3,5-cycloheptatriene
1,3,5-hexatriene

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1,3,5-triMEcyclohexane
1,3,5-triMEcyclohexene
1,3-butadiene
1,3-cycloheptadiene
1,3-cyclohexadiene
1,3-cyclooctadiene
1,3-cyclopentadiene
1,3-dichloropropane
1,3-diME-1-cyclohexene
1,3-dimethylbenzene
1,3-hexadiene
1,3-pentadiene
1,4-cyclohexadiene
1,4-diME-1-cylcohexene
1,4-dimethylbenzene
1,4-hexadiene
1,4-pentadiene
1,5-hexadiene
1,6-heptadiene
1,7-octadiene
1,8-nonadiene
1,C2,T4-triMEcyclopentane
1,T2,C4-triMEcyclopentane
1,trans-3-diMEcyclohexane
1a,2a,3a-triMEcyclopentan
1a,2b,4a-triMEcyclohexane
1a,2b,4b-triMEcyclohexane
1a,3a,5a-triMEcyclohexane
1-butene
1-butyne
1C2T3trimethylcyclopentan
1-chloro-2,2-diMEpropane
1-chloro-2-methylpropane
1-chloro-3-ME-2-butane
1-chlorobutane
1-chlorohexane
1-chloropentane
1-chloropropane
1ethyl-1,4-cyclohexadiene
1-ethyl-1-ME-cyclohexane
1-ethyl-1-MEcylcopentane
1-ethylcyclopentene
1-heptene
1-heptyne
1-hexene
1-hexyne
1-ME-1,3cyclohexadiene

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1-ME-1,3-cyclopentadiene
1-ME-1,4-cyclohexadiene
1-ME-1,4cyclohexadiene
1-ME-1-ethylcyclopentane
1-ME-1-n-propylcyclopenta
1-ME-3-isethylcyclopentan
1-ME-C3-ethylcyclopentane
1-ME-cis3-propylcyclopent
1-ME-T2-ethylcyclopentan
1-ME-T3-ethylcyclopentane
1-methyl-1-cyclohexene
1-methyl-1-cyclopentene
1methylC2ethylcyclopentan
1-methylcyclohexene
1-methylcyclopentene
1-methylcylcopentene
1-ME-trans2-propylcyclope
1-ME-trans3-propylcylcope
1-nonene
1-octene
1-octyne
1-pentene
1-pentyne
1T2C3triMEcyclopentane
2,2,3,3-tetramethylbutane
2,2,3,3tetramethylpentane
2,2,3,4tetramethylpentane
2,2,3-trimethylbutane
2,2,3-trimethylheptane
2,2,3-trimethylhexane
2,2,3-trimethylpentane
2,2,4,4-tetramethylhexane
2,2,4,4tetramethylpentane
2,2,4-triME-2-pentene
2,2,4-trimethylheptane
2,2,4-trimethylhexane
2,2,4-trimethylpentane
2,2,5,5-tetraMEhexane
2,2,5-trimethylhexane
2,2-dichloropropane
2,2-dimethylbutane
2,2-dimethylheptane
2,2-dimethylhexane
2,2-dimethylpentane
2,2-dimethylpropane
2,3,3,4tetramethylpentane
2,3,3-trimethyl-1-butene

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2,3,3-trimethylhexane
2,3,3-trimethylpentane
2,3,4-trimethyl-2-pentene
2,3,4-trimethylhexane
2,3,4-trimethylpentane
2,3,5-trimethylhexane
2,3-dimethyl1,3butadiene
2,3-dimethyl-1-butene
2,3-dimethyl-1-heptene
2,3-dimethyl-1-hexene
2,3-dimethyl-1-pentene
2,3-dimethyl-2-butene
2,3-dimethyl-2-heptene
2,3-dimethyl-2-hexene
2,3-dimethyl-2-pentene
2,3-dimethylbutane
2,3-dimethylheptane
2,3-dimethylhexane
2,3-dimethylpentane
2,3-pentadiene
2,4,4-triemthyl-2-pentene
2,4,4-trimethylhexane
2,4,6-trimethylheptane
2,4-diME-1,3-pentadine
2,4-diME-3-ethylpentane
2,4-dimethyl1,3pentadiene
2,4-dimethyl-1-pentene
2,4-dimethyl-2-pentene
2,4-dimethylheptane
2,4-dimethylhexane
2,4-dimethylpentane
2,5-diME-1,5-hexadiene
2,5-diME-23-diethylhexane
2,5-dimethyl2,4hexadiene
2,5-dimethyl-2-hexene
2,5-dimethylheptane
2,5-dimethylhexane
2,5-eimethyl-2-hexene
2,5-norbornadiene
2,6-dimethylheptane
2-butyne
2-chloro-2-methylbutane
2-chloro-2-methylpentane
2-chloro-2-methylpropane
2-chlorobutane
2-chloroheptane
2-chlorohexane

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2-chloropentane
2-chloropropane
2-ethyl-1-butene
2-ethyl-1-pentene
2-ethyl-3-methyl-1-butene
2-ME-1,3-cyclopentadiene
2-mehyl-3-heptene
2-methyl-1,2-butadiene
2-methyl-1,3-butadiene
2-methyl-1,5-hexadiene
2-methyl-1-butene
2-methyl-1-heptene
2-methyl-1-hexene
2-methyl-1-octene
2-methyl-1-pentene
2-methyl-1-propene
2-methyl-2-butene
2-methyl-2-heptene
2-methyl-2-hexene
2-methyl-2-octene
2-methyl-2-pentene
2-methyl-3-ethylpentane
2-methylbutane
2-methylheptane
2-methylhexane
2-methyloctane
2-methylpentane
2-methylpropane
2-methylpropene
2-norbornadiene
2-pentyne
3,3,4-trimethylhexane
3,3-diethylpentane
3,3-dimethyl-1-butene
3,3-dimethyl-1-butyne
3,3-dimethyl-1-pentene
3,3-dimethylheptane
3,3-dimethylhexane
3,3-dimethylpentane
3,4-dichloro-1-butene
3,4-dimethyl-1-hexene(1)
3,4-dimethyl-1-hexene(2)
3,4-dimethyl-1-pentene
3,4-dimethylheptane(1)
3,4-dimethylheptane(2)
3,4-dimethylhexane(1)
3,4-dimethylhexane(2)

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3,5,5-trimethyl-1-hexene
3,5-dimethylheptane
3,5-dimethylheptane(1)
3,5-dimethylheptane(2)
3-chloro-1-propene
3-ethyl-1-pentene
3-ethyl-2MEpentane
3-ethyl-2-pentene
3-ethyl-3-methylpentane
3-ethylcyclopentene
3-ethylheptane
3-ethylhexane
3-ethylpentane
3-methyl-1,3-pentadiene
3-methyl-1-butene
3-methyl-1-cyclohexene
3-methyl-1-cyclopentene
3-methyl-1-heptene
3-methyl-1-hexene
3-methyl-1-pentene
3-methyl-3-ethylpentane
3-methylcyclohexene
3-methylcyclopentene
3-methyleneheptane
3-methylenepentane
3-methylheptane
3-methylhexane
3-methyloctane
3-methylpentane
4,4-dimethyl-1-pentene
4,4-dimethylheptane
4-ethenylcyclohexene
4-ethylheptane
4-methyl-1,3-pentadiene
4-methyl-1-cyclohexene
4-methyl-1-hexene
4-methyl-1-pentene
4-methylcyclohexene
4-methylheptane
4-methyloctane
4-octyne
4-vinyl-1-cyclohexene
4-vinylcyclohexene
5-chloro-1-pentyne
5-ethylidene-2-norbornene
5-ME-1,3-cyclopentadine
5-methyl-1-hexene

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5-methylene-2-norbornene
5-vinyl-2-norbornene
acetylene
allycyclohexane
benzene
BiCy[2.2.1]hepta-2,5diene
butyne
c-1134-tetraMEcyclopentan
c-1135-tetraMEcyclohexane
c-1-ethyl-3-MEcyclohexane
c-1ME-2propylcyclopropane
cct-1,2,4-triMEcyclopenta
cct-1,3,5-triMEcyclohexan
cct-123-triMEcyclohexane
chlorobenzene
chlorocyclohexane
chlorocyclopentane
chloroethane
cis,trans-2,4-hexadiene
cis-1,2-diethylcyclopropa
cis-1,2-diMEcyclohexane
cis-1,2-diMEcyclopentane
cis-1,2-diMEcyclopropane
cis-1,2-diMEcyclopropane
cis-1,3-diMEcyclohexane
cis-1,3-diMEcyclopentane
cis-1,4-diMEcyclohexane
cis-1-ethyl-2-MEcycloprop
cis-2,2-dimethyl-3-hexene
cis-2-butene
cis-2-heptene
cis-2-hexene
cis-2-methyl-3-hexene
cis-2-octene
cis-2-pentene
cis-3,4dimethyl-2-pentene
cis-3-heptene
cis-3-hexene
cis-3-methyl-2-hexene
cis-3-methyl-2-pentene
cis-3-methyl-3-hexene
cis-3-nonene
cis-3-octene
cis-4,4-diME-2-pentene
cis-4-methyl-2-heptene
cis-4-methyl-2-hexene
cis-4-methyl-2-octene

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cis-4-methyl-2-pentene
cis-4-nonene
cis-4-octene
cis-5-methyl-2-hexene
cis-bicyclo[3.3.0]oct2ene
ctc-1,2,4-triMEcyclopenta
ctct-1234-tetraMEcylclope
ctt-124-triMEcyclohexane
cumene
cycloheptane
cycloheptene
cyclohexane
cyclohexene
cyclooctene
cyclopentane
cyclopentene
ethenylcyclohexane
ethenylcyclopentane
ethylbenzene
ethylcyclohexane
ethylcyclopentane
ethylcyclopropane
ethylene
ethylidenecyclohexane
i-butylcyclopentane
i-propylcyclobutane
i-propylcyclohexane
i-propylcyclopentane
i-propylcyclopropane
isopropylbenzene
isopropylcyclopentane
methylbenzene
methylcycloheptane
methylcyclohexane
methylcyclopentane
methylenecyclobutane
methylenecyclohexane
methylenecyclopentane
m-xylene
n-butylcyclopropane
n-propycyclopentane
n-propylcyclohexane
o-xylene
pentylcyclopropane
phenylacetylene
propene
propyne

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p-xylene
s-butylcyclopropane
styrene
t-1,1,3,4-tetraMEcyclopen
t-1,2-diethylcyclopentane
t-1-ethyl-2-ME-cyclohexan
t-1-ethyl-2-MEcyclopentan
t-1-ethyl-4-MEcyclohexane
toluene
trans,trans-2,4-hexadiene
trans-1,2-dichloroethene
trans-1,2-diMEcyclohexane
trans-1,2diMEcyclopentane
trans-1,2-diMEcylohexane
trans-1,3-diMEcyclohexane
trans-1,3diMEcyclopentane
trans-1,4-diMEcyclohexane
trans-1-Me-1,3-pentadiene
trans-2,2-diME-1-hexene
trans-2,5-diME-3-hexene
trans-2-butene
trans-2-heptene
trans-2-hexene
trans-2-methyl-3-hexene
trans-2-octene
trans-2-pentene
trans-3,4dimethyl2pentene
trans-3-heptene
trans-3-hexene
trans-3-methyl-2-hexene
trans-3-methyl-2-pentene
trans-3-methyl-3-hexene
trans-3-nonene
trans-3-octene
trans-4,4dimethyl2pentene
trans-4-methyl-2-heptene
trans-4-methyl-2-hexene
trans-4-methyl-2-octene
trans-4-methyl-2-pentene
trans-4-nonene
trans-4-octene
trans-5-methyl-2-hexene
trichloroethene
trichloromethane
vinylcyclohexane
vinylcyclopentane

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C1
C2
C3
C4
C5
C6
C7
C8
C9

References for both:
C1-C9 & C9-21 Libraries
HRCC 85 Vol 8 230-242
Hayes & Pitzer
HRCC 82 Vol 10 461-463
Bermejo et al
HRCC 88 Vol 11 649-660
Laub & Purnell
HRCC 83 Vol 6 328-330
HRCC 84 Vol 7 542-544
Lubeck & Sutton
HRCC 92 Vol 15 105-120
White, Hackett etal
HRCC 85 Vol 8 230-242

Library : All-1 Petroleum C9-C21
Phase : 100%MethylSilicone
Copyright : All

(1,1-diMEethyl)benzene
(1-MEethyl)benzene
(1-MEethyl)cyclohexane
(1-methylbutyl)benzene
(1-methylpropyl)benzene
(2-MEbutyl)cyclohexane
(2-MEpropyl)cyclohexane
(2-methylpropyl)benzene
(c)-decalin
(t)-decaline
1-(1-MEethyl)cyclohexene
1,1-diMEcyclooctane
1,2,3,4-tetrahydronaphtha
1,2,3,4-tetramethylbenzen
1,2,3,5-tetramethylbenzen
1,2,3-triethylbenzene
1,2,3-triMEbenzene

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1,2,3-trimethylbenzene
1,2,4,5-tetramethylbenzen
1,2,4-triethylbenzene
1,2,4-trimethylbenzene
1,2-diethylbenzene
1,2-dihexylbenzene
1,2-dihydronaphthalene
1,2-dihydronapthalene
1,2-di-isopropylbenzene
1,2-diME-4-ethylbenzene
1,2-diME4ethylbenzene
1,2-dimethyl-1-octene
1,2-dimethyl-3-ethylbenze
1,2-dimethylnaphthalene
1,2-dimethylnapthalene
1,2-diphenylmethane
1,3,5-triethylbenzene
1,3,5-tri-isopropylbenzen
1,3,5-trimethylbenzene
1,3,7-trimethylnaphthalen
1,3-dichlorobenzene
1,3-diethylbenzene
1,3-di-isopropylbenzene
1,3-diME-2-ethylbenzene
1,3-diME3ethylbenzene
1,3-diME-4-ethylbenzene
1,3-diME-5-tert-butylbenz
1,3-dimethyl-2-ethylbenze
1,3-dimethylnaphthalene
1,3-dimethylnapthalene
1,3-di-vinylbenzene
1,4-dichlorobenzene
1,4-diethylbenzene
1,4-di-isopropylbenzene
1,4-dimethyl-2-ethylbenze
1,4-dimethylnaphthalene
1,4-dimethylnapthalene
1,4-di-vinylbenzene
1,5-cyclooctadiene
1,5-dimethylnapthalene
1,6-dimethylnapthalene
1,7-dimethylnapthalene
1,8-dimethylnaphthalene
1,8-nonadiyne
11335-pentaMEcyclohexane
1234-tetraMEcyclohexane
1235-tetraMEcyclohexane

1235tetraMEcyclohexane
1358tetramethylnaphthalen
13dimethyl5ethylbenzene
1-B-2-benzene
1-butyltetralin
1-chloro-2-methylbenzene
1-chloro-3-methylbenzene
1-chloroheptane
1-decene
1-decyne
1-dodecene
1-ethyl-2-butylbenzene
1-ethyl-2-hexylbenzene
1-ethyl-2-isopropylbenzen
1-ethyl-2-methyl-benzene
1-ethyl-2-methylbenzene
1-ethyl-2-n-propylbenzene
1-ethyl-2-octylbenzene
1-ethyl-2-pentylbenzene
1-ethyl-3-isopropylbenzen
1-ethyl-3-methylbenzene
1-ethyl-3-n-propylbenzene
1-ethyl-4-isopropylbenzen
1-ethyl-4-methylbenzene
1-ethyl-4-n-propylbenzene
1-ethyldecalin 1
1-ethyldecalin 2
1-ethyldecalin 3
1-ethyldecalin 4
1-ethylnaphthalene
1-ethylnapthalene
1-ethyltetralin
1-iso-butylnaphthalene
1ME-1-n-ethylcyclopentane
1-ME-2-butylcyclohexane
1-ME-2-ethylbenzene
1-ME-2-isopropylbenzene
1-ME-2-n-butylbenzene
1-ME-2n-propylbenzene
1-ME-3,5-diethylbenzene
1-ME-3-isopropylbenzene
1-ME-3-n-butylbenzene
1-ME-3n-propylbenzene
1-ME-4-ethylbenzene
1-ME-4-isopropylbenzene
1-ME-4-n-butylbenzene
1-ME-4n-propylbenzene

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1-ME-4-tert-butylbenzene
1ME-cis2-ethylcyclopentan
1-ME-cis2-Prcyclopentane
1ME-cis3-ethylcyclopentan
1-menthene
1-methyl-2-heptylbenzene
1-methyl-2-hexylbenzene
1-methyl-2-nonylbenzene
1-methyl-2-pentylbenzene
1methyl3isopropylbenzene
1-methyl-4-ethyl-benzene
1-methyl-4-propylbenzene
1-methyldecalin 1
1-methyldecalin 2
1-methyldecalin 3
1-methyldecalin 4
1-methyl-indane
1-methylnaphtalene
1-methylnaphthalene
1-methylnapthalene
1-methyltetralin
1ME-trans2-ethylcyclopent
1ME-trans3-ethylcyclopent
1-n-butylnaphthalene
1-nonyne
1-n-propylnaphthalene
1-phenyl-1-butyne
1-phenyl-2-butene
1-propyl-2-hexylbenzene
1-propyl-2-pentylbenzene
1-propyltetralin
1-t-butyl-3,5-diMEbenzene
1-t-butyl-3-MEbenzene
1-t-butyl-4-ethylbenzene
1-t-butyl-4-MEcyclohexane
1-tetradecene
1-tridecene
1-undecene
1-undecyne
2,10-dimethylundecane
2,2,3,4-tetraMEpentane
2,2,3-trimethyloctane
2,2,6,6-trimethylheptane
2,2,7,7-tetramethyloctane
2,2-dimethyldecane
2,2-dimethylnonane
2,2-dimethyloctane

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2,2-dimethylundecane
2,3,4,5-tetramethylhexane
2,3,5-trimethylnaphthalen
2,3,6-triMEnaphthalene
2,3,6-trimethylnaphthalen
2,3-dihydro-indane
2,3-diME-1-ethylbenzene
2,3-dimethyl-2-octene
2,3-dimethyldecane
2,3-dimethylnaphthalene
2,3-dimethylnapthalene
2,3-dimethylnonane
2,3-dimethyloctane
2,3-dimethylundecane
2,4-diME-2,3-diethylhexan
2,4-diME-2,3-isopropylpen
2,4-dimethylnonane
2,4-dimethyloctane
2,4-dimethylstyrene
2,4-dimethylundecane
2,5-dimethylnonane
2,5-dimethylstyrene
2,5-dimethylundecane
2,6-dimethyldecane
2,6-dimethylnaphthalene
2,6-dimethylnapthalene
2,6-dimethyloctane
2,6-dimethylstyrene
2,6-dimethylundecane
2,7-dimethylnaphthalene
2,7-dimethylnapthalene
2,7-dimethyloctane
2,7-dimethylundecane
2,8-dimethylundecane
2,9-dimethylundecane
2233-tetraMEpentane
2244688-heptamethylnonane
22466-pentamethylheptane
2-ethyldecalin 1
2-ethyldecalin 2
2-ethyldecalin 3
2-ethyldecalin 4
2-ethylnaphthalene
2-ethylnapthalene
2-ethyltoluene
2-iso-butylnaphthalene
2-iso-propylnaphthalene

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2-isopropylnapthalene
2-methyl-1-nonene
2-methyl-2-nonene
2methyl3ethylheptane
2-methyldecalin 1
2-methyldecalin 2
2-methyldecalin 3
2-methyldecalin 4
2-methyldecane
2-methylhexadecane
2-methylindene
2-methylnaphthalene
2-methylnapthalene
2-methylnonane
2-methylpentadecane
2-methyltetradecane
2-methyltridecane
2-methylundecane
2-n-butylnaphthalene
2-n-propylnaphthalene
2-phenyloxylene
2-propenylbenzene
2-sec-butylnaphthalene
2-tert-butylnaphthalene
2-vinylnaphthalene
3,3,4,4-tetramethylhexane
3,3,5-trimethylheptane
3,3-dimethyloctane
3,4,5-trimethylheptane
3,4-dimethylhexane
3,4-dimethyloctane
3,4-dimethylundecane
3,5-dimethyloctane(1)
3,5-dimethyloctane(2)
3,5-dimethylundecane
3,6-dimethyloctane(1)
3,6-dimethyloctane(2)
3-ethylnonane
3-ethyloctane
3-ethyltoluene
3-methyl-3-ethylheptane
3-methyl-4-ethyloctane
3-methyl-biphenyl
3-methyldecane
3-methyldodecane
3-methylnonane
3-methylpentadecane

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3-methyltetradecane
3-methyltridecane
3-methylundecane
3-phenyl-octane
4,4-dimethyloctane
4,5-diethyloctane
4,5-diME-2,3-diethylhexan
4,5-dimethylundecane
4,6-dimethylundecane
4ethyl-5methylnonane
4-ethylnonane
4-ethyloctane
4-ethyltoluene
4-iso-propylheptane
4-methyl-biphenyl
4-methyldecane
4-methyldodecane
4-methylnonane
4-methyltetradecane
4-methyltridecane
4-methylundecane
4-phenyl-1-butyne
4-phenyl-2-butene
4-phenyl-octane
4-propylheptane
5,6-dimethyldecane
5,6-dimethylundecane
5,7-dimethylundecane
5-butylindan
5-ethylindan
5-ethylnonane
5-ME-3-ethylheptane
5-methyldecane
5-methyldodecane
5-methylindan
5-methylindane
5-methylnonane
5-methyltetradecane
5-methylundecane
5-propylindan
6-methylpentadecane
6-methylundecane
9,10-dihydroanthracene
9,10-dihydrophenanthrene
acenaphthene
allylbenzene
alpha-methylstyrene

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anthracene
BCY[4.3.0]nona3,6(1)diene
beta-methylstyrene
bicyclo[4.3.0]nona3,6dien
bicyclopentadiene
biphenyl
butylbenzene
butylcyclohexane
butylcyclopentane
c-1,3-diMEcyclooctane
c-1,5-diMEcyclooctane
c-1-ME-4-(1-MEethyl)CYhex
c-5ETideneBI[221]hept2ene
cis-1,2-diMEcyclooctane
cis-1,4-diMEcyclooctane
cis-1-ME-2-propylbenzne
cis-2-decene
cis-2-nonene
cis-2-undecene
cis-3-decene
cis-4-decene
cis-4-methyl-2-nonane
cis-5-decene
cis-cyclodecene
cis-decalin
cis-hydindane
cis-octahydro-1H-indene
cyclodecane
cyclododecane
cyclononane
cyclooctane
cycloundecane
decylbenzene
decylcyclohexane
dibenzofuran
dicylohexyl
dipentene
diphenyl
diphenylmethane
durene
endo-dicyclopentadiene
ethenylcyclooctane
ethylcyclooctane
fluorene
heptylbenzene
heptylcyclohexane
hexamethylbenzene

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hexylbenzene
hexylcyclohexane
indan
indane
indene
isobutylbenzene
iso-butylcyclohexane
isodurene
iso-pentylbenzene
iso-propylcyclopentane
isotetralin
limonene
m-allytoluene
m-diethylbenzene
m-divinylbenzene
methylcyclodecane
methylcyclododecane
methylcyclononane
methylcyclooctane
methylcycloundecane
methyldodecane
m-ethyltoluene
m-ethylvinylbenzene
m-ME-styrene
m-methylstyrene
mycrene
naphthalene
n-butylbenzene
n-butylcyclohexane
n-butylcyclopentane
n-decylbenzene
neopentylbenzene
n-ethylcyclopentane
n-heptylbenzene
n-hexylbenzene
n-octylbenzene
nonylbenzene
nonylcylohexane
n-pentylbenzene
n-propybenzene
n-propylbenzene
o-allytoluene
octahydroanthracene
octahydrophenanthrene
octylbenzene
octylcyclohexane
o-diethylbenzene

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o-divinylbenzene
o-ethyltoluene
o-ethylvinylbenzene
o-ME-styrene
o-methylstyrene
p-allytoluene
p-cymene
p-diethylbenzene
pentachloroethane
pentacyclopentane
pentamethyl-benzene
pentylbenzene
pentylcyclohexane
perhydro2,3benzanthrace 1
perhydro2,3benzanthrace 2
perhydroacenaphthene 1
perhydroacenaphthene 2
perhydroacenaphthene 3
perhydroacenaphthene 4
perhydroacenaphthene 5
perhydroacenaphthene 6
perhydroanthracene 1
perhydroanthracene 2
perhydroanthracene 3
perhydroanthracene 4
perhydroanthracene 5
perhydrochrysene 1
perhydrochrysene 2
perhydrochrysene 3
perhydrochrysene 4
perhydrochrysene 5
perhydrochrysene 6
perhydrochrysene 7
perhydrofluorene 1
perhydrofluorene 2
perhydrofluorene 3
perhydrophenanthrene 1
perhydrophenanthrene 2
perhydrophenanthrene 3
perhydrophenanthrene 4
perhydrophenanthrene 5
perhydrophenanthrene 6
perhydrophenanthrene 7
perhydrophenanthrene 8
perhydrophenanthrene 9
perhydropyrene 1
perhydropyrene 2

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perhydropyrene 3
perhydropyrene 4
perhydropyrene 5
perhydropyrene 6
perhydropyrene 7
perhydropyrene 8
perhydropyrene 9
p-ethyltoluene
p-ethylvinylbenzene
phenanthrene
phenyl-1-cyclohexene
phenylcyclohexane
phenylcyclopentane
p-ME-styrene
p-methylstyrene
propylbenzene
propylcyclohexane
p-tert-butyltoluene
pyrene
s-butylcyclohexane
sec-butylbenzene
sec-ethylcyclopentane
t-1,2-diMEcyclooctane
t-1-ME-2-propylcyclohexan
t-1-ME-4-(1-MEethyl)CYhex
t-decalin
tert-1135tetraMEcyclohexa
tert-butylbenzene
tert-butylcyclohexane
tert-pentylbenzene
tetralin
trans-1,3-diMEcyclooctane
trans-1,4-diMEcyclooctane
trans-1,5-diMEcyclooctane
trans-1-phenyl-1-butene
trans-2-decene
trans-2-nonene
trans-2-undecene
trans-3-decene
trans-4-decene
trans-4-methyl-2-nonane
trans-5-decene
trans-decalin
trans-hydrindane
trans-octahydro-1H-indene
undecylbenzene

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C9
C10
C11
C12
C13
C14
C15
C16
C17
C18
C21

Library : All-5 Petroleum
Phase : 5%Phenyl 95%Methyl
Copyright : All

(-)-a-cedrene
1,1,2trimethylcyclohexane
1,1,3trimethylcyclohexane
1,1,4trimethylcyclohexane
1,12trimethylcyclopentane
1,13trimethylcyclopentane
1,1-dimethylcyclohexane
1,1-dimethylcyclopentane
1,2,3-trimethylbenzene
1,2,4-trimethylbenzene
1,3,5-trimethylbenzene
1,3-cyclopentadiene
1,4-diethylbenzene
1,4-dimethylnaphthalene
1,5,9-cyclododecatriene
123-trimethylcyclohexane
1358tetramethylnaphthalen
13dimethyl5ethylbenzene
1-butene
1-butyltetralin
1C2C3trimethylcyclopentan
1C2-dimethylcyclohexane
1-c2-dimethylcyclopentane
1C2T3trimethylcyclopentan
1C2T4trimethylcyclopentan
1C3-dimethylcyclopentane
1C3dimethylcyclopentane
1C4-dimethylcyclohexane
1Cdimethylcyclopentane
1-decene

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1-dodecene
1-ethyl-3-methylbenzene
1-ethylcyclopentene
1-ethylnnaphthalene
1-ethyltetralin
1-heptene
1-hexene
1methyl1,3cyclopentadiene
1methyl1ethylcyclopentane
1methyl3isopropylbenzene
1methyl4propylbenzene
1methylC2ethylcyclopentan
1methylC3ethylcyclopentan
1-methylcyclohexene
1-methylcyclopentene
1-methylcylcopentene
1-methylnaphthalene
1methylT2ethylcyclopentan
1methylT3ethylcyclopentan
1-methyltetralin
1-nonene
1-octene
1-pentene
1-propyltetralin
1T2C3trimethylcyclopentan
1T2C4trimethylcyclopentan
1T2dimethylcyclopentane
1T3-dimethylcyclohexane
1T3dimethylcyclopentane
1T4-dimethylcyclohexane
1-tetradecene
1-tridecene
1-undecene
2,2,3,3-tetramethylbutane
2,2,3,3tetramethylpentane
2,2,3,4tetramethylpentane
2,2,3-trimethylbutane
2,2,3-trimethylhexane
2,2,3-trimethylpentane
2,2,4,4tetramethylpentane
2,2,4-trimethylhexane
2,2,4-trimethylpentane
2,2,5-trimethylhexane
2,2,7,7-tetramethyloctane
2,2-dimethylbutane
2,2-dimethylheptane
2,2-dimethylhexane

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2,2-dimethyloctane
2,2-dimethylpentane
2,3,3,4tetramethylpentane
2,3,3-trimethyl-1-butene
2,3,3-trimethylhexane
2,3,3-trimethylpentane
2,3,4-trimethylhexane
2,3,4-trimethylpentane
2,3,5-trimethylhexane
2,3-dimethyl-1-butene
2,3-dimethyl-1-hexene
2,3-dimethyl-1-pentene
2,3-dimethyl-2-butene
2,3-dimethyl-2-pentene
2,3-dimethylbutane
2,3-dimethylheptane
2,3-dimethylhexane
2,3-dimethyloctane
2,3-dimethylpentane
2,4,4-trimethylhexane
2,4,6-trimethylheptane
2,4-dimethyl-1-pentene
2,4-dimethyl-2-pentene
2,4dimethyl3ethylpentane
2,4-dimethylbutane
2,4-dimethylheptane
2,4-dimethylhexane
2,5-dimethyl-2-hexene
2,5-dimethylheptane
2,5-dimethylhexane
2,5-norbornadiene
2,6-dimethylheptane
2,6-dimethyloctane
2,7-dimethyloctane
22,4,66pentamethylheptane
2244688-heptamethylnonane
2-ethyl-1-butene
2-ethyl-1-pentene
2-ethyl-3-methyl-1-butene
2-ethyltoluene
2methyl1,3cyclopentadiene
2-methyl-1-butene
2-methyl-1-heptene
2-methyl-1-hexene
2-methyl-1-pentene
2-methyl-2-butene
2-methyl-2-heptene

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2-methyl-2-hexene
2-methyl-2-pentene
2methyl3ethylheptane
2-methyl-3-ethylpentane
2-methyl-cis-3-hexene
2-methyldecane
2-methylheptane
2-methylhexadecane
2-methylhexane
2-methylnonane
2-methyloctane
2-methylpentadecane
2-methylpentane
2-methylpropene
2-methyltetradecane
2-methyl-trans-3-hexene
2-methyltridecane
2-methylundecane
2-norbornadiene
3,3,4-trimethylhexane
3,3-diethylpentane
3,3-dimethyl-1-butene
3,3-dimethyl-1-pentene
3,3-dimethylheptane
3,3-dimethylhexane
3,3-dimethyloctane
3,3-dimethylpentane
3,4,5-trimethylheptane
3,4-dimethyl-1-hexene(1)
3,4-dimethyl-1-hexene(2)
3,4-dimethyl-1-pentene
3,4dimethyl-cis-2-pentene
3,4-dimethylheptane(1)
3,4-dimethylheptane(2)
3,4-dimethylhexane
3,4-dimethylhexane(1)
3,4-dimethylhexane(2)
3,4dimethyl-trans2pentene
3,5-dimethylheptane(1)
3,5-dimethylheptane(2)
3,5-dimethyloctane(1)
3,5-dimethyloctane(2)
3,6-dimethyloctane(1)
3,6-dimethyloctane(2)
3-ethyl-1-pentene
3-ethyl-2-pentene
3-ethyl-3-methylpentane

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3-ethylcyclopentene
3-ethylheptane
3-ethylhexane
3-ethylnonane
3-ethyloctane
3-ethylpentane
3-ethyltoluene
3-methyl-1-butene
3-methyl-1-hexene
3-methyl-1-pentene
3-methyl-3-ethylheptane
3-methyl-3-ethylpentane
3-methyl-cis-2-hexene
3-methyl-cis-2-pentene
3-methyl-cis-3-hexene
3-methylcyclohexene
3-methylcyclopentene
3-methyldecane
3-methyldodecane
3-methylheptane
3-methylhexane
3-methylnonane
3-methyloctane
3-methylpentadecane
3-methylpentane
3-methyltetradecane
3-methyl-trans-2-hexene
3-methyl-trans-2-pentene
3-methyl-trans-3-hexene
3-methyltridecane
4,4-dimethyl-1-pentene
4,4dimethyl-cis-2-pentene
4,4-dimethylheptane
4,4-dimethyloctane
4,4dimethyl-trans2pentene
4-ethylheptane
4-ethyloctane
4-ethyltoluene
4-methyl-1-hexene
4-methyl-1-pentene
4-methyl-cis-2-hexene
4-methyl-cis-2-pentene
4-methylcyclohexene
4-methyldecane
4-methyldodecane
4-methylheptane
4-methylnonane

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4-methyloctane
4-methyltetradecane
4-methyl-trans-2-hexene
4-methyl-trans-2-pentene
4-methyltridecane
4-methylundecane
4-propylheptane
4-vinylcyclohexene
5-butylindan
5-ethylidene-2-norbornene
5-ethylindan
5-methyl-1-hexene
5-methyl-cis-2-hexene
5-methyldecane
5-methyldodecane
5-methylene-2-norbornene
5-methylindan
5-methylnonane
5-methyltetradecane
5-methyl-trans-2-hexene
5-methylundecane
5-propylindan
5-vinyl-2-norbornene
6-methylpentadecane
benzene
bicyclo[4.3.0]nona3,6dien
butylbenzene
butylcyclohexane
c-1,3-dimethylcyclohexane
c-decalin
cis-2-butene
cis-2-heptene
cis-2-hexene
cis-2-octene
cis-2-pentene
cis-3-heptene
cis-3-hexene
cis-3-octene
cis-4-octene
cis-bicyclo[3.3.0]oct2ene
cis-cyclodecene
cumene
cyclohexane
cyclohexene
cyclopentane
cyclopentene
decylbenzene

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decylcyclohexane
endo-dicyclopentadiene
ethylbenzene
ethylcyclohexane
ethylcyclopentane
ethylidenecyclohexane
heptylbenzene
heptylcyclohexane
hexylbenzene
hexylcyclohexane
indan
isobutylbenzene
isopropylcyclopentane
methylbenzene
methylcyclohexane
methylcyclopentane
methylenecyclohexane
methylenecyclopentane
m-xylene
naphthalene
n-butylcyclopentane
neopentylbenzene
nonylbenzene
nonylcylohexane
n-propylbenzene
n-propylcyclohexane
octylbenzene
octylcyclohexane
o-xylene
pentylbenzene
pentylcyclohexane
propylbenzene
propylcyclohexane
p-tert-butyltoluene
p-xylene
sec-butylbenzene
t-decalin
tert-butylbenzene
tert-pentylbenzene
tetralin
toluene
trans-2-butene
trans-2-heptene
trans-2-hexene
trans-2-octene
trans-2-pentene
trans-3-heptene

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trans-3-hexene
trans-3-octene
trans-4-octene
undecylbenzene
vinylcyclohexane

C3
C4
C5
C6
C7
C8
C9
C10
C11
C12
C13
C14
C15
C16
C17
C18

References:

HRCC 1984
Vol 6 542-544
Vol 6 38-330
Lubeck & Sutton

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Pro ezGC® Thermodynamic Retention Index Database - Solvents and Chemicals

Library : Industrial Solvents
Phases : Rtx-1, Rtx-502.2, Stabilwax
Copyright : Restek Corp.

Group 1 - alcohols, aldehydes, ketones

acetone
tert-amyl alcohol
benzyl acetone
benzyl alcohol
2,3-butanediol
1-butanol
2-butanol
2-butanone (MEK)
3-buten-1-ol
cis-2-buten-1-ol
3-buten-2-ol
2-butenal(crotonaldehyde)
2-butoxyethanol
2-(2-butoxyethoxy)ethanol
tert-butyl alcohol
butyrolactone
crotonaldehyde(2-butenal)
cyclohexanone
cyclopentanol
cyclopentanone
decanal
decane
1-decanol
2-decanol
2-decanone
diacetone alcohol
2,2-dimethyl-1-pentanol
2,2-dimethyl-1-propanol
2,4-dimethyl-2-pentanol
2,4-dimethyl-3-pentanol
2,4-dimethyl-3-pentanone

Analytical Innovations Innovative Solutions for Analytical Chemistry
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2,6-dimethyl-4-heptanone
2,2-dimethyl-3-pentanol
docosane
dodecane
1-dodecanol
2-dodecanone
eicosane
ethanol
2-ethoxyethanol
2(2-ethoxyethoxy)ethanol
2-ethyl-1-butanol
2-ethyl-1-hexanol
3-ethyl-3-pentanol
heneicosane
heptadecane
heptanal
heptane
1-heptanol
2-heptanol
4-heptanol
2-heptanone
3-heptanone
4-heptanone
hexadecane
hexanal
hexane
1-hexanol
2-hexanol
3-hexanol
2-hexanone
3-hexanone
trans-2-hexen-1-ol
cis-3-hexen-1-ol
4-hexen-3-one
tetra-hydro-2-furan-metol
4hydroxy4methyl2pentanone
isobutyl alcohol
isobutyraldehyde
isopropyl alcohol
mesityl oxide
methanol
methylethylketone (MEK)
2-methoxyethanol
2(2-methoxyethoxy)ethanol
2-methyl-1-butanol
3-methyl-1-butanol
2-methyl-1-pentanol

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2-methyl-1-propanol
2-methyl-2-butanol
3-methyl-2-butanol
3-methyl-2-butanone
3-methyl-2-buten-1-ol
5-methyl-2-hexanone
4-methyl-2-pentanol
2-methyl2propanol(t-buty)
1-methyl-2-pyrrolidinone
2-methyl-3-buten-2-ol
5-methyl-3-heptanone
2-methyl-3-pentanol
3-methyl-3-pentanol
2-methyl-3-pentanone
4-methyl-2-pentanone
4-methyl-3-penten-2-one
2methylpropanal(isobutyr)
methylisobutylketone MIBK
alpha methylbenzylalcohol
neopentanol (22dimet1pro)
nonadecane
nonanal
nonane
1-nonanol
2-nonanol
2-nonanone
3-nonanone
5-nonanone
octanal
octadecane
octane
1-octanol
2-octanol
2-octanone
3-octanone
pentadecane
pentanal
pentane
1-pentanol
2-pentanol
2-pentanone
3-pentanone
cis-2-penten-1-ol
3-penten-2-one
2-phenoxyethanol
4-phenyl-2-butanone
1,2-propanediol

propanal
1-propanol
2-propanol
2-propanone (acetone)
propargyl alcohol
2-propen-1-ol
propional(propanal)
2-propyn-1-ol(propargyl)
tetradecane
tetraethylene glycol
tricosane
tridecane
triethylene glycol
2,2,2-trifluoroethanol
undecanal
1-undecanol
undecane
2-undecanone
water

Group 2 - aromatics, esters, ethers

allyl acetate
allyl ether
amyl acetate
benzene
benzyl acetate
benzyl ether
bibenzyl
2-butoxyethyl acetate
butyl acetate
tert-butyl acetate
butylbenzene
sec-butylbenzene
tert-butylbenzene
butyl butyrate
butyl ether
butyl propionate
m-cresol
o-cresol
p-cresol
cumene
cymene
cis-decahydronaphthalene
trans-decahydronaphthalen
1,2-diethylbenzene

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1,3-diethylbenzene
1,4-diethylbenzene
diisopropylbenzene
1,2-dimethoxy ethane
1,4-dioxane
1,3-dioxolane
1,2-ethanediol diacetate
1,2-ethanediol monoacetat
2-ethoxyethyl acetate
2-ethoxyethyl ether
ethyl acetate
ethyl acrylate
ethylbenzene
ethyl benzoate
ethyl butyrate
ethyl caproate
ethyl decanoate
ethyl ether
ethyl formate
ethyl hexanoate
ethyl isobutyrate
ethyl-2-methylbutyrate
ethyl pentanoate
ethyl propionate
ethylene glycol diacetate
ethylene glycol monoaceta
hexyl acetate
2-hydroxyethyl acetate
isoamyl acetate
isobutylbenzene
isobutyl acetate
isobutyl isobutyrate
isopropyl acetate
isopropylbenzene
isopropyl butyrate
isopropyl ether
isopropyltoluene
1,2-bis(2-methxyethx)etha
bis2(2metxyetxy)ethlether
2-methoxyethyl acetate
2-methoxyethyl ether
p-methoxyphenol
methyl acetate
methyl benzoate
methyl butyrate
methyl decanoate
methyl ether

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methyl formate
methyl hexanoate
methyl isobutyrate
methyl octanoate
methyl pentanoate
methyl propionate
methyl valerate
alpha-methylstyrene
naphthalene
nitrobenzene
phenol
propyl acetate
propylbenzene
propyl benzoate
propyl butyrate
propyl formate
propyl propionate
pyridine
styrene
tetrahydrofurfuryl acetat
tetrahydro-2-methyl furan
1,2,3,4-tetrahydronaphtha
toluene
triethylbenzene
triethlenglycoldimthether
tetethlenglycoldimthether
1,2,3-trimethylbenzene
1,2,4-trimethylbenzene
1,3,5-trimethylbenzene
vinyl acetate
1,2-xylene
1,3-xylene
1,4-xylene

Methods:
alcohols
aldehydes
ketones
aromatics
esters
ethers

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Pro ezGC® Thermodynamic Retention Index Database - FAMEs

Library : FAMEs
Phases : StabilWax, Rtx-2330
Copyright : Restek Corp.

C4:0
C5:0
C6:0
C7:0
C8:0
C9:0
C10:0
C11:0
C11:1 n1 cis
C12:0
C12:1 n1 cis
C13:0
C13:1 n1 cis
C14:0
C14:1 n5 cis
C14:1 n5 trans
C15:0
C15:1 n5
C16:0
C16:1 n7 cis
C16:1 n7 trans
C16:2 n4 cis
C16:3 n4 cis
C16:4 n1 cis
C17:0
C17:1 n7 cis
C17:1 n7 trans
C18:0
C18:1 n12 cis
C18:1 n12 trans
C18:1 n9 cis
C18:1 n9 trans
C18:1 n7 cis

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C18:1 n7 trans
C18:1 n5 cis
C18:2 n6 cis
C18:2 n6 trans
C18:2 n4 cis
C18:3 n6 cis
C18:3 n4 cis
C18:3 n3 cis
C18:4 n3 cis
C18:4 n1 cis
C19:0
C19:1 n12 cis
C19:1 n9 cis
C19:1 n9 trans
C19:2 n6 cis
C19:2 n6 trans
C20:0
C20:1 n15 cis
C20:1 n11 cis
C20:1 n9 cis
C20:1 n9 trans
C20:1 n7 cis
C20:2 n6 cis
C20:2 n6 trans
C20:3 n6 cis
C20:3 n3 cis
C20:4 n6 cis
C20:4 n3 cis
C20:5 n3 cis
C21:0
C21:1 n9 cis
C21:5 n3 cis
C22:0
C22:1 n11 cis
C22:1 n9 cis
C22:1 n9 trans
C22:2 n6 cis
C22:3 n3 cis
C22:4 n6 cis
C22:5 n6 cis
C22:5 n3 cis
C22:6 n3 cis
C23:0
C23:1 n9 cis
C23:1 n9 trans
C24:0
C24:1 n9 cis

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me butyrate
me valerate
me caproate
me enanthioate
me caprylate
me pelargonate
me caprate
me hendecanoate
me hendecenoate
me laurate
me myristate
me myristoleate
me myristelaidate
me palmitate
me palmitoleate
me palmitelaidate
me margarate
me stearate
me petroselinate
me petroselaidate
me oleate
me elaidate
me vaccenate
me transvaccenate
me linoleate
me linoelaidate
me linolenate
me gamma linolenate
me arachidate
me homogamma linolenate
me arachidonate
me behenate
me erucate
me brassidate
me lignocerate
me nervonate
me butanoate
me pentanoate
me hexanoate
me heptanoate
me octanoate
me nonanoate
me decanoate
me undecanoate
me 10-undecenoate
me dodecanoate
me 11-dodecenoate

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me tridecanoate
me 12-tridecenoate
me tetradecanoate
me 9-tetradecenoate
me 9-transtetradecenoate
me pentadecanoate
me 10-pentadecenoate
me hexadecanoate
me 9-hexadecenoate
me 9-transhexadecenoate
me 9,12-hexadecadienoate
me 6,9,12-hexadecatrienoa
me 6,9,12,15-hexadecatetr
me heptadecanoate
me 10-heptadecenoate
me 10-transheptadecenoate
me octadecanoate
me 6-octadecenoate
me 6-transoctadecenoate
me 9-octadecenoate
me 9-transoctadecenoate
me 11-octadecenoate
me 11-transoctadecanoate
me 13-octadecenoate
me 9,12-octadecadienoate
me 9,12-transoctadecadien
me 11,14-octadecadienoate
me 6,9,12-octadecatrienoa
me 8,11,14-octadecatrieno
me 9,12,15-octadecatrieno
me 6,9,12,15-octadecatetr
me 8,11,14,17-octadecatet
me nonadecanoate
me 7-nonadecenoate
me 10-nonadecenoate
me 10-transnonadecenoate
me 10,13-nonadecadienoate
me 10,13-transnonadecadie
me eicosanoate
me 5-eicosenoate
me 9-eicosenoate
me 11-eicosenoate
me 11-transeicosenoate
me 13-eicosenoate
me 11,14-eicosadienoate
me 11,14-transeicosadieno
me 8,11,14-eicosatrienoat

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me 11,14,17-eicosatrienoa
me 5,8,11,14-eicosatetrae
me 8,11,14,17-eicosatetra
me 5,8,11,14,17-eicosapen
me heneicosanoate
me 12-heneicosenoate
me 6,9,12,15,18-heneicosa
me docosanoate
me 11-docosenoate
me 13-docosenoate
me 13-transdocosenoate
me 13,16-docosadienoate
me 13,16,19-docosatrienoa
me 7,10,13,16-docosatetra
me 4,7,10,13,16-docosapen
me 7,10,13,16,19-docosape
me4,7,10,13,16,19-docohex
me tricosanoate
me 14-tricosenoate
me 14-transtricosenoate
me tetracosanoate
me 15-tetracosenoate
nonane
decane
undecane
dodecane
tridecane
tetradecane
pentadecane
hexadecane
heptadecane
octadecane
nonadecane
eicosane
heneicosane
docosane
tricosane
tetracosane
hexacosane

Methods:
AOCS#1:corn,sunflower oil
AOCS#2:linseed,perilla oi
AOCS#3:peanut,rapeseed oi
AOCS#4:olive,teaseed oils
AOCS#5:coconut,palm kerna
AOCS#6:lard,palm,tallows

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Pro ezGC® Thermodynamic Retention Index Database
Abbreviations used in the Database

1>5 is 1,2,3,4,5
ME is methyl

At beginning of names:
c is cis
t is trans

At end of names:
pr,pro etc is propane
p,pe,pen etc is pentane
he,hex etc is hexane
hep,hept etc is heptane
ben,benz etc is benzene
na,nap etc is napthanlene
ph,phe etc is phenanthrene
ch,chr etc is chrysene
flu,fluo etc is fluorene
qu,qui etc is quinoline
T,Thi etc is thiophene

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