



# GC Optimization Just Got "EZ"er!

- Prices slashed!
- Simplify column selection.
- Reduce analysis times and improve sample resolution.
- Optimize dual column run conditions.
- Master Library Set now included FREE!

Many analysts are following methods or using columns and run conditions they know could be optimized. But, who has time to make the hundreds of injections necessary to optimize the temperatures, ramp rates, flow rates, pressures, and column

parameters to get the perfect chromatogram? No one!

Let *Pro ezGC*™ for Windows® do the work for you. *Pro ezGC*™ for Windows® makes GC optimization a breeze. By using a computer algorithm to predict thermodynamic retention indices for sample components, the software predicts the best combinations of column dimensions, temperature program, and flow conditions for your analysis. It can decrease your analysis time and help you obtain key separations for single column, dual column, and dual detector analyses. What could be easier?

*Pro ezGC*™ for Windows™ is now more affordable than ever. In addition to the lower price, Restek is now including the entire Master Set of Retention Index Libraries at no extra charge! These libraries contain more than 3000 compounds on the most commonly used stationary phases in 10 different application areas including: pesticides, PCBs, flavor &

fragrance compounds, drugs of abuse, FAMES, semi-volatile pollutants, volatile pollutants, and solvents & chemicals.

*Pro ezGC* will save you time and money by greatly enhancing your productivity and increasing sample throughput. Take advantage of this powerful GC optimization tool today!

## Prices Reduced!

Pro ezGC for Windows, Cat.# 21487  
Upgrade Pro ezGC version 1.5 (DOS) to  
Pro ezGC for Windows, Cat.# 21486  
Pro ezGC Ver.1.5 for DOS, Cat.# 21481



# THE RESTEK

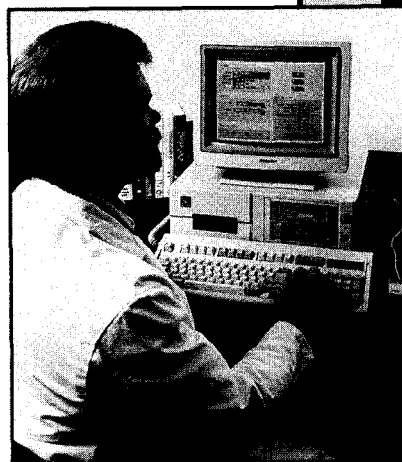
## ADVANTAGE

### Sneak Preview! ezGC™ Software Simplifies GC Method Development

- Saves time and money by reducing analysis times and improving sample resolution.
- Automatically determines optimum temperature program rates and column flow rates.
- Works with constant flow, constant pressure, or electronic pressure/ flow programming.
- Visually demonstrates changes in resolution when the column parameters and operating conditions are changed.
- Easy to use, mouse driven software with built in help menus.
- Takes the guesswork out of capillary column selection.
- Easy to install and works on all DOS operating systems with 5 12K of free RAM.
- Costs about the same as a 30-meter column.

Did you ever work with a chromatographer who seems to know how to pick the best temperature program and flow conditions? After years and years of experience they seem to inherently know which GC parameters work best. They have learned how parameters such as temperature, flow, and distribution coefficients affect a separation. Why wait years? Use ezGC™ and quickly become a master at capillary column selection and optimization.

**Before ezGC™**  
*time consuming GC  
method development  
guesswork*



**After ezGC™**  
*accurate predictions of  
GC separations in  
minutes*

#### In this Issue...

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Even experienced chromatographers will benefit by using ezGCTM. Restek's applications department was hard at work trying to optimize the temperature program rate for the 60 compounds in EPA Method 502.2. They tried 4, 10, 12, and 16°C/min., but there were so many compounds that new coelutions occurred at each temperature program ramp. The separations were so complex that they couldn't figure out whether faster or

slower program rates were better. After several frustrating days of working on the project, they tried ezGC™. They entered the retention times into the ezGC™ program and let the software do the optimization. ezGC™ predicted 7S°C/min. as the optimum temperature program rate and printed a simulated chromatogram illustrating the expected separations. They were impressed but still not convinced. Actual chromatograms were then generated at 7 and 8°C/min., but only 7S°C gave the best separation, just as the program predicted. Now our applications department is so convinced of the power of ezGC™ that they use it for all optimization work.

You can save time and money in your laboratory by using ezGC™ to optimize all your analyses. If you have a simple analysis with no coelutions, you can use the software to predict the fastest temperature program and flow conditions while

maintaining baseline resolution (R2 1.5). And, if your sample contains compounds which may switch elution orders at the new optimized conditions, ezGC will list the new elution order.

Did you ever wonder how your sample would look on a different film thickness? If you are using a 0.25um film and you suspect that a 0.5um film would improve resolution, use ezGC to print a simulated chromatogram with the 0.5um film. In fact, you can try any other film thickness and ezGC will provide simulated chromatograms at optimized run conditions. How about a longer length or different inside diameter? Enter the desired column dimensions into the ezGC program and it will provide a simulated chromatogram for visual examination. Now you don't have to waste your time or money buying experimental columns to optimize your analysis, ezGC can do it for you.

How does ezGC work?

In the past 20 years, several attempts have been made to predict retention and elution in gas chromatography. Initially, elution order was predicted by Kovats indices (1). However, Kovats indices are restricted to isothermal conditions. With the increasing use of temperature programming, Kovats indices were not applicable in many situations. A modified retention index equation was developed by Van den Dool and Kratz<sup>2</sup> that incorporated Kovats indices into temperature programming. This modified retention index works relatively well, as was demonstrated in *The Restek Advantage* (January 1992). However, neither the Kovats or Van den Dool and Kratz methods account for changes in carrier gas viscosity, linear velocity, film thickness, etc. Recently, advances have been made in developing a more sophisticated method to predict GC behavior. Several researchers, Dose<sup>3</sup>; Curvers and Rijks<sup>4</sup>; and Snow and McNair<sup>5</sup> have contributed to a method for calculating temperature programmed or isothermal retention from thermodynamic parameters. The distribution coefficient *K*, is

related to the Gibbs free energy of gases in solution by the following equation:

$$AG = RT \ln K_D \text{ and since } AG = AH - TAS$$

substituting  $K_D = k * \beta$ , the following equation can be derived:

$$\ln k = \left( \frac{\Delta H}{R} \right) * \left( \frac{1}{T} \right) + \ln \left( \frac{a}{\beta} \right)$$

where

$$a = \left( \frac{\Delta S}{R} \right)$$

This new equation is in the form of  $y = mx + b$  where  $\frac{\Delta H}{R}$  is the slope of the line and the quantity  $\ln(a/\beta)$  is the y intercept. The ezGC software incorporates these fundamental concepts into a computer algorithm that makes it possible to accurately predict GC retention times routinely to within 2 %.

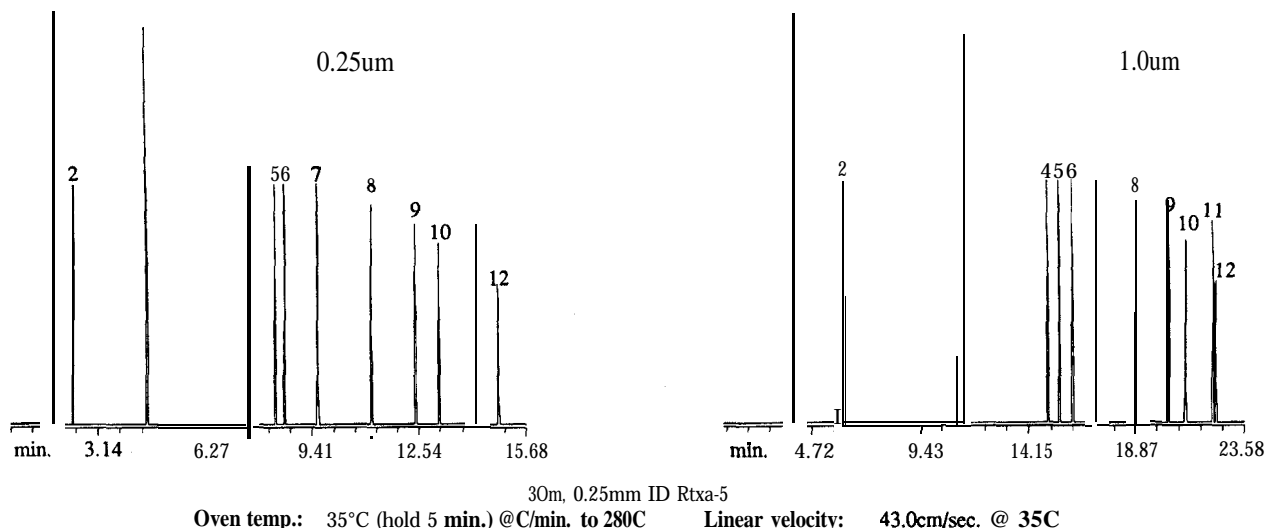
How hard is it to use ezGC?

By following a few simple steps, optimum operating conditions can easily be predicted for any analysis. To utilize ezGC simply obtain an accurate dead time and run your sample at fast and slow temperature program ramps. Enter the retention times for both runs in the program and you are ready to try new temperature program rates, flow rates, column IDs, film thicknesses, or column lengths. An on-line help manual is available at any time to answer questions, and in those rare cases when you need extra help, experienced Restek technical service chemists will be available to assist you with your more detailed questions.

Ways to generate optimum conditions

Optimum temperature programmed run conditions can be generated two ways. In one case, a specific set of GC conditions is entered and under those conditions, the ezGC program will predict the retention times of the components.

Figure 1 - ezGC quickly predicts actual peak resolution when increasing the film thickness from 0.25 to 1.0um when using the same temperature program.



**Table I - Comparison of Experimental vs. Calculated Retention Times**

#	Component Name	Exp. tR (min.)	Calc. tR (min.)	Exp. Calc. Error (min.)	(Exp.-Calc.) /Exp. % Error (min.)
1	hexane	3.891	3.900	-0.009	-0.2
2	benzene	6.032	6.117	-0.085	-1.4
3	toluene	11.001	11.076	-0.075	-0.7
4	chlorobenzene	15.002	14.991	0.011	0.1
5	ethylbenzene	15.500	15.495	0.005	0.0
6	m-xylene	16.184	16.059	0.125	0.8
7	styrene	17.395	17.129	0.266	1.5
8	isopropylbenzene	19.082	18.861	0.221	1.2
9	n-propylbenzene	20.517	20.345	0.172	0.8
10	1,3,5-trimethylbenzene	21.202	21.07	0.131	0.6
11	tert-butylbenzene	22.385	22.259	0.126	0.6
12	decane	22.501	22.364	0.137	0.6
Average error 0.7					

Predicted results can be viewed in either a table format or a computer simulated chromatogram. Figure 1 shows simulated chromatograms demonstrating how the analysis would look if the stationary phase film thickness was increased from 0.25 to 1.0µm with the same program conditions. The 30m, 1.0µm film thickness increases the analysis times from approximately 14 to 22 minutes. Figure 2 shows the predicted optimum temperature program ramp for the 5m, 11.0µm column to maximize resolution and minimize analysis times. Baseline resolution is obtained in under 6 minutes with the 5m column.

Another way to generate the optimum conditions is by entering a range of desirable temperature program conditions into the program. The optimum conditions, yielding the shortest analysis time with the best resolution, will be listed first with other possibilities listed sequentially. Computing time varies with the number of permutations requested.\*

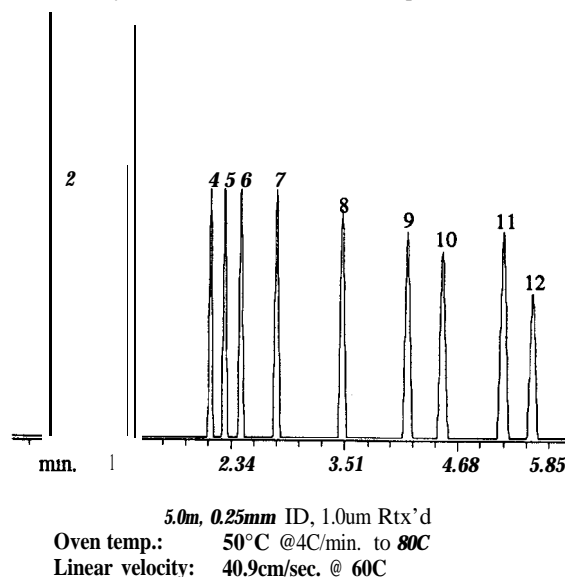
#### Quickly compare differences in analysis and resolution changes when varying linear velocity, ID, film thickness, length, or theoretical plates

ezGC permits a visual comparison of analysis times and resolution when column parameters such as linear velocity (including electronic pressure or flow programming), column diameter, theoretical plates, film thickness, and/or the column length are varied. Table I shows the predicted vs. actual retention times for a 1.0µm Rtx-5 using data generated on a 0.25µm capillary column. The absolute error is approximately 2%.

#### ezGC simplifies method development

ezGC greatly reduces the workload of GC method development. It also insures the best resolution and analysis time conditions for existing methods. This versatile program allows any parameter or combination of parameters to be changed and

**Figure 2 - ezGC predicts the optimum resolution and fastest analysis times with a 5.0m, 1.0µm column.**



quickly viewed in either a table format or simulated chromatogram. ezGC can be installed on any IBM PC or compatible system with a hard drive and 512K of free memory.

After reading about ezGC, you may ask, "How could method development be easier?" The answer is, by having Restek generate thousands of thermodynamic retention index libraries on volatile organics, industrial solvents, pharmaceutical compounds, and flavors/fragrances using a wide variety of bonded phases. Restek has dedicated a large portion of our application chemists' time towards generating extensive libraries that interface to ezGC. See the July 1993 issue of The Restek Advantage for information on Restek's thermodynamic retention index libraries. ■

#### References

- (1) Kovzits, E., Giddings, J.C., and Keller, R.A., *Advances in Chromatography*, Volume 1, Chapter 7. New York: Marcel Dekker (1965).
- (2) Van den Dool, H. and Kratz, P.D., *Journal of Chromatography*, Volume 11, pp.463-471, (1963).
- (3) Dose, E.V., *Anal. Chem.*, 1987, 59, 2414-2419.
- (4) Curvers, J., Rijks, J., Cramers, C., Knauss, K., Larson, P., *HRC & CC*, Vol. 8, Sept. 1985.
- (5) Snow, N.H. and McNair, H.M., *J. of Chrom. Sci.*, Vol. 30, July 1992.

### ezGC Software

(includes 5 1/4" and 3 1/2" disks)

cat.# 21480, 21495

ezGC will be available for shipment in May 1993.

ezGC™ was developed jointly by Analytical Innovation, Inc. in cooperation with Restek Corporation.

\*A 386SX-25 without a coprocessor was able to evaluate 350 temperature programs for 12 components in under 1 minute.

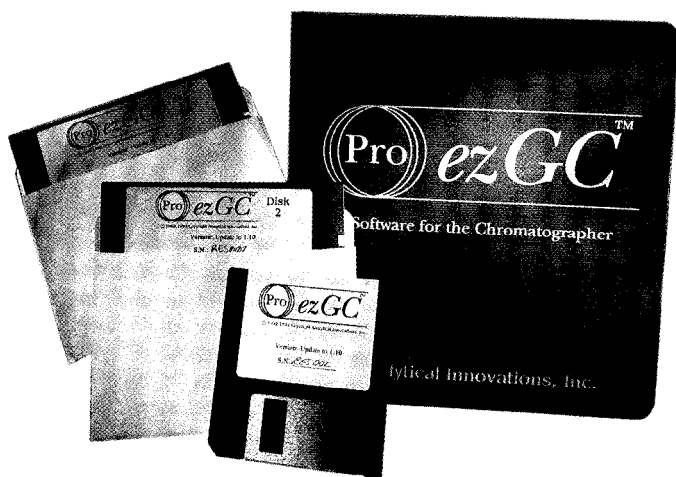
# Pro ezGC Software (Ver 2,0) for Windows,



***The most powerful GC optimization software has new features!***

by Mike Feeney

- Optimize temperature and flow programs from a single analysis.
- Model retention gap and guard column applications including Restek's Integra-Guard™ columns.
- Model columns in series for process GC and multi-dimensional GC analyses.
- Software routines expanded for Fast GC and Windows® 95.



Pro ezGC™ software is a powerful optimization software and retention index database for gas chromatography. This program accurately predicts GC separations on any capillary column and is useful for selecting the best column and conditions for your GC analysis. Pro ezGC™ software utilizes either your chromatographic retention data or you can use the extensive library containing thousands of commonly analyzed compounds. From this data, it is possible to automatically evaluate thousands of combinations of column dimensions, oven temperature program, and carrier gas pressure program to determine

the best separation with the fastest analysis time. This saves days of method development time for new analyses and can decrease analyses times of existing analyses by more than 50%. Several new features incorporated into version 2.0 make Pro ezGC™ software for Windows® even more powerful and easy to use.

## **Optimize separation and analysis time from a single GC run**

In order to accurately simulate separations and analysis time, the software requires either selecting a compound from an existing library or entering retention times from a GC analysis. This new version of

Pro ezGC™ software for Windows® can calculate the thermodynamic retention indices from a single chromatographic run. This analysis can be your current method, retention data from a scientific journal, or retention times from publications such as Restek's chromatography products catalog. This makes it possible to select a GC column for your analysis and estimate the separation quickly and easily.

## **Model GC separation including guard columns and capillary restrictors**

The analysis of contaminated samples often requires the use of a guard column to minimize contamination of the analytical column. Cool on-column injection often utilizes retention gaps to improve peak widths and to facilitate injection using standard gauge syringes. These "precolumns" can either be connected using a low-volume union or built-in as with Restek's Integra-Guard™ columns. In GUMS applications, a length of deactivated tubing is sometimes added to the end of the analytical column to either increase the GC inlet pressure or to decrease background bleed from the transfer line tube. Pro ezGC™ software for Windows® now permits accurate modeling when these types of columns are used, even when the diameters are not identical to the analytical column.

**Pro ezGC™ for Windows®  
version 2.0**  
cat.# 21487

## **Predict the optimum column for dual columns connected in series or parallel**

Many times, resolution of all components in a sample is not possible using a single column. This is where the power of Pro ezGC™ software becomes especially obvious because the program can either model two columns connected in parallel to two separate detectors or two columns connected in series. With series connections, the lengths of the two columns are often cut to give the best combination. This approach would be costly and time consuming without Pro ezGC™ software. Now, any laboratory can quickly evaluate whether serially coupled columns will give the separation without cutting up valuable capillary columns.

Take the guesswork out of selecting the best column and conditions for your GC analysis with Pro ezGC™ software for Windows®. Increase the productivity of your existing gas chromatographs by improving separations and shortening analysis time with optimized temperature and carrier gas programs. For more information, download a copy of the demo software directly from Restek's website at <http://www.restekcorp.com> or call your local distributor and request a demo disk of Pro ezGC™ software for Windows®.

**Upgrade from Pro ezGC™ for  
DOS to Pro ezGC™ for  
Windows®**  
cat.# 21486

# Pro ezGC

## Method Development Software Updates

### *Pro ezGC" has become more powerful with new Version 1.5*

- . Increase your labs' competitive advantage!
- . Optimize temperature and pressure programming parameters to decrease analysis times and increase sample throughput.
- . Improve resolution to meet or exceed method protocols.
- . Optimize column length, diameter and film thickness before purchasing the column.
- . Import data from ASCII or AIA(AND1) formats to reduce data entry time.
- . Calculate Kovats and Linear Temperature Program Indices, as well as Equivalent Chain Length (ECL) values, for qualitative analysis.

The addition of several new features allows simultaneous optimization of column length, internal diameter, and film thickness, as well as pressure programming. These features are added to the temperature program optimization features already in place. By using **Pro ezGC**, you can improve the resolution of your analysis, shorten analysis times, increase sample throughput, and save money.

**Pro ezGC** uses thermodynamic retention indices (TRIs) to calculate retention times and elution characteristics for a set of components on a given stationary phase. By entering a column dead time and two temperature programmed runs of experimental data, the user can calculate TRIs. TRIs are then used to predict the performance of these components when any of the column parameters (length, ID, film thickness, carrier gas, or flow control) are changed. By using component libraries and

TRIs generated by Restek, you can pick the best column and run conditions without ever installing a column. GC method development and analysis optimization couldn't be easier.



Version 1.5 now allows simultaneous optimization of temperature programs, column length, ID, film thickness and flow or pressure parameters. New component libraries include FAMES, Pesticides, and PCBs. Call your local distributor to request a complete listing of all the component libraries.

**Pro ezGC Software ver. 1.5:**  
cat# 21481, \$1495

**Pro ezGC" ver. 1.0 to  
Pro ezGC" ver. 1.5:**  
cat.# 21485, \$595

**ezGC" ver. 1.0 or 1.5 to  
Pro ezGC" ver. 1.5:**  
cat.# 21482, \$1095

## Three New Retention Index Libraries Available

### **Fatty Acid Methyl Ester (FAME) cat.# 21455**

FAME thermodynamic retention index libraries are now available for 70 compounds on the Rtx@-2330 and Stabilwax" stationary phases. All straight chain saturates from methyl butanoate(C4:O) to methyl tetradocosanoate(C24:O) are included, along with unsaturates ranging from monounsaturate methyl undecenoate (C 11: 1) to the polyunsaturate methyl docosahexanoate(C226).

### **Environmental - Pesticides/Herbicides (Part 1) cat.# 21456**

A collection of 62 chlorinated pesticides from EPA methods 505,507,508,608.1, 608.2, 1618, and CLP Pesticides, as well as 19 derivatized phenoxy-acids found in EPA methods 515.1,815OB, and 615 are included in this library. Thermodynamic retention indices are provided on the Rtx@-5, Rtx@-35, and Rtx"-1701 stationary phases.

### **Environmental - PCBs cat# 21454**

A complete collection of retention indices for the 209 polychlorinated biphenyls (PCBs) on the Rtxa-5 stationary phase are included in this library.

### **Other Retention Index Libraries Available:**

**Food and Flavor Volatiles (cat3 21451)**

**Drugs & Pharmaceuticals (cat9 21453)**

**Environmental - Volatiles (cat.# 21452)**

**Solvents & Chemicals - Part 1 (cat.# 21450)**

**Please call your local distributor for  
additional information.**

# ezGC and Pro ezGC

## for Fast, Economical GC Method Development

The March 1993 issue of *The Restek Advantage* previewed ezGC™, a new software program that uses computer modeling to accurately simulate changes to a GC analysis. The software calculates the peak widths and retention times for a given set of chromatographic conditions and then displays the resulting chromatogram. In addition, the software predicts the optimum temperature program for a given analysis that provides baseline resolution in the shortest time. A chromatographer can see, within seconds, the effect of changes in column dimensions, carrier gas, and operating conditions instead of spending hours or days in the laboratory. The ezGC™ software improves column selection, optimizes peak resolution, minimizes analysis times, and greatly increases laboratory productivity. Both method development labs and analytical labs performing routine analysis can benefit from ezGC™. The following examples demonstrate the capabilities of ezGC™ using a typical set of columns and chromatographic conditions.

### Let ezGC™ optimize your GC method for resolution in the shortest analysis time

To begin optimizing a GC method, first obtain two sets of retention times for the components of interest at two different temperature programs. In the following example, retention times were collected from two injections of a volatile fragrance mixture using temperature program rates of 3 and 8°C/min. Next, the chromatographic conditions and retention times were entered using the menu driven screens of the ezGC™ program.

Figure 1 - Easily enter information into ezGC™ from menu driven screens.

Pro ezGC 1.07b

Operating Conditions Solutions

Column

Name: Rtx-1 OK

Comment: Food Volatiles #10120

Length: 30.00 meters Cancel

Diameter: 0.320 mm

Film: 1.000 microns Help

Carrier

Gas: Helium

Control: Constant Pressure

Pressure Units

( ) kPa ( ) PSI ( ) atm

What if ?

Gauge Pressure: 7.34 PSI

Flow Rate: 1.311 ml/min

Dead Time: 2.000 min

Linear Velocity: 25.00 cm/sec

Test Temp: 65.00 °C

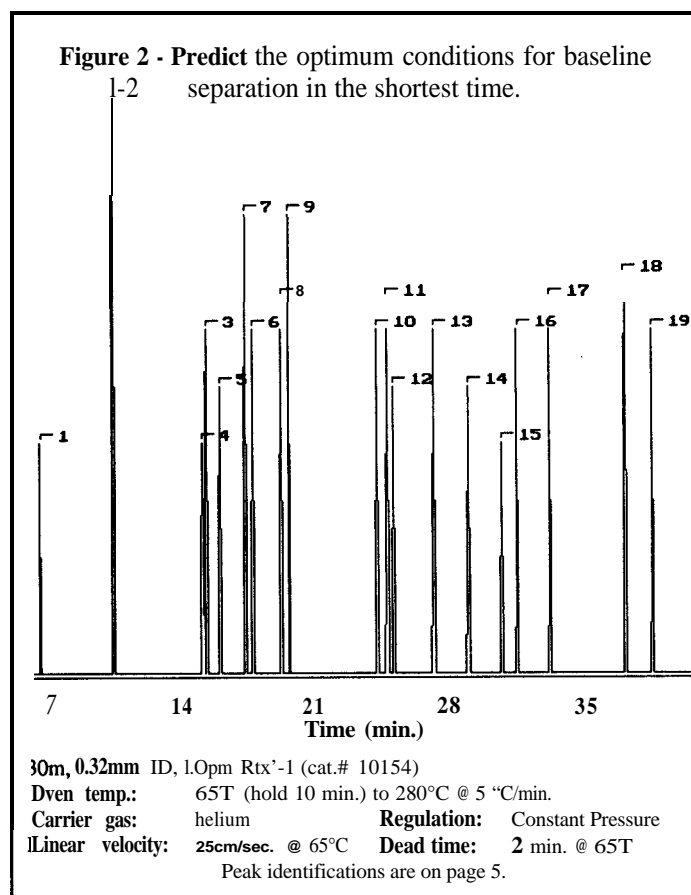
Atm. Pressure: 14.69 PSI

Outlet Pressure: 14.69 PSI

View Summary

Figure 1 shows the screen used to input the retention time data. The first scenario we will investigate is where a particular column is already installed and the chromatographer wants to determine the conditions that will separate all components with the shortest analysis time. The ezGC™ software can be set to automatically evaluate different temperature programs and print a solution list. The solution list is prioritized according

to the temperature(s) that resolve the most components in the shortest time. A resolution factor can be specified, or defaulted to a value of 1 S, which approximates baseline separation. Figure 2 illustrates the predicted chromatogram obtained for 19 flavor and fragrance compounds using a 30 meter, Rtx®-1 column with a 1.0µm film thickness. The program predicted a 10 minute initial hold at 65°C, providing baseline resolution in under 40 minutes.



### Determine how changes in column and carrier gas will improve separations

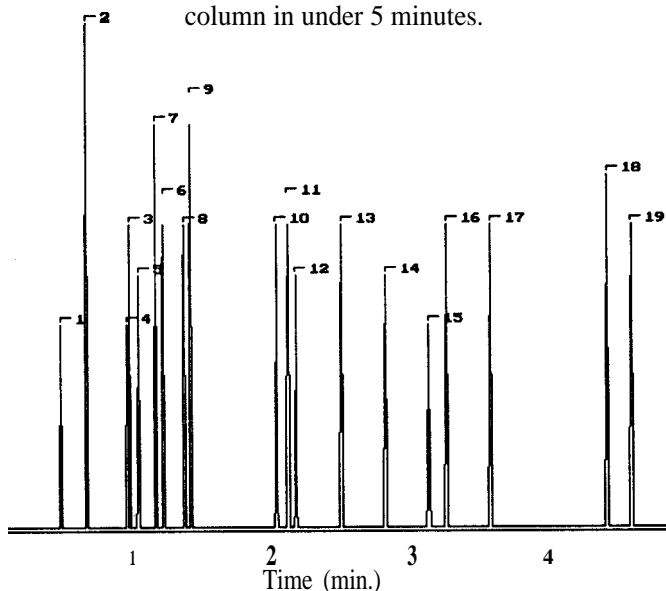
GC method development can be very costly when considering the expense of evaluating different stationary phases, column dimensions, and oven temperatures. Many chromatographers empirically optimize their chromatographic conditions for a particular column and then accept these as the "best separation" achievable. This is understandable considering the cost of buying and installing new columns. With ezGC™ you can determine within minutes how changes in the column and operating conditions will effect separations. (Table I). All that is needed are the retention times for your components from two temperature programs using any column which has the same stationary phase. Previously calculated indices can be retrieved either from disk or loaded from a commercial data base or library.

**Table I - Parameters that can be optimized using ezGC**

oven temperature and program rate (multi-ramp)  
 minimum analysis time  
 maximum resolution  
 column length  
 film thickness  
 internal diameter  
 carrier gas type (He, H<sub>2</sub>, N<sub>2</sub>, Ar)  
 carrier gas flow or velocity  
 constant pressure or pressure program

To illustrate how ezGC™ can be used to quickly determine the optimum analysis time for a particular sample, Restek's applications group optimized each of the parameters listed in Table I for the flavor and fragrance compounds shown in Figure 1. ezGC™ predicted that a 15-meter column, 0.25mm ID, a 0.25µm film thickness, in conjunction with a 25°C/min. temperature program would greatly decrease the analysis time without sacrificing resolution. The new optimum analysis was obtained using a lower-cost 15-meter column with an analysis time under 5 minutes with 1/10 the analysis time and 1/2 the column length originally used (Figure 3). ezGC™ more than pays for itself.

**Figure 3 - Complete separation obtained using a 15-meter column in under 5 minutes.**



15m, 0.25mm ID, 0.25µm Rtx@-1 (cat.# 10120)  
 Oven temp.: 5X to 230°C @ 25 °T/min.  
 Carrier gas: hydrogen Regulation: constant F%eswre  
 Linear velocity: 89.1cm/sec. @ WC Dead time: 0.281 min. @ 55T

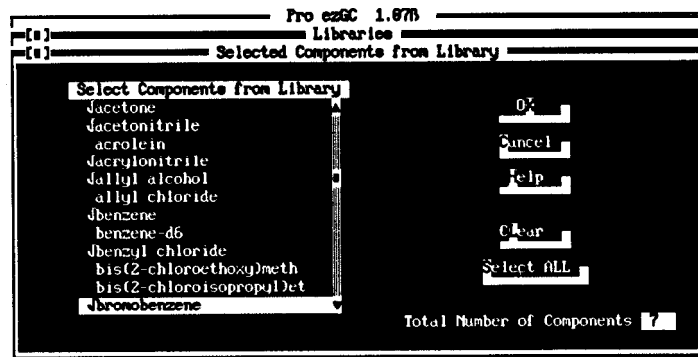
**Peak Identification for Figures 2 & 3.**

1	ethyl butyrate	15	eugenol
2	trans-2-hexenol	9	D-limonene
4	benzaldehyde	10	methone
3	a-pinene	11	menthofurao
5	camphene	12	menthol
7	fi-pinene	13	carvone
6	octanal	14	cinnamic alcohol
		16	vanillin
		17	ethyl vanillin
		18	ethyl lamate
		19	anily cinnamic aldehyde

Do method development without installing a column. Method optimization is much faster using ezGC™, but is it possible to make column selection easier? Restek now offers data bases of thermodynamic retention indices called libraries, making it possible to select a column and predict chromatographic separations without even installing a column. These libraries contain hundreds of commonly analyzed components. These libraries have been generated in Restek's Applications Laboratory using the most appropriate stationary phases. Entries are added to the library after certifying each identification using GC/MS. Once the libraries are complete, it is possible to select components by simply choosing the entry from the library section of either ezGC™ or **Pro ezGC™**. Figure 4 is an example of the select menu, showing a portion of the Environmental Volatiles library. This library currently contains 138 organic components (along with surrogates and internal standards) commonly analyzed in water and solid wastes, analyzed on three different stationary phases (Rtx@-502.2, Rtx™-1 and Rtx™-624). Furthermore, using **Pro ezGC™** makes it possible for each laboratory to create their own "User" libraries, adding compounds which can be modeled along with library data supplied by Restek. Restek now offers five libraries and plans to introduce several more libraries in the upcoming months. We also have plans to continue expanding the number of compounds offered and the number of stationary phases in each library.

Almost every chromatographic method currently in use could be made more efficient by separating the components of interest in less time. The thought of spending days of additional method time and/or purchasing columns which may not give better results often keeps analysts from investigating these options. With ezGC™ it is possible to quickly and easily determine: "What is the best column?" and "What is the optimum temperature program and carrier flow?". The advanced features of **Pro ezGC™** make GC computer modeling

**Figure 4 - Select the specific components for a stationary phase to separate and then optimize your method for any column, oven temperature and carrier gas parameters.**



*(ezGC™ article is continued on page 6.)*



FREE  
**Master Library**  
 contains over 3,000  
 compounds!

*Pro ezGC™ now includes the entire Master Set of Retention Index Libraries at no extra charge! These libraries contain more than 3000 compounds on the most commonly used stationary phases in ten different application areas including pesticides, PCBs, dioxins/furans, flavor & fragrance compounds, drugs of abuse, FAMES, semi-volatile pollutants, volatile pollutants, petroleum hydrocarbons, and solvents & chemicals. These libraries permit computer simulation without entering actual laboratory data.*

### *Pro ezGC™ Methods Development Software*

*The most powerful GC optimization software has new features!*

- Simplify column selection.
- Optimize temperature and flow programs from a single analysis.
- Reduce analysis times and improve sample resolution.
- Model retention gap and guard column applications including Restek's Integra-Guard™ columns.
- Model columns in parallel or in series for process GC and multi-dimensional GC analyses.
- Software routines expanded for Fast GC, Windows@ 95, and Windows@ NT.
- Optimize dual-column run conditions.
- FREE Master Library Set!



Many analysts are following methods or using columns and run conditions they know could be optimized. But who has time to make the hundreds of injections necessary to optimize the temperatures, ramp rates, flow rates, pressures, and column parameters to get the perfect chromatogram? No one!

Let **Pro ezGC™** for Windows@ do the work for you. **Pro ezGC™** software is a powerful optimization software and retention index database for gas chromatography. This program accurately predicts GC separations on any capillary column and is useful for selecting the best column and conditions for your GC analysis. **Pro ezGC™** software utilizes either your chromatographic retention data or you can use the extensive library containing thousands of commonly analyzed compounds. From this data, it is possible to automatically evaluate thousands of combinations of column dimensions, oven temperature program, and carrier gas pressure program to determine the best separation with the fastest analysis time. This saves days of method development time for new analyses and can decrease analyses times of existing analyses by more than 50%. Several new features incorporated into Version 2 make **Pro ezGC™** for Windows@ even more powerful and easy to use.

#### **Optimize separation and analysis time from a single GC run**

In order to accurately simulate separations and analysis time, the software requires either selecting a compound from an existing library or entering retention times from a GC analysis. This new version of **Pro ezGC™** for Windows@ can calculate the thermodynamic retention indices from a single chromatographic run. This analysis can be your current method, retention data from a scientific journal, or retention times from publications such as this catalog, making it possible to select a GC column for your analysis and estimate the separation quickly and easily.

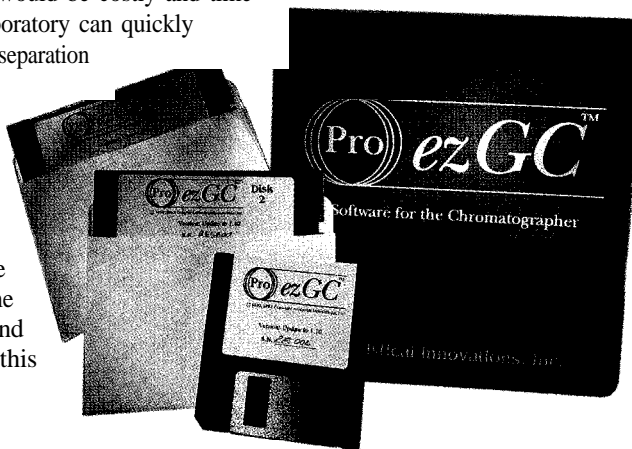
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The analysis of contaminated samples often requires the use of a guard column to minimize contamination of the analytical column. Cool on-column injection often utilizes retention gaps to improve peak widths and to facilitate injection using standard gauge syringes. These "precolumns" can either be connected using a low-volume union or built-in as with Restek's Integra-Guard™ columns. In GUMS applications, a length of deactivated tubing is sometimes added to the end of the analytical column to either increase the GC inlet pressure or to decrease background bleed from the transfer line tube. **Pro ezGC™** for Windows@ now permits accurate modeling when these types of columns are used, even when the diameters are not identical to the analytical column.

## Predict the optimum column for dual columns connected in series or parallel

Many times, resolution of all components in a sample is not possible using a single column. This is where the power of **Pro ezGC™** software becomes especially obvious because the program can either model two columns connected in parallel to two separate detectors or two columns connected in series. With series connections, the lengths of the two columns are often cut to give the best combination. This approach would be costly and time consuming without **Pro ezGC™** software. Now, any laboratory can quickly evaluate whether serially coupled columns will give the separation without cutting up valuable capillary columns.

Take the guesswork out of selecting the best column and conditions for your GC analysis with **Pro ezGC** for Windows®. Increase the productivity of your existing gas chromatographs by improving separations and shortening analysis time with optimized temperature and carrier gas programs. **Pro ezGC™** will save you time and money by greatly enhancing your productivity and increasing sample throughput. Take advantage of this powerful GC optimization tool today!



**Pro ezGC™ Method Development Software**

**Pro ezGC™ for Windows® ver. 2:** cat.# 21487, ea.

**Pro ezGC™ (DOS) to Pro ezGC™ for Windows® ver. 2 Upgrade:** cat.# 21486, ea.

## Attention EPC users!

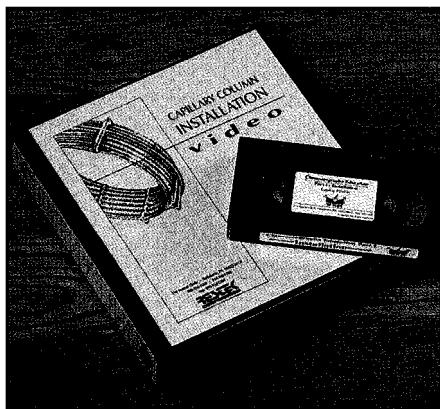
**Learn how to best use EPC with Pro ezGCM software. This software allows chromatogram optimization using constant flow, constant pressure, and pressure programming.**

## Capillary Column Installation Video

The technical wizards at Restek produced an instructional video that takes the mystery and frustration out of capillary column installation. This essential resource covers critical points in the proper installation of a capillary column such as:

- Choice of carrier gas
- Instrument preparation
- Trouble-free installation
- Leak checking
- Setting carrier and detector gas flows
- Column conditioning

The installation sequence allows you to install your capillary column correctly, minimize downtime, and get your GC up and running quickly. The video follows ASTM Method E1510-93 for installing fused silica open tubular capillary columns in gas chromatographs to ensure your lab conforms with industry standards.



## Ideal Training Tool

**We guarantee this video will be the most useful instructional tool you'll ever use or we'll refund your money!**

**VHS:** cat.# 20490, ea.

**PAL:** cat.# 20491, ea.

**Educational Materials**

# Solvents & Chemicals Library Cotipound

## Index - Part 1

Version 1.0-cat#21450

Benzyl alkohol	2-(2-Ethoxyethoxy)ethanol	2-(2-Methoxyethoxy)ethanoi	2-Octanol
2,3-Butanediol	2-Ethyl-1-butanol	a-Methyl-1-butanol	2-Gctanone
1-Butanol	2-Ethyl-1-hexanol	3-Methyl-1-butanol	3-Gctanone
2-Butanol	3-Ethyl-3-pentanol	2-Methyl-2-butanol	Pentadecane
2-Butanone	Heptadecane	3-Methyl-2-butanol	Pentanal
3-Buten-1-ol	Heptanal	3-Methyl-2-buten-1-ol	Pentane
3-Buten-2-ol	Heptane	S-Methyl-3-heptanone	1-Pentanol
cis-2-Buten-1-ol	1-Heptanol	5-Methyl-2-hexanone	2-Pentanol
2-Butenal	2-Heptanol	2-Methyl-1-pentanol	t-Pentanone
2-Butoxyethanol	CHeptanol	4-Methyl-2-pentanol	3-Pentanone
t-(2-Butoxyethoxy)ethanol	2-Heptanone	2-Methyl-3-pentanol	cis-2-Penten-1-ol
Butyrlactone ;	3-lieptanone	3-Methyl-3-pentanol	3-Penten-2-one
Cyclopentanol	CHeptanone	t-Methyl-3-pentanone	2-Phenoxyethanol
Decanal	Hexanal	2-Methyl-pmpanal	CPhenyl-2-butanone
Decane	Hexadecane	2-Methyl-1-propanol	1b-Pmpanediol
1-Decanol	Hexane	1-Methyl-2-pyrrolidinone	1-Propanol
2-Decanol	1-Hexanol	a-Methyl benzyl alcohol	2-Propanone
2-Decanone	2-Hexanol	Methyilisobutylketone	2-Pmpen-1-ol
2,6-Dimethyl-1-heptanone	3-Hexanol	4-Methyl-j-penten-2-one	Propionai
2,4-Dimethyl-2-pentanol	t-Hexanone	Nonanal	2-Pmpyn-1-ol
2,4-Dimethyl-3-pentanol	3-Hexanone	Nonane	Tetradecane
2,2-Dimethyl-3-pentanol	cis-3-Hexen-1-ol	1-Nonanol	Tetraethylene glycol
2,2-Dimethyl-1-pentanol	trans-tlexen-1-ol	t-Nonanol	Tridecane
2,4-Dimethyl-3-pentanone	4-Hexen-3-one	2-Nonanone	Triethylene glycol
Dodecane	tetra-Hydro-tfuran-methanol	3-Nonanone	2,2,2-Trifluoroethanol
1-Dodecanol	4-Hydmxyl-methyl-2-pentanone	5-Nonanone	Undecrme
t-Dodecanone	Isopropyl alcohol	Octanal	1-Undecanol
Ethanol	Methanol	Octane	2-Undecanone
2-Ethoxyethanol	2-Methoxyethanol	1-Octanol	

### Conditions:

Column 1 10Sm, 0.3mm ID, 3.0um Rtx\*-I (cat.# 10189)  
 Slow run: 35°C (hold 10 min.) to 270°C @ 4°C/min. (hold 20 min.)  
 Fast run: 40°C (hold 10 min.) to 275°C @ 12°C/min. (hold 20 min.)

Column 2 105m, 0.53mm ID, 3.0um RtxO-502.2 (cat.# 10910)  
 Slow run: 35°C (hold 10 min.) to 265°C @ 4°C/min.  
 Fast run: 40°C (hold 10 min.) to 270°C @ 12°C/min. (hold 10 min.)

Column 3 60m, 0.53mm ID, 1.0um Stabiiwax™ (cat.# 10658)  
 Slow run: 40°C (hold 10 min.) to 245°C @ 4°C/min. (hold 20 min.)  
 Fast run: 45°C (hold 10 min.) to 250°C @ 12°C/min. (hold 20 min.)

Carrier: Helium  
 Instrument: HP 589011 GC and HP5971A MSD  
 Outlet: Vacuum (MSD), 0.00 psi

Note: ***Some stationary phases may contain species not common to all libraries.***

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# Drugs & Pharmaceuticals Library

## Compound Index

VersionL0-cat#21453

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 Fiunitrazepam Fluazepam Glutethimide Haloperidol Hexobarbital Hydrocodone Hydromorphone Imipramine Ketamine L-evorphanol Lidocaine	Lorazepam Maprotyline Medazepam Meperidine Mephobarbital Meprobamate Methadone Methapyriline Methaqualone Methypylon Nalorphine Nicotine Norcodeine Nortriptyline Papaverine Pentazocine Pentobarbital Phencyclidine Pheniramine Phenobarbital Phenothiazine Phenylbutazone Phenyltoloxamine Prazepam Primidone	Procainamide Prochlorperazine Promazine Propoxyphene Pyrilamine Scopolamine Secobarbital Strychnine Temazepam Tetracaine Thiamylal Thiopental Thioridazine Trazodone Triazolam Trifluoperazine Trimeprazine Trimipramine Tripeleminamine Triprolidine Valproic Acid Verapamil
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Conditions:	Experimental Runs:
Column 1: 30m, 0.25mm ID, 0.25µm Rtx*-5, cat.# 10223 Column 2: 30m.0.25mm ID. 0.25µm Rtx*-50, cat.# 10523 Column 3: 30m. 0.25mm ID, 0.25µm RtxO-200, cat.# 15023 Inlet: Constant pressure      Outlet: Vacuum (0.00 psi) Linear velocity: 35cm/sec.      Dead time: 1.4 min. Carrier gas: Helium	<b>Slow Temperature Program:</b> 50°C (hold 0 min.) to 325°C @ 4°C/min. (hold 20 min.)  <b>Fast Temperature Program:</b> 100°C (hold 0 min.) to 325°C @ 12°C/min_ (hold 20 min.)

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# Environmental Volatiles Library

## Compound Index

Version 1.0 - cat.# 21452

Acetone Acetonitrile Acrolein Acrylonitrile Allyl alcohol Allyl chloride Benzene Benzene-d6 <b>Benzyl chloride</b> Bis(2-chloroethoxy)methane Bis(2-chloroisopropyl)ether Bromobenzene Bromochloroacetonitrile 2-Bromochlorobenzene 3-Bromochlorobenzene 4-Bromochlorobenzene Bromochloromethane Bromochloromethane CBromofluorobenzene Bromoform Bromomethane 2-Bromo-1-Chloropropane t-Butyl alcohol n-Butylbenzene sec-Butylbenzene tert-Butylbenzene Carbon disulfide Carbon tetrachloride Chloroacetonitrile Chlorobenzene Chlorobenzene-d5 1-Chlorobutane Chloroethane 2-Chloroethanol 2-Chloroethyl vinyl ether	Chloroform 1-Chlorohexane Chloromethane 3-Chloropropionitrile 2-Chlorotoluene 4-chlorotoluene 1-Chloro-2-Fluorobenzene Cyclohexane Dibromoacetonitrile Dibromochloromethane 1,2-Dibromoethane Dibromofluoromethane Dibromomethane 1,2-Dibromo-3-chloropropane Dichloroacetonitrile 1,2-Dichlorobenzene 1,3-Dichlorobenzene 1,4-Dichlorobenzene 1,2-Dichlorobenzene-d4 1,4-Dichlorobenzene-d4 1,2-Dichlorobutane Dichlorodifluoromethane 1,1-Dichloroethane 1,2-Dichloroethane 1,2-Dichloroethane-d4 1,1-Dichloroethene cis- 1,2-Dichloroethene trans- 1,2-Dichloroethene Dichloromethane (CH2Cl2) 1,2-Dichloropropane 1,2-Dichloropropane 2,2-Dichloropropane 1,1-Dichloropropane 1,1-Dichloropropene cis-1,3-Dichloropropane	trans- 1,3-Dichloropropene cis- 1,4-Dichloro-2-butene trans- 1,4-Dichloro-2-butene 1,3-Dichloro-2-propanol Diethyl ether 1,4-Difluorobenzene 1,4-Dioxane Epichlorohydrin Ethanol Ethyl methacrylate Ethylbenzene Ethylbenzene-d10 Ethylbenzene-d5 Ethylene oxide Fluorobenzene Hexachlorobutadiene Hexachloroethane 2-Hexanone Iodomethane Isobutyl alcohol Di-isopropyl ether Isopropylbenzene p-Isopropyltoluene Malononitrile Methacrylonitrile Methyl ethyl ketone (MEK) Methyl isobutyl ketone (MIBK) Methyl methacrylate Methyl tertiary butyl ether Methylacrylate Naphthalene Nitrobenzene 2-Nitropropane Pentachloroethane	Pentafluorobenzene ZPicoline Propargyl alcohol Propionitrile n-Propylamine n-Propylbenzene Pyridine Styrene 1,1,1,2-Tetrachloroethane 1,1,2,2-Tetrachloroethane Tetramethylethylene THP Thiophenol (Benzenethiol) Toluene Toluene-d8 Trichloroacetonitrile 1,2,3-Trichloroethene 1,2,4-Trichlorobenzene 1,1,1-Trichloroethane 1,1,2-Trichloroethane Trichloroethene Trichlorofluoromethane 1,2,3-Trichloropropane 1,1,1-Trichloro-2-propanone 1,1,2-Trichloro-1,2,2-trifluoroethane (FIF1) 1,2,4-Trimethylbenzene 1,3,5-Trimethylbenzene Vinyl acetate Vinyl chloride m-Xylene o-Xylene p-Xylene
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Conditions:			Experimental Runs:
Column 1: IOSm, 0.53mm ID, 3.0pm R&-1 cat4 10189	Column 2: 105m, 0.53mm ID, 3.0pm Rtx*-502.2 cat.# 10910		Slow Temperature Program: 35°C (hold 10 min.) to 220°C @ 4°C/min. (hold 3 min.)  Fast Temperature Program: 40°C (hold 10 min.) to 230°C @ 12°C/min. (hold 3 min.)
Carrier: Helium	Dead time: 3.16 min. @ 50°C		
Instrument: HP 589011 GC and HP 5971 MSD			
Inlet: constant pressure	Column 3: 105m. 0.53mm ID. 3.0pm R&-624 cat.# 10975		
Dead time: 3.03 min. @ 5WC	Dead time: 3.31 min. @ 50°C		
Outlet: Vacuum (MSD), atmospheric			

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# Flavor & Fragrance Library Compound Index

Version 1.0-cat.#21451

4-ylblllSOIC amyl cinnamic aldehyde trans-anethole alpha-angelicalactone anisaldehyde anisole benzaldehyde borneol bomyl acetate camphene camphor 3-carene catvacrol carveol r-carvone s-carvone carvone acetate catvone hydrate cis-carvyl acetate trans-carvyl acetate cis-carvyl propionate trans-catvyl propionate alpha-znyophyllene beta-caryophyllene caryophyllene oxide 1.8-cineole trans-cinnamic acid cinnamic alcohol trans-cinnamaldehyde cinnamide cinnamyl acetate citral a citral b citronellal beta-citronelloi citronellyl acetate citronellyl formate coumarin cumin acid cumin alcohol	cuminaldehyde para-cymene dihydCaNeo1 cisdiidrcarvone transdihydrocarvone dihydrocoumarin dihydrojasmone 2,3-dimethylkisol 2.4dimethylanisoIe 2,5diethylankole 2,6-diiethylanisole 2..5diiethylfuran 2,3dimethyl-p-anisaldehyde 2,5-dimethyl-panisaldehyde D-n-menthol estragole ethyl butyrate ethyl laurate ethyl vanillin 2-ethylKuran eucalyptol eugenol cis-famesol trans-famesol fenchone tiufurai furfuryl acetate furfuryl alcohol geranial geraniol geranyl acetate guaiaxulene tmns-2-hexenal trans-2-hexenol alpha-humulene indole alpha-ionone beta-ionone isobomeol isoeugenol	cis-jasmone liionene linalool linalyl acetate maltol menthofuran +/- menthol menthone cis-menthyl acetate tram+menthyl acetate methyl cinnamate 2-methylutisole 3-methylanisole 4-methylanisole alpha-methylcinnamic acid 6-methylcoumarin 7-methylcoumarin 2-methylfumn S-methylfufural 3-methyl-p-anisaldehyde 2-methyl-trans-cinnamic aldehyde myrcene neral cis-nerol netyl acetate nootketone cis-ocimene trans-ocimene octaral l-octen-3-ol perillaldehyde perillyl alcohol phellandrene pinacol pinacoi alcohol pinacolone alpha-pinene beta-pinene pulegone trans-sabinene hydrate	salicaldehyde alpha-terpinene gamma-terpinene terpirlen4ol alpha-terpineol alpha-terpinolene terpinyl acetate thiazole thiophene alpha-thujone beta-thujone thymol triacetin tricyclene valencene deha-valerolactone gamma-vaierolactone vanillin vanillin acetate <b>verbeneone</b>  C!honane C10:decane C 11 :undecane C1Z:dodecane C13:tridecane C14:tetradecane C1S:pentadecane C16:hexadecane C 17:heptadecane C18:octadecane C 19:nonadecane C20:eicosane C21:heneicosane C22:docosane C23:tricosane C24:tetracosane CZkhexacosane
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Conditions:			Experimenthl Runs:
Column 1: 60m, 0.25mm ID, 0.2.5pm RtxO- 1 cat.# 10126 Carrier: Helium Instrument: HP 589011 GC and HP5971A MSD Inlet: Constant Pressure, 18.74 psi Dead time: 3.988 min. at 50°C Outlet: Vacuum (MSD), 0.00 psi	Column 2: 60m. 0.25mm ID. 0.25um StabilwaxO cat.# 10626 Carrier: Helium Instrument: HP 589011 GC and HP5971A MSD Inlet: Constant Pressure, 16.21 psi Dead time: 4.110 min. at 50°C Outlet: Vacuum (MSD), 0.00 psi		Slow Temperature Program: 35°C (hold 0 min.) to 250°C @ 3°C/min. (hold 15 min.)  Fast Temperature Program: 50°C (hold 0 min.) to 280°C @ 8°C/min. (hold 15 min.)

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