# Will Pro *EZGC* Chromatography Modeling Software Work For You? We Put It to the Test!

Method development is hard. As any analyst will tell you, it takes time—and a lot of trial and error—even for the most experienced chromatographer. Wouldn't it be convenient if there were a tool that allowed you to develop optimized GC methods in just a matter of seconds? Restek's Pro *EZGC* chromatogram modeling software is just such a tool! It provides GC column recommendations as well as the tailored set of conditions you need without the hours of experimentation, saving you time, material costs, and lots of frustration.

To demonstrate the power of the Pro *EZGC* chromatogram simulator, we used a few examples of analyses conducted in our labs to test the accuracy of the GC modeling software's predictions. Using the same analytical run conditions as in the empirical work, will the modeler produce a simulated chromatogram that matches real-world results? Our examples span a variety of chemical classes and column phases to demonstrate how the Pro *EZGC* modeling software is valid for a wide range of applications.

While these examples pit the performance of the Pro *EZGC* chromatogram simulator against experimentally established instrumental conditions with the goal of showing just how closely the modeled results match the data generated empirically, the real power of the Pro *EZGC* modeler is its ability to provide optimized analytical conditions using only a list of compounds. The demonstration presented here illustrates the accuracy of the underlying principles that power the modeler, so that when using the Pro *EZGC* chromatogram simulator to create your next method from scratch, you will have confidence it's predictions will be remarkably close to the actual chromatography you'll obtain when you try it out on your GC.

Before we get started, there are a few things to keep in mind when comparing empirical results to modeled chromatograms. First, any differences in peak heights are due to the model's random generation of height; without information regarding compound concentrations and detector sensitivities it is impossible to accurately predict the relative peak heights for the compounds modeled. Second, the software ideally predicts resolutions (R) of 1.5 or higher because an R of 1.5 means two peaks have been baseline resolved. In instances where it isn't possible to have baseline resolution, the model highlights those resolution values in either yellow or red in the peak table list, depending on how far the predicted value is from an ideal R of 1.5. Figure 1 illustrates the typical output that is provided by the modeling software.
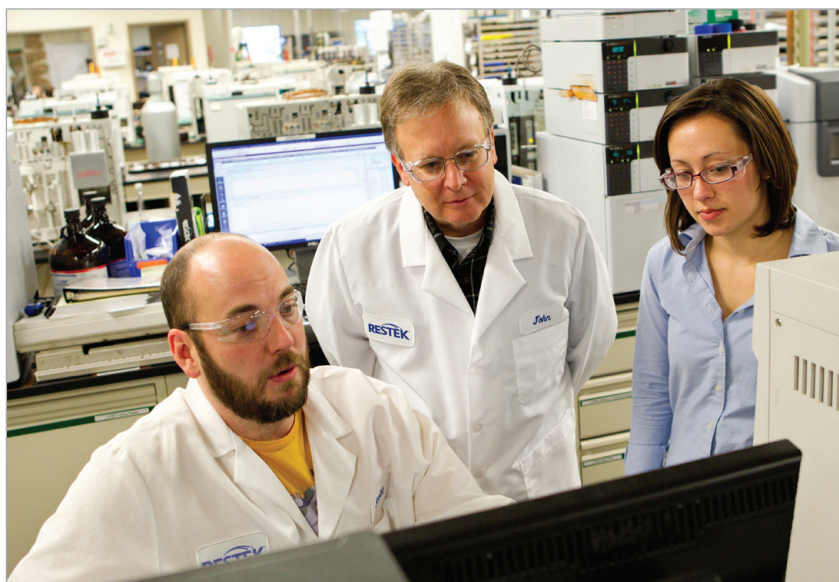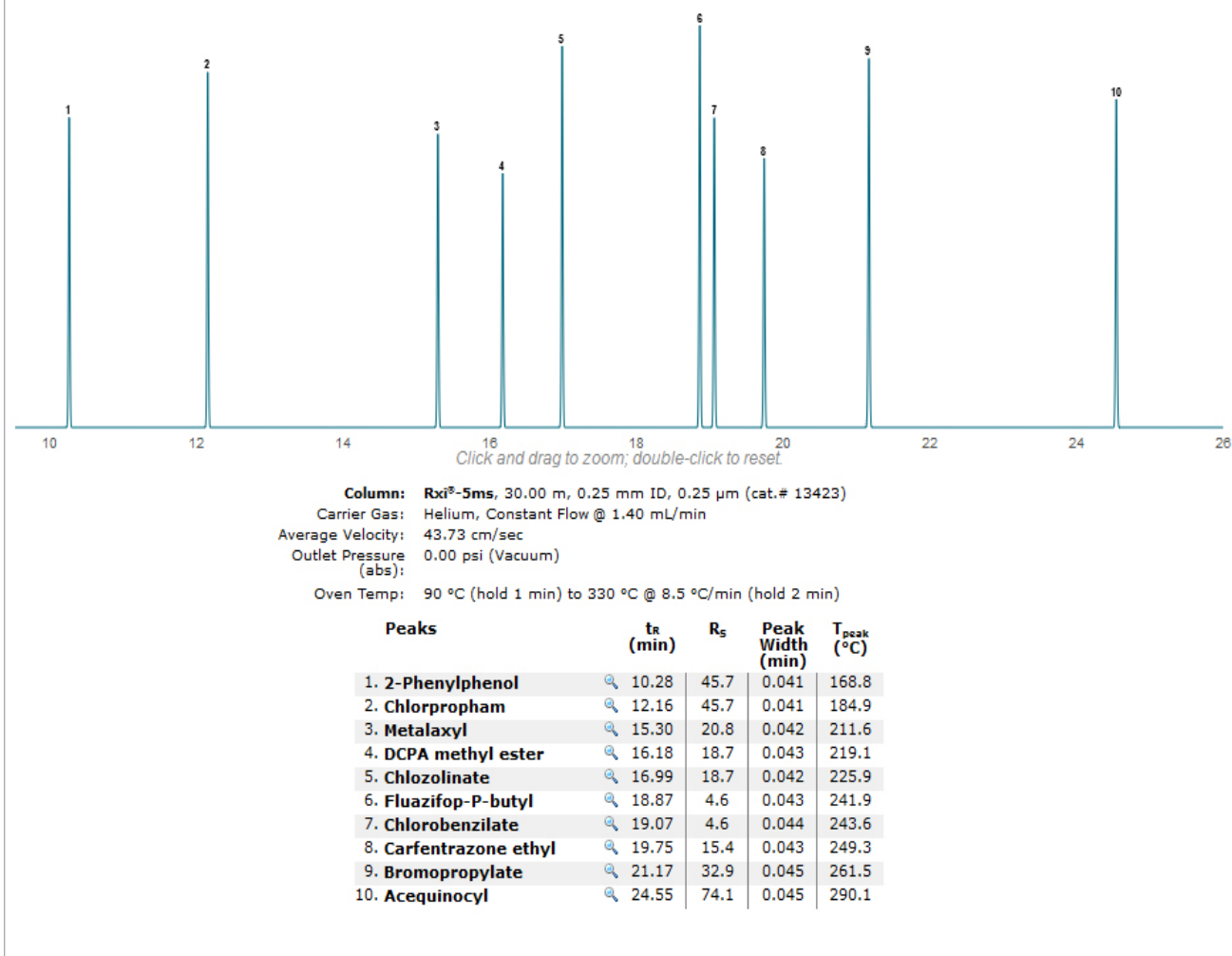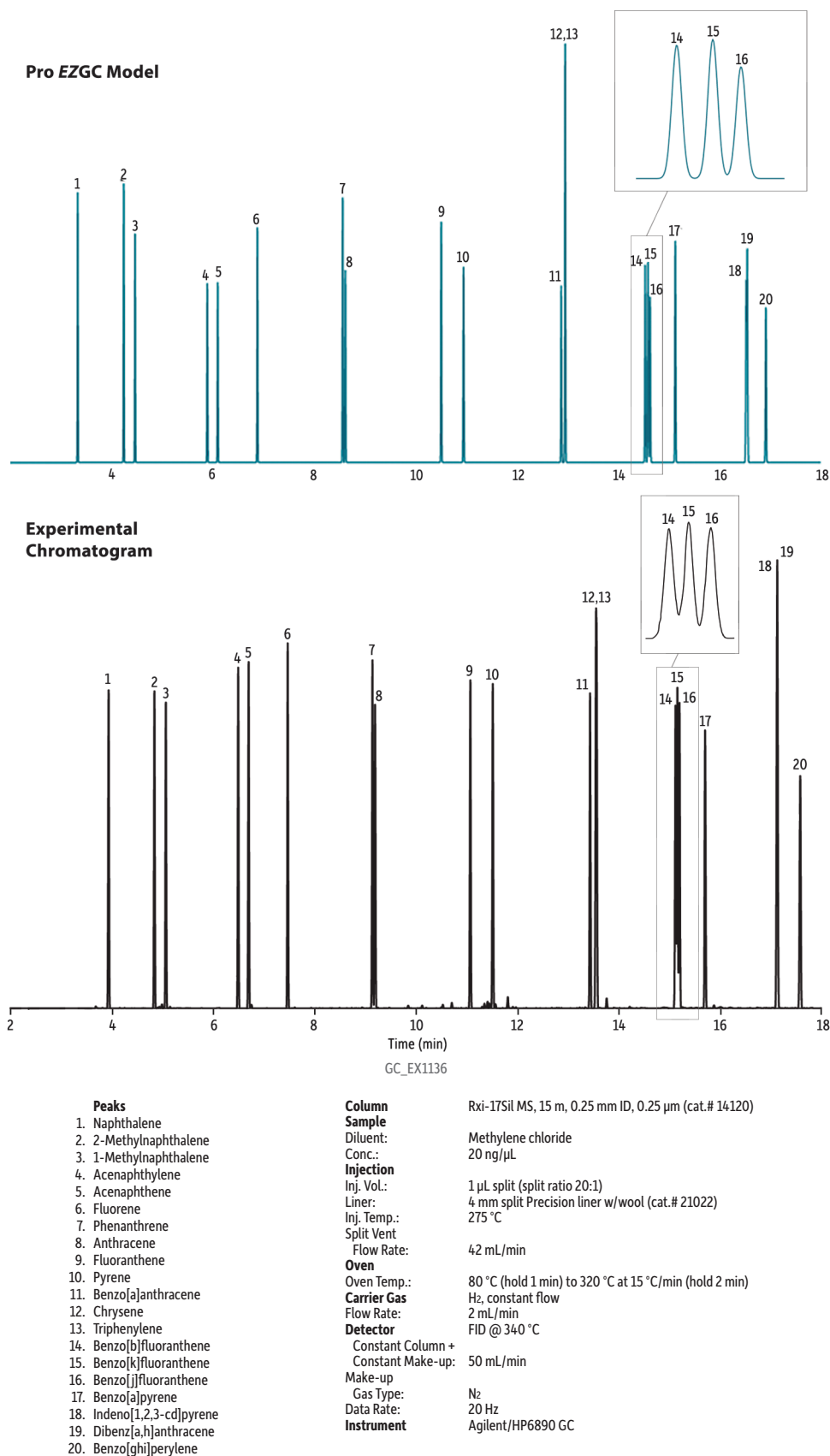
Figure 1: Just input your analyte list and the Pro *EZGC* chromatogram simulator delivers a customized, interactive model chromatogram that provides a specific phase, column dimension, and conditions. You can change columns, modify conditions, zoom in, view chemical structures, and even overlay mass spectra of coeluting compounds.

Click and drag to zoom; double-click to reset.

Column: Rxi®-5ms, 30.00 m, 0.25 mm ID, 0.25 µm (cat.# 13423)
Carrier Gas: Helium, Constant Flow @ 1.40 mL/min
Average Velocity: 43.73 cm/sec
Outlet Pressure (abs): 0.00 psi (Vacuum)
Oven Temp: 90 °C (hold 1 min) to 330 °C @ 8.5 °C/min (hold 2 min)

Peaks		t_R (min)	R_S	Peak Width (min)	T_{peak} (°C)
1. 2-Phenylphenol	🔍	10.28	45.7	0.041	168.8
2. Chlorpropham	🔍	12.16	45.7	0.041	184.9
3. Metalaxyl	🔍	15.30	20.8	0.042	211.6
4. DCPA methyl ester	🔍	16.18	18.7	0.043	219.1
5. Chlozolinate	🔍	16.99	18.7	0.042	225.9
6. Fluazifop-P-butyl	🔍	18.87	4.6	0.043	241.9
7. Chlorobenzilate	🔍	19.07	4.6	0.044	243.6
8. Carfentrazone ethyl	🔍	19.75	15.4	0.043	249.3
9. Bromopropylate	🔍	21.17	32.9	0.045	261.5
10. Acequinocyl	🔍	24.55	74.1	0.045	290.1

Example 1: Ensure the Separation of Critical Compounds with Pro *EZGC* Simulations

Some compounds are difficult to separate because they are very similar, yet their chromatographic resolution may be required. For example, the isomers benzo[b]fluoranthene, benzo[k]fluoranthene, and benzo[j]fluoranthene coelute on many stationary phases, but they must be resolved chromatographically for accurate reporting because the mass spectrometer can't distinguish them spectrally. In Figure 2, you can see that the modeled results closely match the empirical results in terms of relative peak resolution. Actual retention times may shift slightly due to differences in the temperature calibration between the experimental instrument and the one used to develop the modeler's compound libraries; however, even with small retention time shifts, the Pro *EZGC* chromatogram modeler accurately predicted this critical resolution under the same conditions. Imagine the method development time that could be saved by using GC modeling software to establish conditions that ensure key separations instead of spending time testing conditions in the lab!
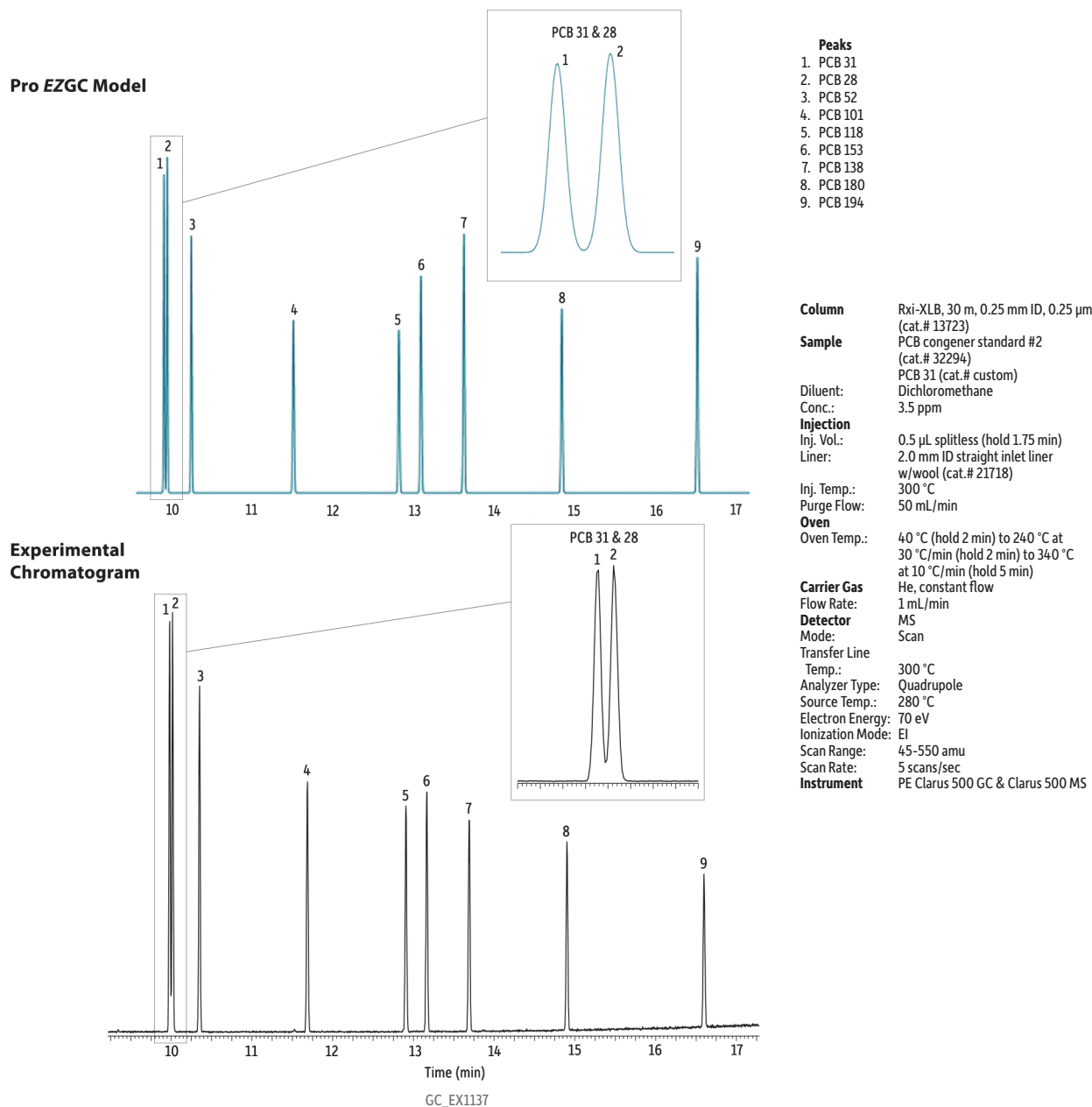
Figure 2: The Pro *EZ*GC chromatogram simulator correctly models critical separations.

Peaks
1. Naphthalene
2. 2-Methylnaphthalene
3. 1-Methylnaphthalene
4. Acenaphthylene
5. Acenaphthene
6. Fluorene
7. Phenanthrene
8. Anthracene
9. Fluoranthene
10. Pyrene
11. Benzo[a]anthracene
12. Chrysene
13. Triphenylene
14. Benzo[b]fluoranthene
15. Benzo[k]fluoranthene
16. Benzo[j]fluoranthene
17. Benzo[a]pyrene
18. Indeno[1,2,3-cd]pyrene
19. Dibenz[a,h]anthracene
20. Benzo[ghi]perylene

Column Rxi-17Sil MS, 15 m, 0.25 mm ID, 0.25 µm (cat.# 14120)
Sample
Diluent: Methylene chloride
Conc.: 20 ng/µL
Injection
Inj. Vol.: 1 µL split (split ratio 20:1)
Liner: 4 mm split Precision liner w/wool (cat.# 21022)
Inj. Temp.: 275 °C
Split Vent
 Flow Rate: 42 mL/min
Oven
Oven Temp.: 80 °C (hold 1 min) to 320 °C at 15 °C/min (hold 2 min)
Carrier Gas H_2, constant flow
Flow Rate: 2 mL/min
Detector FID @ 340 °C
 Constant Column +
 Constant Make-up: 50 mL/min
Make-up
 Gas Type: N_2
Data Rate: 20 Hz
Instrument Agilent/HP6890 GC

GC_EX1136

Example 2: Determine if QC Requirements Can Be Met

Performance-based requirements are critical and finding method conditions that meet them during development can be a challenge. For instance, if you are developing a GC-MS method for a list of compounds that contain isobaric analytes, chromatographic resolution is essential. In the example shown in Figure 3, the polychlorinated biphenyl (PCB) congeners PCB 28 and PCB 31 must be resolved in order to be detected because the mass spectrometer would not be able to distinguish one from the other. You can see that the Pro *EZGC* modeling software predicted the necessary separation shown in the empirical data. The Pro *EZGC* chromatogram simulator even accurately accounts for the vacuum the mass spectrometer is drawing at the end of the column. Using GC modeling software during method development to simulate critical separations helps ensure that QC performance requirements will be met during actual sample analysis.
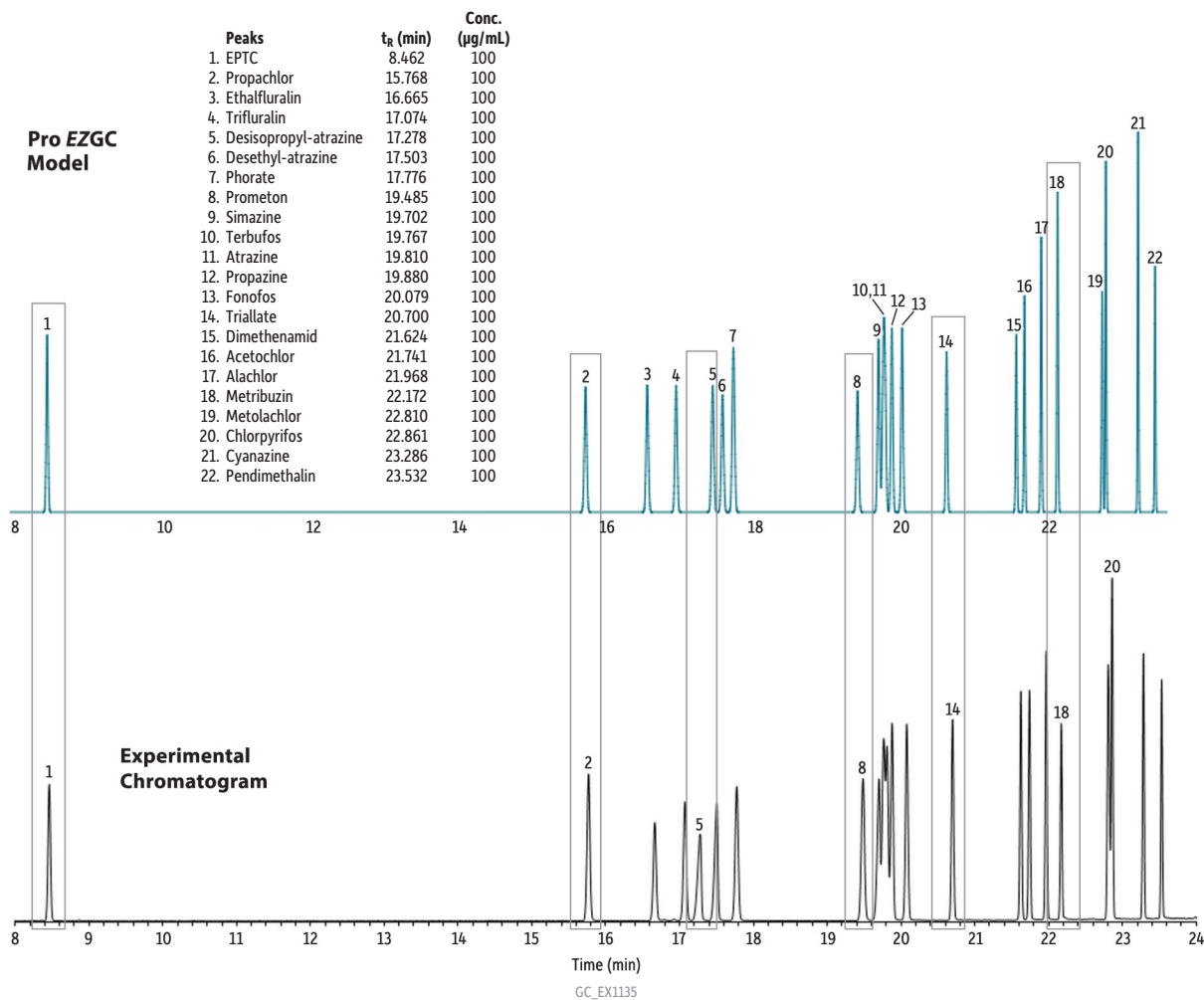
Figure 3: Using GC modeling software for method development assures performance criteria will be met.

Pro *EZGC* Model

Experimental Chromatogram

Time (min)

GC_EX1137

Peaks
1. PCB 31
2. PCB 28
3. PCB 52
4. PCB 101
5. PCB 118
6. PCB 153
7. PCB 138
8. PCB 180
9. PCB 194

Column	Rxi-XLB, 30 m, 0.25 mm ID, 0.25 µm (cat.# 13723)
Sample	PCB congener standard #2 (cat.# 32294) PCB 31 (cat.# custom)
Diluent:	Dichloromethane
Conc.:	3.5 ppm
Injection	
Inj. Vol.:	0.5 µL splitless (hold 1.75 min)
Liner:	2.0 mm ID straight inlet liner w/wool (cat.# 21718)
Inj. Temp.:	300 °C
Purge Flow:	50 mL/min
Oven	
Oven Temp.:	40 °C (hold 2 min) to 240 °C at 30 °C/min (hold 2 min) to 340 °C at 10 °C/min (hold 5 min)
Carrier Gas	He, constant flow
Flow Rate:	1 mL/min
Detector	MS
Mode:	Scan
Transfer Line Temp.:	300 °C
Analyzer Type:	Quadrupole
Source Temp.:	280 °C
Electron Energy:	70 eV
Ionization Mode:	EI
Scan Range:	45-550 amu
Scan Rate:	5 scans/sec
Instrument	PE Clarus 500 GC & Clarus 500 MS

PCB 31 & 28

Example 3: Pro *EZ*GC Software Predicts Correct Elution Order and Relative Retention Times, Even for Sensitive Compounds

The elution of some compounds is very sensitive to column characteristics and conditions. Can GC modeling software accurately simulate elution order and relative retention times in these cases? The example in Figure 4 demonstrates that the Pro *EZ*GC chromatogram simulator predicted the correct elution order and relative retention times for a set of pesticides that are notoriously sensitive to column conditions. The Pro *EZ*GC software even achieves very similar resolution values compared to the experimental data. For GC method development, this means that method performance can be accurately predicted in minutes from your desk instead of by spending hours fine-tuning separations at the bench.

Figure 4: The elution of sensitive compounds can be accurately predicted using Restek's Pro *EZ*GC chromatogram simulator.

Peaks	t_R (min)	Conc. (µg/mL)
1. EPTC	8.462	100
2. Propachlor	15.768	100
3. Ethalfluralin	16.665	100
4. Trifluralin	17.074	100
5. Desisopropyl-atrazine	17.278	100
6. Desethyl-atrazine	17.503	100
7. Phorate	17.776	100
8. Prometon	19.485	100
9. Simazine	19.702	100
10. Terbufos	19.767	100
11. Atrazine	19.810	100
12. Propazine	19.880	100
13. Fonofos	20.079	100
14. Triallate	20.700	100
15. Dimethenamid	21.624	100
16. Acetochlor	21.741	100
17. Alachlor	21.968	100
18. Metribuzin	22.172	100
19. Metolachlor	22.810	100
20. Chlorpyrifos	22.861	100
21. Cyanazine	23.286	100
22. Pendimethalin	23.532	100

GC_EX1135

Column	Rtx-440, 30 m, 0.25 mm ID, 0.25 µm (cat.# 12923)
Sample	Minnesota Ag List 1 pesticide kit (cat.# 32408)
Diluent:	Acetone
Conc.:	100 ppm
Injection	
Inj. Vol.:	1 µL split (split ratio 25:1)
Liner:	Premium 4 mm Precision liner w/wool (cat.# 23305.1)
Inj. Temp.:	300 °C
Oven	
Oven Temp.:	100 °C (hold 0.5 min) to 175 °C at 4 °C/min to 250 °C at 14.5 °C/min
Carrier Gas	He, constant flow
Flow Rate:	2.0 mL/min
Detector	MS
Mode:	Scan

Scan Program:

	Group	Start Time (min)	Scan Range (amu)	Scan Rate (scans/sec)
	1	1.6	40-350	5

Transfer Line Temp.:	300 °C
Analyzer Type:	Quadrupole
Source Type:	Inert
Drawout Plate:	6 mm ID
Source Temp.:	250 °C
Quad Temp.:	180 °C
Electron Energy:	70 eV
Solvent Delay Time:	1.6 min
Tune Type:	PFTBA
Ionization Mode:	EI
Instrument	Agilent 7890A GC & 5975C MSD

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Example 4: Wide Variety of Column Phases in the Pro EZGC Modeler Lets You Try before Buying

Numerous GC column stationary phases have been developed over the years because their distinct selectivities provide important differences in separations. Different phases can provide improved chromatographic performance for specific analytes and, in some cases, initial results must be confirmed via an analysis on a secondary column of different selectivity. Confirmation analysis with a second column that provides retention time and elution order changes is often performed when using some detectors, such as FIDs or ECDs, because a greater degree of confidence is achieved when target analytes are observed in both analyses.

The Pro *EZ*GC chromatogram simulator includes a wide range of column phases (Table I) that differ significantly in selectivity. Because Pro *EZ*GC modeling software includes a diverse range of compound libraries and column phases, GC method developers can use the tool to test the performance of different columns, and buy only the ones that provide optimal selectivity for their own specific target analytes.

Table I: Current phases and compound libraries available in the Pro *EZ*GC chromatogram modeler.

Phases	Compound Classes
Rxi-17	Flavors & Fragrances
Rxi-17Sil MS	Polycyclic Aromatic Hydrocarbons (PAHs), Flavors & Fragrances
Rxi-35Sil MS	Phthalates
Rxi-5Sil MS	Polychlorinated Biphenyls (PCBs), Semivolatile Organic Compounds (SVOCs)
Rxi-5ms	Semivolatile Organic Compounds (SVOCs), Pesticides
Rxi-624Sil MS	Volatile Organic Compounds (VOCs)
Rxi-PAH	Polycyclic Aromatic Hydrocarbons (PAHs)
Rxi-XLB	Polychlorinated Biphenyls (PCBs)
Rtx-1	Solvents, Flavors & Fragrances, Drugs, Pesticides, Volatile Organic Compounds (VOCs)
Rtx-1614	Flame Retardants (FRs)
Rtx-1701	Pesticides, Herbicides
Rtx-200	Drugs
Rtx-35	Drugs, Pesticides, Herbicides, Polychlorinated Biphenyls (PCBs)
Rtx-440	Pesticides & Herbicides, Polychlorinated Biphenyls (PCBs)
Rtx-5	Drugs, Pesticides, Herbicides, Semivolatile Organic Compounds (SVOCs)
Rtx-50	Drugs, Pesticides, Polychlorinated Biphenyls (PCBs)
Rtx-502.2	Volatile Organic Compounds (VOCs), Solvents
Rtx-624	Volatile Organic Compounds (VOCs)
Rtx-CLPesticides	Pesticides
Rtx-CLPesticides2	Pesticides
Rtx-OPPesticides	Organophosphorus Pesticides (OPPs)
Rtx-OPPesticides2	Organophosphorus Pesticides (OPPs)
Rtx-PCB	Polychlorinated Biphenyls (PCBs), Pesticides
Rtx-VMS	Volatile Organic Compounds (VOCs), Halocarbons, Hydrocarbons, Alcohols, Aldehydes, Ethers & Esters, "Acetates Plus," Glycol Ethers, Alkanes
Rtx-VRX	Volatile Organic Compounds (VOCs)
Rtx-XLB	Pesticides & Semivolatile Organic Compounds (SVOCs)
Rt-2560	Food Fatty Acid Methyl Esters (FAMEs)
RT-2330	Fatty Acid Methyl Esters (FAMEs)
Stabilwax	Solvents, Flavors & Fragrances, Fatty Acid Methyl Esters (FAMEs)

Example 5: Pro EZGC Chromatogram Simulator Gives an Excellent Overall Match, Even for Different Experimental Setups

This final example illustrates that some experimental setups will generate slightly different results than the Pro *EZ*GC model but, even in these situations, the match is excellent and provides a great starting place for GC method development. The Pro *EZ*GC modeling software assumes an ideal split/splitless sample introduction onto the column, so in a case where the actual sample was introduced via headspace with a sampling loop, there are differences in retention time that result from the additional time required to transfer the sample to the column. Peak widths may also increase due to band broadening that occurs during the sample introduction process. As shown in Figure 5, despite these differences, the Pro *EZ*GC chromatogram simulator produces a very close match to the experimental separation in terms of relative peak resolution. This allows method developers, who will ultimately use a different sample introduction technique, to still benefit from using Pro *EZ*GC modeling software.

Figure 5: While exact retention times shifted due to the use of a headspace sampling loop, the overall separation predicted by the Pro *EZ*GC chromatogram modeler is very close to the actual experimental results.

Pro *EZ*GC Model

Experimental Chromatogram

Time (min)

GC_EX1138
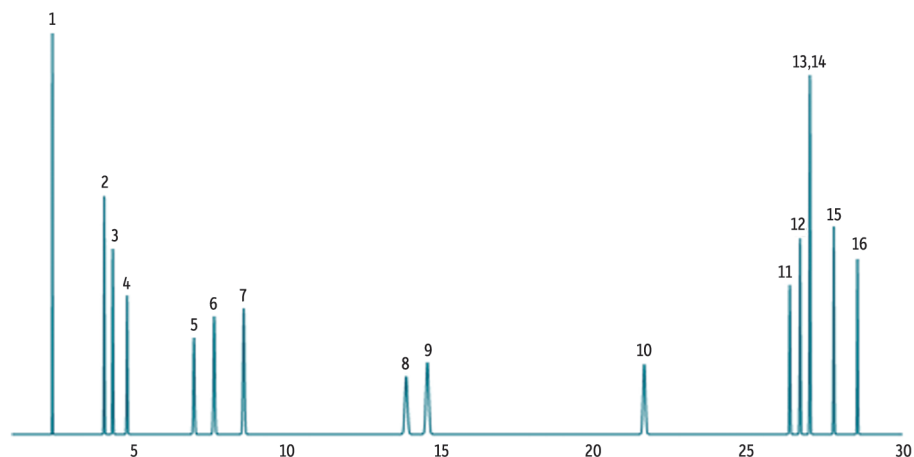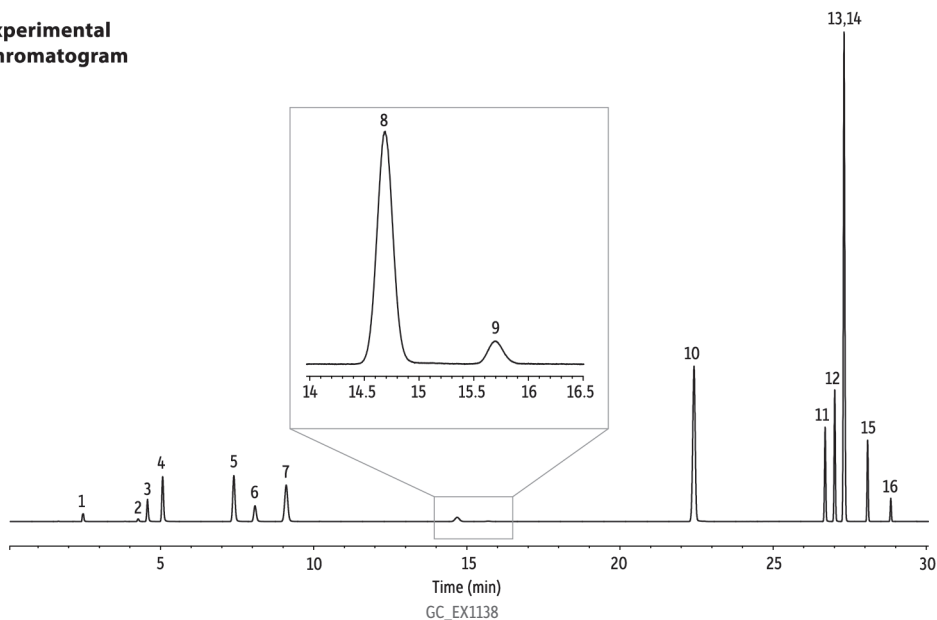
Peaks
1. Methanol
2. Acetonitrile
3. Methylene chloride
4. *trans*-1,2-Dichloroethene
5. *cis*-1,2-Dichloroethene
6. Tetrahydrofuran
7. Cyclohexane
8. Methylcyclohexane
9. 1,4-Dioxane
10. Toluene
11. Chlorobenzene
12. Ethylbenzene
13. *m*-Xylene
14. *p*-Xylene
15. *o*-Xylene
16. Cumene

Column — Rxi-624Sil MS, 30 m, 0.32 mm ID, 1.80 µm (cat.# 13870)
Sample — Residual solvents Class 2 — Mix A (2013 Rev) (cat.# 36012)
Diluent: Water
Injection
Inj. Vol.: 1,000 µL headspace-loop split (split ratio 5:1)
Liner: Premium 1.0 mm ID straight inlet liner (cat.# 23333.1)

Headspace-Loop
Inj. Port Temp.: 140 °C
Instrument: Tekmar HT-3
Inj. Time: 1.0 min
Transfer Line Temp.: 105 °C
Valve Oven Temp.: 105 °C
Needle Temp.: 85 °C
Sample Temp.: 80 °C
Sample Equil. Time: 60 min
Mixer time: 5.0 min
Mixing level: 5
Mixer stabilize time: 0.50 min

Vial Pressure: 10 psi
Pressurize Time: 5.0 min
Pressure Equilibration
 Time: 0.20 min
Loop Pressure: 5.0 psi
Loop Fill Time: 2.0 min
Oven
Oven Temp.: 40 °C (hold 20 min) to 240 °C at 10 °C/min (hold 20 min)
Carrier Gas He, constant flow
Flow Rate: 2.2 mL/min
Detector FID @ 250 °C
Make-up Gas
 Flow Rate: 45 mL/min
Make-up Gas
 Type: N₂
Hydrogen flow: 40 mL/min
Air flow: 450 mL/min
Data Rate: 20 Hz
Instrument Agilent/HP6890 GC

When Models Meet Reality

When it comes to accurately predicting the chromatographic performance of a set of compounds on a given GC column under certain conditions, nothing beats Pro *EZGC* modeling software. Restek's chemists use it extensively to develop applications and, despite the fact that some real-world situations, such as sample introduction via headspace transfer lines or inaccurate flow rates, introduce variables that may require slight adjustments from the modeled results, the Pro *EZGC* chromatogram simulator still arrives at a modeled chromatogram and a set of conditions that serve as excellent starting conditions for any further method refinement that may be necessary.

Try it yourself for free!

All of the examples shown here are cases where the model was able to replicate empirical results with impressive accuracy. If you have a list of compounds, get started using our free Pro *EZGC* modeling software, and let Restek's years of chromatographic experience do the work for you! GC method development has never been so easy.

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