How to Develop GC Methods That Meet Both Technical and Business Demands

Use Pro *EZ*GC Software to Quickly Compare Columns, Conditions, and MS versus Non-MS Detection

Related Products

- *Rtx-VMS cat.# 19915*

Many factors go into GC method development: fast run times, adequate separations, symmetric peak shapes, good sensitivity, and many other chromatographic issues that need to be optimized. But business factors also need to be considered. Lab managers need to budget time for method development and weigh which instruments they want to use for specific methods in order to maximize productivity and profitability. Fortunately, using Restek's free Pro *EZ*GC chromatogram modeling software makes it easy to quickly evaluate methods virtually without tying up an instrument in the lab. And now it can also be used to help lab managers decide whether an MS or non-MS platform will be used.

Getting Started

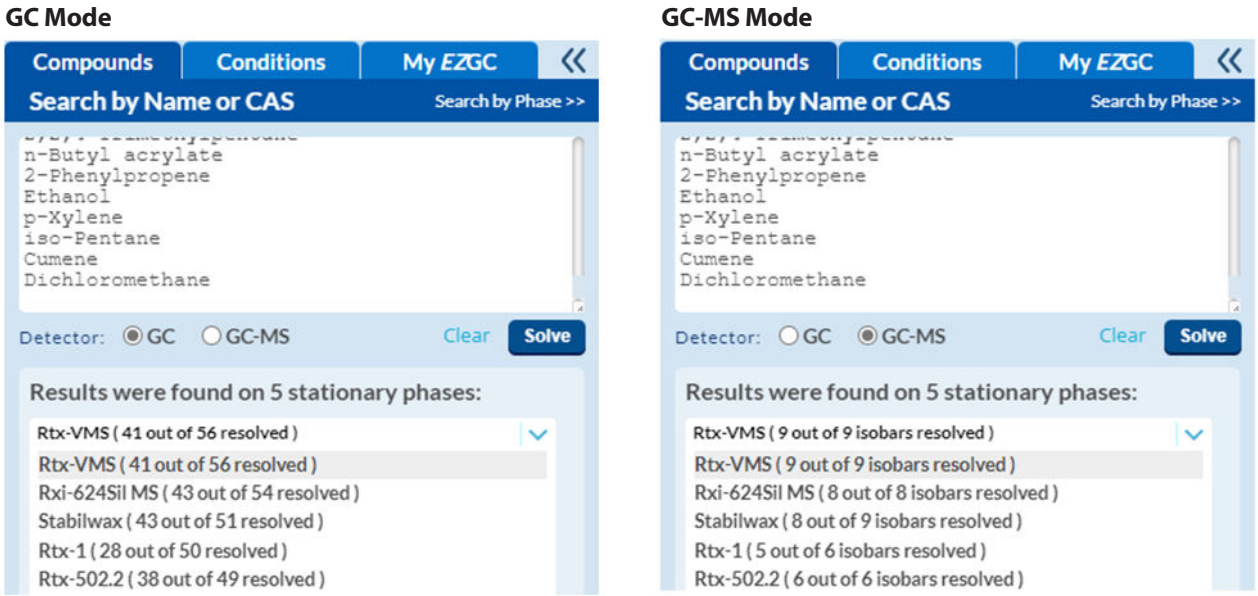
Let's say, for example, that we need to develop a new method for the 56 volatile compounds listed below, and we also want to determine whether GC-MS or GC with a non-MS detector is the best approach for our lab. Simulating separations with different columns and conditions using Pro *EZ*GC software has been a useful tool for evaluating chromatographic parameters for years, but a new GC-MS mode that automatically targets isobaric compounds for separation allows us to more efficiently compare MS and non-MS methods.

Target Analytes

- 2-Propanol
- 1-Methoxypropan-2-ol
- Octanal
- Diisopropyl ether
- Heptane
- Cyclohexane
- Ethyl Acetate
- Allyl alcohol
- 2-(2-Butoxyethoxy)ethanol
- 1,2-Dichlorobenzene
- Methyl ethyl ketone
- Toluene
- Acetone
- Limonene
- Benzene
- Pentyl acetate
- Chloroform
- Naphthalene
- 1-Propanol
- Decane
- 2-(2-Methoxyethoxy)ethanol
- Octane
- Isopropyl acetate
- Benzyl Alcohol
- Ethyl methacrylate
- Pyridine
- 2-Chlorotoluene
- Isobutanol
- Vinyl acetate
- Acetonitrile
- Methyl acrylate
- Bromobenzene
- n-Butyl acetate
- 2-Butoxyethyl acetate
- Pentane
- Tetrahydrofuran
- Nonane
- Methylcyclohexane
- o-Xylene
- 4-Ethyltoluene
- Ethylbenzene
- 2-Hexanone
- Acrylonitrile
- Carbon Tetrachloride
- Propyl acetate
- 1,1-Dichloroethane
- 2-Butoxyethanol
- Hexane
- 2,2,4-Trimethylpentane
- n-Butyl acrylate
- 2-Phenylpropene
- Ethanol
- p-Xylene
- iso-Pentane
- Cumene
- Dichloromethane

To get started, we go to ez.restek.com/proezgc; enter our analyte list in the Compounds tab (no experimental data needed); select a detection mode; and click the Solve button. GC mode will attempt to separate all compounds and will produce modeled results and conditions that could be used with a non-MS detector (e.g., FID or ECD). In contrast, GC-MS mode will automatically target only isobars because, when using MS, they are the only compounds that require chromatographic resolution. In both cases, the software will generate a list summarizing which column stationary phases could be used and how many compounds (GC) or isobars (GC-MS) they will separate (Figure 1).

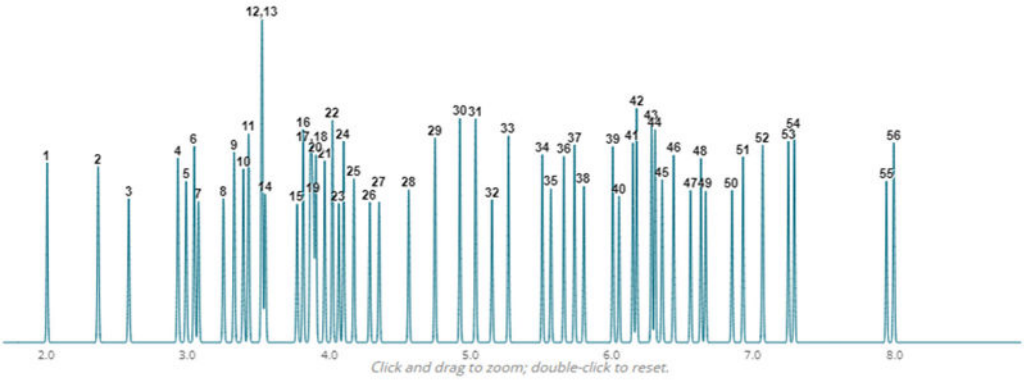
Figure 1: In the Compounds tab, enter your analytes, select a detection mode, and click Solve to generate a list of stationary phases and a summary of the compounds they will separate.



Evaluating Initial Results

Initial results for the non-MS model show 41 out of 56 compounds can be fully resolved (Rs ≥1.5) on an Rtx-VMS column in an eight-minute run (Figure 2). This may be acceptable depending on which specific compounds individual labs are analyzing, what degree of resolution is needed, and whether a screening or quantitative method is being developed. For the MS model, nine isobaric ions are present, and the compounds sharing them are all resolved to baseline in a slightly longer nine-minute analysis (Figure 3). As shown in Figure 4, individual isobaric ions can be selected, and the modeler will highlight the separation of all compounds sharing that ion.

Figure 2: GC Model–Initial

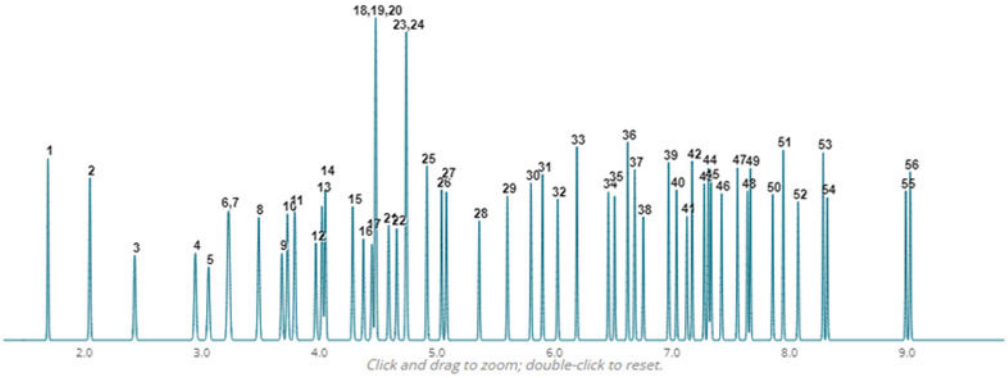


Column: **Rtx-VMS**, 30 m, 0.25 mm ID, 1.4 µm (cat.# 19915)
Carrier Gas: Helium, Constant Flow @ 2.00 mL/min
Average Velocity: 40.97 cm/sec
Outlet Pressure (abs): 14.70 psi
Oven Temp.: 35 °C (hold 1 min) to 60 °C @ 16 °C/min to 225 °C @ 30 °C/min

Peaks	t_R (min)	R_s	Peak Width (min)	T_{peak} (°C)
1. iso-Pentane	2.00	14.7	0.021	51.1
2. Pentane	2.37	9	0.025	56.9
3. Ethanol	2.58	9	0.024	60.6
4. Dichloromethane	2.93	2.3	0.025	71.1
5. Acetone	2.99	2.3	0.025	72.8
6. 2-Propanol	3.05	1.2	0.024	74.5
7. Hexane	3.08	1.2	0.024	75.4
8. Acetonitrile	3.25	3.1	0.025	80.7
9. Diisopropyl ether	3.33	2.6	0.024	83.0
10. 1,1-Dichloroethane	3.39	1.5	0.025	85.0
11. Acrylonitrile	3.43	1.5	0.024	86.1
12. Vinyl acetate	3.52	0.1	0.024	88.8
13. Allyl alcohol	3.53	0.1	0.023	88.9
14. 1-Propanol	3.55	0.9	0.023	89.6
15. Cyclohexane	3.77	1.7	0.024	96.4
16. Chloroform	3.82	1.7	0.024	97.6
17. Ethyl Acetate	3.87	0.4	0.023	99.1
18. Methyl acrylate	3.88	0.4	0.023	99.5
19. Carbon Tetrachloride	3.89	0.5	0.024	99.8
20. Tetrahydrofuran	3.91	0.6	0.024	100.3
21. Methyl ethyl ketone	3.97	2.3	0.024	102.2
22. 2,2,4-Trimethylpentane	4.02	1.9	0.023	103.8
23. Heptane	4.07	1.4	0.023	105.2
24. Benzene	4.10	1.4	0.024	106.2
25. Isobutanol	4.18	3.3	0.022	108.4
26. Isopropyl acetate	4.29	2.8	0.022	111.8
27. Methylcyclohexane	4.35	2.8	0.023	113.7
28. 1-Methoxypropan-2-ol	4.56	8.3	0.023	120.1

Peaks	t_R (min)	R_s	Peak Width (min)	T_{peak} (°C)
29. Propyl acetate	4.75	8	0.022	125.6
30. Octane	4.93	4.8	0.022	130.9
31. Toluene	5.04	4.8	0.023	134.2
32. Pyridine	5.15	5	0.023	137.7
33. Ethyl methacrylate	5.27	5.3	0.022	141.2
34. n-Butyl acetate	5.51	2.7	0.022	148.4
35. 2-Hexanone	5.57	2.7	0.022	150.2
36. Nonane	5.66	3.3	0.022	153.0
37. Ethylbenzene	5.74	2.9	0.022	155.2
38. p-Xylene	5.80	2.9	0.022	157.2
39. o-Xylene	6.01	2	0.022	163.3
40. n-Butyl acrylate	6.05	2	0.021	164.7
41. Cumene	6.15	1.2	0.022	167.6
42. Pentyl acetate	6.18	1.2	0.021	168.4
43. 2-Butoxyethanol	6.28	1.1	0.022	171.6
44. Decane	6.31	1.1	0.021	172.3
45. Bromobenzene	6.36	2.1	0.023	173.8
46. 2-Chlorotoluene	6.44	3.5	0.023	176.3
47. 2-Phenylpropene	6.56	3.3	0.022	179.9
48. 2-(2-Methoxyethoxy)ethanol	6.63	1.5	0.022	182.1
49. Limonene	6.66	1.5	0.022	183.1
50. 4-Ethyltoluene	6.85	3.5	0.023	188.7
51. Octanal	6.93	3.5	0.022	191.0
52. 1,2-Dichlorobenzene	7.07	6	0.023	195.2
53. 2-Butoxyethyl acetate	7.25	1.8	0.021	200.6
54. Benzyl Alcohol	7.29	1.8	0.022	201.9
55. 2-(2-Butoxyethoxy)ethanol	7.94	2.2	0.022	221.4
56. Naphthalene	8.00	2.2	0.023	223.0

Figure 3: GC-MS Model–Initial



Available Isobars: Select an Isobar Reset

Column: **Rtx-VMS**, 30 m, 0.25 mm ID, 1.4 µm (cat.# 19915)
Carrier Gas: Helium, Constant Flow @ 2.00 mL/min
Average Velocity: 50.96 cm/sec
Outlet Pressure (abs): 0.00 psi
Oven Temp.: 35 °C (hold 3 min) to 225 °C @ 30 °C/min

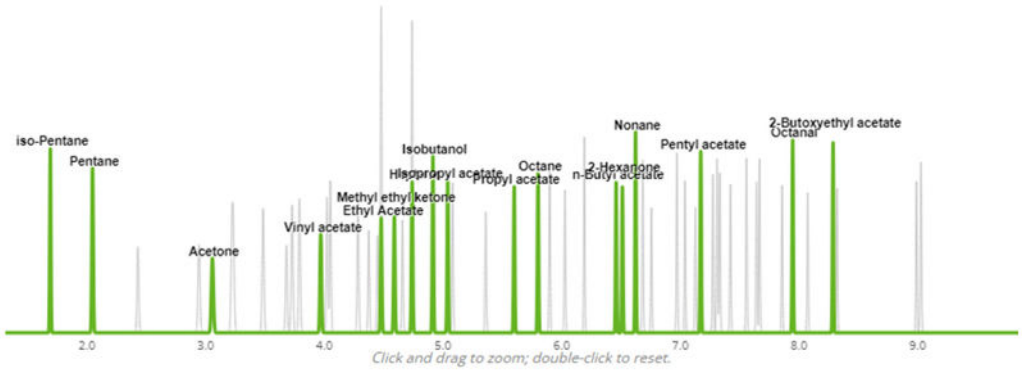
Peaks	t_R (min)	R_s	Peak Width (min)	T_{peak} (°C)	Quantifier Ion	Secondary Ion
1. **iso-Pentane**	1.69	13.4	0.021	35.0	43.0	42.0
2. **Pentane**	2.05	13.4	0.026	35.0	43.0	42.0
3. **Ethanol**	2.43	21.4	0.032	35.0	45.0	46.0
4. **Dichloromethane**	2.94	--	0.039	35.0	49.0	84.0
5. **Acetone**	3.06	25.8	0.039	36.7	43.0	58.0
6. **2-Propanol**	3.22	14.3	0.037	41.6	45.0	43.0
7. **Hexane**	3.23	27.3	0.037	42.0	57.0	43.0
8. **Acetonitrile**	3.48	--	0.035	49.5	41.0	40.0
9. **Diisopropyl ether**	3.68	14.3	0.032	55.4	45.0	43.0
10. **1,1-Dichloroethane**	3.73	--	0.033	56.9	63.0	65.0
11. **Acrylonitrile**	3.79	--	0.032	58.7	53.0	52.0
12. **Vinyl acetate**	3.97	19	0.030	64.1	43.0	86.0
13. **Allyl alcohol**	4.02	23.8	0.029	65.7	57.0	39.0
14. **1-Propanol**	4.05	15.3	0.029	66.5	42.0	59.0
15. **Cyclohexane**	4.28	--	0.029	73.5	56.0	84.0
16. **Chloroform**	4.38	27.9	0.028	76.2	83.0	85.0
17. **Carbon Tetrachloride**	4.45	--	0.028	78.5	117.0	119.0
18. **Methyl acrylate**	4.48	120	0.027	79.3	55.0	85.0
19. **Ethyl Acetate**	4.48	4.1	0.027	79.4	43.0	61.0
20. **Tetrahydrofuran**	4.48	15.3	0.028	79.4	42.0	41.0
21. **Methyl ethyl ketone**	4.59	4.1	0.027	82.7	43.0	72.0
22. **2,2,4-Trimethylpentane**	4.66	23.8	0.027	84.8	57.0	56.0
23. **Heptane**	4.74	5.7	0.026	87.2	43.0	41.0
24. **Benzene**	4.74	--	0.027	87.2	78.0	77.0
25. **Isobutanol**	4.92	5.1	0.024	92.5	43.0	41.0
26. **Isopropyl acetate**	5.04	5.1	0.024	96.2	43.0	61.0
27. **Methylcyclohexane**	5.08	27.9	0.025	97.4	83.0	55.0
28. **1-Methoxypropan-2-ol**	5.36	69.9	0.024	105.8	45.0	47.0
29. **Propyl acetate**	5.60	8.8	0.023	113.0	43.0	61.0
30. **Octane**	5.80	8.8	0.023	119.0	43.0	41.0

(Continued on page 5.)

Figure 3: Continued

31. **Toluene**	5.90	34.7	0.023	122.0	91.0	92.0
32. **Pyridine**	6.03	106	0.024	125.8	79.0	52.0
33. **Ethyl methacrylate**	6.19	--	0.022	130.7	69.0	41.0
34. **n-Butyl acetate**	6.46	2.3	0.022	138.8	43.0	56.0
35. **2-Hexanone**	6.51	2.3	0.022	140.4	43.0	58.0
36. **Nonane**	6.62	5	0.022	143.7	43.0	57.0
37. **Ethylbenzene**	6.68	3.2	0.023	145.5	91.0	106.0
38. **p-Xylene**	6.76	3.2	0.022	147.7	91.0	106.0
39. **o-Xylene**	6.97	9.6	0.022	154.2	91.0	106.0
40. **n-Butyl acrylate**	7.04	120	0.021	156.2	55.0	56.0
41. **Cumene**	7.13	32.8	0.022	158.8	105.0	120.0
42. **Pentyl acetate**	7.17	25.8	0.021	160.2	43.0	70.0
43. **2-Butoxyethanol**	7.28	1.5	0.022	163.3	57.0	45.0
44. **Decane**	7.31	1.5	0.021	164.3	57.0	43.0
45. **Bromobenzene**	7.33	--	0.023	165.0	77.0	156.0
46. **2-Chlorotoluene**	7.42	19.9	0.023	167.7	91.0	126.0
47. **2-Phenylpropene**	7.56	--	0.022	171.7	118.0	117.0
48. **2-(2-Methoxyethoxy)ethanol**	7.64	62.1	0.022	174.3	45.0	59.0
49. **Limonene**	7.67	--	0.022	175.0	68.0	93.0
50. **4-Ethyltoluene**	7.86	32.8	0.022	180.7	105.0	120.0
51. **Octanal**	7.95	16.1	0.022	183.4	43.0	44.0
52. **1,2-Dichlorobenzene**	8.07	--	0.023	187.2	146.0	148.0
53. **2-Butoxyethyl acetate**	8.29	16.1	0.021	193.6	43.0	57.0
54. **Benzyl Alcohol**	8.32	106	0.022	194.6	79.0	108.0
55. **2-(2-Butoxyethoxy)ethanol**	8.99	62.1	0.022	214.7	45.0	57.0
56. **Naphthalene**	9.03	--	0.023	215.8	128.0	129.0

Figure 4: Selecting an ion from the Available Isobars field highlights the separation of compounds sharing that ion (e.g., m/z 43) and gives the resolution value of the closest eluting pair.



Available Isobars: m/z 43 Critical Pair 34,35 Rs 2.39 Reset

Column: **Rtx-VMS**, 30 m, 0.25 mm ID, 1.4 µm (cat.# 19915)
Carrier Gas: Helium, Constant Flow @ 2.00 mL/min
Average Velocity: 50.96 cm/sec
Outlet Pressure (abs): 0.00 psi
Oven Temp.: 35 °C (hold 3 min) to 225 °C @ 30 °C/min

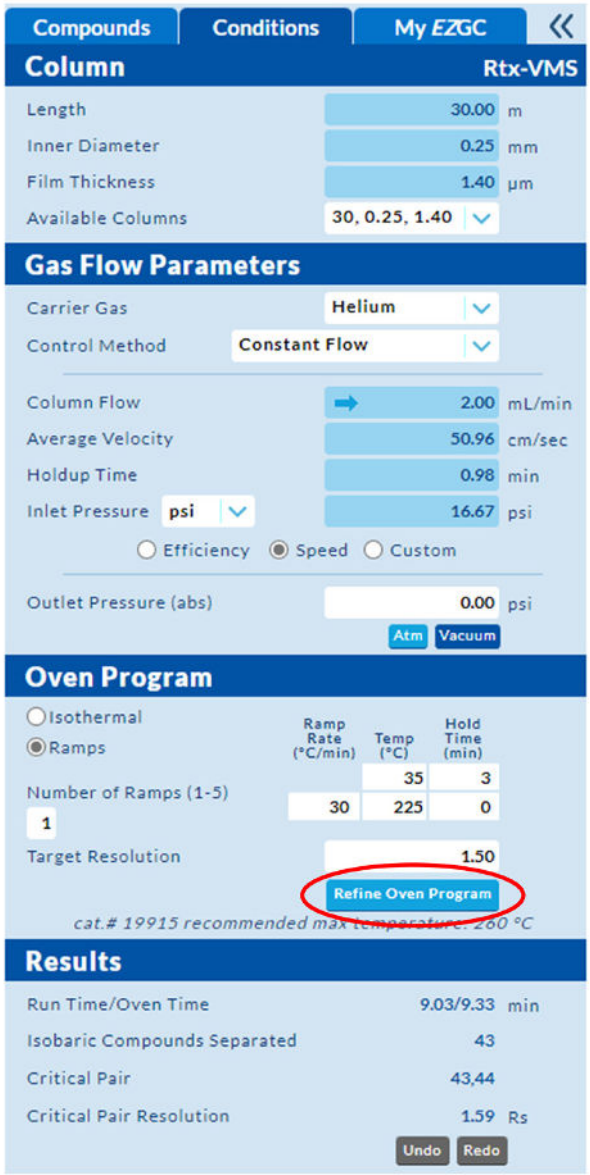
From the initial simulated chromatogram results, we could select GC-MS for developing our final method in the lab since all the isobars are resolved in a reasonable analysis time, but what if we prefer to use a non-MS method for business reasons (e.g., the GC-MS is often unavailable, or we want to keep it open for more profitable samples)? Using the Pro *EZ*GC chromatogram modeler, we can further optimize both methods to better inform our decision.

Fine-Tuning Methods

For our purposes, we will select the Rtx-VMS column recommended by the software on the Compounds tab for both the GC and GC-MS models before we optimize them, but it is important to note that users can choose other columns from that list if desired. This can be useful if you want to evaluate columns that you already have, or if you want to see results on a different stationary phase before buying a new column.

To further refine our methods, we will now move to the Conditions tab. Here, models can be fine-tuned manually by adding gradients and/or modifying any of the input fields, but the simplest way to optimize a method is to use the Refine Oven Program button (Figure 5). As method parameters are changed, the results summary at the bottom of the Conditions tab and the simulated chromatogram and peak information are automatically updated. Users can also save models for easy reference and comparison.

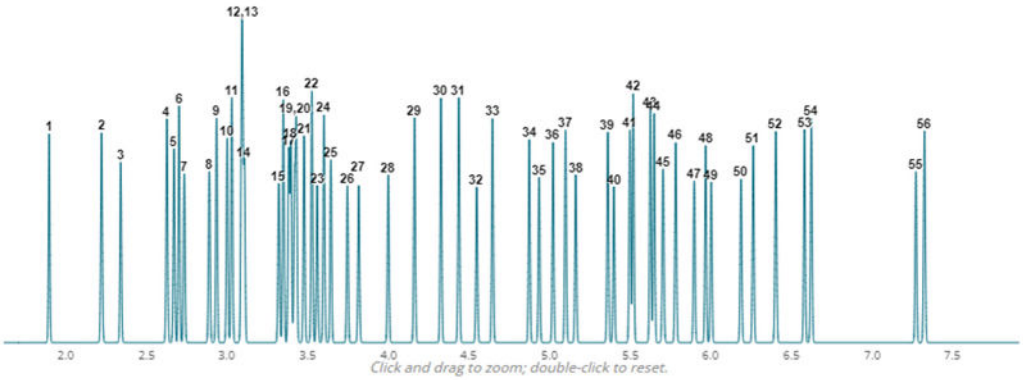
Figure 5: Change parameters on the Conditions tab to optimize your separations (example shown is in GC-MS mode).



For our purposes, we used the Refine Oven Program button to generate the final optimized models shown in Figures 6 (GC mode) and 7 (GC-MS mode). The Refine Oven Program button can be clicked multiple times if run time or resolution can be improved with different temperature ramps, and it will disable and turn gray when no further automatic refinements are available.

Comparing the initial and final GC mode models, we can see that a slightly faster overall run time was achieved in the final optimized model and resolution was improved for some compounds but diminished for others. For example, 2-propanol and hexane (peaks 6 and 7) were not adequately resolved (Rs = 1.2) under the initial modeled conditions but were separated to baseline (Rs = 1.5) using the optimized conditions. In contrast, resolution between cyclohexane and chloroform (peaks 15 and 16) passed in the initial model (Rs = 1.7) but decreased in the optimized model (Rs = 1.2), highlighting the importance of labs evaluating results for their specific analyte lists against their own chromatographic requirements.

Figure 6: GC Model–Optimized



Column: **Rtx-VMS**, 30.00 m, 0.25 mm ID, 1.40 µm (cat.# 19915)
Carrier Gas: Helium, Constant Flow @ 2.00 mL/min
Average Velocity: 40.97 cm/sec
Outlet Pressure (abs): 14.70 psi
Oven Temp.: 35 °C (hold 0.5 min) to 60 °C @ 18 °C/min to 225 °C @ 30 °C/min

Peaks	t_R (min)	R_s	Peak Width (min)	T_{peak} (°C)	Peaks	t_R (min)	R_s	Peak Width (min)	T_{peak} (°C)
1. iso-Pentane	1.90	14.9	0.019	60.2	29. Propyl acetate	4.16	7.6	0.021	128.2
2. Pentane	2.22	5.8	0.022	70.0	30. Octane	4.33	5	0.021	133.1
3. Ethanol	2.34	5.8	0.020	73.5	31. Toluene	4.44	4.9	0.022	136.4
4. Dichloromethane	2.63	2	0.021	82.1	32. Pyridine	4.55	4.6	0.022	139.8
5. Acetone	2.67	1.5	0.022	83.4	33. Ethyl methacrylate	4.65	4.6	0.021	142.7
6. 2-Propanol	2.70	1.5	0.021	84.4	34. n-Butyl acetate	4.87	2.8	0.021	149.5
7. Hexane	2.73	1.5	0.021	85.4	35. 2-Hexanone	4.93	2.8	0.022	151.4
8. Acetonitrile	2.89	2	0.022	90.0	36. Nonane	5.02	3.5	0.021	154.0
9. Diisopropyl ether	2.93	2	0.021	91.3	37. Ethylbenzene	5.10	2.8	0.022	156.3
10. 1,1-Dichloroethane	3.00	1.3	0.022	93.3	38. p-Xylene	5.16	2.8	0.022	158.2
11. Acrylonitrile	3.03	1.3	0.022	94.2	39. o-Xylene	5.36	1.7	0.022	164.2
12. Allyl alcohol	3.09	0.3	0.021	96.0	40. n-Butyl acrylate	5.40	1.7	0.021	165.3
13. Vinyl acetate	3.10	0.3	0.022	96.2	41. Cumene	5.50	0.9	0.022	168.3
14. 1-Propanol	3.11	0.5	0.021	96.5	42. Pentyl acetate	5.52	0.9	0.021	168.9
15. Cyclohexane	3.32	1.2	0.022	102.9	43. 2-Butoxyethanol	5.63	1	0.022	172.1
16. Chloroform	3.35	1.2	0.022	103.8	44. Decane	5.65	1	0.021	172.8
17. Ethyl Acetate	3.38	0.6	0.021	104.8	45. Bromobenzene	5.70	2.4	0.023	174.4
18. Methyl acrylate	3.40	0.6	0.022	105.2	46. 2-Chlorotoluene	5.78	3.4	0.023	176.8
19. Carbon Tetrachloride	3.42	0.5	0.022	105.9	47. 2-Phenylpropene	5.90	3.2	0.022	180.3

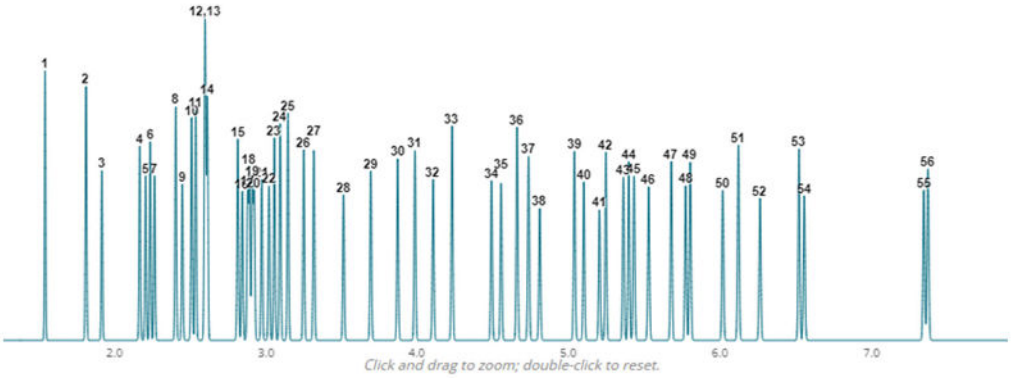
(Continued on page 8.)

Figure 6: Continued

20. Tetrahydrofuran	3.43	0.5	0.022	106.2
21. Methyl ethyl ketone	3.48	2.1	0.022	107.7
22. 2,2,4-Trimethylpentane	3.52	1.5	0.022	109.1
23. Heptane	3.56	1.5	0.022	110.1
24. Benzene	3.60	1.8	0.022	111.3
25. Isobutanol	3.64	2	0.021	112.6
26. Isopropyl acetate	3.75	3.1	0.021	115.7
27. Methylcyclohexane	3.82	3.1	0.022	117.8
28. 1-Methoxypropan-2-ol	4.00	7.6	0.022	123.3
48. 2-(2-Methoxyethoxy)ethanol	5.97	1.5	0.022	182.4
49. Limonene	6.00	1.5	0.022	183.4
50. 4-Ethyltoluene	6.19	3.4	0.022	188.9
51. Octanal	6.26	3.4	0.022	191.2
52. 1,2-Dichlorobenzene	6.40	6.1	0.023	195.4
53. 2-Butoxyethyl acetate	6.58	1.9	0.021	200.8
54. Benzyl Alcohol	6.62	1.9	0.022	202.0
55. 2-(2-Butoxyethoxy)ethanol	7.27	2.2	0.022	221.5
56. Naphthalene	7.33	2.2	0.023	223.1

Similarly, the GC-MS model was further optimized using the Refine Oven Program button. In this case, as shown in Figure 7, baseline resolution was maintained for all the isobaric compounds, and the overall analysis time (termed "oven time" in the Results section of the Conditions tab) was reduced from 9.33 minutes to 8.10 minutes. While there are some coeluting compounds (e.g., allyl alcohol and vinyl acetate) in this model, it is not a concern because none of the coeluting compounds are isobars so the MS detector will be able to distinguish them.

Figure 7: GC-MS Model–Optimized



Available Isobars: Select an Isobar Reset

Column: **Rtx-VMS**, 30.00 m, 0.25 mm ID, 1.40 µm (cat.# 19915)
Carrier Gas: Helium, Constant Flow @ 2.00 mL/min
Average Velocity: 50.96 cm/sec
Outlet Pressure (abs): 0.00 psi
Oven Temp.: 35 °C (hold 0.5 min) to 225 °C @ 25 °C/min

Peaks	t_R (min)	R_s	Peak Width (min)	T_{peak} (°C)	Quantifier Ion	Secondary Ion
1. iso-Pentane	1.54	13.9	0.016	61.1	43.0	42.0
2. Pentane	1.81	13.9	0.019	67.8	43.0	42.0
3. Ethanol	1.92	16.3	0.018	70.5	45.0	46.0
4. Dichloromethane	2.17	--	0.020	76.7	49.0	84.0
5. Acetone	2.21	18.9	0.020	77.7	43.0	58.0
6. 2-Propanol	2.24	10.4	0.020	78.5	45.0	43.0
7. Hexane	2.27	16.2	0.020	79.2	57.0	43.0
8. Acetonitrile	2.41	--	0.021	82.7	41.0	40.0
9. Diisopropyl ether	2.45	10.4	0.020	83.8	45.0	43.0
10. 1,1-Dichloroethane	2.51	--	0.021	85.3	63.0	65.0

(Continued on page 9.)

Figure 7: Continued

11. Acrylonitrile	2.54	--	0.021	85.9	53.0	52.0
12. Allyl alcohol	2.60	16.2	0.021	87.4	57.0	39.0
13. Vinyl acetate	2.60	13.1	0.021	87.6	43.0	86.0
14. 1-Propanol	2.62	14	0.021	87.9	42.0	59.0
15. Cyclohexane	2.82	--	0.022	92.9	56.0	84.0
16. Chloroform	2.85	21	0.022	93.6	83.0	85.0
17. Ethyl Acetate	2.88	4.2	0.021	94.5	43.0	61.0
18. Methyl acrylate	2.89	95.4	0.022	94.8	55.0	85.0
19. Carbon Tetrachloride	2.91	--	0.022	95.3	117.0	119.0
20. Tetrahydrofuran	2.92	14	0.022	95.6	42.0	41.0
21. Methyl ethyl ketone	2.97	3.8	0.022	96.8	43.0	72.0
22. 2,2,4-Trimethylpentane	3.02	19.3	0.022	98.0	57.0	56.0
23. Heptane	3.06	3.8	0.022	98.9	43.0	41.0
24. Benzene	3.10	--	0.022	99.9	78.0	77.0
25. Isobutanol	3.15	4.2	0.021	101.2	43.0	41.0
26. Isopropyl acetate	3.25	4.7	0.022	103.8	43.0	61.0
27. Methylcyclohexane	3.32	21	0.022	105.5	83.0	55.0
28. 1-Methoxypropan-2-ol	3.51	47.4	0.022	110.4	45.0	47.0
29. Propyl acetate	3.69	7.9	0.022	114.8	43.0	61.0
30. Octane	3.87	7.9	0.022	119.3	43.0	41.0
31. Toluene	3.98	31.4	0.023	122.1	91.0	92.0
32. Pyridine	4.11	101	0.024	125.1	79.0	52.0
33. Ethyl methacrylate	4.23	--	0.023	128.2	69.0	41.0
34. n-Butyl acetate	4.49	2.7	0.023	134.8	43.0	56.0
35. 2-Hexanone	4.55	2.7	0.023	136.3	43.0	58.0
36. Nonane	4.66	4.5	0.023	139.0	43.0	57.0
37. Ethylbenzene	4.74	3.1	0.024	140.9	91.0	106.0
38. p-Xylene	4.81	3.1	0.024	142.7	91.0	106.0
39. o-Xylene	5.04	9.5	0.024	148.4	91.0	106.0
40. n-Butyl acrylate	5.10	95.4	0.023	150.0	55.0	56.0
41. Cumene	5.20	32.9	0.024	152.6	105.0	120.0
42. Pentyl acetate	5.25	25.4	0.023	153.6	43.0	70.0
43. 2-Butoxyethanol	5.36	1.5	0.024	156.5	57.0	45.0
44. Decane	5.40	1.5	0.023	157.4	57.0	43.0
45. Bromobenzene	5.43	--	0.025	158.3	77.0	156.0
46. 2-Chlorotoluene	5.53	19.8	0.025	160.7	91.0	126.0
47. 2-Phenylpropene	5.68	--	0.024	164.4	118.0	117.0
48. 2-(2-Methoxyethoxy)ethanol	5.77	63.9	0.024	166.8	45.0	59.0
49. Limonene	5.80	--	0.024	167.5	68.0	93.0
50. 4-Ethyltoluene	6.02	32.9	0.025	172.9	105.0	120.0
51. Octanal	6.12	17	0.024	175.5	43.0	44.0
52. 1,2-Dichlorobenzene	6.26	--	0.025	179.1	146.0	148.0
53. 2-Butoxyethyl acetate	6.52	17	0.024	185.5	43.0	57.0
54. Benzyl Alcohol	6.55	101	0.024	186.4	79.0	108.0
55. 2-(2-Butoxyethoxy)ethanol	7.34	63.9	0.025	206.1	45.0	57.0
56. Naphthalene	7.37	--	0.026	206.8	128.0	129.0

Choosing a Method

Deciding on a final method to establish in the lab should factor in both chromatographic performance and business interests. In our examples, the non-MS method was faster but contained coeluting compounds. If these compounds are critical analytes for a quantitative method, then the GC-MS method may be the preferred technical choice because it separates all isobars in a similar analysis time. However, if more profitable samples can be run on GC-MS instruments and labs can accept the degree of coelution among target compounds, developing the method on a non-MS instrument instead may be the better business decision. Using Pro *EZ*GC chromatogram modeling software to examine different options before making a final decision allows labs to quickly and efficiently balance all interests and choose a sound method that meets technical requirements and business goals.

Rtx-VMS GC Capillary Column

- Unique, proprietary polymer designed for excellent retention and better separation of volatile organic compounds.
- Temperature range: -40 °C to 260 °C.

Catalog No.	Product Name	Units
19915	Rtx-VMS GC Capillary Column, 30 m, 0.25 mm ID, 1.40 µm	ea.

Restek Electronic Leak Detector

Prevent small leaks from causing big problems with a Restek leak detector.

- Detects a broad range of gases and indicates leak severity with both an LED display and audible tone.
- No more waiting for a full charge—can be operated during charging or used up to 12 hours between charges.

Catalog No.	Product Name	Units
28500	Restek Electronic Leak Detector (includes carrying case; universal AC power adaptor [U.S., UK, Europe, Australia, Japan]; 6-ft USB charging cable)	ea.

Restek ProFLOW 6000 Electronic Flowmeter

State-of-the-art features include:

- Measures volumetric flow for gases across a range of 0.5–500 mL/min.
- NIST traceable calibration.
- Ex rating (electrical apparatus for explosive gas atmospheres) for hydrogen and related gas types.

Catalog No.	Product Name	Units
22656	Restek ProFLOW 6000 Electronic Flowmeter	ea.

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