Detection of Lung Cancer: Concomitant Volatile Organic Compounds and Metabolomics profiling of six cancer cell lines of different histological origins

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Disclosure of Potential Conflicts of Interest

No potential conflicts of interest were disclosed.

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Figure Captions

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Figure S2. PCA score plot of metabolites profiling shows QC samples are clustered together.

Figure S3. Features detected in blank SPME fiber. (TIC chromatogram with labelled compound ID, followed with a table showing the retention time, mass, compound, CAS number, match score, reverse match score and probability of each peak.)

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Figure S8. ROC analysis of a) cancer vs normal cell b) large cell vs. other NSCLC. c) SCLC vs NSCLC

Table S1. m/z, CAS number, and retention time of 20 statistically differential VOCs.

m/z	CAS	Retention Time (min)	Compound
57.0685	123-38-6	1.6	Propanal
58.0387	67-64-1	1.62	Acetone
45.03243	78-92-2	1.64	2-Butanol
71.0826	107-83-5	1.87	Pentane,2-methyl
91.05265	108-88-3	4.59	Toluene
83.04758	625-65-0	5.5	2-Pentene, 2,4-dimethyl-
56.0998	66-25-1	5.61	Hexanal
91.05268	100-41-4	7.54	Ethylbenzene
91.05264	95-47-6	7.86	o-xylene
91.0571	108-38-3,106-42-3	7.92	m & p-Xylene
57.03459	108-93-0	8.52	Cyclohexanol
104.0602	100-42-5	8.61	Styrene
105.0375	100-52-7	11.09	Benzaldehyde
105.0779	95-63-6	11.33	1,2,4-Trimethylbenzene
57.06854	104-76-7	13.47	2-Ethyl-1-Hexanol
55.05294	14507-02-9	13.47	2,4-Decadien-1-ol
98.1042	124-19-6	15.94	Nonanal
128.0648	91-20-3	18.05	Naphthalene
91.05252	1014-60-4	19.25	Benzene, 1,3-bis(1,1-dimethylethyl)-
91.05247	96-76-4	21.89	Phenol, 2,4-bis(1,1-dimethylethyl)-

Table S2. Comparison of match, reverse match and probability scores of the 13 VOCs confirmed with standards.

	Compound	Sample			Standards		
		Match	Reverse Match	Probability	Match	Reverse Match	Probability
1	Acetone	712	765	50	703	802	45.3
2	Pentane,2-methyl	706	732	6.5	704	737	7.58
3	Propanal	703	712	12.3	713	725	25.9
4	Toluene	866	895	34	795	850	24.1
5	Hexanal	727	804	14.9	706	812	16.7
6	Ethylbenzene	878	901	60.4	903	925	67.2
7	o-xylene	868	914	29	894	913	28.4
8	m & p-Xylene	849	909	32.4	890	910	28.3
9	Styrene	707	856	19.4	726	877	14.1
10	1,2,4-Trimethylbenzene	721	877	14.3	810	907	22.8
11	2-Ethyl-1-Hexanol	785	820	14.6	742	849	9.9
12	Nonanal	768	806	13.5	726	815	10.9
13	Naphthalene	919	942	55	939	950	45.1

Table S3. Retention time and m/z values of identified statistically differential non-volatile metabolites.

	RT (min)	M/Z	Compound
1	4.069	73	Acetamide
2	4.427	145	Dimethylurea
3	4.8	144	Valine
4	5.008	174	Phenylethanolamine
5	5.441	158	Leucine
6	5.7	73,158	Isoleucine
7	5.789	73,142	Proline
8	5.9	73,147,174	Glycine
9	5.98	75,117,132,199	Cyclohexaneacetic acid
10	6.263	73,99,147,241	Pyrimidine
11	6.439	73,147,245	3-Ketovaleric acid
12	6.531	73,204,218	Serine
13	6.891	73,117,218,219	Threonine
14	7.55	73,147,174,248	Alanine
15	8.16	73,147,218	Aminomalonic acid
16	8.451	73,147	Butanedioic acid
17	8.98	73,100,232	Aspartic acid
18	10.58	73,142	Ornithine
19	10.64	73,128,246	Glutamic acid
20	10.756	73,192,218	Phenylalanine
21	11.5	73,116,231	Asparagine
22	12.42	73,147,217	Ribitol
23	13.72	73,265,280	Purine
24	14.54	117,285	Tetradecanoic acid
25	14.8	73,217,307	Fructose
26	15.1	319	mannose
27	15.58	73,147,205,319	Glucose
28	15.7	73,174,317	Lysine
29	15.9	73,218	Tyrosine
30	17.7	117,313	Hexadecanoic acid
31	18.31	73,147,217,305	Inositol
32	18.95	73,147,319	Allose
33	20.238	117,339	Oleic acid
34	20.64	117,341	Octadecanoic acid
35	23.37	73,217	Uridine
36	26.47	73,204,361	Lactose
37	31.028	129,329,368	Cholesterol

Table S4. Comparison of match, reverse match and probability scores of the 20 non-volatile metabolites confirmed with standards.

		Chemical Standards			Sample		
	Compounds	**Match**	**Reverse Match**	**Probability (%)**	**Match**	**Reverse Match**	**Probability (%)**
1	Valine	879	879	74	877	880	76.1
2	Leucine	887	887	41.1	852	862	38.9
3	Isoleucine	899	911	63	908	927	62.9
4	Proline	882	885	94.1	876	886	95.6
5	Glycine	904	904	87.4	889	899	86.7
6	Serine	902	904	84.2	892	895	81.3
7	Threonine	911	912	94.2	893	913	95.7
8	Phenylalanine	902	902	55.9	890	891	59.4
9	Asparagine	890	911	81.9	823	867	78.5
10	Ornithine	851	852	93.2	837	851	92.7
11	Lysine	755	795	92.8	764	809	92.8
12	Tyrosine	925	941	86.2	907	933	77.2
13	Hexadecanoic acid	837	844	84.3	848	850	94
14	Glutamic acid	901	903	92.5	898	898	90.8
15	Oleic acid	874	875	15.7	862	869	19.1
16	Octadecanoic acid	853	855	85.2	846	848	93.9
17	Inositol	906	906	72.6	909	909	77.3
18	Mannose	879	879	11.2	861	862	9.6
19	Glucose	899	899	21	855	897	13.2
20	Fructose	868	868	20	845	842	12.7

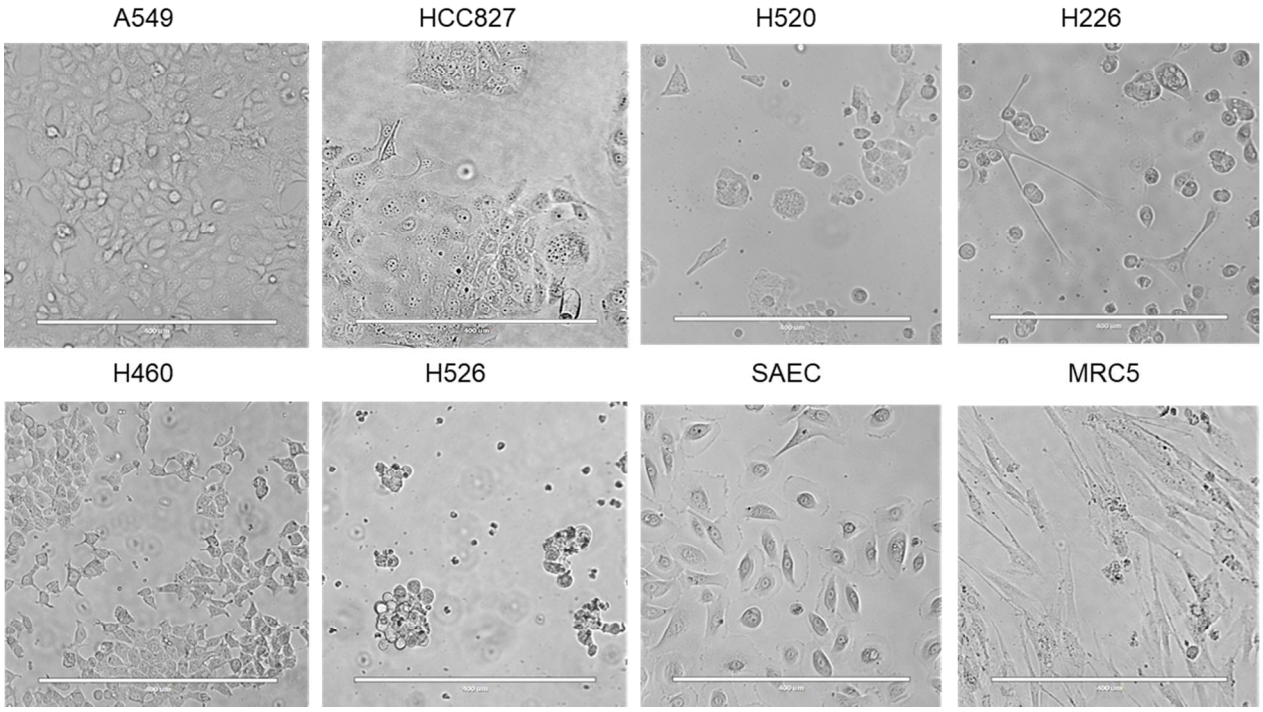


Figure S1. Morphology of eight lung cell lines when cultured in supplier recommended medium

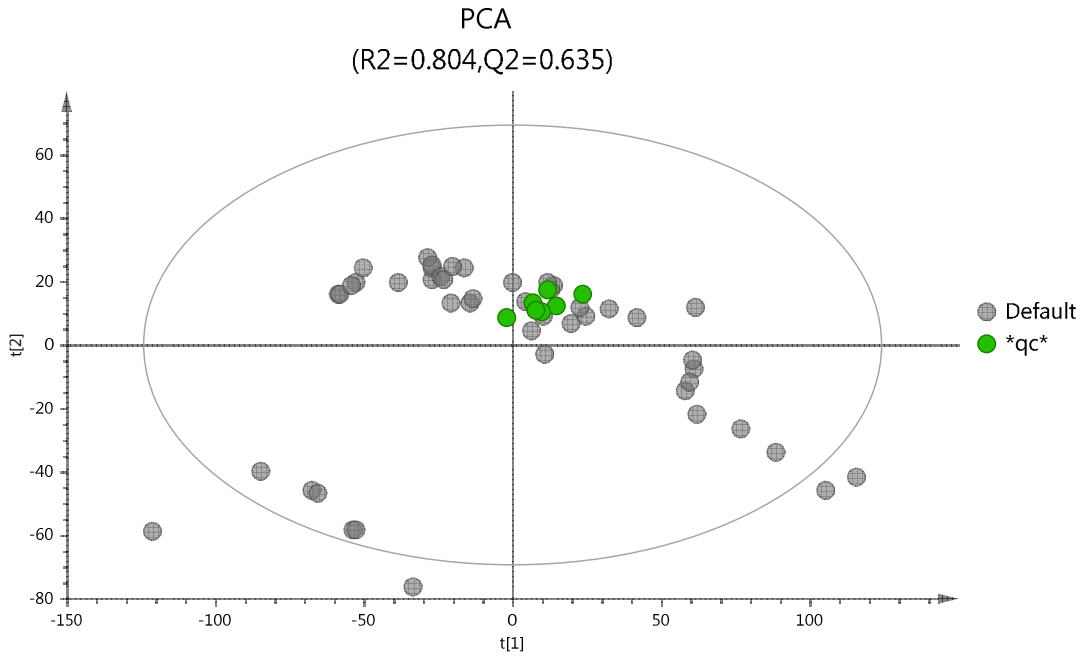
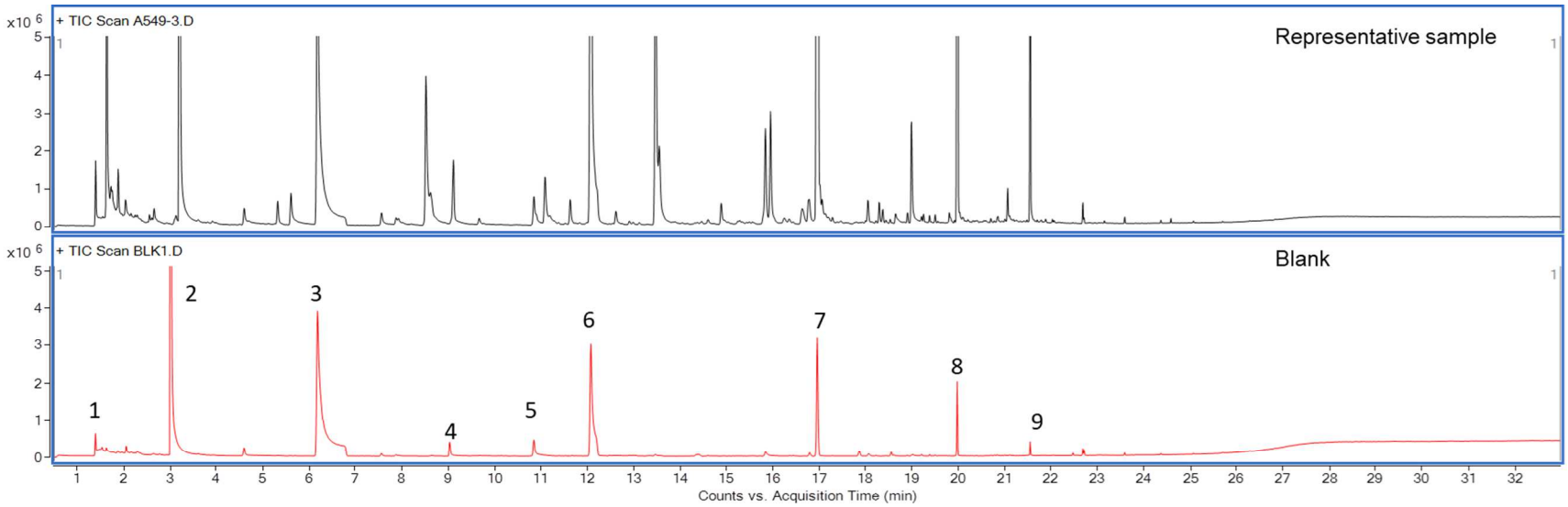


Figure S2. PCA score plot of metabolites profiling shows QC samples are clustered together.



	RT (min)	Mass	Compound	CAS	Match	Reverse Match	Probability
1	1.384	43.98	carbon dioxide	124-38-9	829	850	28.4
2	3.309	77	Silanediol, dimethyl-	1066-42-8	876	876	93.6
3	6.215	207.03	Cyclotrisiloxane, hexamethyl-	541-05-9	897	898	83.8
4	9.04	133	Oxime-, methoxy-phenyl-	NIST#: 222866	760	780	71.7
5	10.83	192.97	Vanillin, tert-butyldimethylsilyl ether	NIST#: 352846	681	684	25.6
6	12.1	281.05	Cyclotetrasiloxane, octamethyl-	556-67-2	907	912	90.3
7	16.96	267.001	Cyclopentasiloxane, decamethyl-	541-02-6	914	916	39.8
8	19.967	341.0185	Cyclohexasiloxane, dodecamethyl-	540-97-6	939	963	45.3
9	21.54	281.0504	Cycloheptasiloxane, tetradecamethyl-	107-50-6	802	811	89.9

Figure S3. Features detected in blank SPME fiber. (TIC chromatogram with labelled compound ID, followed with a table showing the retention time, mass, compound, CAS number, match score, reverse match score and probability of each peak.)

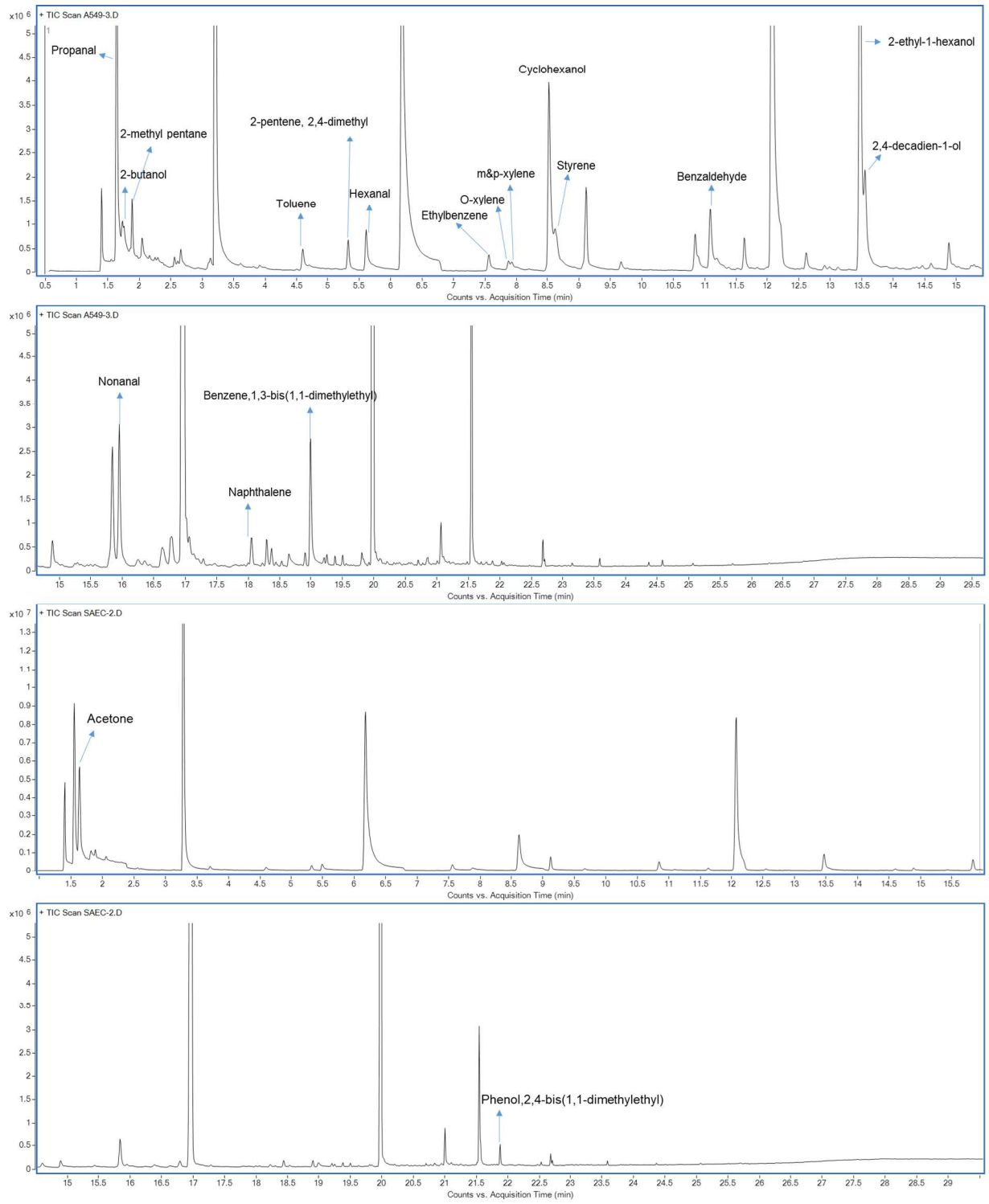
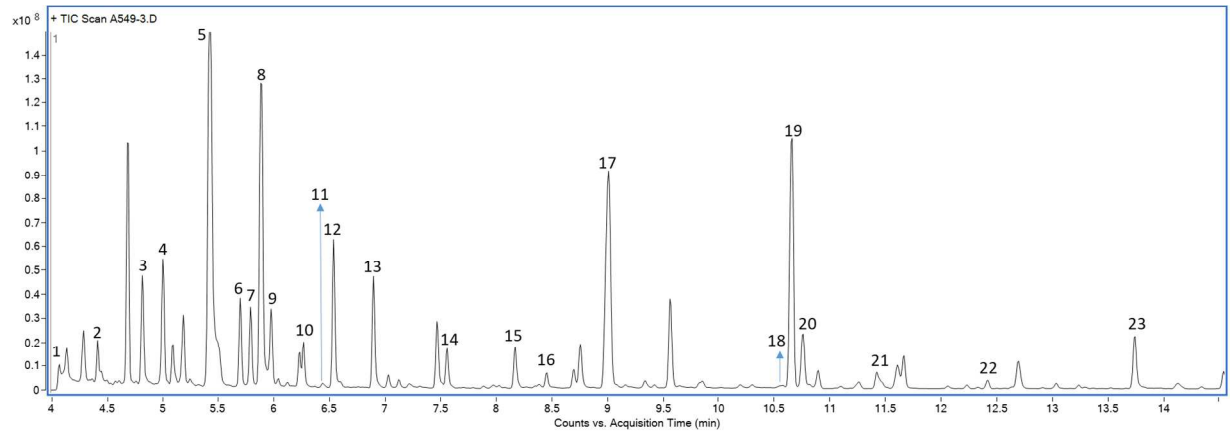
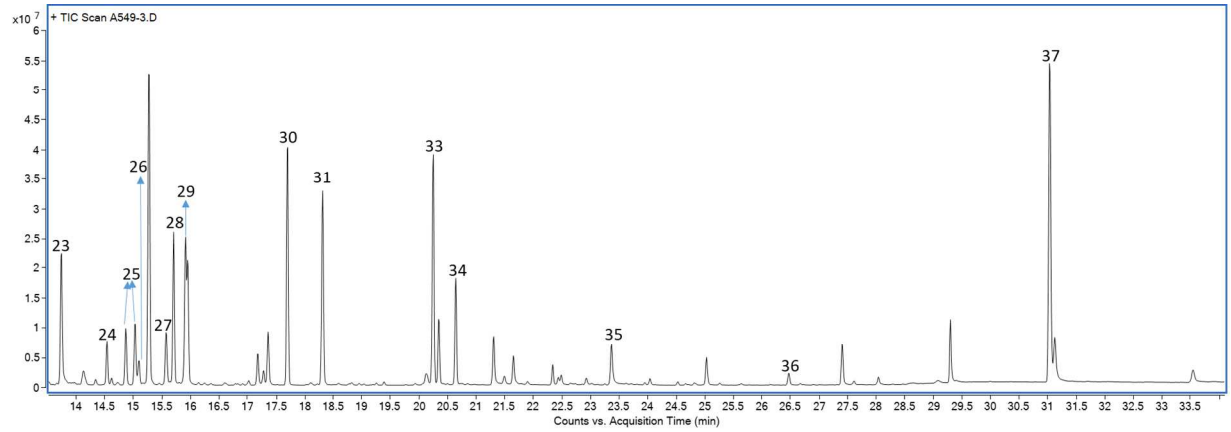


Figure S4. TIC of 20 VOCs in two representative samples. (acetone and phenol,2,4-bis(1,1-eimethylethyl) were shown in sample SAEC-2, the rest were shown in sample A549-3)

a)



b)



c)

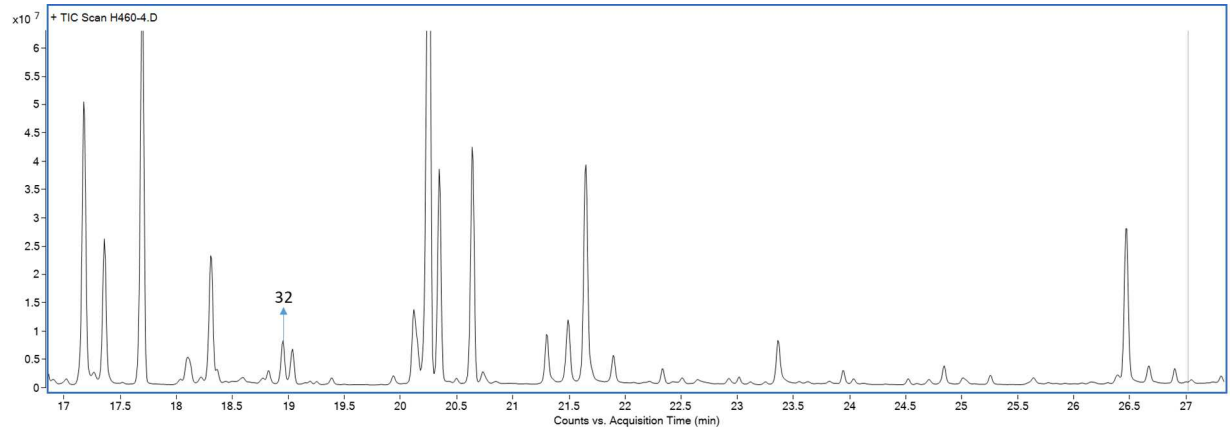
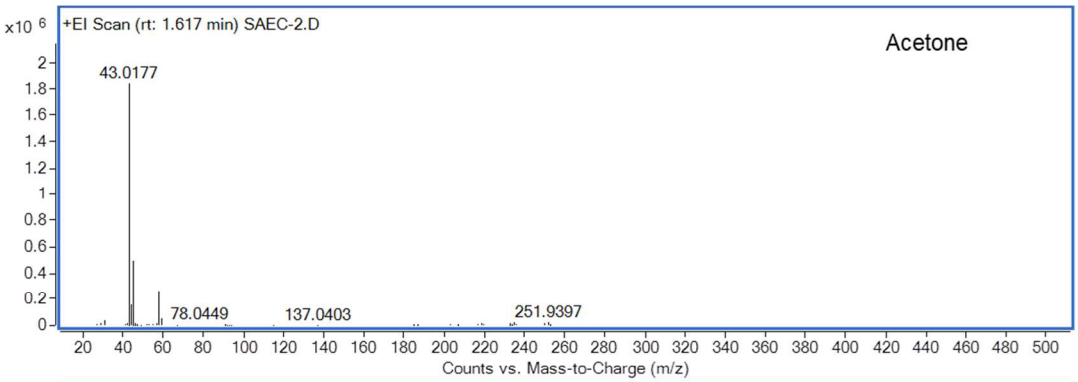
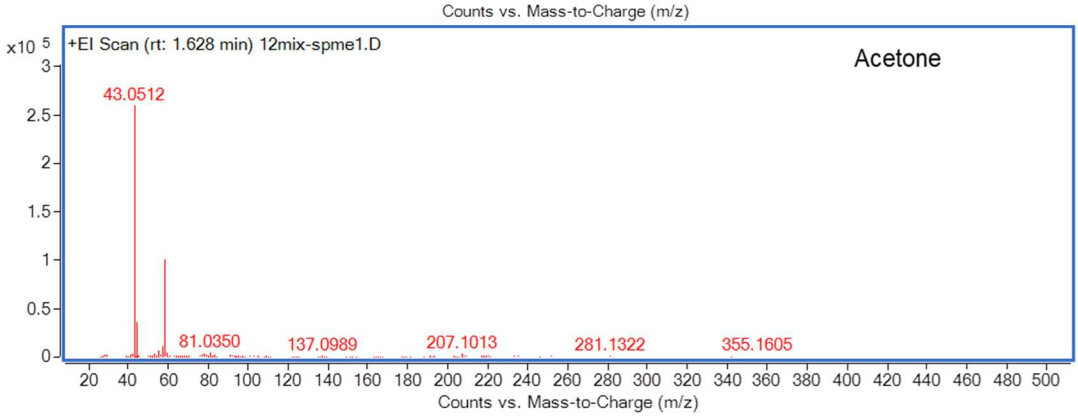
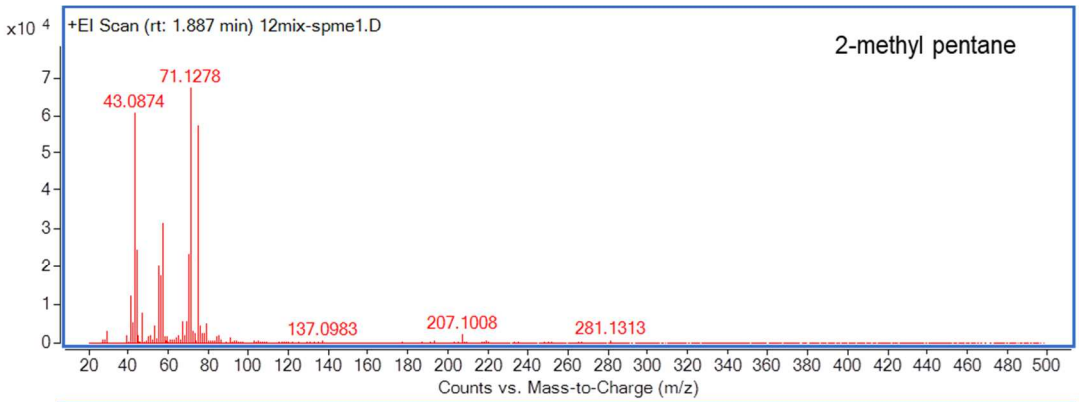


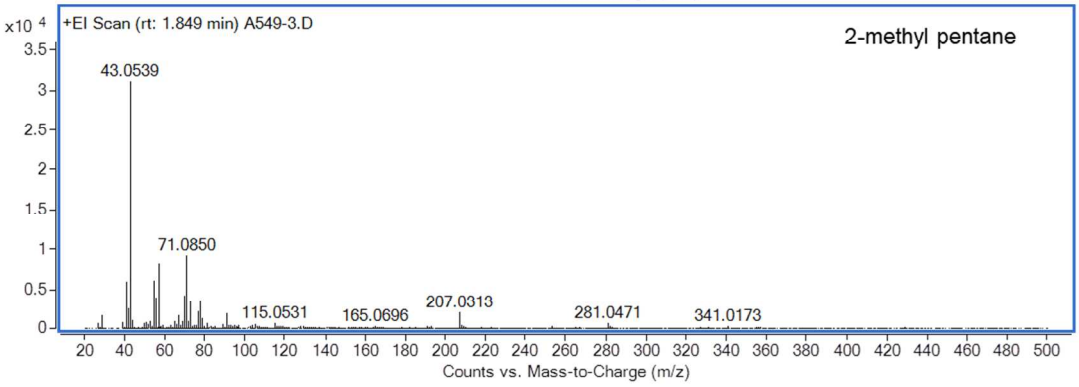
Figure S5. Total Ion Chromatogram of 37 non-volatile metabolites in a representative sample. a).4-14 mins. (1: Acetamide; 2: Dimethylurea; 3: Valine;4: Phenylethanolamine;5: Leucine;6: Isoleucine;7: Proline;8: Glycine;9: Cyclohexaneacetic acid;10: Pyrimidine;11: 3-Ketovaleric acid;12: Serine;13: Threonine;14: Alanine;15: Aminomalonic acid;16: Butanedioic acid;17: Aspartic acid;18: Ornithine;19: Glutamic acid;20: Phenylalanine;21: Asparagine;22: Ribitol;23: Purine;) b). 14-34 mins. (24: Tetradecanoic acid;25: Fructose;26:Mannose;27: Glucose;28: Lysine;29: Tyrosine;30: Hexadecanoic acid;31: Inositol;33: Oleic acid;34: Octadecanoic acid;35: Uridine;36: Lactose;37: Cholesterol) c).

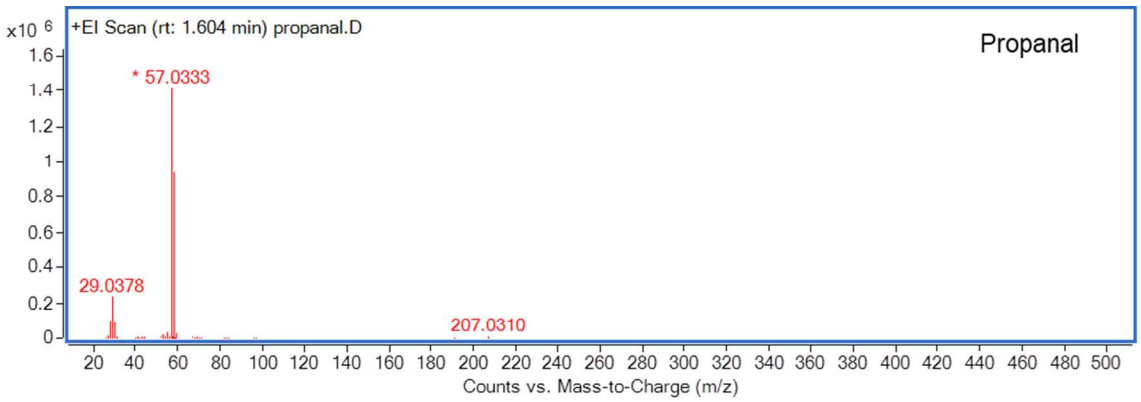
Compound 32 Allose is of very low level in the selected sample (A549-3), therefore its TIC peak was shown in another sample (H460-4)

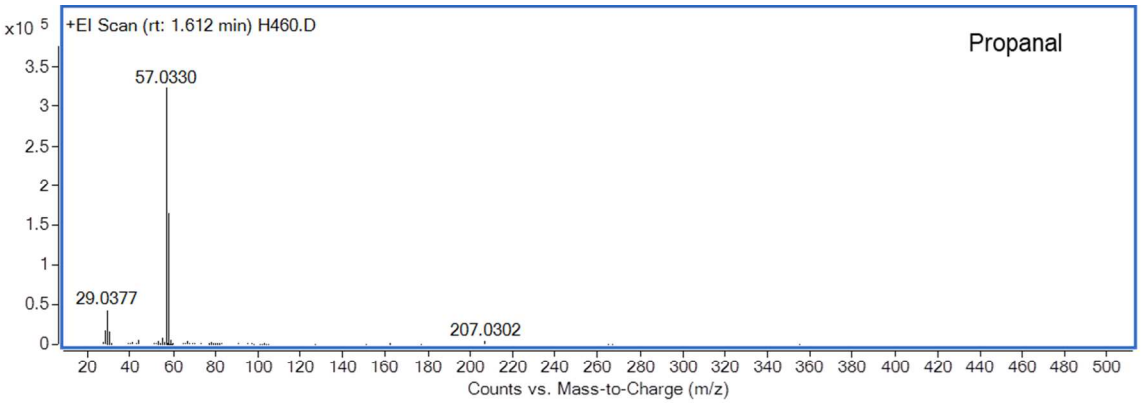

x10 6
+EI Scan (rt: 1.617 min) SAEC-2.D
Acetone
43.0177
78.0449
137.0403
251.9397
Counts vs. Mass-to-Charge (m/z)

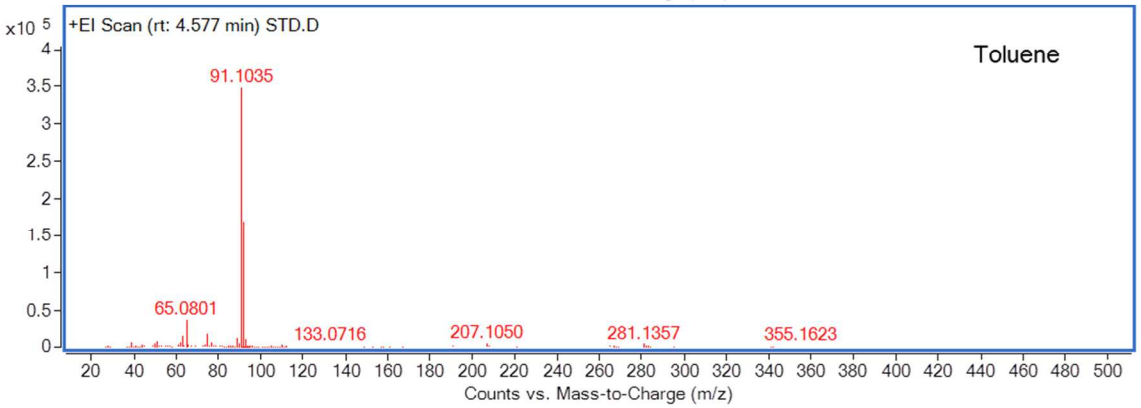

x10 5
+EI Scan (rt: 1.628 min) 12mix-spme1.D
Acetone
43.0512
81.0350
137.0989
207.1013
281.1322
355.1605
Counts vs. Mass-to-Charge (m/z)


x10 4
+EI Scan (rt: 1.887 min) 12mix-spme1.D
2-methyl pentane
71.1278
43.0874
137.0983
207.1008
281.1313
Counts vs. Mass-to-Charge (m/z)


x10 4
+EI Scan (rt: 1.849 min) A549-3.D
2-methyl pentane
43.0539
71.0850
115.0531
165.0696
207.0313
281.0471
341.0173
Counts vs. Mass-to-Charge (m/z)


x10 6
+EI Scan (rt: 1.604 min) propanal.D
Propanal
* 57.0333
29.0378
207.0310
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 1.612 min) H460.D
Propanal
57.0330
29.0377
207.0302
Counts vs. Mass-to-Charge (m/z)


x10 5
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Toluene
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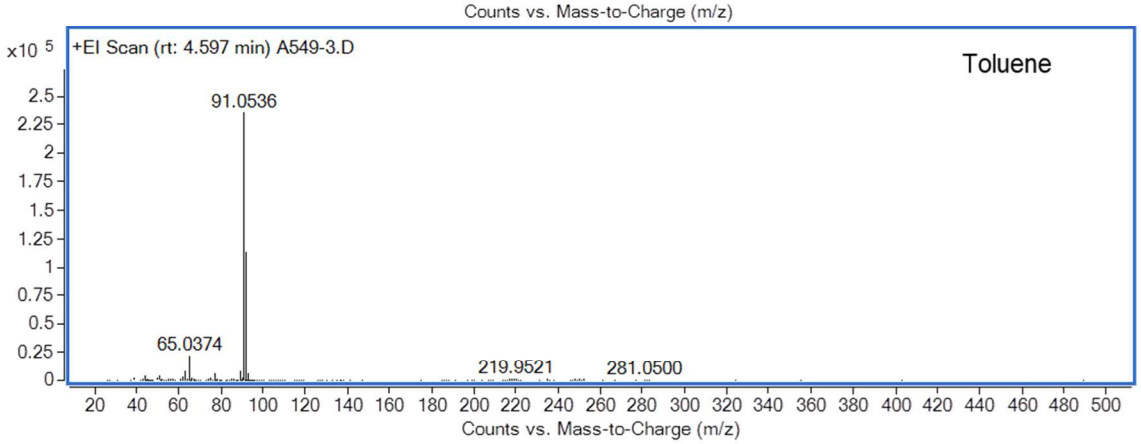
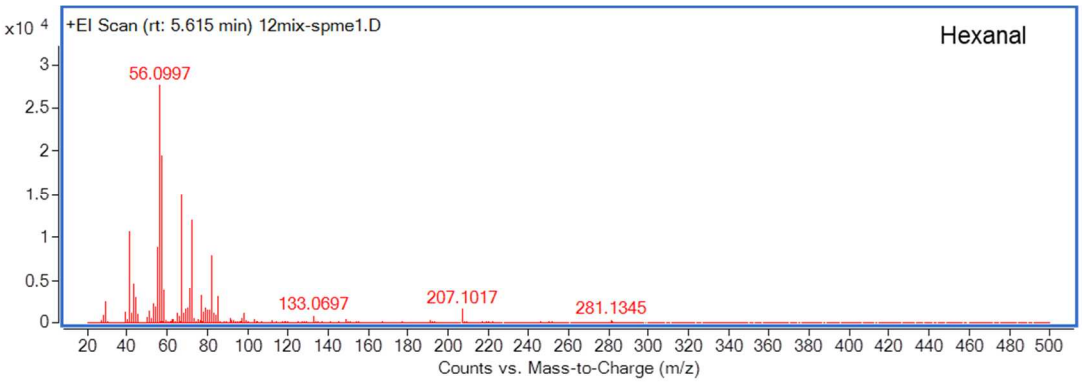
133.0716
207.1050
281.1357
355.1623
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 4.597 min) A549-3.D
Toluene
91.0536
65.0374
219.9521
281.0500
Counts vs. Mass-to-Charge (m/z)


x10 4
+EI Scan (rt: 5.615 min) 12mix-spme1.D
Hexanal
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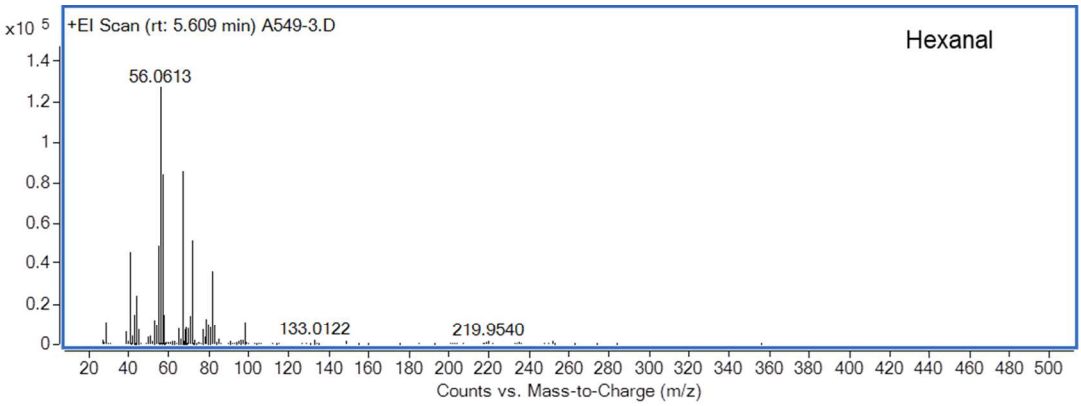
133.0697
207.1017
281.1345
Counts vs. Mass-to-Charge (m/z)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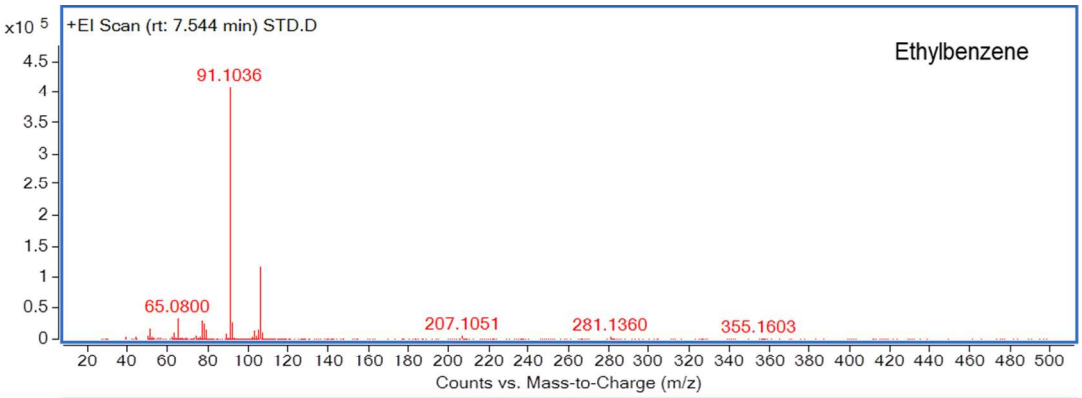
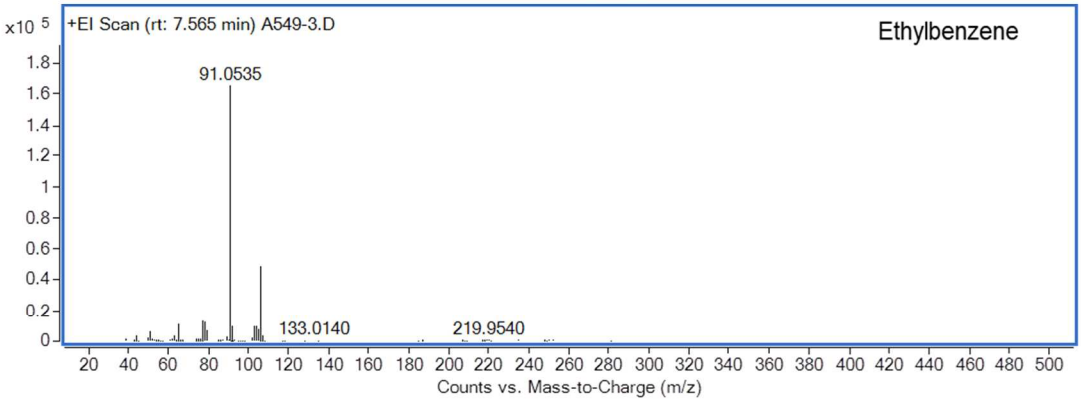
Hexanal
56.0613
133.0122
219.9540
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 7.544 min) STD.D
Ethylbenzene
91.1036
65.0800
207.1051
281.1360
355.1603
Counts vs. Mass-to-Charge (m/z)


x10 5
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Ethylbenzene
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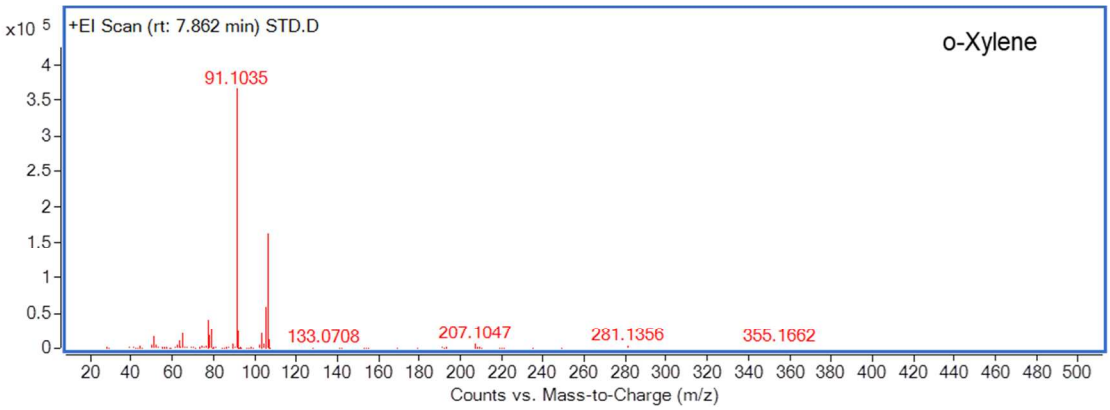
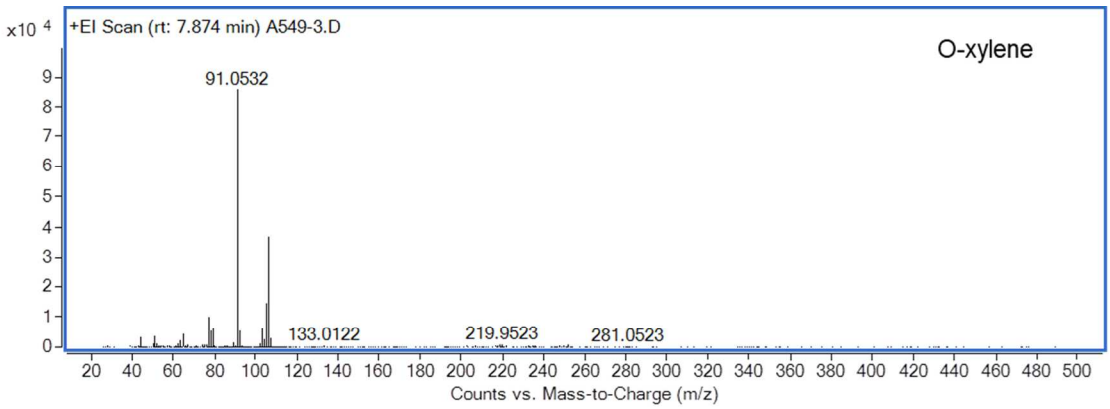
133.0140
219.9540
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 7.862 min) STD.D
o-Xylene
91.1035
133.0708
207.1047
281.1356
355.1662
Counts vs. Mass-to-Charge (m/z)


x10 4
+EI Scan (rt: 7.874 min) A549-3.D
O-xylene
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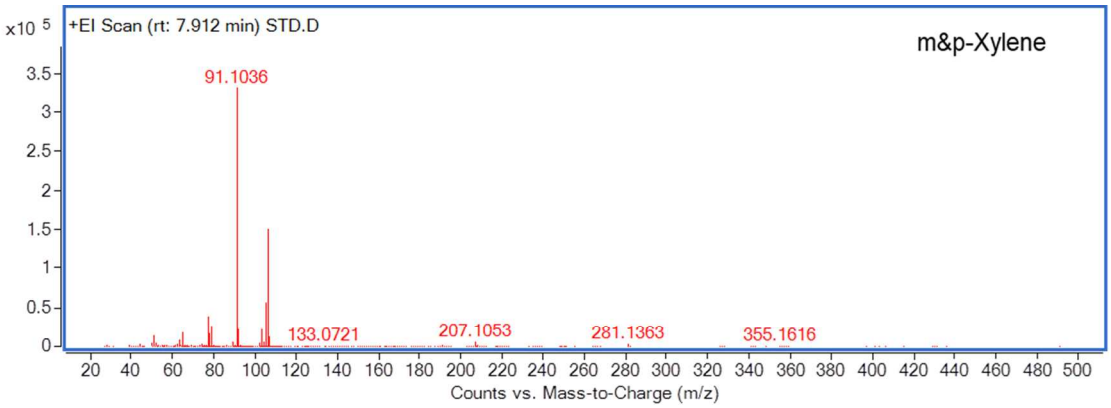
133.0122
219.9523
281.0523
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 7.912 min) STD.D
m&p-Xylene
91.1036
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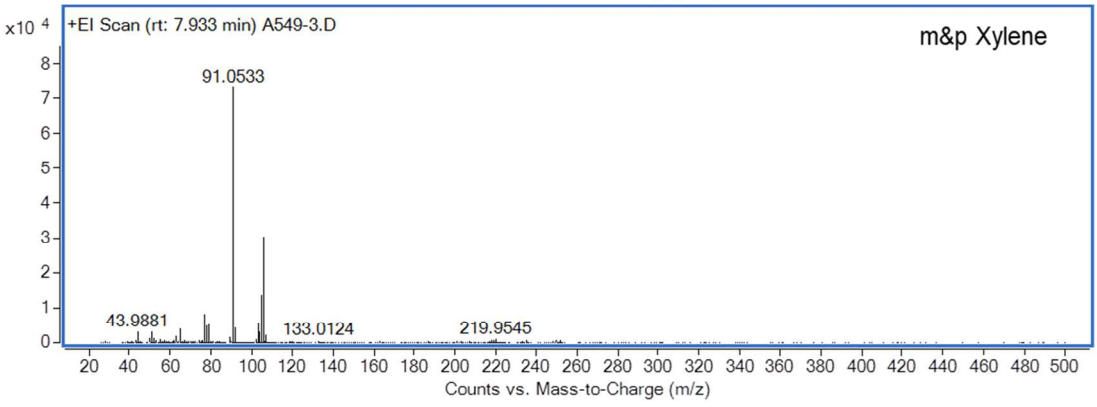
207.1053
281.1363
355.1616
Counts vs. Mass-to-Charge (m/z)


x10 4
+EI Scan (rt: 7.933 min) A549-3.D
m&p Xylene
91.0533
43.9881
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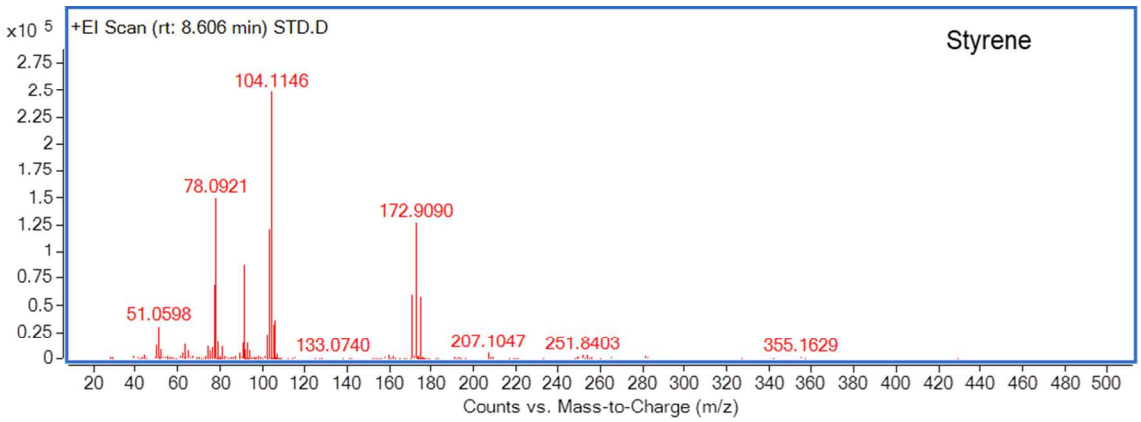
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 8.606 min) STD.D
Styrene
104.1146
78.0921
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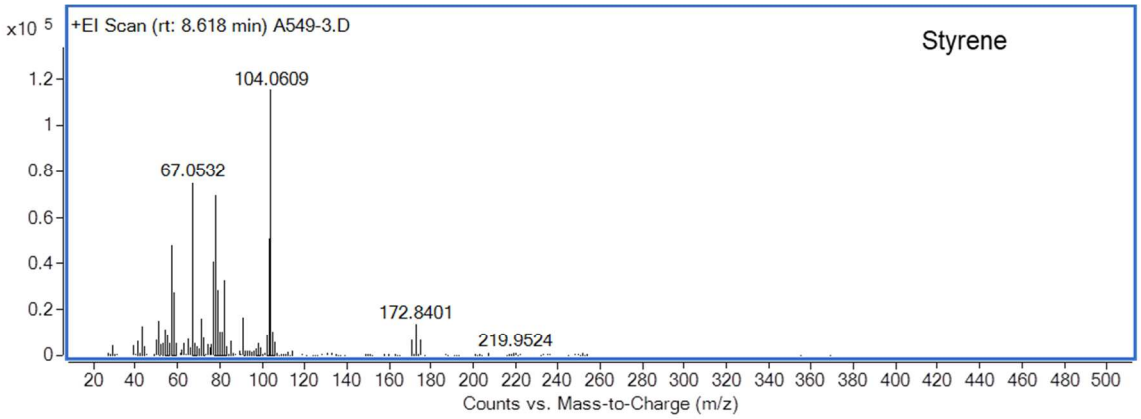
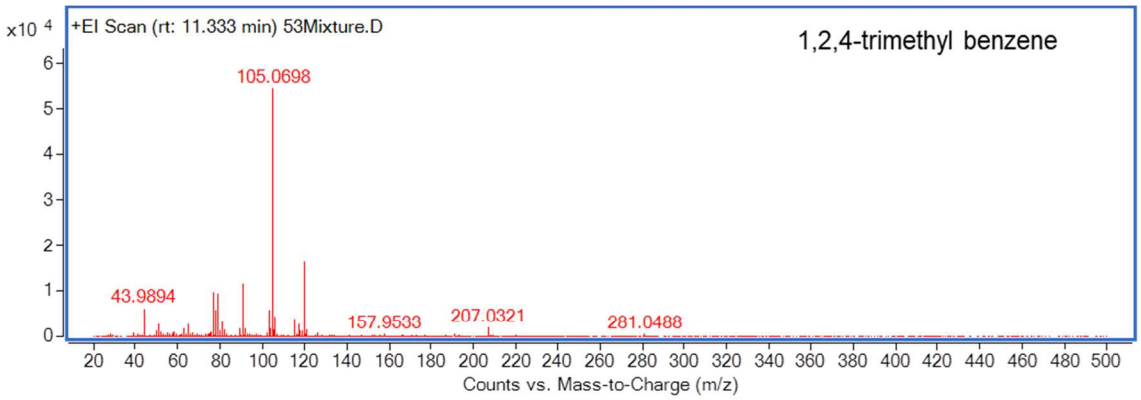
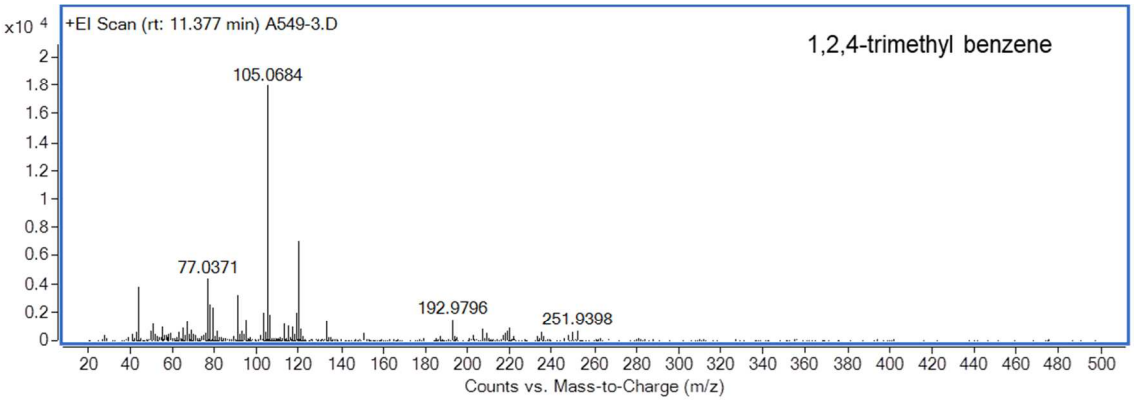
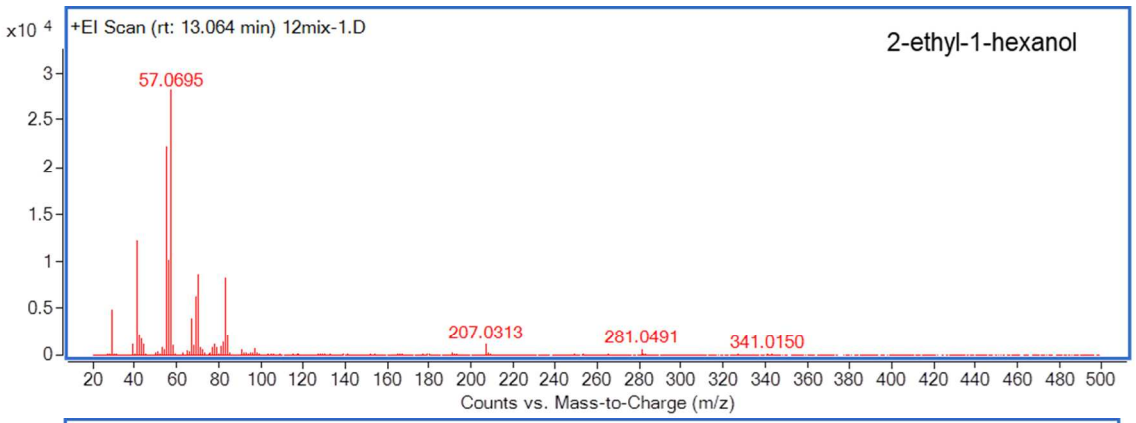
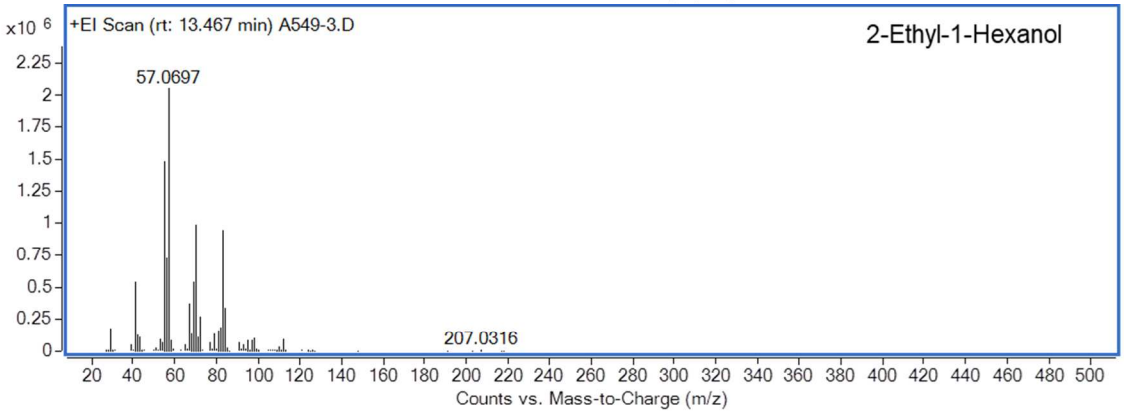
51.0598
133.0740
207.1047
251.8403
355.1629
Counts vs. Mass-to-Charge (m/z)

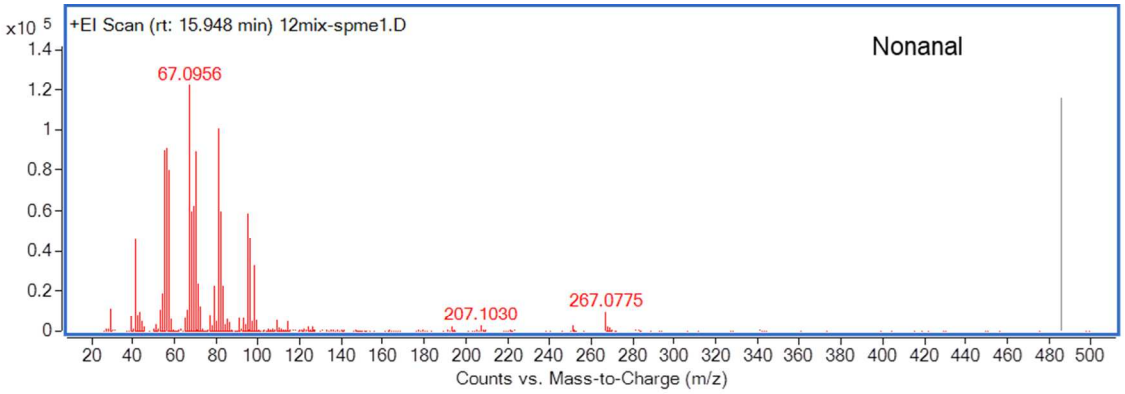

x10 5
+EI Scan (rt: 8.618 min) A549-3.D
Styrene
104.0609
67.0532
172.8401
219.9524
Counts vs. Mass-to-Charge (m/z)

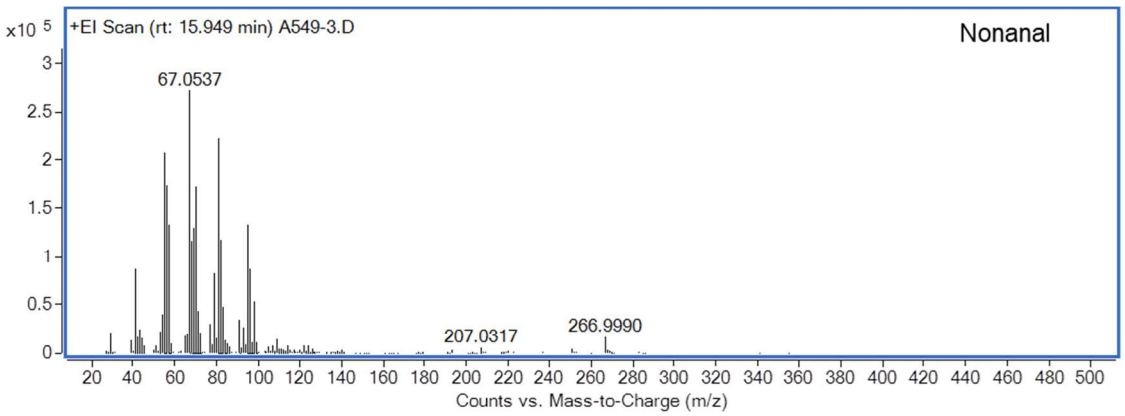

x10 4
+EI Scan (rt: 11.333 min) 53Mixture.D
1,2,4-trimethyl benzene
105.0698
43.9894
157.9533
207.0321
281.0488
Counts vs. Mass-to-Charge (m/z)


x10 4
+EI Scan (rt: 11.377 min) A549-3.D
1,2,4-trimethyl benzene
105.0684
77.0371
192.9796
251.9398
Counts vs. Mass-to-Charge (m/z)


x10 4
+EI Scan (rt: 13.064 min) 12mix-1.D
2-ethyl-1-hexanol
57.0695
207.0313
281.0491
341.0150
Counts vs. Mass-to-Charge (m/z)


x10 6
+EI Scan (rt: 13.467 min) A549-3.D
2-Ethyl-1-Hexanol
57.0697
207.0316
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 15.948 min) 12mix-spme1.D
Nonanal
67.0956
207.1030
267.0775
Counts vs. Mass-to-Charge (m/z)


x10 5
+EI Scan (rt: 15.949 min) A549-3.D
Nonanal
67.0537
207.0317
266.9990
Counts vs. Mass-to-Charge (m/z)

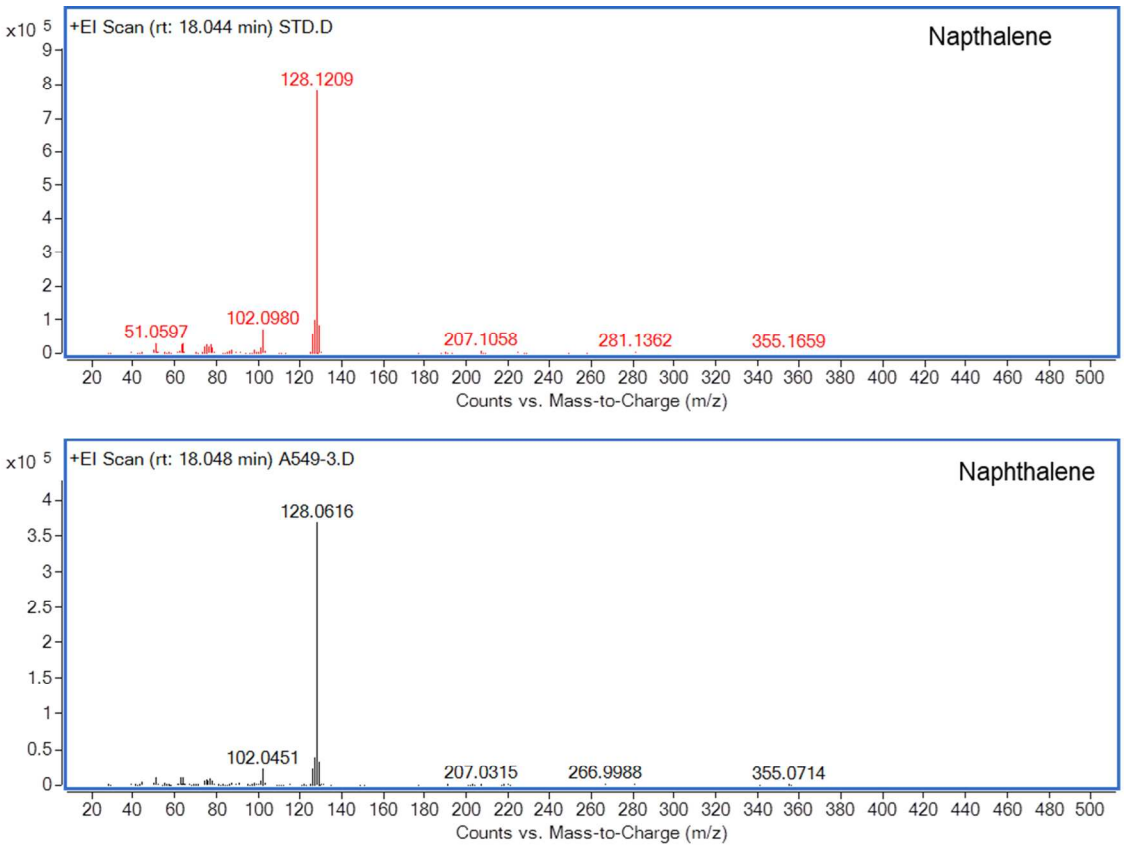
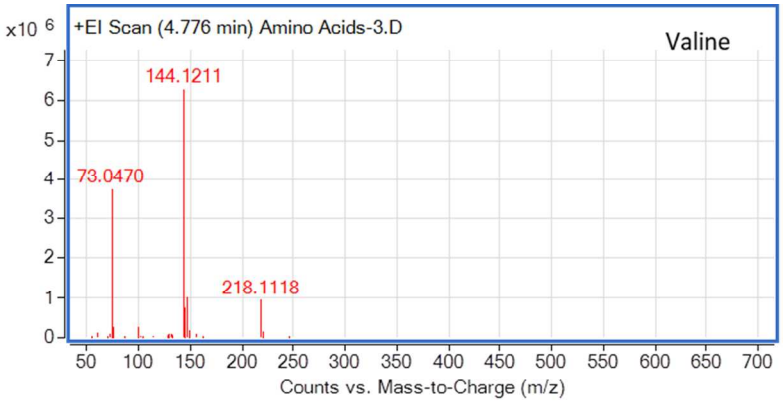
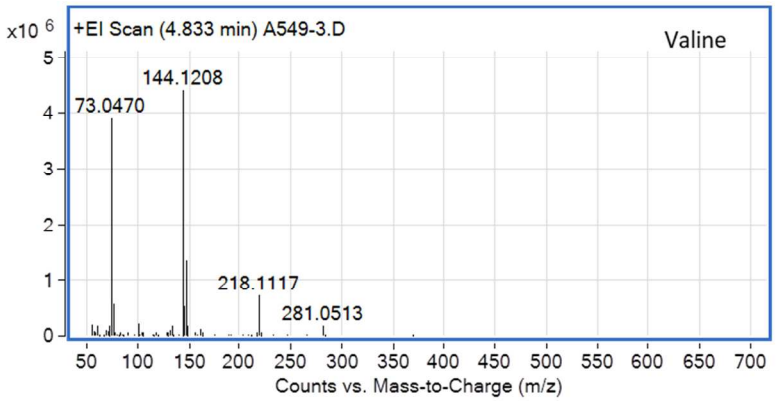
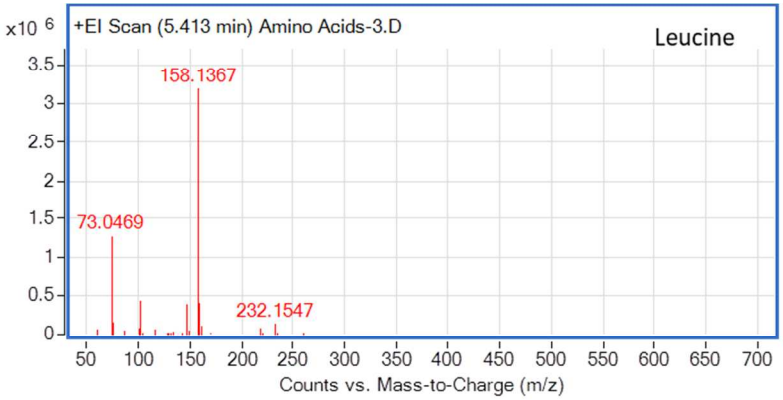
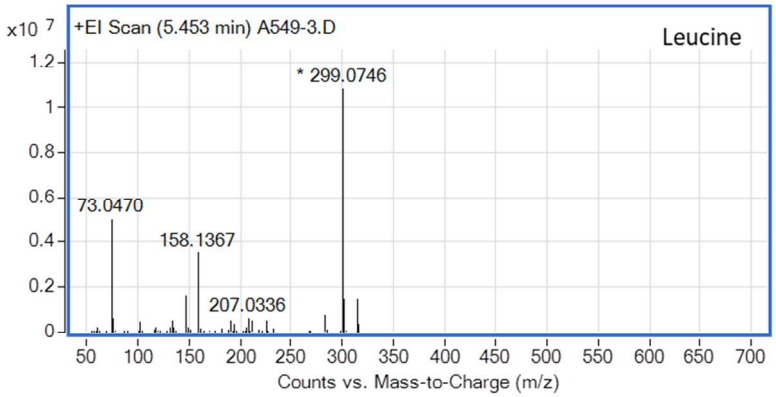


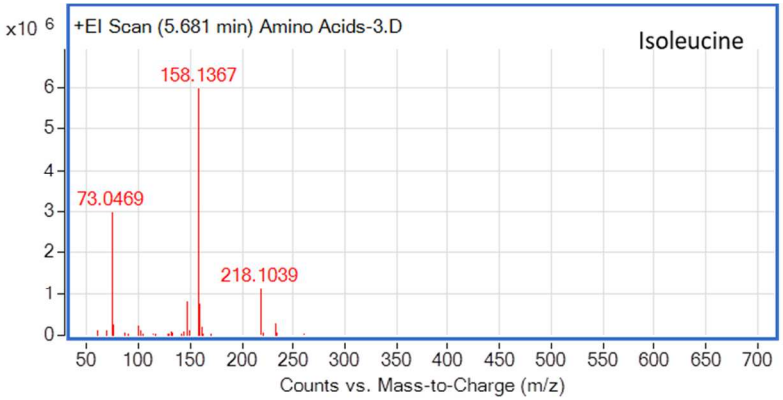
Figure S6. Parallel comparisons of spectrums of 13 VOCs in sample and in standards. Spectrum of standard is in red, spectrum of sample is in black.

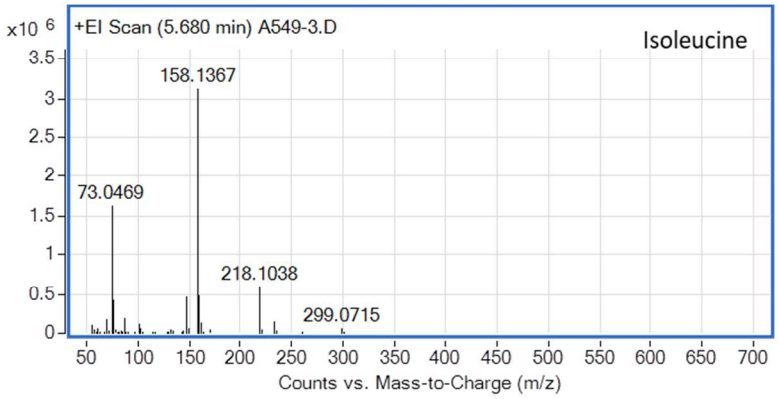

x10 6
+EI Scan (4.776 min) Amino Acids-3.D
Valine
144.1211
73.0470
218.1118
Counts vs. Mass-to-Charge (m/z)

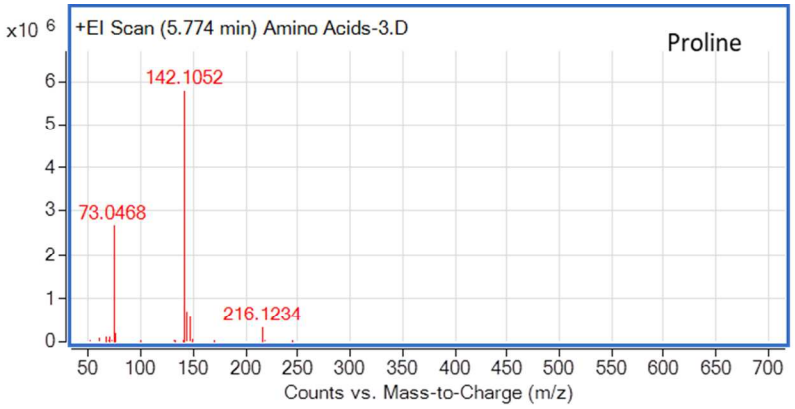

x10 6
+EI Scan (4.833 min) A549-3.D
Valine
144.1208
73.0470
218.1117
281.0513
Counts vs. Mass-to-Charge (m/z)

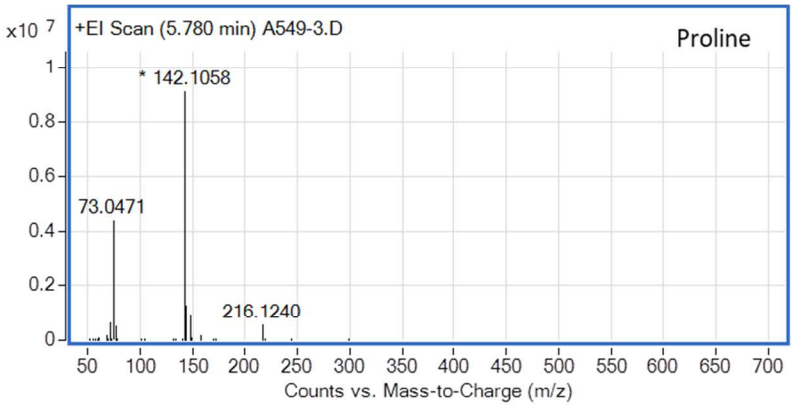

x10 6
+EI Scan (5.413 min) Amino Acids-3.D
Leucine
158.1367
73.0469
232.1547
Counts vs. Mass-to-Charge (m/z)

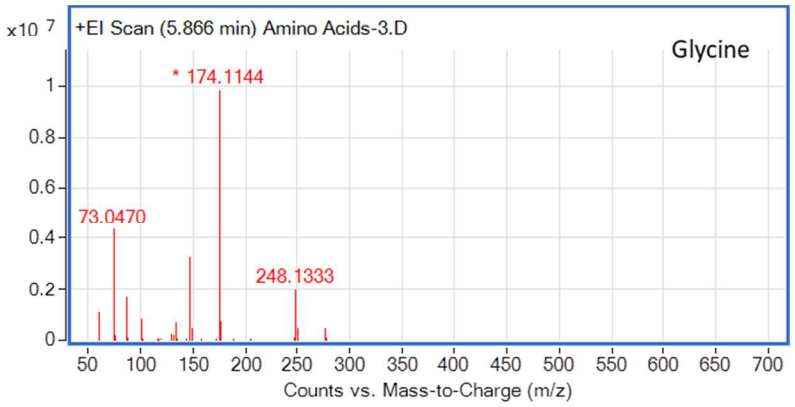

x10 7
+EI Scan (5.453 min) A549-3.D
Leucine
* 299.0746
73.0470
158.1367
207.0336
Counts vs. Mass-to-Charge (m/z)

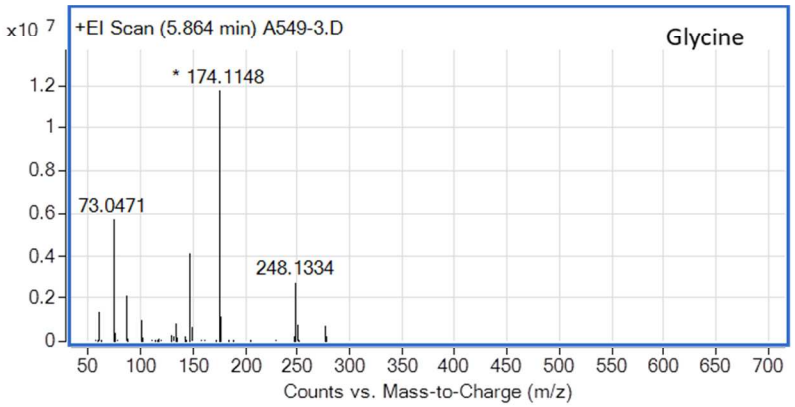

x10 6
+EI Scan (5.681 min) Amino Acids-3.D
Isoleucine
158.1367
73.0469
218.1039
Counts vs. Mass-to-Charge (m/z)

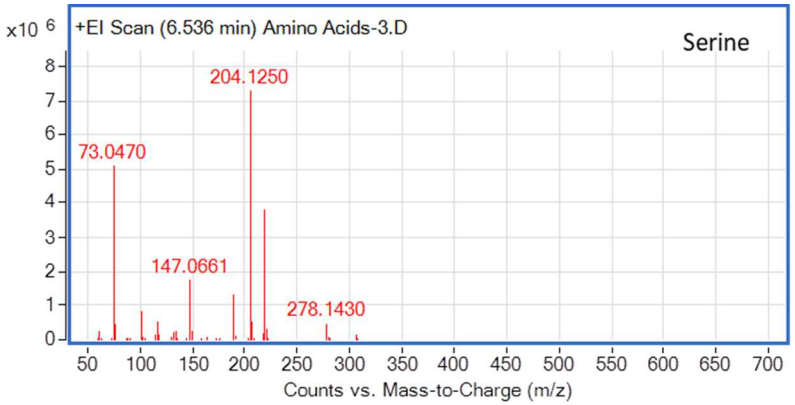

x10 6
+EI Scan (5.680 min) A549-3.D
Isoleucine
158.1367
73.0469
218.1038
299.0715
Counts vs. Mass-to-Charge (m/z)

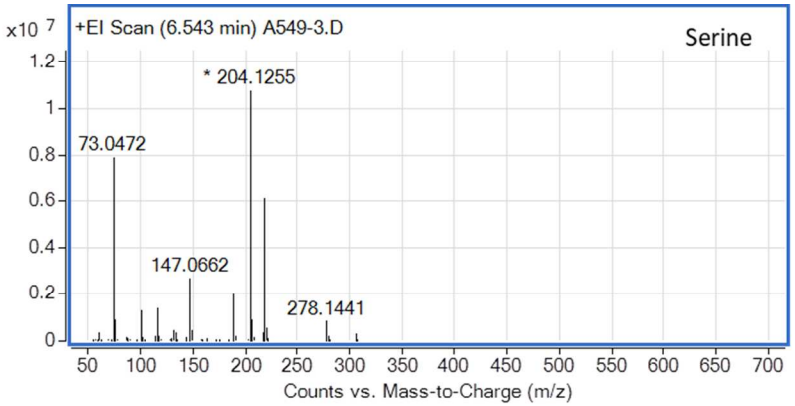

x10 6
+EI Scan (5.774 min) Amino Acids-3.D
Proline
142.1052
73.0468
216.1234
Counts vs. Mass-to-Charge (m/z)

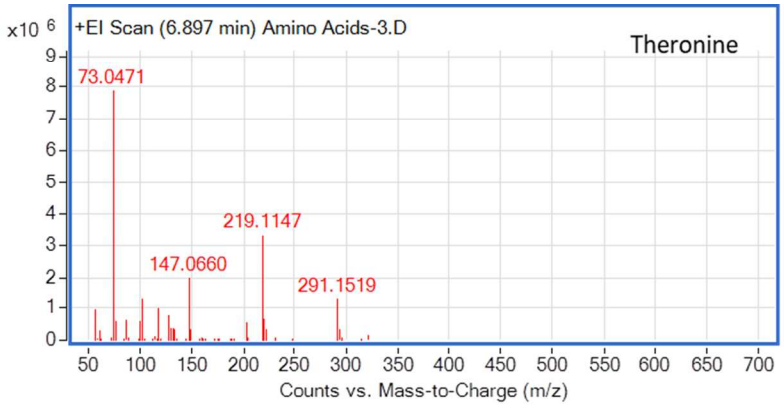

x10 7
+EI Scan (5.780 min) A549-3.D
Proline
* 142.1058
73.0471
216.1240
Counts vs. Mass-to-Charge (m/z)

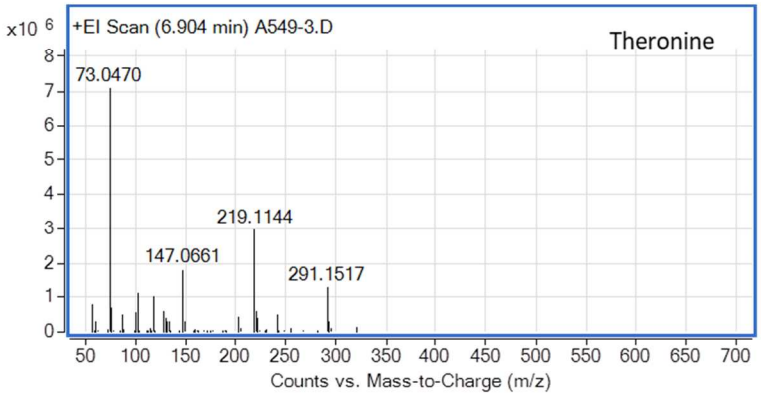

x10 7
+EI Scan (5.866 min) Amino Acids-3.D
Glycine
* 174.1144
73.0470
248.1333
Counts vs. Mass-to-Charge (m/z)

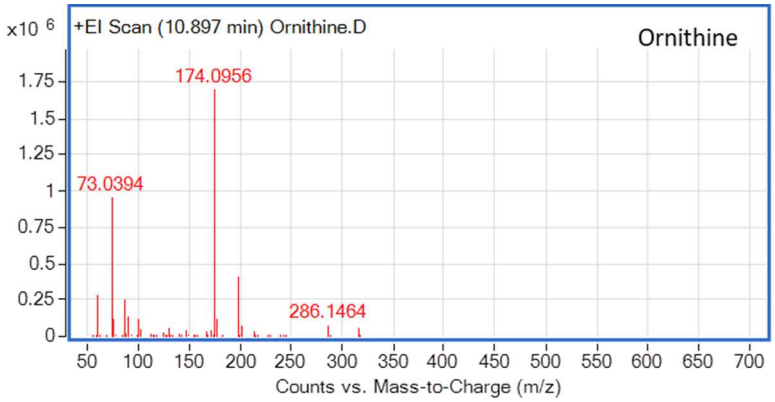

x10 7
+EI Scan (5.864 min) A549-3.D
Glycine
* 174.1148
73.0471
248.1334
Counts vs. Mass-to-Charge (m/z)

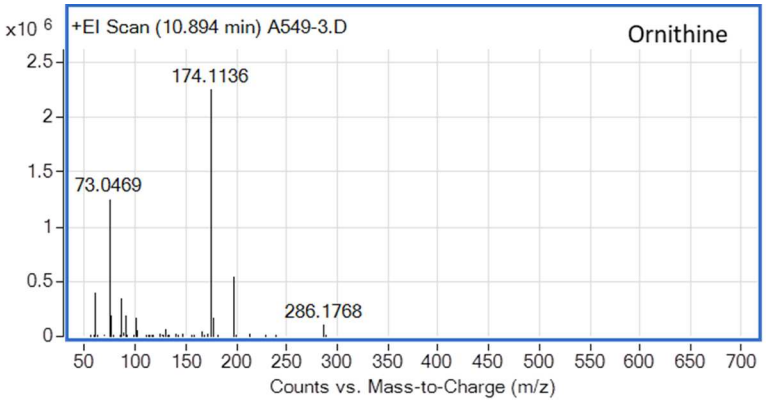

x10 6
+EI Scan (6.536 min) Amino Acids-3.D
Serine
204.1250
73.0470
147.0661
278.1430
Counts vs. Mass-to-Charge (m/z)

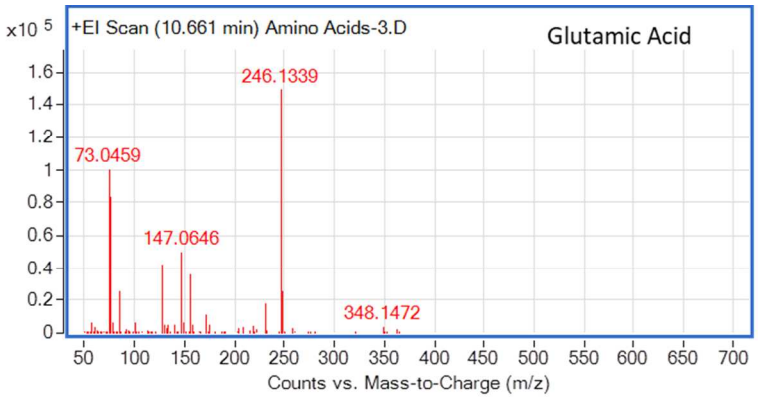

x10 7
+EI Scan (6.543 min) A549-3.D
Serine
* 204.1255
73.0472
147.0662
278.1441
Counts vs. Mass-to-Charge (m/z)

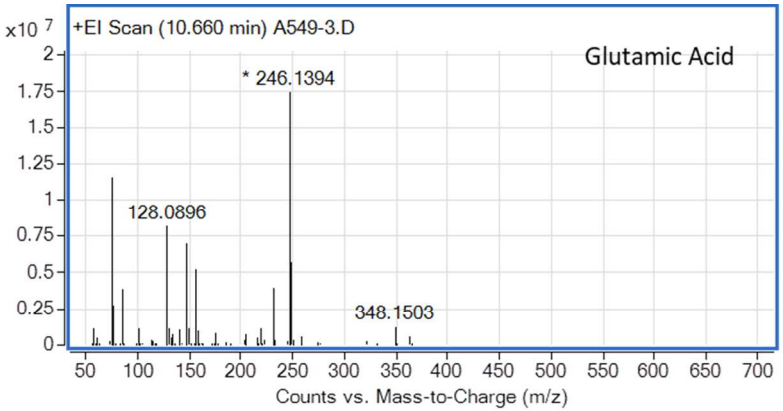

x10 6
+EI Scan (6.897 min) Amino Acids-3.D
Theronine
73.0471
219.1147
147.0660
291.1519
Counts vs. Mass-to-Charge (m/z)

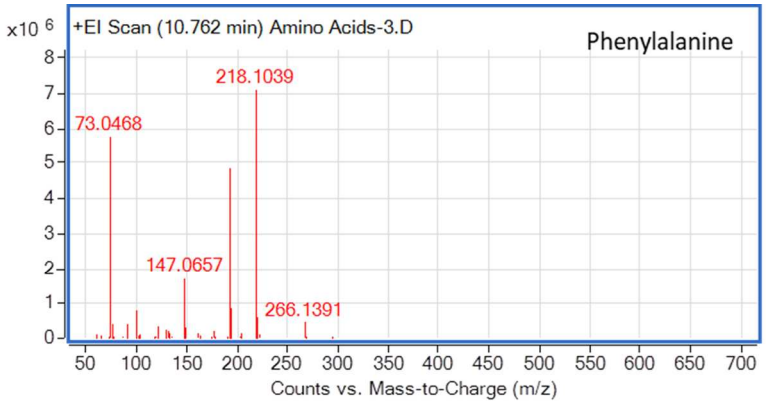

x10 6
+EI Scan (6.904 min) A549-3.D
Theronine
73.0470
219.1144
147.0661
291.1517
Counts vs. Mass-to-Charge (m/z)

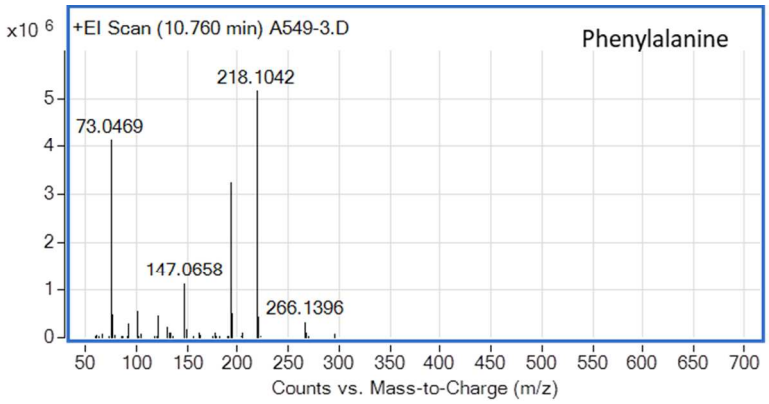

x10 6
+EI Scan (10.897 min) Ornithine.D
Ornithine
174.0956
73.0394
286.1464
Counts vs. Mass-to-Charge (m/z)

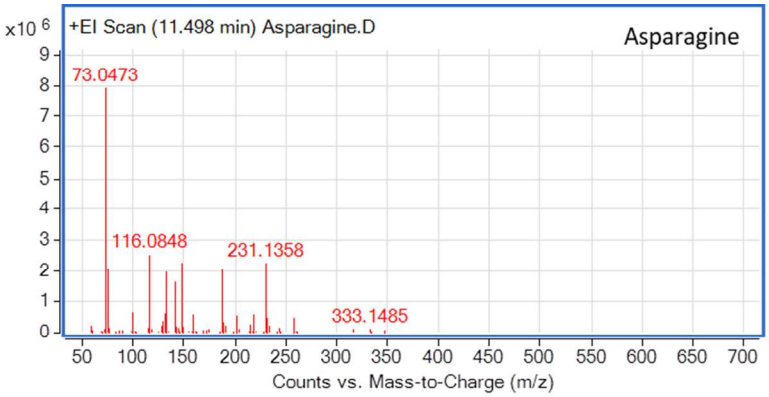

x10 6
+EI Scan (10.894 min) A549-3.D
Ornithine
174.1136
73.0469
286.1768
Counts vs. Mass-to-Charge (m/z)

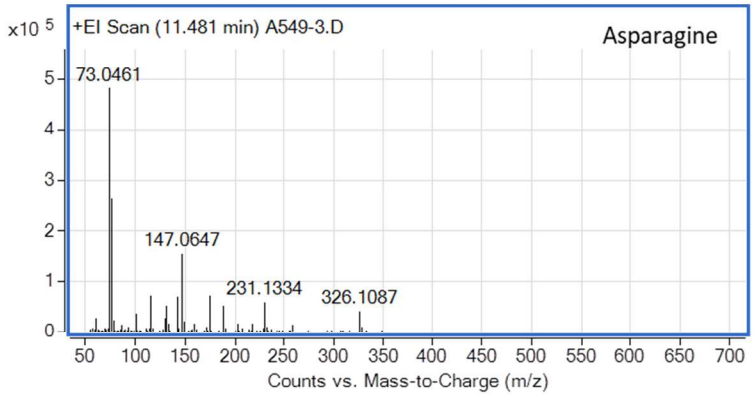

x10 5
+EI Scan (10.661 min) Amino Acids-3.D
Glutamic Acid
246.1339
73.0459
147.0646
348.1472
Counts vs. Mass-to-Charge (m/z)

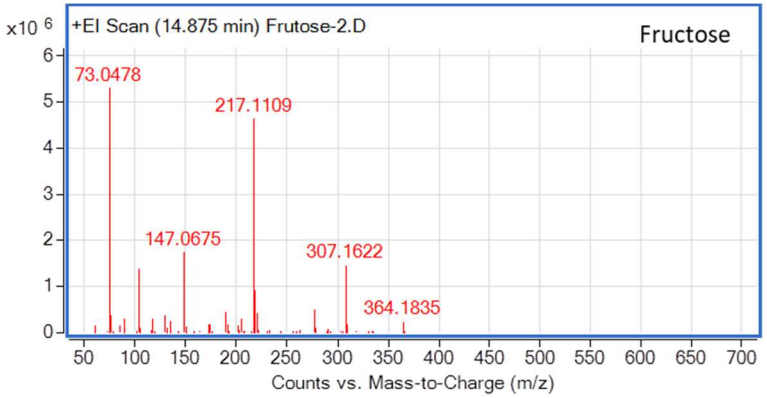

x10 7
+EI Scan (10.660 min) A549-3.D
Glutamic Acid
* 246.1394
128.0896
348.1503
Counts vs. Mass-to-Charge (m/z)

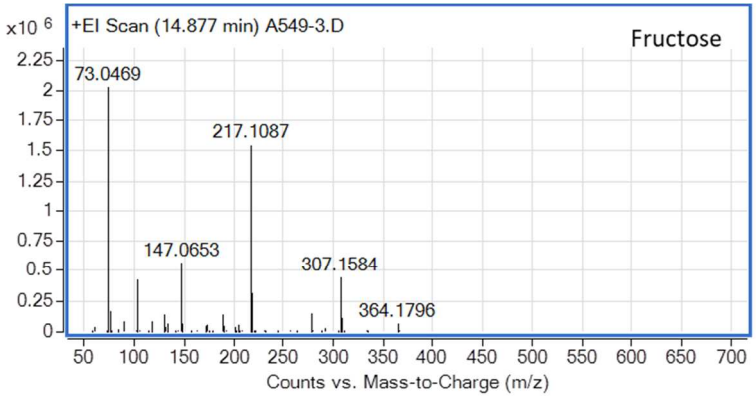

x10 6
+EI Scan (10.762 min) Amino Acids-3.D
Phenylalanine
218.1039
73.0468
147.0657
266.1391
Counts vs. Mass-to-Charge (m/z)

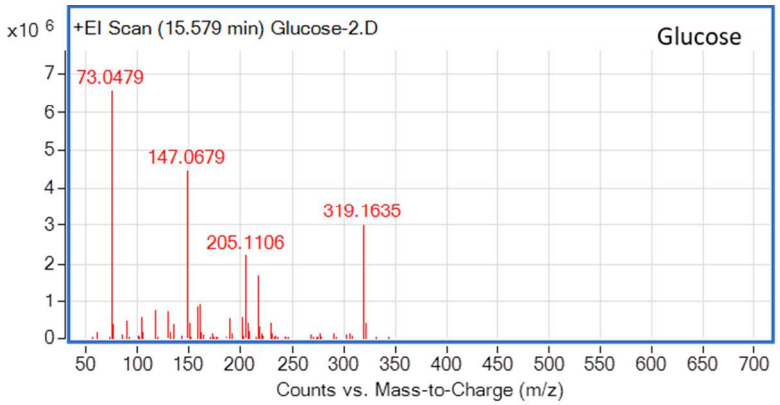

x10 6
+EI Scan (10.760 min) A549-3.D
Phenylalanine
218.1042
73.0469
147.0658
266.1396
Counts vs. Mass-to-Charge (m/z)

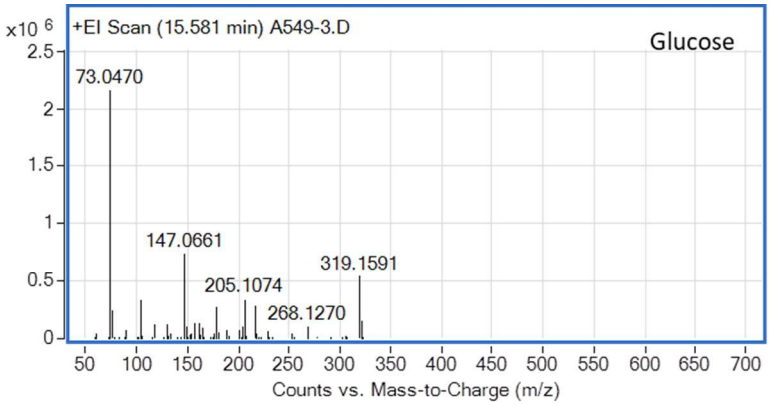

x10 6
+EI Scan (11.498 min) Asparagine.D
Asparagine
73.0473
116.0848
231.1358
333.1485
Counts vs. Mass-to-Charge (m/z)

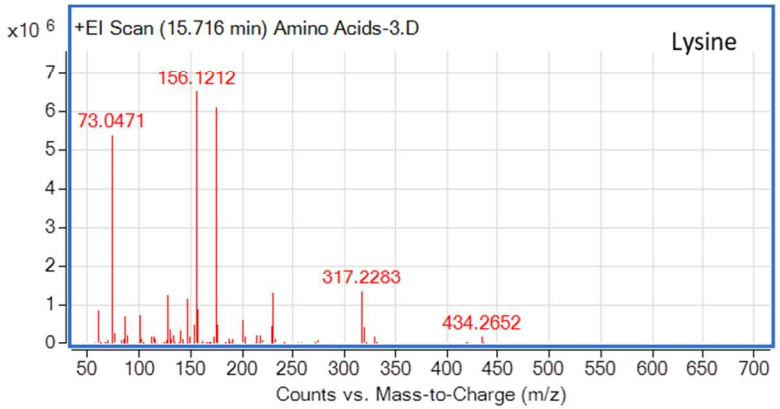

x10 5
+EI Scan (11.481 min) A549-3.D
Asparagine
73.0461
147.0647
231.1334
326.1087
Counts vs. Mass-to-Charge (m/z)

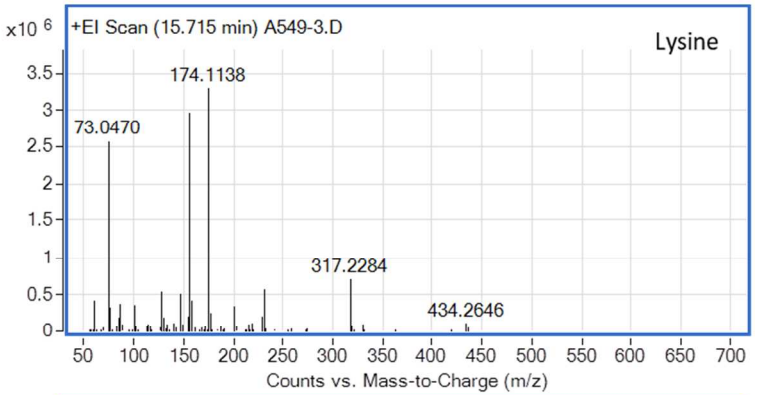

x10 6
+EI Scan (14.875 min) Frutose-2.D
Fructose
73.0478
217.1109
147.0675
307.1622
364.1835
Counts vs. Mass-to-Charge (m/z)

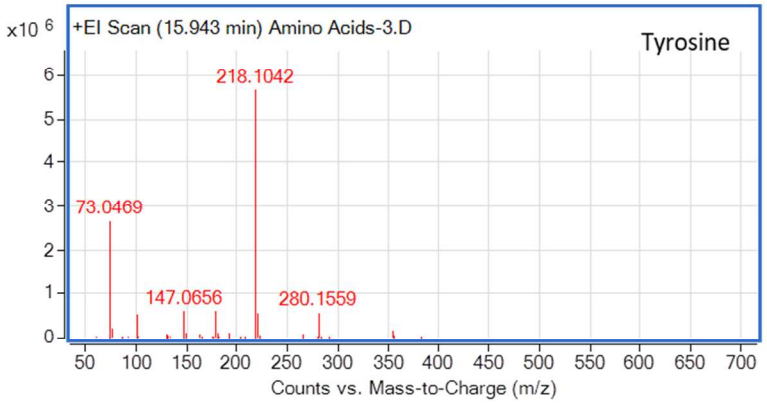

x10 6
+EI Scan (14.877 min) A549-3.D
Fructose
73.0469
217.1087
147.0653
307.1584
364.1796
Counts vs. Mass-to-Charge (m/z)

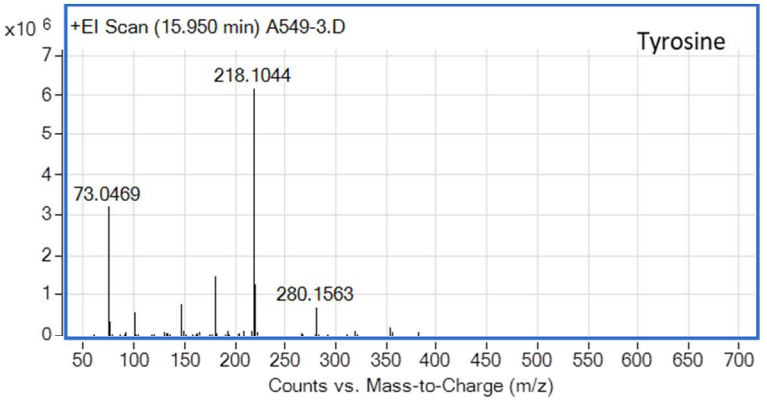

x10 6
+EI Scan (15.579 min) Glucose-2.D
Glucose
73.0479
147.0679
205.1106
319.1635
Counts vs. Mass-to-Charge (m/z)

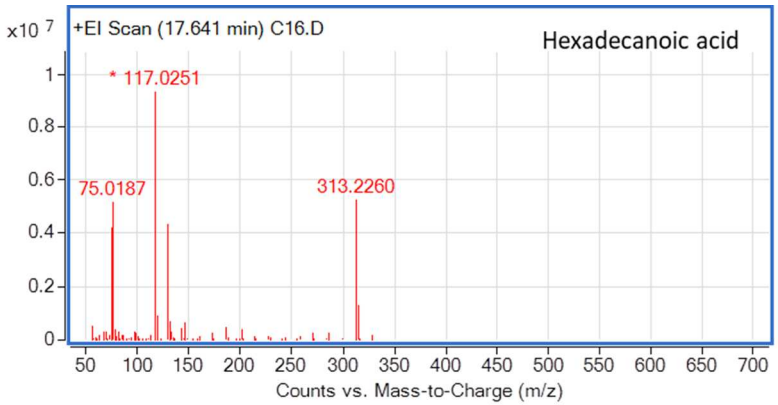

x10 6
+EI Scan (15.581 min) A549-3.D
Glucose
73.0470
147.0661
205.1074
268.1270
319.1591
Counts vs. Mass-to-Charge (m/z)

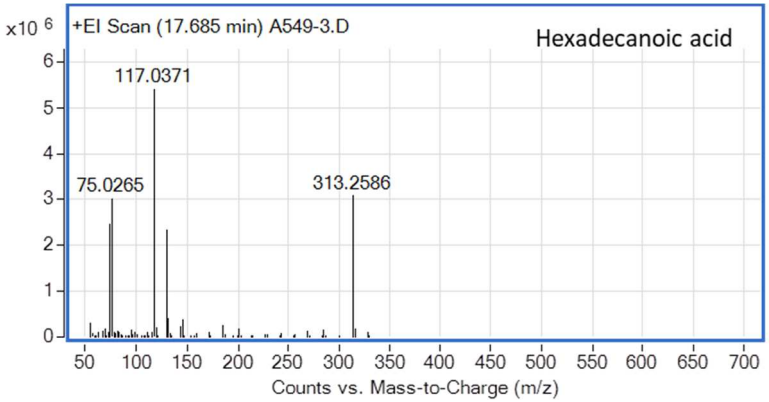

x10 6
+EI Scan (15.716 min) Amino Acids-3.D
Lysine
156.1212
73.0471
317.2283
434.2652
Counts vs. Mass-to-Charge (m/z)

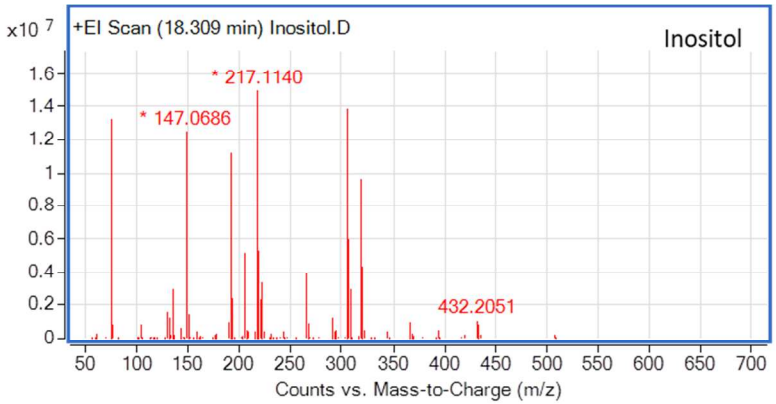

x10 6
+EI Scan (15.715 min) A549-3.D
Lysine
174.1138
73.0470
317.2284
434.2646
Counts vs. Mass-to-Charge (m/z)

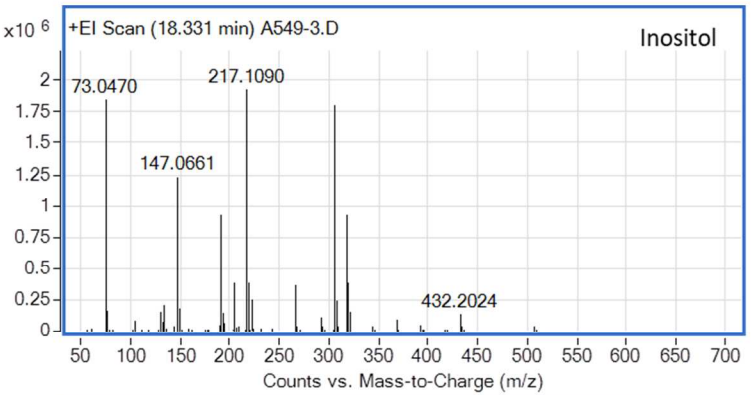

x10 6
+EI Scan (15.943 min) Amino Acids-3.D
Tyrosine
218.1042
73.0469
147.0656
280.1559
Counts vs. Mass-to-Charge (m/z)

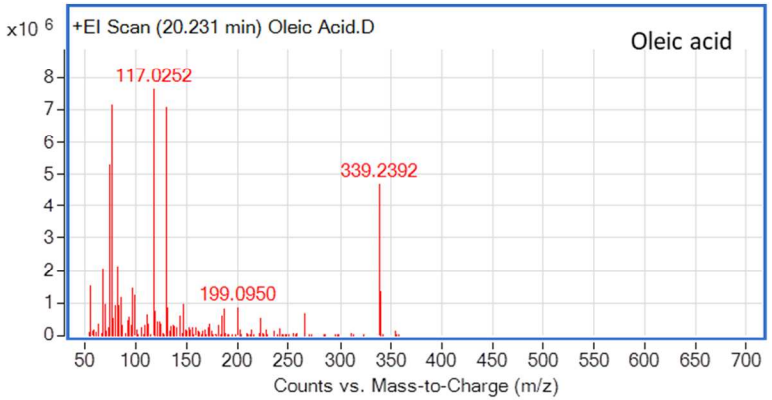

x10 6
+EI Scan (15.950 min) A549-3.D
Tyrosine
218.1044
73.0469
280.1563
Counts vs. Mass-to-Charge (m/z)

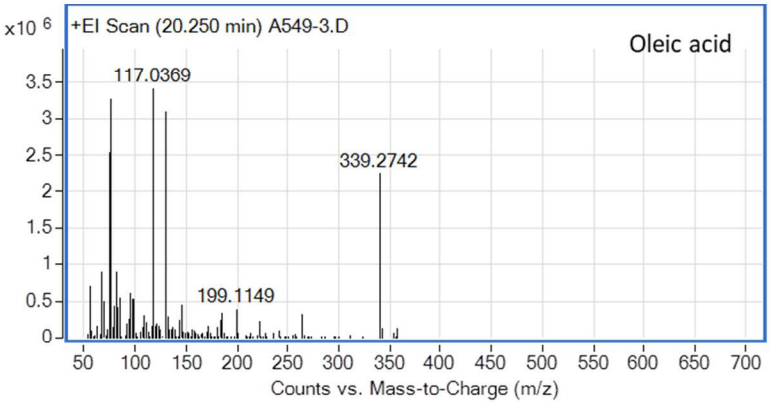

x10 7
+EI Scan (17.641 min) C16.D
Hexadecanoic acid
* 117.0251
75.0187
313.2260
Counts vs. Mass-to-Charge (m/z)

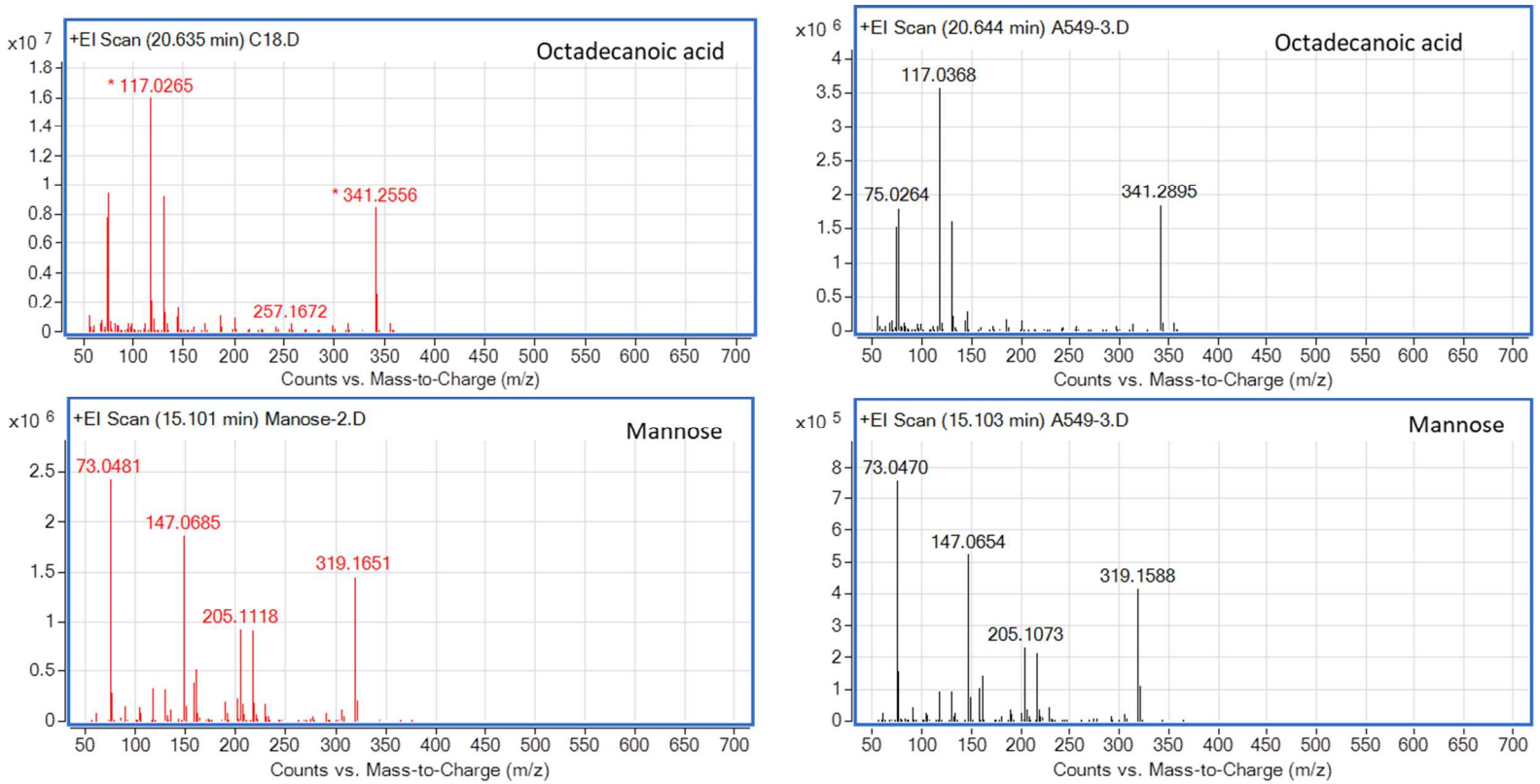

x10 6
+EI Scan (17.685 min) A549-3.D
Hexadecanoic acid
117.0371
75.0265
313.2586
Counts vs. Mass-to-Charge (m/z)


x10 7
+EI Scan (18.309 min) Inositol.D
Inositol
* 217.1140
* 147.0686
432.2051
Counts vs. Mass-to-Charge (m/z)


x10 6
+EI Scan (18.331 min) A549-3.D
Inositol
73.0470
217.1090
147.0661
432.2024
Counts vs. Mass-to-Charge (m/z)

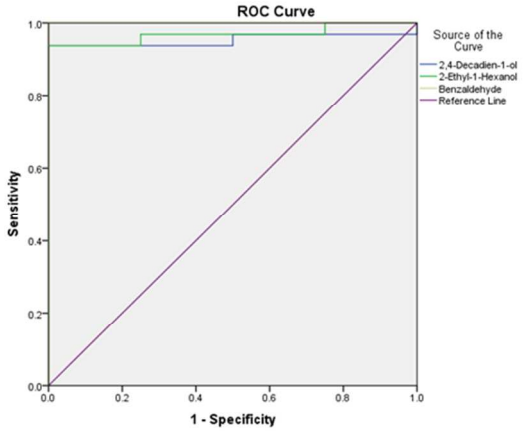

x10 6
+EI Scan (20.231 min) Oleic Acid.D
Oleic acid
117.0252
339.2392
199.0950
Counts vs. Mass-to-Charge (m/z)


x10 6
+EI Scan (20.250 min) A549-3.D
Oleic acid
117.0369
339.2742
199.1149
Counts vs. Mass-to-Charge (m/z)



Figue S7. Parallel comparison of spectrums of 20 non-volatile metabolites in sample and in standards. Spectrum of standard is in red, spectrum of sample is in black

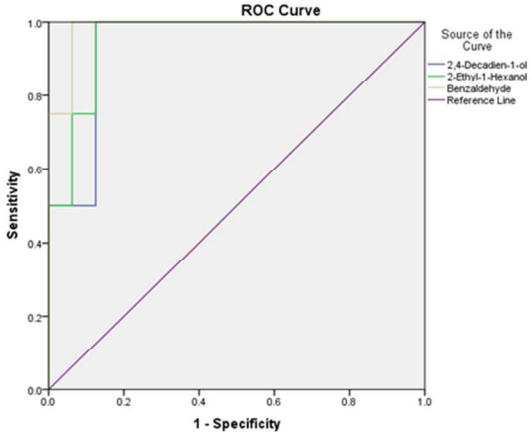
a)



Area Under the Curve

Test Result Variable(s)	Area
2,4-Decadien-1-ol	.953
2-Ethyl-1-Hexanol	.969
Benzaldehyde	1.000

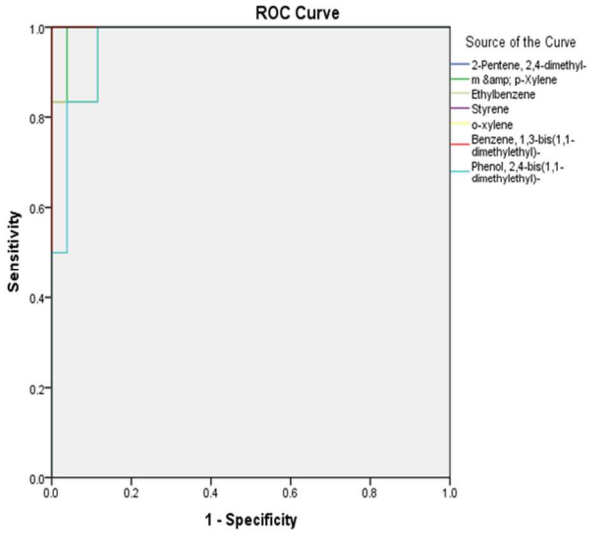
b)



Area Under the Curve

Test Result Variable(s)	Area
2,4-Decadien-1-ol	.938
2-Ethyl-1-Hexanol	.953
Benzaldehyde	.984

c)



Area Under the Curve

Test Result Variable(s)	Area
2-Pentene, 2,4-dimethyl-	1.000
m & p-Xylene	.994
Ethylbenzene	.981
Styrene	1.000
o-xylene	1.000
Benzene, 1,3-bis(1,1-dimethylethyl)-	1.000
Phenol, 2,4-bis(1,1-dimethylethyl)-	.968

Figure S8. ROC analysis of a) cancer vs normal cell b) large cell vs. other NSCLC. c) SCLC vs NSCLC