

## Library Search Results - NonTarget Hits with Details



Trusted Answers

Batch Path	D:\MassHunter\GCMS\1\data\RBEL\240501 scan	Analysis Time	5/2/2024 11:31:09 AM
Analysis File Name	240502 data.uaf		
Analyst Name	admin		
File Name	1.D	Path Name	D:\MassHunter\GCMS\1\data\RBEL\240501 scan
Sample Name	1	Sample Type	Sample
Acq. Method File	240501 scan	Acq. Method Path	D:\MassHunter\GCMS\1\methods\RBEL\
Acq. Date-Time	5/1/2024 1:36:47 PM	Acq. Operator	
Instrument Name	GCMSD	Dil.	1

Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
6.9745	3-Furaldehyde	498-60-2	C5H4O2	234391.9	95.7	
7.2735	1,3-Propanediol	504-63-2	C3H8O2	1263556.9	96.0	
10.1875	Ethanedioic acid, diethyl ester	95-92-1	C6H10O4	478276.3	75.0	
11.5784	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	1041610.3	78.5	
12.3947	Butyrolactone	96-48-0	C4H6O2	12958594.4	97.7	
12.3974	2-Propenal	107-02-8	C3H4O	2114377.4	78.1	
12.7378	(S)-(+)-1,2-Propanediol	4254-15-3	C3H8O2	1369287.5	79.3	
12.7378	Acetoin	513-86-0	C4H8O2	1449576.9	79.2	
13.2773	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	922641.6	76.5	
13.2773	Ethanol, 2-(1,1-dimethylethoxy)-	7580-85-0	C6H14O2	817371.6	76.0	
16.4438	Ethane, 1,1,1-triethoxy-	78-39-7	C8H18O3	399182.1	75.5	
16.4440	Ethyl 2,2-diethoxypropionate	7476-20-2	C9H18O4	399225.1	75.8	
17.0180	Acetoin	513-86-0	C4H8O2	690174.9	79.6	
17.9778	Phenol	108-95-2	C6H6O	254152.5	93.3	
18.6438	Diisoamyl ether	544-01-4	C10H22O	3396460.2	98.2	
20.0201	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	703403.8	95.0	
21.1093	1,3,5-Trioxane	110-88-3	C3H6O3	4648194.3	77.4	
23.0255	Octanol	111-87-5	C8H18O	3779230.8	98.4	
23.5574	Phenol, 2-methoxy-	90-05-1	C7H8O2	8383926.4	98.5	
23.6130	Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	3230331.3	82.1	
24.6682	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	3228314.2	87.8	
25.1522	1,3,5,7-Tetroxane	293-30-1	C4H8O4	648304.1	78.0	
26.6801	2-Propanone, 1-hydroxy-	116-09-6	C3H6O2	22515463.1	80.1	
26.6803	Glycerin	56-81-5	C3H8O3	37962614.8	80.5	
27.7058	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	1010279.2	81.3	
29.1581	Creosol	93-51-6	C8H10O2	525521.9	97.3	
30.4598	1,3-Dioxolane, 2-butyl-4-methyl-	74094-60-3	C8H16O2	834040.1	79.0	
30.7535	Catechol	120-80-9	C6H6O2	925875.3	86.6	
31.1051	1-Propanone, 1-(5-methyl-2-thienyl)-	59303-13-8	C8H10O5	343736.1	76.1	
32.0956	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	234475.9	90.1	
32.4794	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	538517.7	94.6	
33.3274	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	2832530.1	97.6	
35.0048	Ethylene glycol Formate Isobutyrate	1000458-48-0	C7H12O4	17452974.0	83.5	
35.3071	2,3-dihydroxypropyl isobutyrate	1010458-45-6	C7H14O4	17670321.0	79.5	
35.3074	Butanoic acid, 2-methylpropyl ester	539-90-2	C8H16O2	17616193.8	78.2	
36.1579	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	4021958.6	82.2	
36.7946	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	16652182.6	97.9	
37.4113	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	240330.3	80.4	
38.9840	Vanillin	121-33-5	C8H8O3	9553029.9	99.0	
39.4888	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	C8H8O2	227800.9	89.7	
40.8720	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	776796.4	92.5	
42.5978	Apocynin	498-02-2	C9H10O3	5395989.4	99.2	
44.0450	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	2188782.0	97.5	
44.2850	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	7255885.9	93.9	
44.2924	4-[2-(2-Propenyl)-1,3-dioxolan-2-yl]-1H-pyrazole	98816-47-8	C9H12N2O2	329057.9	75.7	
44.3268	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6825508.8	94.9	
45.6164	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	3757-32-2	C9H16O3	991790.5	85.1	
46.0282	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	913799.3	90.7	
46.4726	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9	C10H12O3	384241.8	83.3	
46.6327	Butyrovanillone	64142-23-0	C11H14O3	10320359.6	95.3	
47.0806	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	352815.4	82.6	
47.3445	Homosyringaldehyde	87345-52-6	C10H12O4	249662.5	83.0	
48.9790	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	6788098.5	96.4	
49.3444	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	2605242.4	96.7	
49.4061	7-Methoxy-1-naphthol	67247-13-6	C11H10O2	366053.3	84.2	
49.4209	2,6-Dimethoxyhydroquinone	15233-65-5	C8H10O4	383468.5	78.5	
50.4127	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	326279.1	80.6	
50.6291	Phenylacetylformic acid, 4-hydroxy-3-methoxy-	1081-71-6	C10H10O5	303107.7	79.6	
51.0371	Butanoic acid, (tetrahydro-2-furanyl)methyl ester	2217-33-6	C9H16O3	665275.7	77.4	
51.9859	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	6385500.3	97.5	
52.1417	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	553692.7	76.7	
53.2264	Syringylacetone	19037-58-2	C11H14O4	5978717.1	97.7	
53.5885	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	308310.5	79.4	
54.9294	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	530-57-4	C9H10O5	621745.1	85.0	

## Library Search Results - NonTarget Hits with Details

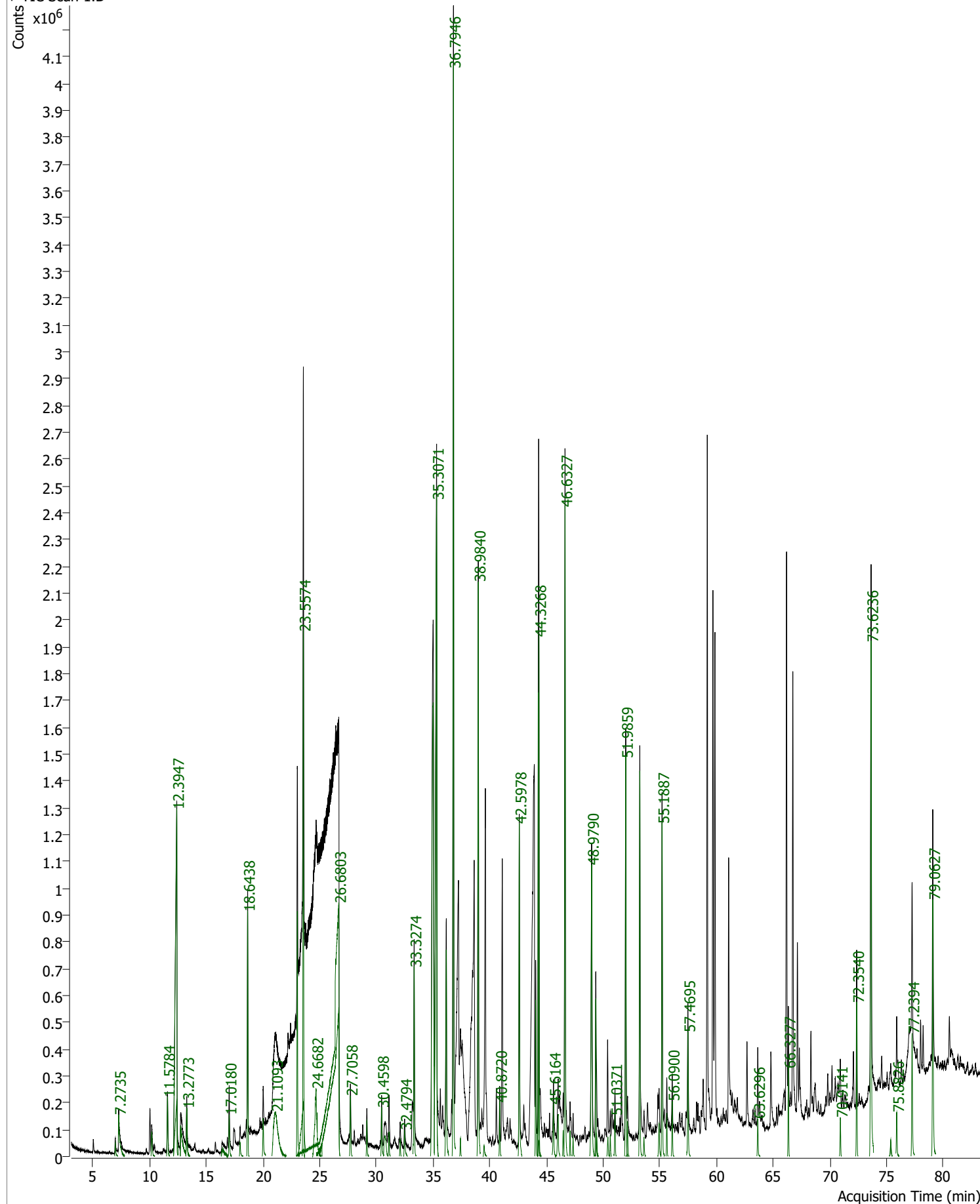


Trusted Answers

Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
55.1887	Butylsyringone	69271-91-6	C12H16O4	5238788.3	92.8	
55.6079	Acetyl syringic acid, ethyl ester	1000454-70-9	C13H16O6	586028.4	87.9	
56.0900	2,3-Dimethoxy-5-aminocinnamitrile	1000214-46-5	C11H12N2O2	821559.2	79.6	
57.4695	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	2046714.7	92.7	
63.6296	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	592568.4	76.5	
66.3277	(E)-9-Octadecenoic acid ethyl ester	6114-18-7	C20H38O2	1204905.9	89.6	
70.9141	Methyl dehydroabietate	1235-74-1	C21H30O2	544068.0	83.3	
72.3540	Methyl dehydroabietate	1235-74-1	C21H30O2	2231742.9	76.5	
73.6236	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-	5155-70-4	C20H28O2	10413462.8	93.3	
75.3528	Cyclotetradecane	295-17-0	C14H28	268574.4	84.5	
75.3538	Undecane, 4-cyclohexyl-	13151-79-6	C17H34	316799.7	84.8	
75.8826	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	771065.1	92.0	
77.2394	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	2195585.6	76.2	
79.0627	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	4958162.3	92.6	

## Sample Chromatogram

+ TIC Scan 1.D



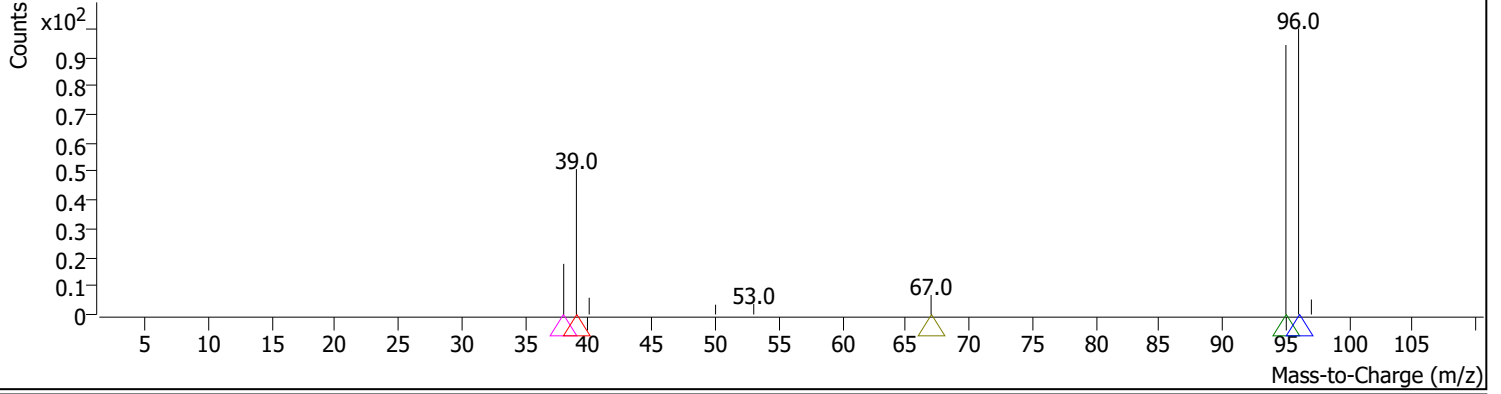
# Library Search Results - NonTarget Hits with Details



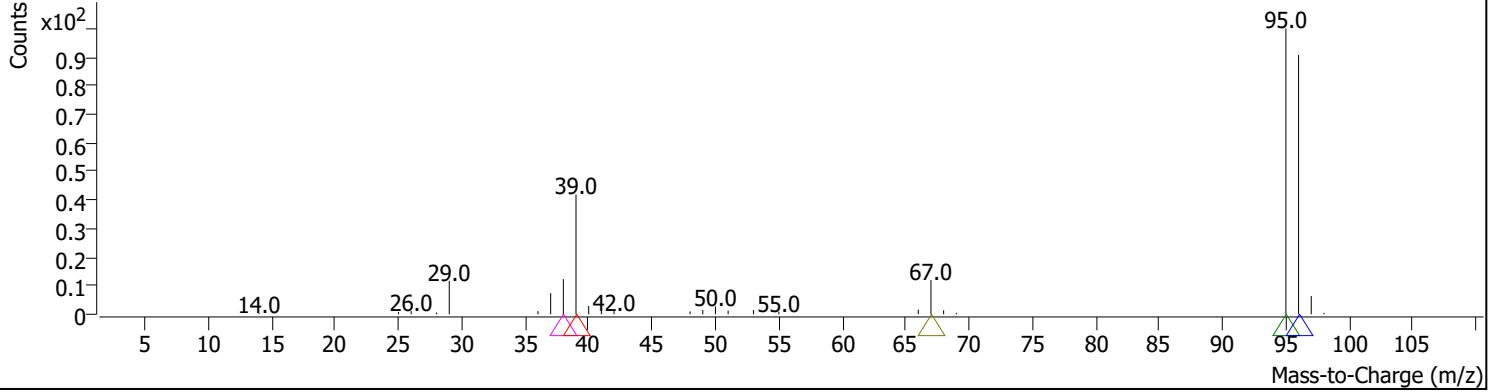
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
6.9745	3-Furaldehyde	234391.9	95.7	498-60-2	C5H4O2	

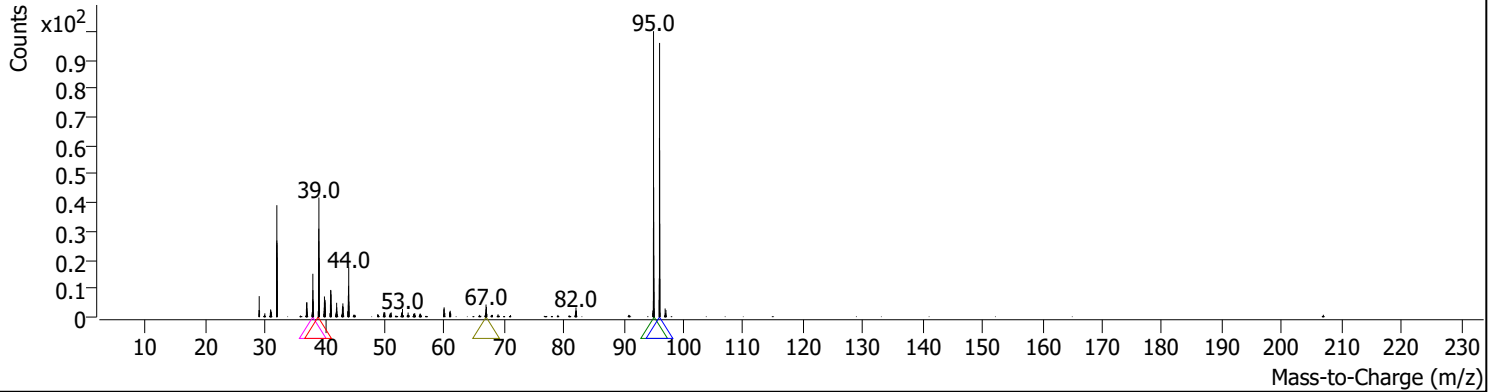
Component RT: 6.9745



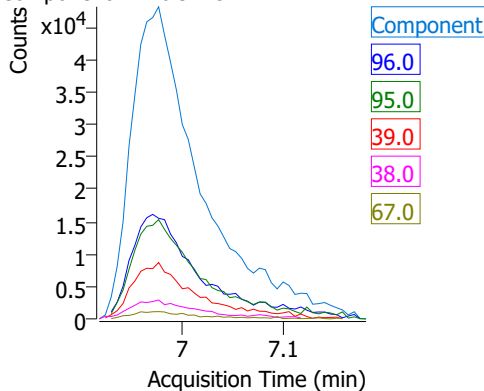
3-Furaldehyde (NIST20.L)



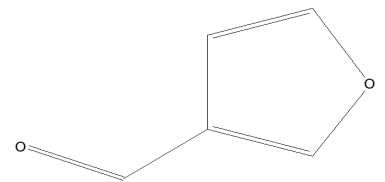
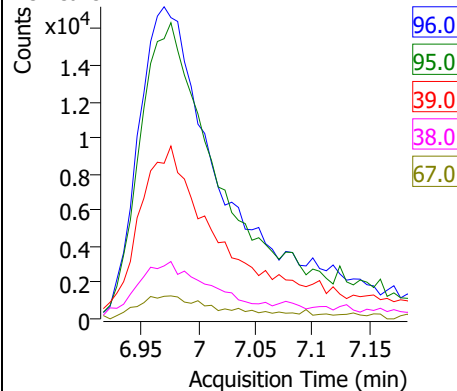
+ Scan (6.9236-7.1780 min, 43 scans) 1.D



Component RT: 6.9745



EIC Peaks



# Library Search Results - NonTarget Hits with Details

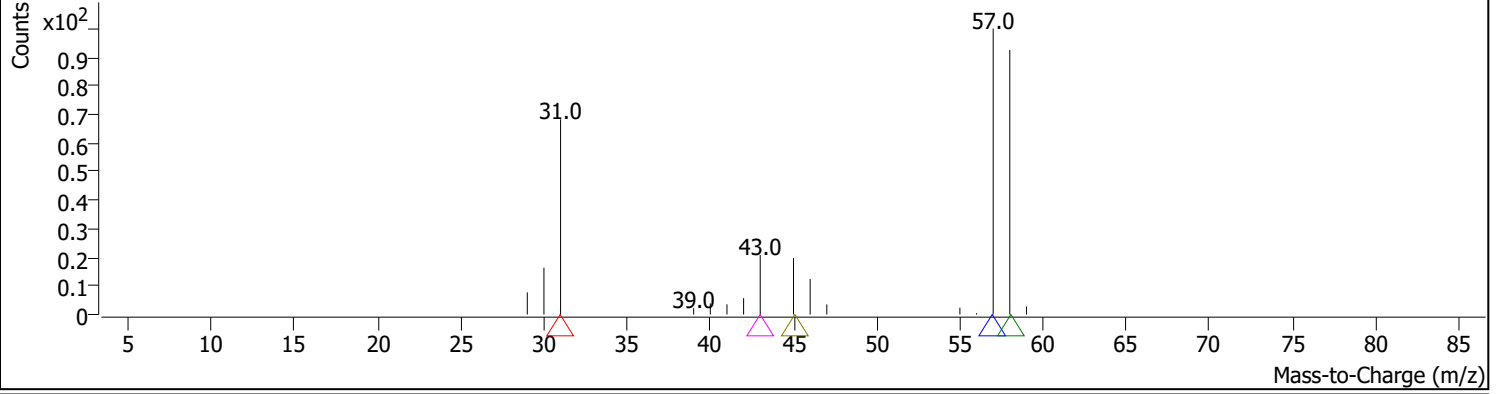


Agilent

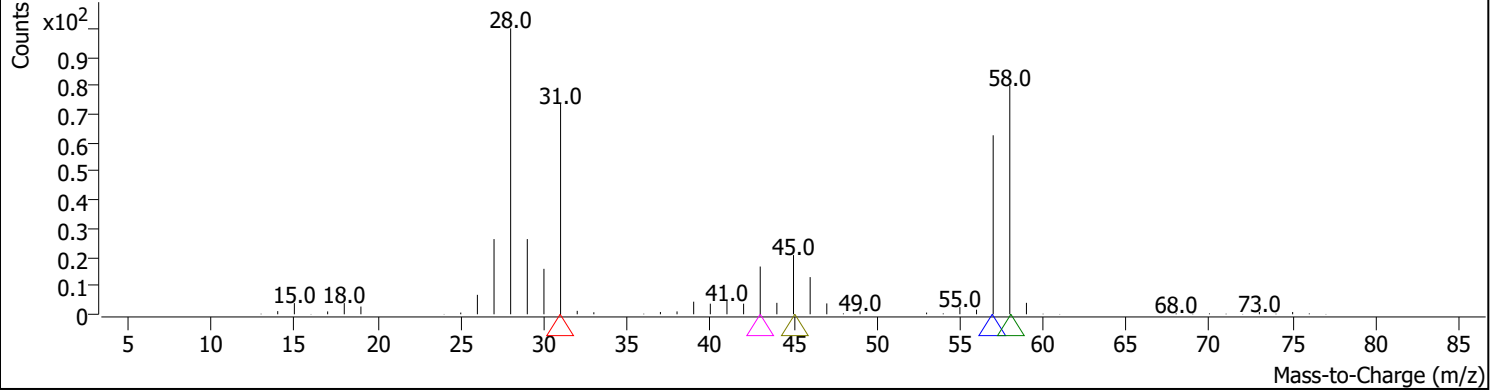
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
7.2735	1,3-Propanediol	1263556.9	96.0	504-63-2	C3H8O2	

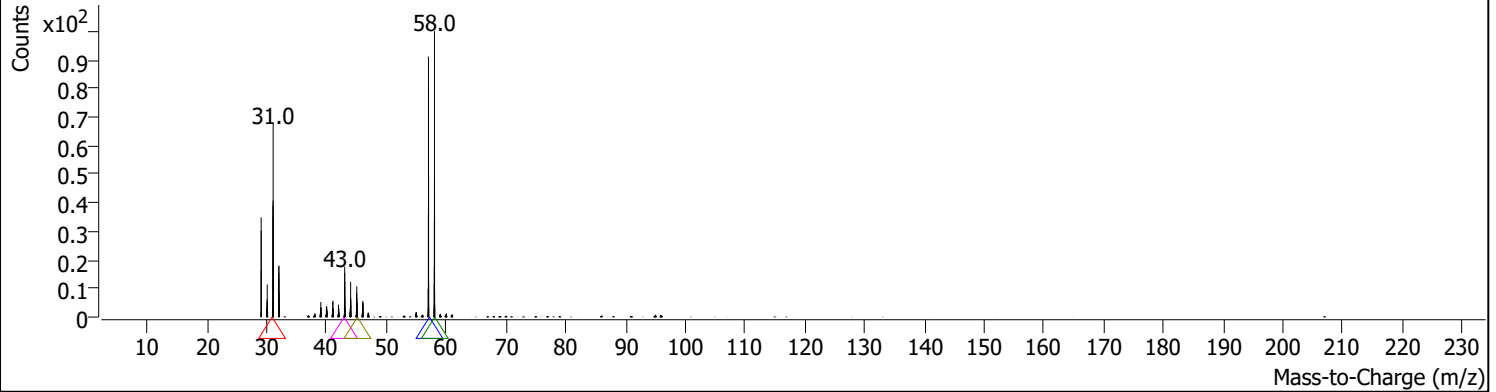
Component RT: 7.2735



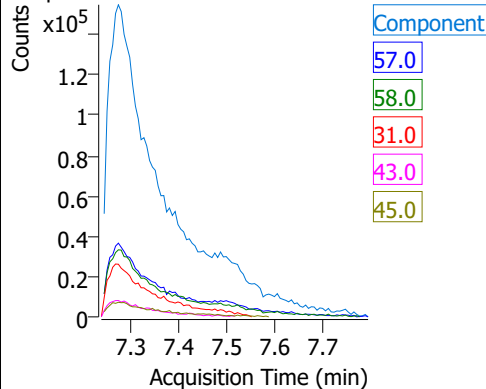
1,3-Propanediol (NIST20.L)



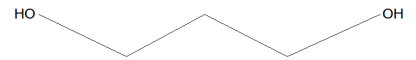
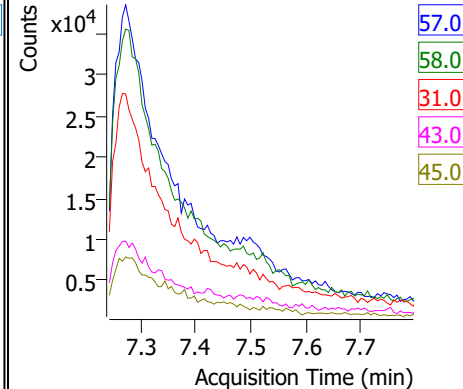
+ Scan (7.2376-7.7786 min, 91 scans) 1.D



Component RT: 7.2735



EIC Peaks



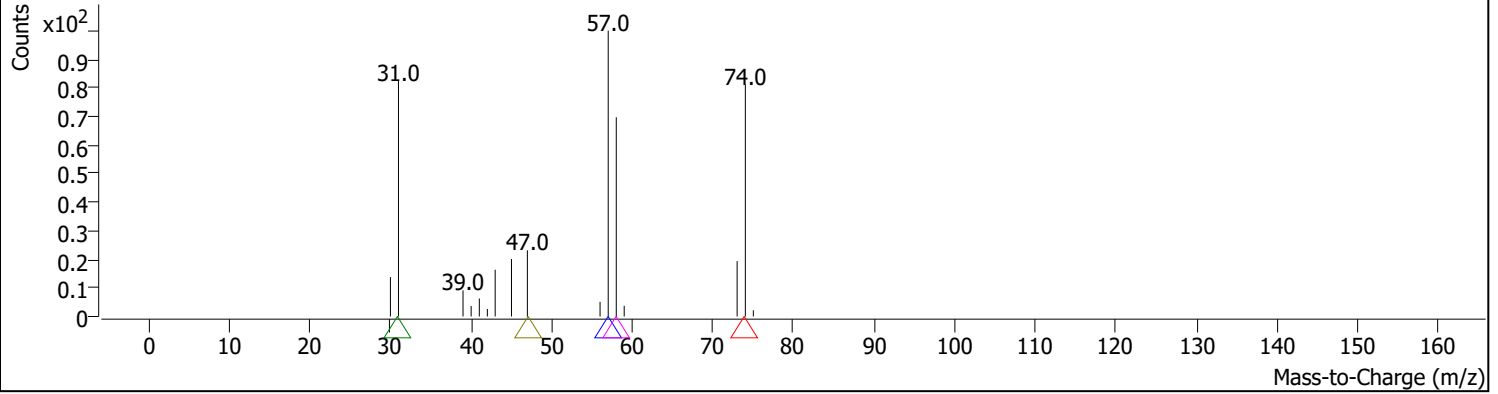
## Library Search Results - NonTarget Hits with Details



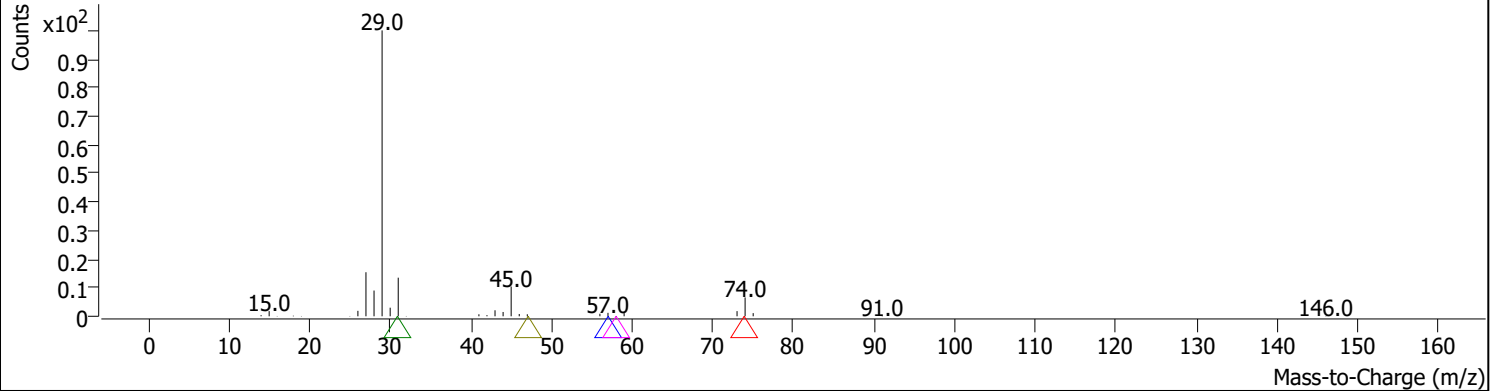
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
10.1875	Ethanedioic acid, diethyl ester	478276.3	75.0	95-92-1	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>	

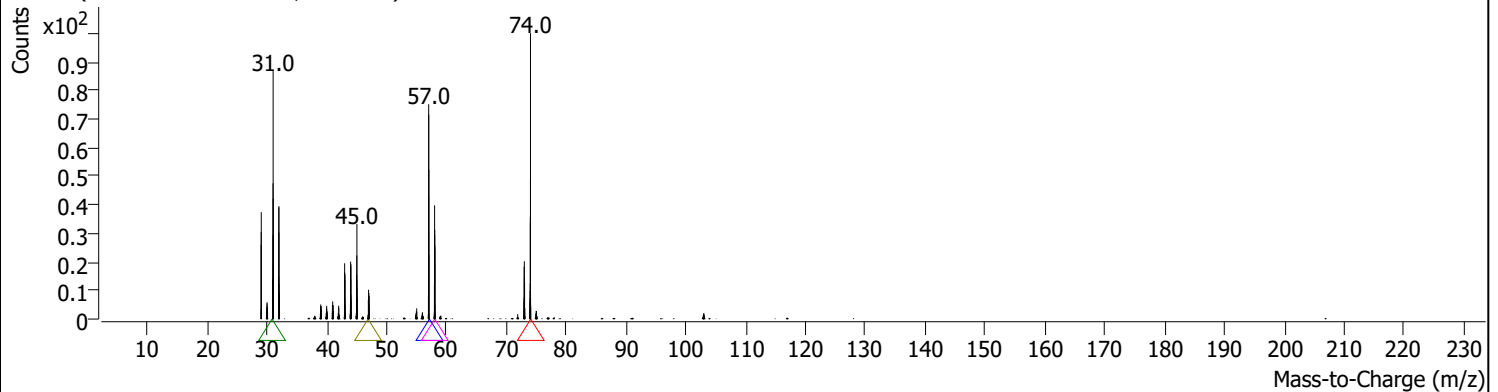
Component RT: 10.1875



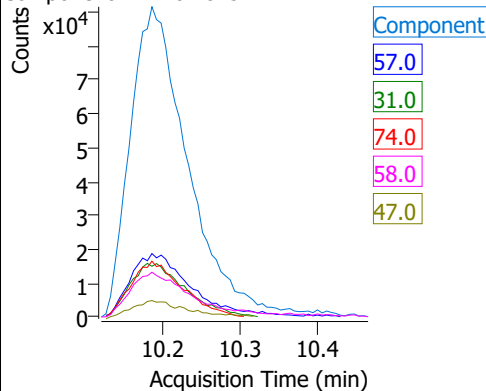
Ethanedioic acid, diethyl ester (NIST20.L)



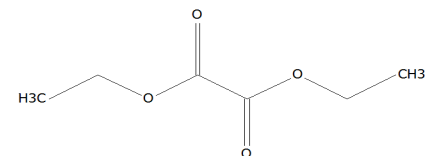
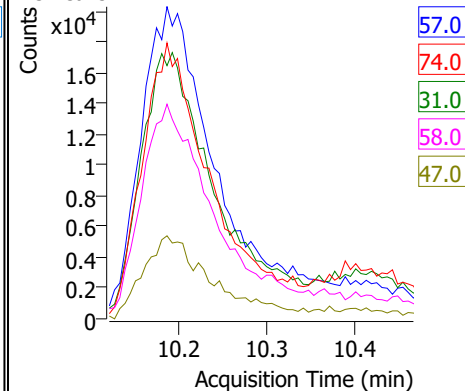
+ Scan (10.1257-10.4677 min, 58 scans) 1.D



Component RT: 10.1875



EIC Peaks



## Library Search Results - NonTarget Hits with Details

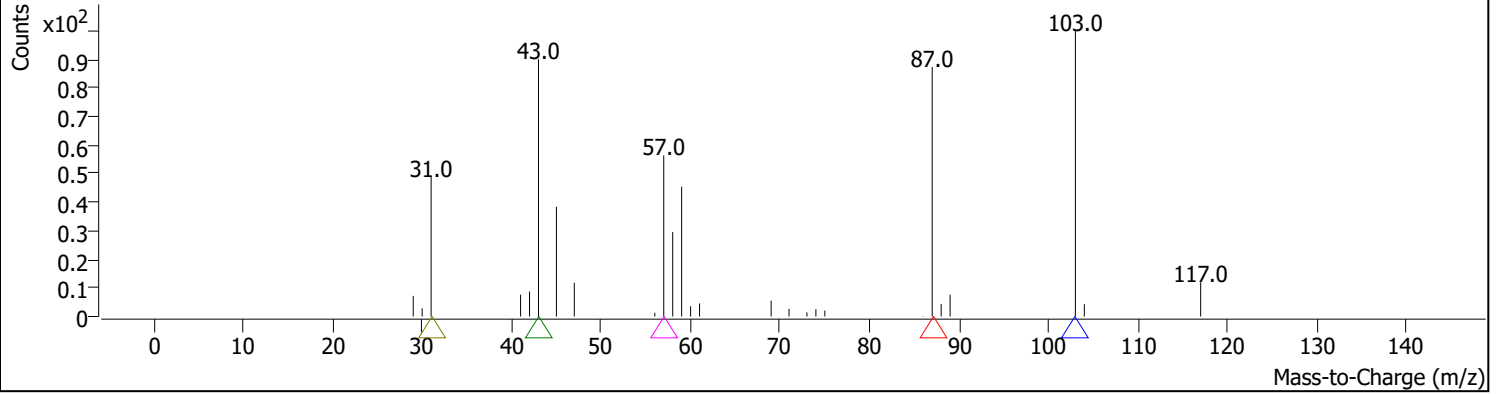


Agilent

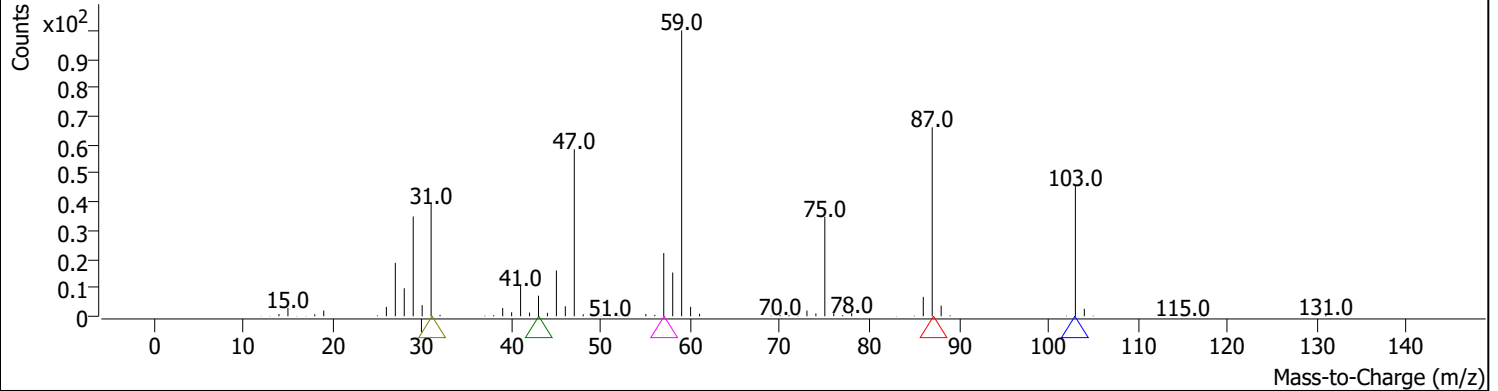
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
11.5784	Propane, 1,1-diethoxy-	1041610.3	78.5	4744-08-5	C7H16O2	

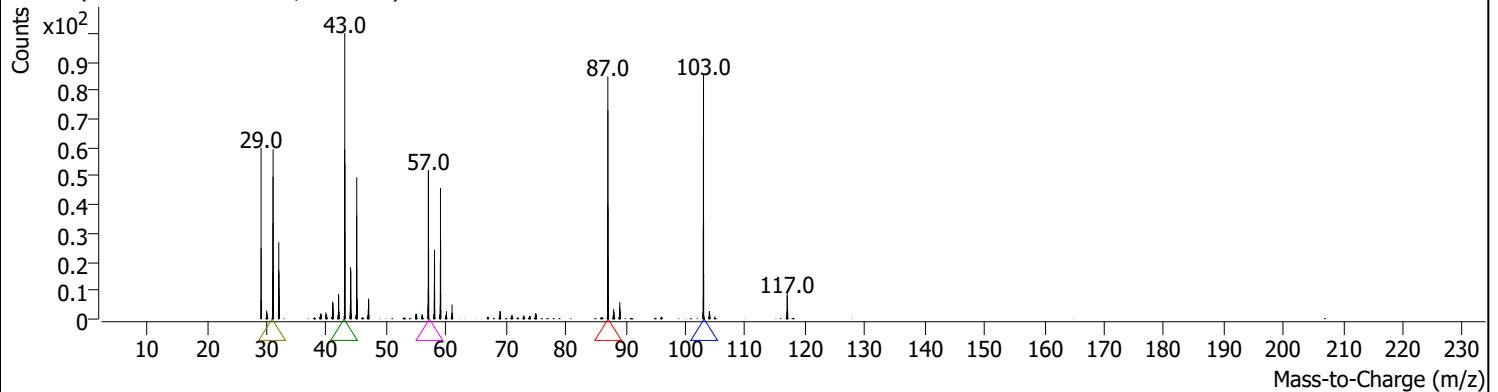
Component RT: 11.5784



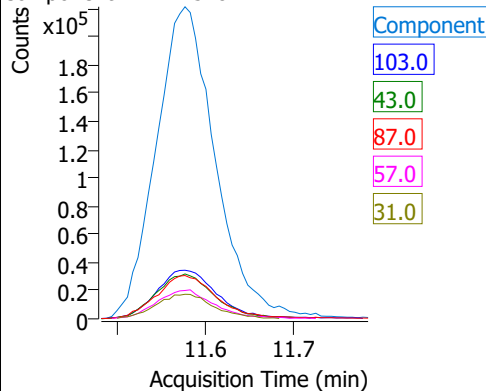
Propane, 1,1-diethoxy- (NIST20.L)



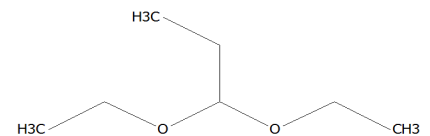
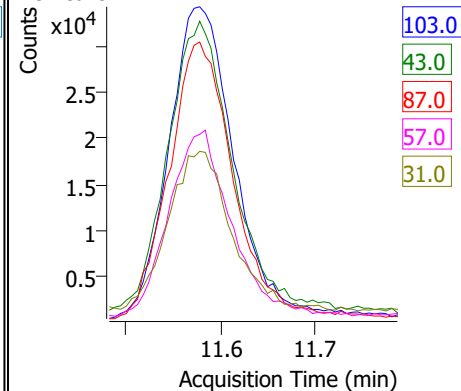
+ Scan (11.4925-11.7327 min, 41 scans) 1.D



Component RT: 11.5784



EIC Peaks



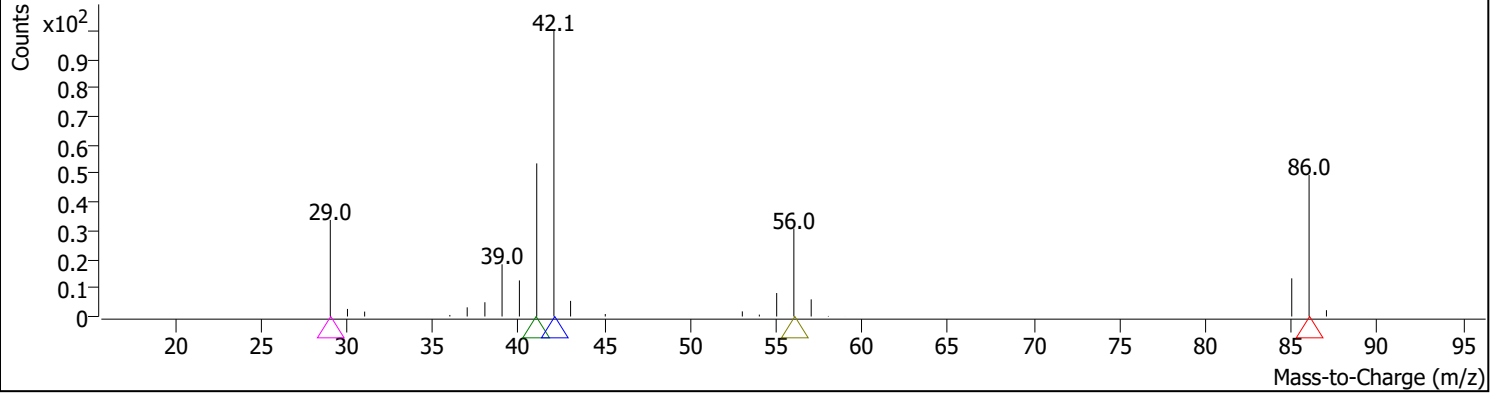
## Library Search Results - NonTarget Hits with Details



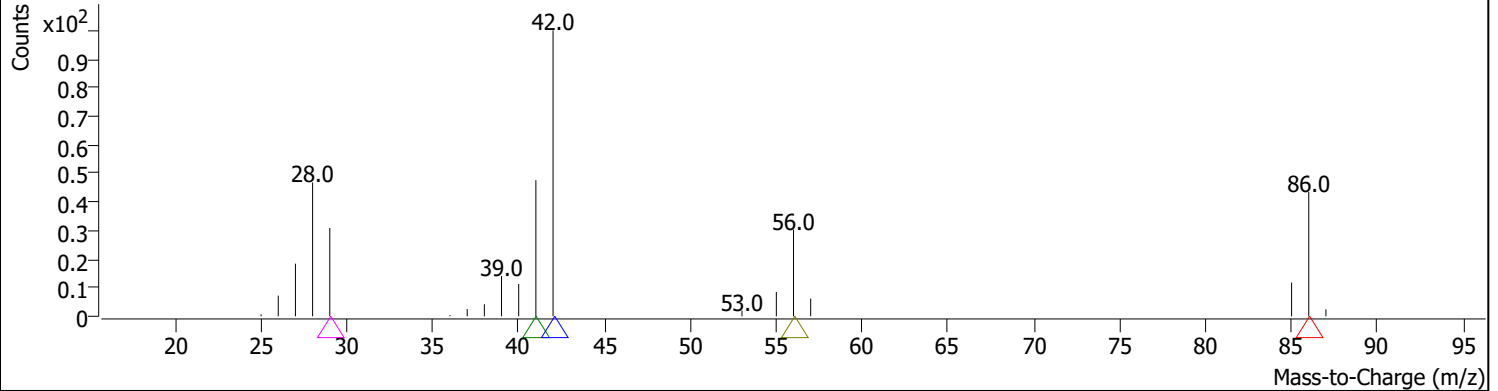
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
12.3947	Butyrolactone	12958594.4	97.7	96-48-0	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	

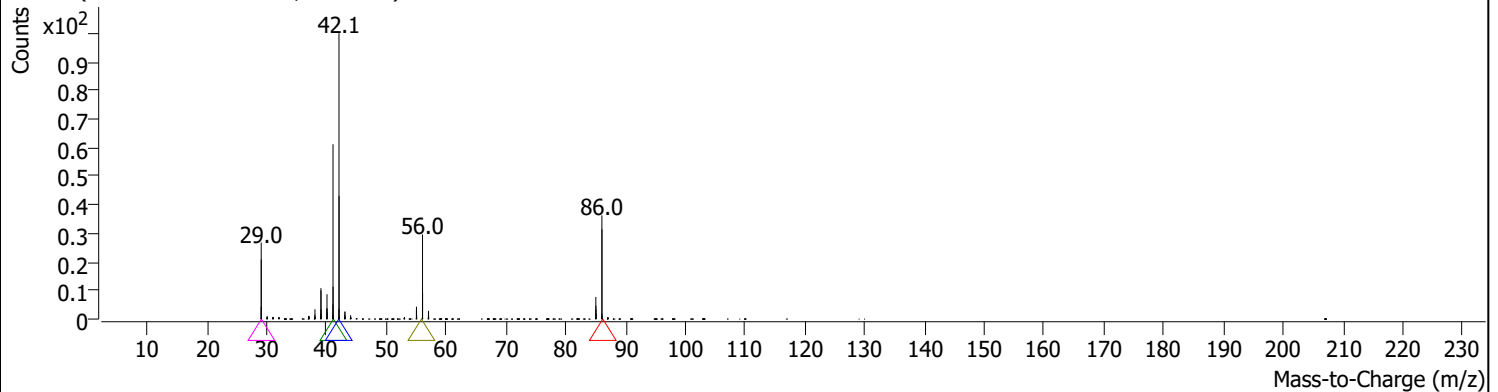
Component RT: 12.3947



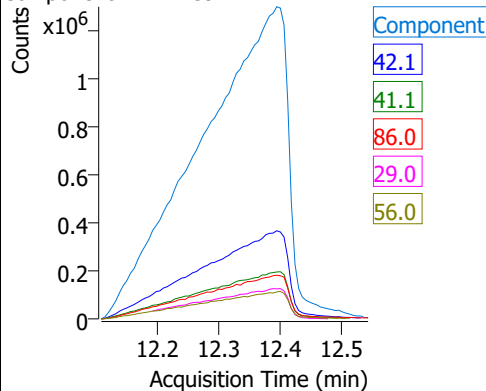
Butyrolactone (NIST20.L)



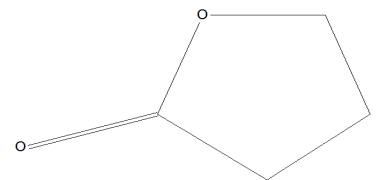
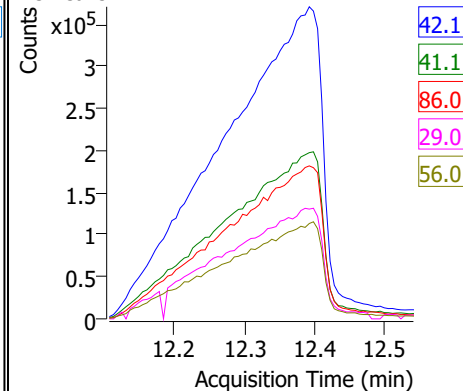
+ Scan (12.1015-12.5414 min, 74 scans) 1.D



Component RT: 12.3947



EIC Peaks





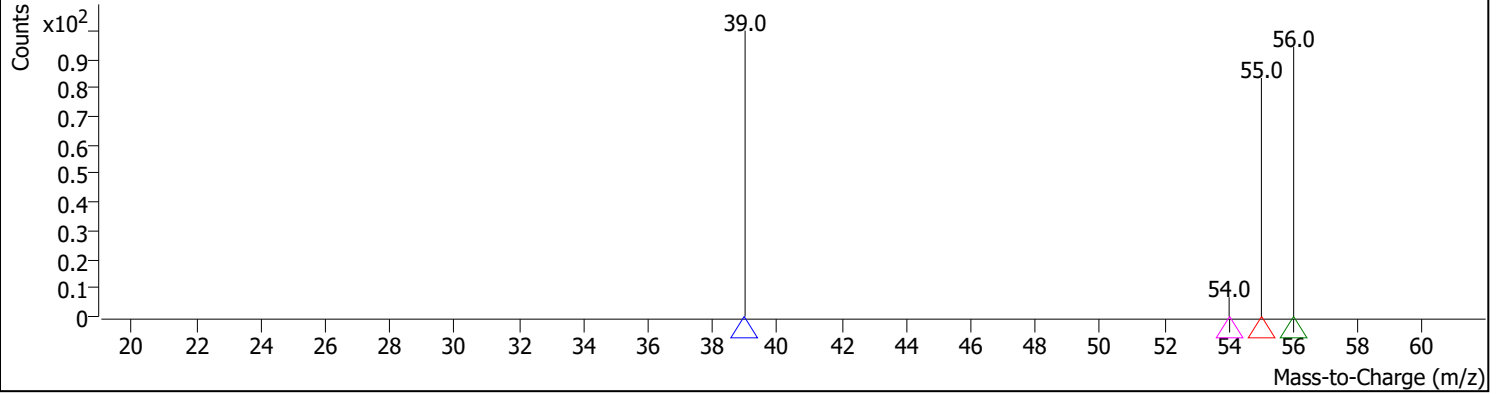
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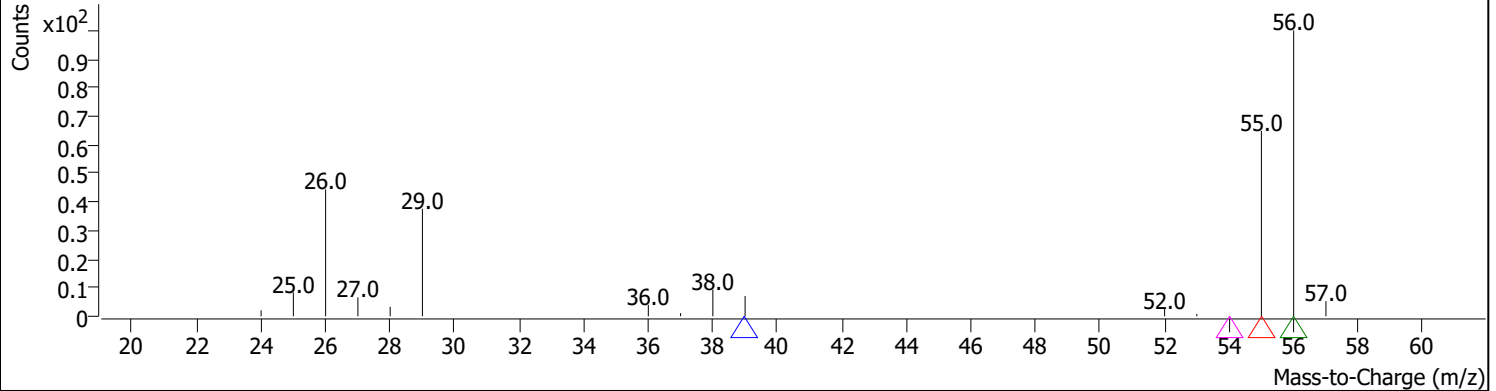
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
12.3974	2-Propenal	2114377.4	78.1	107-02-8	C <sub>3</sub> H <sub>4</sub> O	

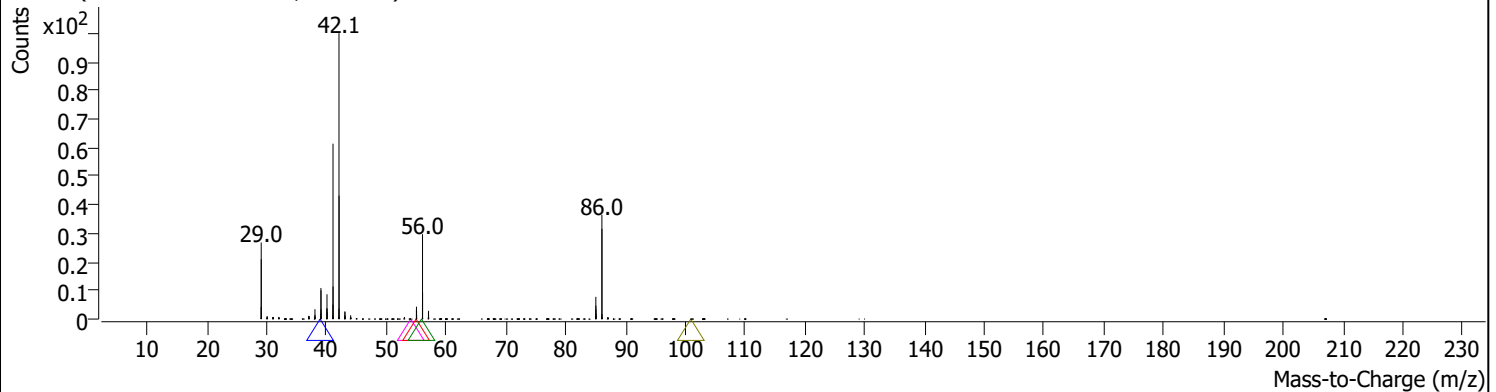
Component RT: 12.3974



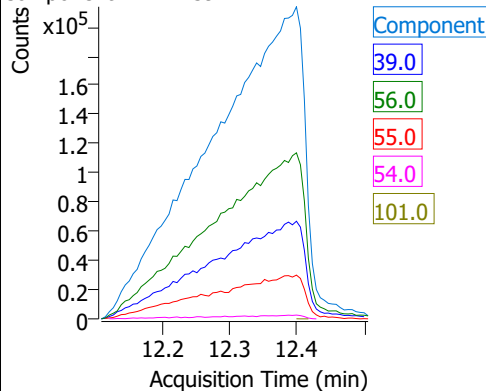
2-Propenal (NIST20.L)



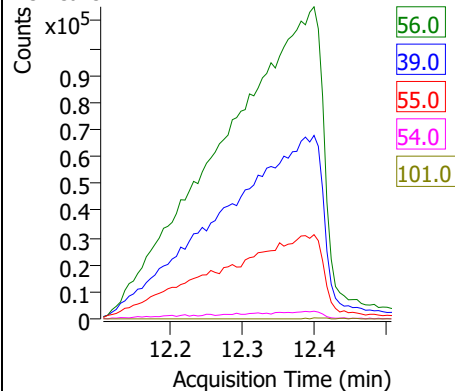
+ Scan (12.1023-12.5057 min, 68 scans) 1.D



Component RT: 12.3974



EIC Peaks



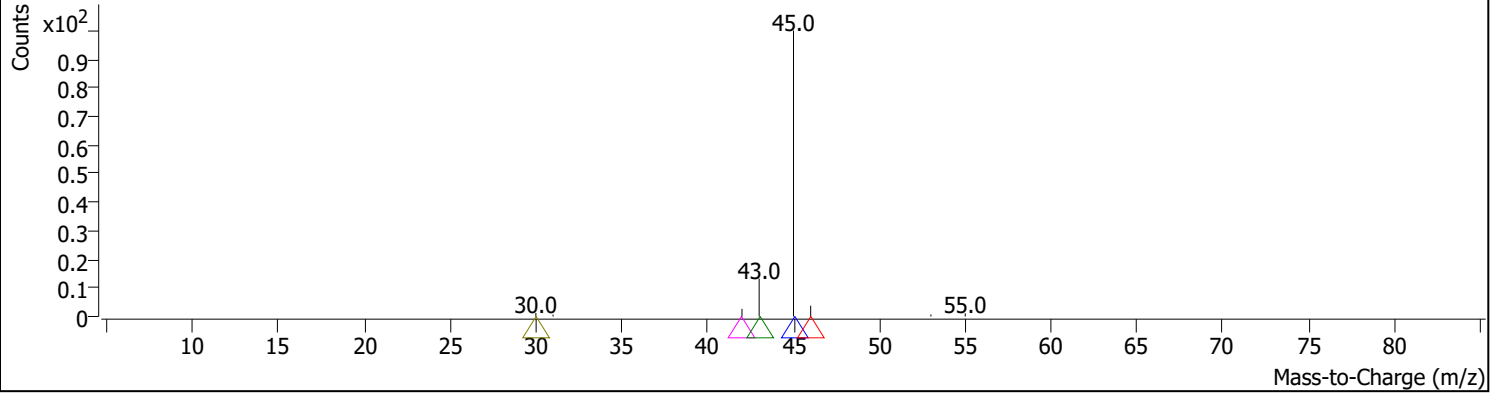
## Library Search Results - NonTarget Hits with Details



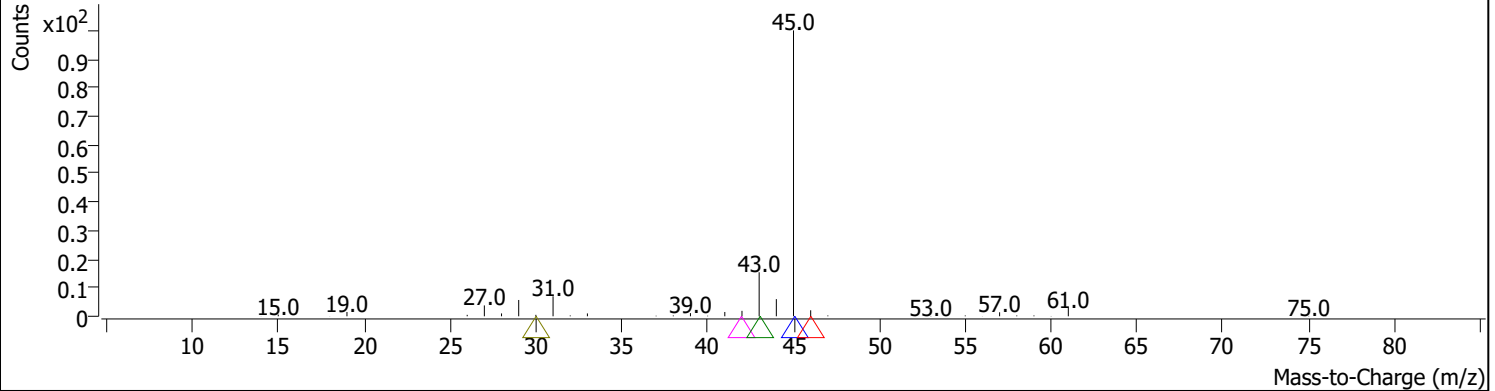
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
12.7378	(S)-(+)-1,2-Propanediol	1369287.5	79.3	4254-15-3	C3H8O2	

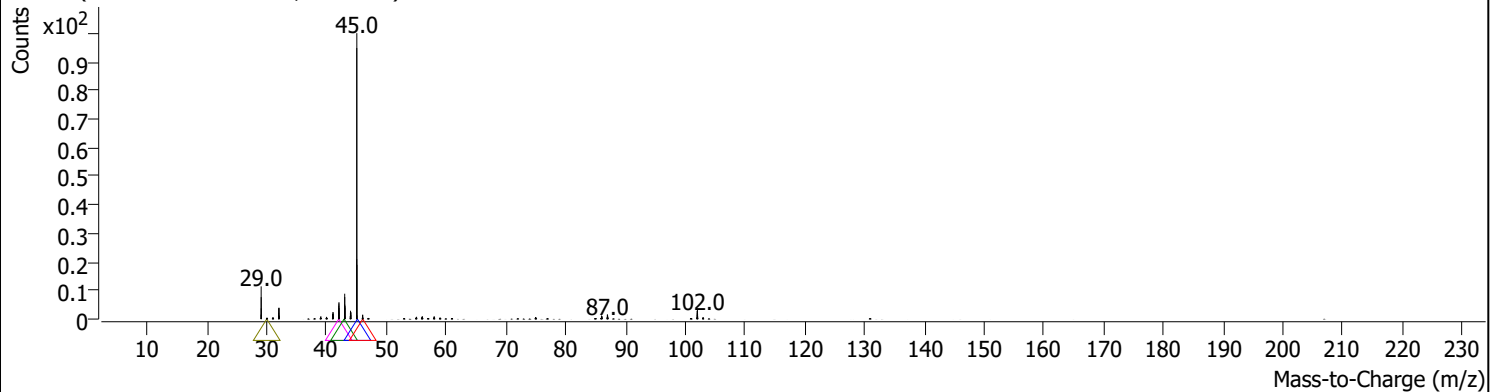
Component RT: 12.7378



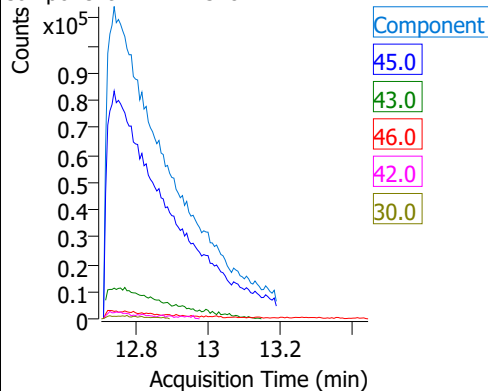
(S)-(+)-1,2-Propanediol (NIST20.L)



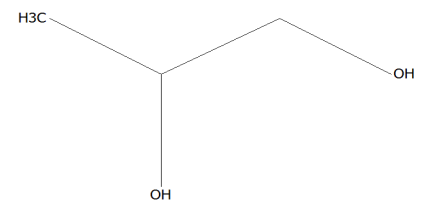
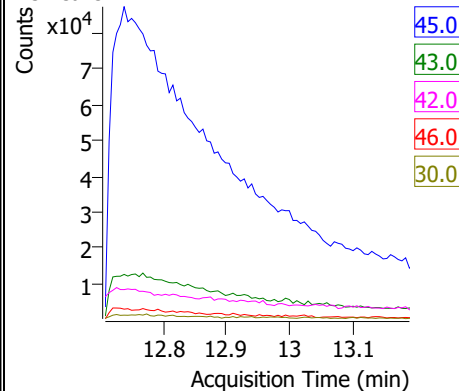
+ Scan (12.7050-13.1895 min, 82 scans) 1.D



Component RT: 12.7378



EIC Peaks



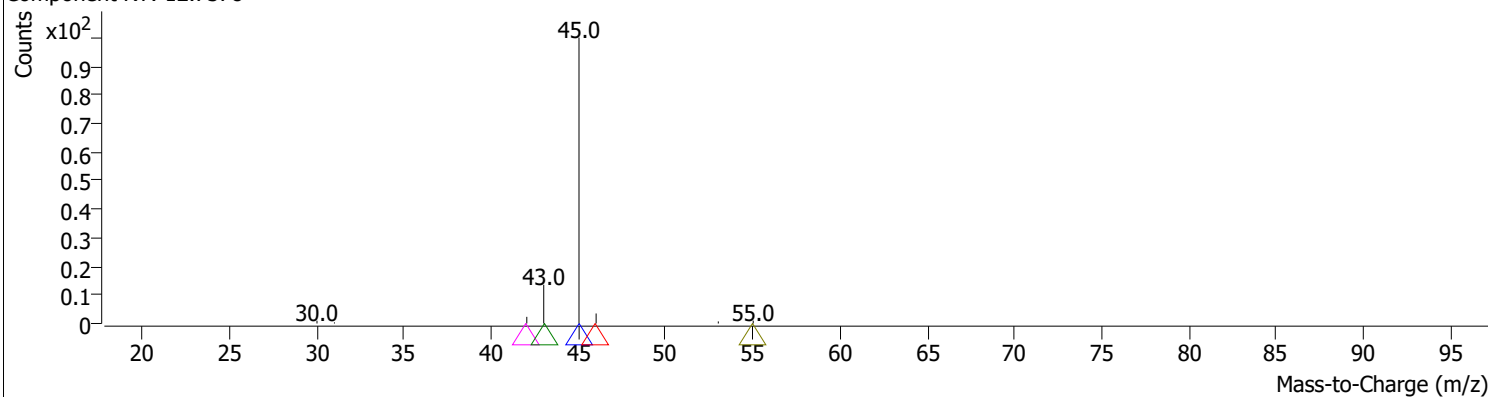
## Library Search Results - NonTarget Hits with Details



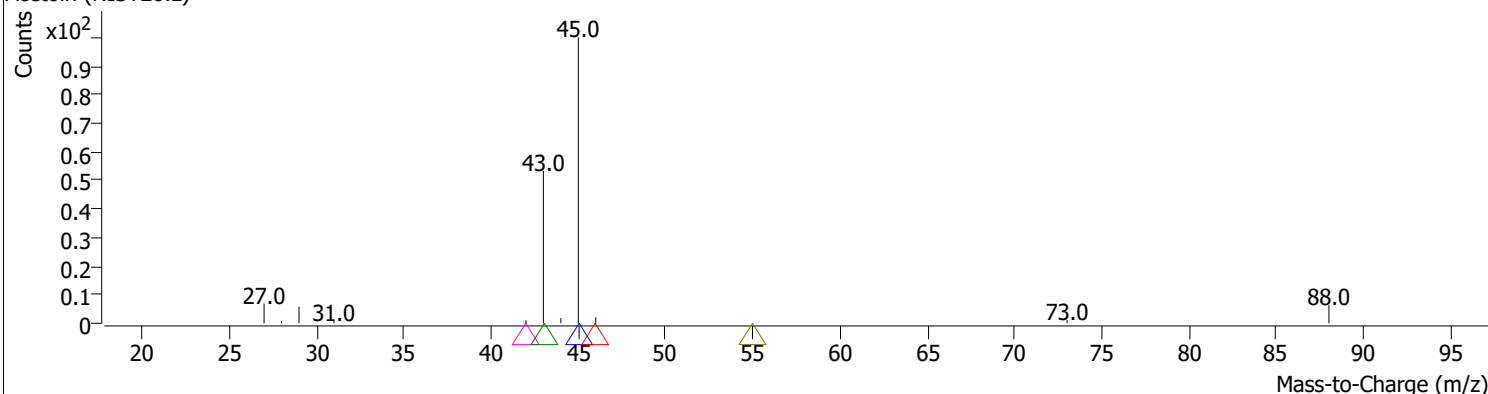
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
12.7378	Acetoin	1449576.9	79.2	513-86-0	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	

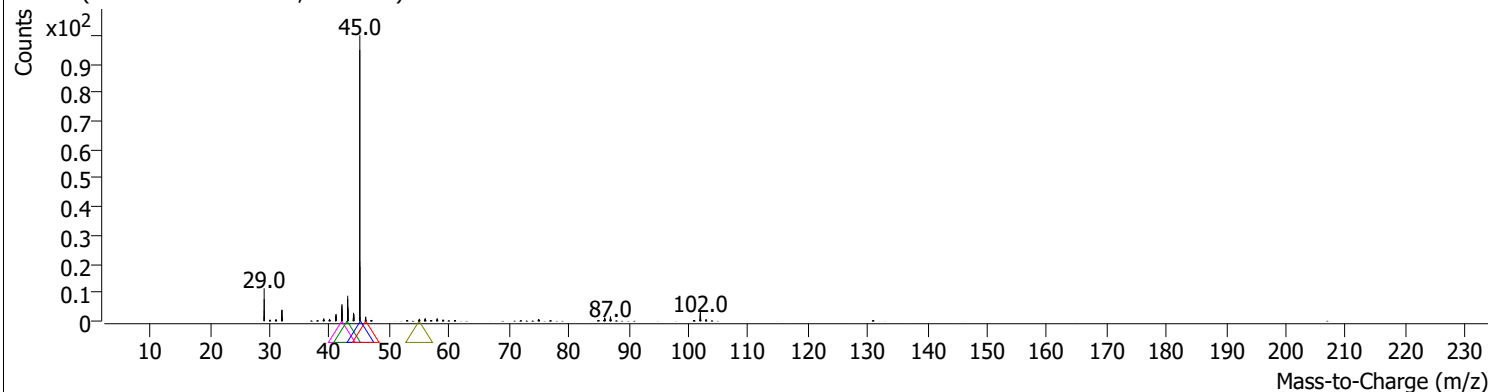
Component RT: 12.7378



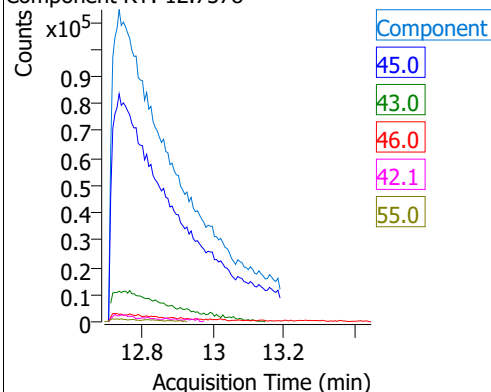
Acetoin (NIST20.L)



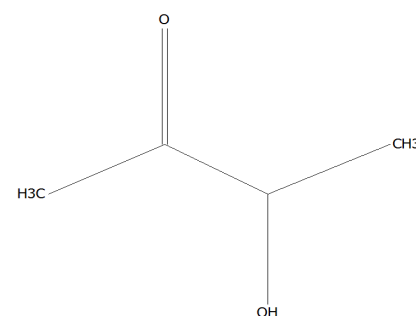
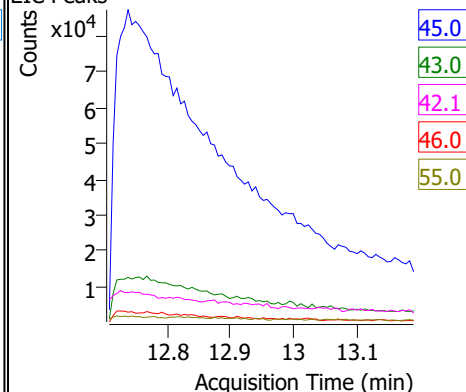
+ Scan (12.7029-13.1895 min, 82 scans) 1.D



Component RT: 12.7378



EIC Peaks



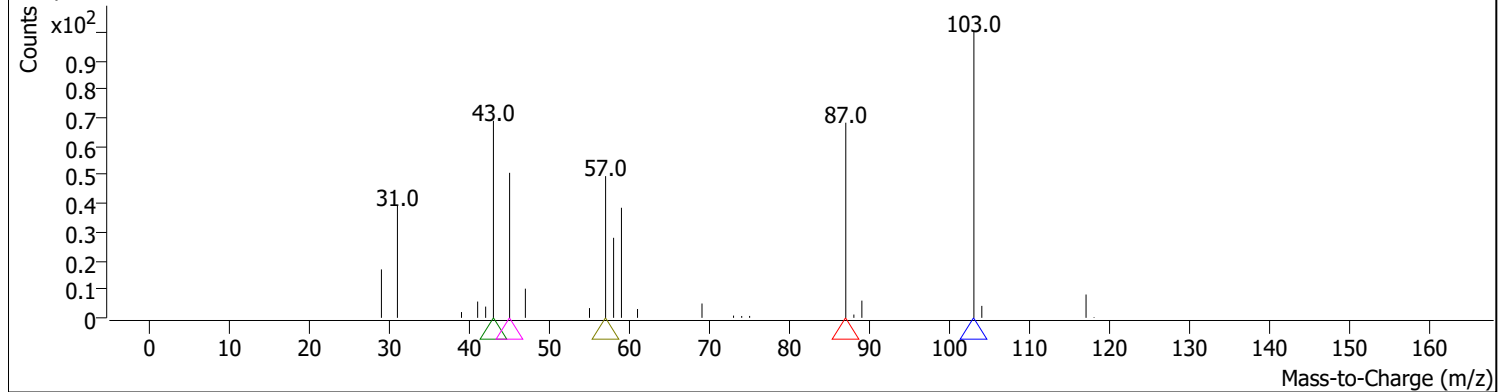
## Library Search Results - NonTarget Hits with Details



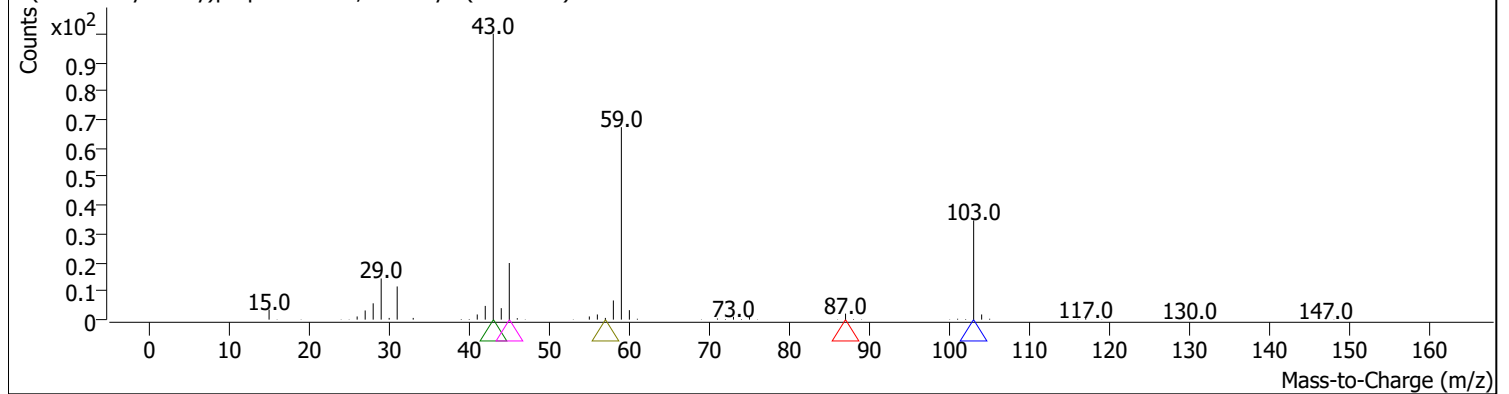
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
13.2773	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	922641.6	76.5	1000506-61-7	C8H14O5	

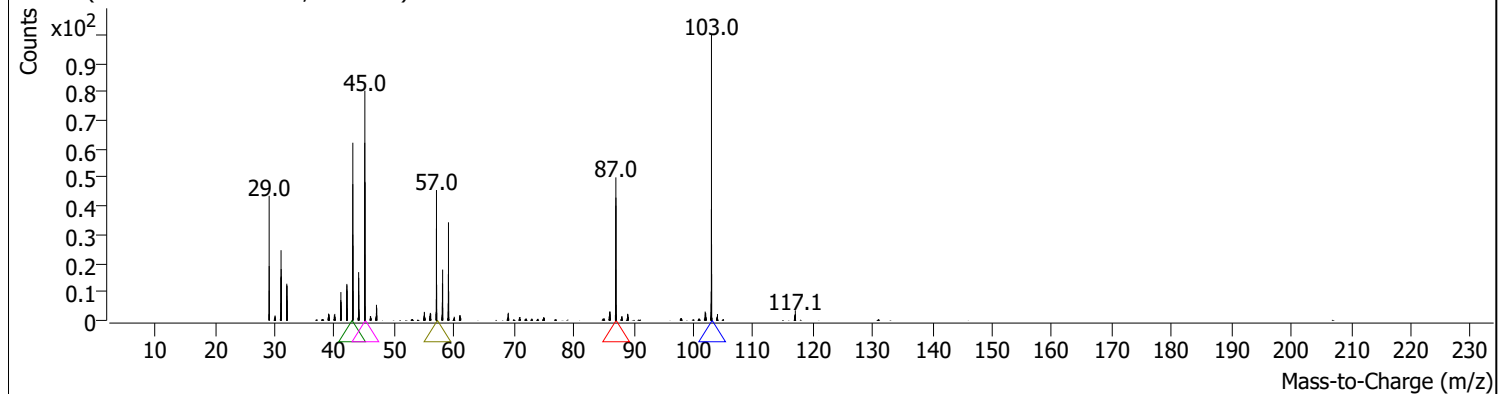
Component RT: 13.2773



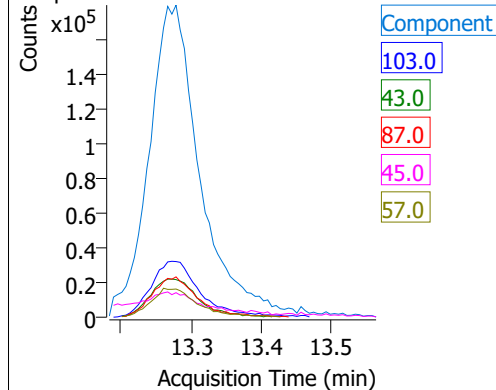
2-(2-methoxyethoxy)propanoic acid, O-acetyl- (NIST20.L)



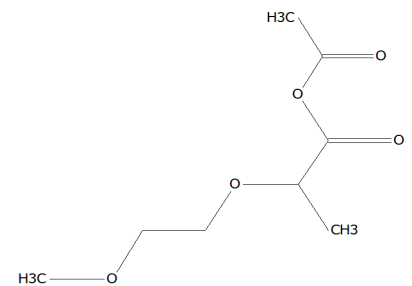
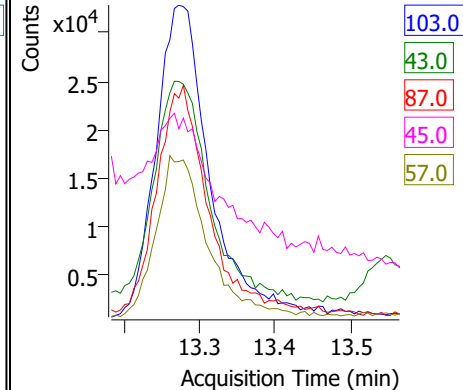
+ Scan (13.1957-13.4333 min, 40 scans) 1.D



Component RT: 13.2773



EIC Peaks



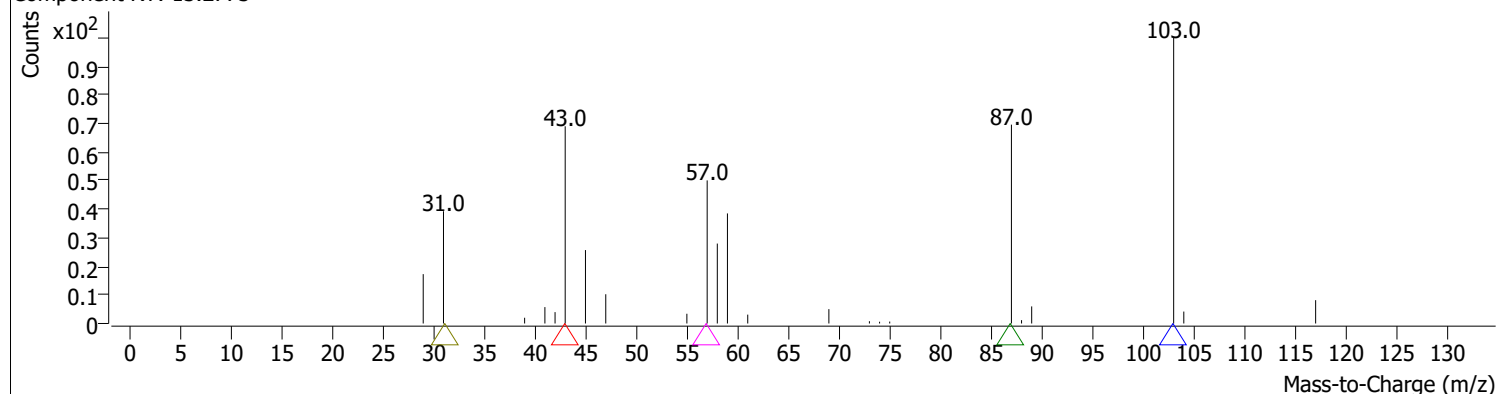
## Library Search Results - NonTarget Hits with Details



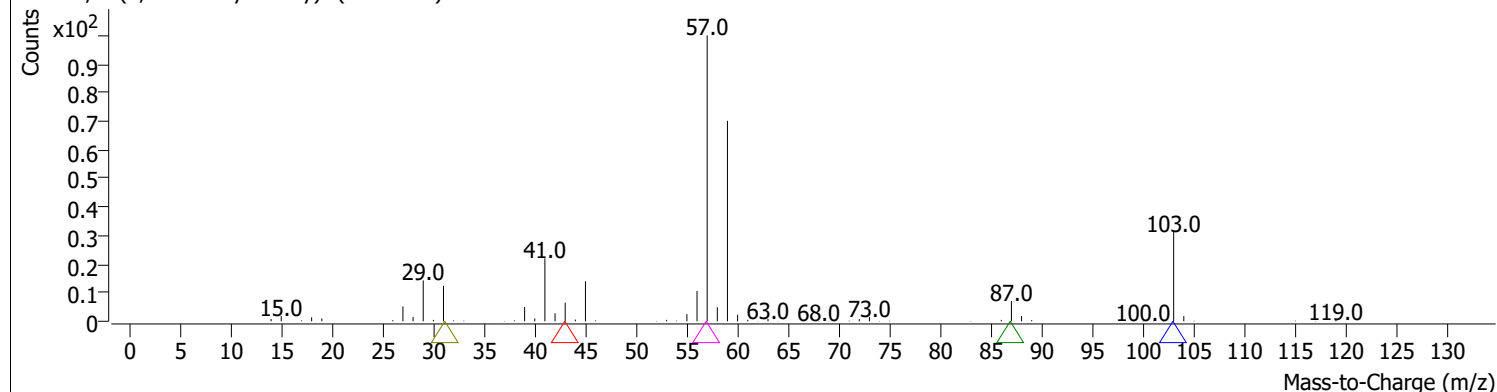
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
13.2773	Ethanol, 2-(1,1-dimethylethoxy)-	817371.6	76.0	7580-85-0	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	

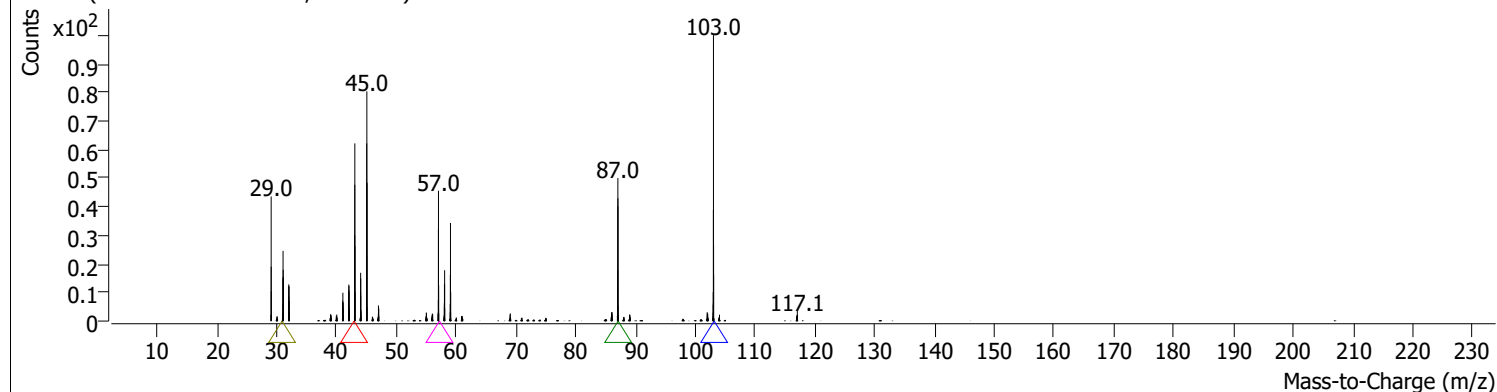
Component RT: 13.2773



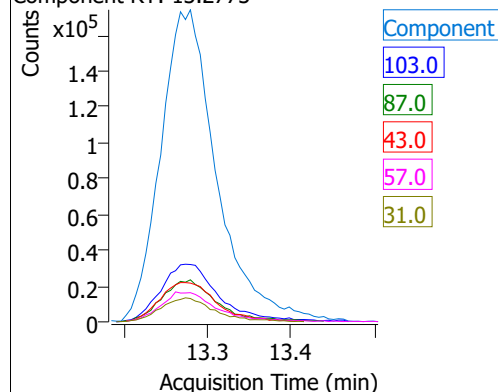
Ethanol, 2-(1,1-dimethylethoxy)- (NIST20.L)



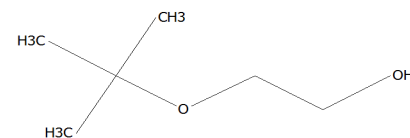
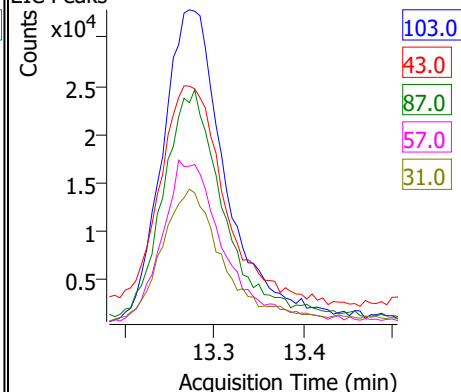
+ Scan (13.1957-13.4333 min, 40 scans) 1.D



Component RT: 13.2773



EIC Peaks



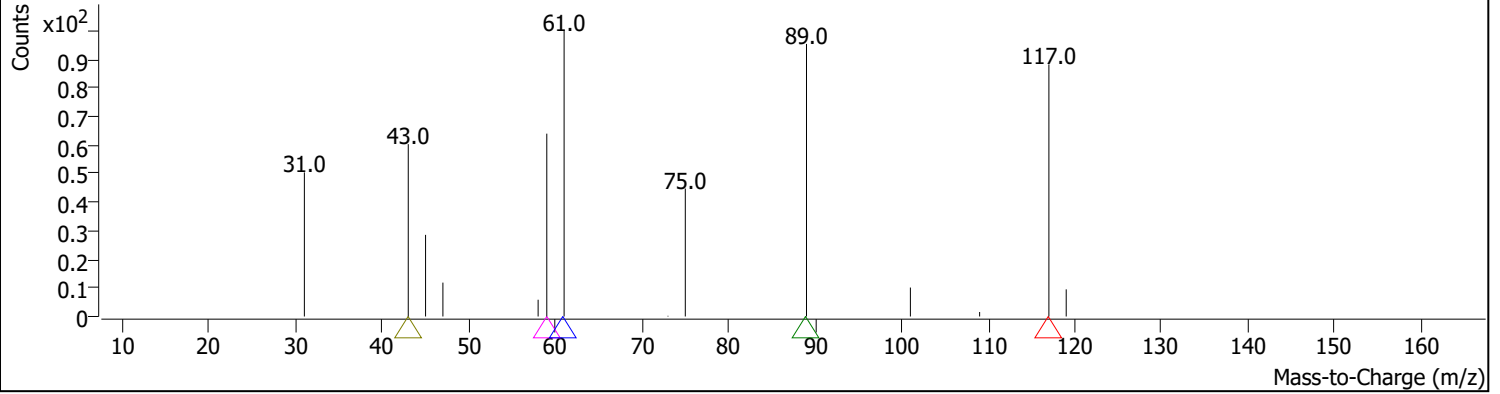
## Library Search Results - NonTarget Hits with Details



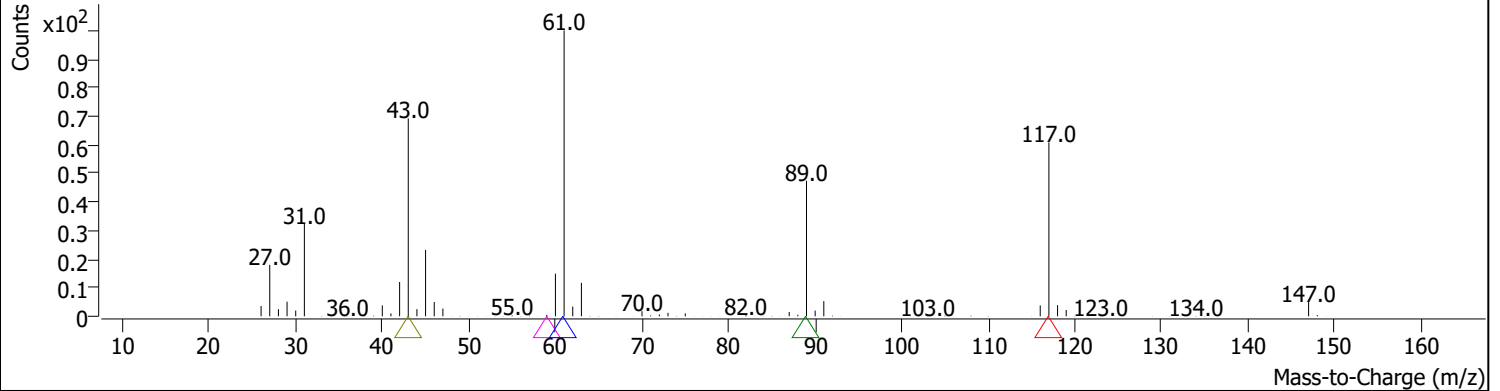
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
16.4438	Ethane, 1,1,1-triethoxy-	399182.1	75.5	78-39-7	C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>	

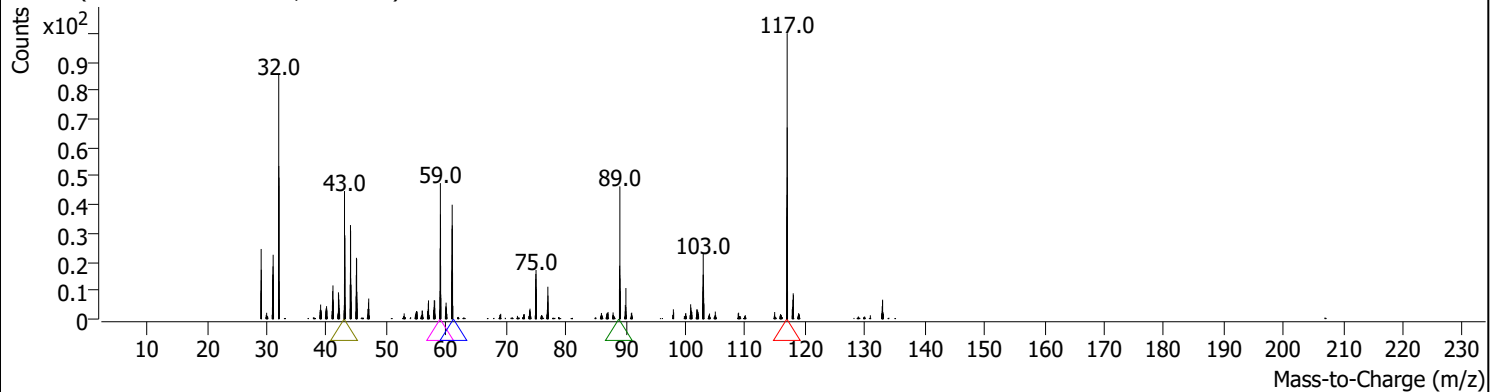
Component RT: 16.4438



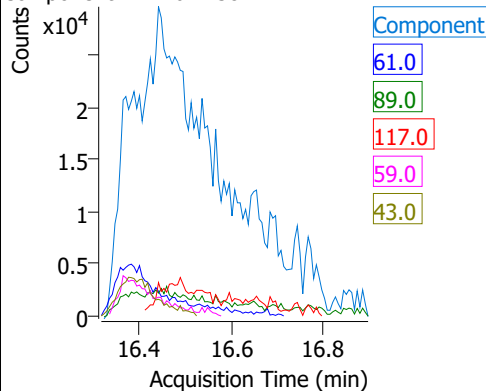
Ethane, 1,1,1-triethoxy- (NIST20.L)



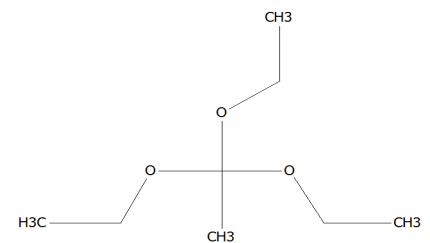
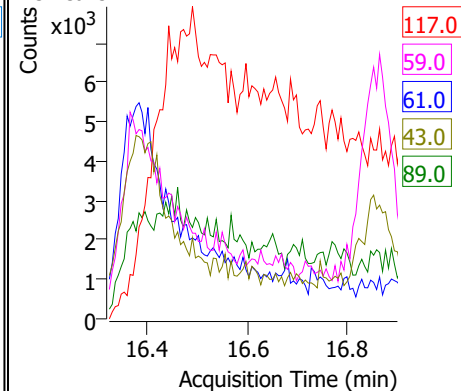
+ Scan (16.3310-16.5787 min, 42 scans) 1.D



Component RT: 16.4438



EIC Peaks



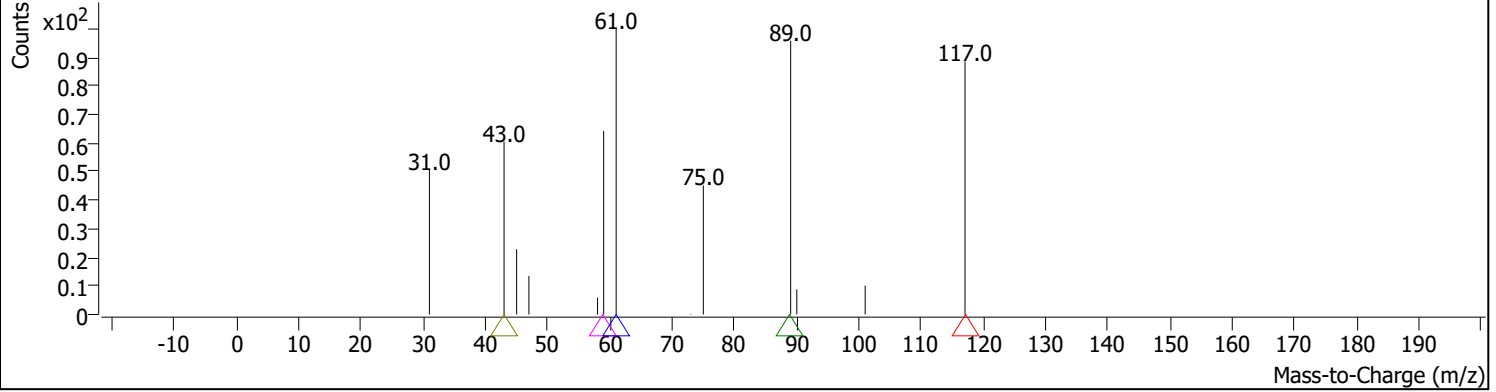
# Library Search Results - NonTarget Hits with Details



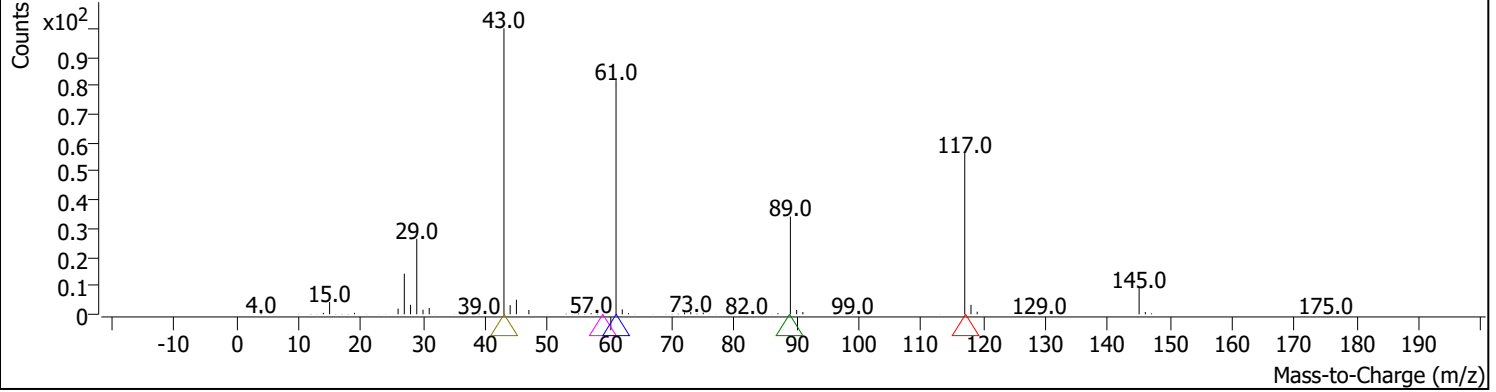
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
16.4440	Ethyl 2,2-diethoxypropionate	399225.1	75.8	7476-20-2	C9H18O4	

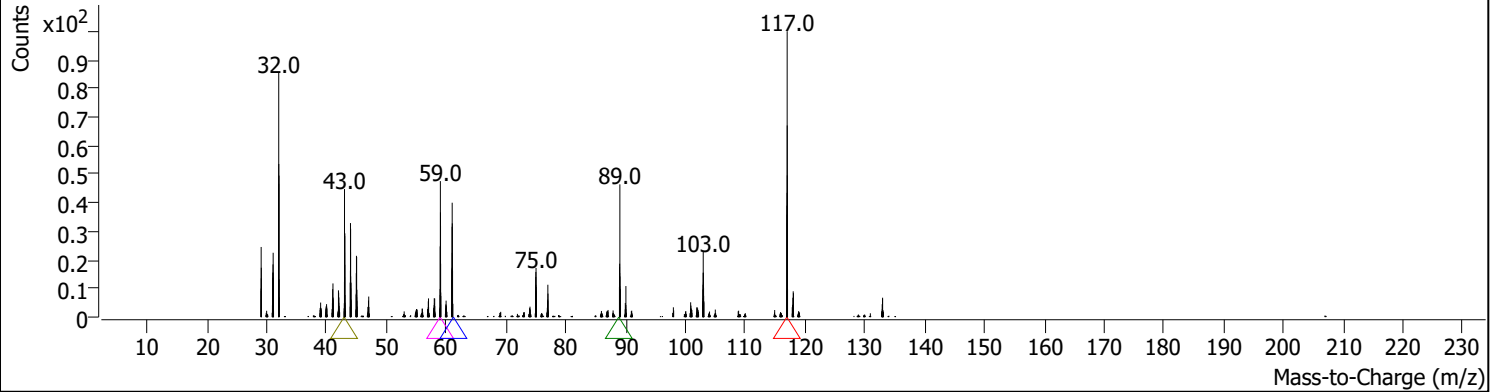
Component RT: 16.4440



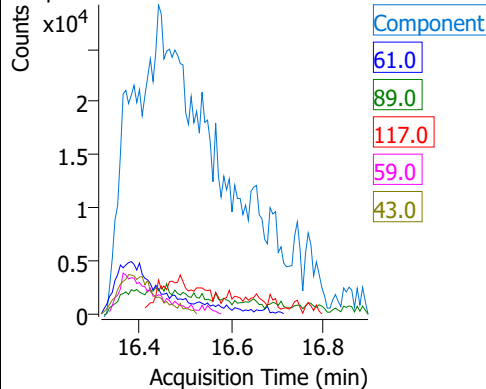
Ethyl 2,2-diethoxypropionate (NIST20.L)



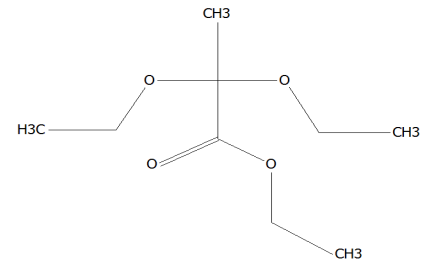
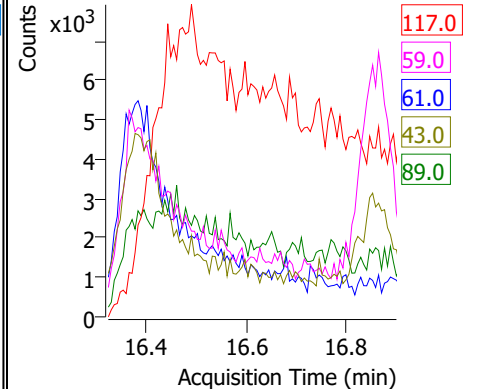
+ Scan (16.3310-16.5787 min, 42 scans) 1.D



Component RT: 16.4440



EIC Peaks



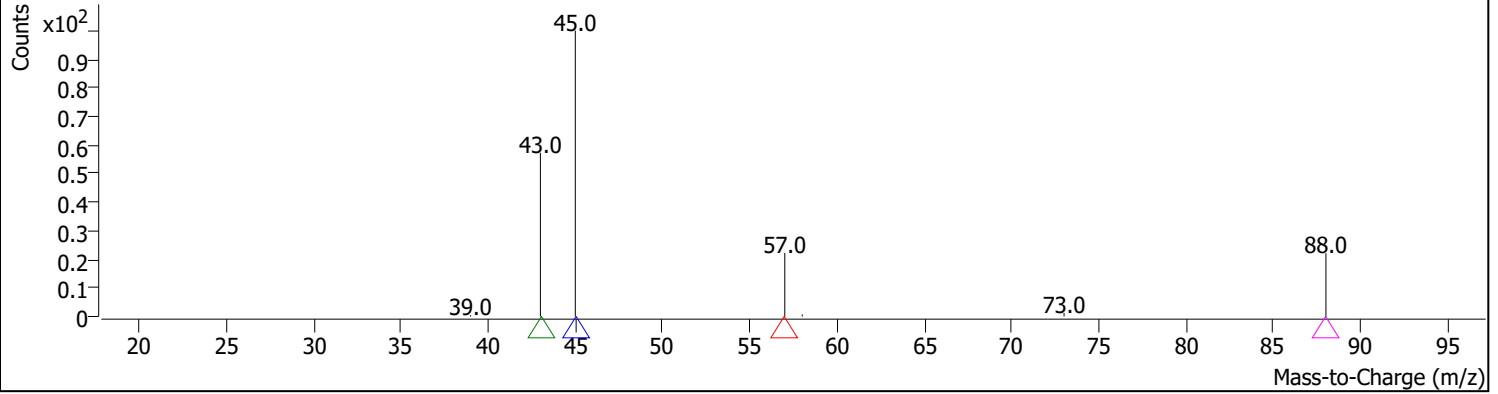
## Library Search Results - NonTarget Hits with Details



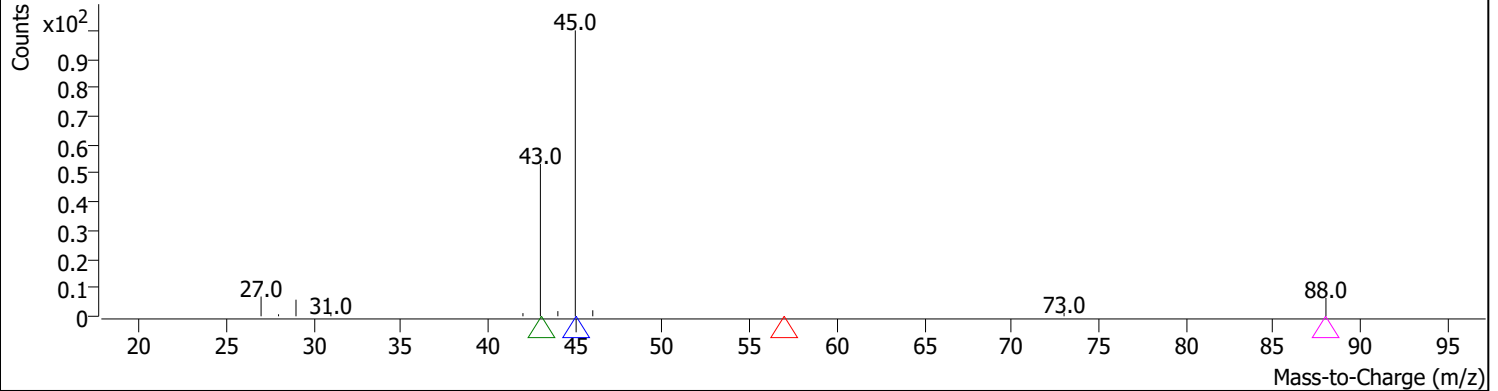
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
17.0180	Acetoin	690174.9	79.6	513-86-0	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	

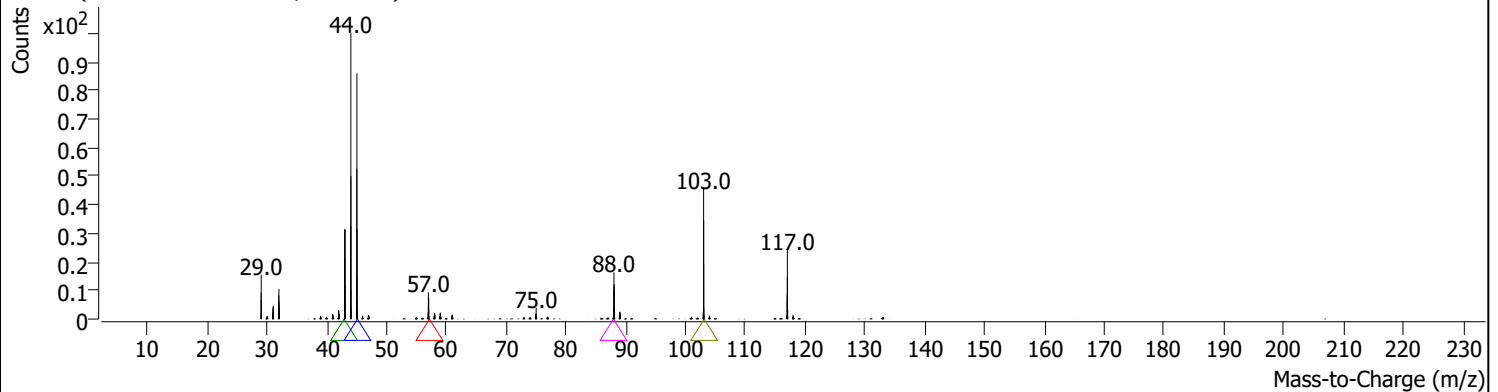
Component RT: 17.0180



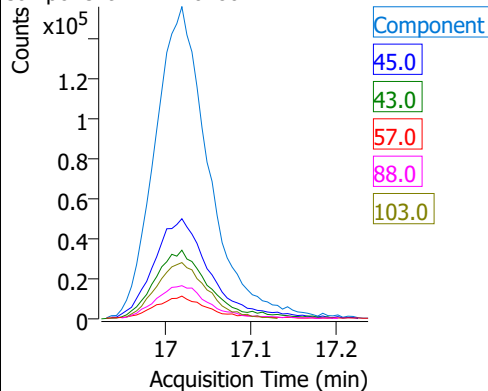
Acetoin (NIST20.L)



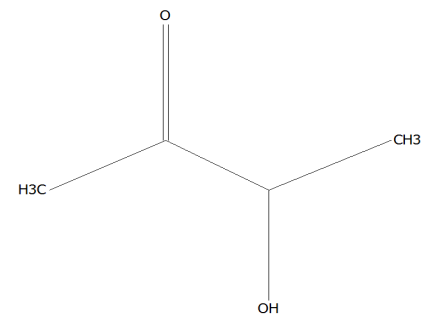
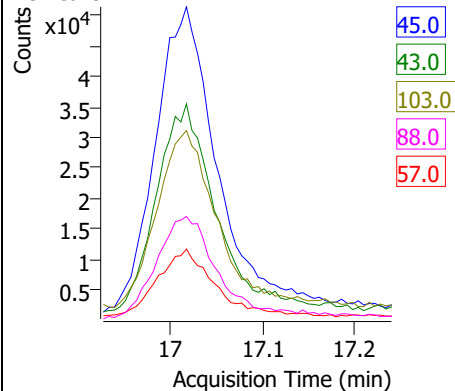
+ Scan (16.9297-17.2298 min, 50 scans) 1.D



Component RT: 17.0180



EIC Peaks





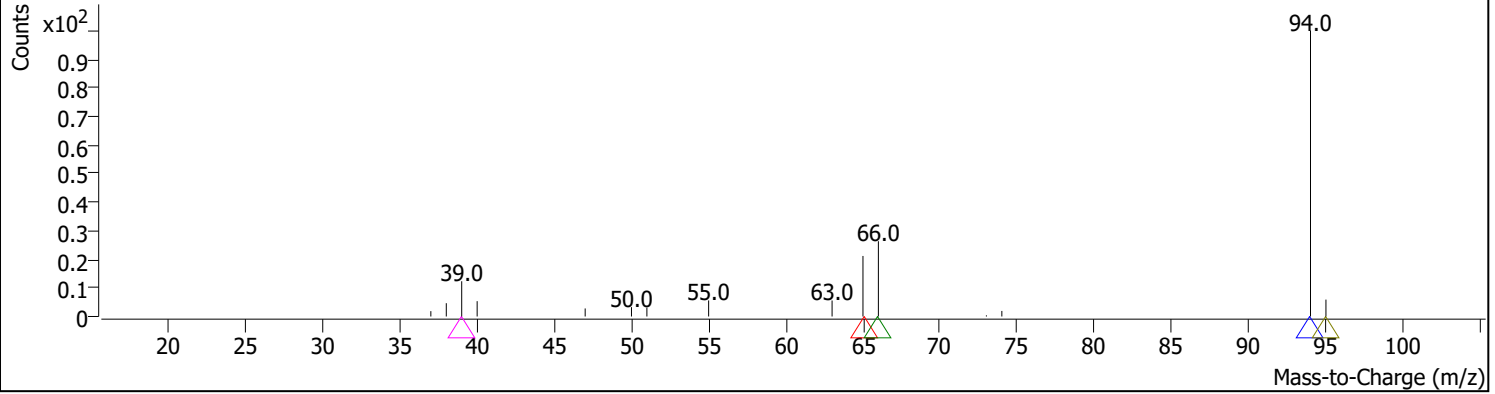
## Library Search Results - NonTarget Hits with Details



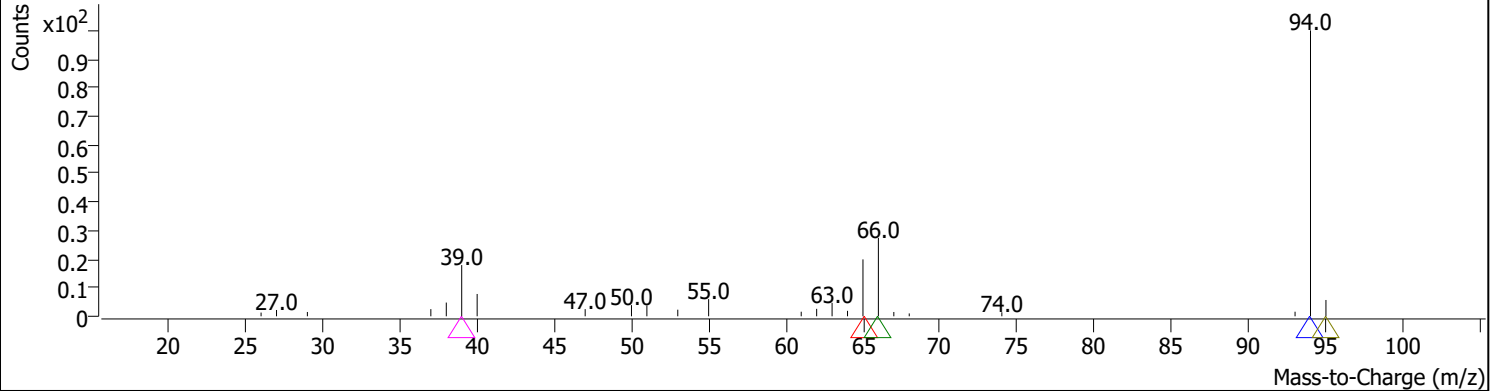
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
17.9778	Phenol	254152.5	93.3	108-95-2	C <sub>6</sub> H <sub>6</sub> O	

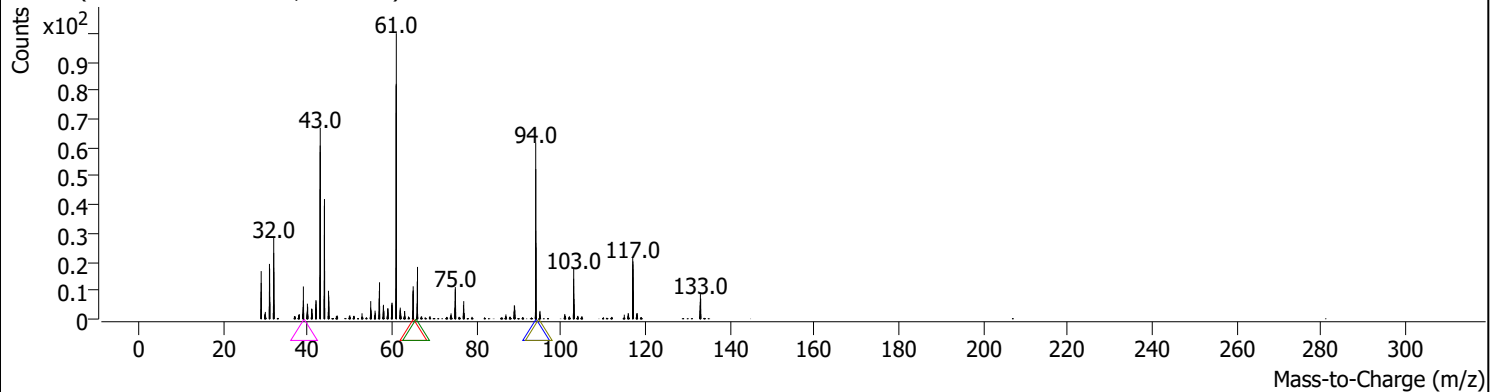
Component RT: 17.9778



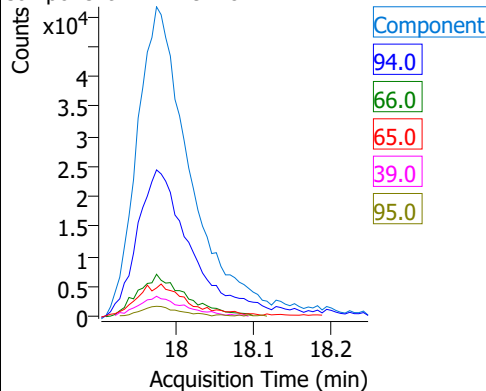
Phenol (NIST20.L)



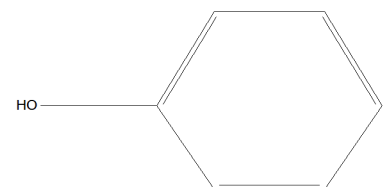
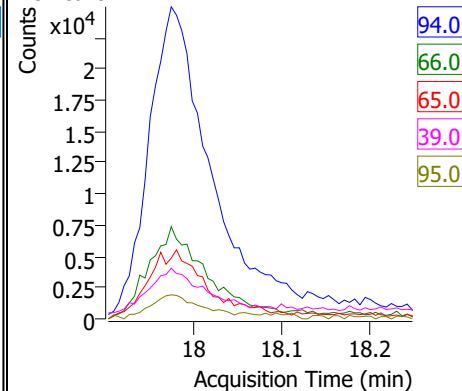
+ Scan (17.9089-18.2496 min, 58 scans) 1.D



Component RT: 17.9778



EIC Peaks



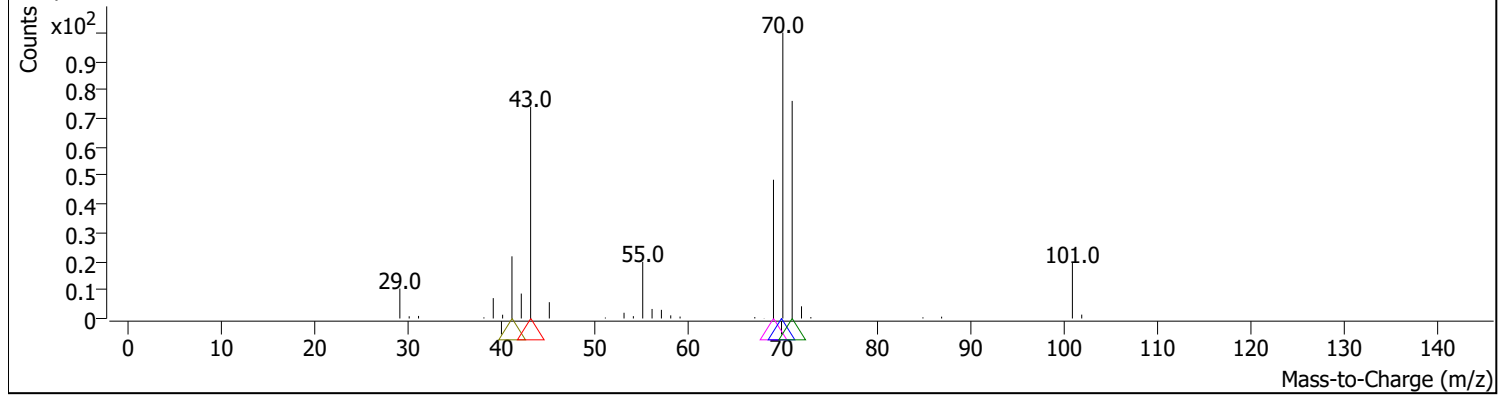
## Library Search Results - NonTarget Hits with Details



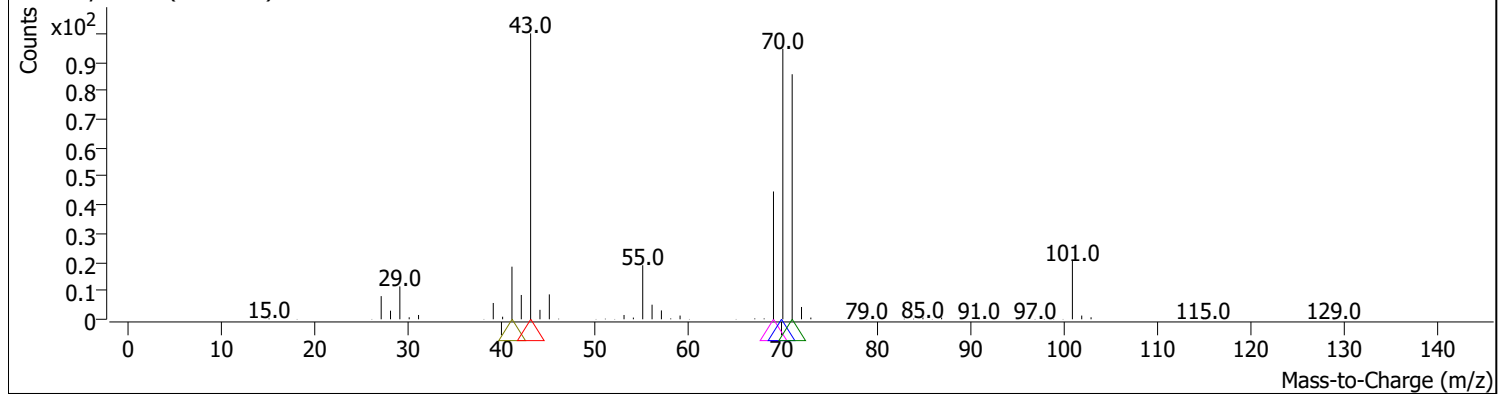
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
18.6438	Diisoamyl ether	3396460.2	98.2	544-01-4	C <sub>10</sub> H <sub>22</sub> O	

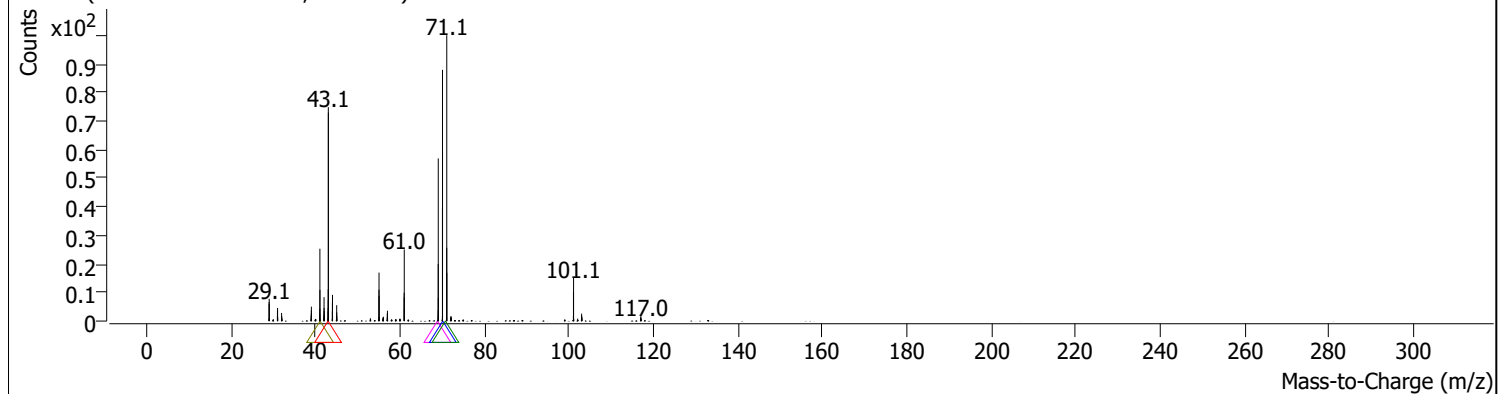
Component RT: 18.6438



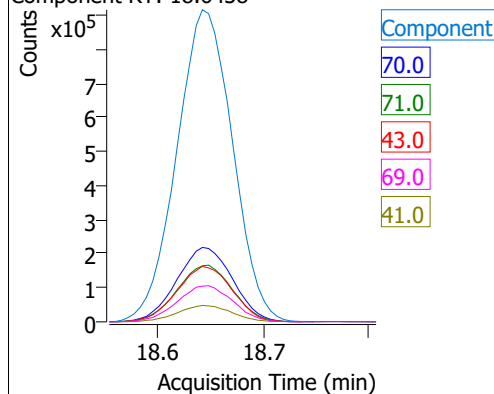
Diisoamyl ether (NIST20.L)



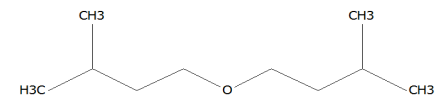
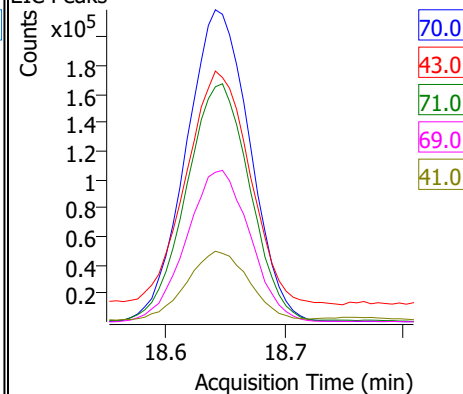
+ Scan (18.5528-18.7490 min, 34 scans) 1.D



Component RT: 18.6438



EIC Peaks



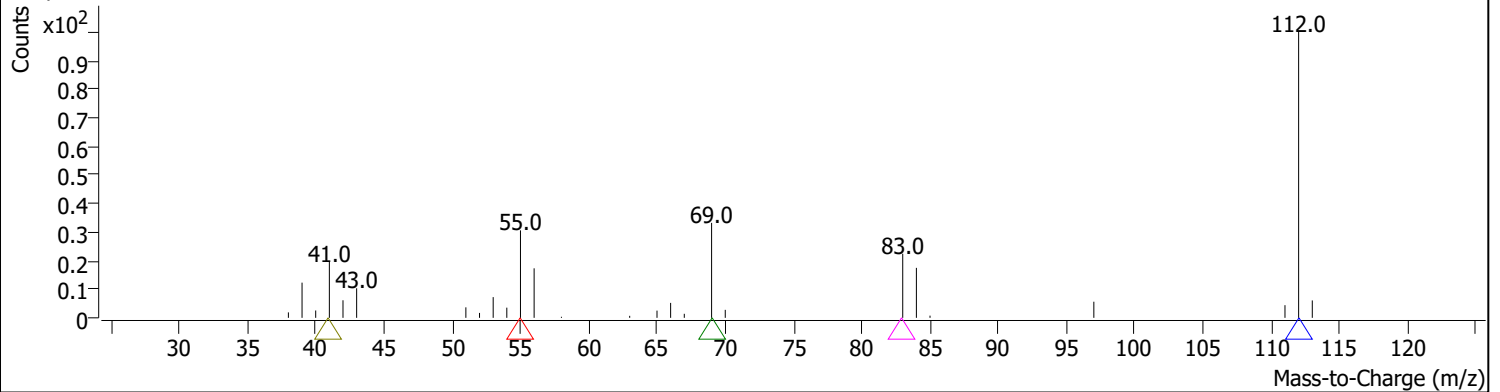
## Library Search Results - NonTarget Hits with Details



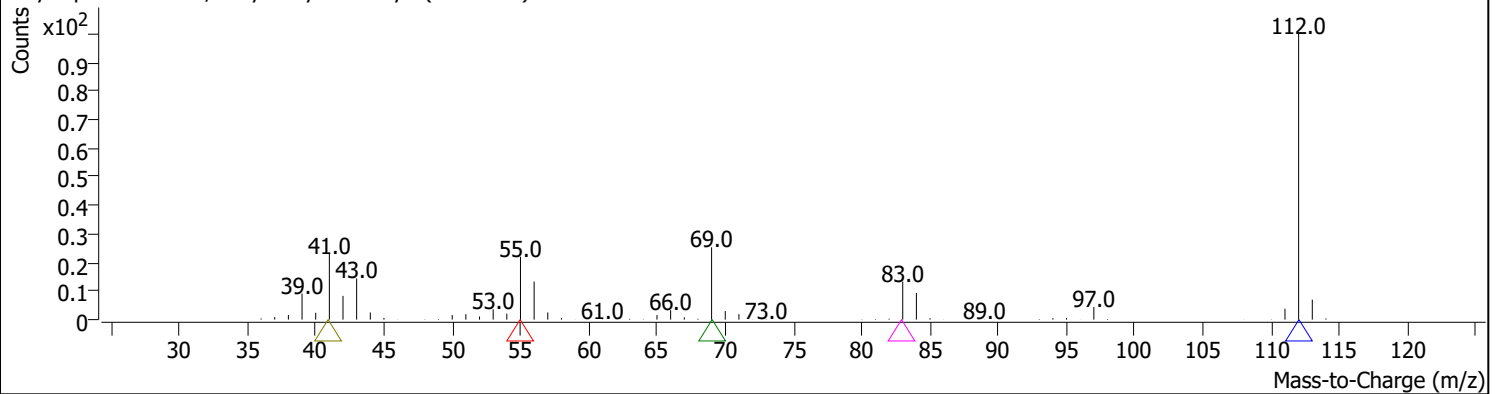
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
20.0201	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	703403.8	95.0	80-71-7	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	

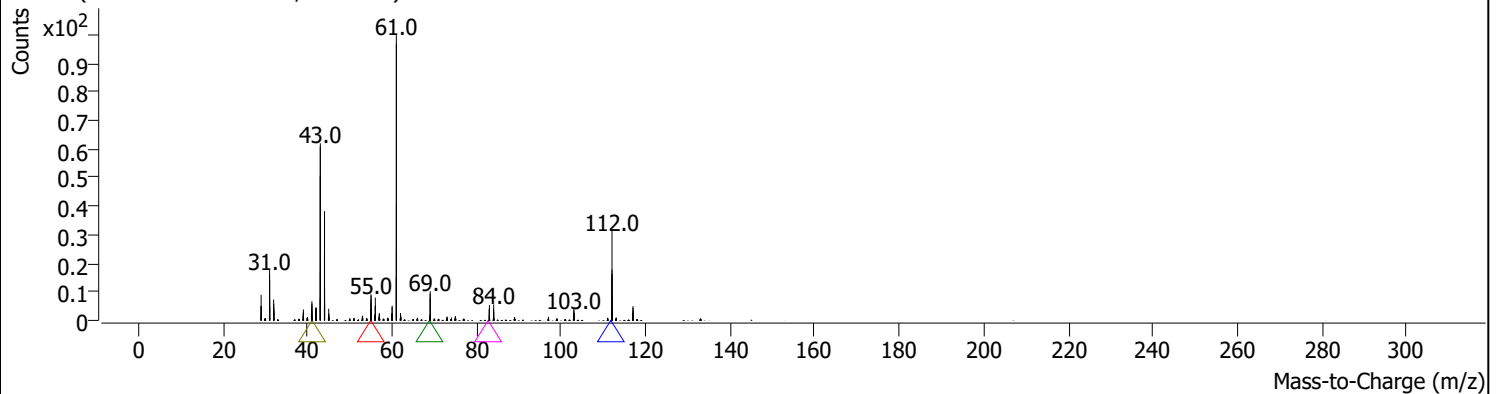
Component RT: 20.0201



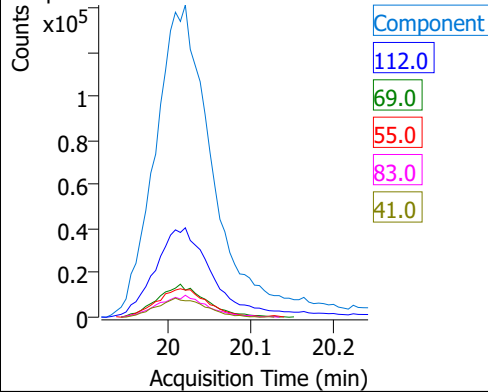
2-Cyclopenten-1-one, 2-hydroxy-3-methyl- (NIST20.L)



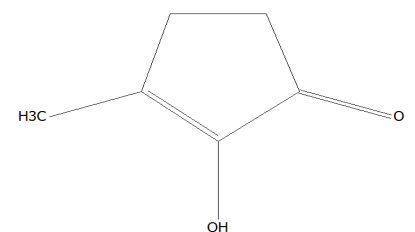
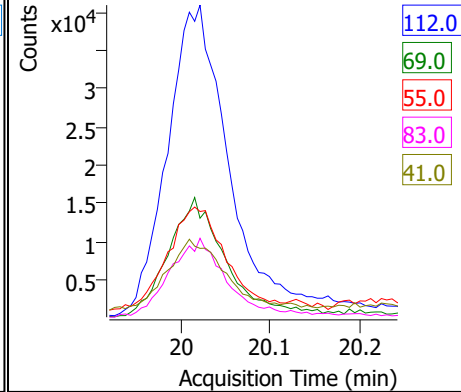
+ Scan (19.9156-20.2415 min, 55 scans) 1.D



Component RT: 20.0201



EIC Peaks



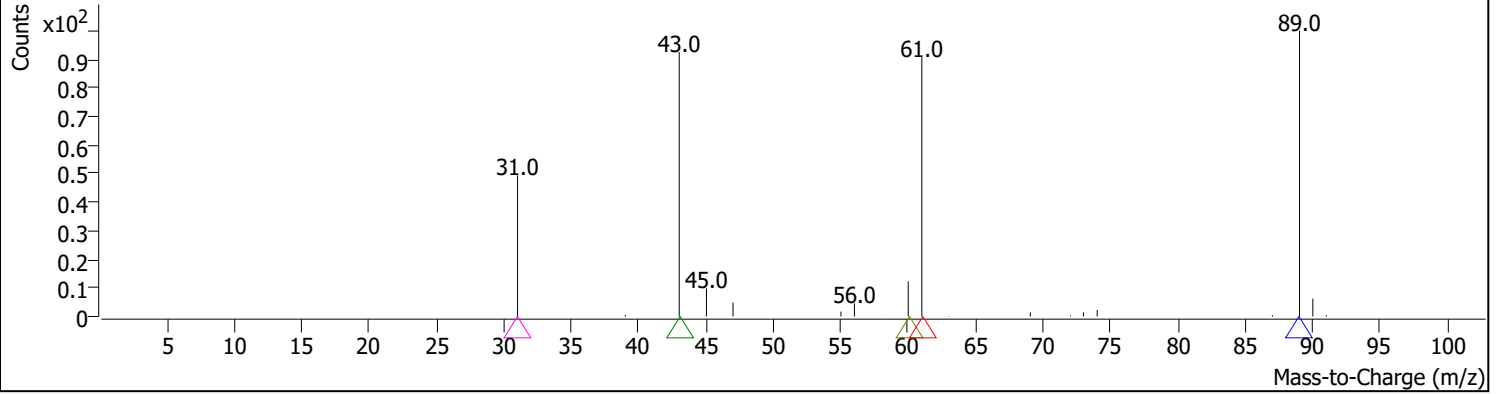
## Library Search Results - NonTarget Hits with Details



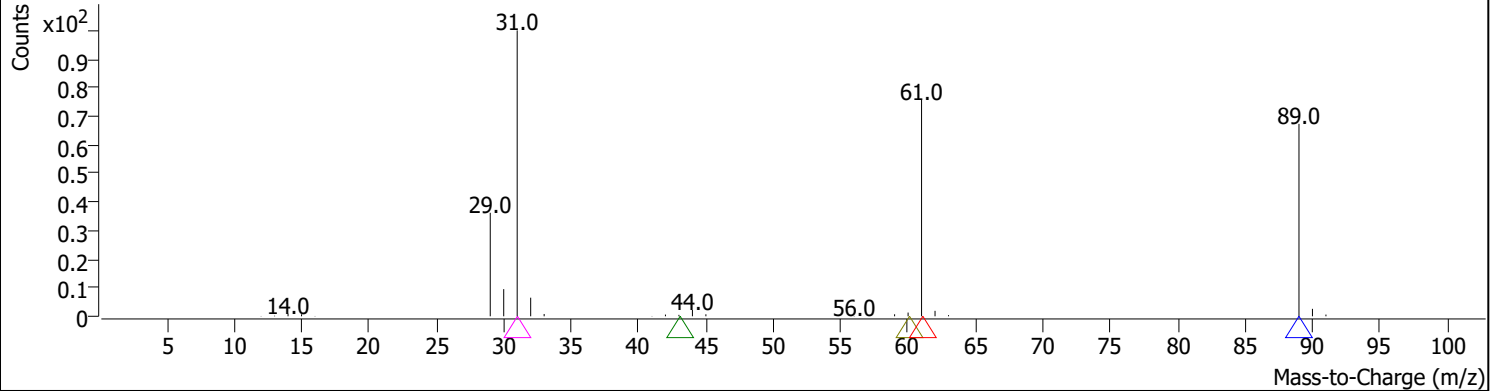
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
21.1093	1,3,5-Trioxane	4648194.3	77.4	110-88-3	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	

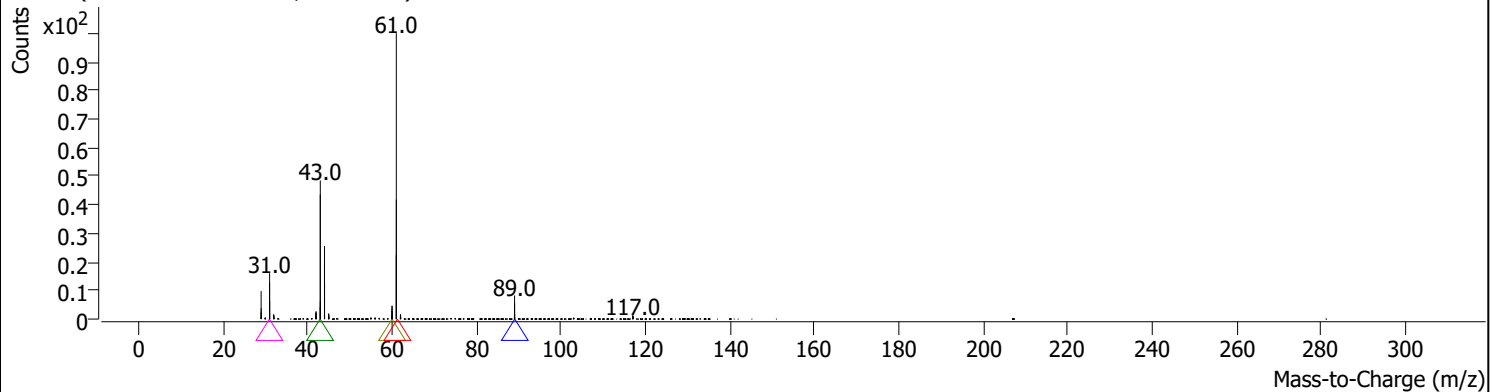
Component RT: 21.1093



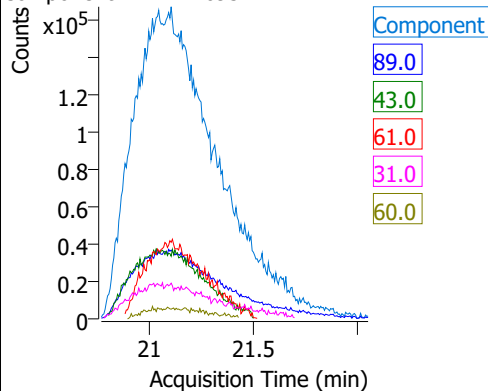
1,3,5-Trioxane (NIST20.L)



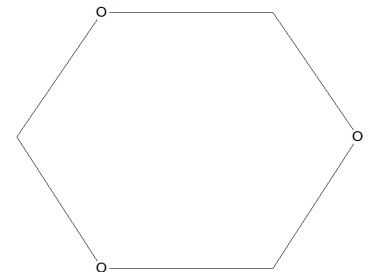
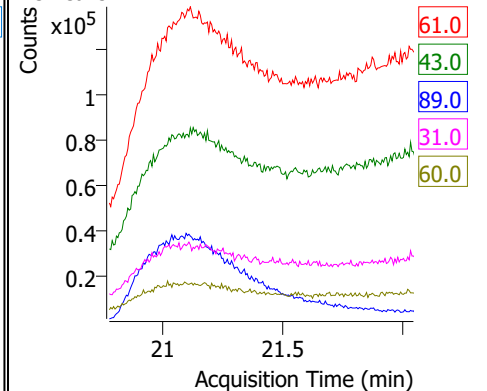
+ Scan (20.7715-22.0548 min, 215 scans) 1.D



Component RT: 21.1093



EIC Peaks



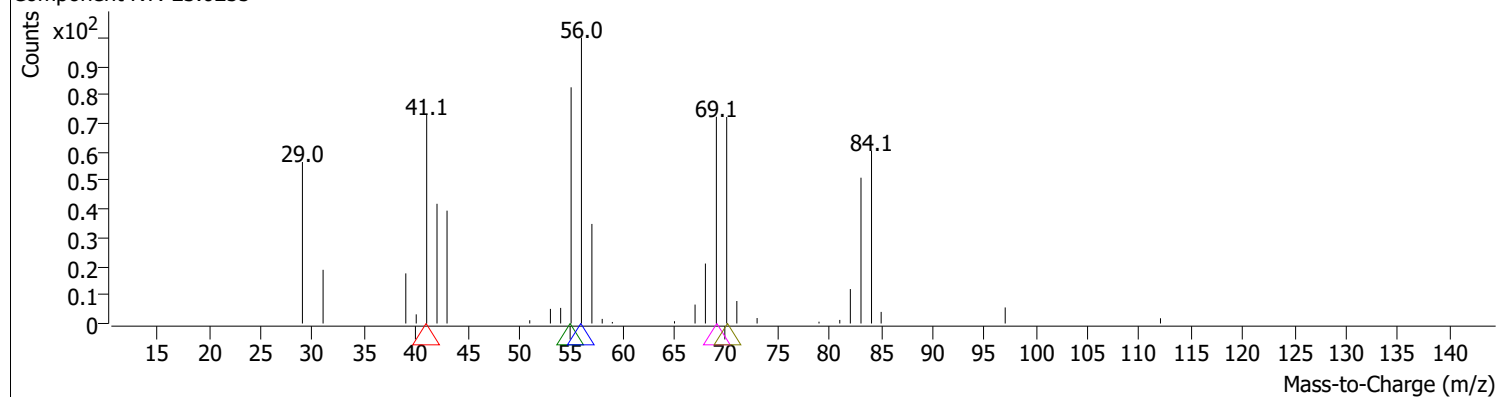
## Library Search Results - NonTarget Hits with Details



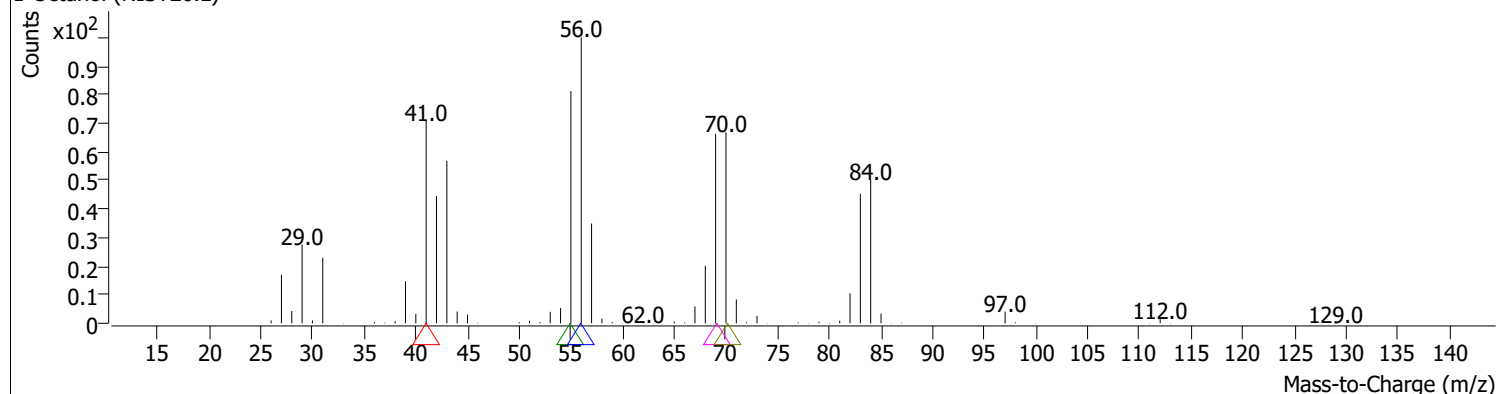
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
23.0255	1-Octanol	3779230.8	98.4	111-87-5	C <sub>8</sub> H <sub>18</sub> O	

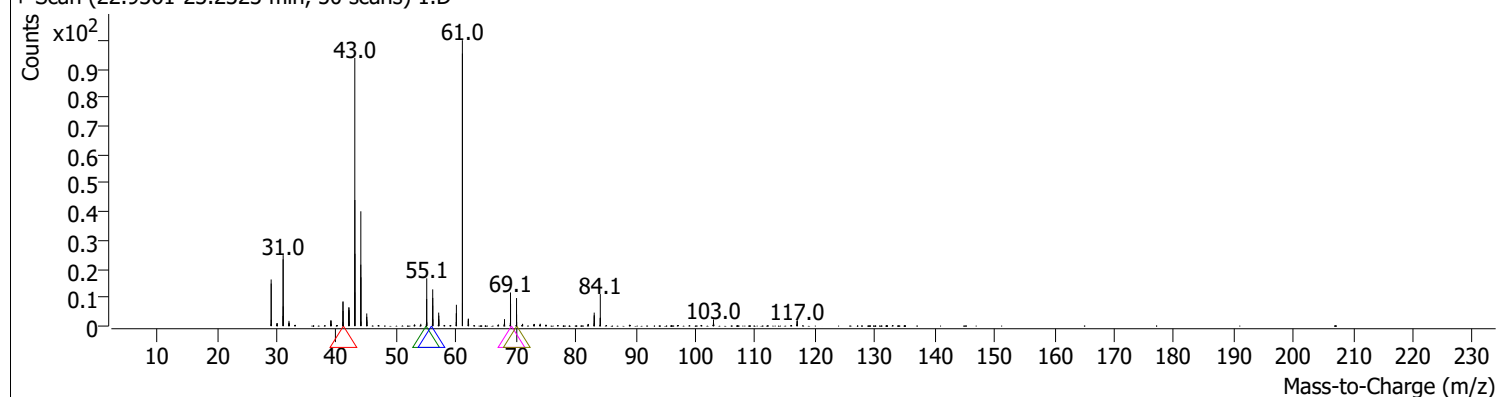
Component RT: 23.0255



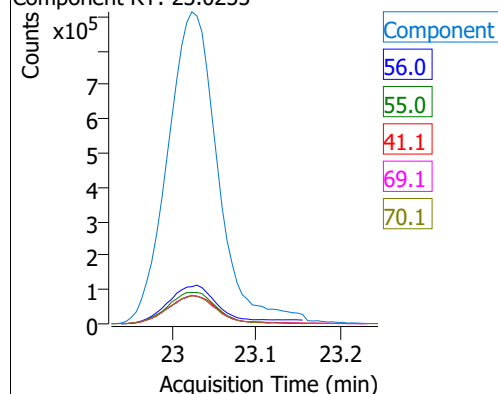
1-Octanol (NIST20.L)



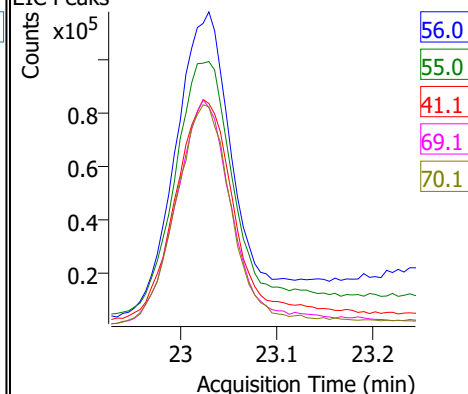
+ Scan (22.9361-23.2323 min, 50 scans) 1.D



Component RT: 23.0255



EIC Peaks



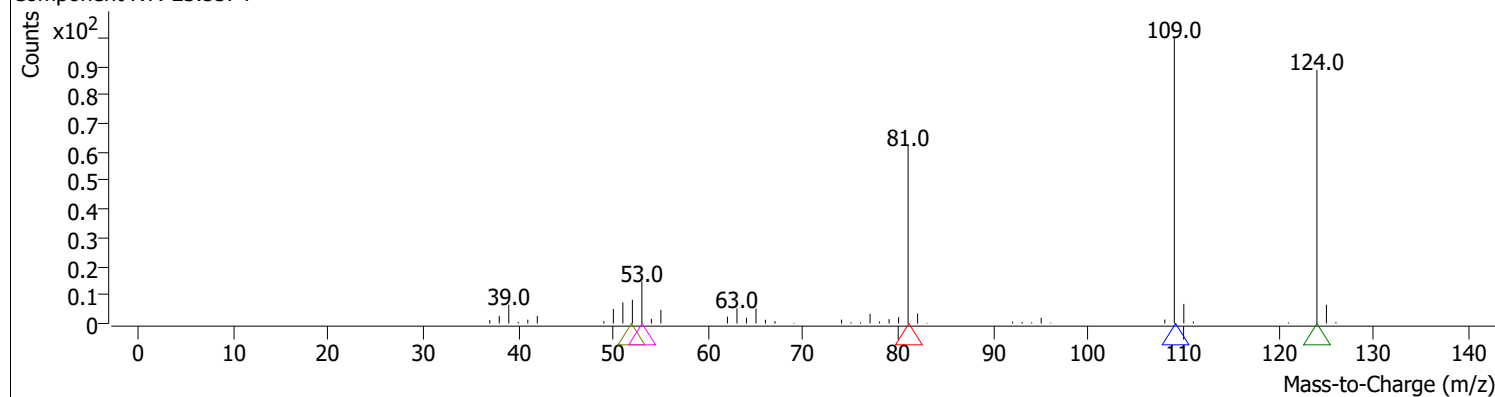
## Library Search Results - NonTarget Hits with Details



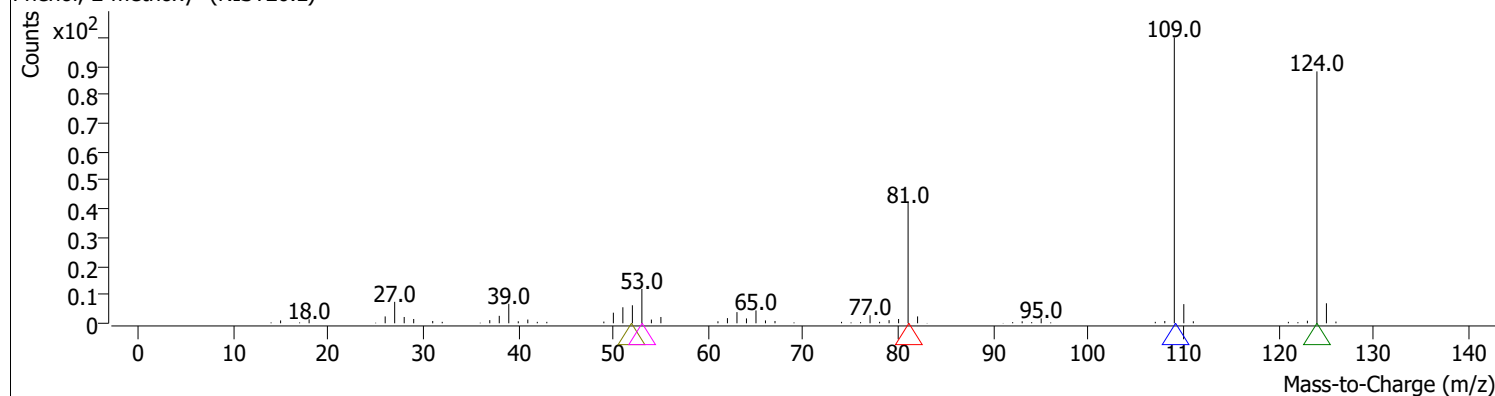
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
23.5574	Phenol, 2-methoxy-	8383926.4	98.5	90-05-1	C7H8O2	

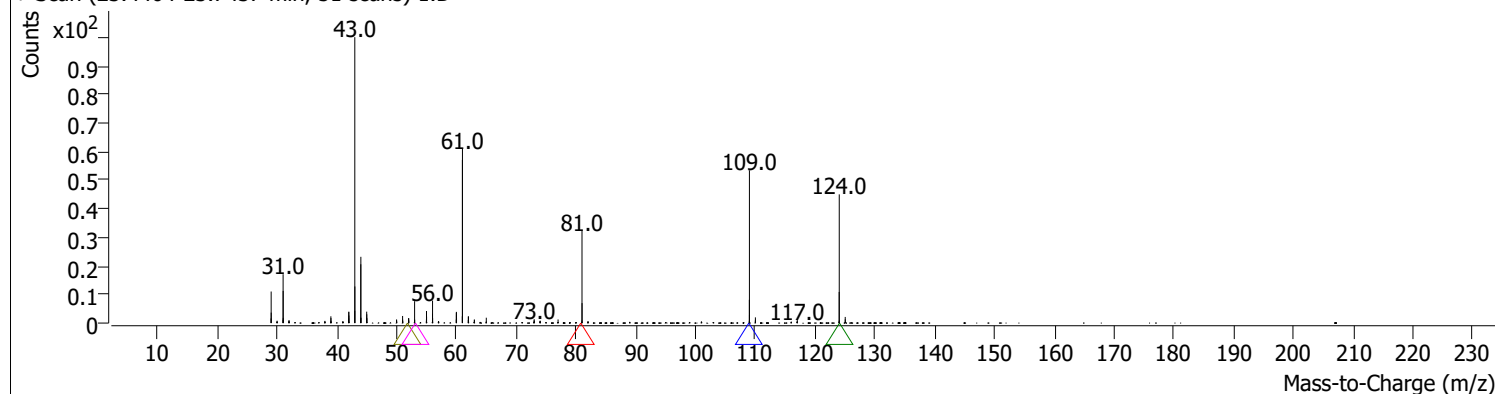
Component RT: 23.5574



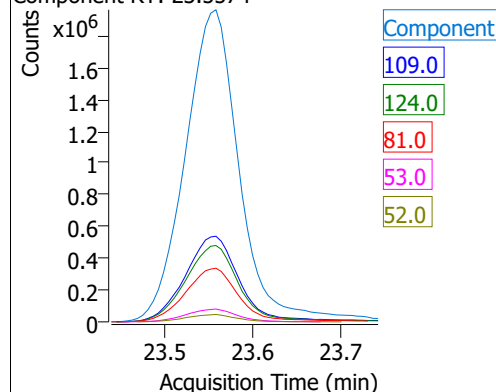
Phenol, 2-methoxy- (NIST20.L)



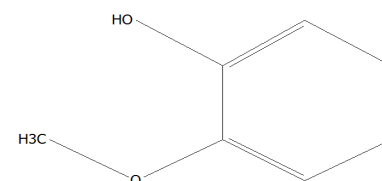
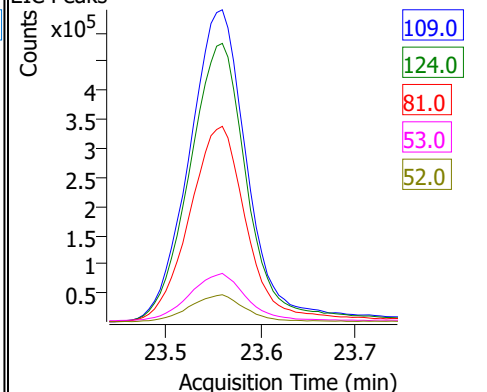
+ Scan (23.4464-23.7437 min, 51 scans) 1.D



Component RT: 23.5574



EIC Peaks



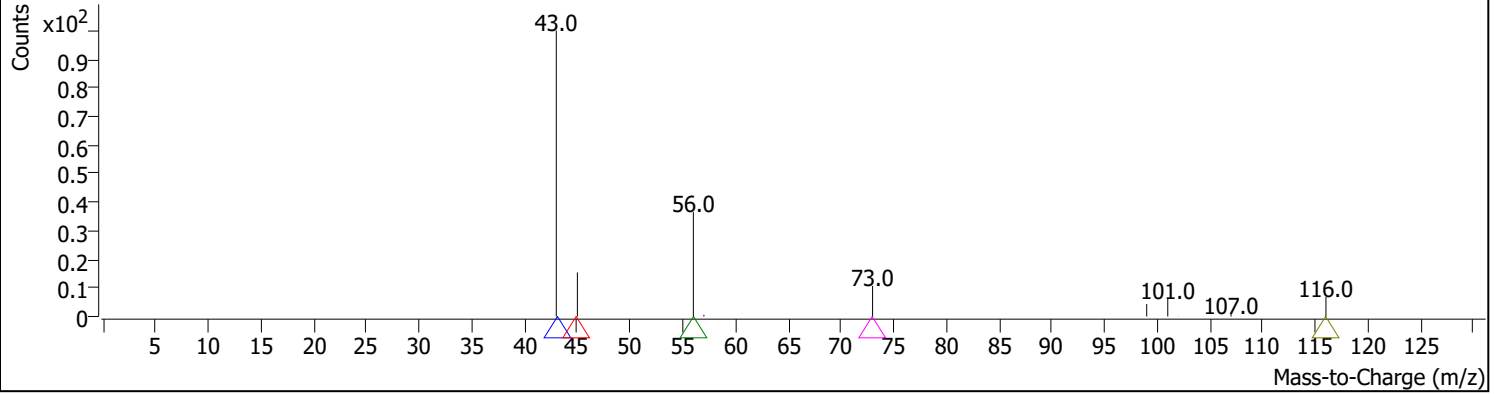
## Library Search Results - NonTarget Hits with Details



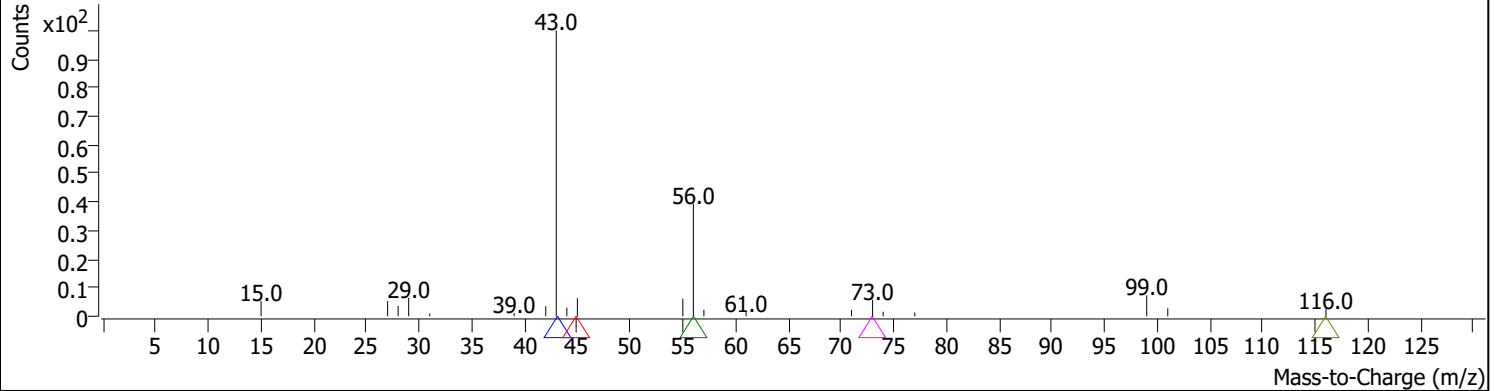
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
23.6130	Pentanoic acid, 4-oxo-	3230331.3	82.1	123-76-2	C5H8O3	

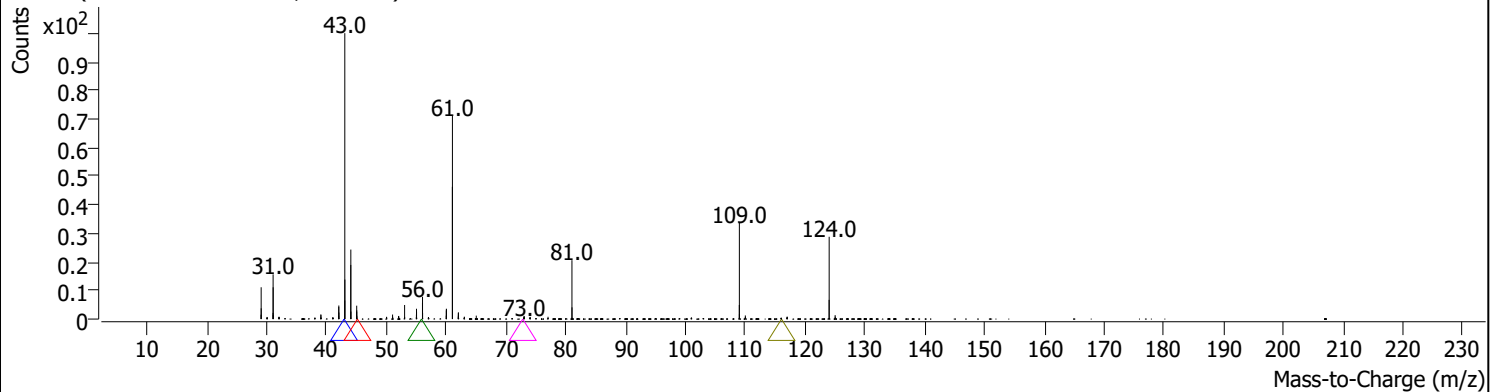
Component RT: 23.6130



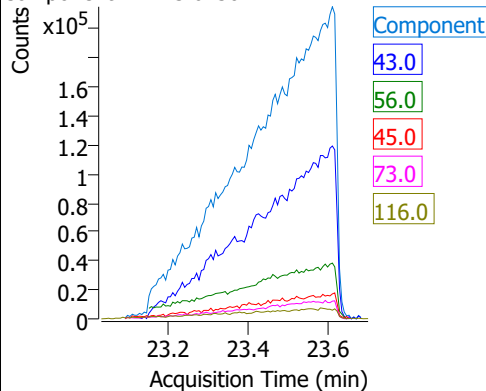
Pentanoic acid, 4-oxo- (NIST20.L)



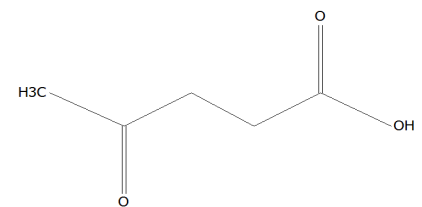
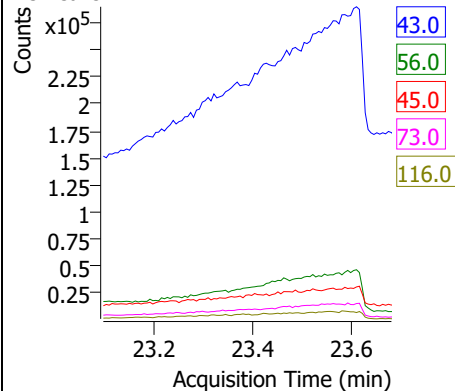
+ Scan (23.1550-23.6486 min, 84 scans) 1.D



Component RT: 23.6130



EIC Peaks



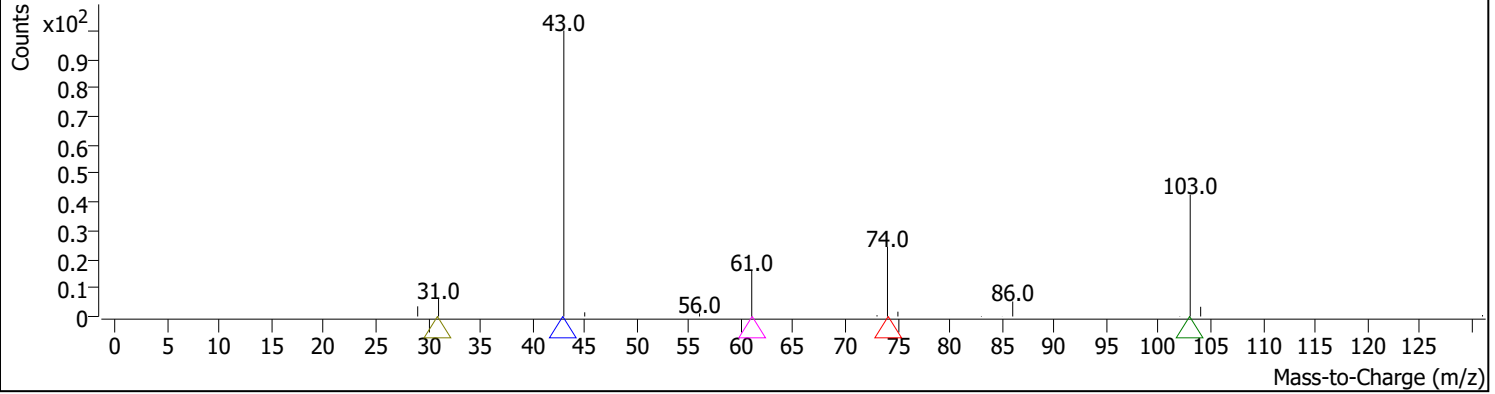
## Library Search Results - NonTarget Hits with Details



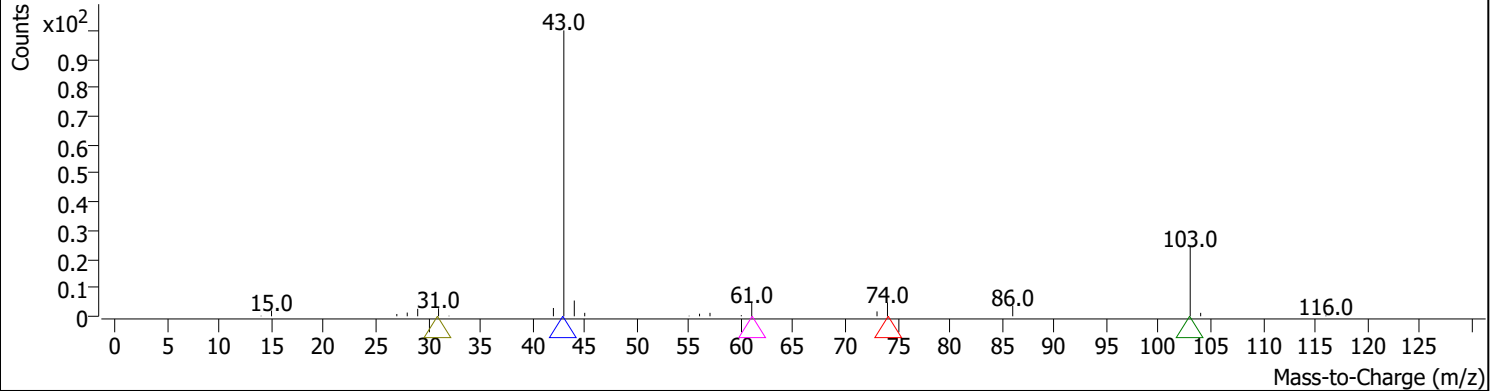
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
24.6682	1,2,3-Propanetriol, 1-acetate	3228314.2	87.8	106-61-6	C <sub>5</sub> H <sub>10</sub> O <sub>4</sub>	

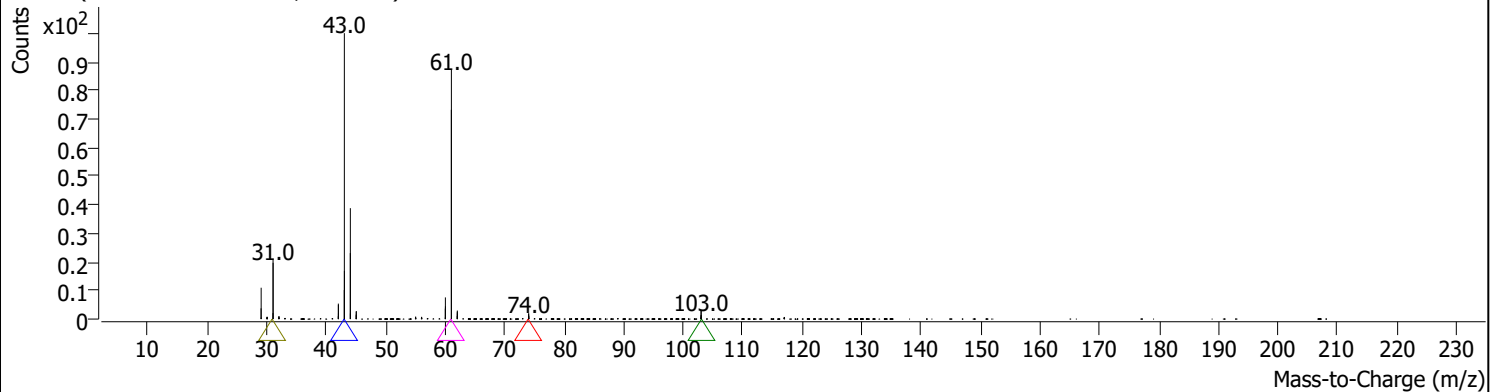
Component RT: 24.6682



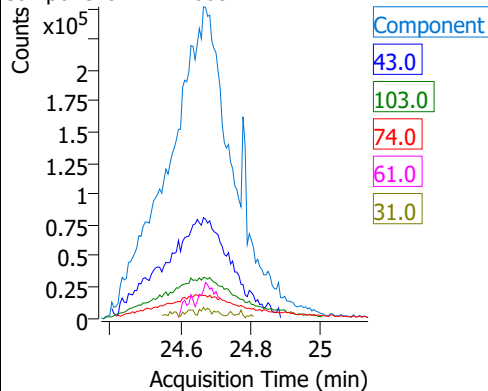
1,2,3-Propanetriol, 1-acetate (NIST20.L)



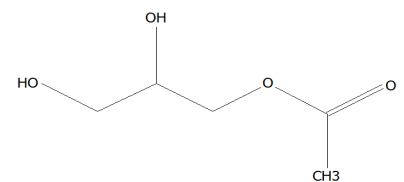
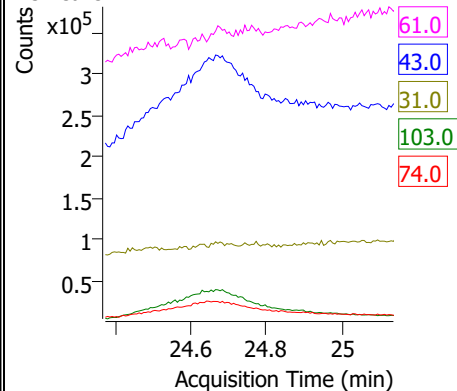
+ Scan (24.3859-24.9686 min, 99 scans) 1.D



Component RT: 24.6682



EIC Peaks





# Library Search Results - NonTarget Hits with Details

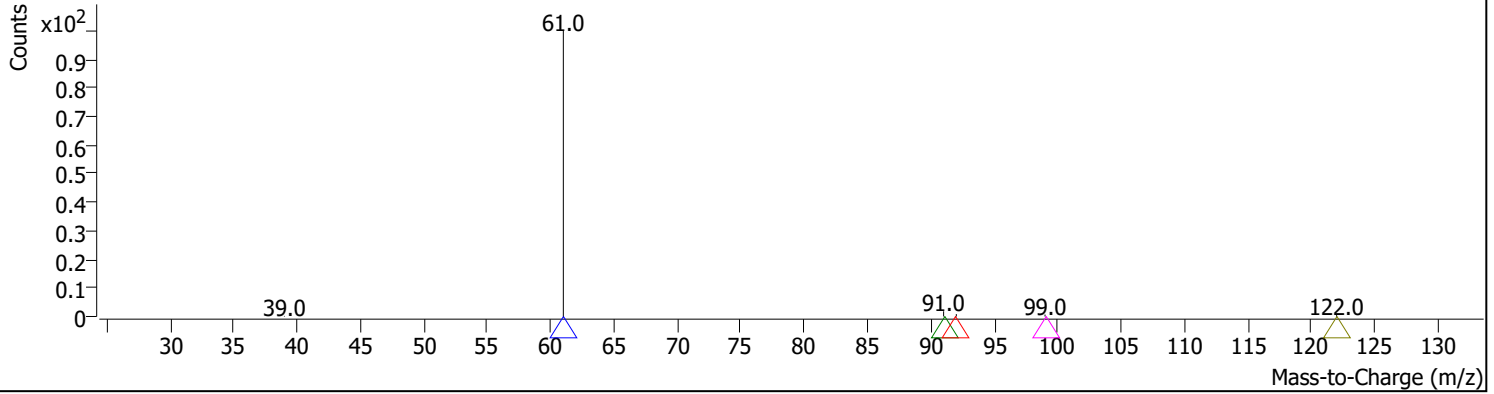


Agilent

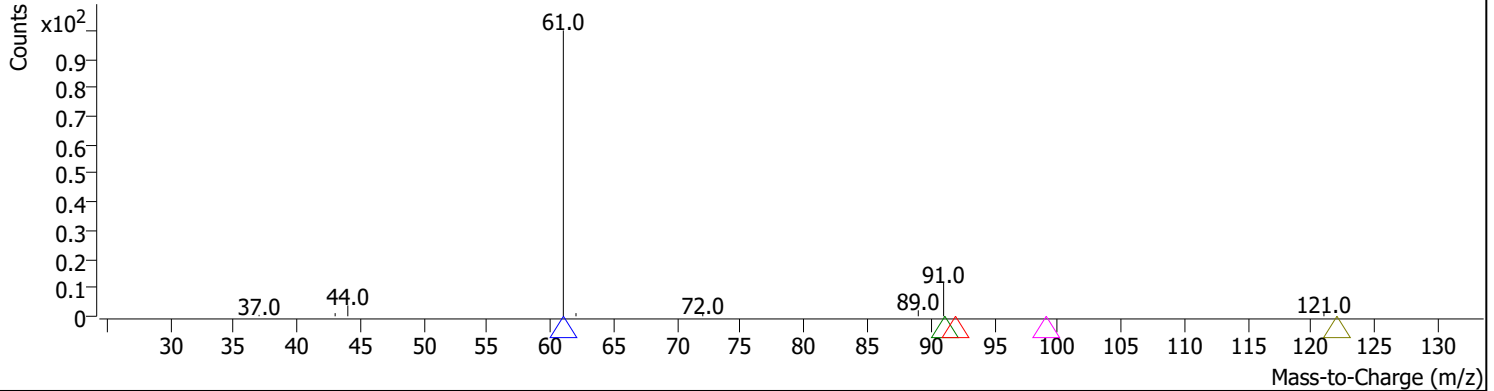
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
25.1522	1,3,5,7-Tetroxane	648304.1	78.0	293-30-1	C <sub>4</sub> H <sub>8</sub> O <sub>4</sub>	

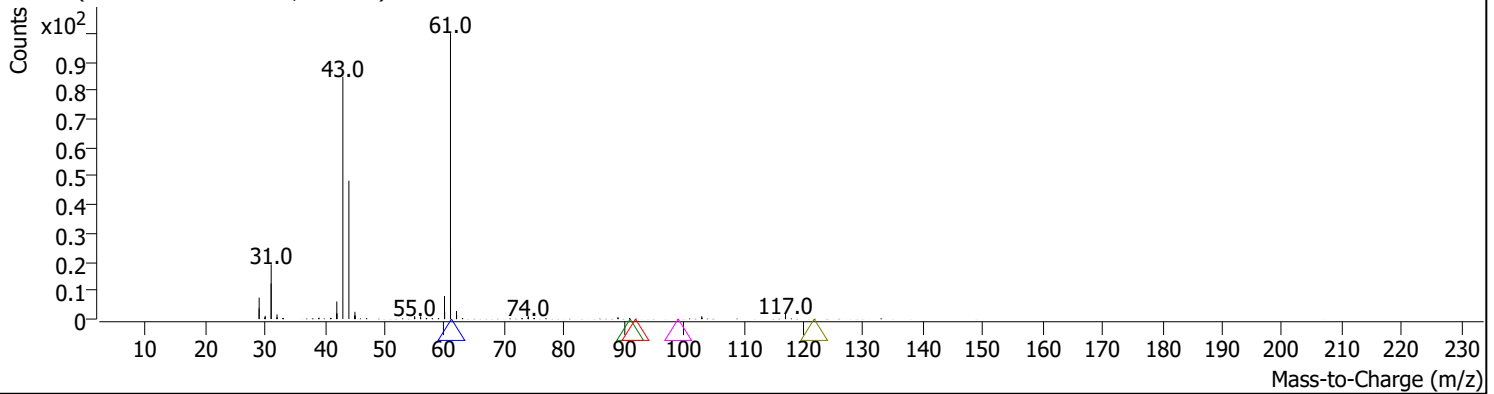
Component RT: 25.1522



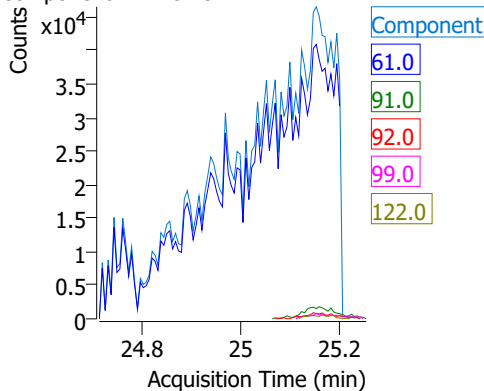
1,3,5,7-Tetroxane (NIST20.L)



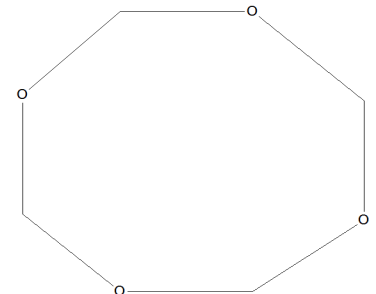
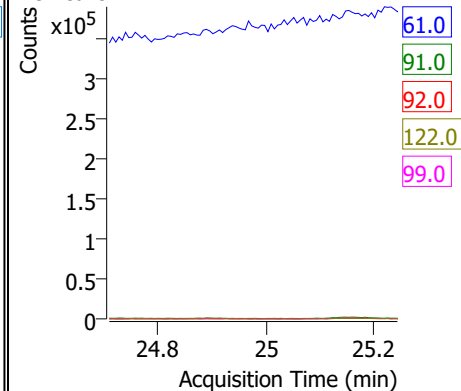
+ Scan (25.1470-25.1708 min, 5 scans) 1.D



Component RT: 25.1522



EIC Peaks



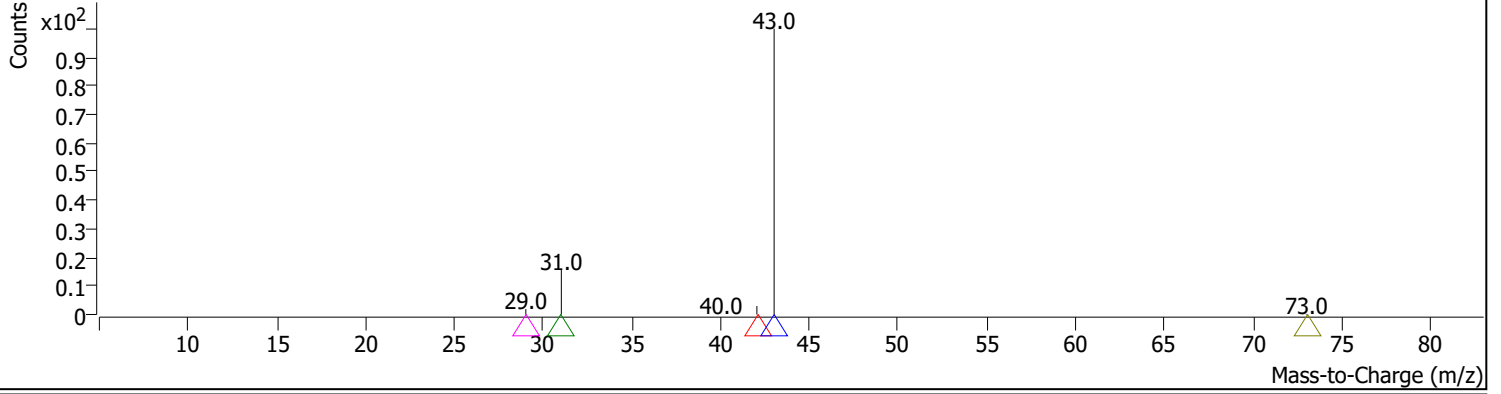
# Library Search Results - NonTarget Hits with Details



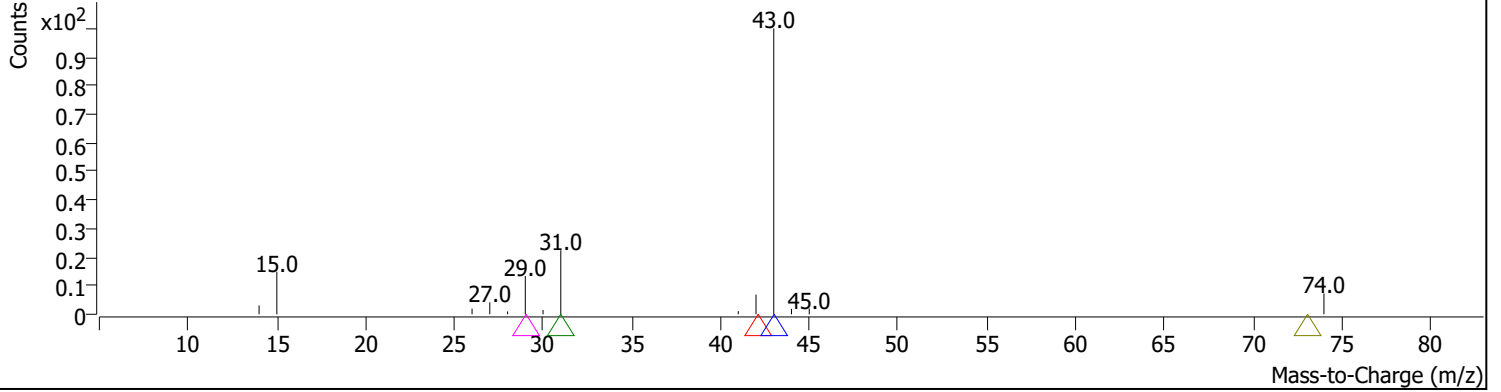
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
26.6801	2-Propanone, 1-hydroxy-	22515463.1	80.1	116-09-6	C3H6O2	

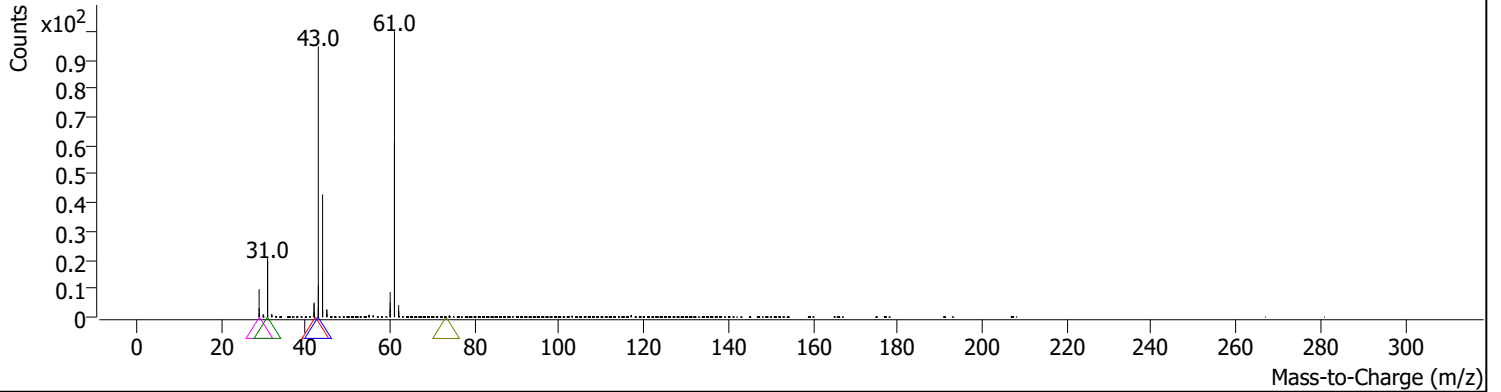
Component RT: 26.6801



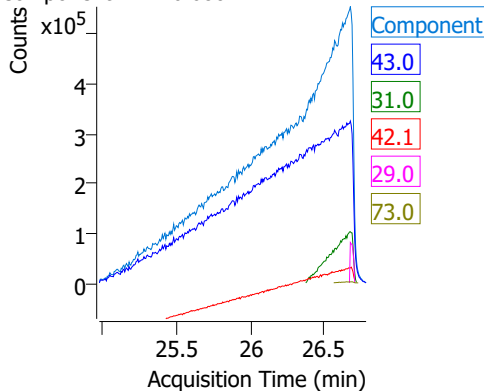
2-Propanone, 1-hydroxy- (NIST20.L)



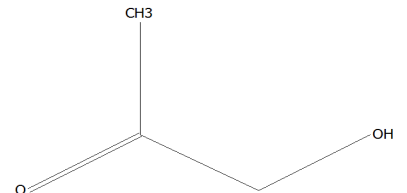
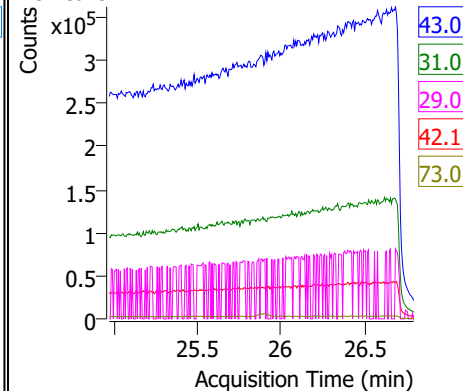
+ Scan (24.9745-26.7893 min, 306 scans) 1.D



Component RT: 26.6801



EIC Peaks



# Library Search Results - NonTarget Hits with Details

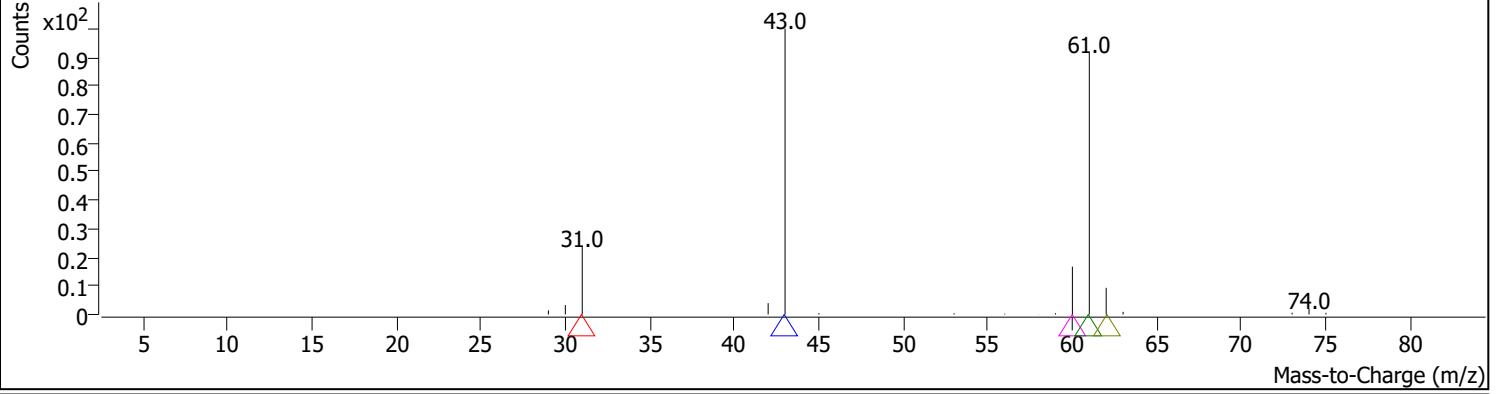


Agilent

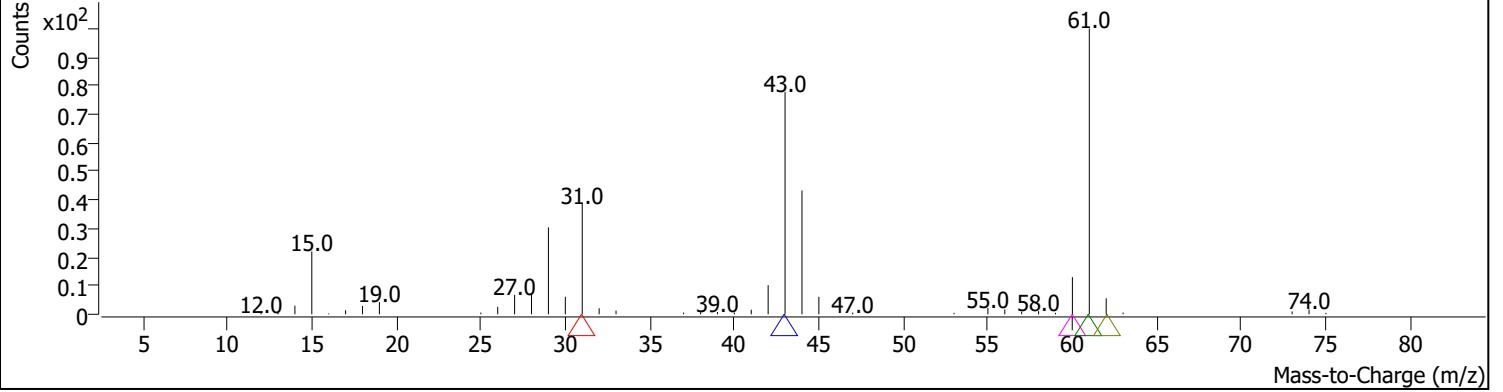
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
26.6803	Glycerin	37962614.8	80.5	56-81-5	C3H8O3	

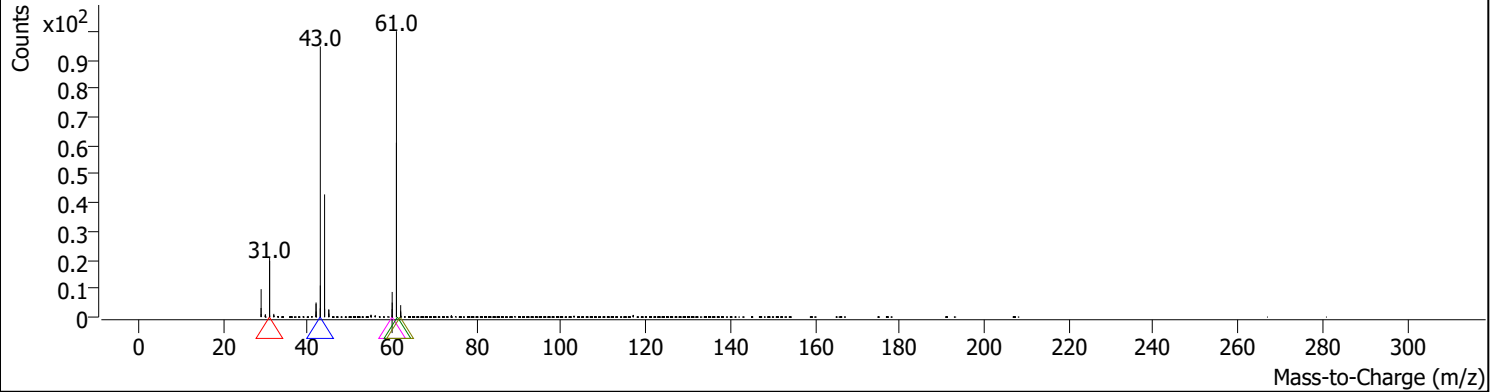
Component RT: 26.6803



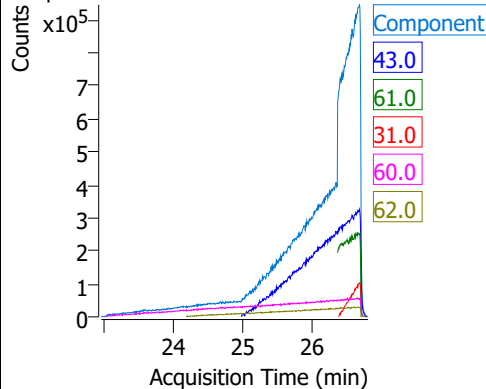
Glycerin (NIST20.L)



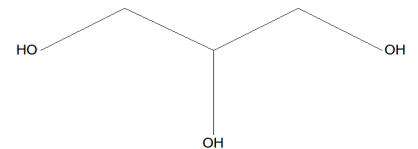
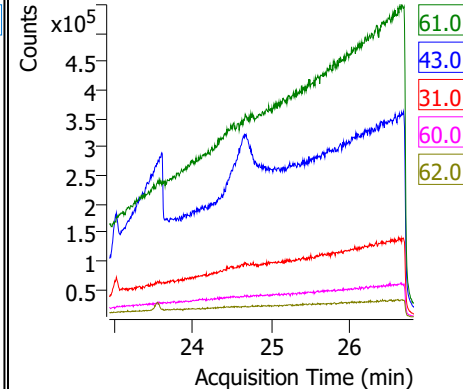
+ Scan (24.9745-26.7893 min, 306 scans) 1.D



Component RT: 26.6803



EIC Peaks



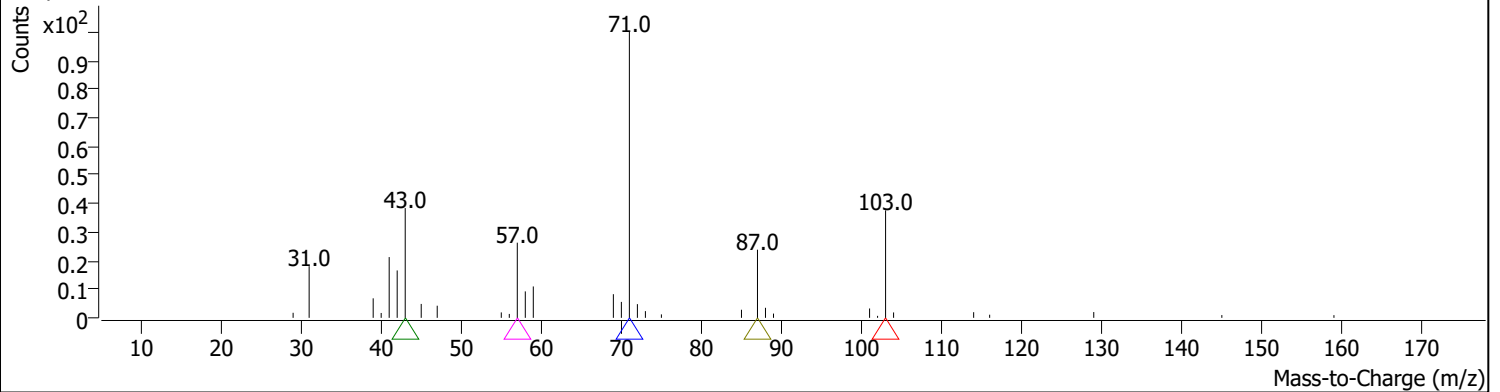
## Library Search Results - NonTarget Hits with Details



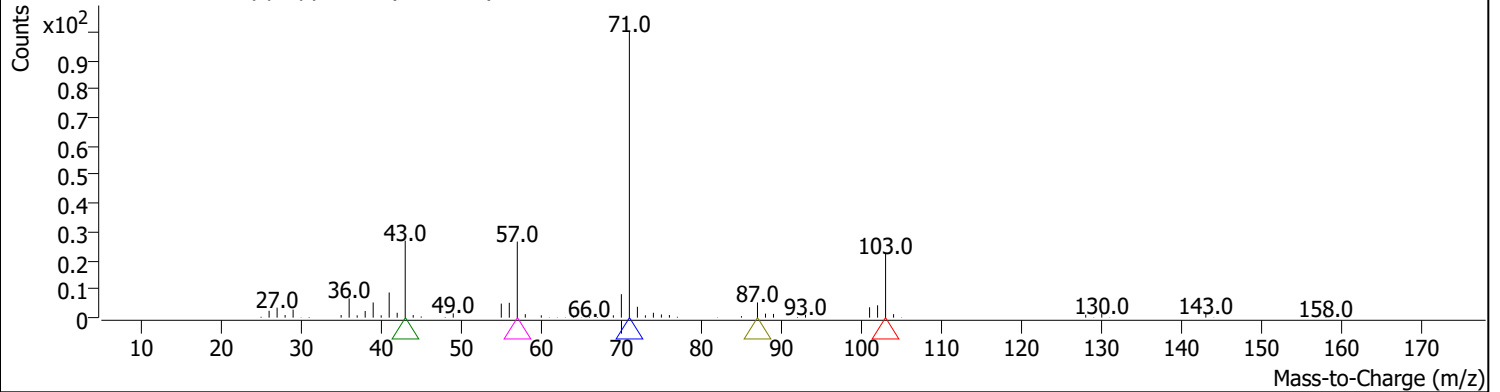
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
27.7058	Butanoic acid, 2,2-dimethylpropyl ester	1010279.2	81.3	23361-69-5	C9H18O2	

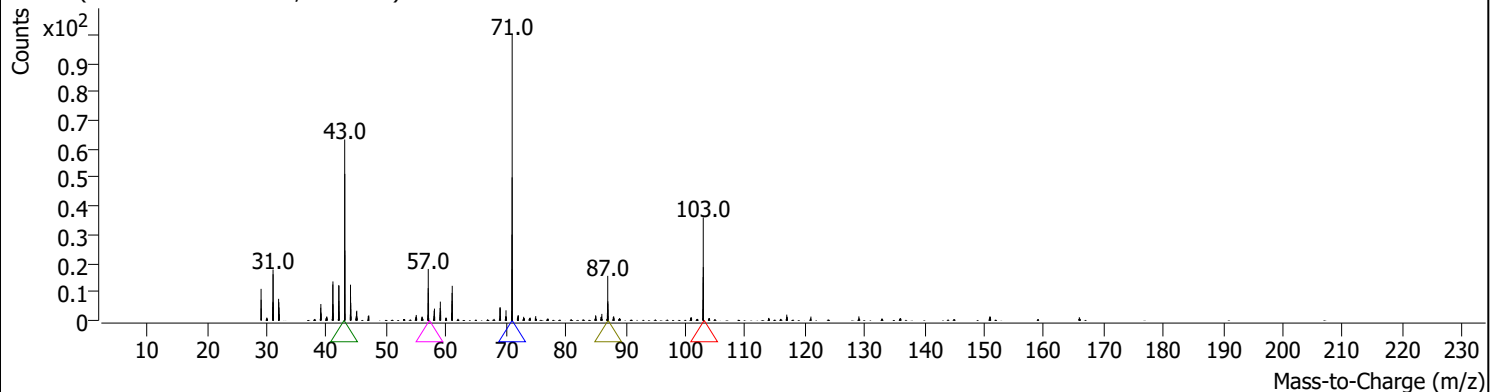
Component RT: 27.7058



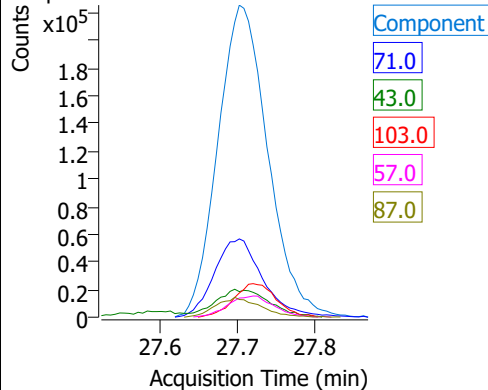
Butanoic acid, 2,2-dimethylpropyl ester (NIST20.L)



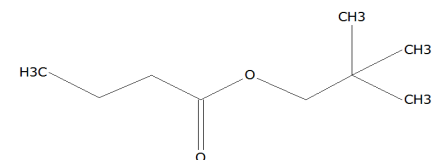
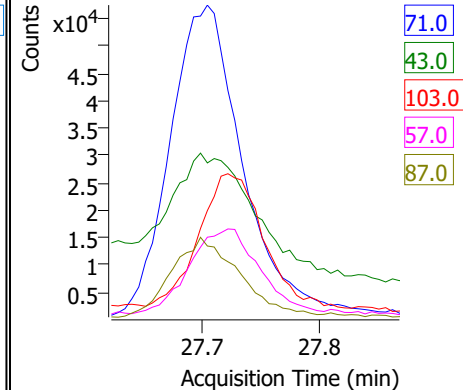
+ Scan (27.6293-27.8393 min, 35 scans) 1.D



Component RT: 27.7058



EIC Peaks



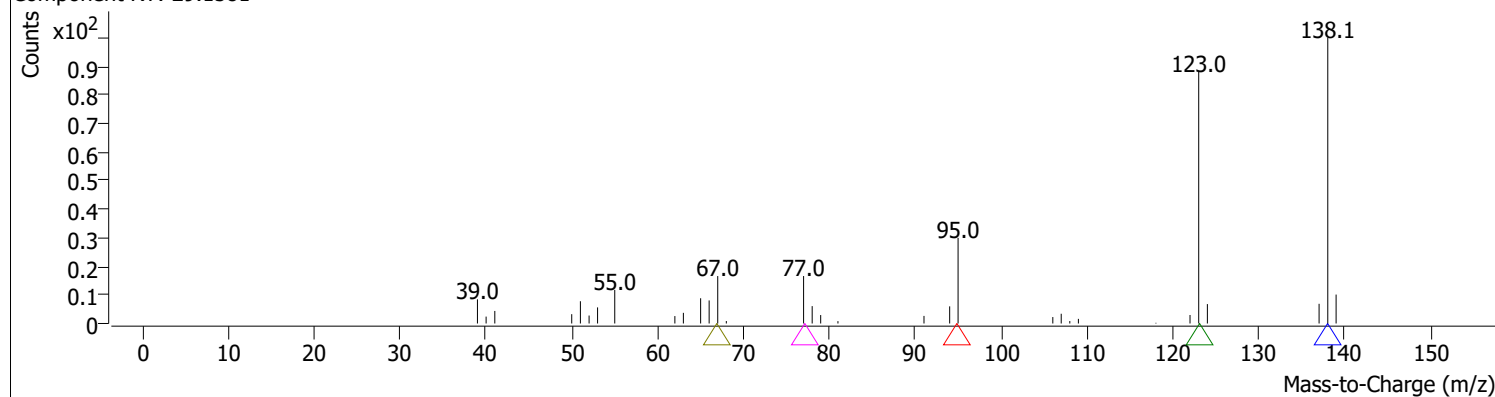
## Library Search Results - NonTarget Hits with Details



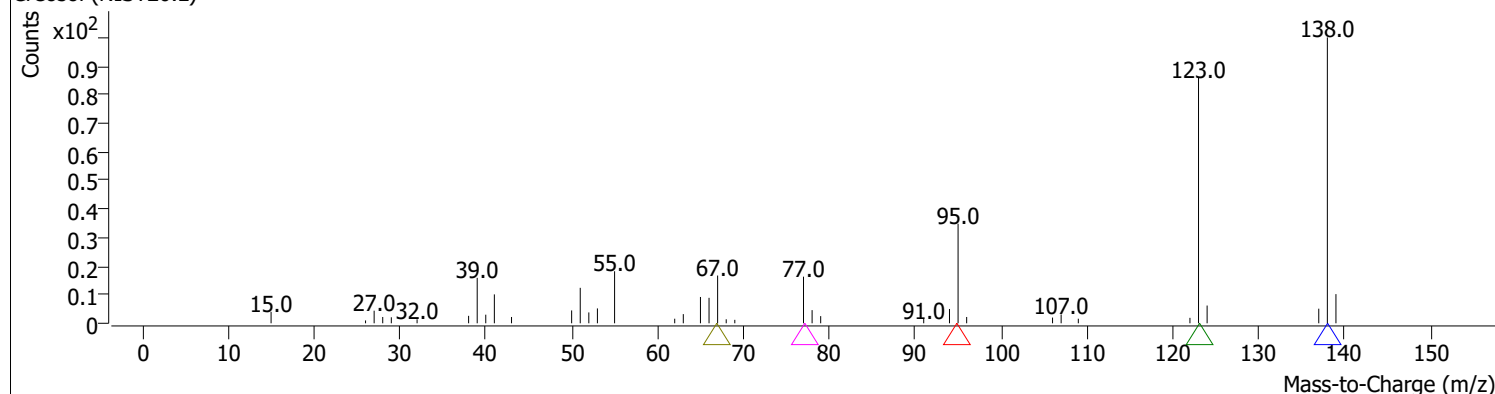
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
29.1581	Creosol	525521.9	97.3	93-51-6	C8H10O2	

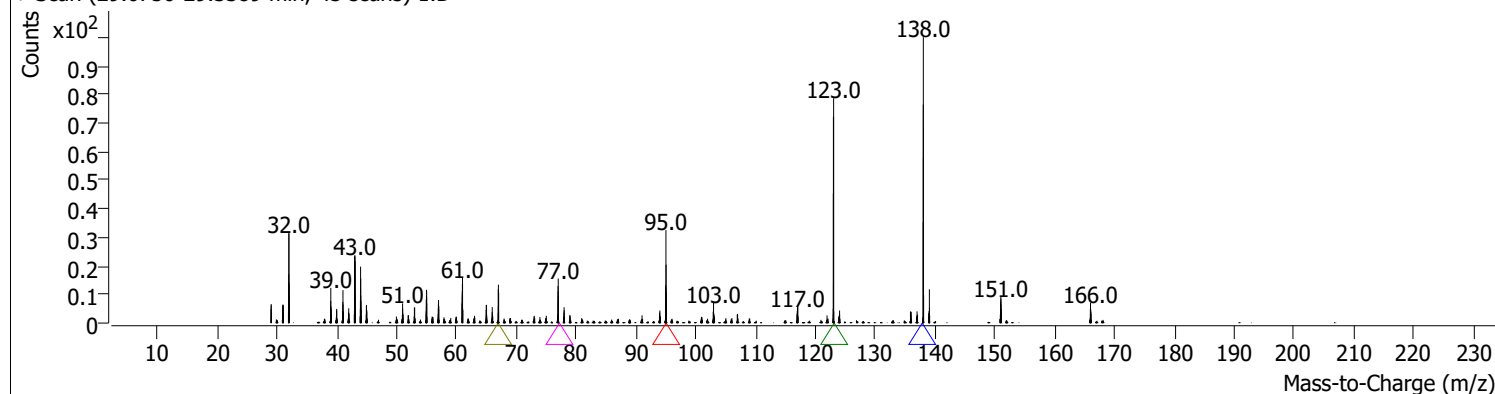
Component RT: 29.1581



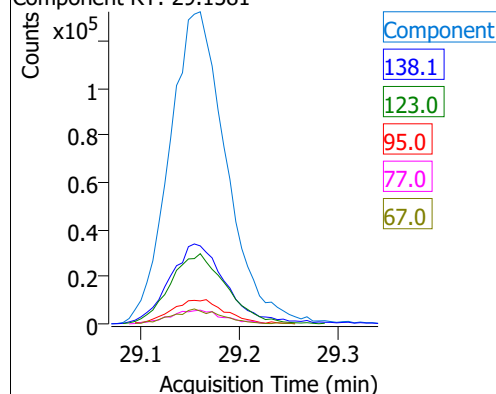
Creosol (NIST20.L)



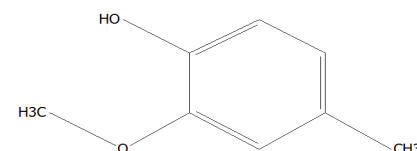
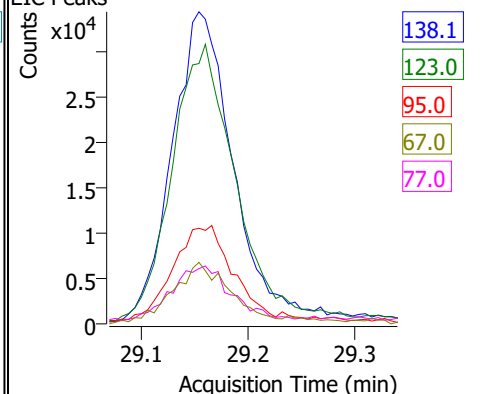
+ Scan (29.0750-29.3389 min, 45 scans) 1.D



Component RT: 29.1581



EIC Peaks



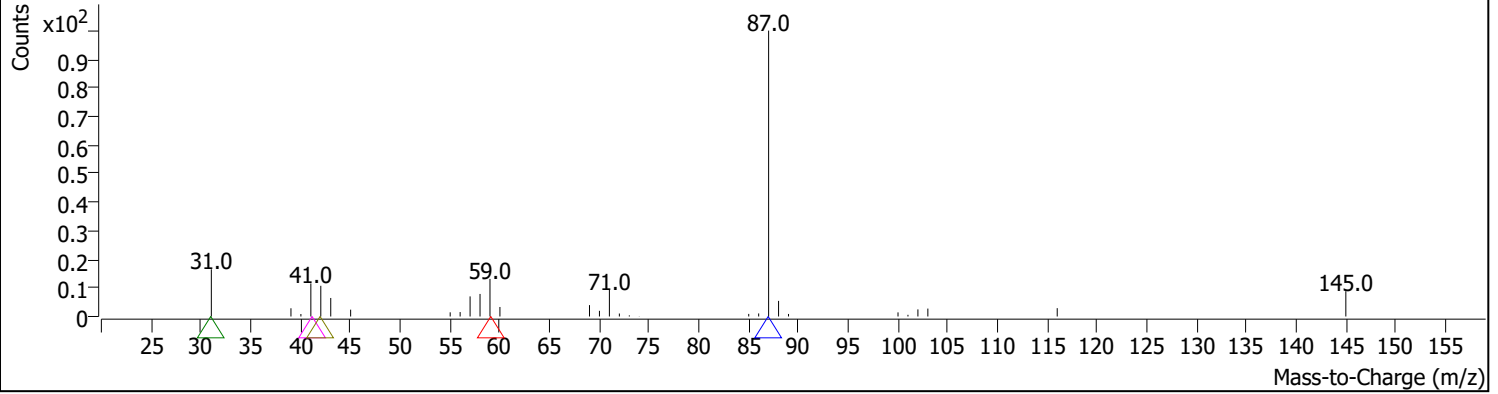
## Library Search Results - NonTarget Hits with Details



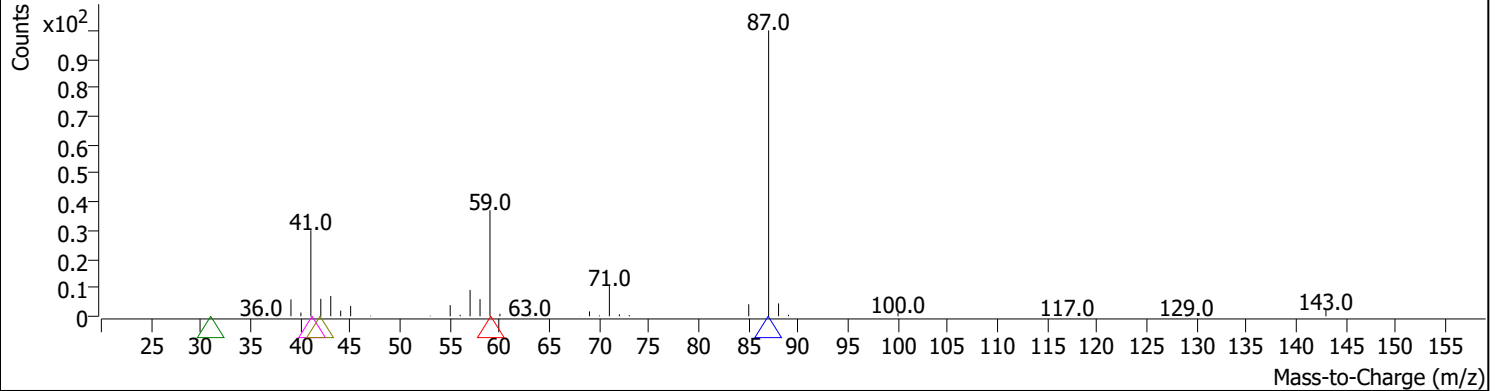
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
30.4598	1,3-Dioxolane, 2-butyl-4-methyl-	834040.1	79.0	74094-60-3	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	

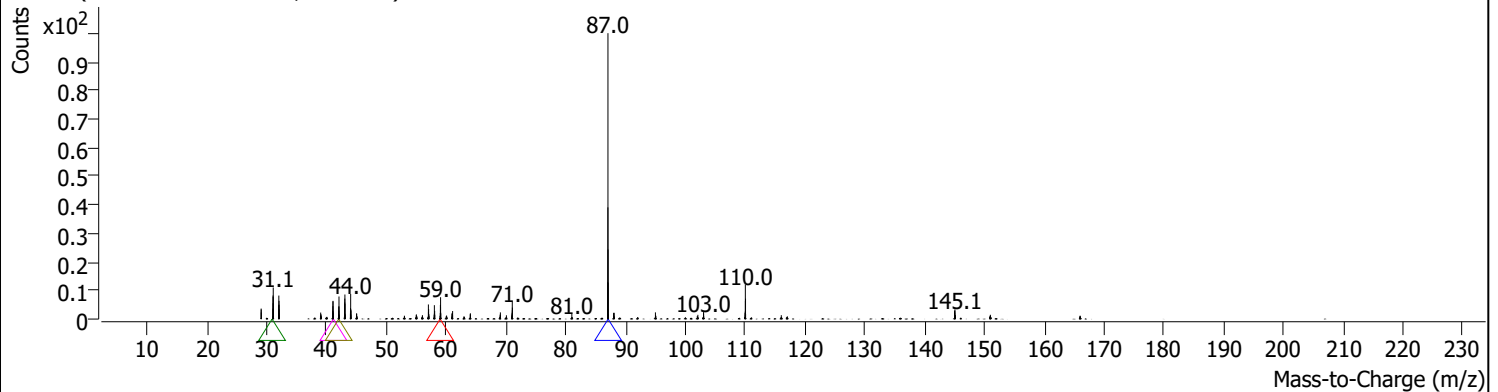
Component RT: 30.4598



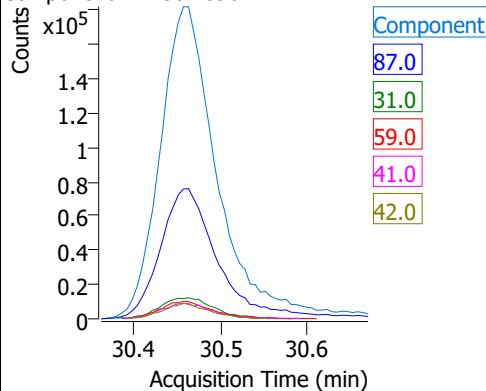
1,3-Dioxolane, 2-butyl-4-methyl- (NIST20.L)



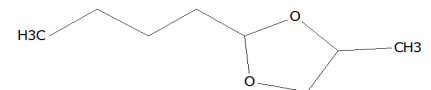
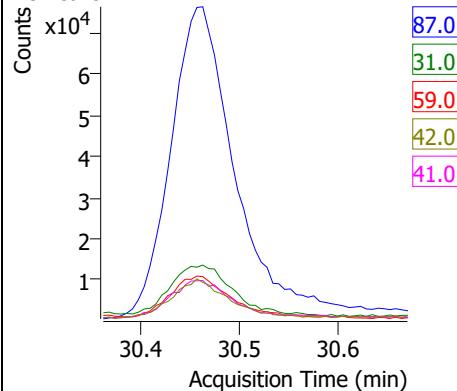
+ Scan (30.3581-30.6708 min, 53 scans) 1.D



Component RT: 30.4598



EIC Peaks



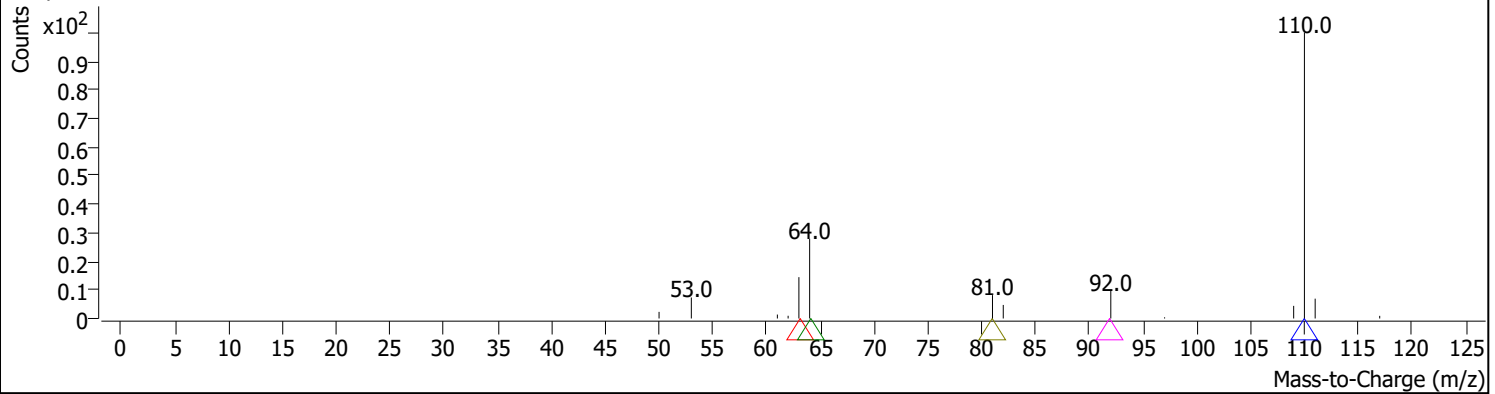
## Library Search Results - NonTarget Hits with Details



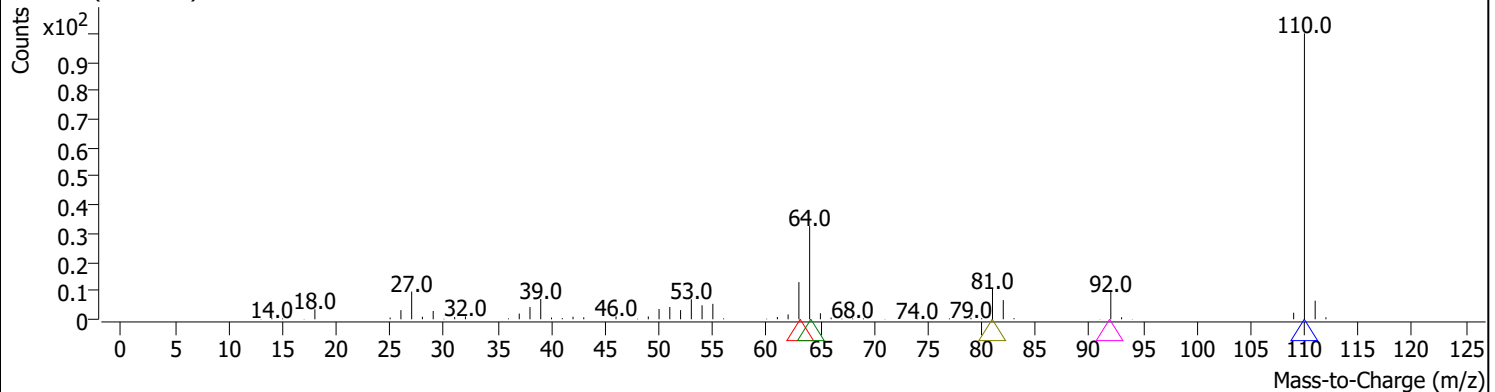
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
30.7535	Catechol	925875.3	86.6	120-80-9	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	

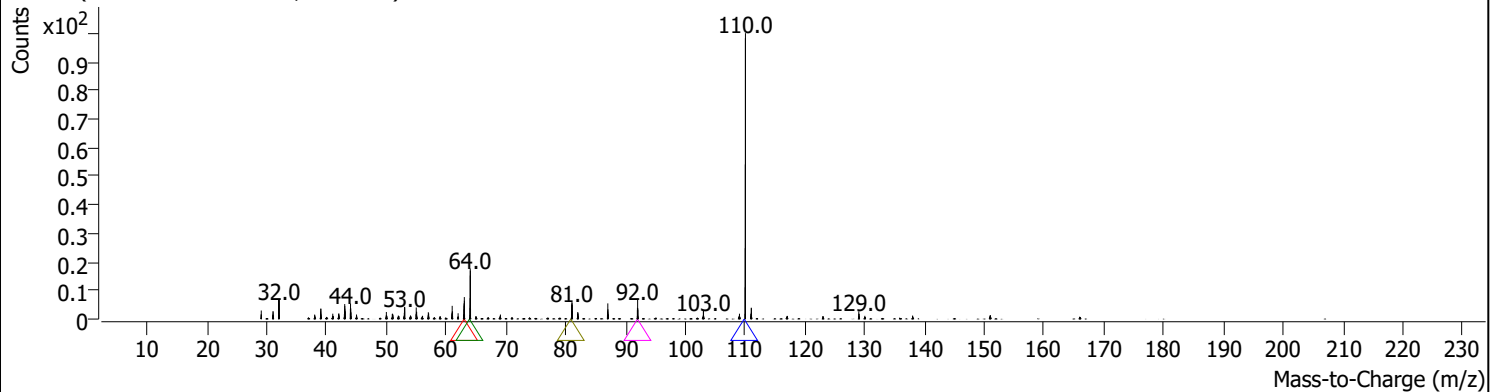
Component RT: 30.7535



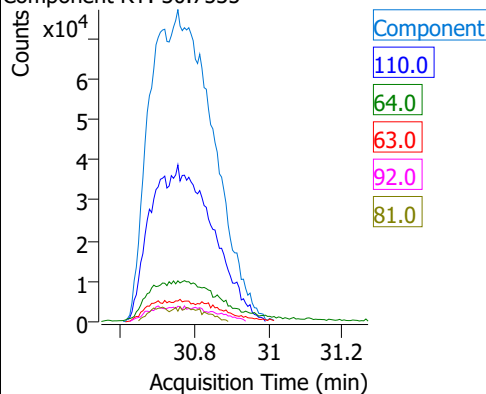
Catechol (NIST20.L)



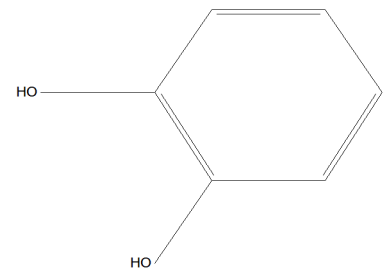
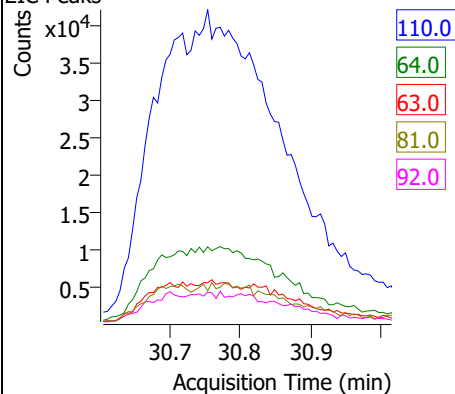
+ Scan (30.6115-30.9919 min, 64 scans) 1.D



Component RT: 30.7535



EIC Peaks



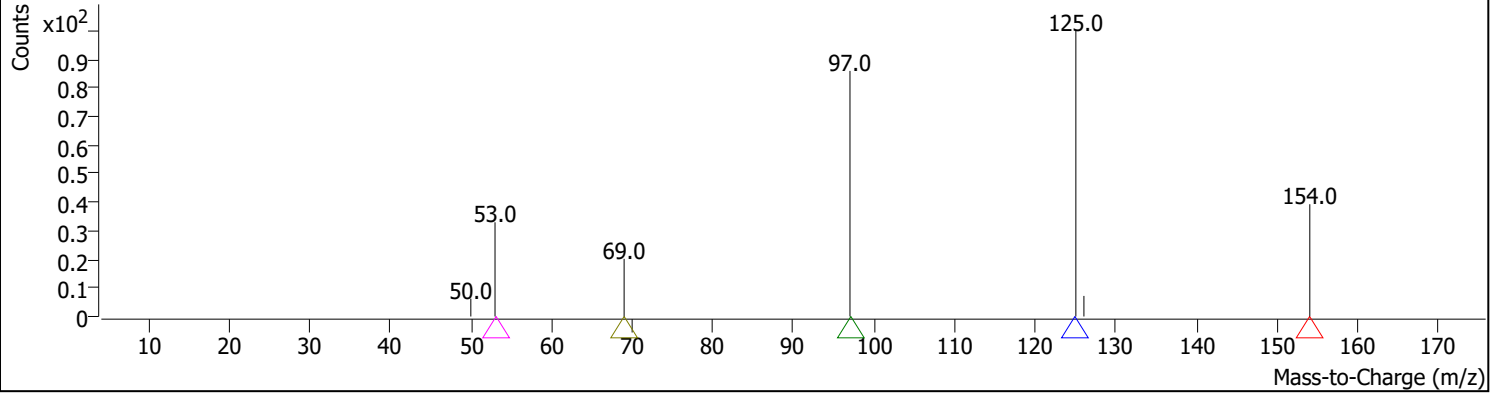
## Library Search Results - NonTarget Hits with Details



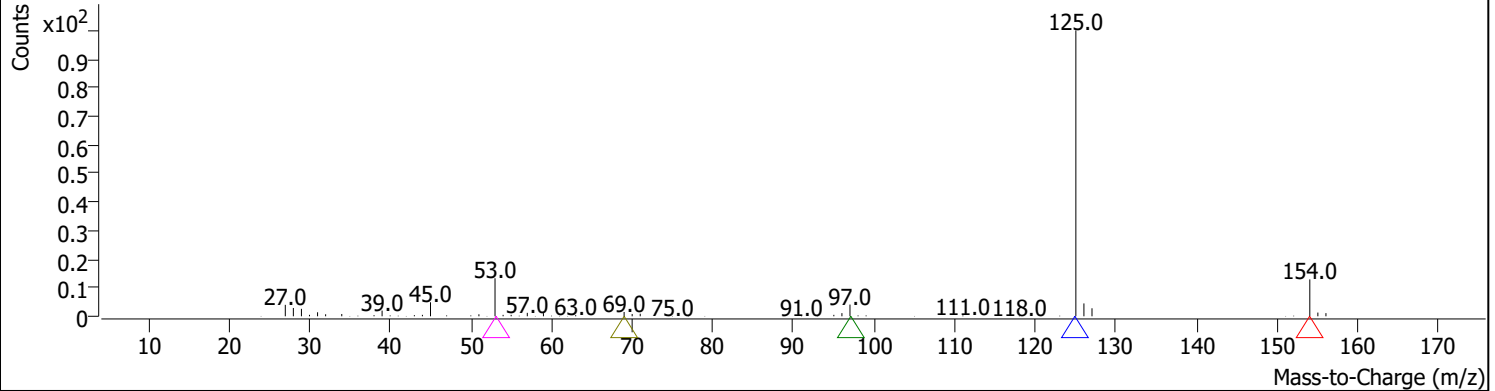
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
31.1051	1-Propanone, 1-(5-methyl-2-thienyl)-	343736.1	76.1	59303-13-8	C8H10OS	

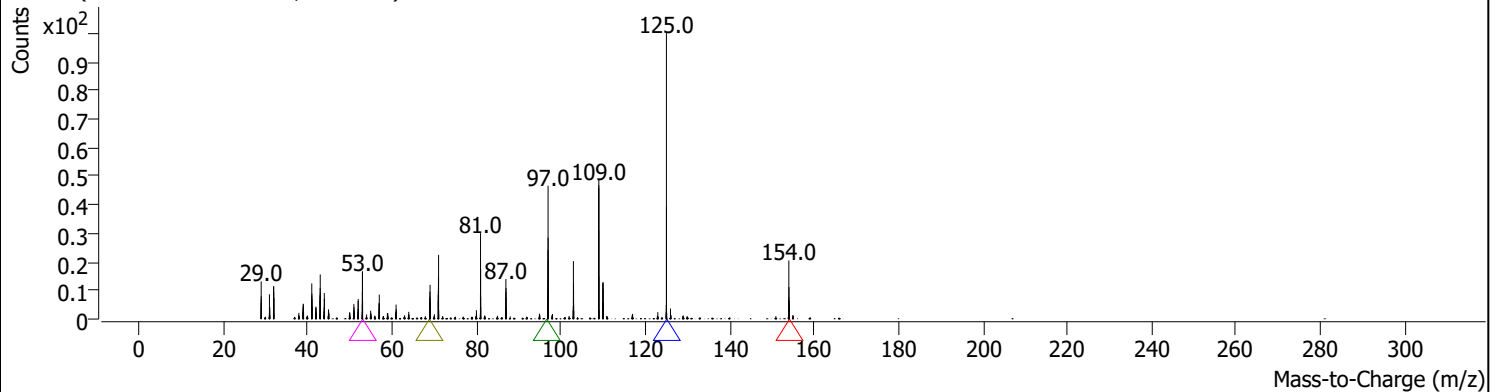
Component RT: 31.1051



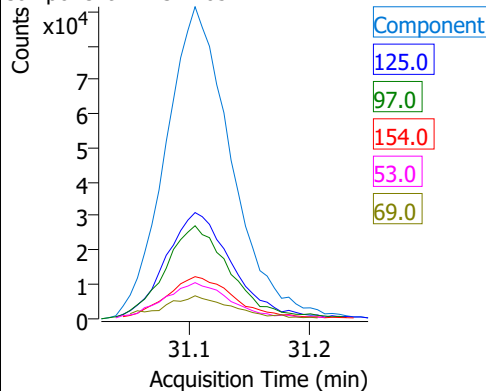
1-Propanone, 1-(5-methyl-2-thienyl)- (NIST20.L)



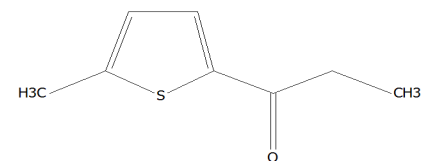
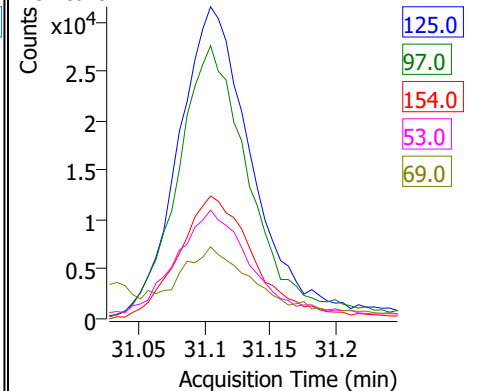
+ Scan (31.0326-31.2298 min, 34 scans) 1.D



Component RT: 31.1051



EIC Peaks





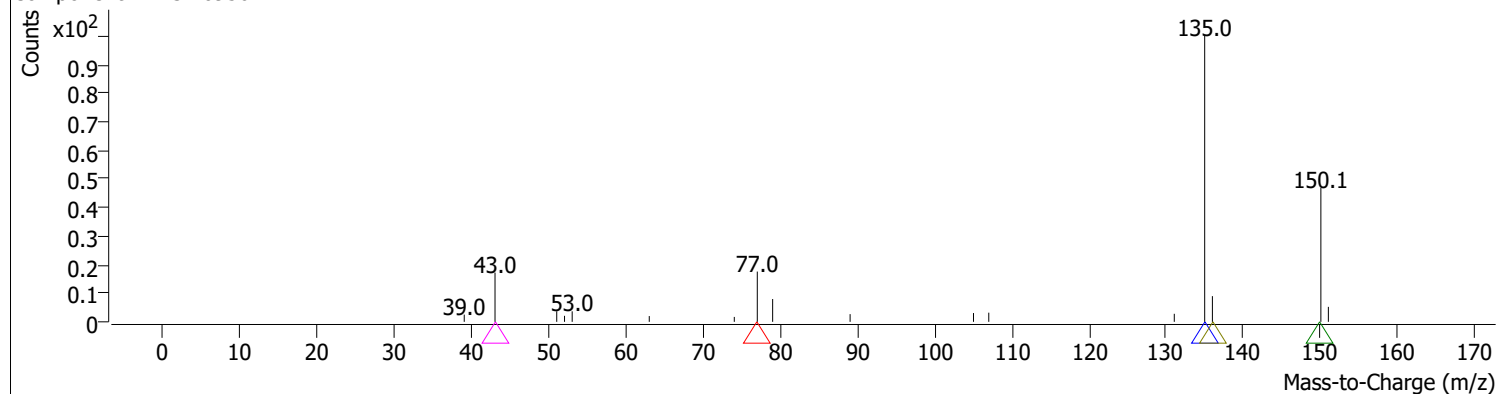
## Library Search Results - NonTarget Hits with Details



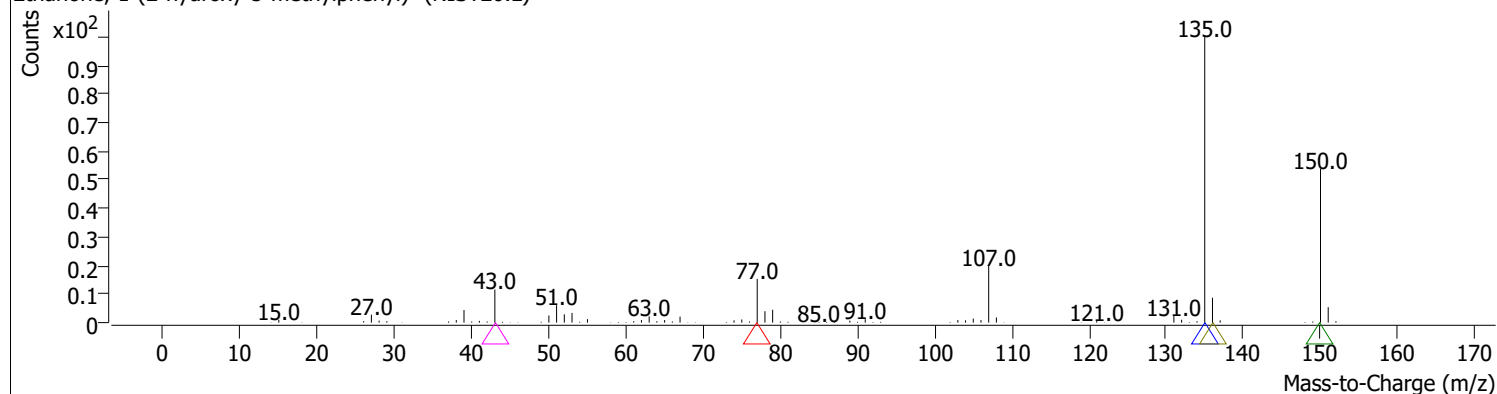
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
32.0956	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	234475.9	90.1	1450-72-2	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	

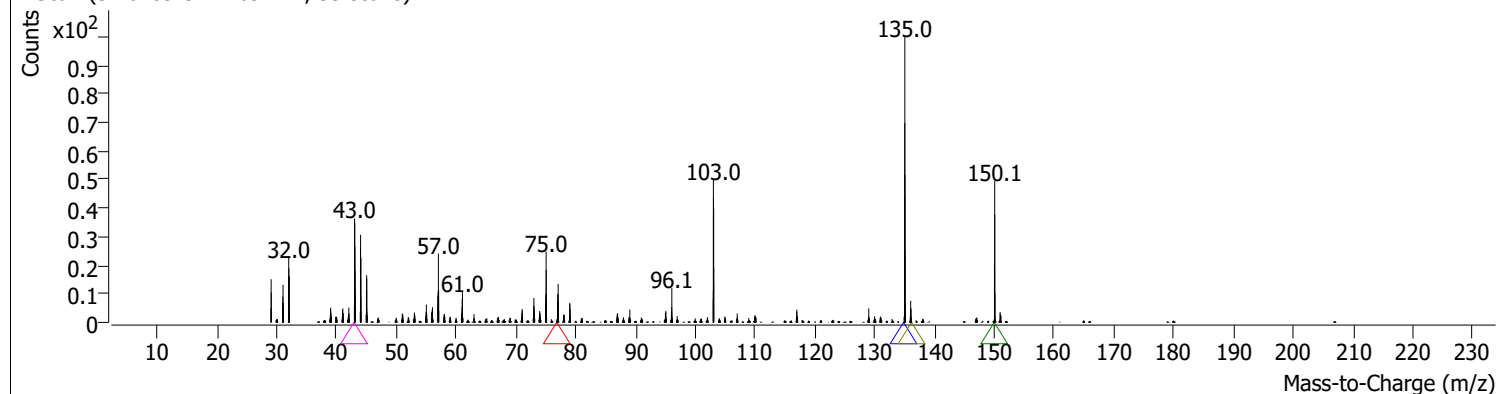
Component RT: 32.0956



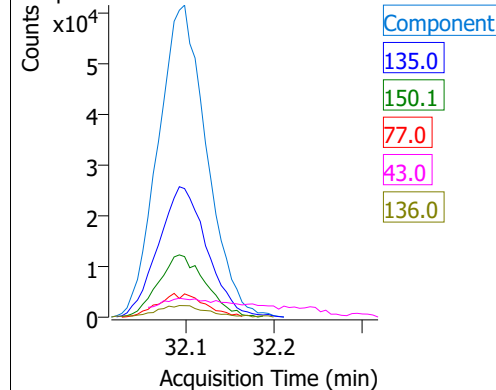
Ethanone, 1-(2-hydroxy-5-methylphenyl)- (NIST20.L)



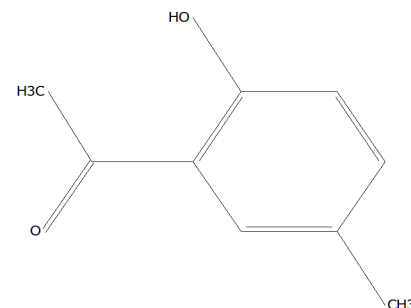
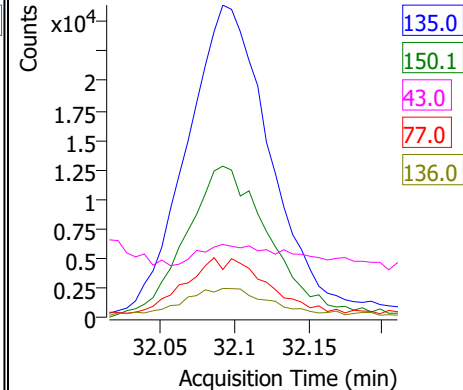
+ Scan (32.0159-32.2109 min, 33 scans) 1.D



Component RT: 32.0956



EIC Peaks



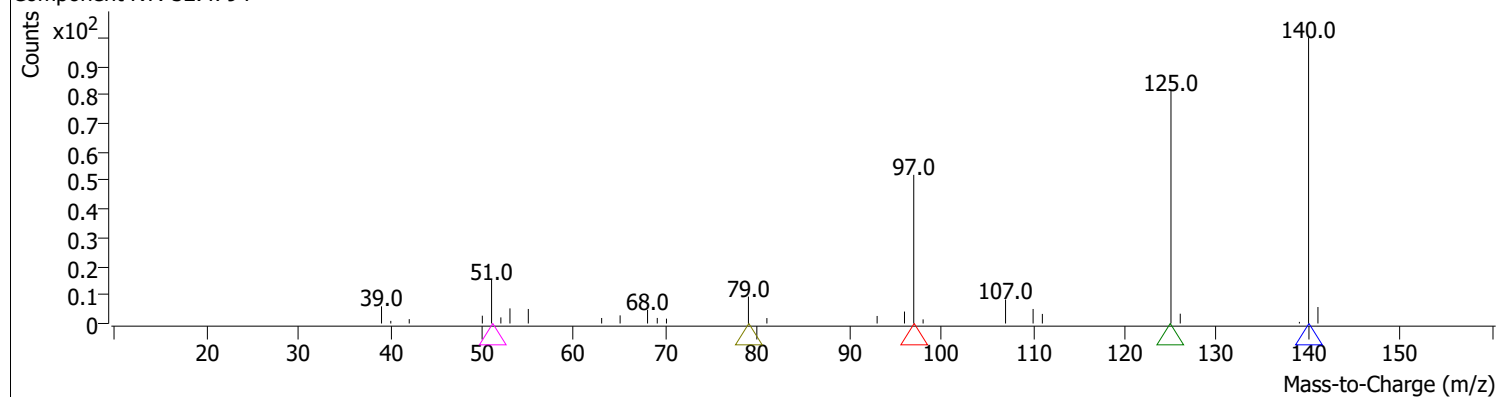
## Library Search Results - NonTarget Hits with Details



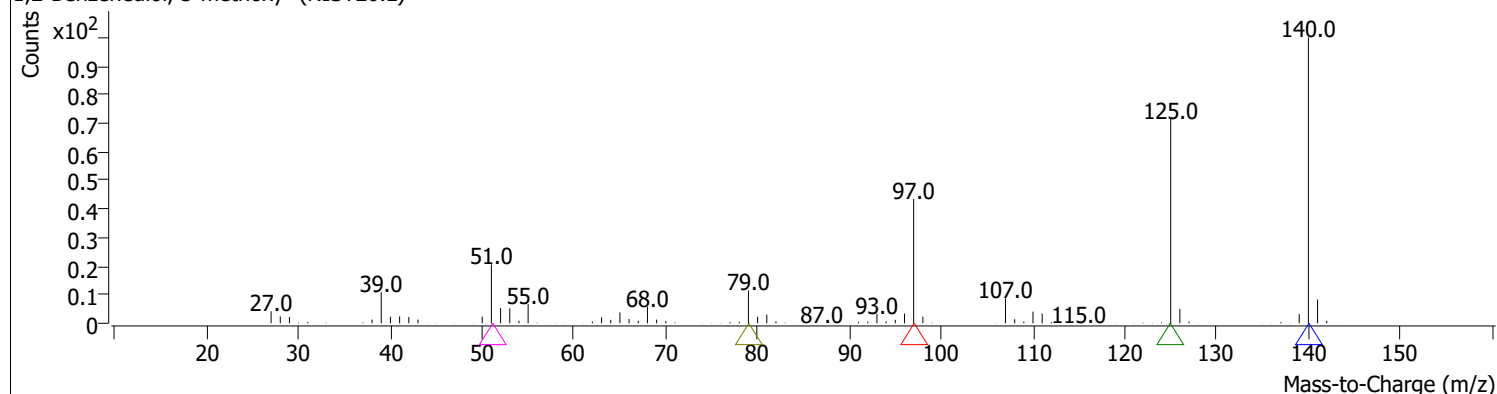
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
32.4794	1,2-Benzenediol, 3-methoxy-	538517.7	94.6	934-00-9	C7H8O3	

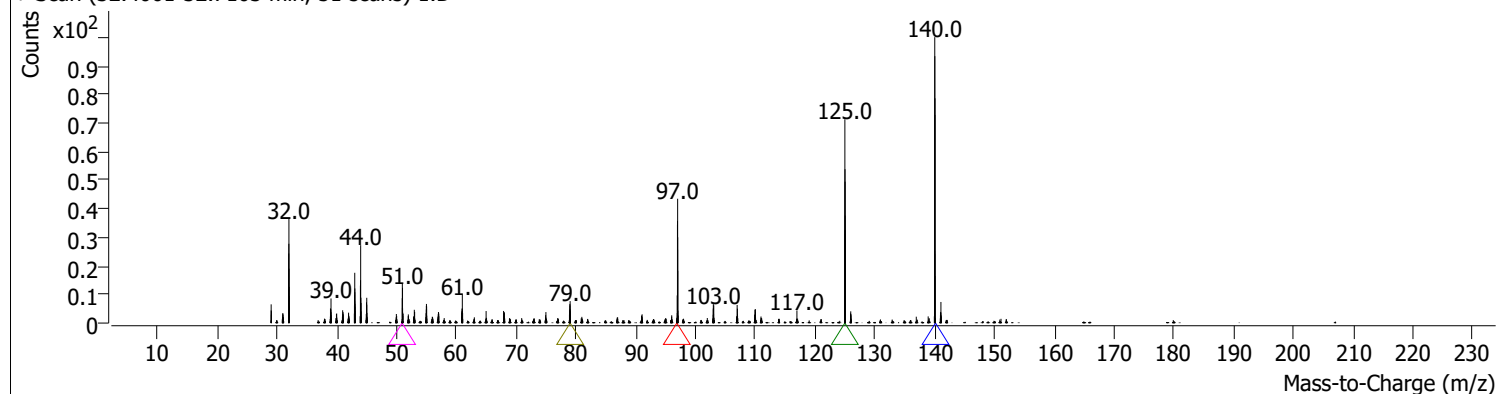
Component RT: 32.4794



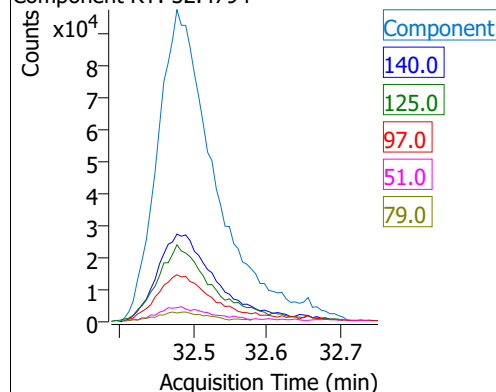
1,2-Benzenediol, 3-methoxy- (NIST20.L)



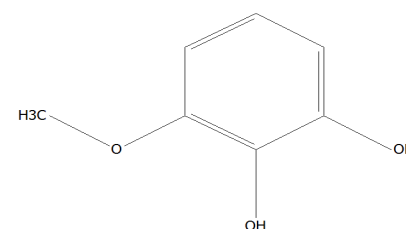
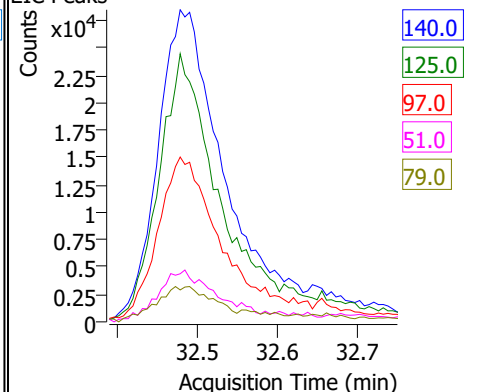
+ Scan (32.4061-32.7103 min, 51 scans) 1.D



Component RT: 32.4794



EIC Peaks



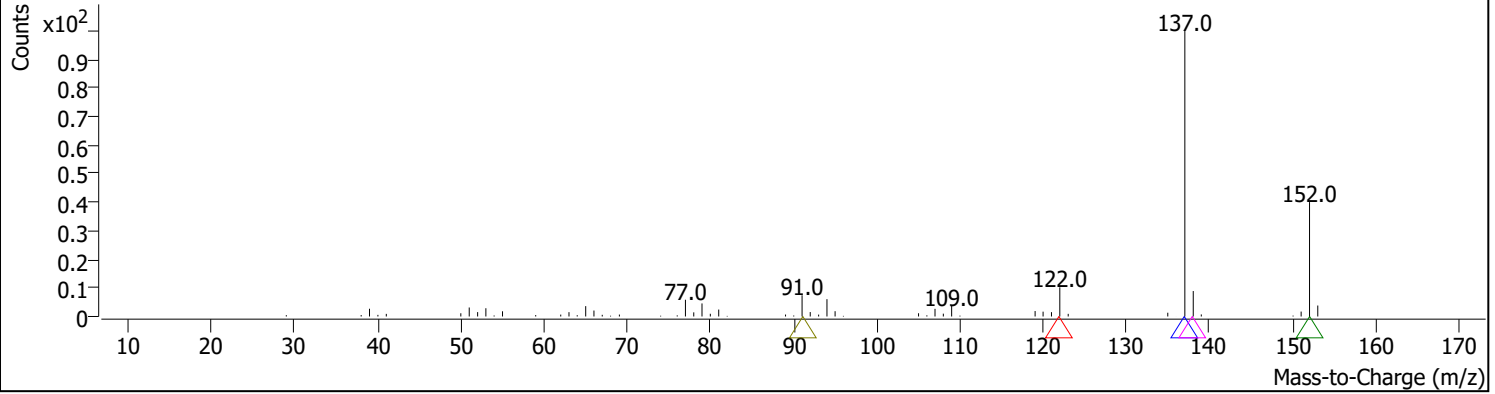
## Library Search Results - NonTarget Hits with Details



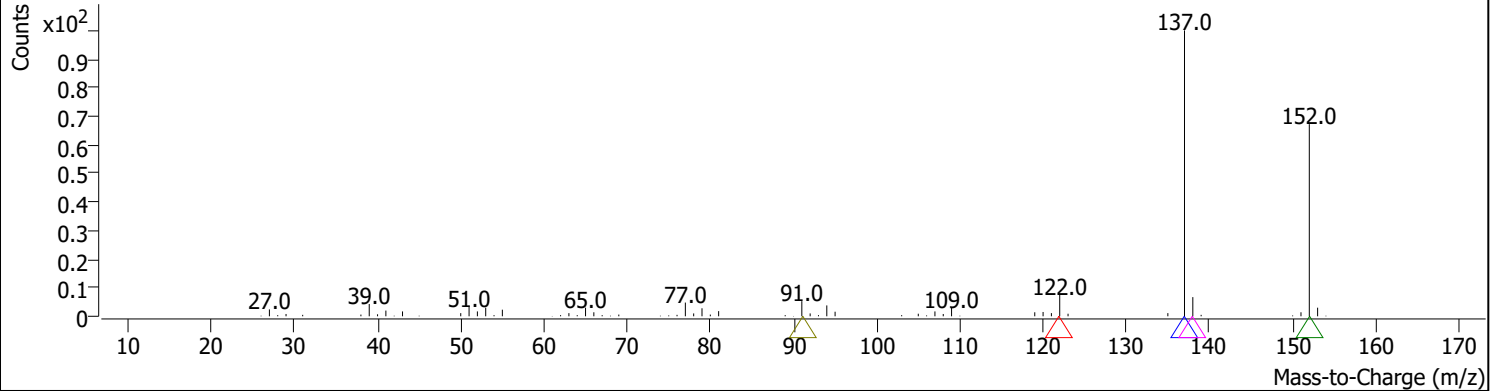
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
33.3274	Phenol, 4-ethyl-2-methoxy-	2832530.1	97.6	2785-89-9	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	

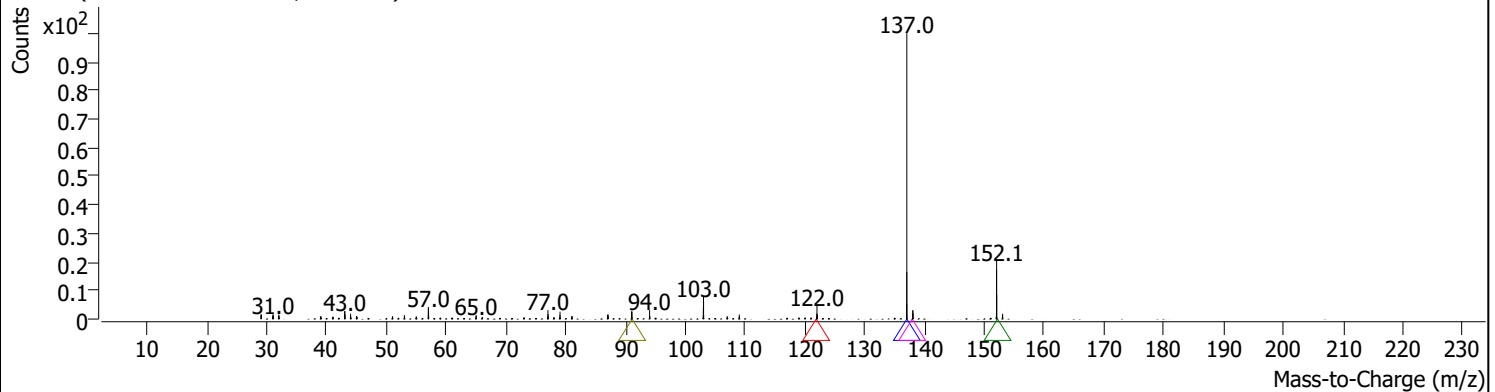
Component RT: 33.3274



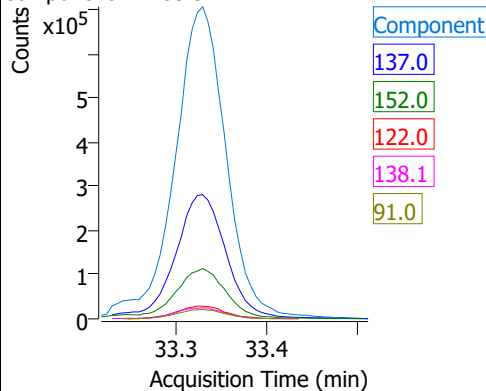
Phenol, 4-ethyl-2-methoxy- (NIST20.L)



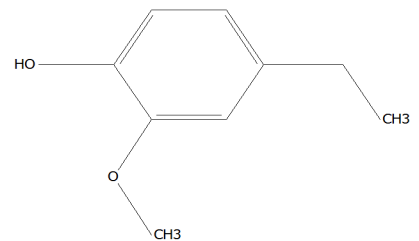
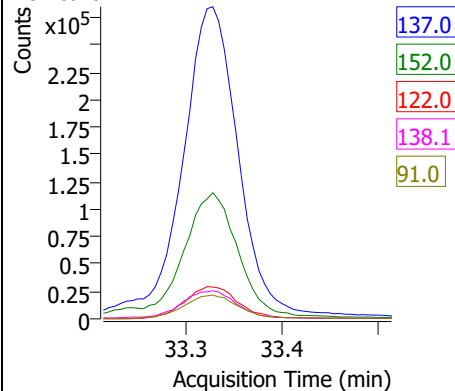
+ Scan (33.2157-33.5071 min, 50 scans) 1.D



Component RT: 33.3274



EIC Peaks



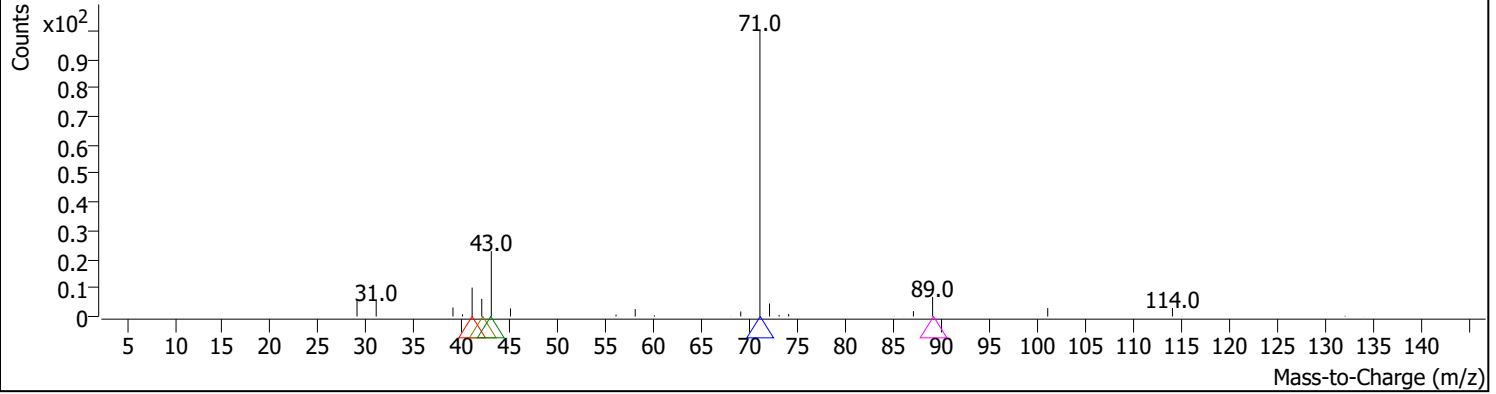
# Library Search Results - NonTarget Hits with Details



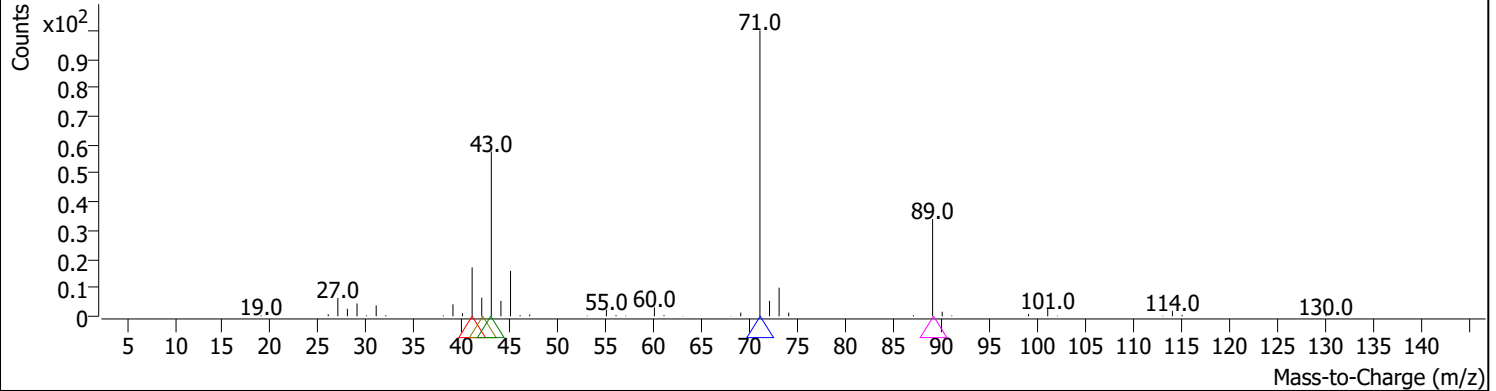
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
35.0048	Ethylene glycol Formate Isobutyrate	17452974.0	83.5	1000458-48-0	C7H12O4	

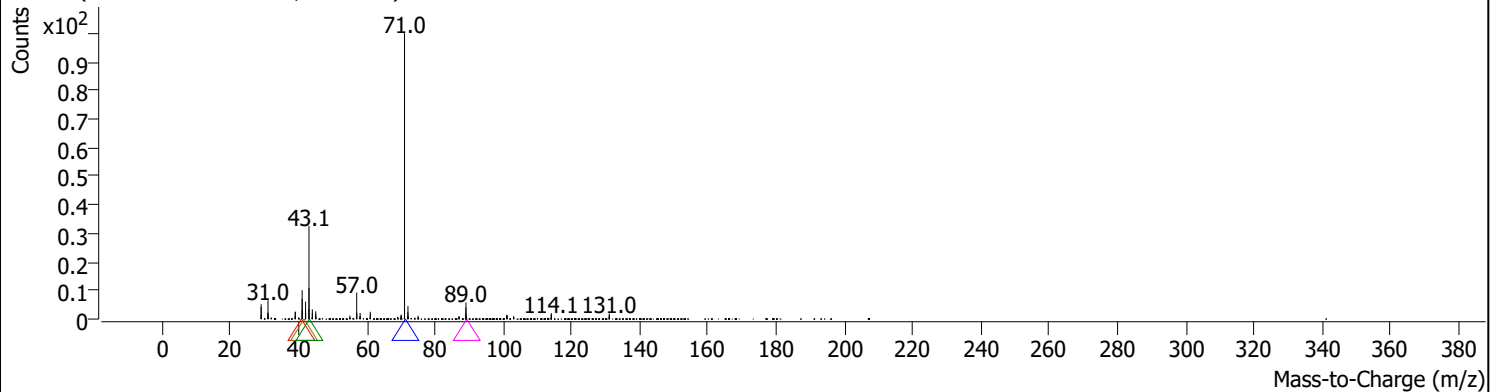
Component RT: 35.0048



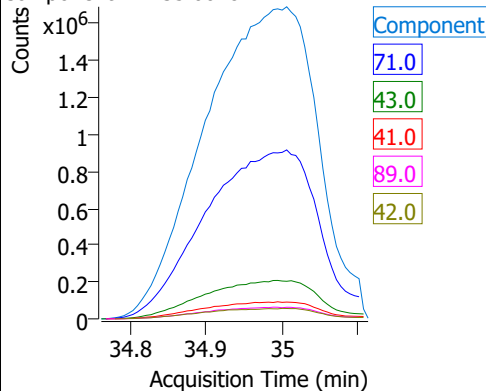
Ethylene glycol Formate Isobutyrate (NIST20.L)



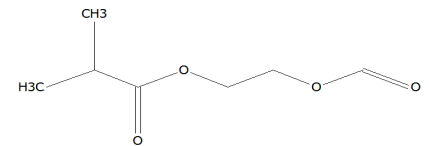
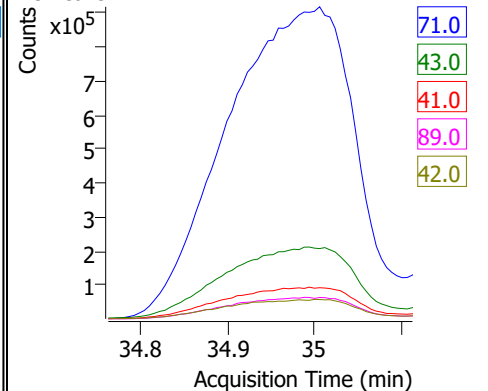
+ Scan (34.7677-35.1006 min, 57 scans) 1.D



Component RT: 35.0048



EIC Peaks



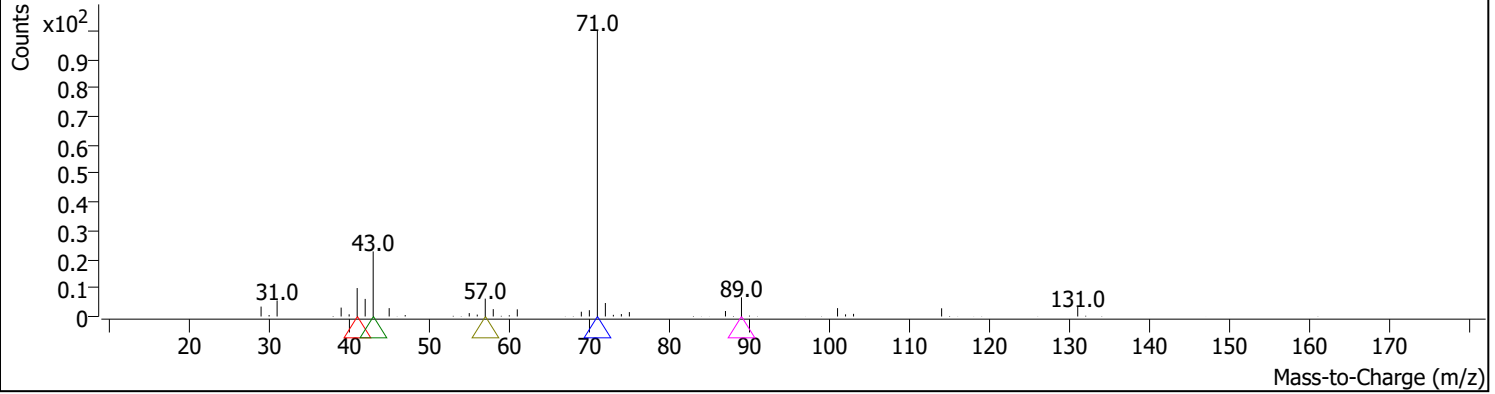
## Library Search Results - NonTarget Hits with Details



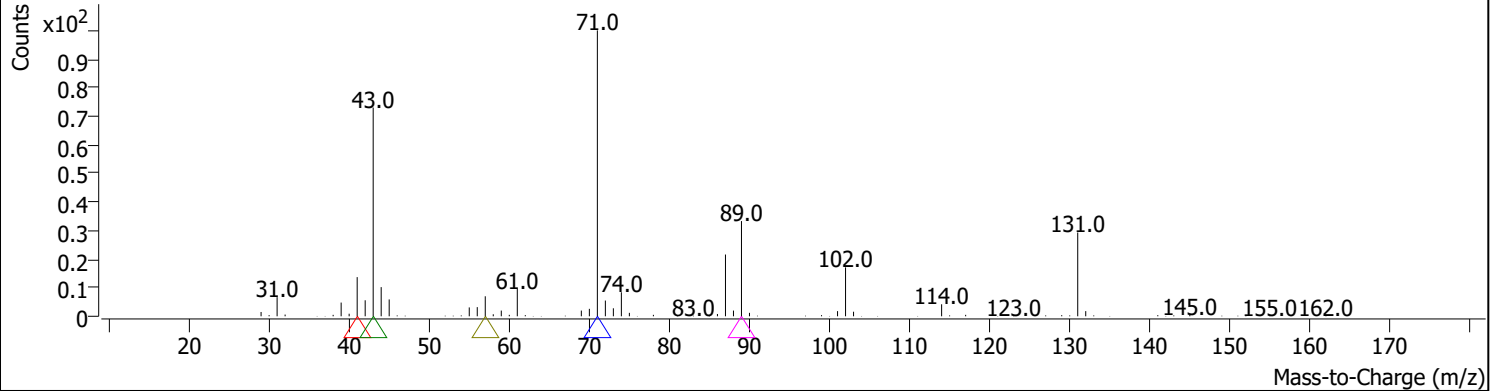
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
35.3071	2,3-dihydroxypropyl isobutyrate	17670321.0	79.5	1010458-45-6	C7H14O4	

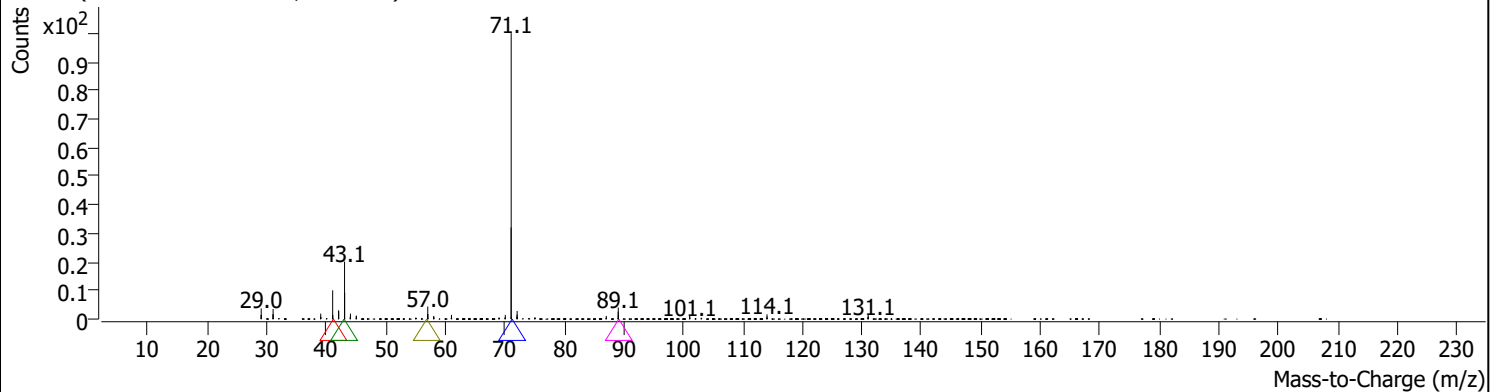
Component RT: 35.3071



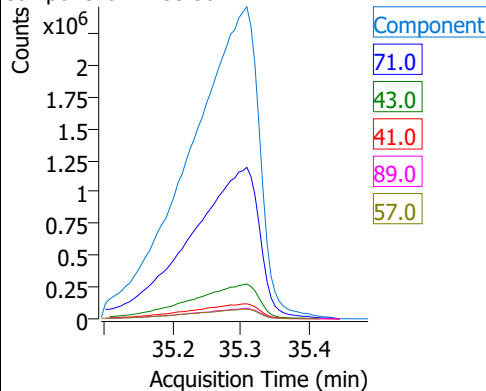
2,3-dihydroxypropyl isobutyrate (NIST20.L)



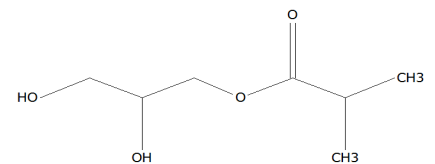
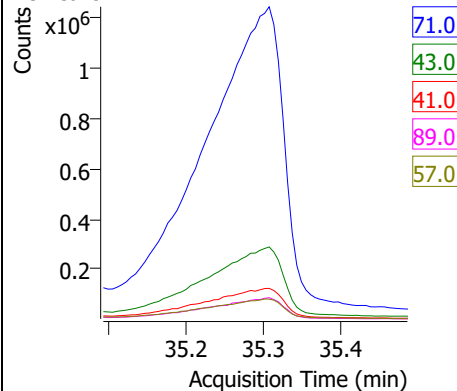
+ Scan (35.1006-35.4455 min, 59 scans) 1.D



Component RT: 35.3071



EIC Peaks



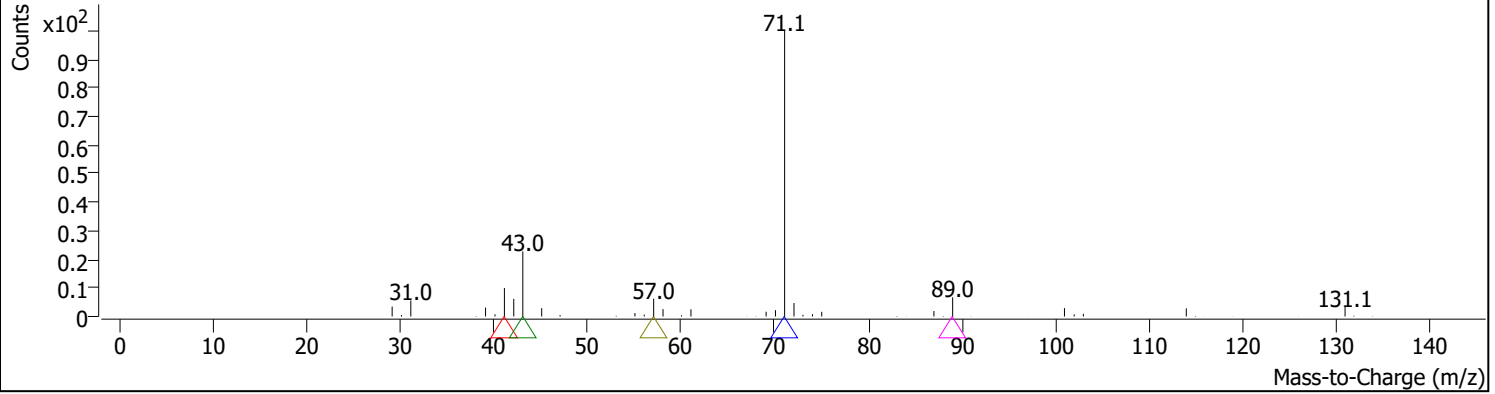
## Library Search Results - NonTarget Hits with Details



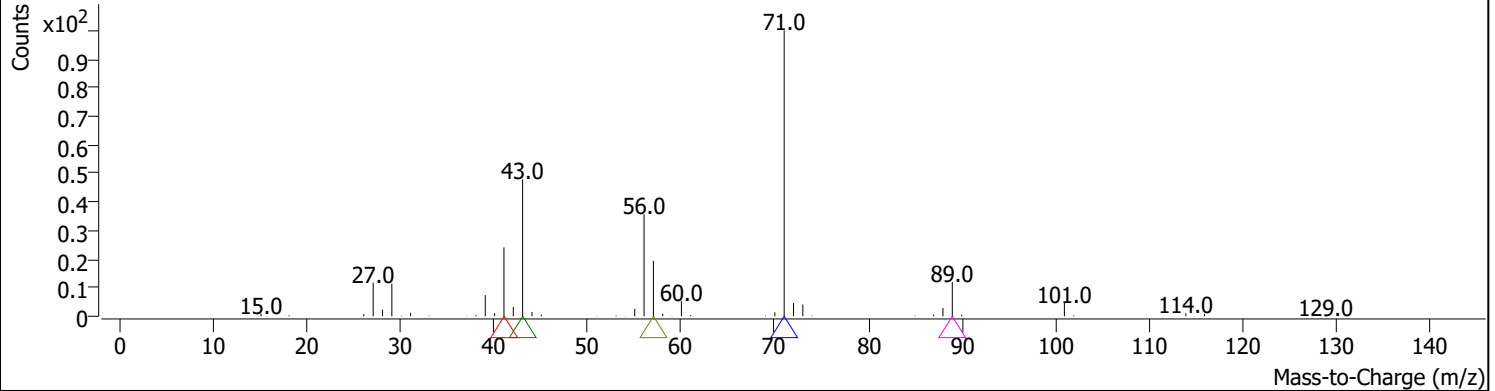
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
35.3074	Butanoic acid, 2-methylpropyl ester	17616193.8	78.2	539-90-2	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	

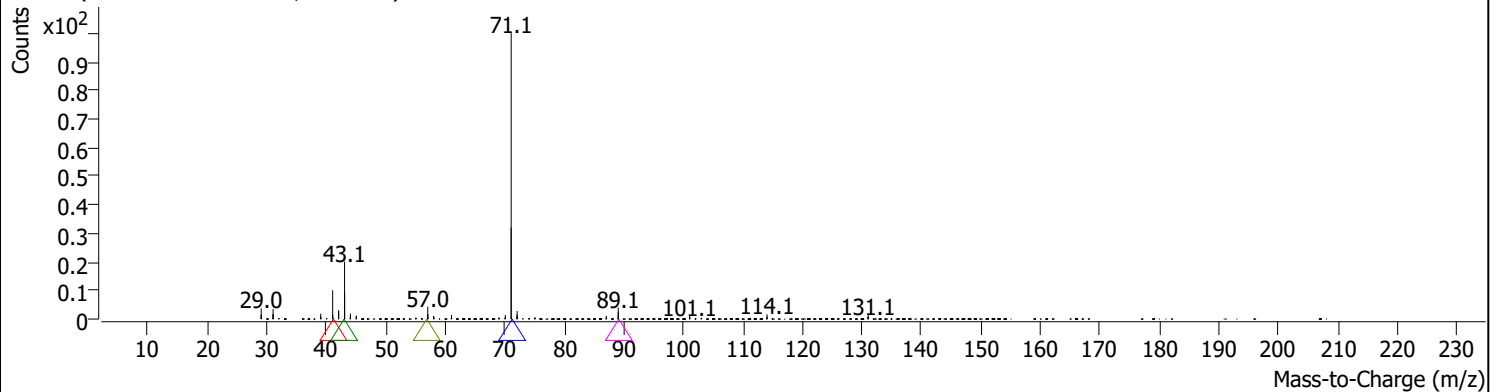
Component RT: 35.3074



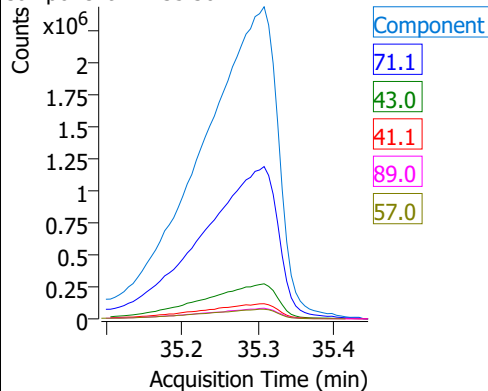
Butanoic acid, 2-methylpropyl ester (NIST20.L)



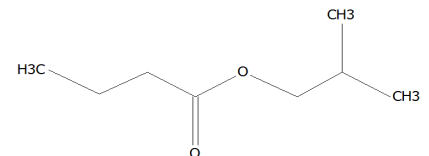
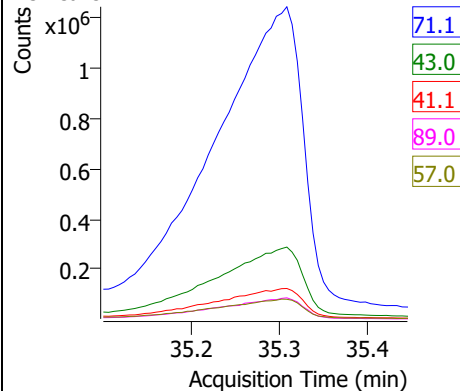
+ Scan (35.1006-35.4455 min, 59 scans) 1.D



Component RT: 35.3074



EIC Peaks



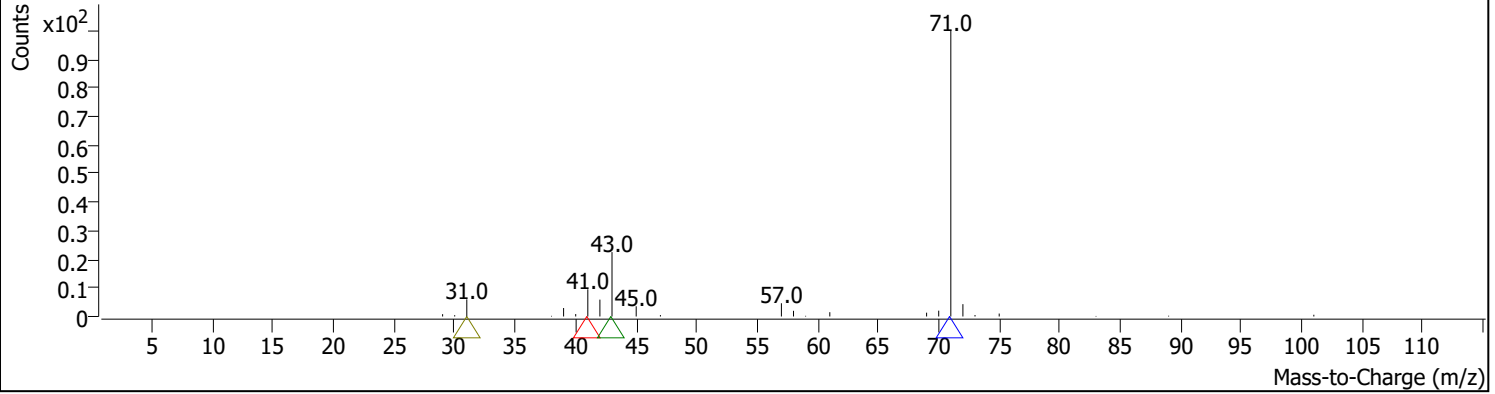
## Library Search Results - NonTarget Hits with Details



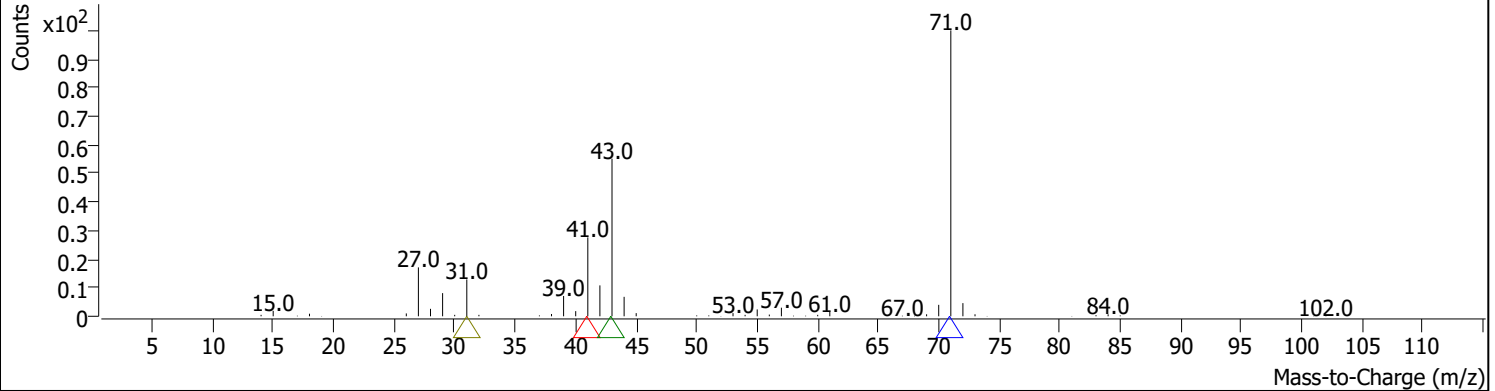
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
36.1579	2-Furanmethanol, tetrahydro-	4021958.6	82.2	97-99-4	C5H10O2	

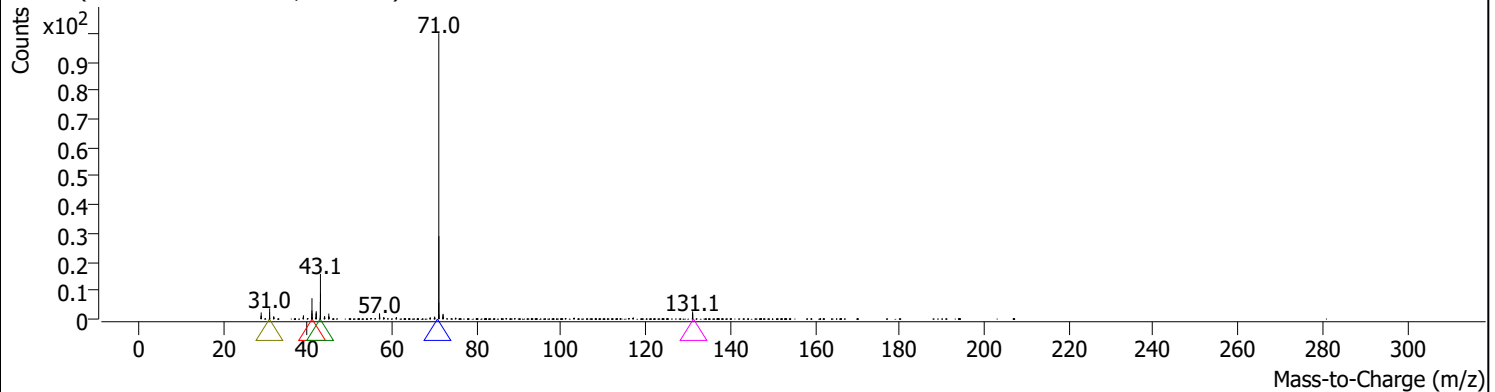
Component RT: 36.1579



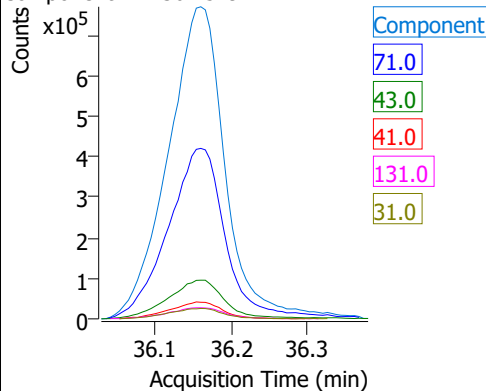
2-Furanmethanol, tetrahydro- (NIST20.L)



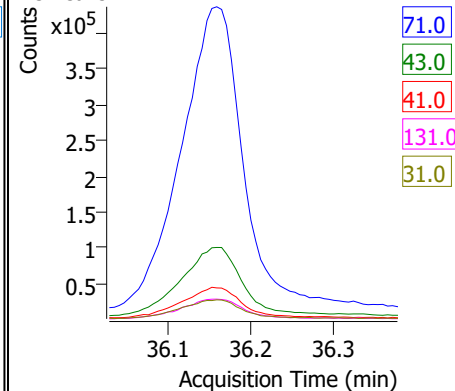
+ Scan (36.0342-36.3672 min, 57 scans) 1.D



Component RT: 36.1579



EIC Peaks



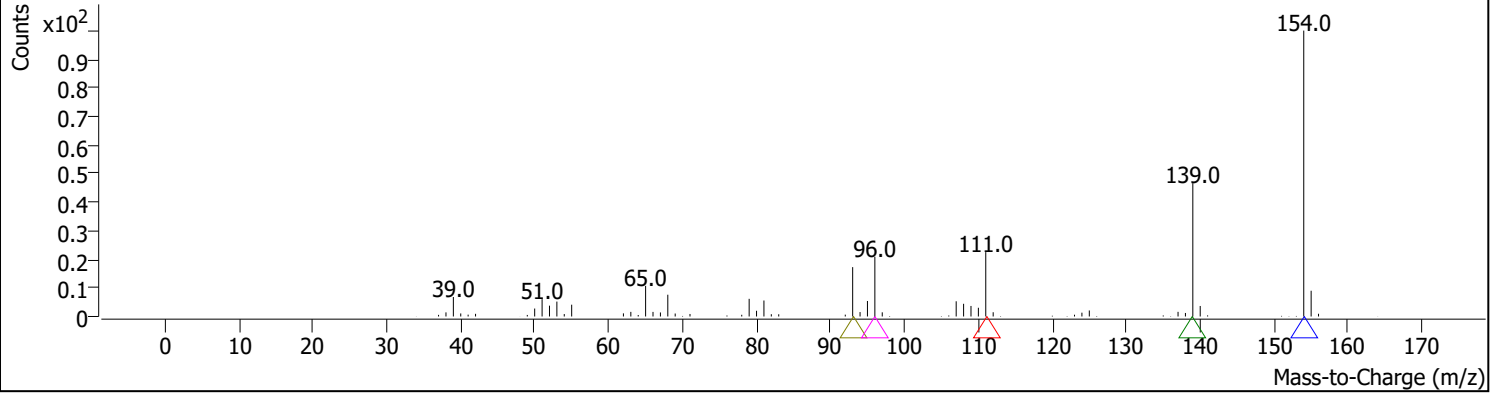
## Library Search Results - NonTarget Hits with Details



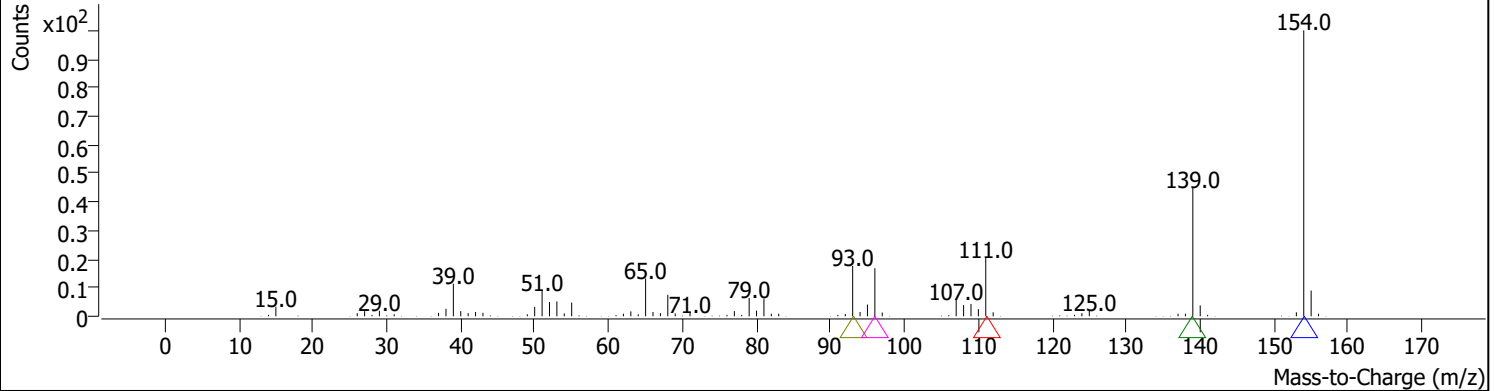
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
36.7946	Phenol, 2,6-dimethoxy-	16652182.6	97.9	91-10-1	C8H10O3	

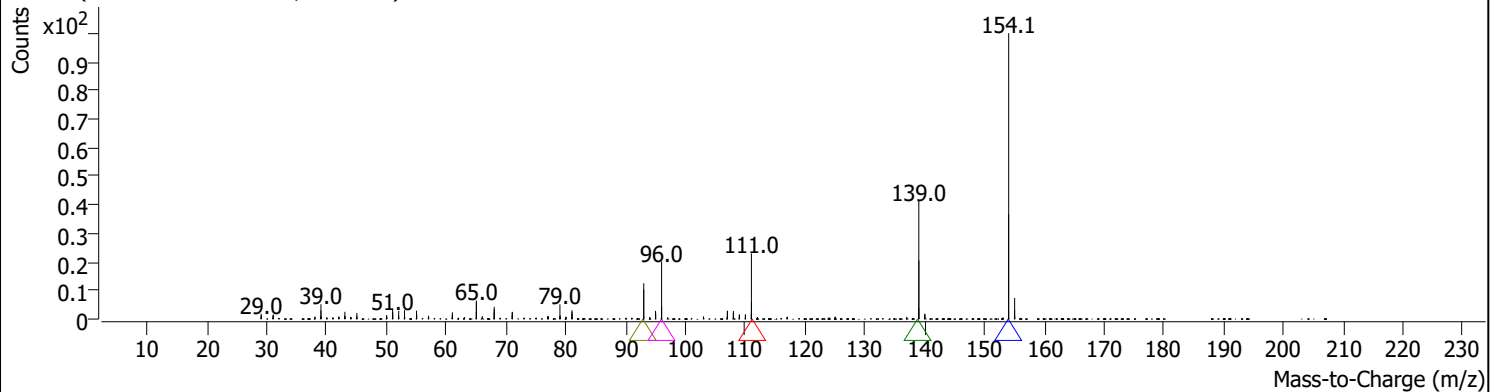
Component RT: 36.7946



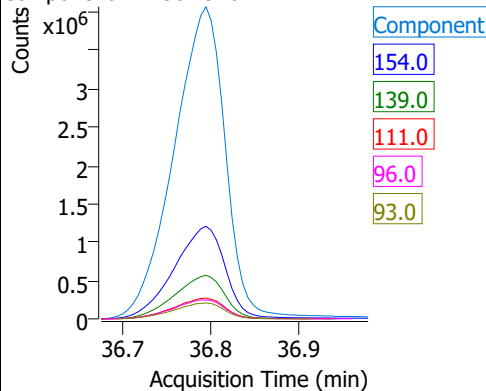
Phenol, 2,6-dimethoxy- (NIST20.L)



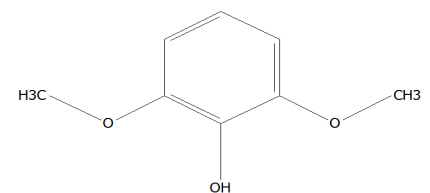
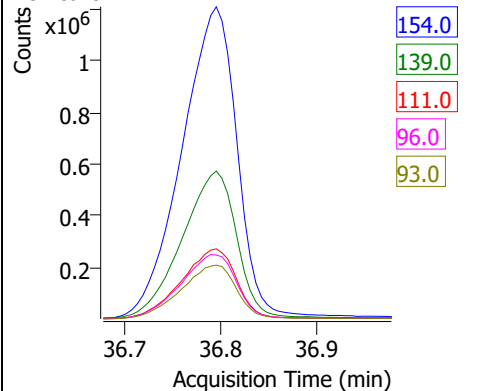
+ Scan (36.6724-36.9796 min, 52 scans) 1.D



Component RT: 36.7946



EIC Peaks





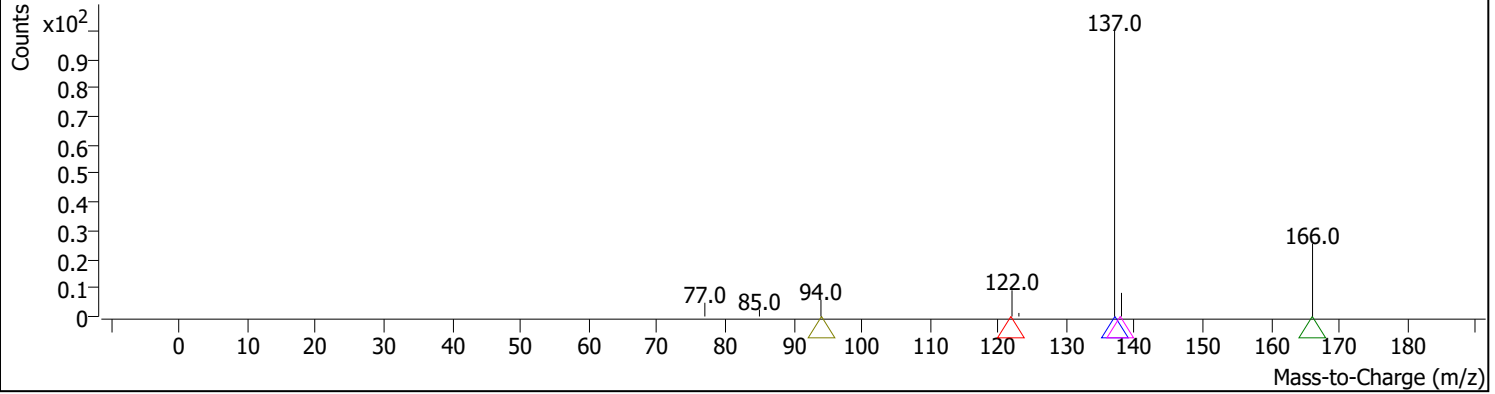
## Library Search Results - NonTarget Hits with Details



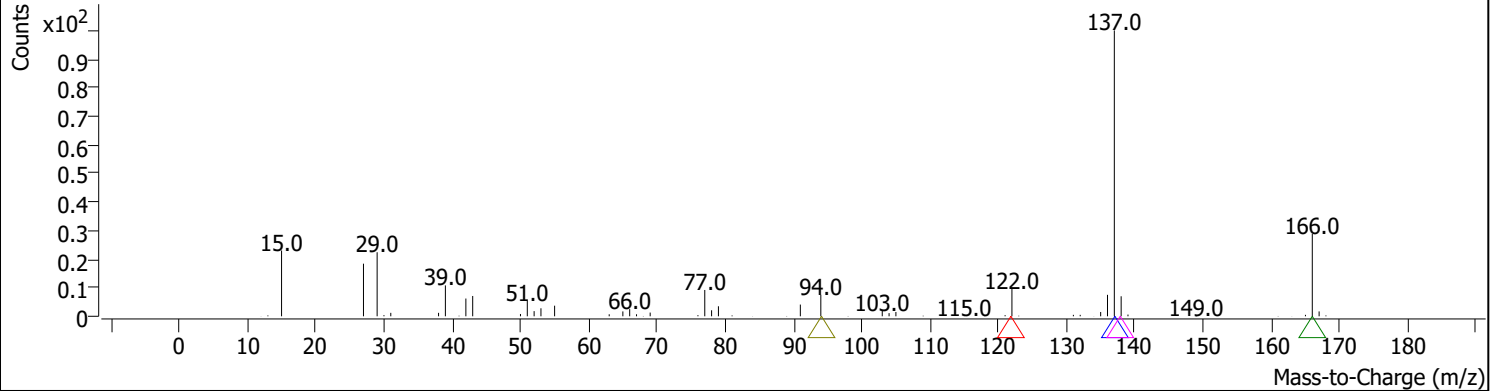
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
37.4113	Phenol, 2-methoxy-4-propyl-	240330.3	80.4	2785-87-7	C10H14O2	

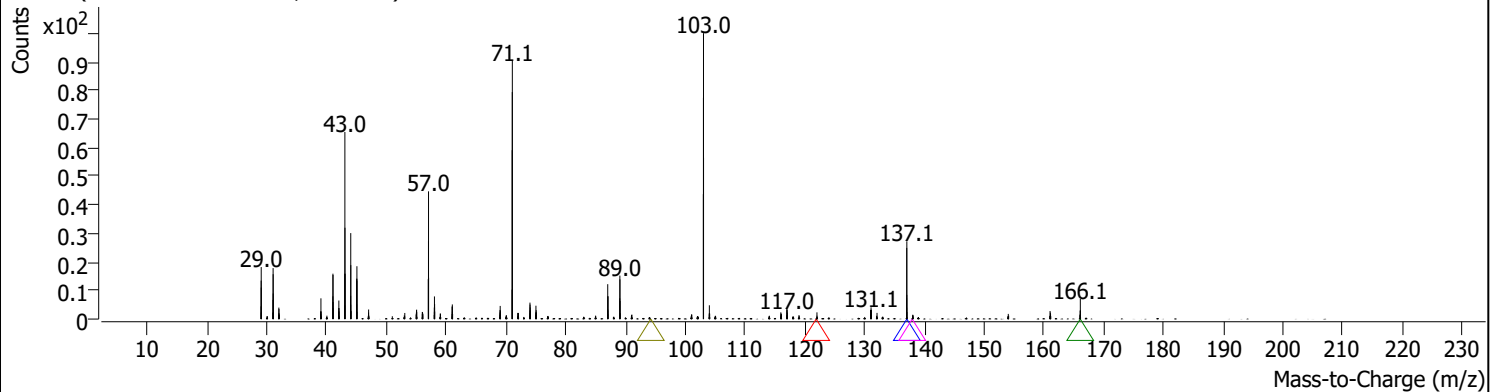
Component RT: 37.4113



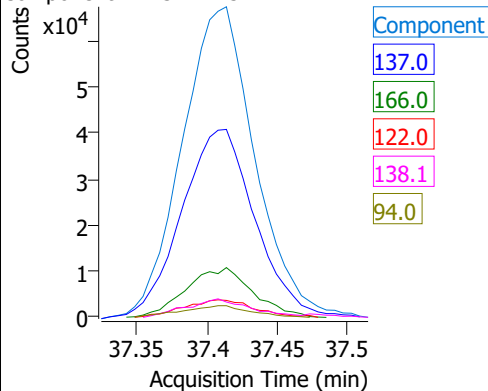
Phenol, 2-methoxy-4-propyl- (NIST20.L)



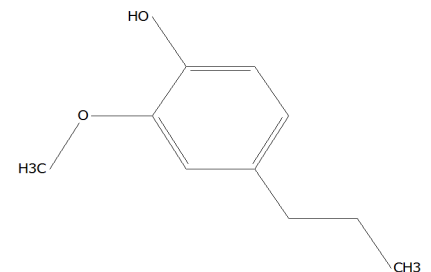
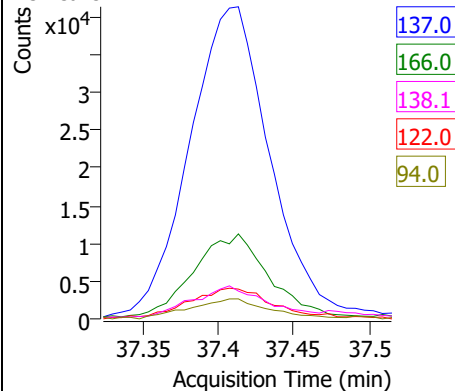
+ Scan (37.3380-37.4850 min, 25 scans) 1.D



Component RT: 37.4113



EIC Peaks



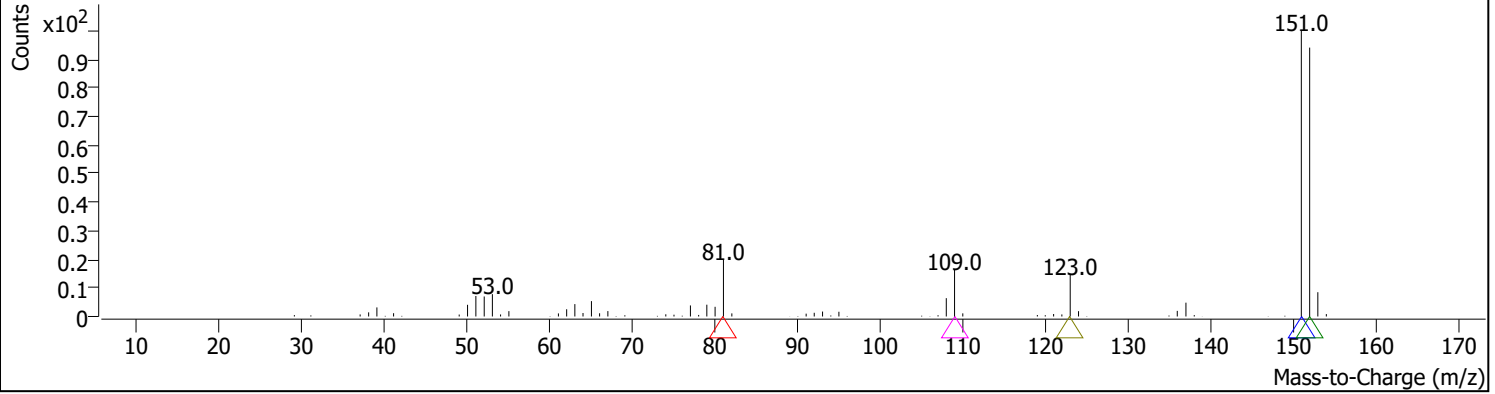
## Library Search Results - NonTarget Hits with Details



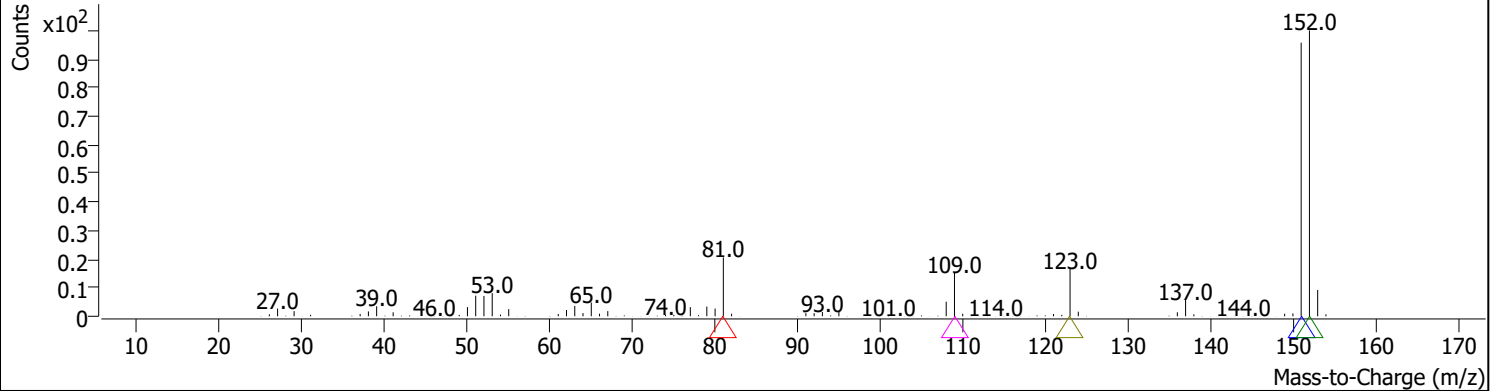
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
38.9840	Vanillin	9553029.9	99.0	121-33-5	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	

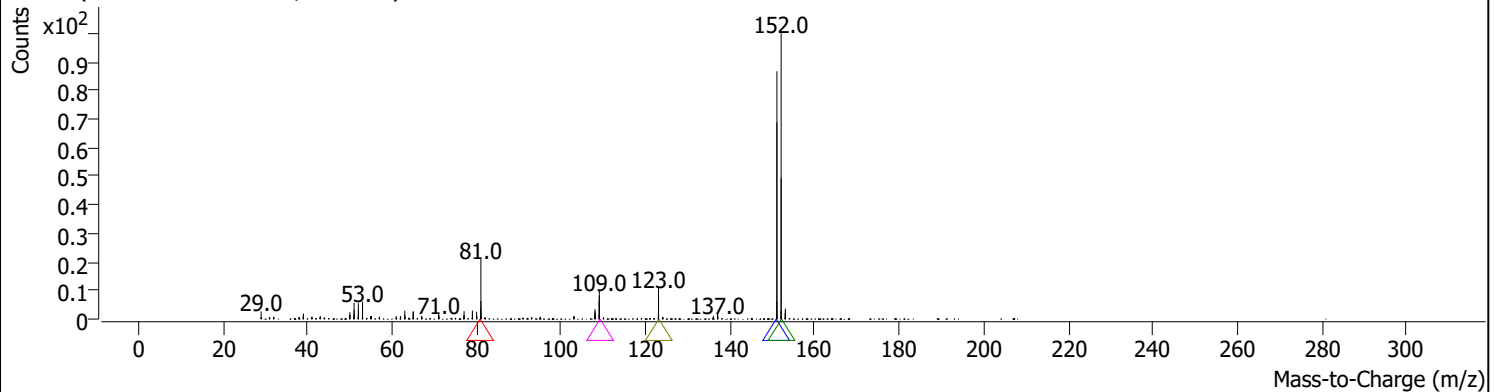
Component RT: 38.9840



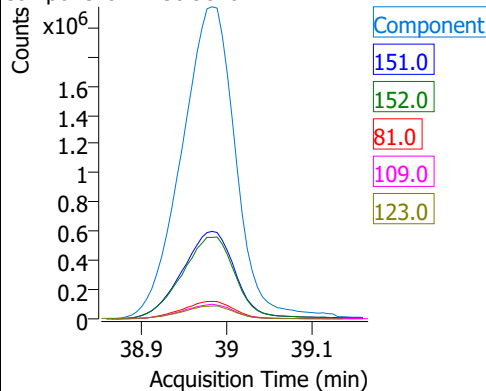
Vanillin (NIST20.L)



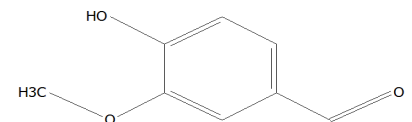
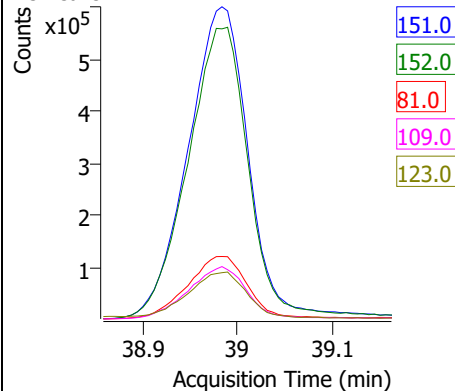
+ Scan (38.8585-39.1261 min, 46 scans) 1.D



Component RT: 38.9840



EIC Peaks



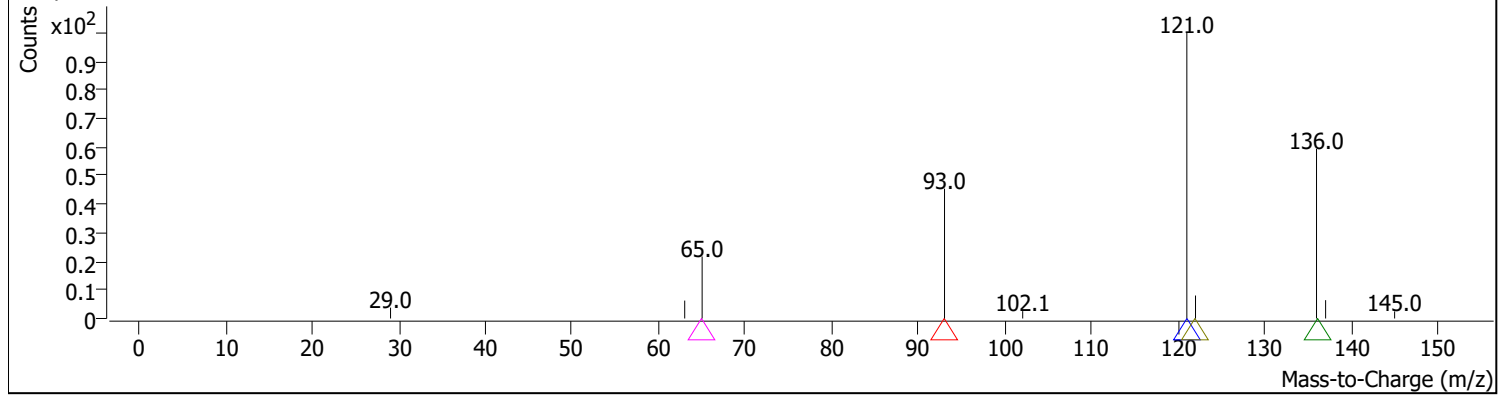
## Library Search Results - NonTarget Hits with Details



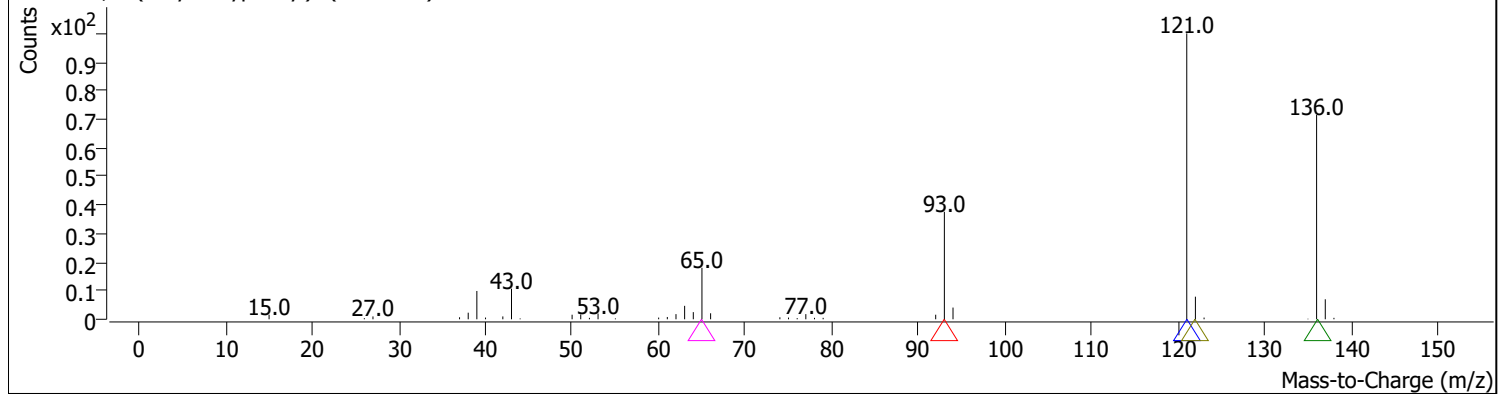
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
39.4888	Ethanone, 1-(3-hydroxyphenyl)-	227800.9	89.7	121-71-1	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	

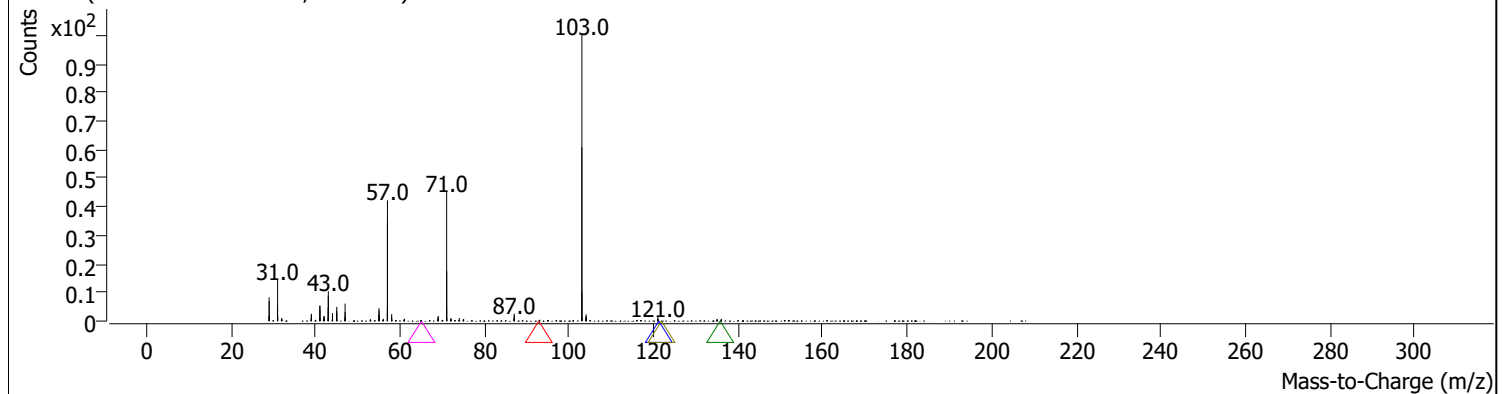
Component RT: 39.4888



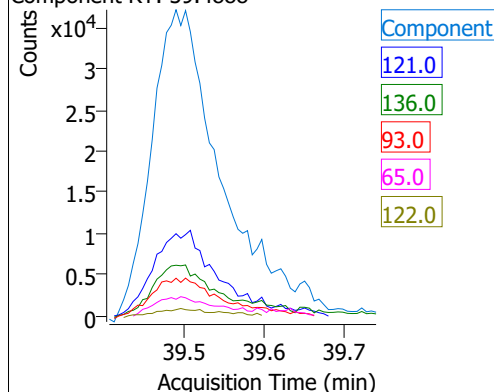
Ethanone, 1-(3-hydroxyphenyl)- (NIST20.L)



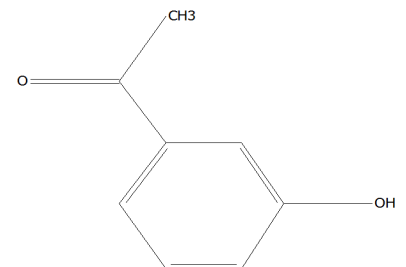
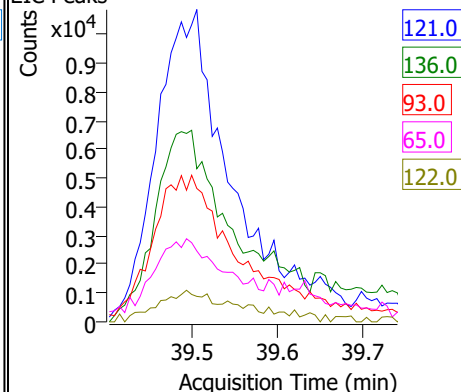
+ Scan (39.4077-39.6791 min, 46 scans) 1.D



Component RT: 39.4888



EIC Peaks



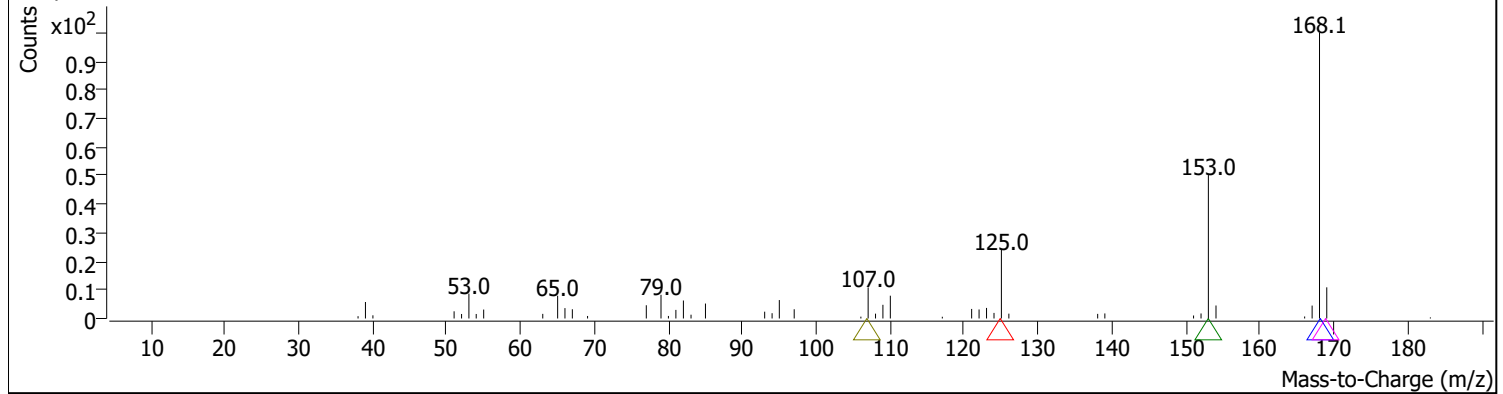
## Library Search Results - NonTarget Hits with Details



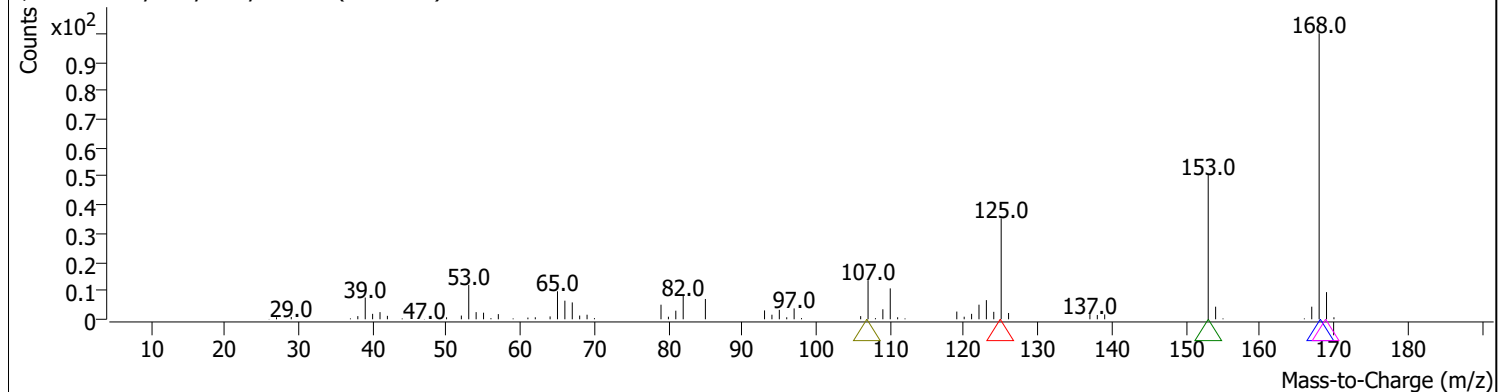
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
40.8720	3,5-Dimethoxy-4-hydroxytoluene	776796.4	92.5	6638-05-7	C9H12O3	

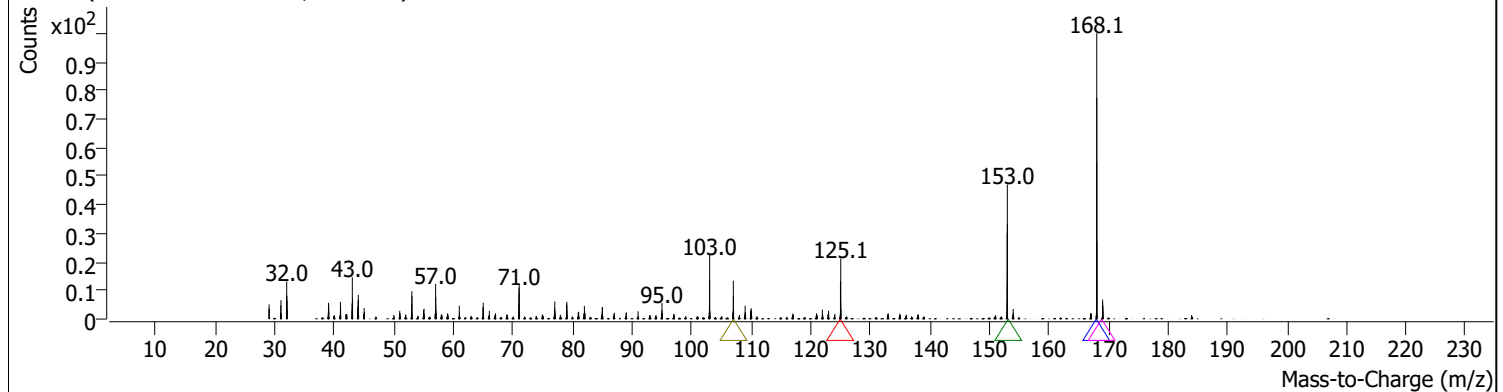
Component RT: 40.8720



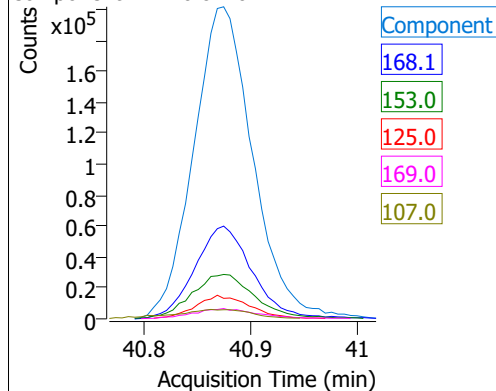
3,5-Dimethoxy-4-hydroxytoluene (NIST20.L)



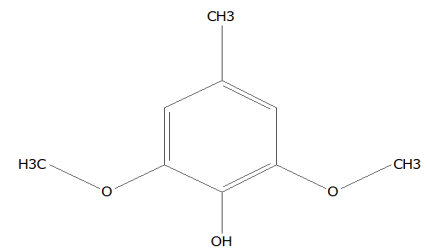
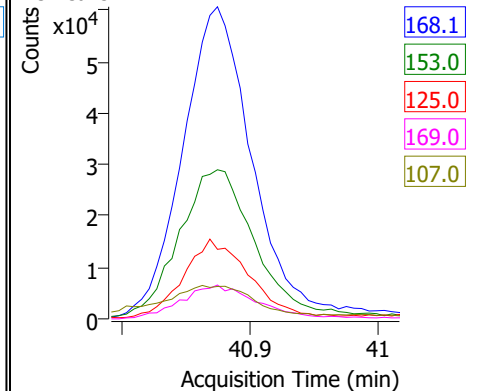
+ Scan (40.7968-41.0170 min, 38 scans) 1.D



Component RT: 40.8720



EIC Peaks



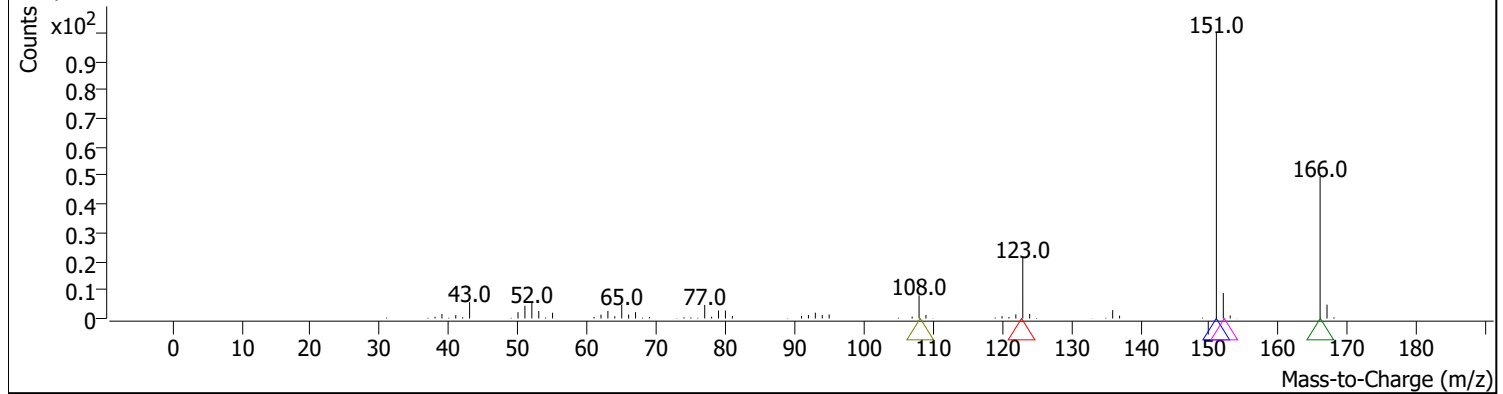
## Library Search Results - NonTarget Hits with Details



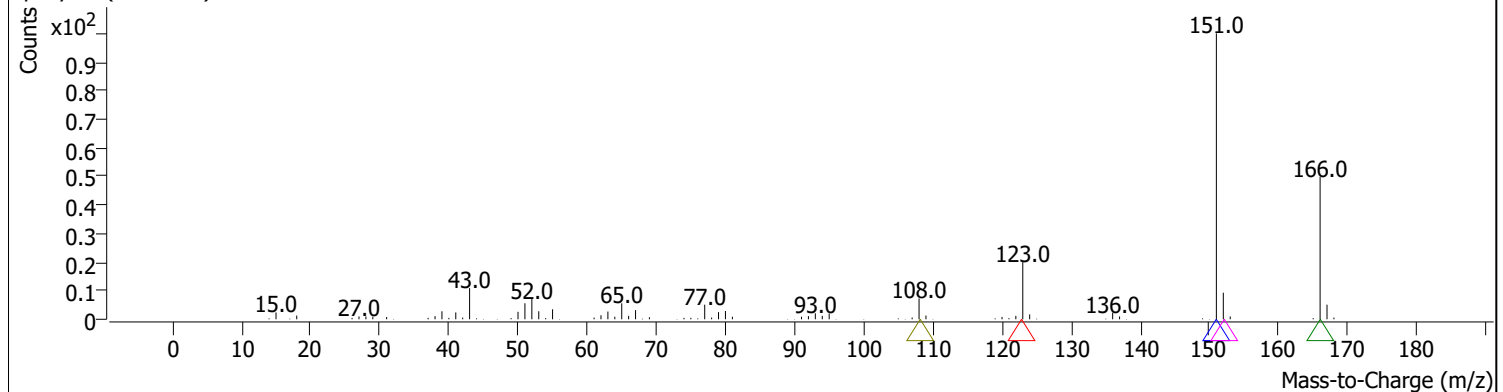
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
42.5978	Apocynin	5395989.4	99.2	498-02-2	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	

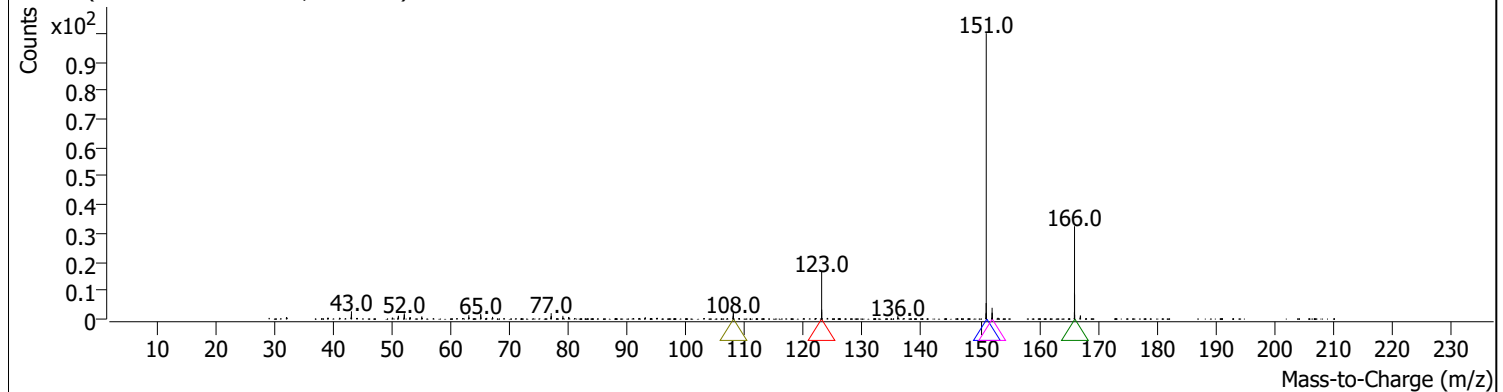
Component RT: 42.5978



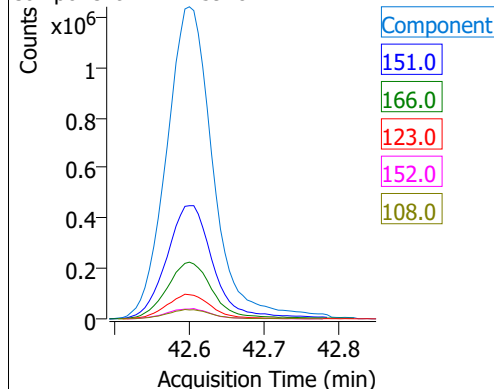
Apocynin (NIST20.L)



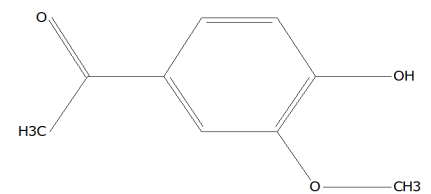
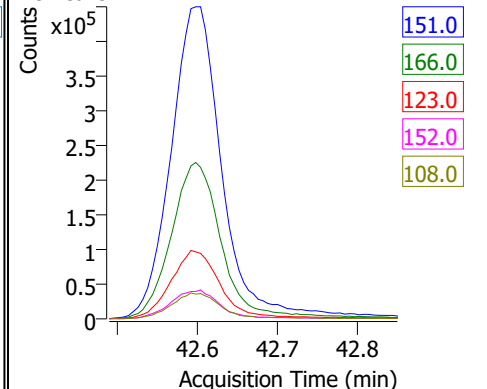
+ Scan (42.4916-42.8186 min, 56 scans) 1.D



Component RT: 42.5978



EIC Peaks



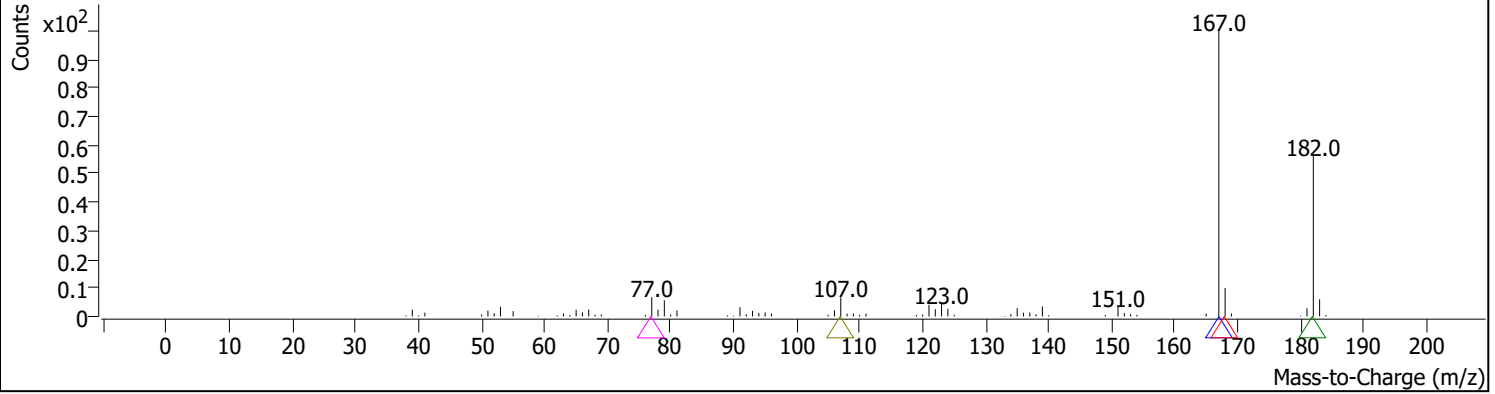
## Library Search Results - NonTarget Hits with Details



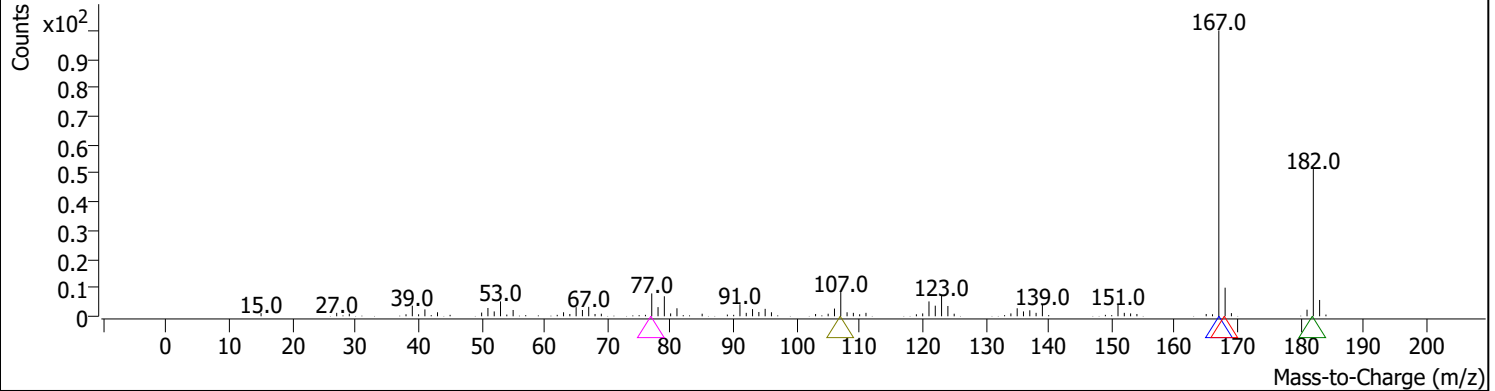
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
44.0450	4-Ethyl-2,6-dimethoxyphenol	2188782.0	97.5	14059-92-8	C <sub>10</sub> H <sub>14</sub> O <sub>3</sub>	

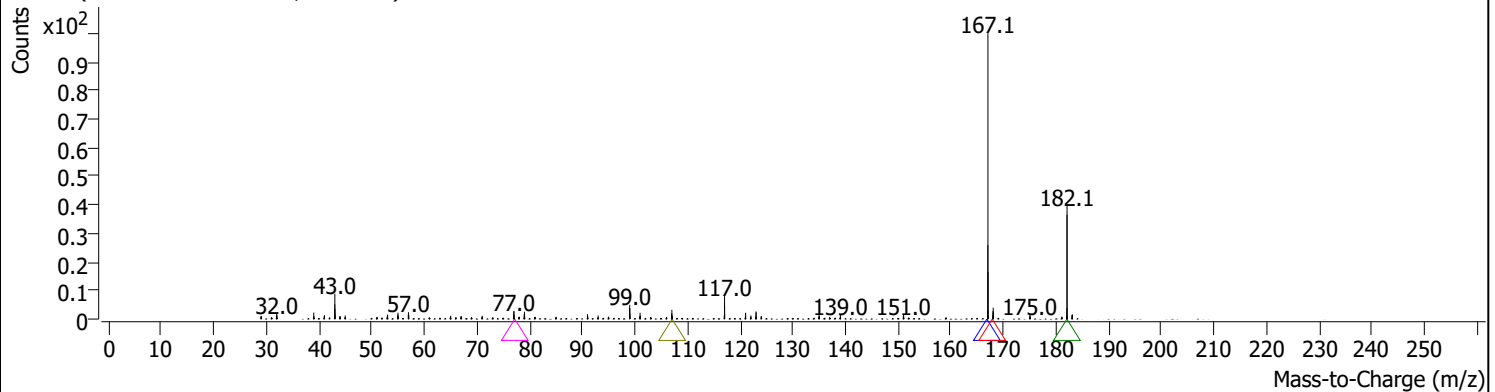
Component RT: 44.0450



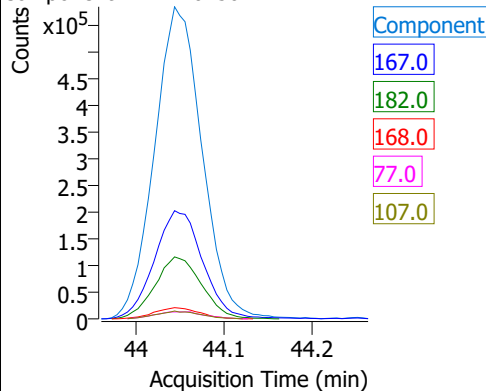
4-Ethyl-2,6-dimethoxyphenol (NIST20.L)



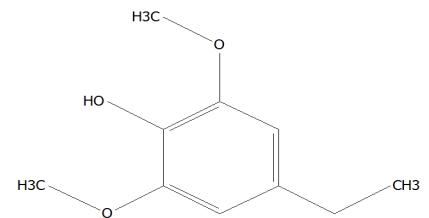
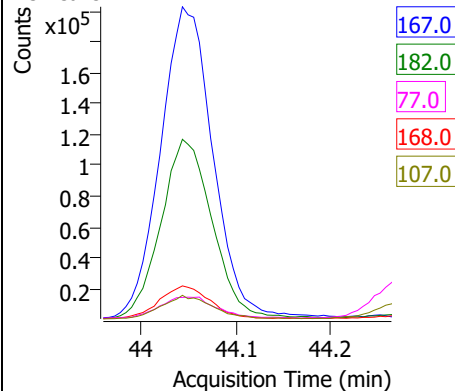
+ Scan (43.9703-44.1624 min, 33 scans) 1.D



Component RT: 44.0450



EIC Peaks



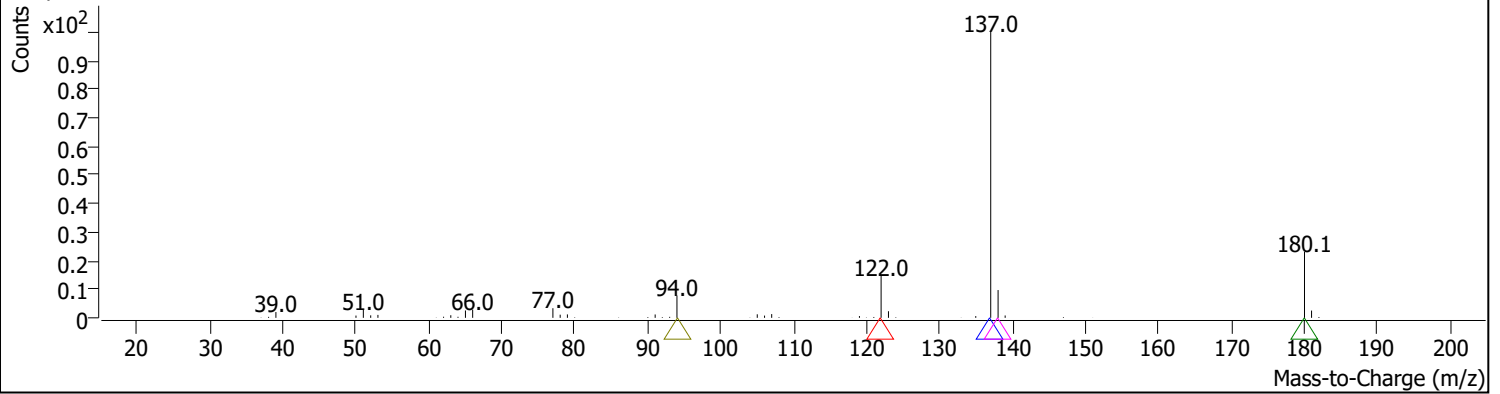
## Library Search Results - NonTarget Hits with Details



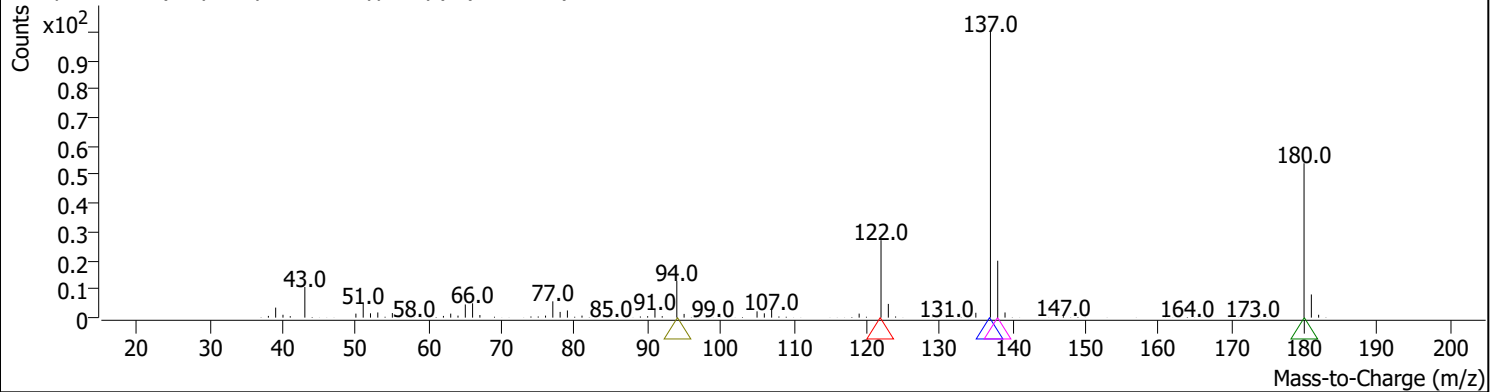
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
44.2850	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	7255885.9	93.9	2503-46-0	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	

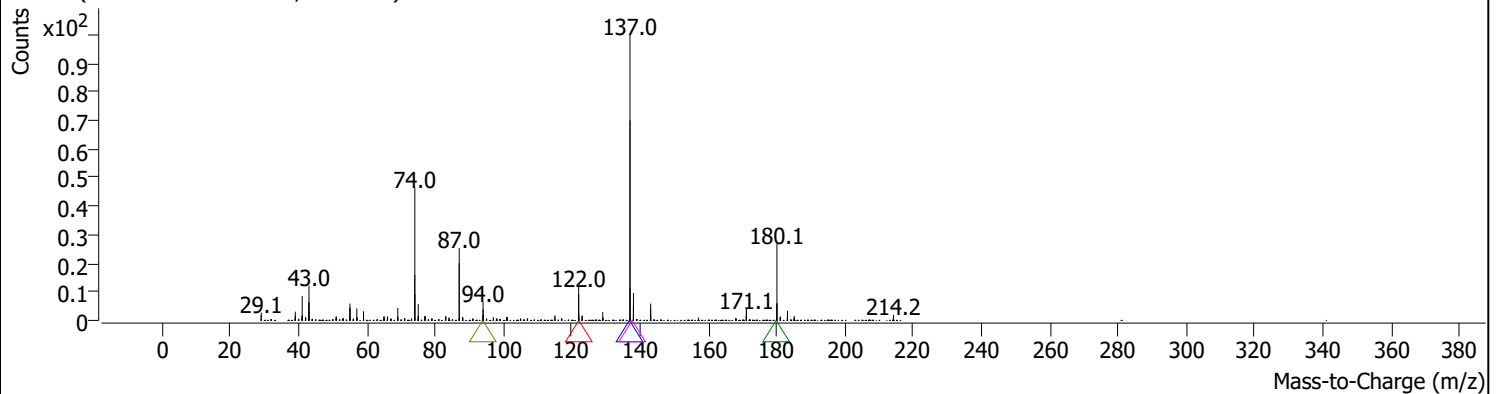
Component RT: 44.2850



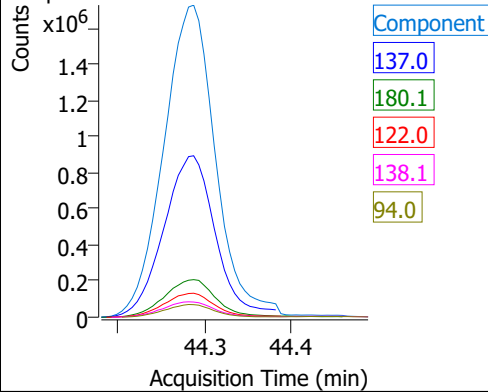
2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L)



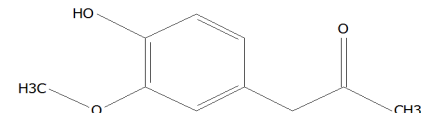
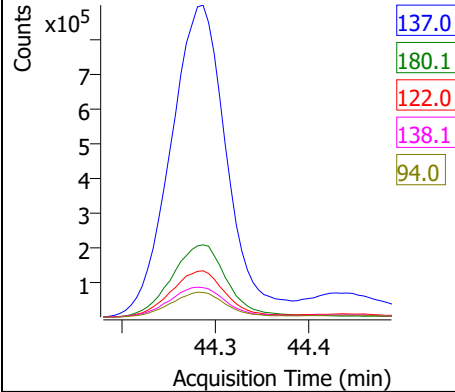
+ Scan (44.1803-44.4597 min, 48 scans) 1.D



Component RT: 44.2850



EIC Peaks



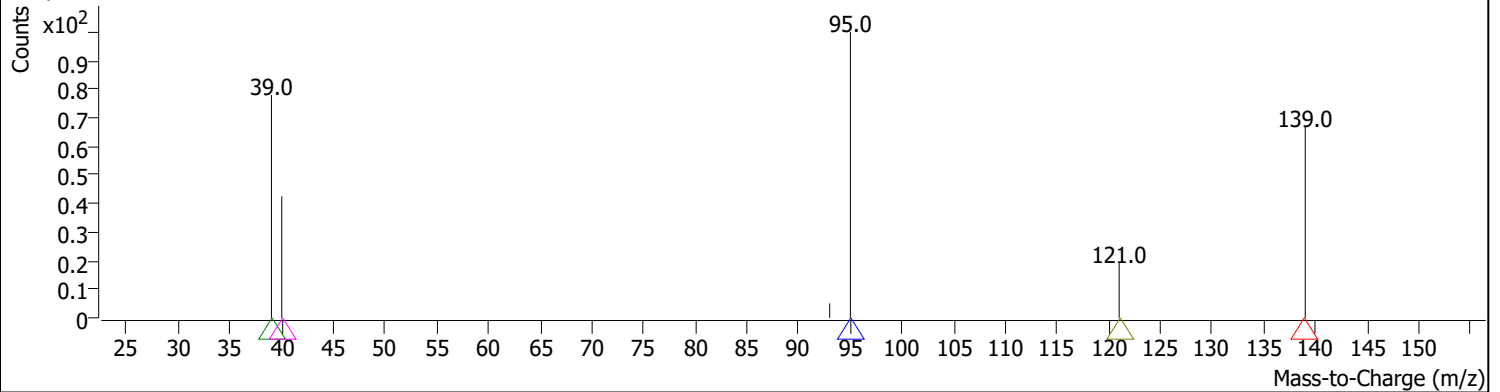
## Library Search Results - NonTarget Hits with Details



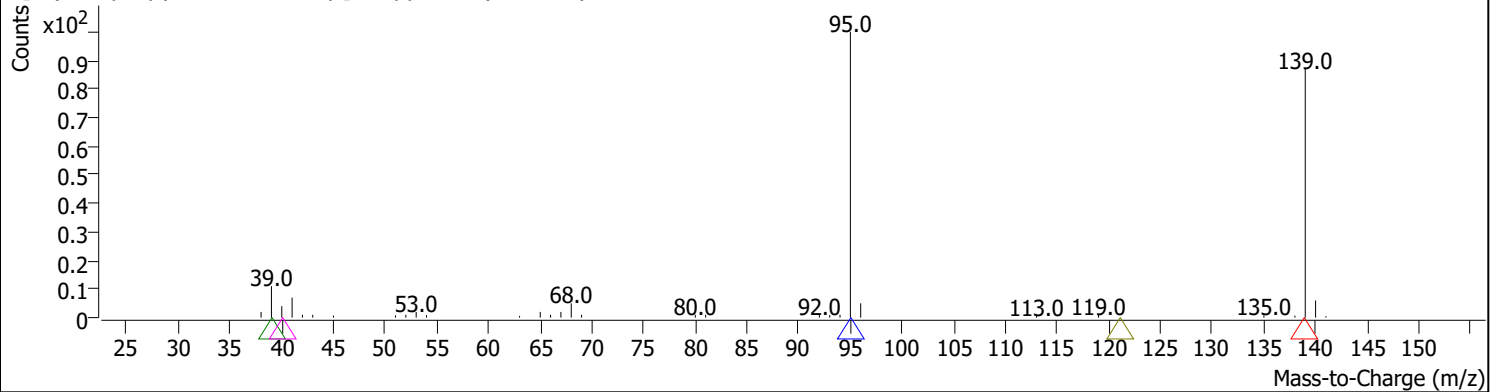
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
44.2924	4-[2-(2-Propenyl)-1,3-dioxolan-2-yl]-1H-pyrazole	329057.9	75.7	98816-47-8	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	

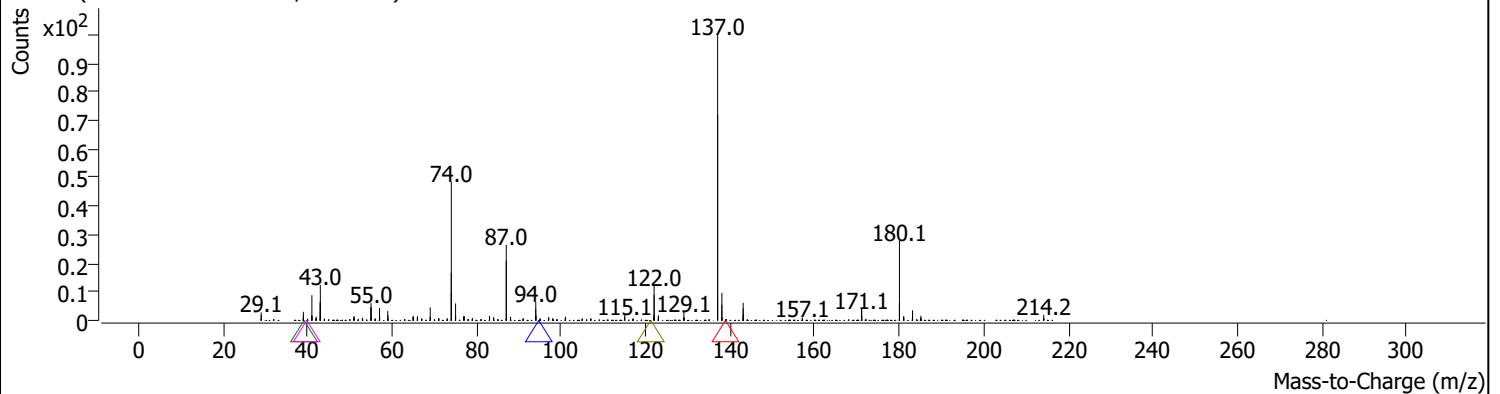
Component RT: 44.2924



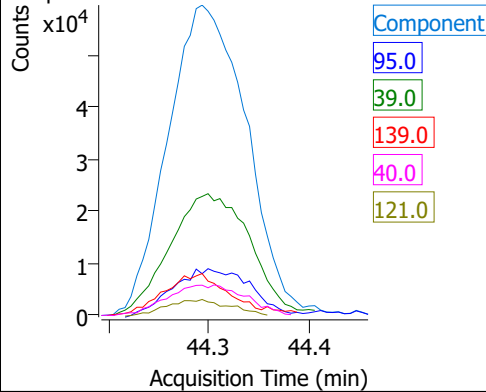
4-[2-(2-Propenyl)-1,3-dioxolan-2-yl]-1H-pyrazole (NIST20.L)



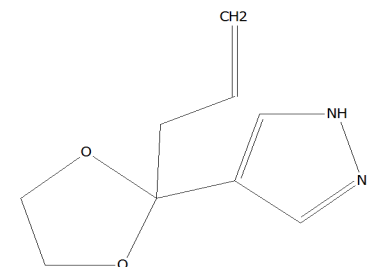
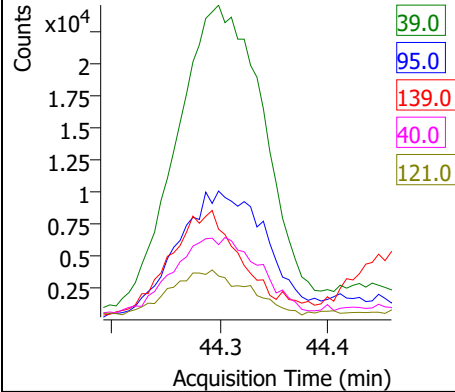
+ Scan (44.2040-44.4062 min, 35 scans) 1.D



Component RT: 44.2924



EIC Peaks





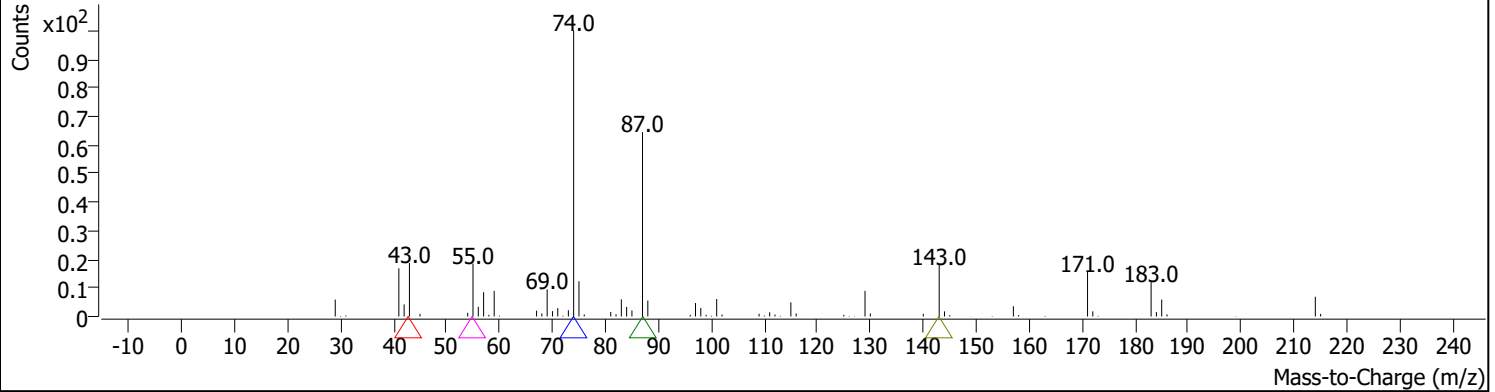
## Library Search Results - NonTarget Hits with Details



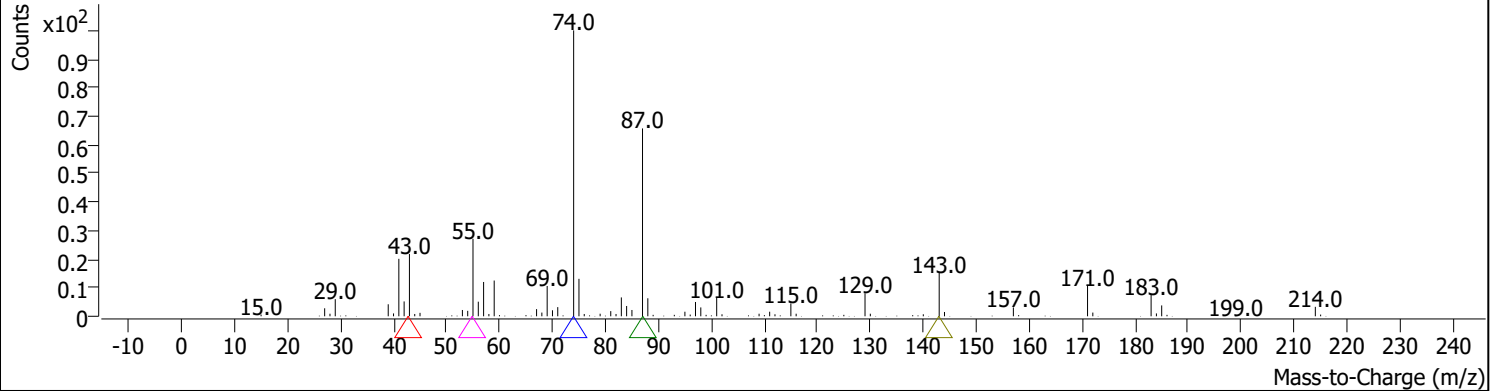
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
44.3268	Dodecanoic acid, methyl ester	6825508.8	94.9	111-82-0	C13H26O2	

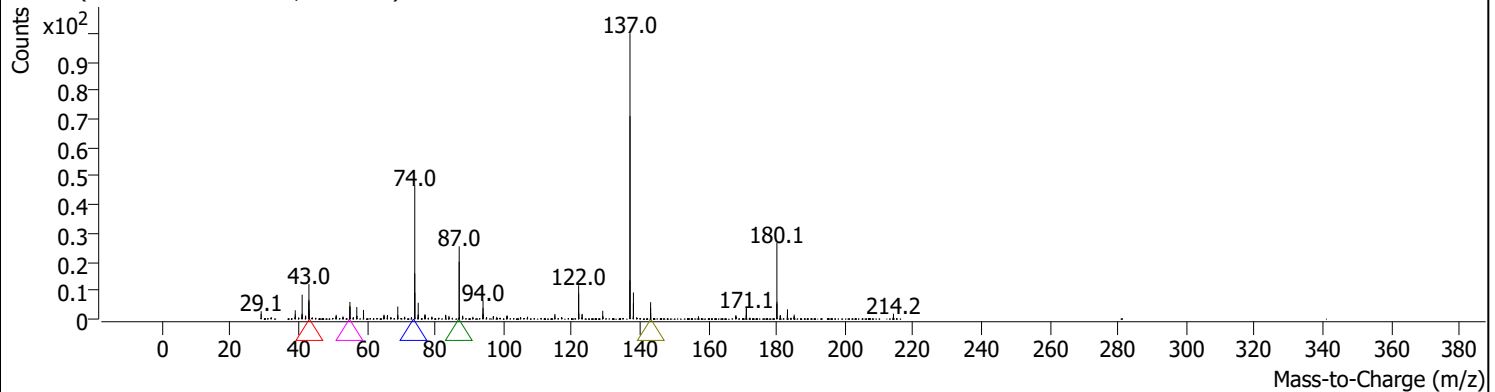
Component RT: 44.3268



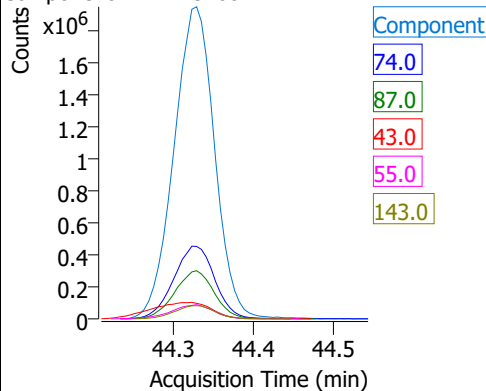
Dodecanoic acid, methyl ester (NIST20.L)



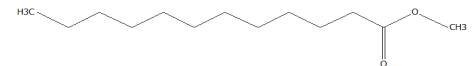
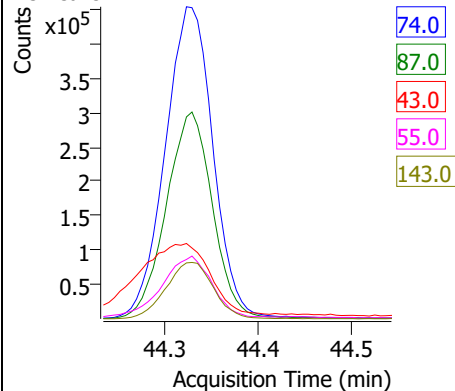
+ Scan (44.2338-44.5430 min, 53 scans) 1.D



Component RT: 44.3268



EIC Peaks



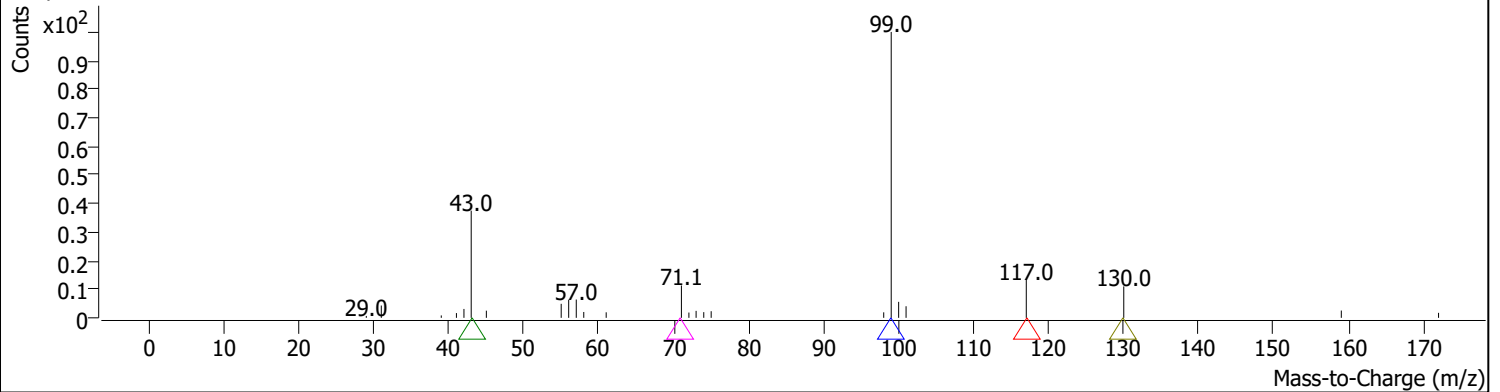
## Library Search Results - NonTarget Hits with Details



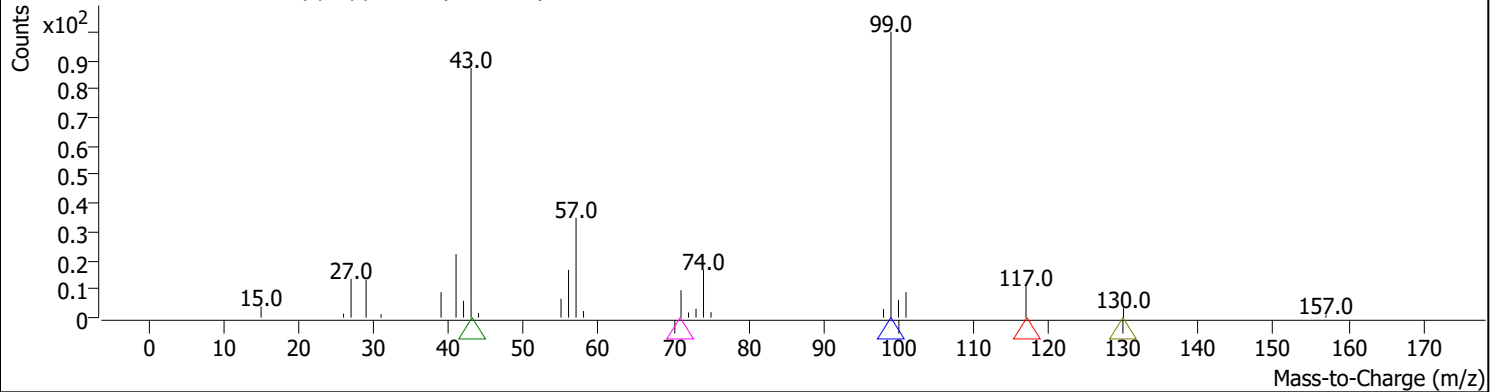
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
45.6164	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	991790.5	85.1	3757-32-2	C9H16O3	

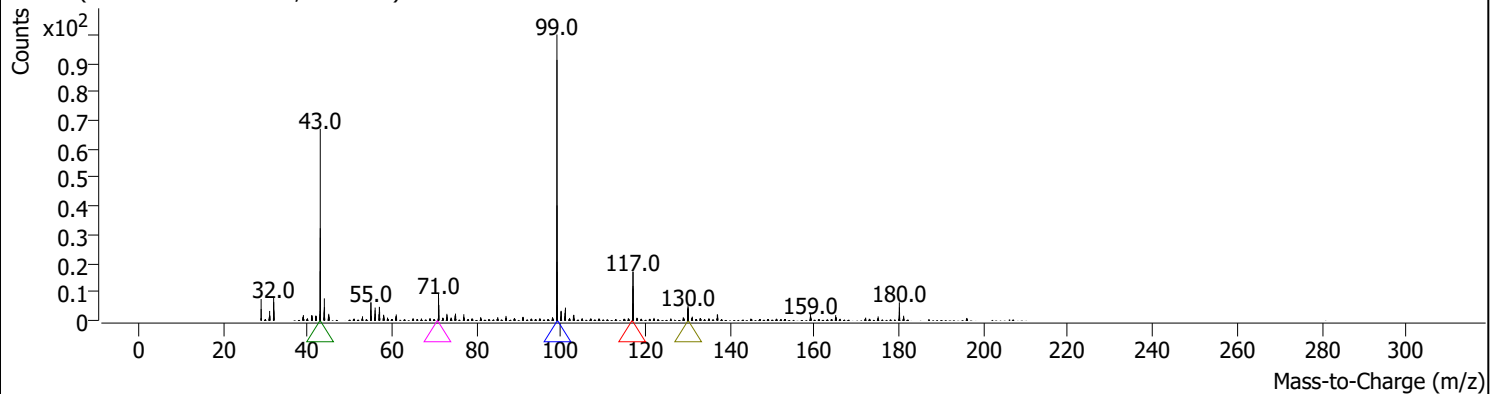
Component RT: 45.6164



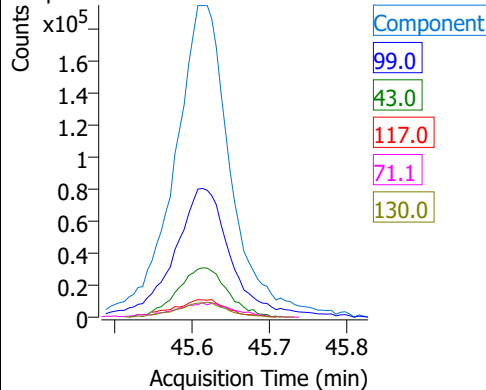
Pentanoic acid, 4-oxo-, 2-methylpropyl ester (NIST20.L)



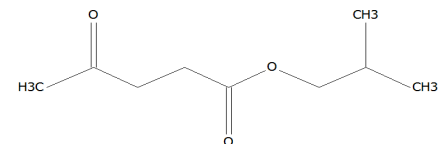
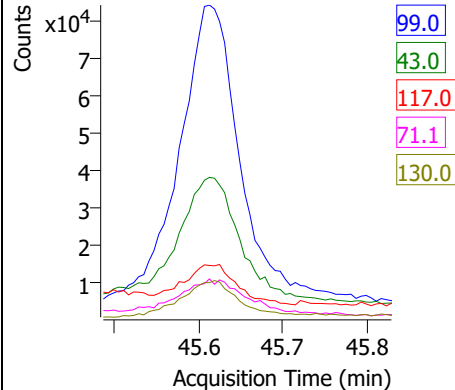
+ Scan (45.4884-45.8273 min, 58 scans) 1.D



Component RT: 45.6164



EIC Peaks



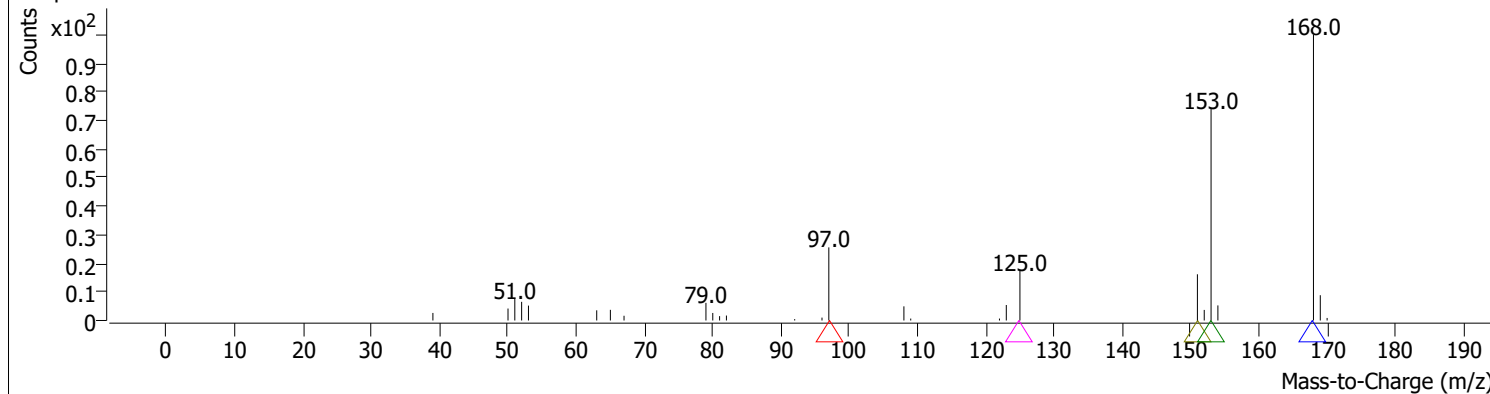
# Library Search Results - NonTarget Hits with Details



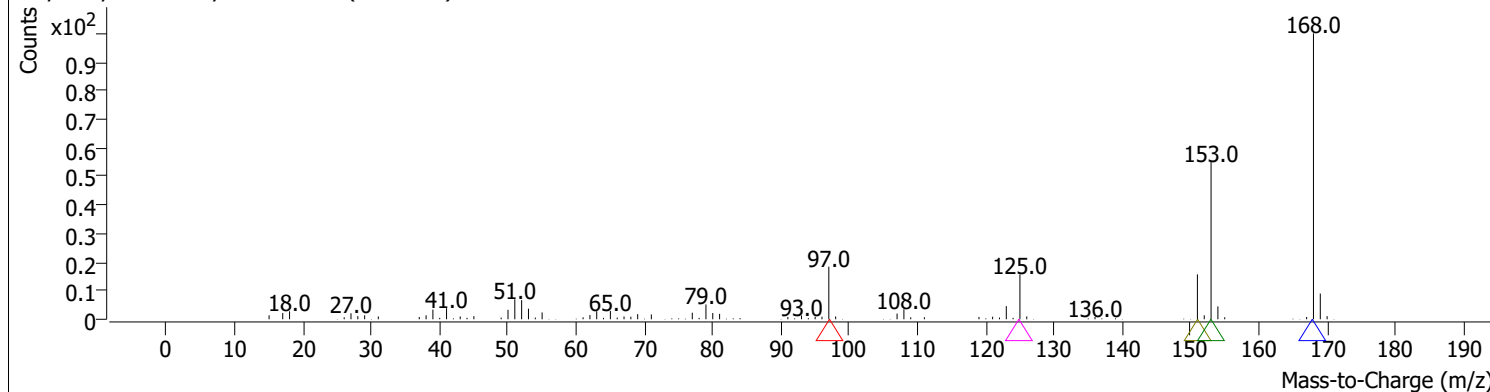
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.0282	3-Hydroxy-4-methoxybenzoic acid	913799.3	90.7	645-08-9	C <sub>8</sub> H <sub>8</sub> O <sub>4</sub>	

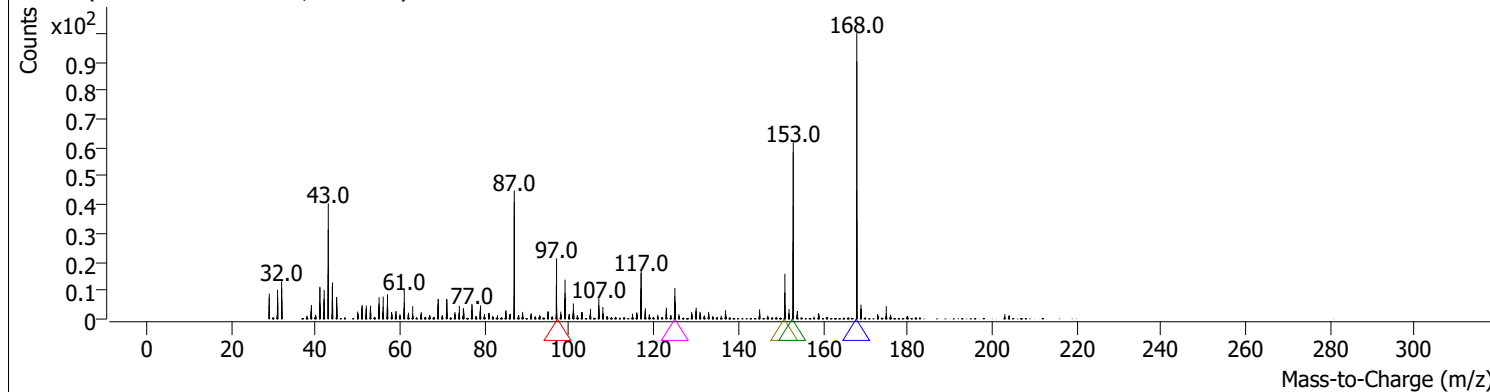
Component RT: 46.0282



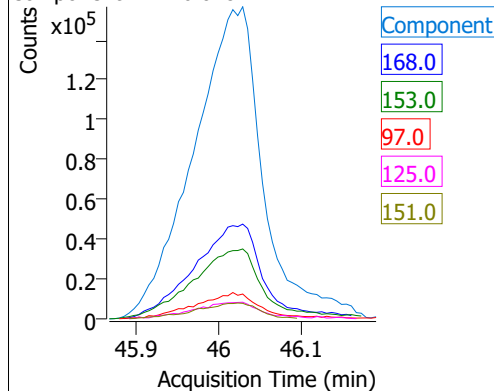
3-Hydroxy-4-methoxybenzoic acid (NIST20.L)



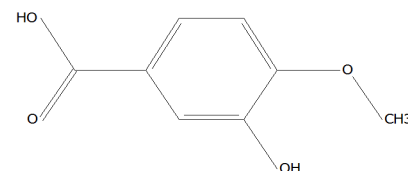
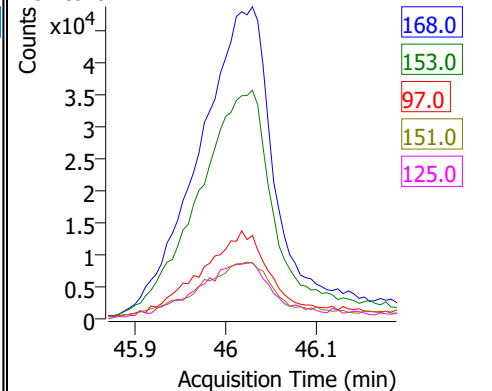
+ Scan (45.8817-46.1603 min, 47 scans) 1.D



Component RT: 46.0282



EIC Peaks



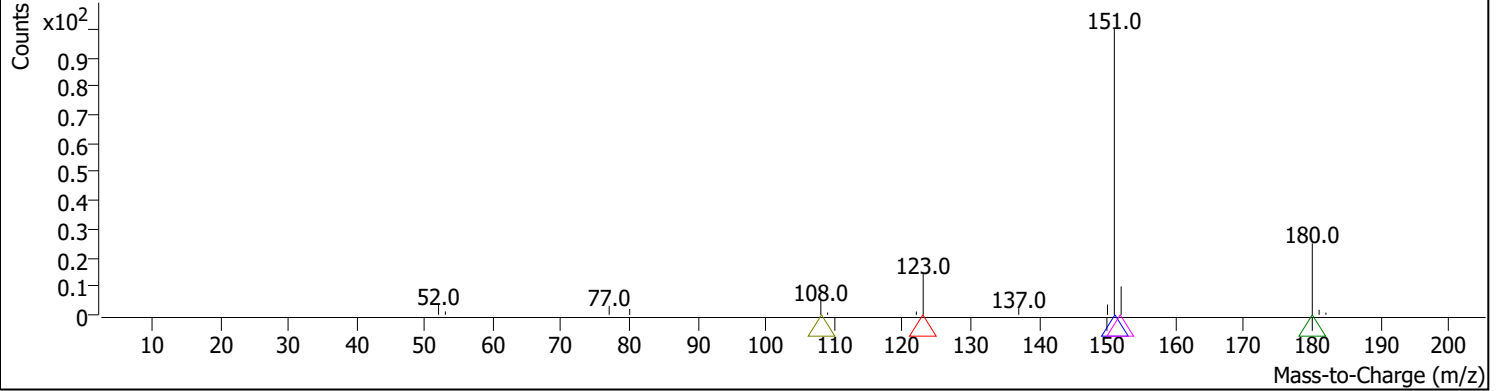
## Library Search Results - NonTarget Hits with Details



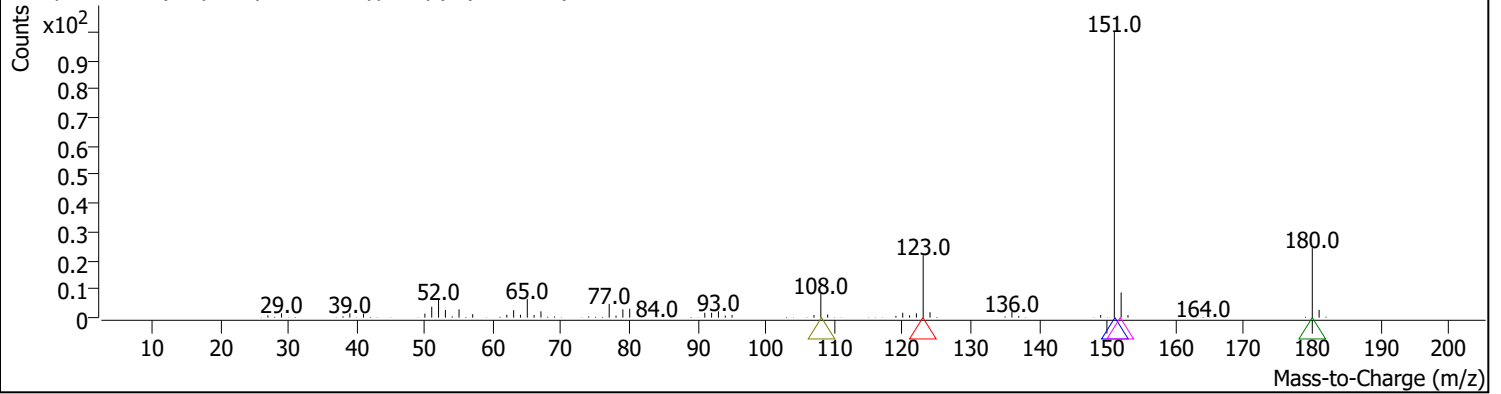
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.4726	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	384241.8	83.3	1835-14-9	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	

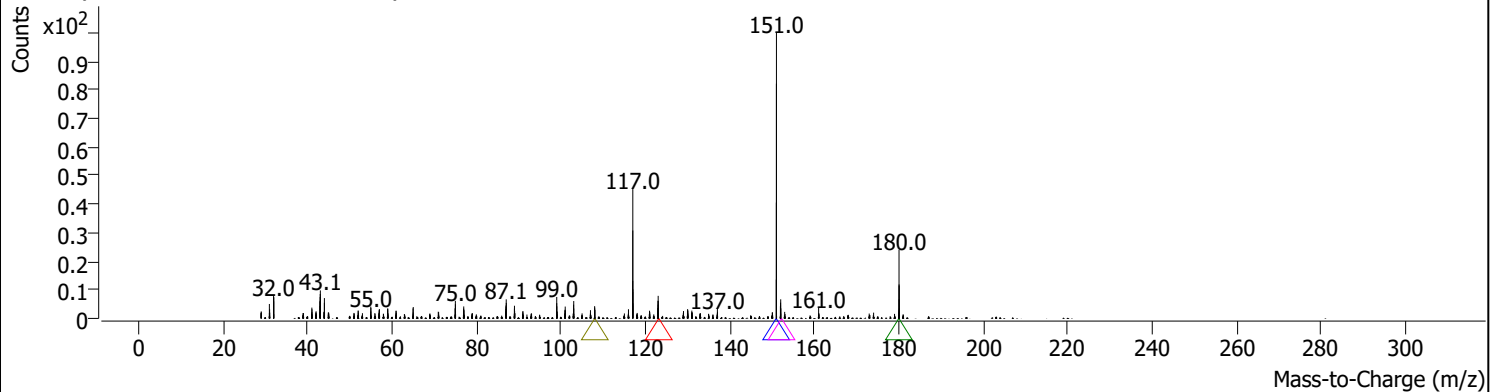
Component RT: 46.4726



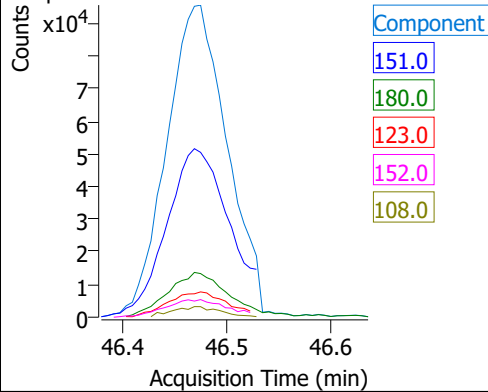
1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L)



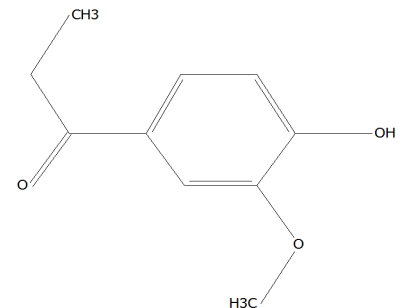
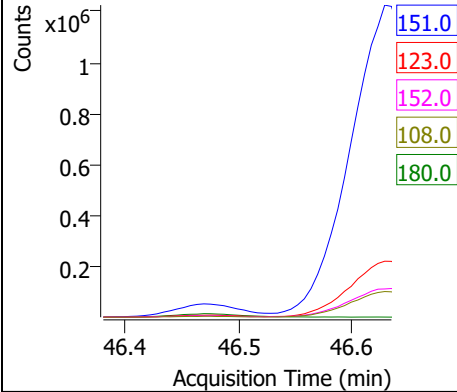
+ Scan (46.3803-46.5289 min, 26 scans) 1.D



Component RT: 46.4726



EIC Peaks



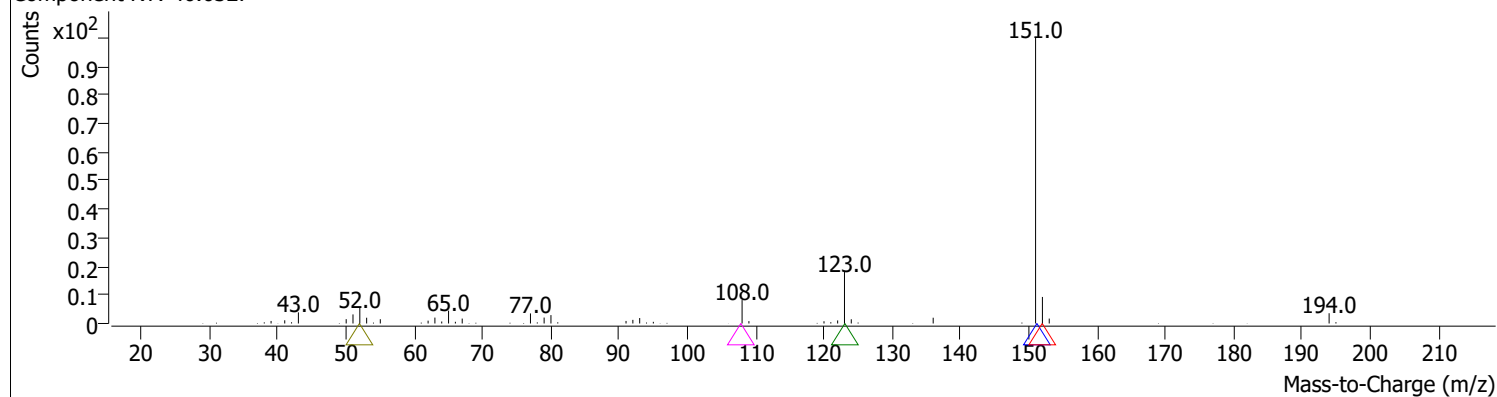
## Library Search Results - NonTarget Hits with Details



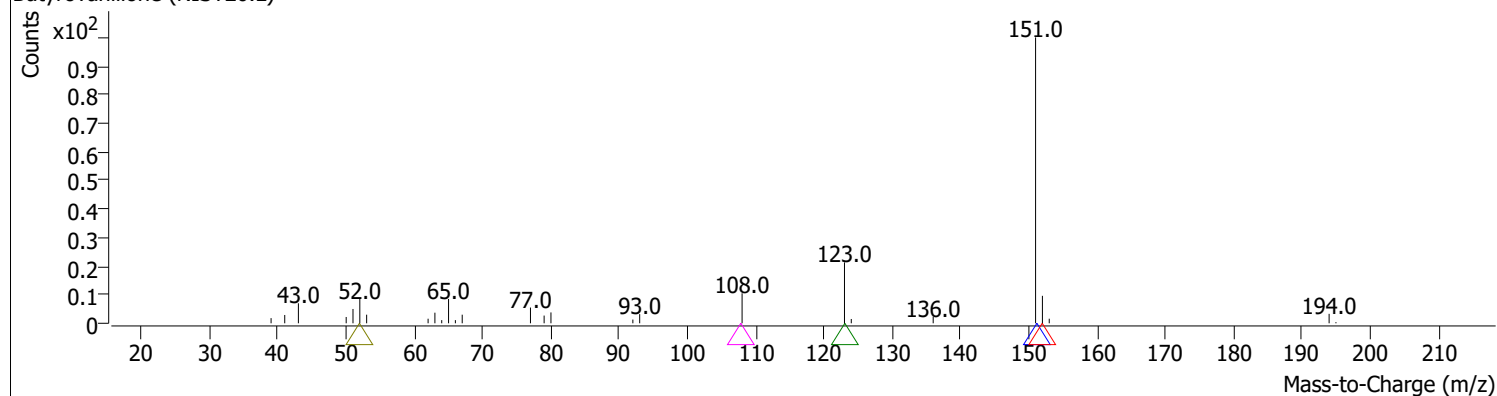
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.6327	Butyrovanihone	10320359.6	95.3	64142-23-0	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	

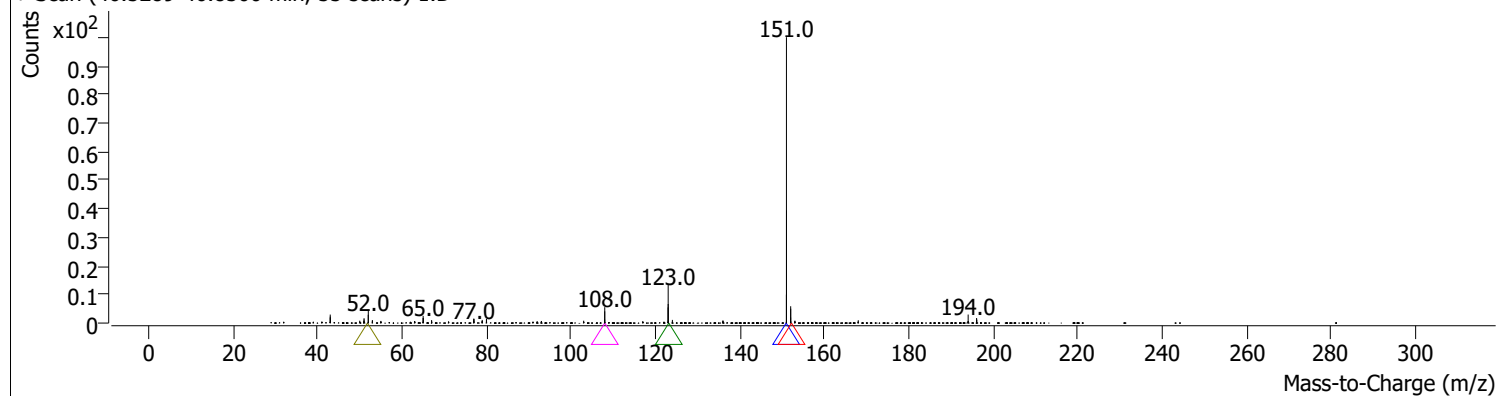
Component RT: 46.6327



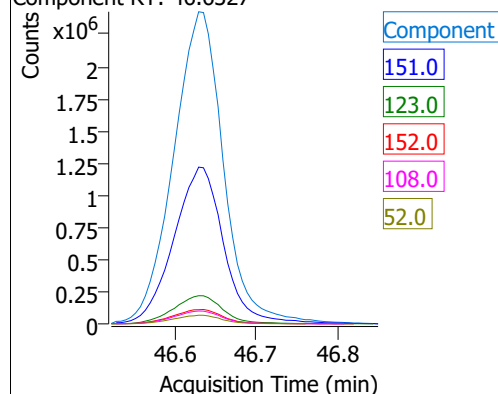
Butyrovanihone (NIST20.L)



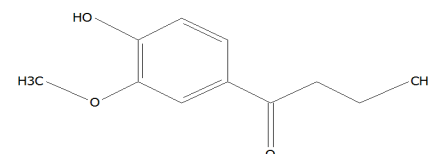
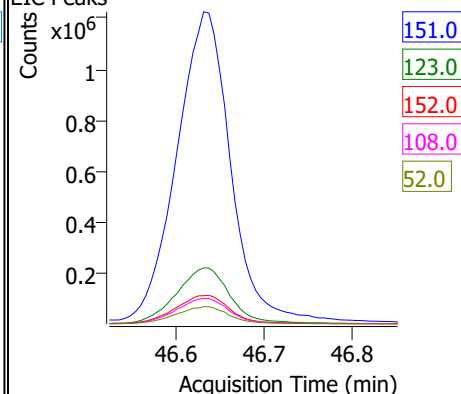
+ Scan (46.5289-46.8500 min, 55 scans) 1.D



Component RT: 46.6327



EIC Peaks



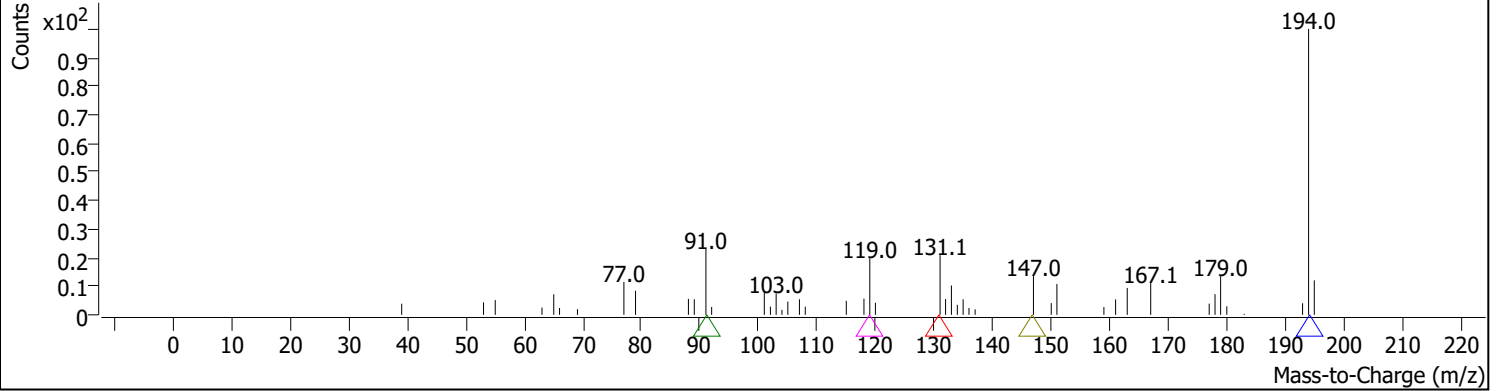
## Library Search Results - NonTarget Hits with Details



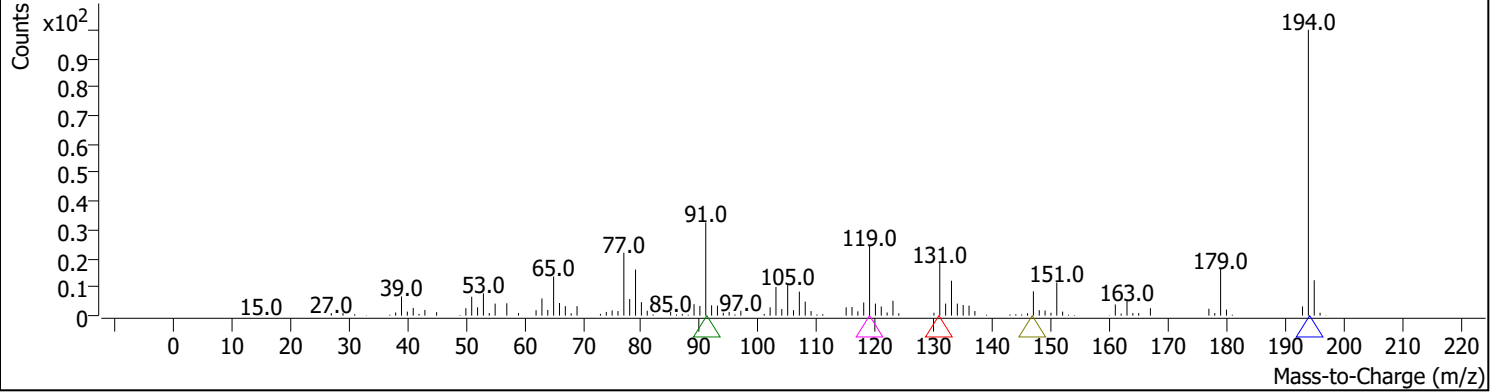
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
47.0806	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	352815.4	82.6	20675-95-0	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	

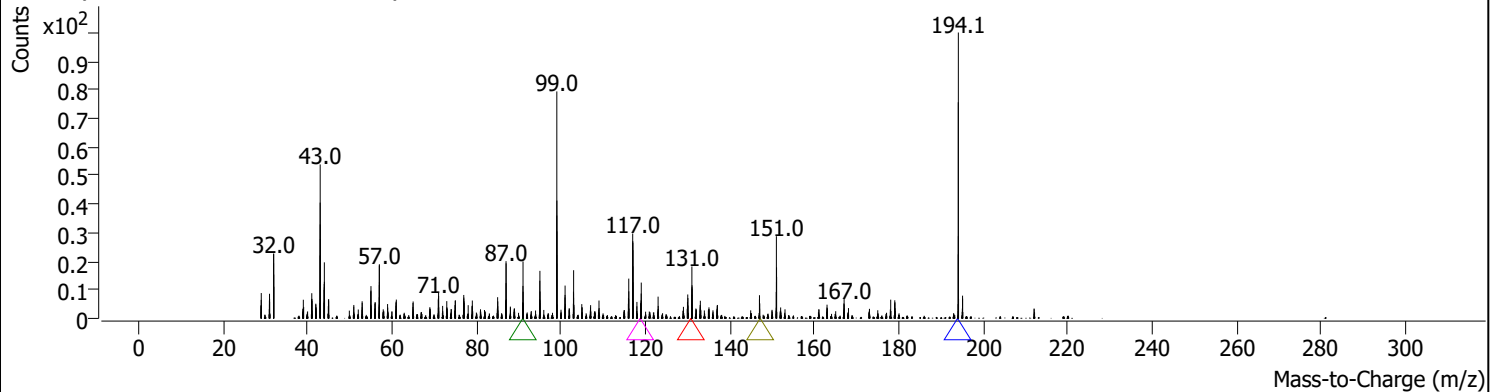
Component RT: 47.0806



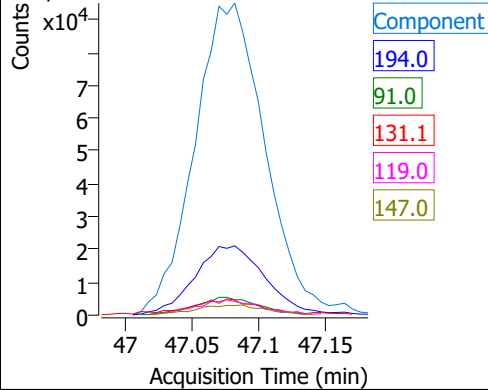
(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L)



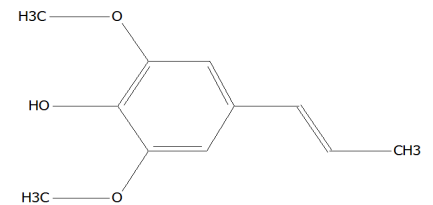
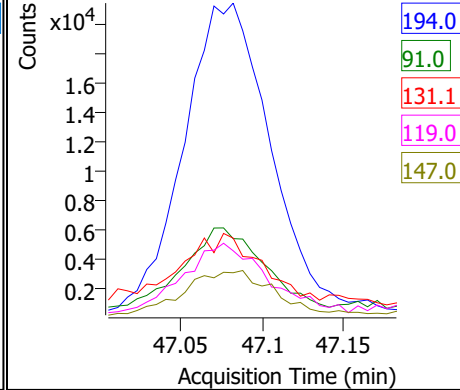
+ Scan (47.0058-47.1830 min, 30 scans) 1.D



Component RT: 47.0806



EIC Peaks



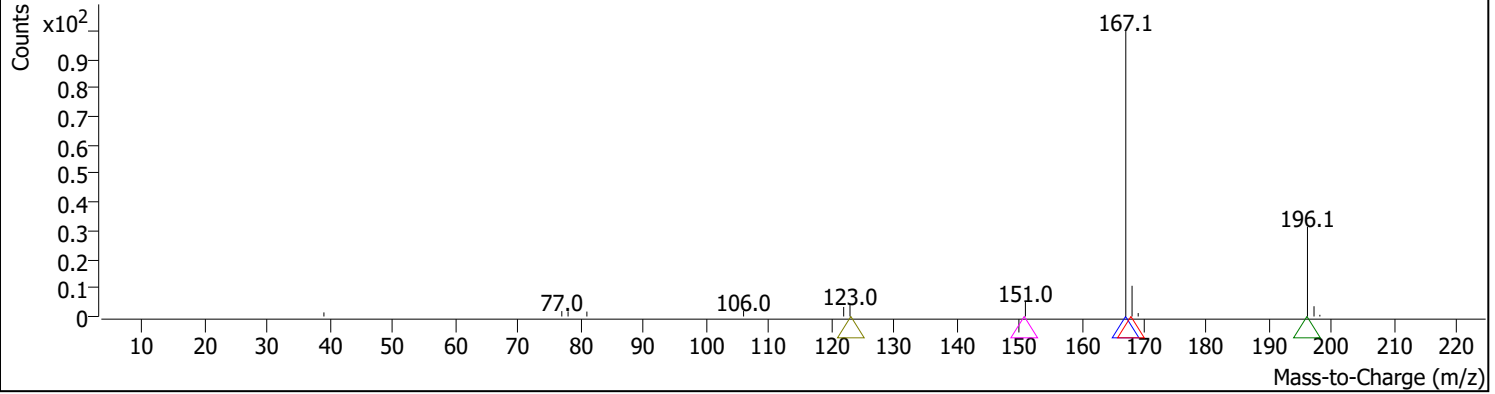
## Library Search Results - NonTarget Hits with Details



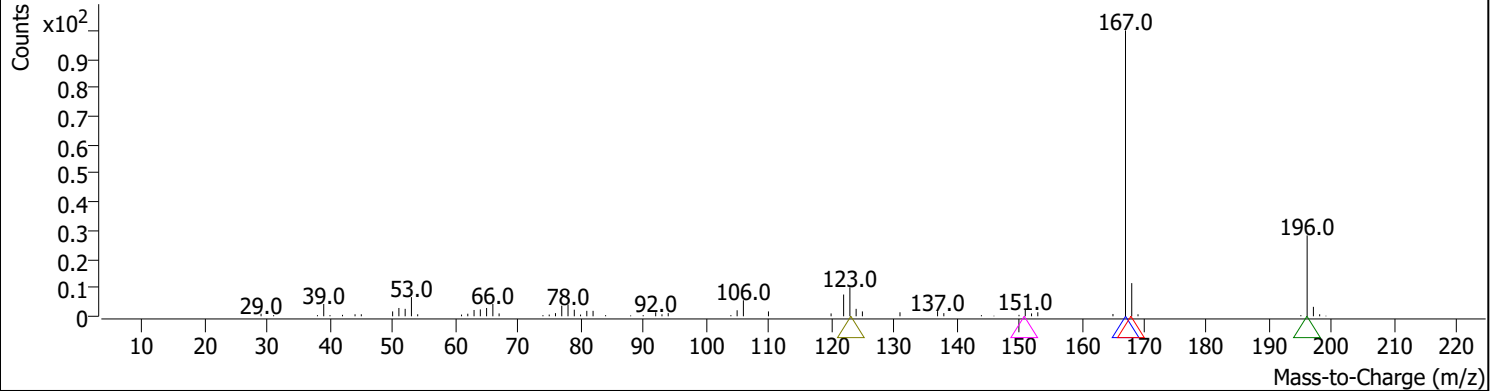
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
47.3445	Homosyringaldehyde	249662.5	83.0	87345-52-6	C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>	

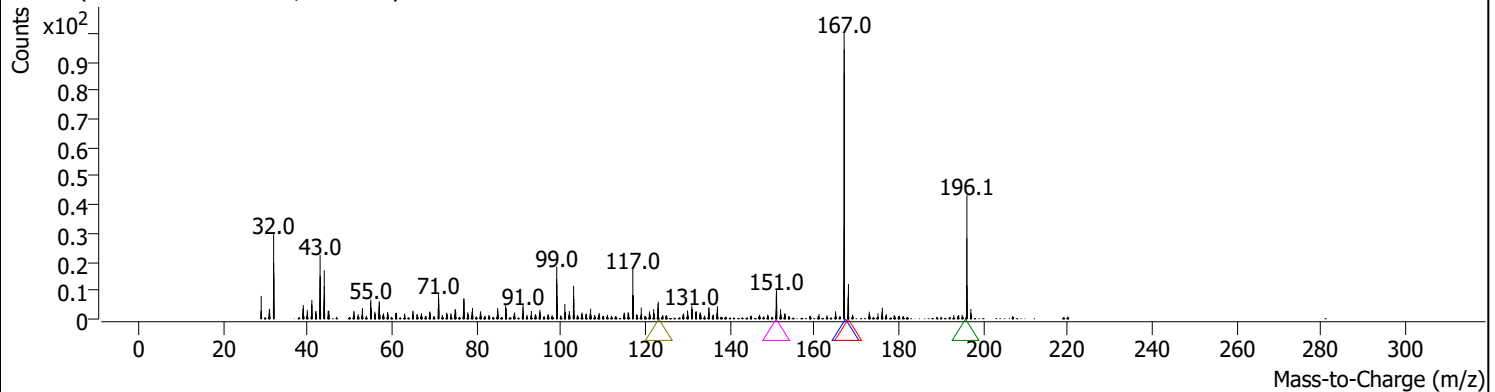
Component RT: 47.3445



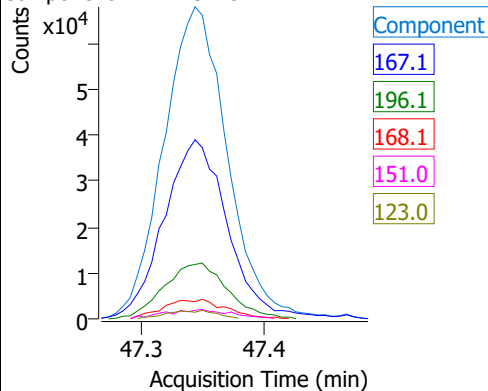
Homosyringaldehyde (NIST20.L)



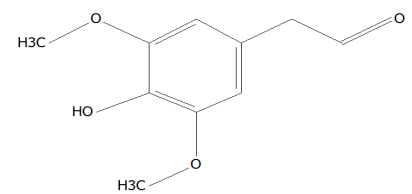
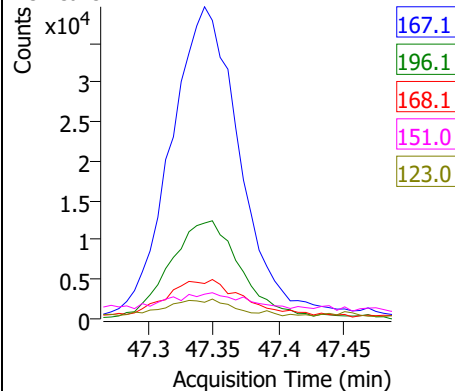
+ Scan (47.2613-47.4862 min, 38 scans) 1.D



Component RT: 47.3445



EIC Peaks



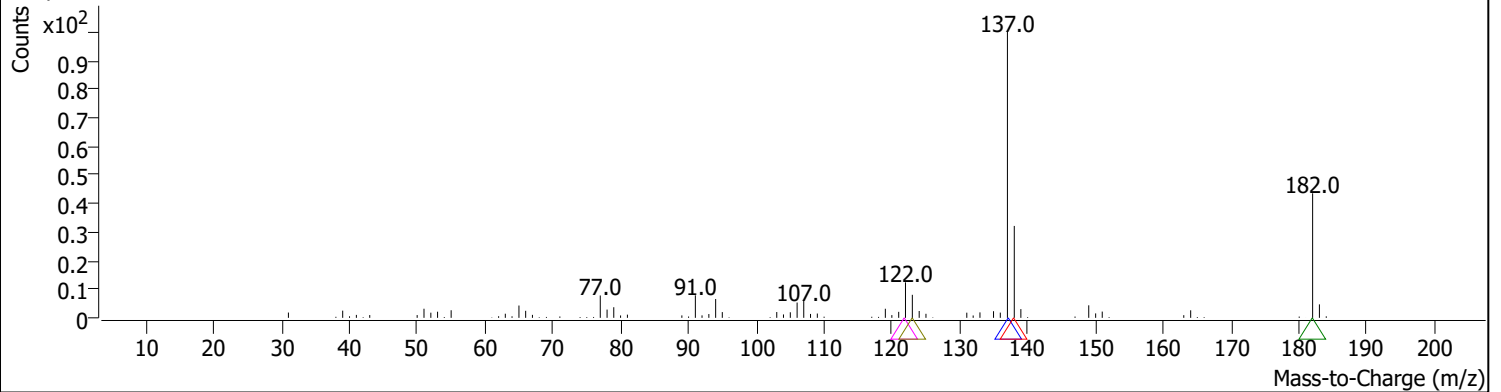
## Library Search Results - NonTarget Hits with Details



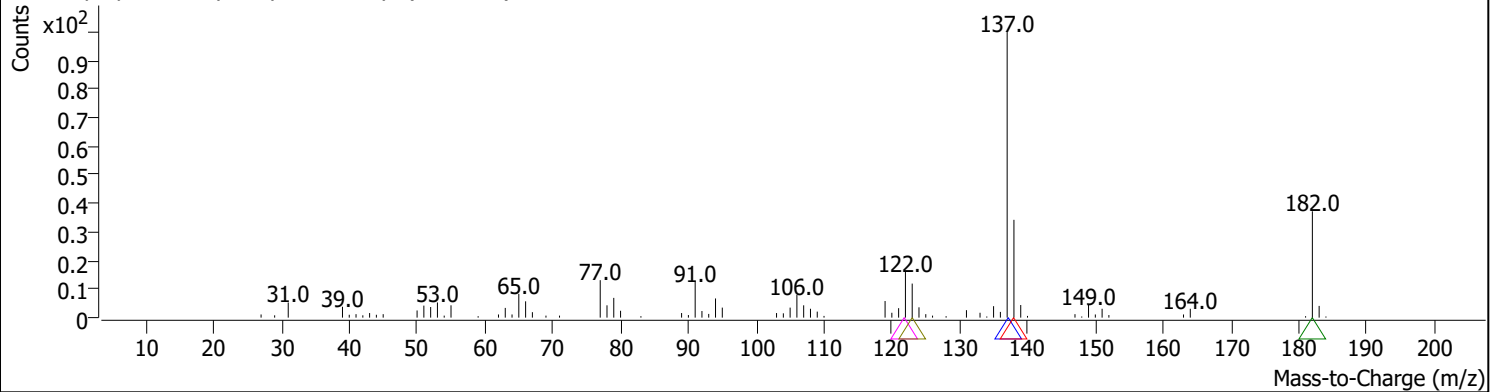
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
48.9790	Benzenepropanol, 4-hydroxy-3-methoxy-	6788098.5	96.4	2305-13-7	C10H14O3	

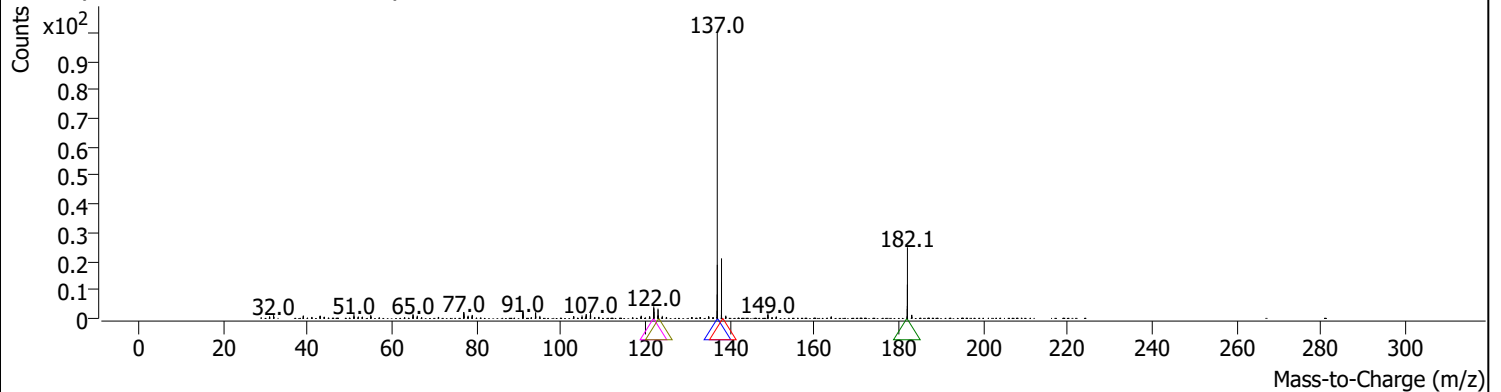
Component RT: 48.9790



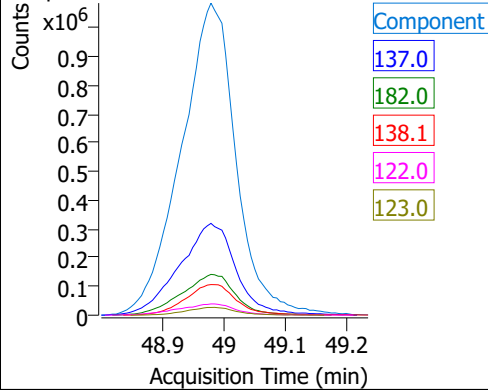
Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L)



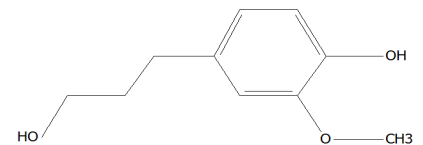
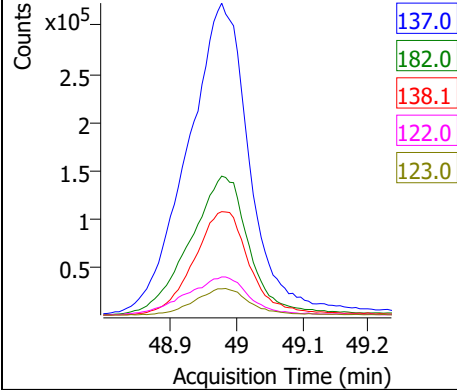
+ Scan (48.8136-49.1806 min, 61 scans) 1.D



Component RT: 48.9790



EIC Peaks





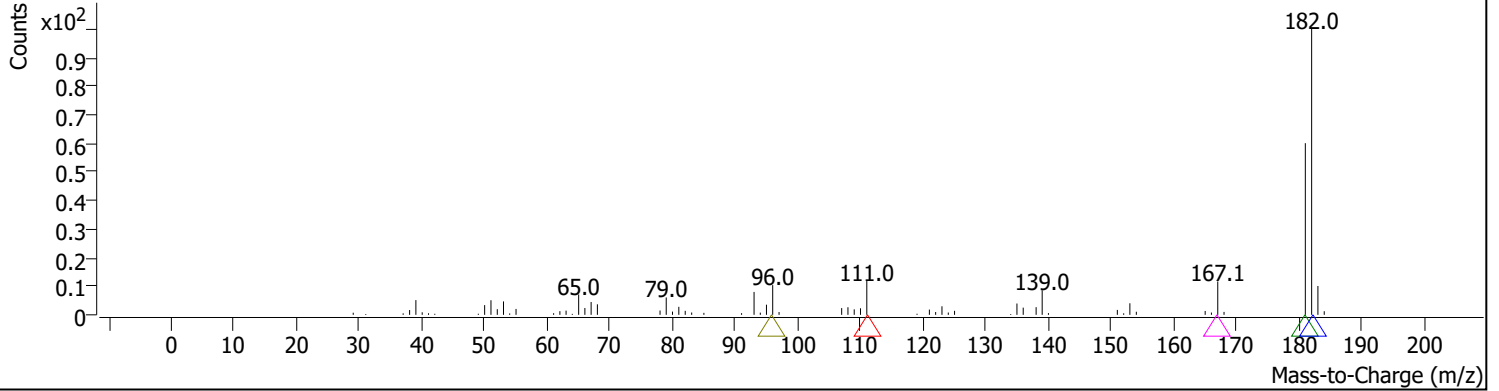
# Library Search Results - NonTarget Hits with Details



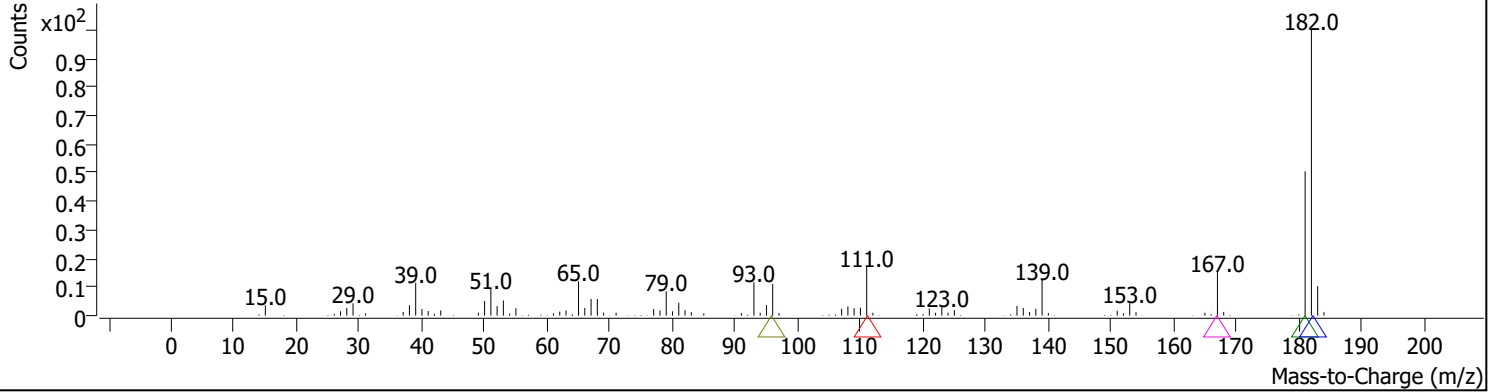
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
49.3444	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	2605242.4	96.7	134-96-3	C9H10O4	

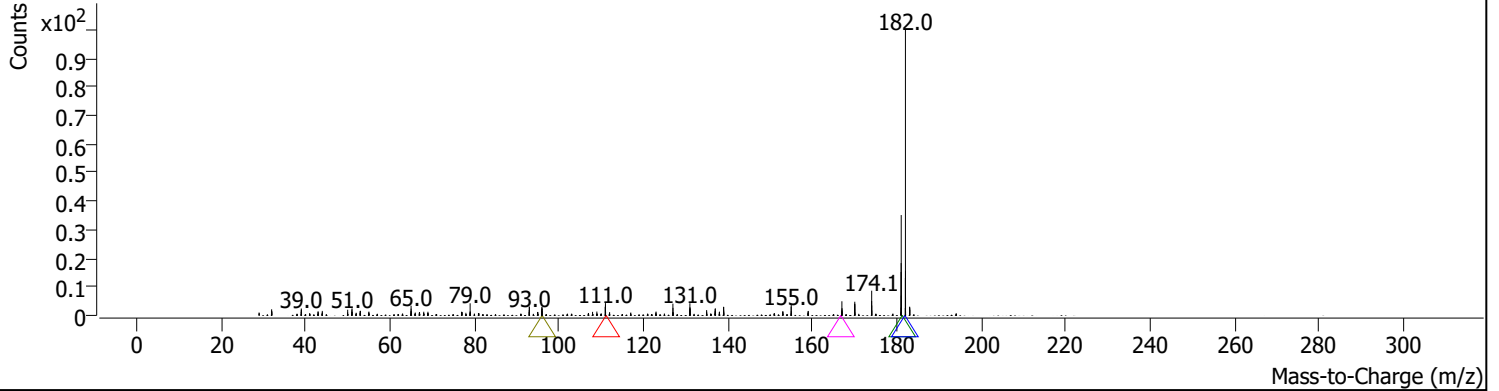
Component RT: 49.3444



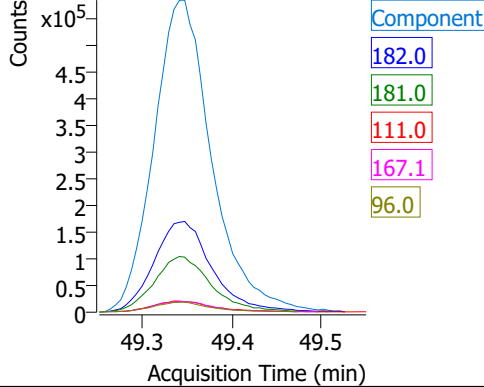
Benzaldehyde, 4-hydroxy-3,5-dimethoxy- (NIST20.L)



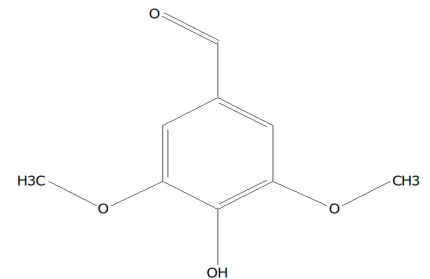
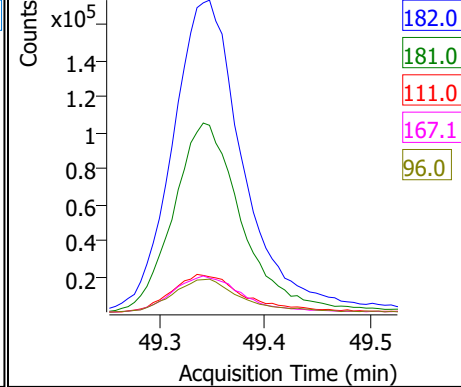
+ Scan (49.2586-49.5257 min, 45 scans) 1.D



Component RT: 49.3444



EIC Peaks



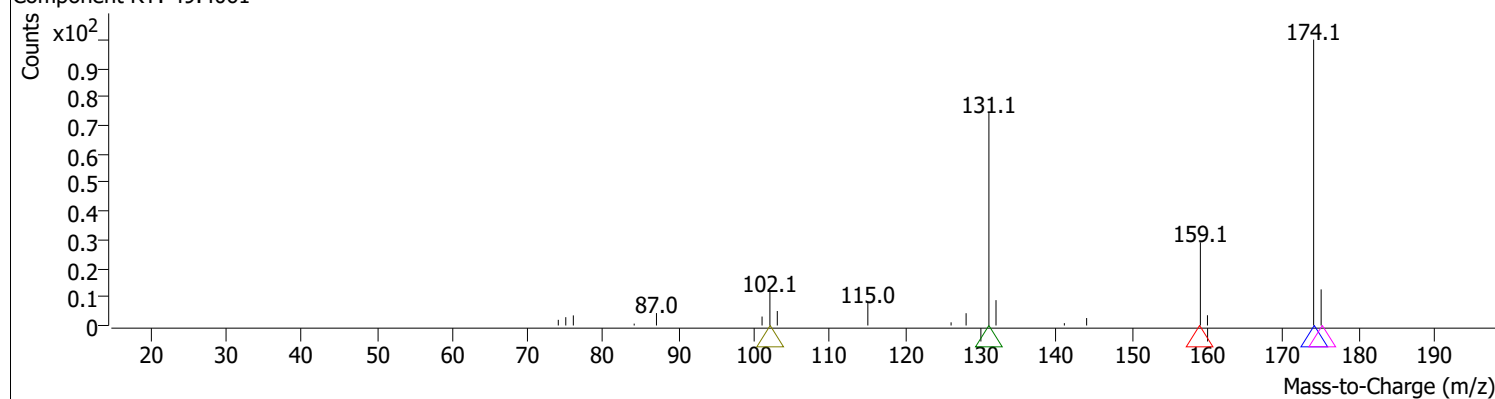
## Library Search Results - NonTarget Hits with Details



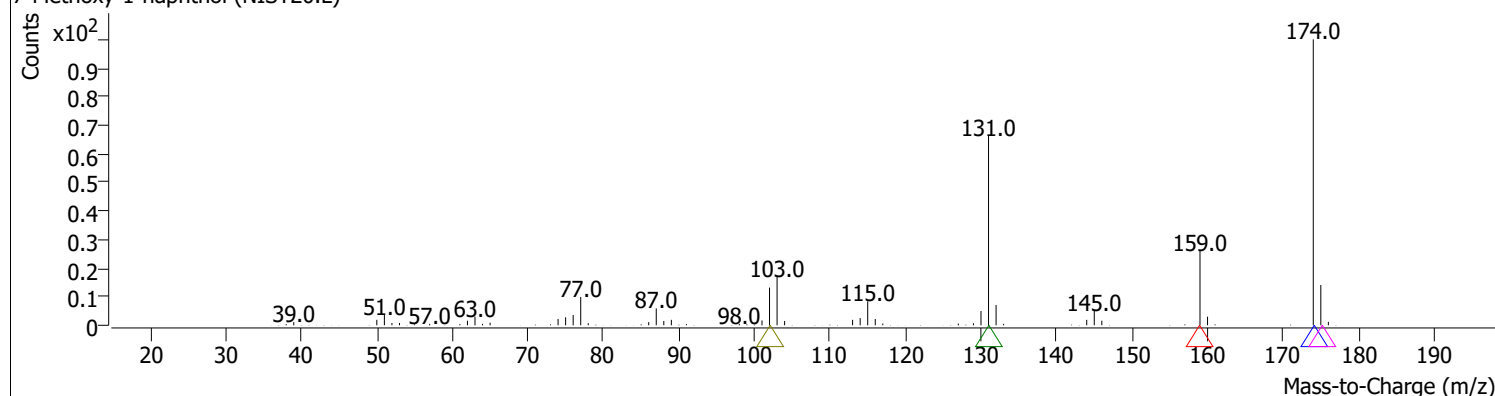
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
49.4061	7-Methoxy-1-naphthol	366053.3	84.2	67247-13-6	C <sub>11</sub> H <sub>10</sub> O <sub>2</sub>	

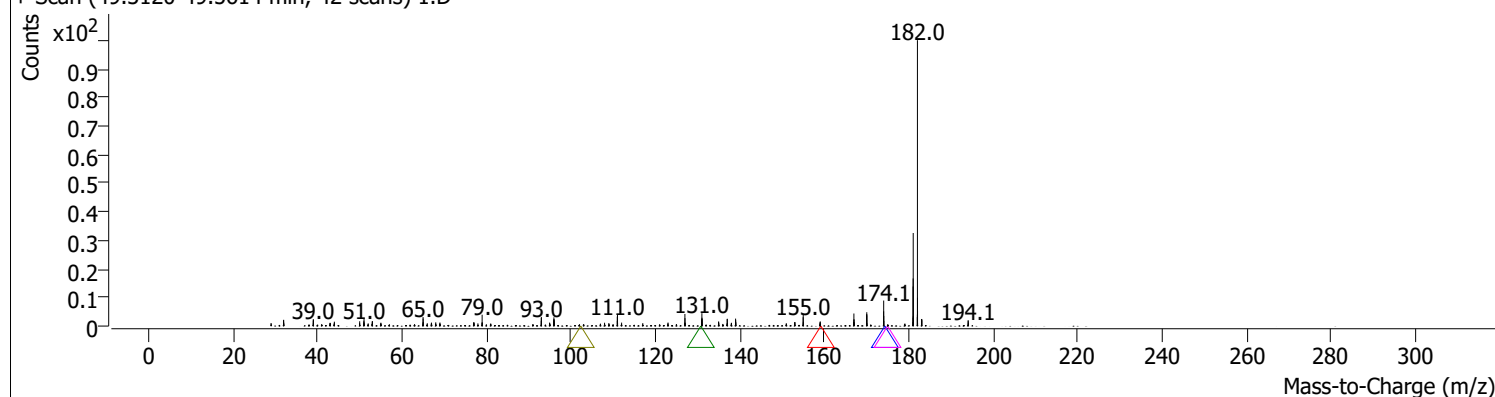
Component RT: 49.4061



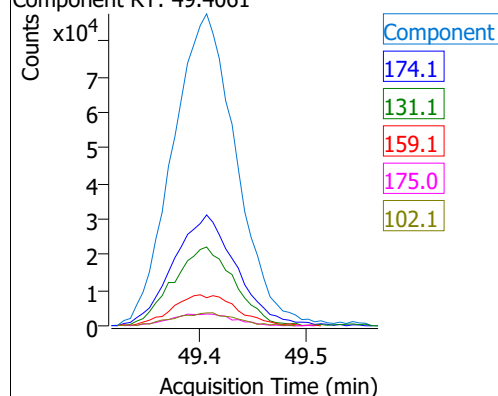
7-Methoxy-1-naphthol (NIST20.L)



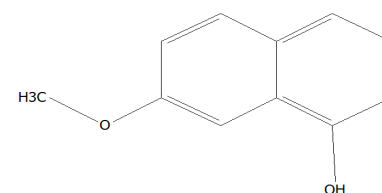
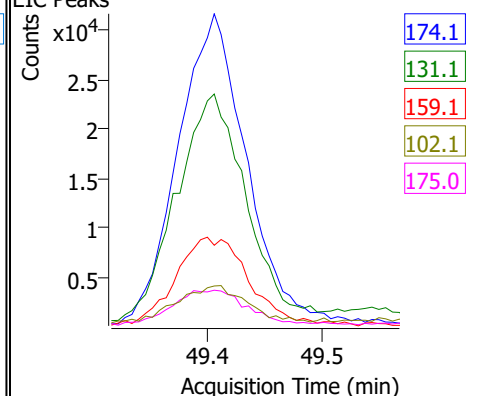
+ Scan (49.3120-49.5614 min, 42 scans) 1.D



Component RT: 49.4061



EIC Peaks



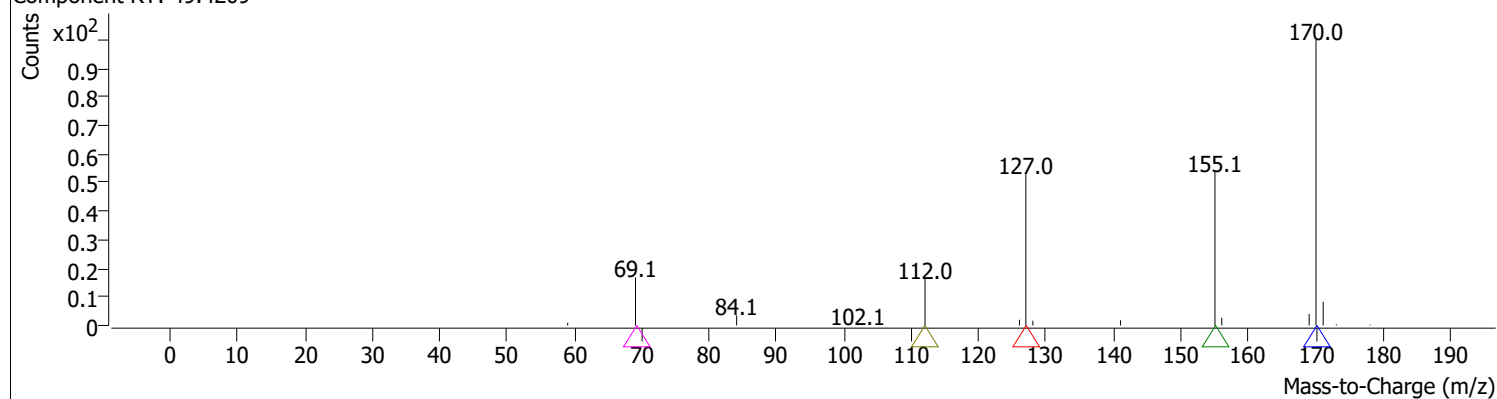
## Library Search Results - NonTarget Hits with Details



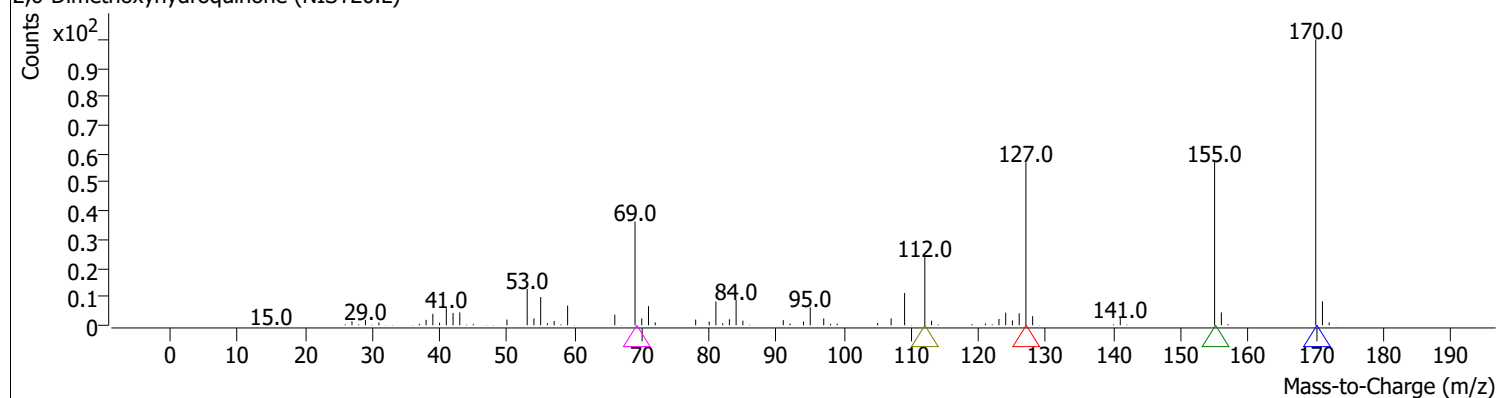
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
49.4209	2,6-Dimethoxyhydroquinone	383468.5	78.5	15233-65-5	C <sub>8</sub> H <sub>10</sub> O <sub>4</sub>	

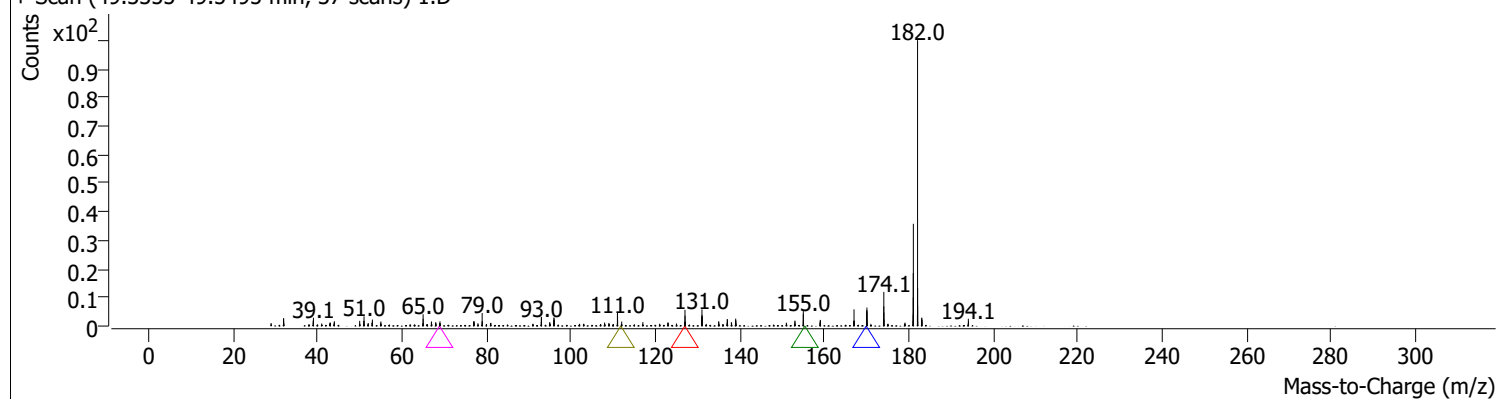
Component RT: 49.4209



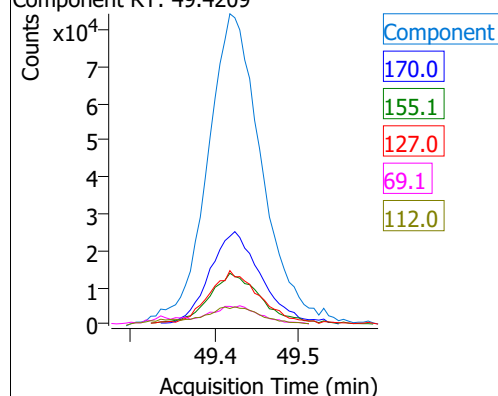
2,6-Dimethoxyhydroquinone (NIST20.L)



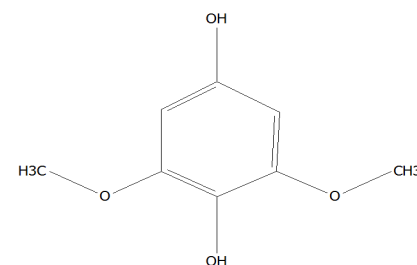
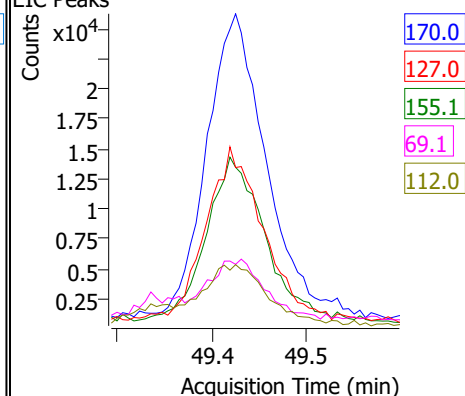
+ Scan (49.3355-49.5495 min, 37 scans) 1.D



Component RT: 49.4209



EIC Peaks



## Library Search Results - NonTarget Hits with Details

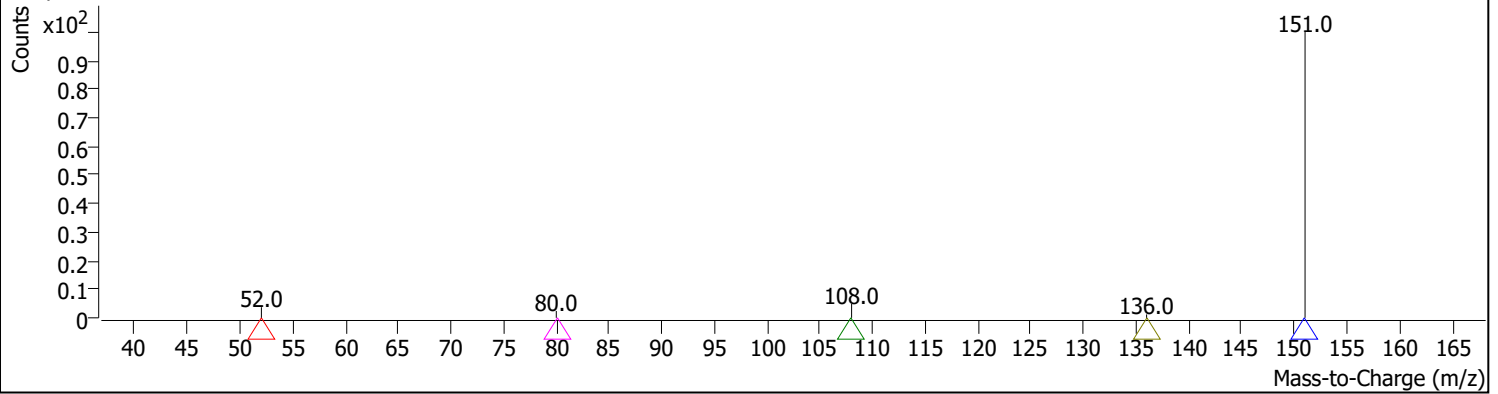


Agilent

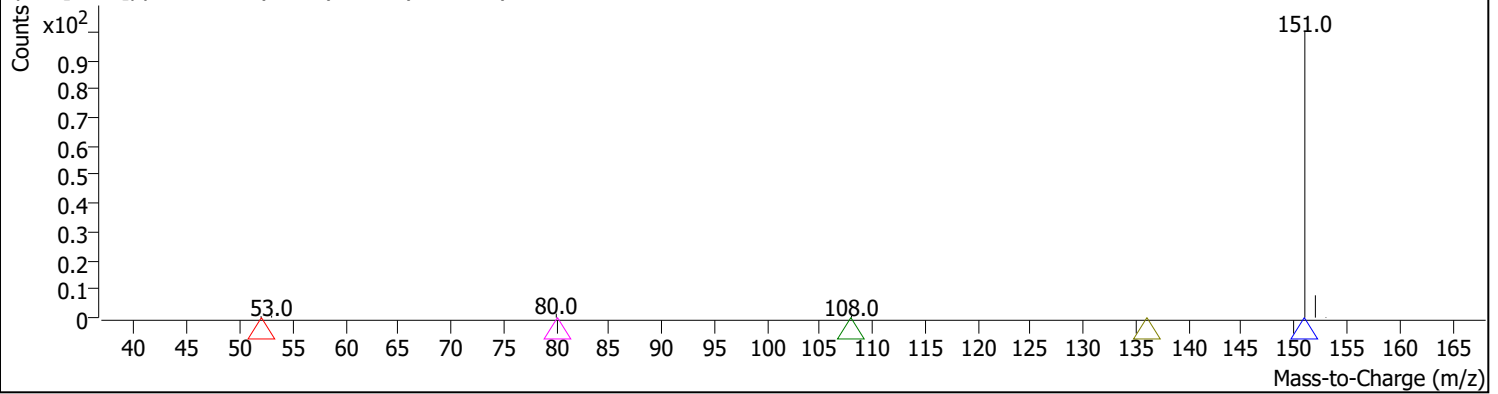
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
50.4127	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	326279.1	80.6	65996-50-1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	

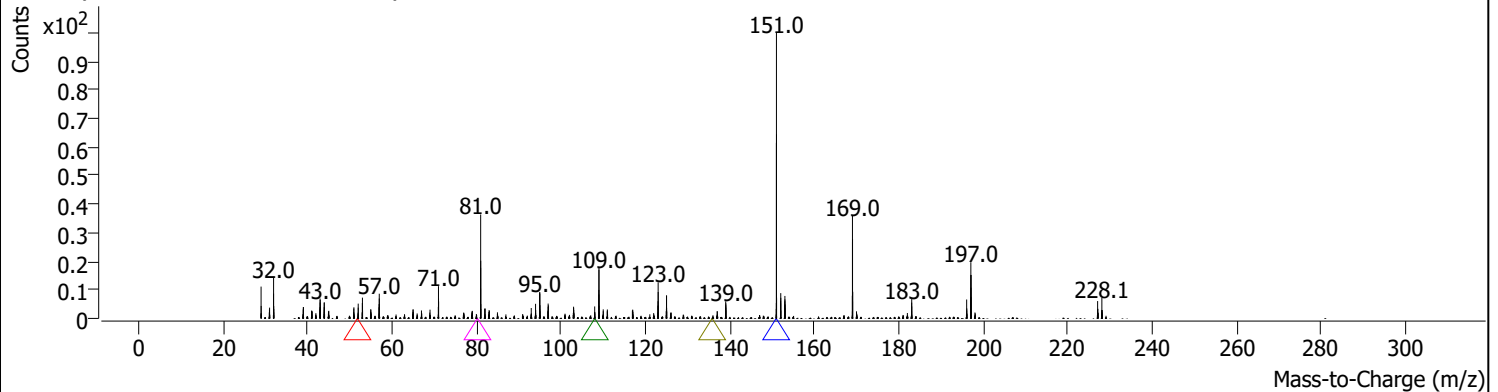
Component RT: 50.4127



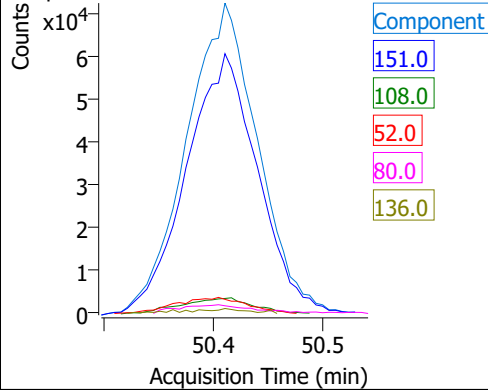
Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)



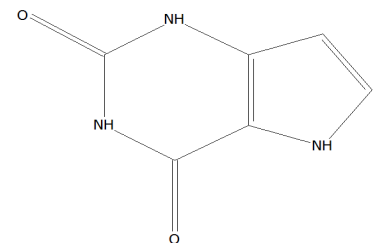
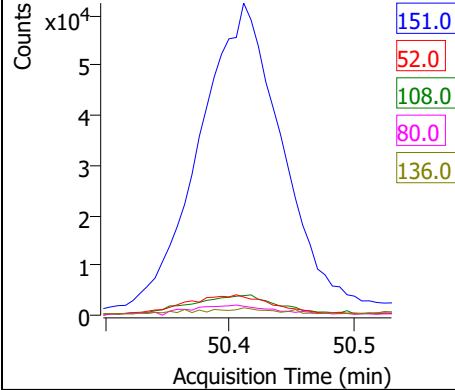
+ Scan (50.3047-50.5350 min, 39 scans) 1.D



Component RT: 50.4127



EIC Peaks



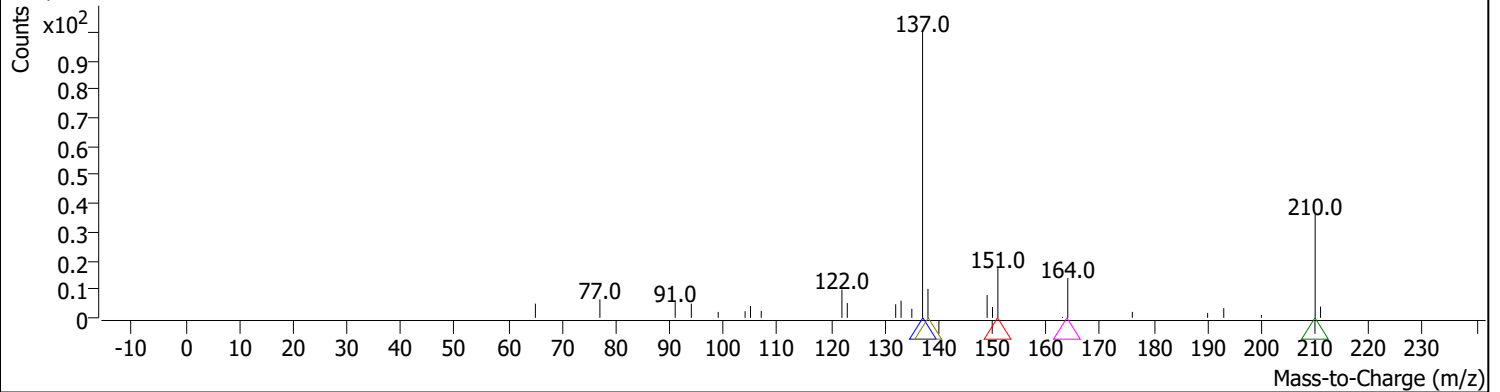
## Library Search Results - NonTarget Hits with Details



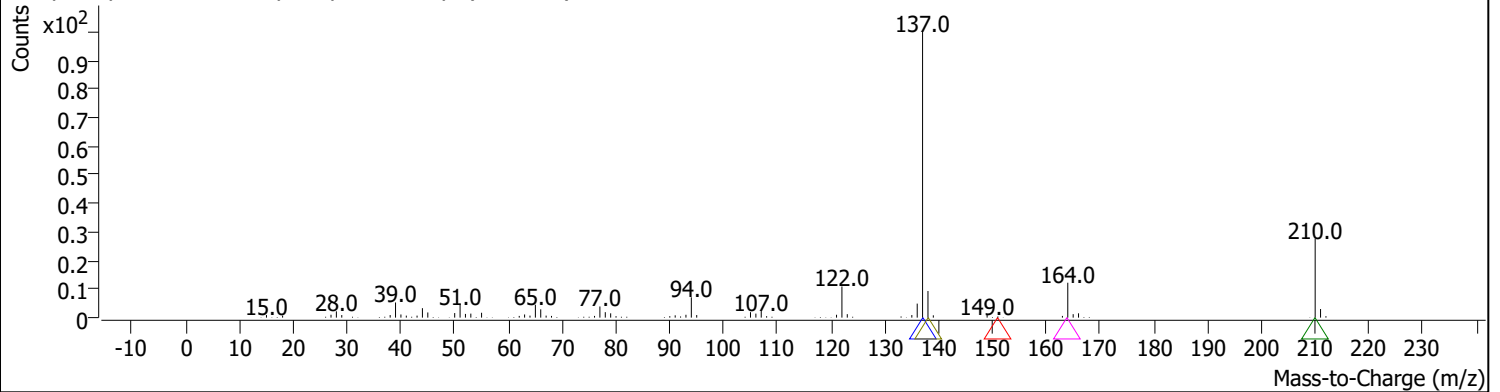
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
50.6291	Phenylacetylformic acid, 4-hydroxy-3-methoxy-	303107.7	79.6	1081-71-6	C10H10O5	

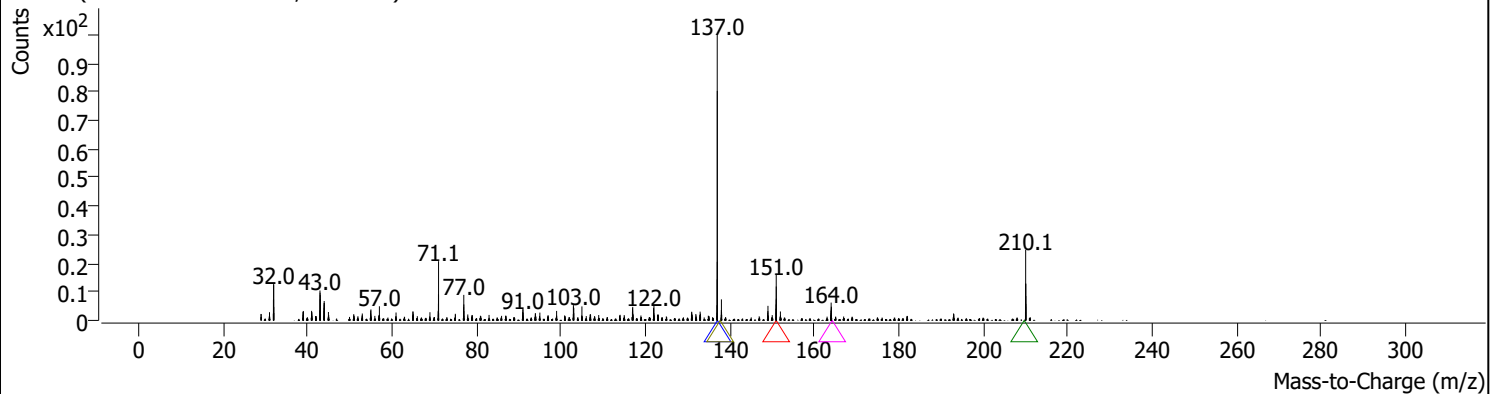
Component RT: 50.6291



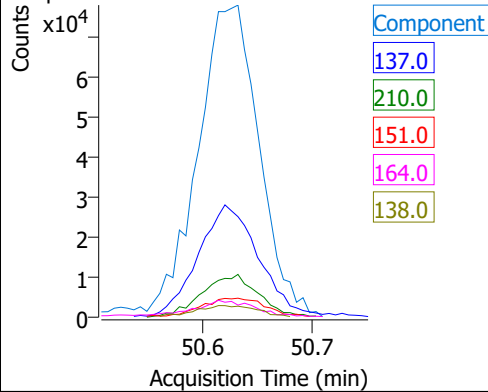
Phenylacetylformic acid, 4-hydroxy-3-methoxy- (NIST20.L)



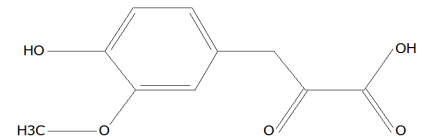
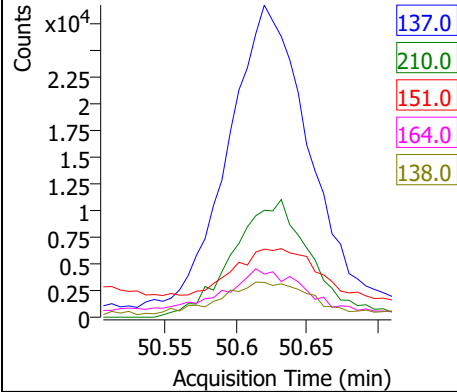
+ Scan (50.5524-50.7059 min, 26 scans) 1.D



Component RT: 50.6291



EIC Peaks



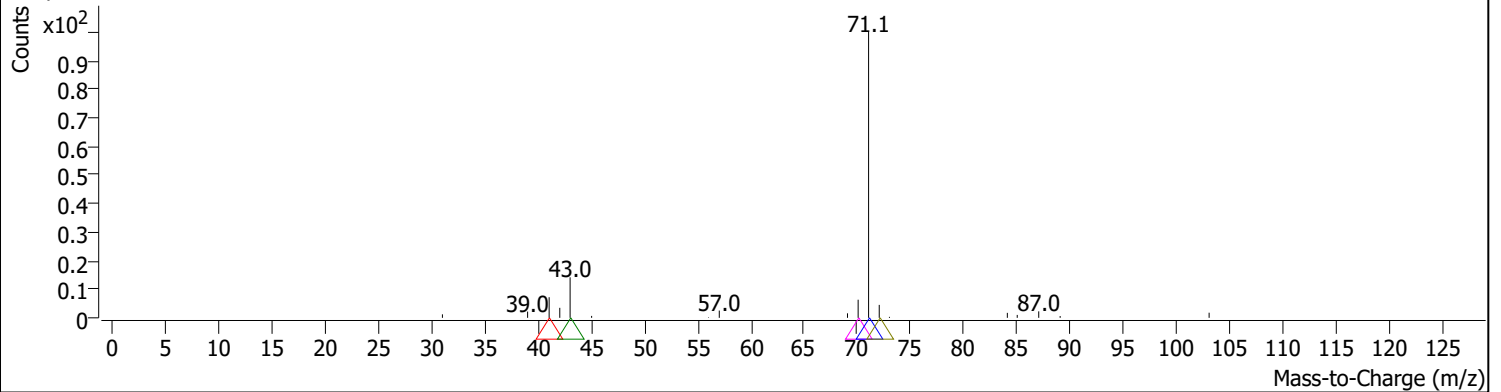
## Library Search Results - NonTarget Hits with Details



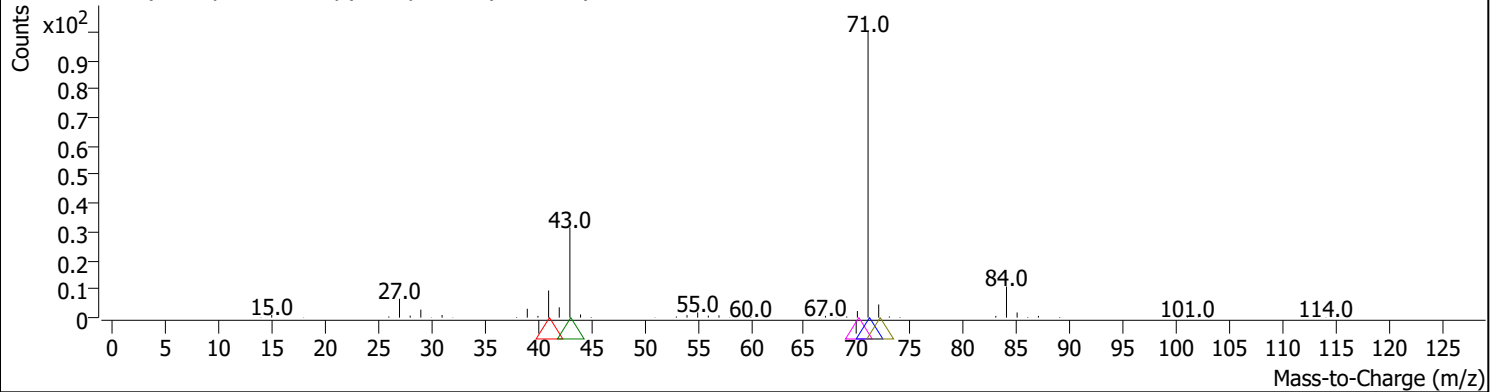
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
51.0371	Butanoic acid, (tetrahydro-2-furanyl)methyl ester	665275.7	77.4	2217-33-6	C9H16O3	

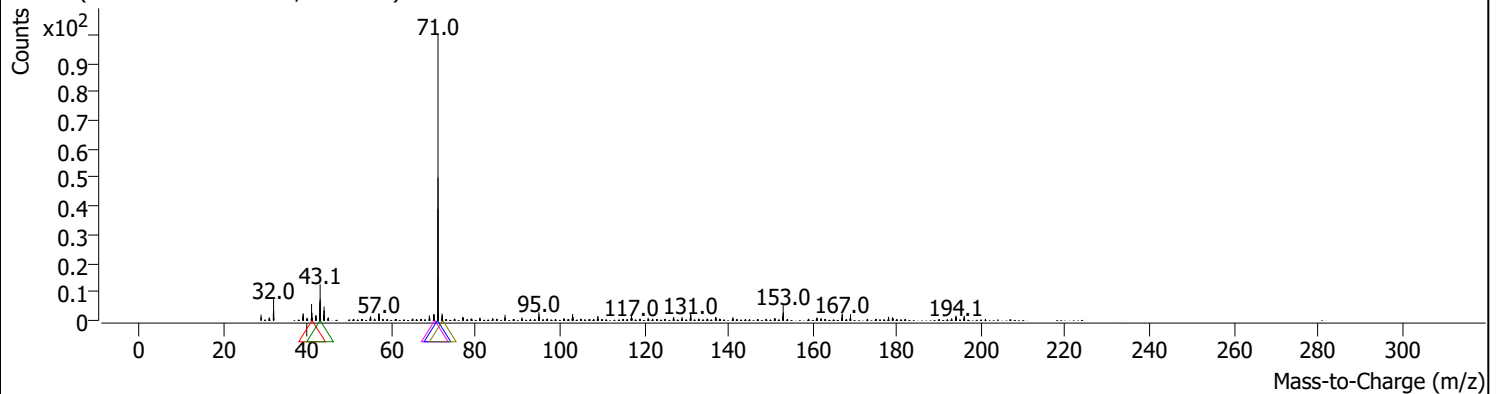
Component RT: 51.0371



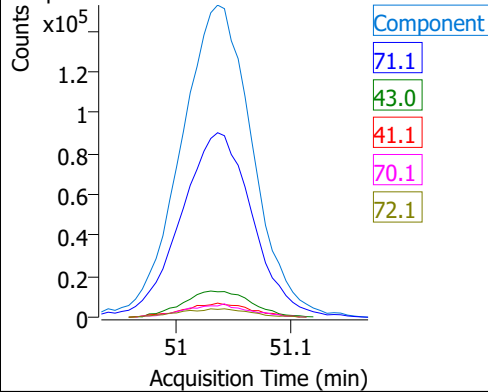
Butanoic acid, (tetrahydro-2-furanyl)methyl ester (NIST20.L)



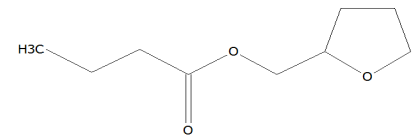
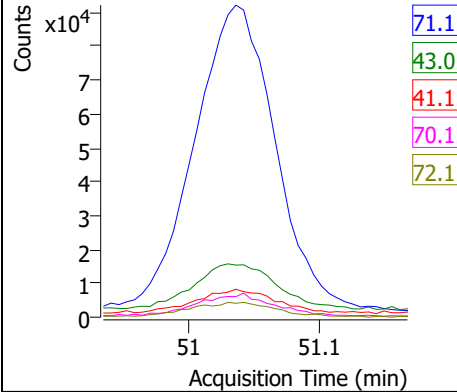
+ Scan (50.9350-51.1669 min, 40 scans) 1.D



Component RT: 51.0371



EIC Peaks



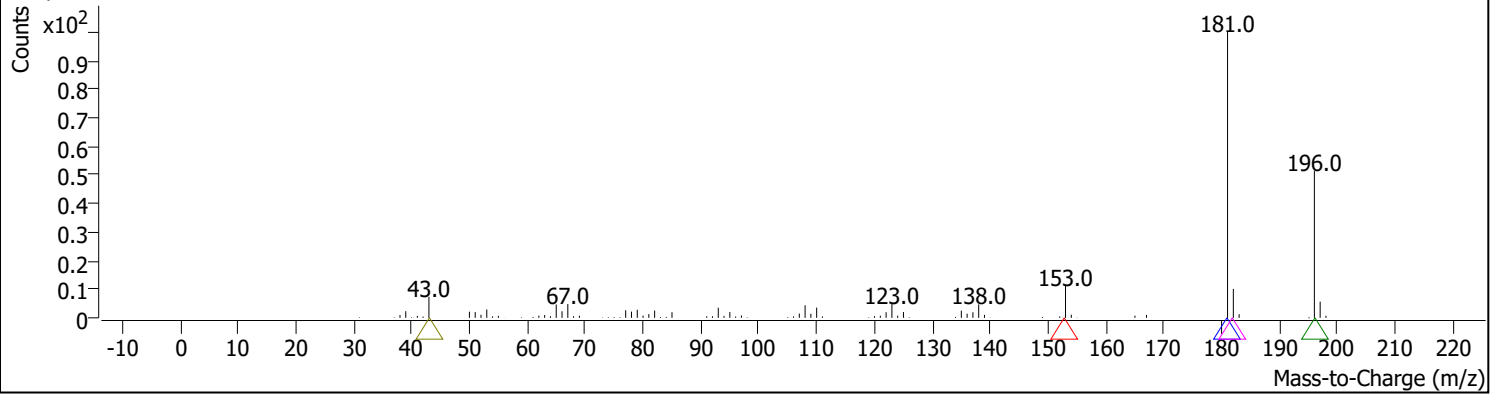
## Library Search Results - NonTarget Hits with Details



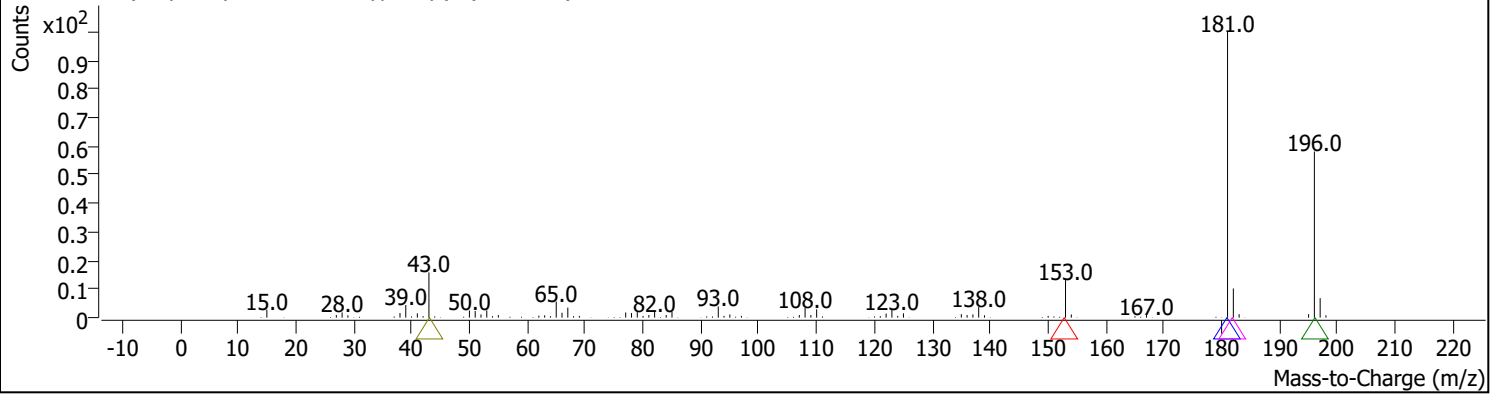
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
51.9859	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	6385500.3	97.5	2478-38-8	C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>	

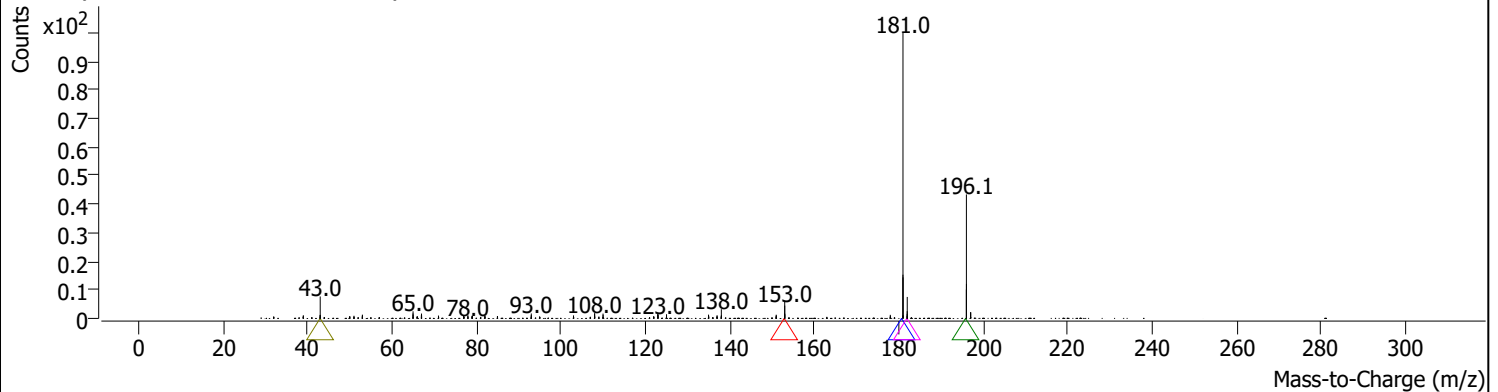
Component RT: 51.9859



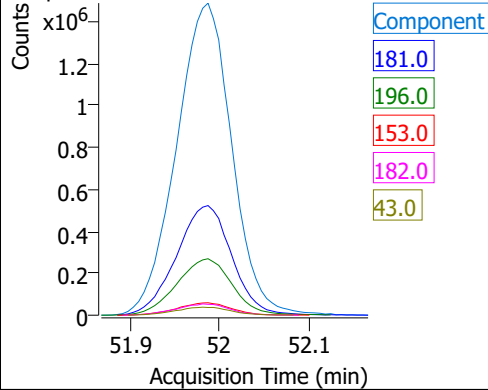
Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)- (NIST20.L)



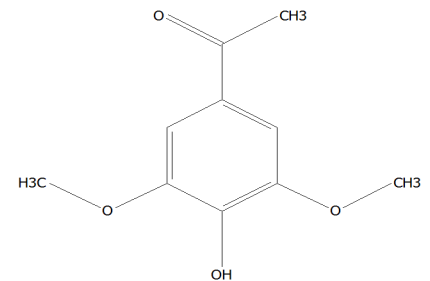
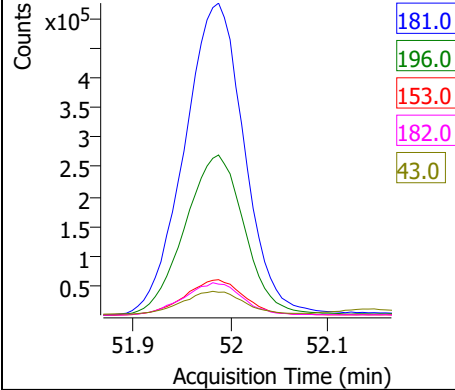
+ Scan (51.8685-52.1242 min, 44 scans) 1.D



Component RT: 51.9859



EIC Peaks



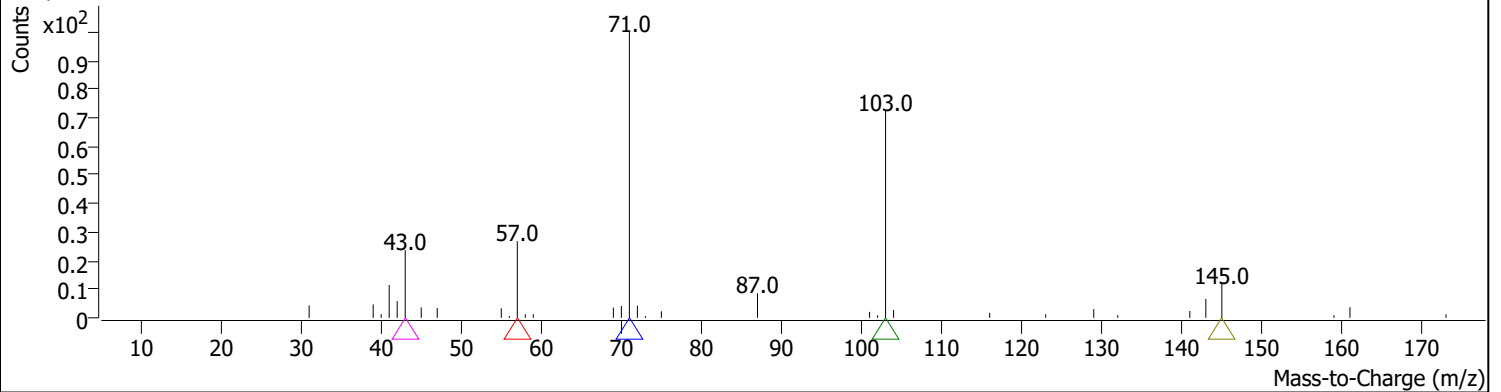
## Library Search Results - NonTarget Hits with Details



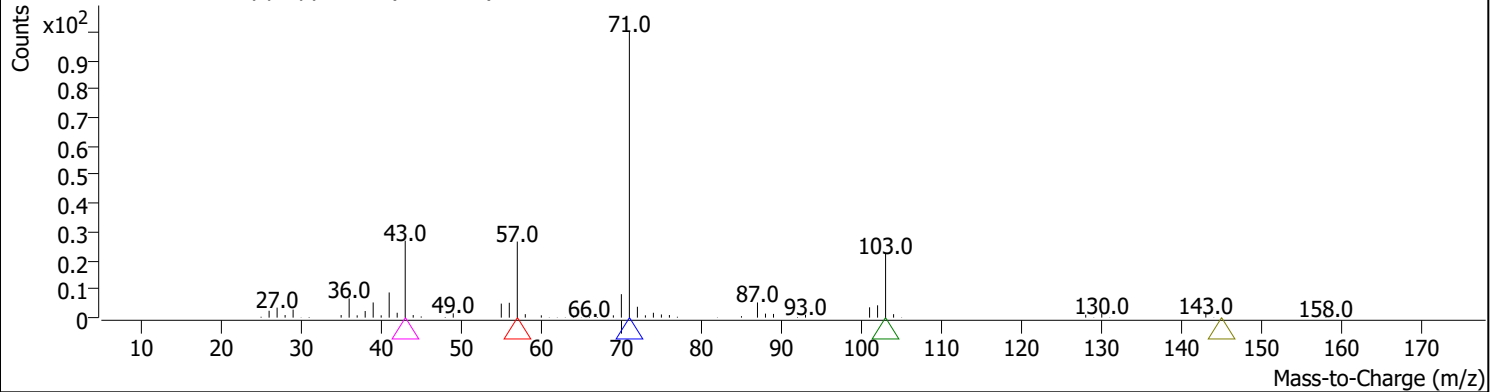
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
52.1417	Butanoic acid, 2,2-dimethylpropyl ester	553692.7	76.7	23361-69-5	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	

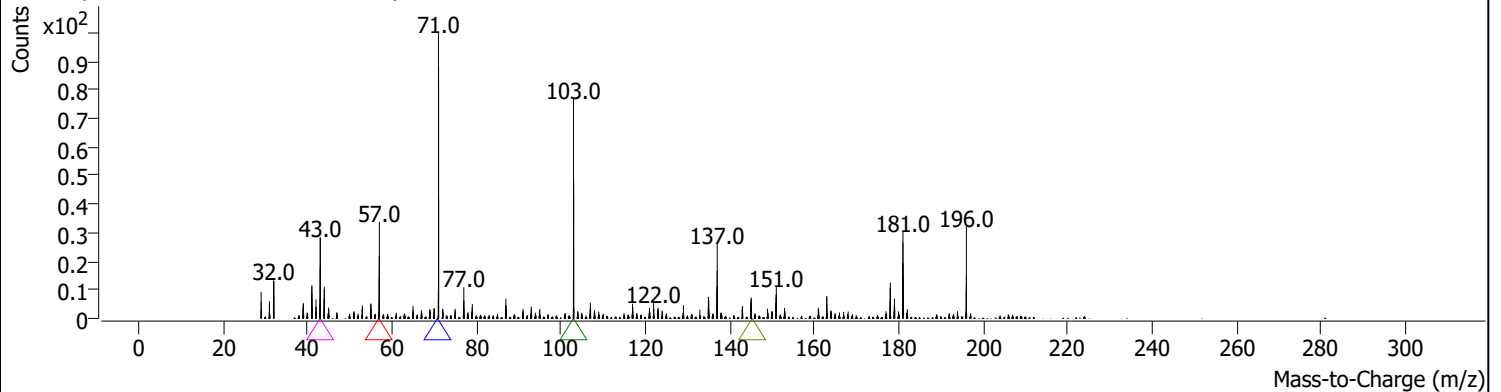
Component RT: 52.1417



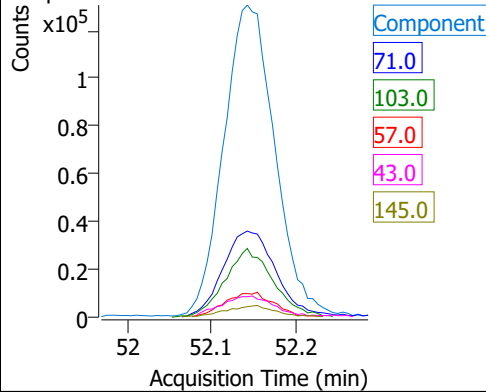
Butanoic acid, 2,2-dimethylpropyl ester (NIST20.L)



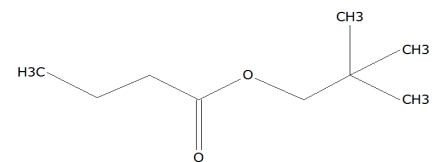
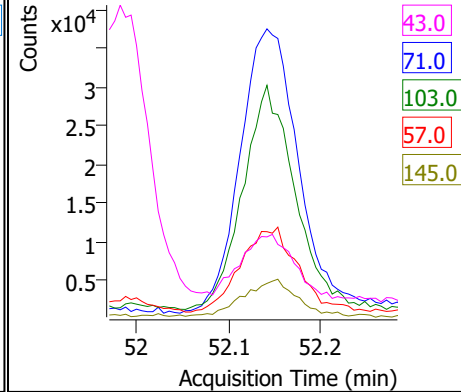
+ Scan (52.0575-52.2431 min, 32 scans) 1.D



Component RT: 52.1417



EIC Peaks





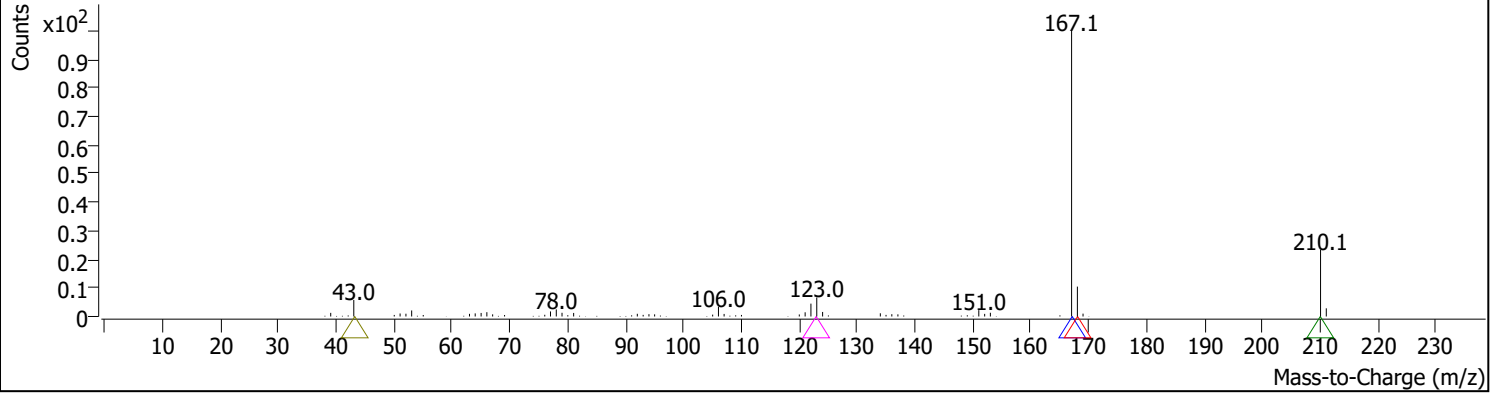
## Library Search Results - NonTarget Hits with Details



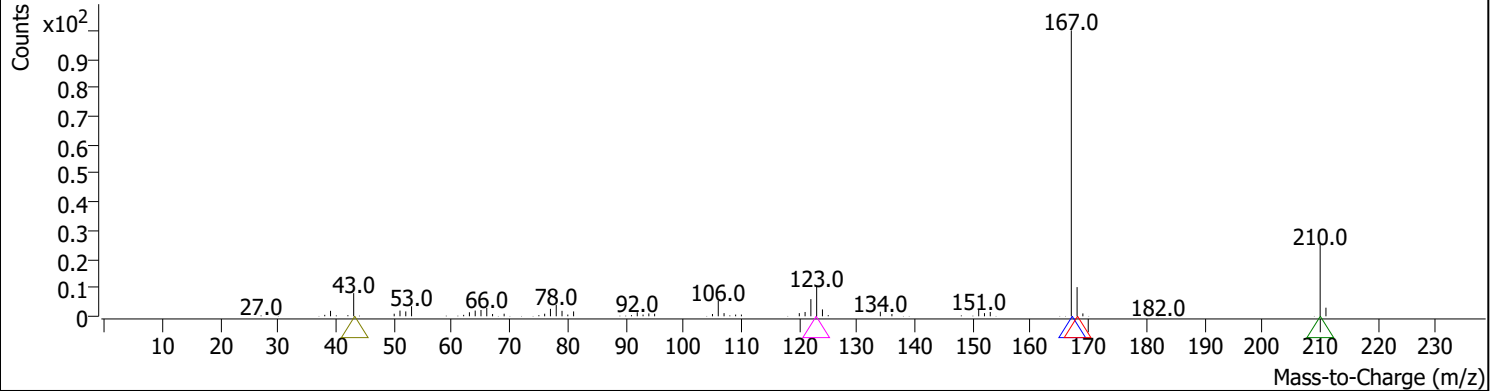
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
53.2264	Syringylacetone	5978717.1	97.7	19037-58-2	C <sub>11</sub> H <sub>14</sub> O <sub>4</sub>	

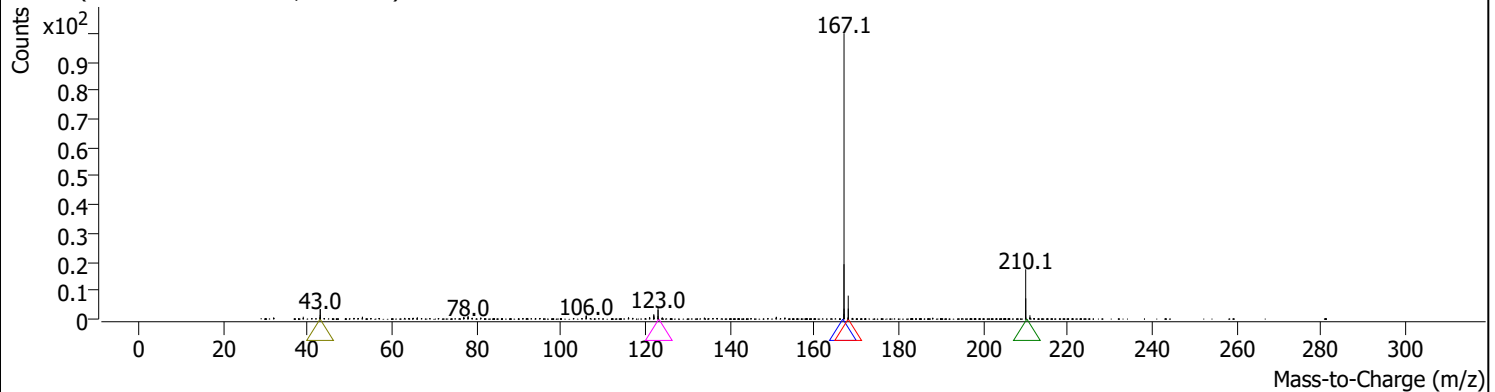
Component RT: 53.2264



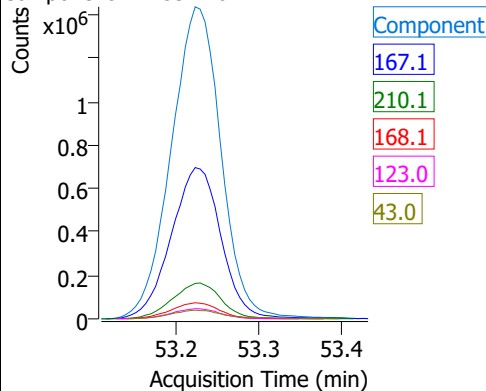
Syringylacetone (NIST20.L)



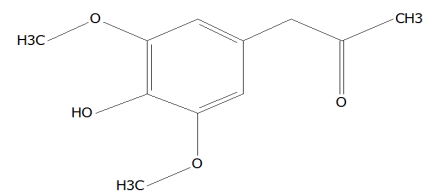
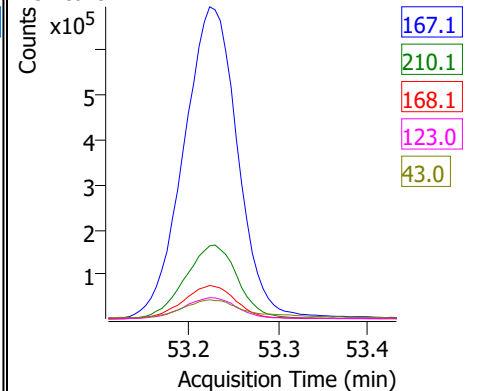
+ Scan (53.1112-53.4145 min, 52 scans) 1.D



Component RT: 53.2264



EIC Peaks



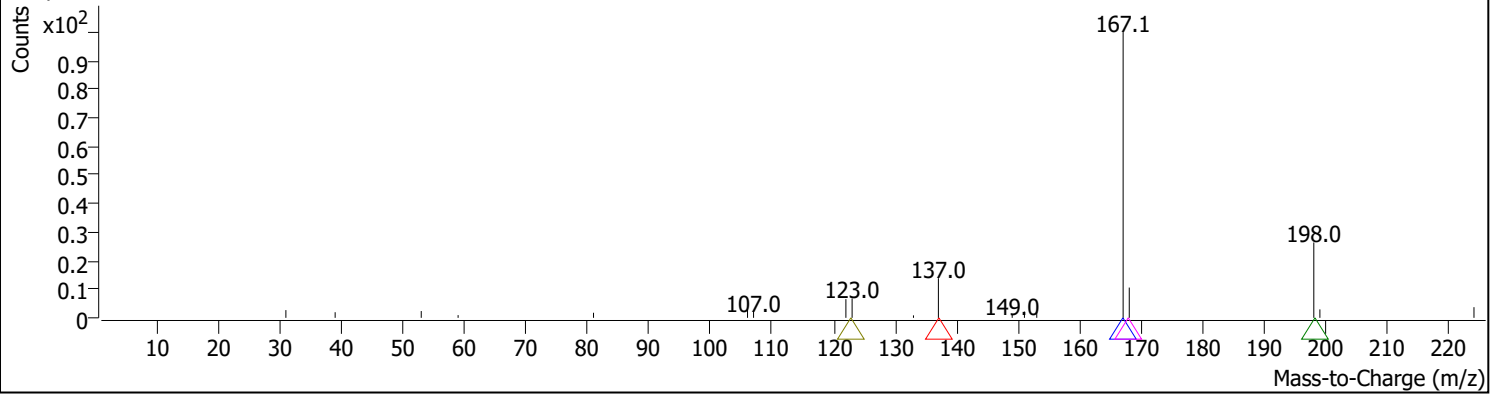
## Library Search Results - NonTarget Hits with Details



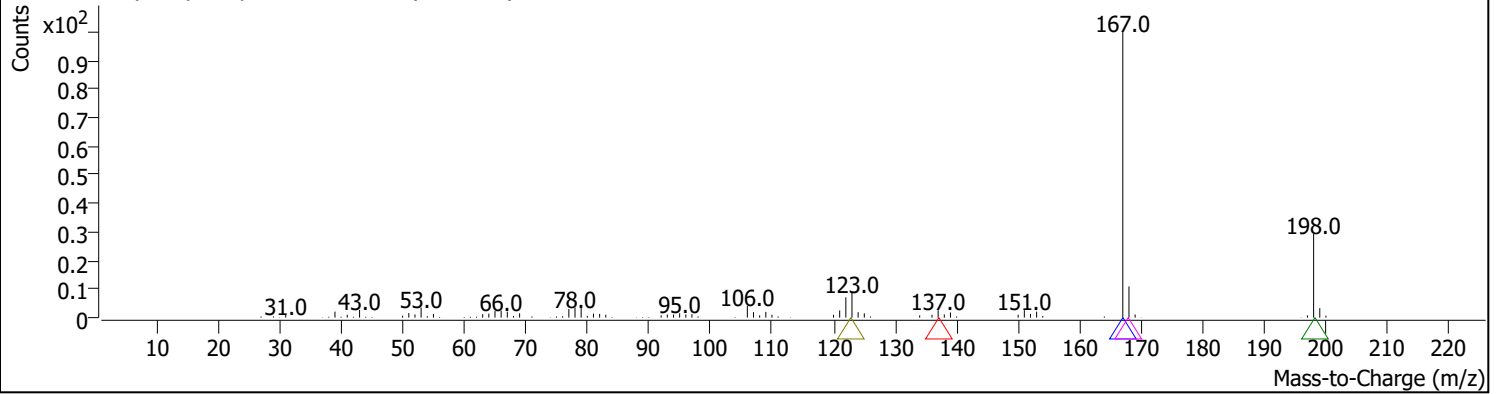
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
53.5885	3,5-Dimethoxy-4-hydroxybenzeneethanol	308310.5	79.4	20824-45-7	C10H14O4	

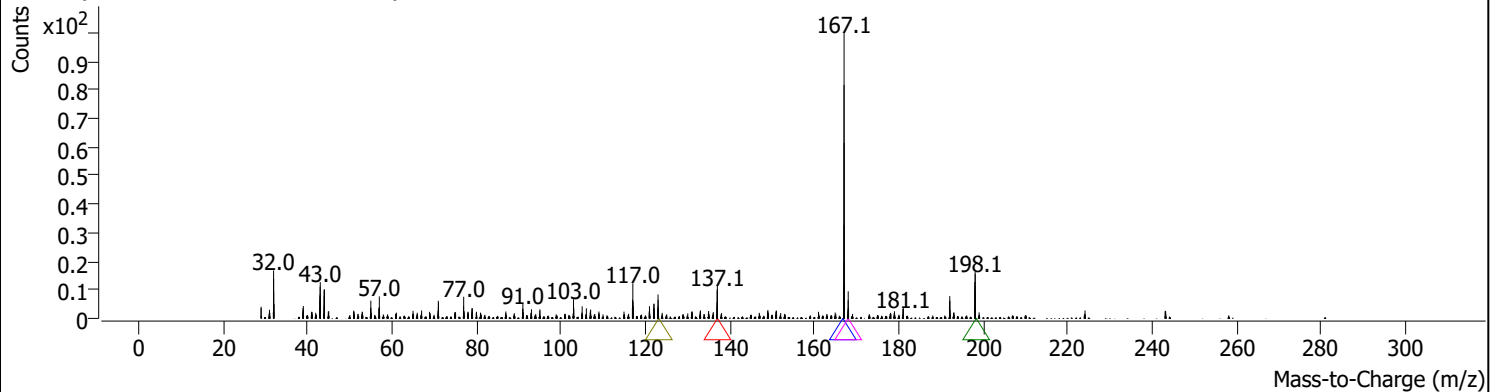
Component RT: 53.5885



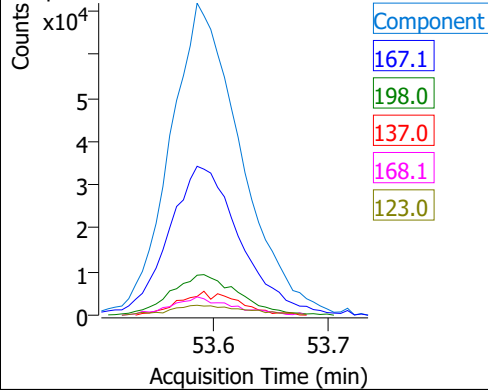
3,5-Dimethoxy-4-hydroxybenzeneethanol (NIST20.L)



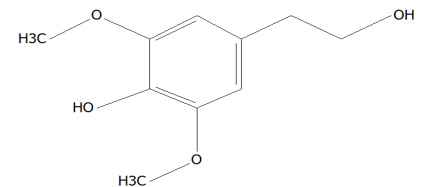
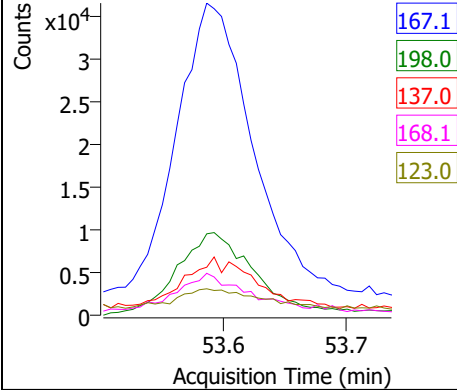
+ Scan (53.5076-53.7058 min, 34 scans) 1.D



Component RT: 53.5885



EIC Peaks



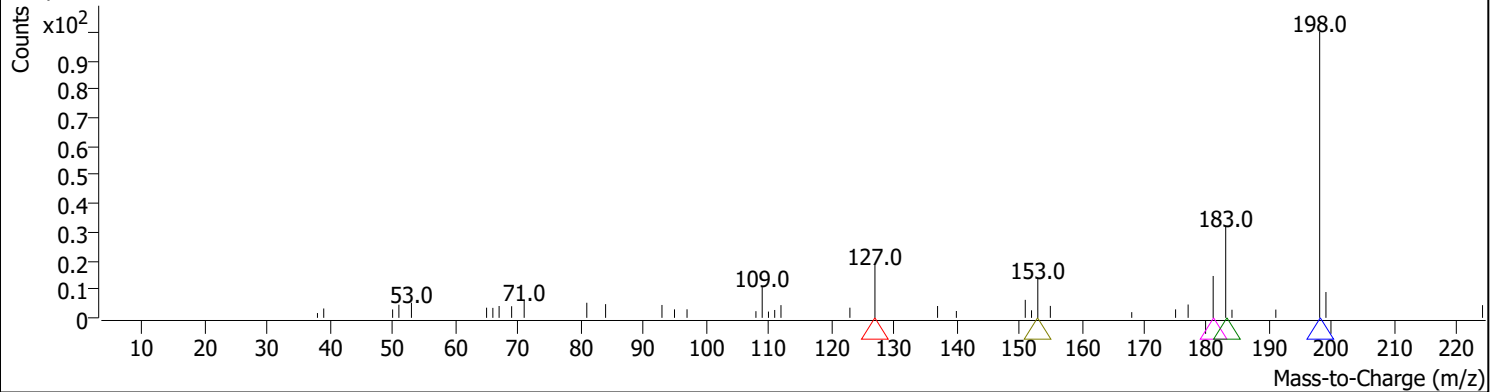
## Library Search Results - NonTarget Hits with Details



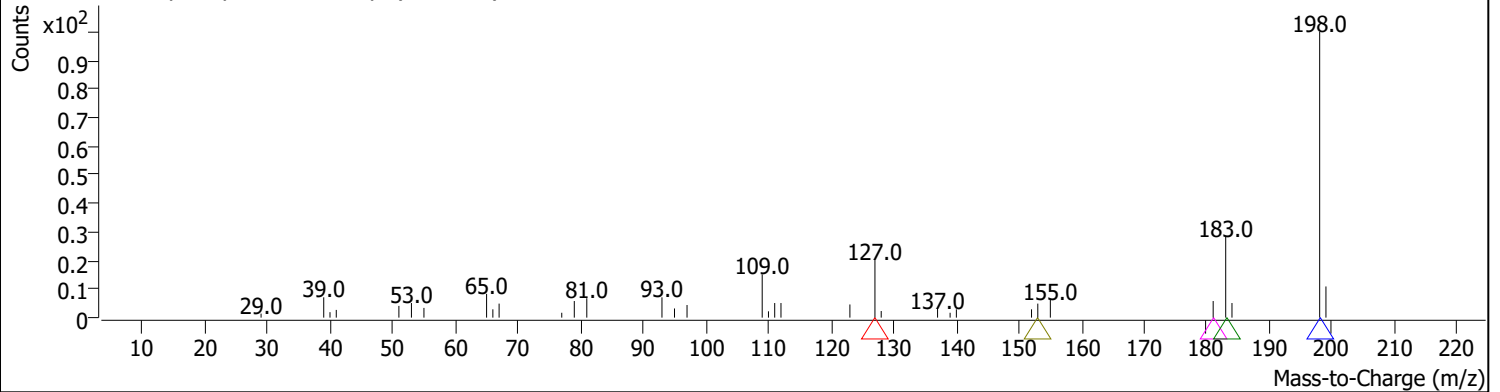
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
54.9294	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	621745.1	85.0	530-57-4	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	

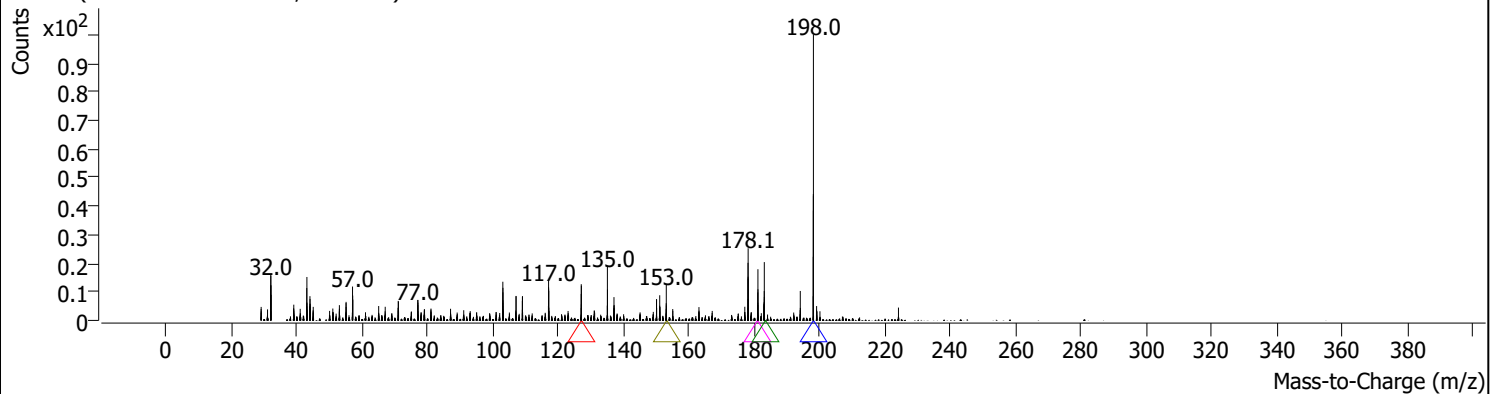
Component RT: 54.9294



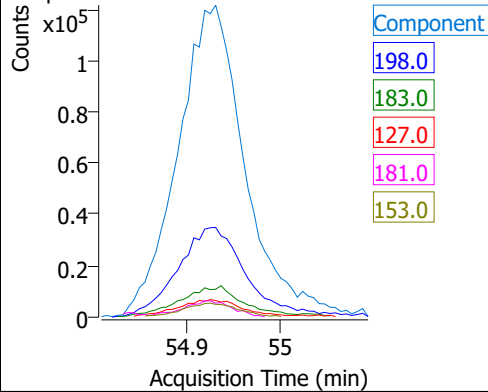
Benzoic acid, 4-hydroxy-3,5-dimethoxy- (NIST20.L)



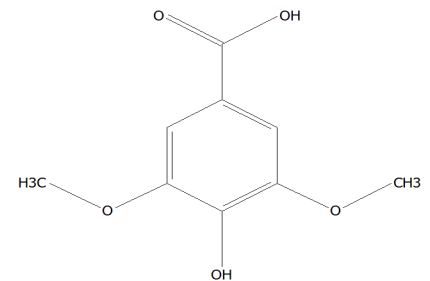
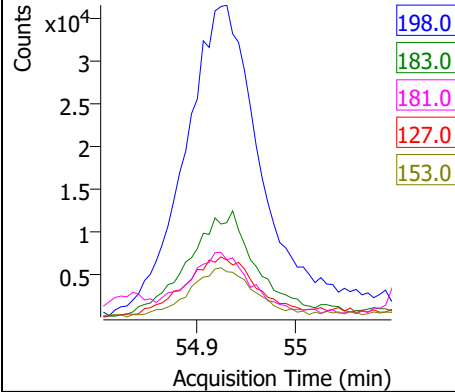
+ Scan (54.8217-55.0972 min, 47 scans) 1.D



Component RT: 54.9294



EIC Peaks



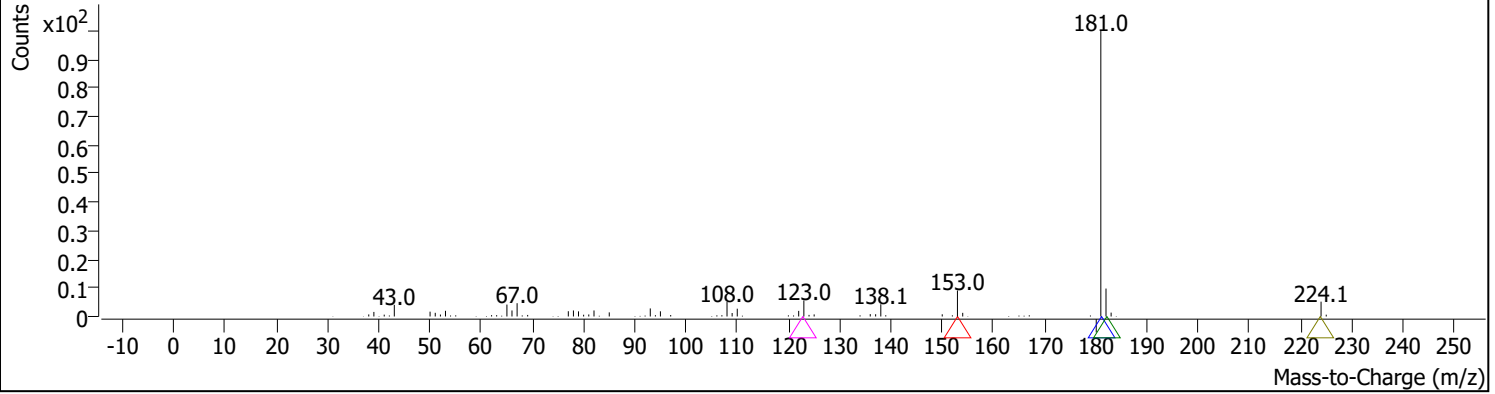
## Library Search Results - NonTarget Hits with Details



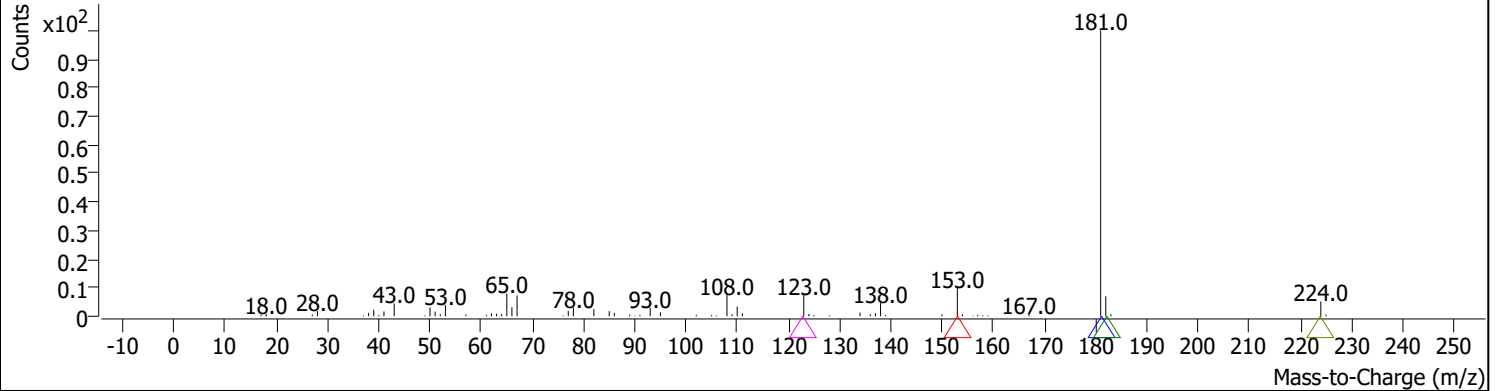
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
55.1887	Butylsyringone	5238788.3	92.8	69271-91-6	C <sub>12</sub> H <sub>16</sub> O <sub>4</sub>	

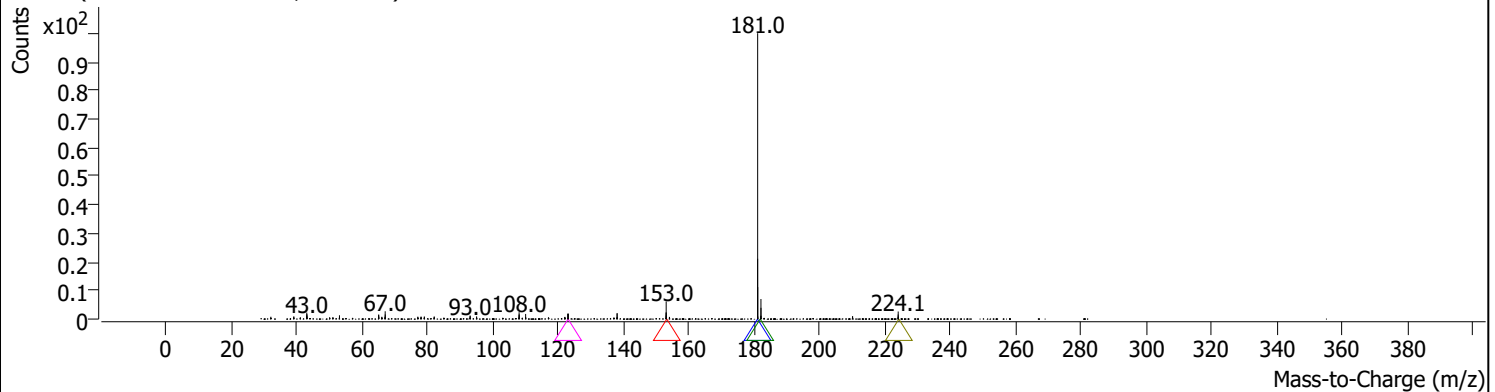
Component RT: 55.1887



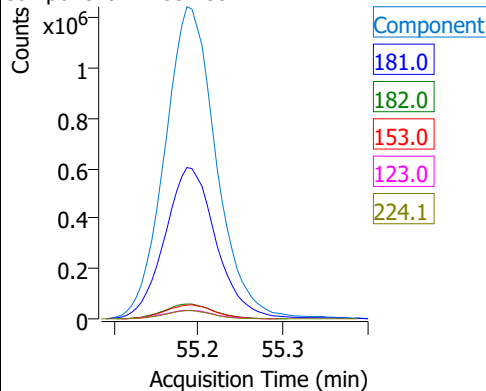
Butylsyringone (NIST20.L)



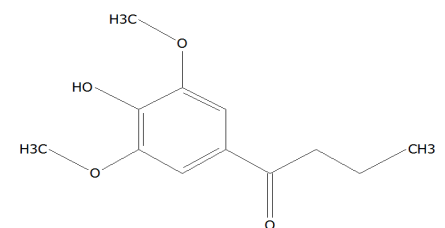
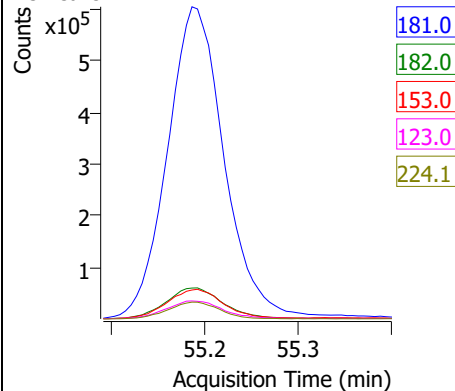
+ Scan (55.0912-55.4004 min, 53 scans) 1.D



Component RT: 55.1887



EIC Peaks



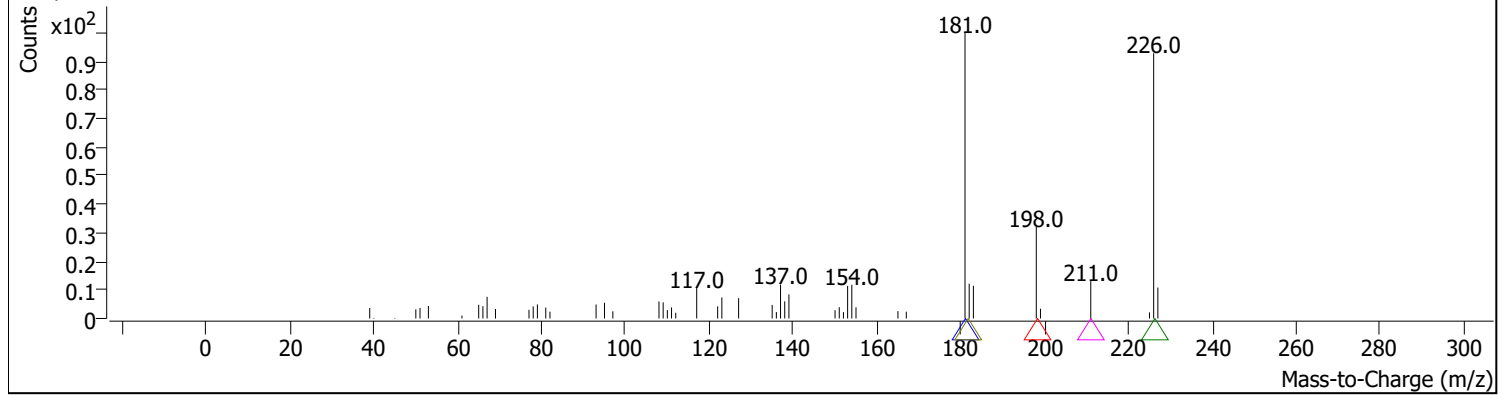
## Library Search Results - NonTarget Hits with Details



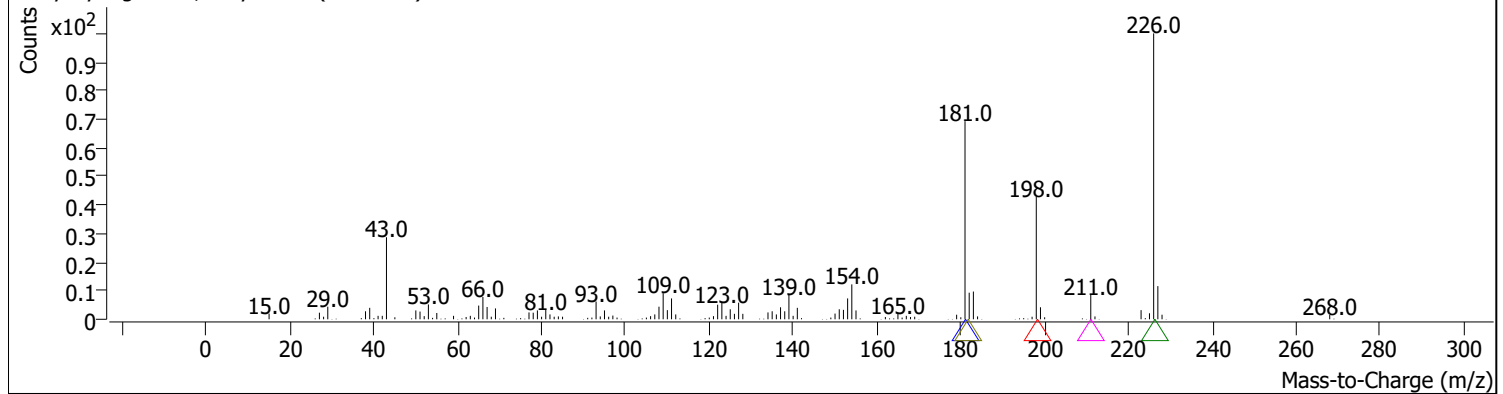
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
55.6079	Acetyl syringic acid, ethyl ester	586028.4	87.9	1000454-70-9	C <sub>13</sub> H <sub>16</sub> O <sub>6</sub>	

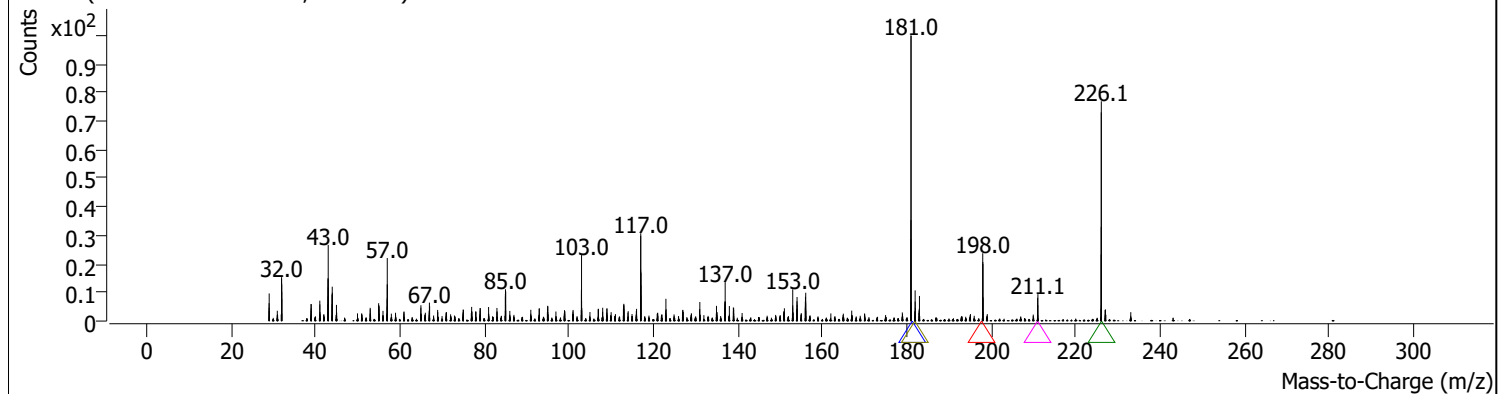
Component RT: 55.6079



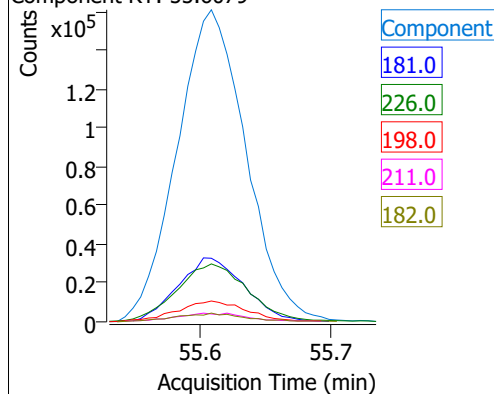
Acetyl syringic acid, ethyl ester (NIST20.L)



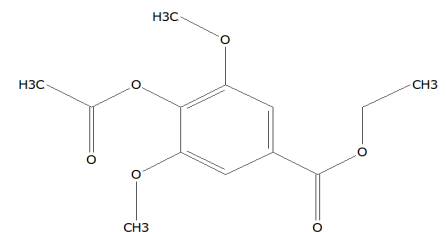
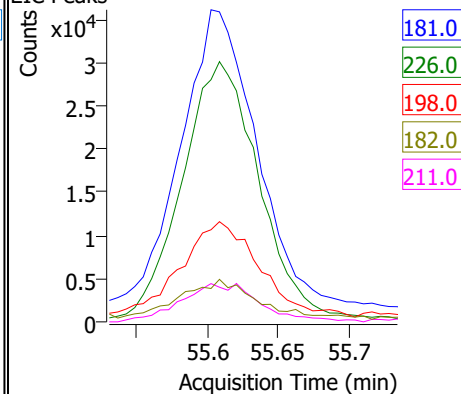
+ Scan (55.5259-55.7334 min, 35 scans) 1.D



Component RT: 55.6079



EIC Peaks



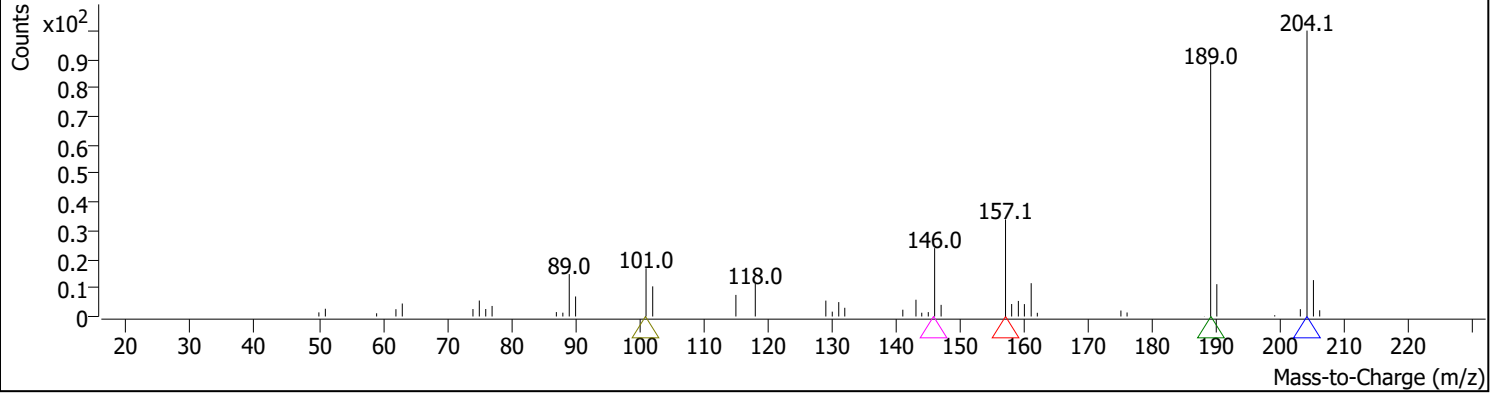
## Library Search Results - NonTarget Hits with Details



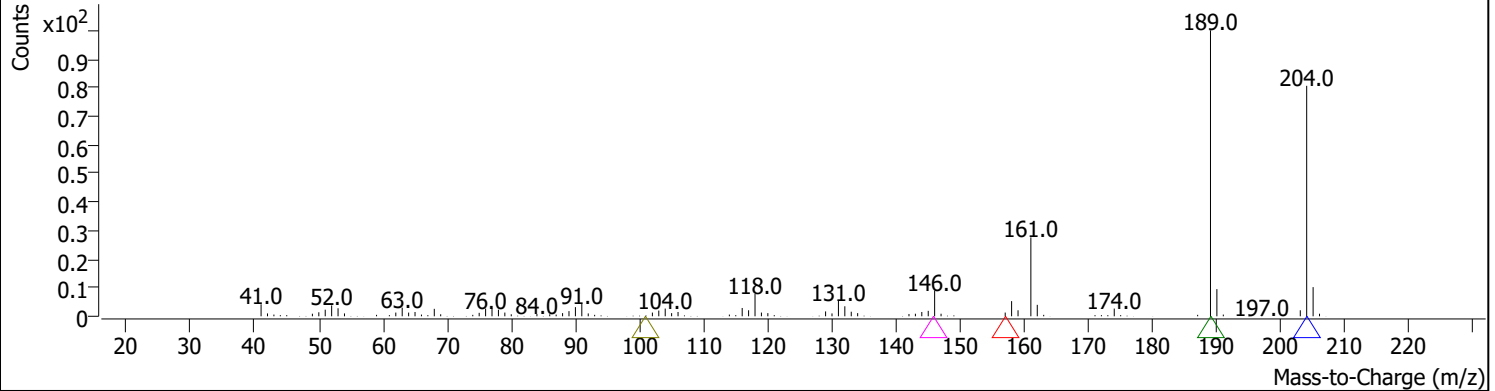
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
56.0900	2,3-Dimethoxy-5-aminocinnamionitrile	821559.2	79.6	1000214-46-5	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	

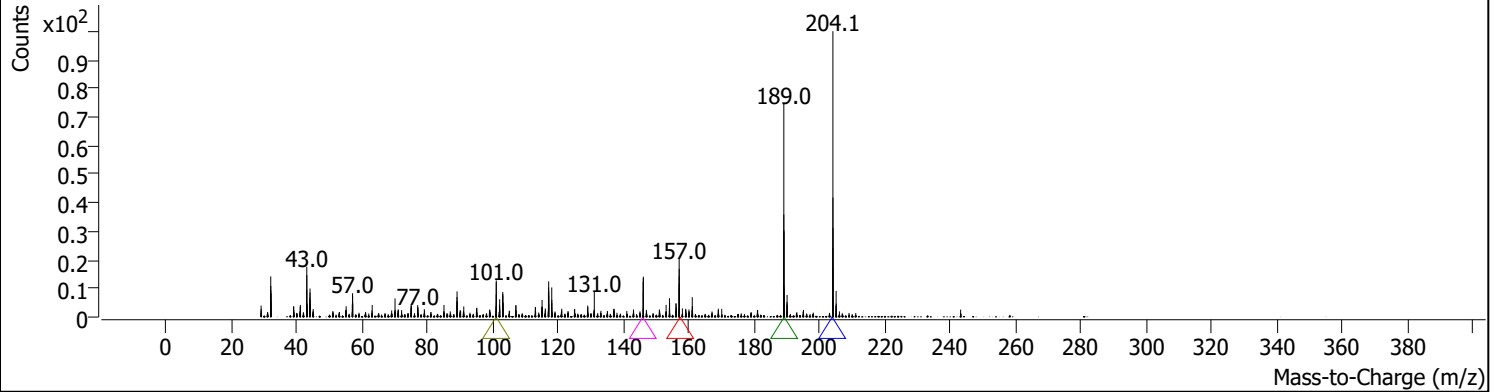
Component RT: 56.0900



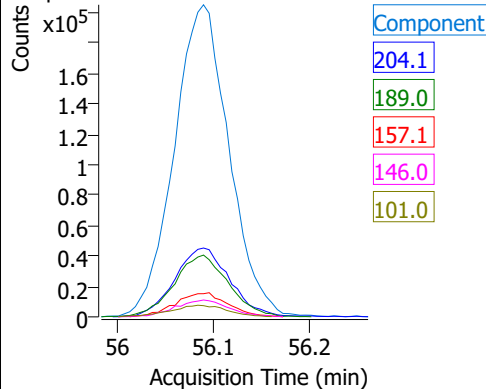
2,3-Dimethoxy-5-aminocinnamionitrile (NIST20.L)



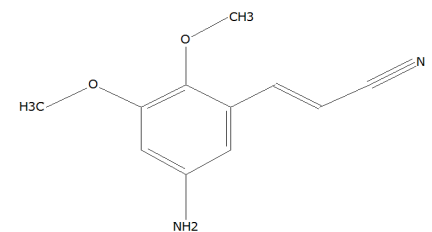
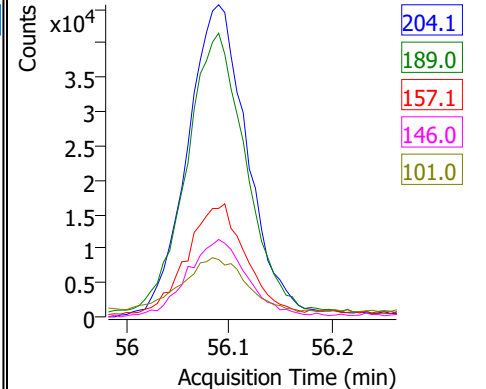
+ Scan (55.9924-56.2626 min, 46 scans) 1.D



Component RT: 56.0900



EIC Peaks



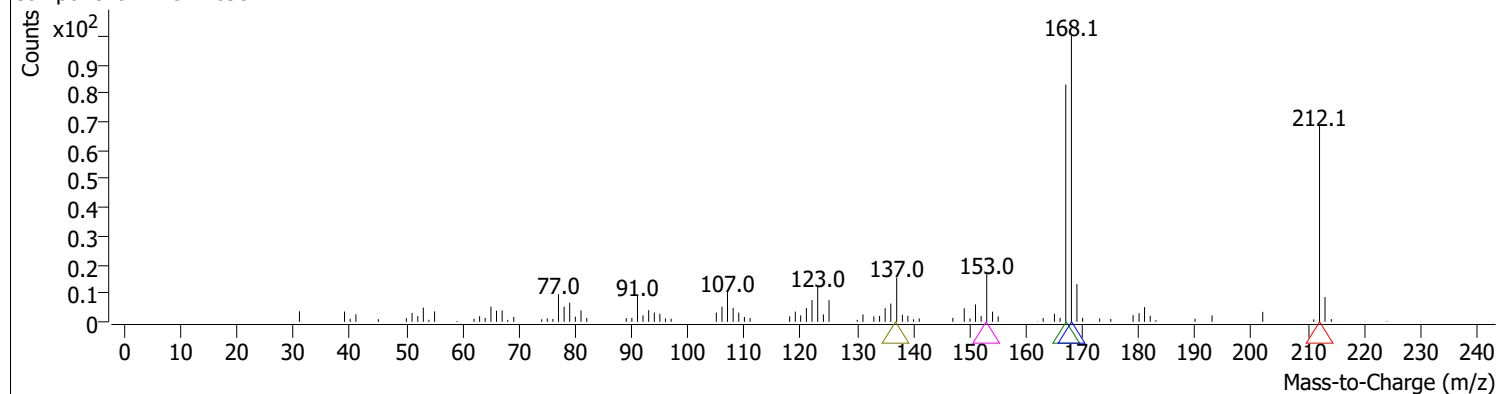
## Library Search Results - NonTarget Hits with Details



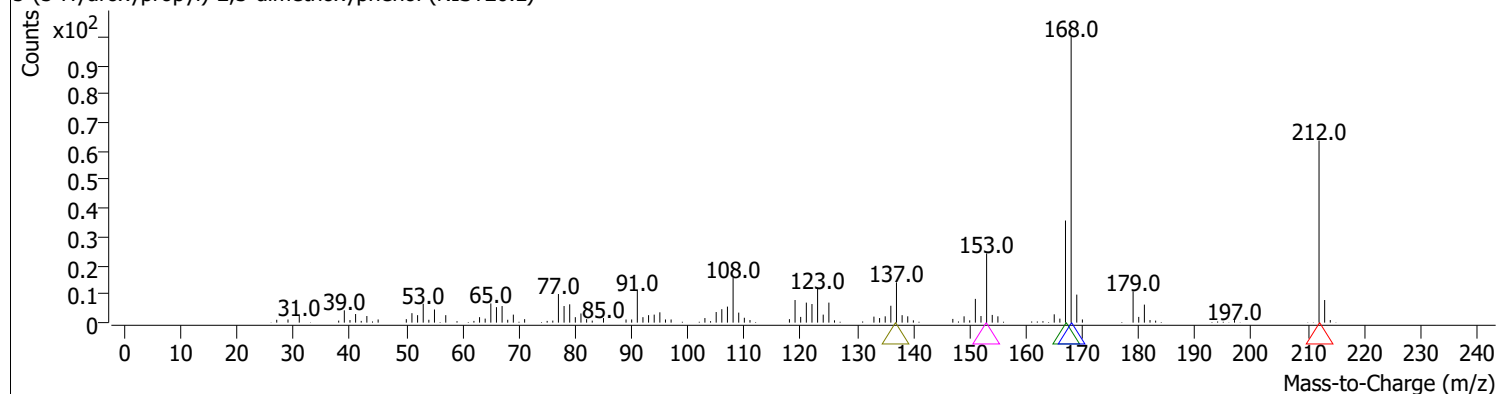
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
57.4695	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	2046714.7	92.7	63543-12-4	C11H16O4	

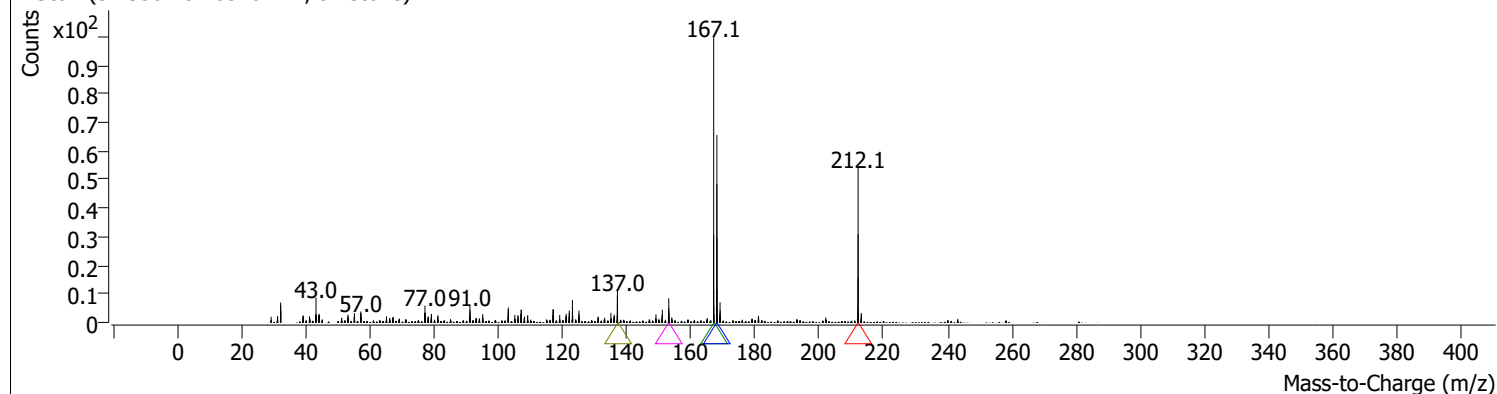
Component RT: 57.4695



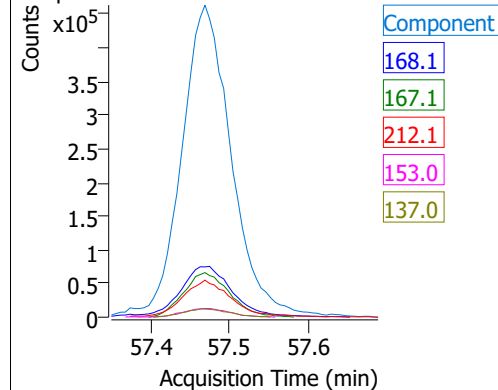
5-(3-Hydroxypropyl)-2,3-dimethoxyphenol (NIST20.L)



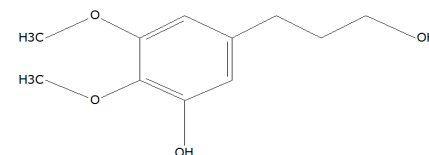
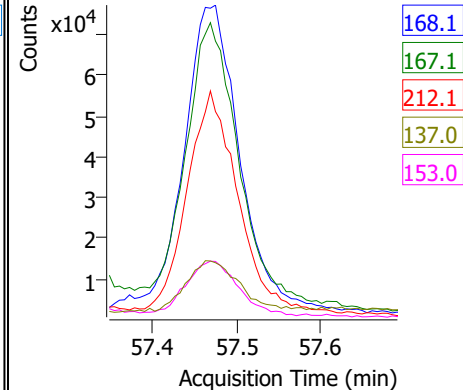
+ Scan (57.3507-57.6540 min, 52 scans) 1.D



Component RT: 57.4695



EIC Peaks



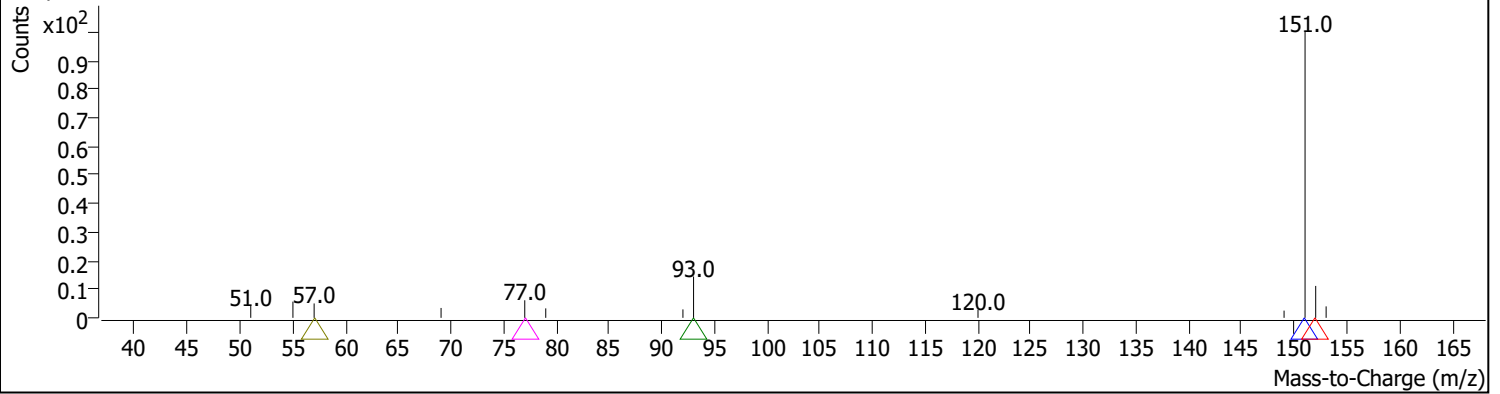
## Library Search Results - NonTarget Hits with Details



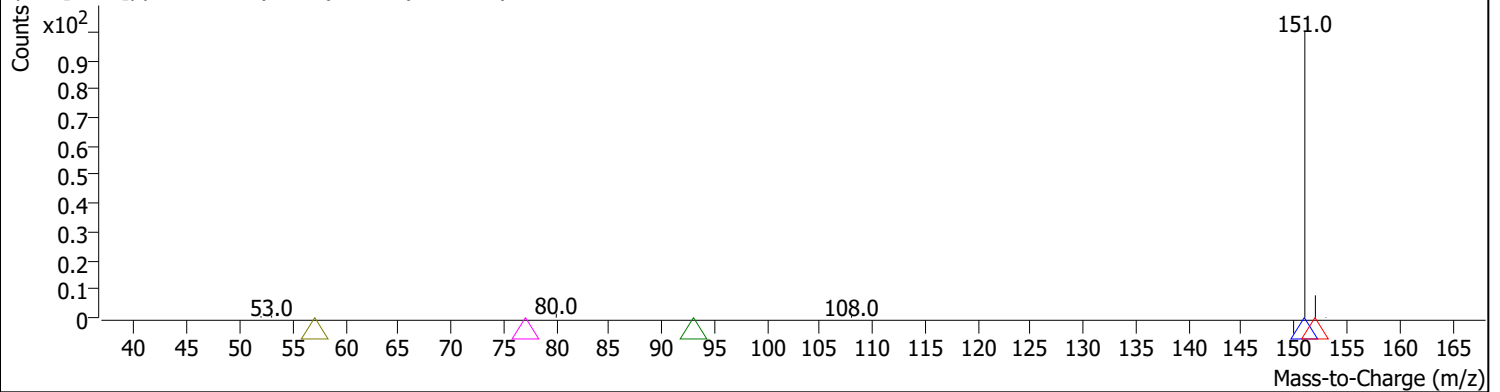
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
63.6296	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	592568.4	76.5	65996-50-1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	

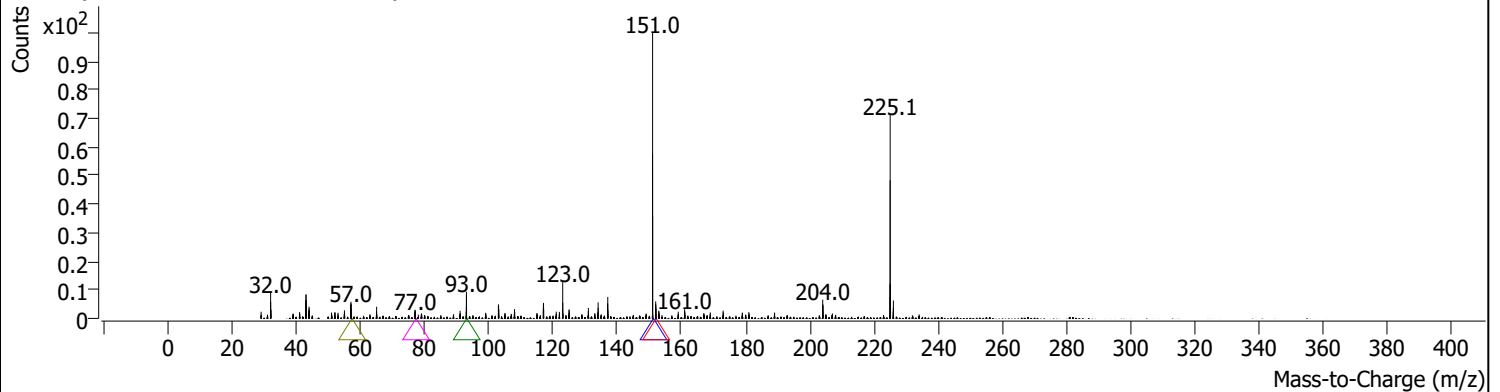
Component RT: 63.6296



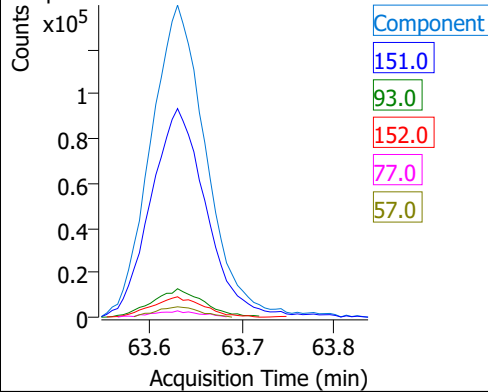
Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)



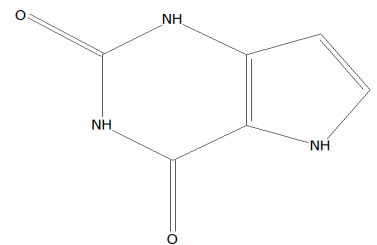
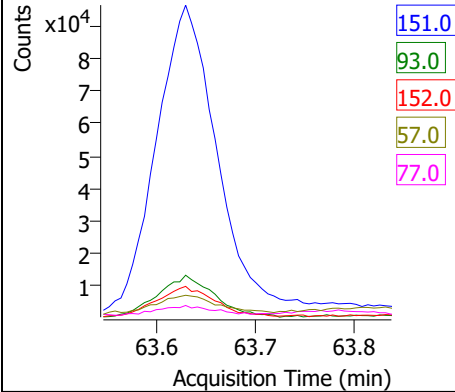
+ Scan (63.5413-63.8429 min, 50 scans) 1.D



Component RT: 63.6296



EIC Peaks





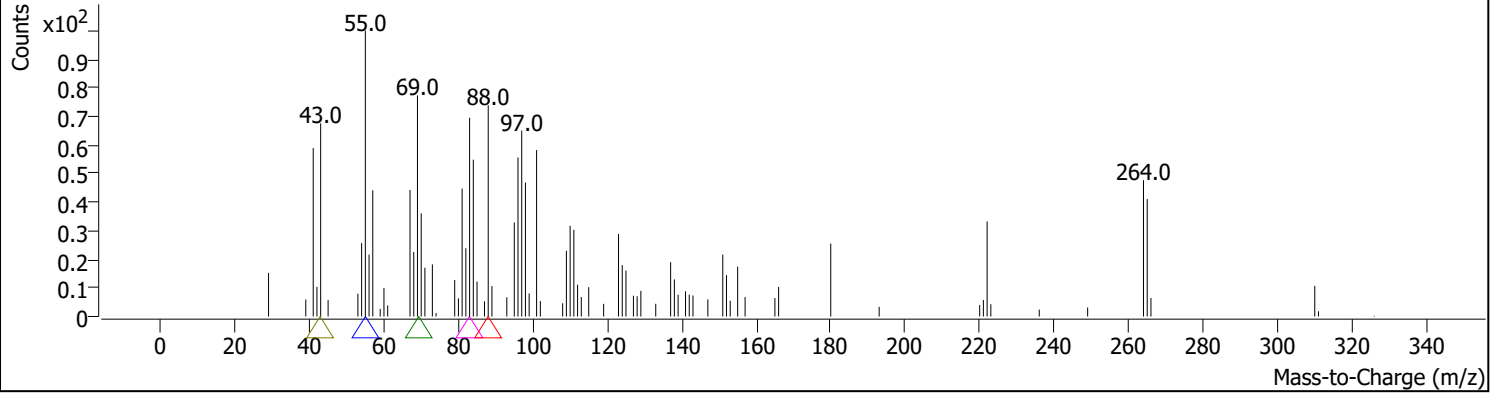
## Library Search Results - NonTarget Hits with Details



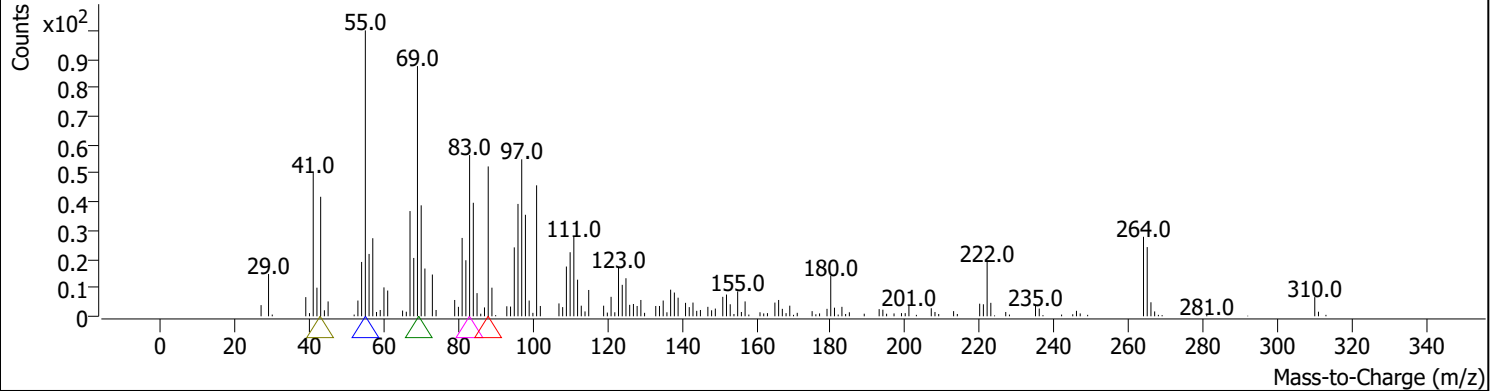
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
66.3277	(E)-9-Octadecenoic acid ethyl ester	1204905.9	89.6	6114-18-7	C20H38O2	

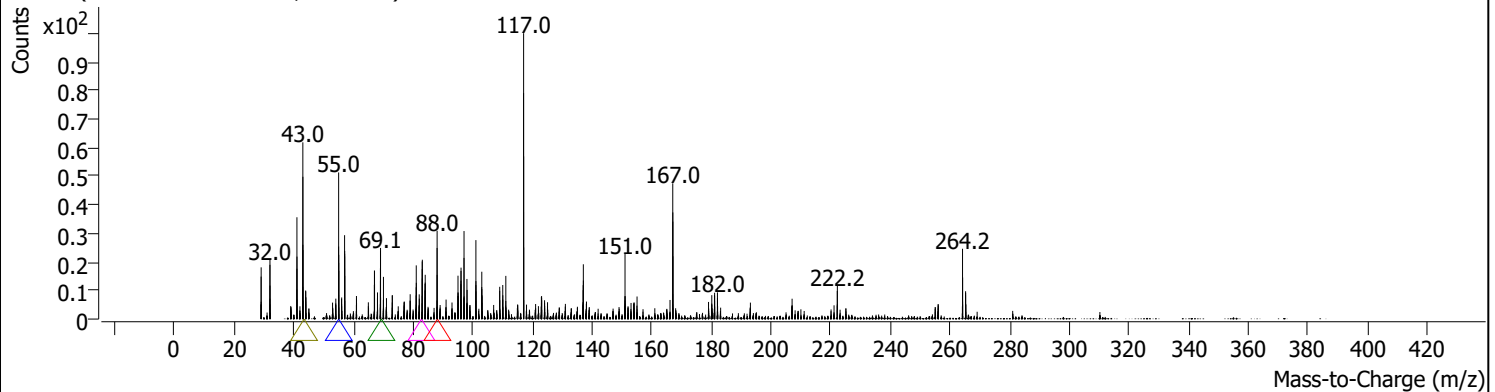
Component RT: 66.3277



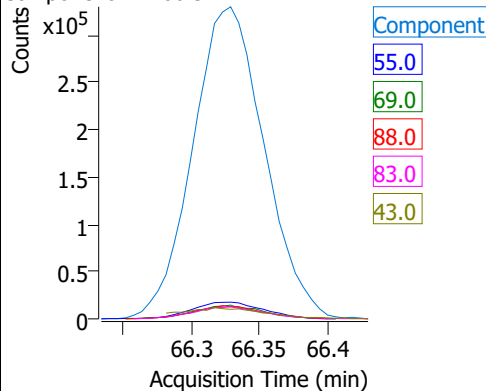
(E)-9-Octadecenoic acid ethyl ester (NIST20.L)



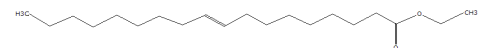
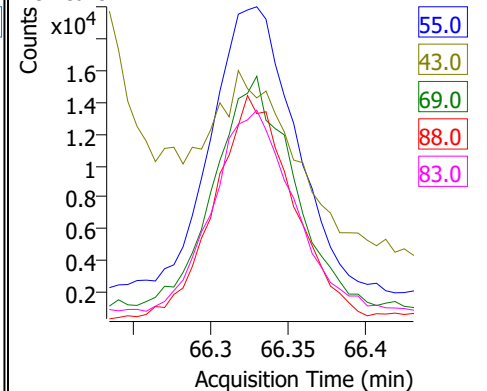
+ Scan (66.2501-66.4285 min, 30 scans) 1.D



Component RT: 66.3277



EIC Peaks



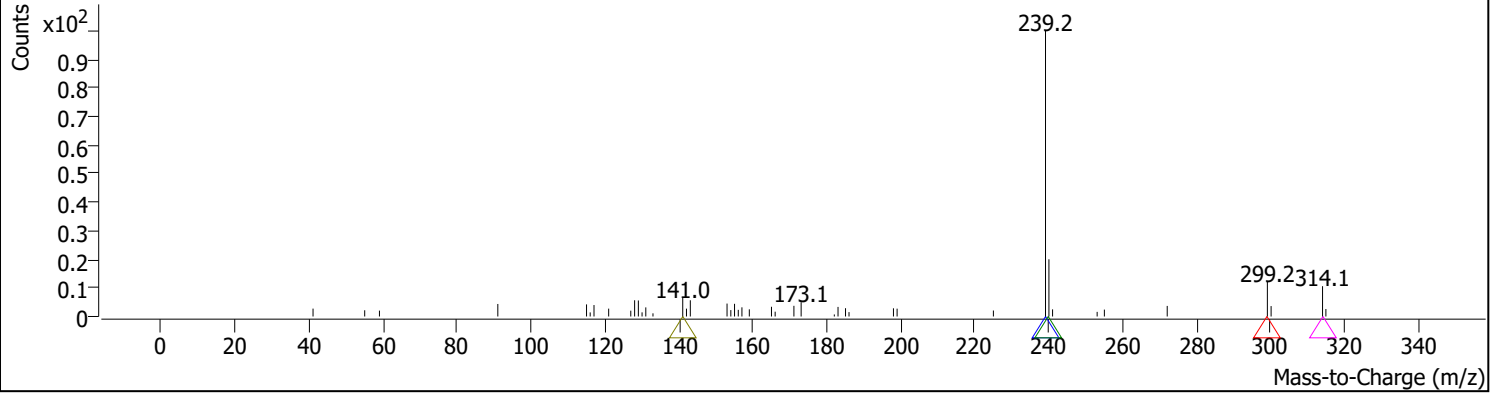
## Library Search Results - NonTarget Hits with Details



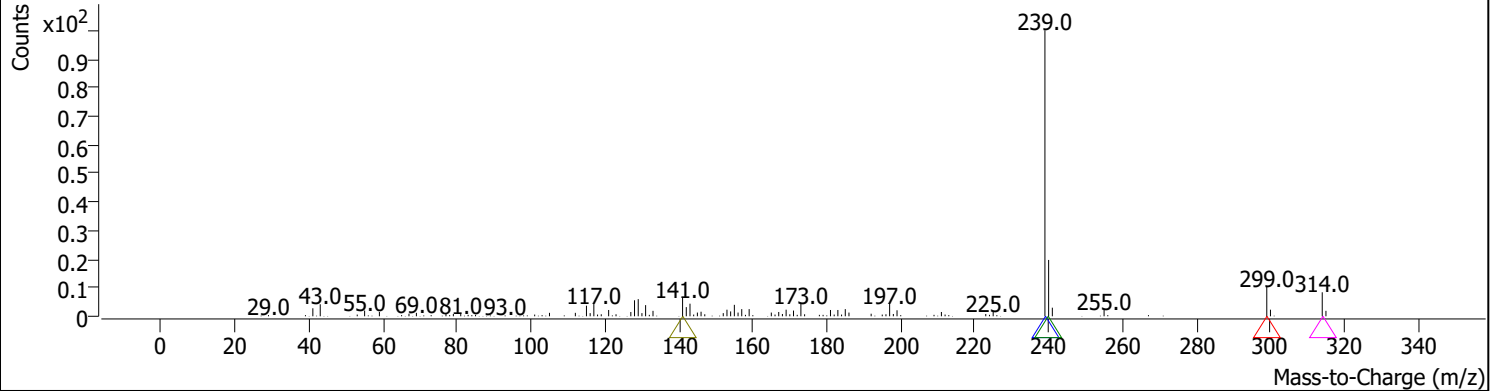
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
70.9141	Methyl dehydroabietate	544068.0	83.3	1235-74-1	C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>	

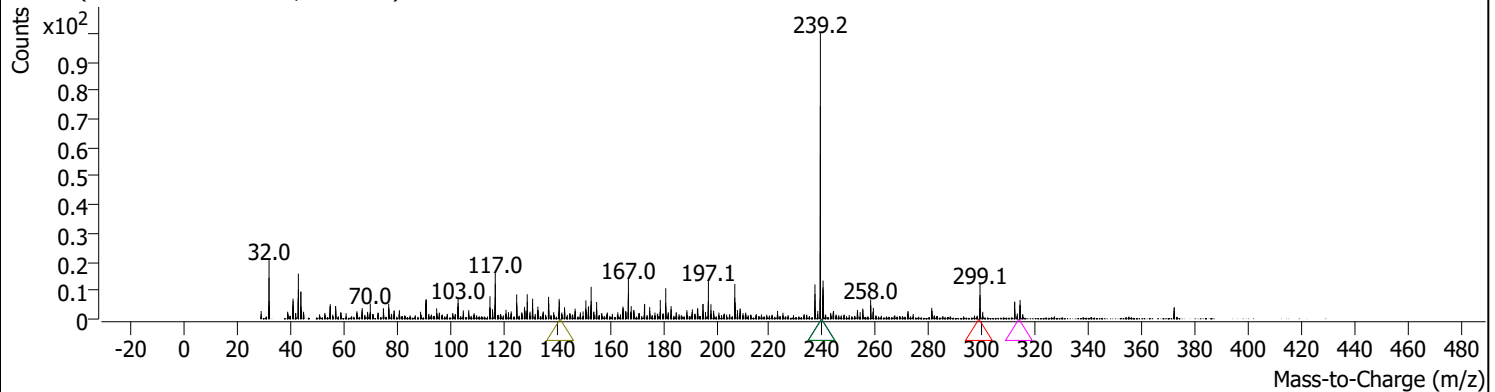
Component RT: 70.9141



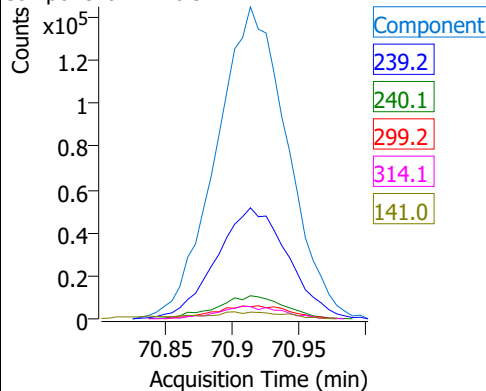
Methyl dehydroabietate (NIST20.L)



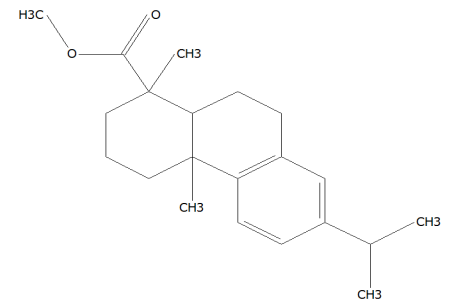
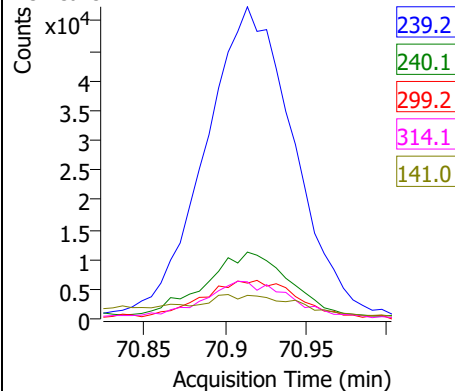
+ Scan (70.8245-71.0036 min, 31 scans) 1.D



Component RT: 70.9141



EIC Peaks



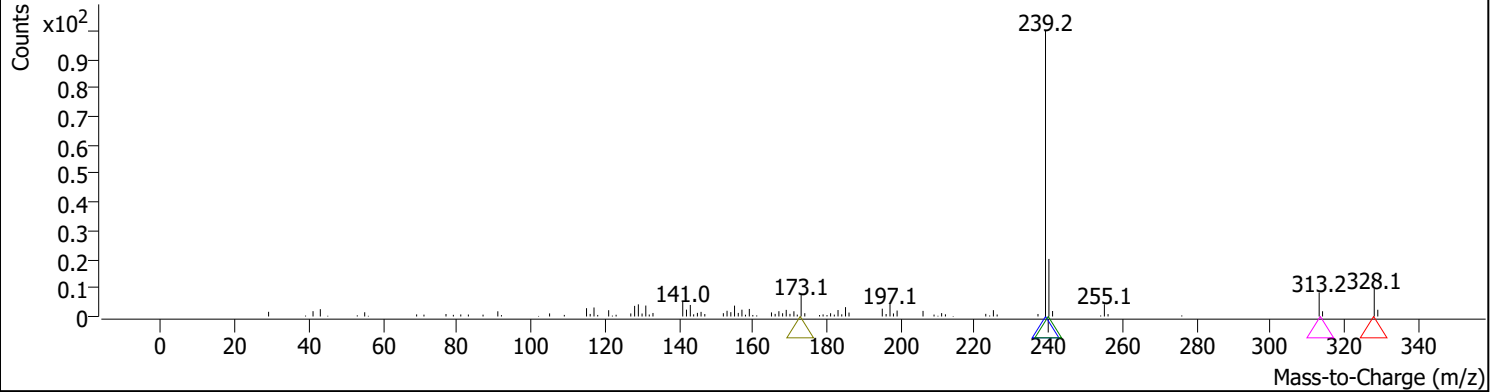
## Library Search Results - NonTarget Hits with Details



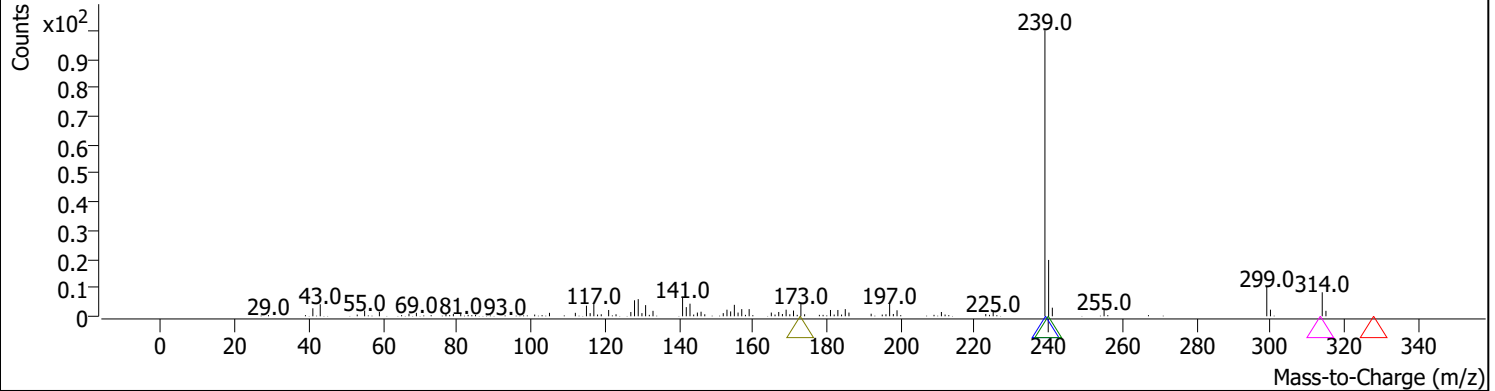
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
72.3540	Methyl dehydroabietate	2231742.9	76.5	1235-74-1	C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>	

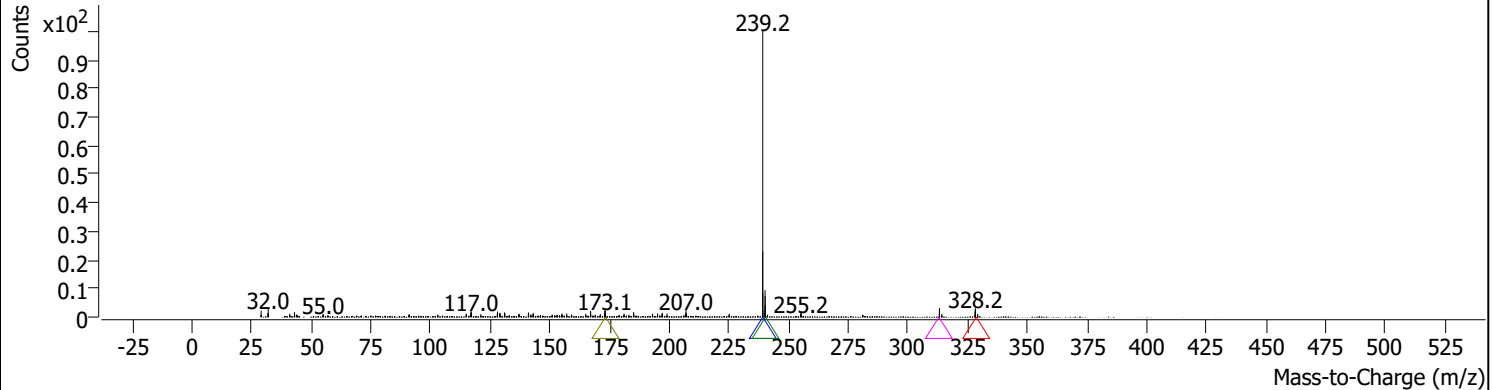
Component RT: 72.3540



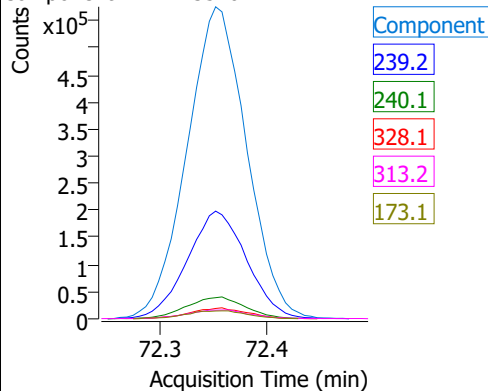
Methyl dehydroabietate (NIST20.L)



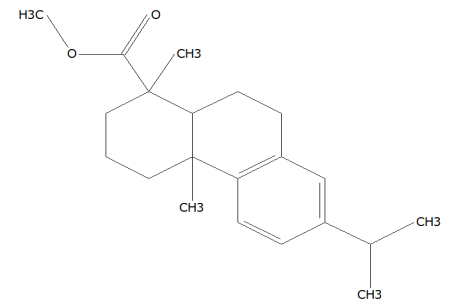
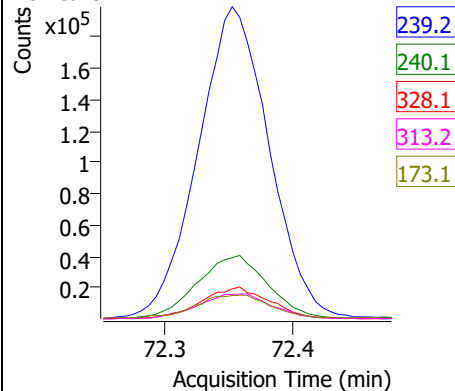
+ Scan (72.2575-72.4775 min, 38 scans) 1.D



Component RT: 72.3540



EIC Peaks



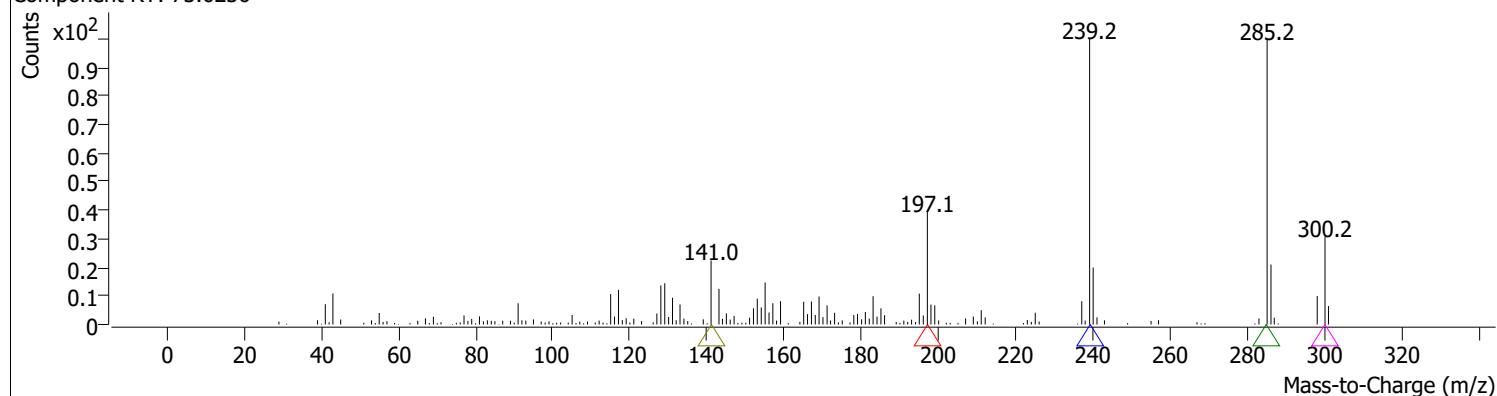
## Library Search Results - NonTarget Hits with Details



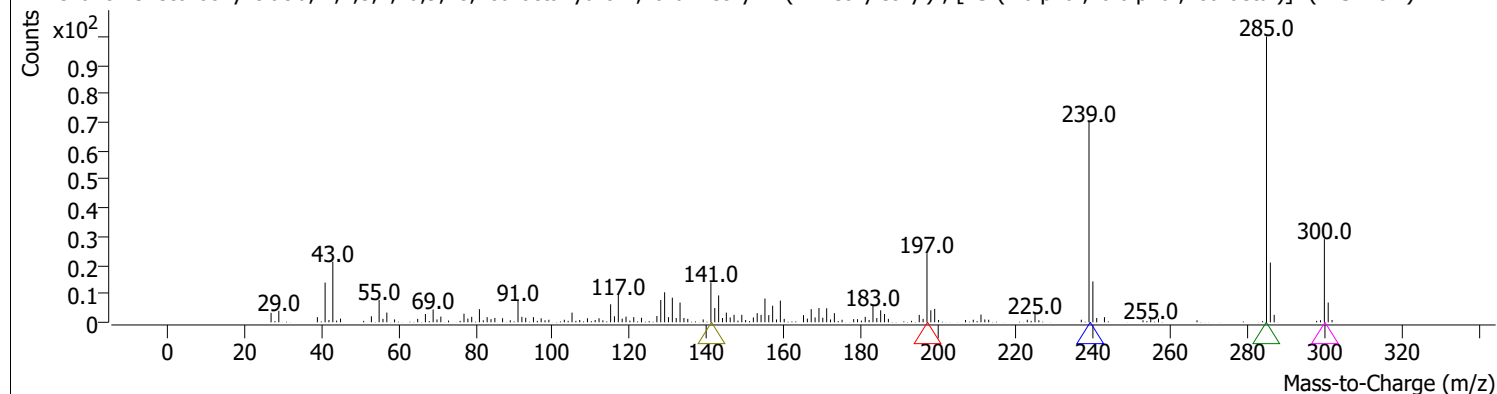
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
73.6236	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-	10413462.8	93.3	5155-70-4	C20H28O2	

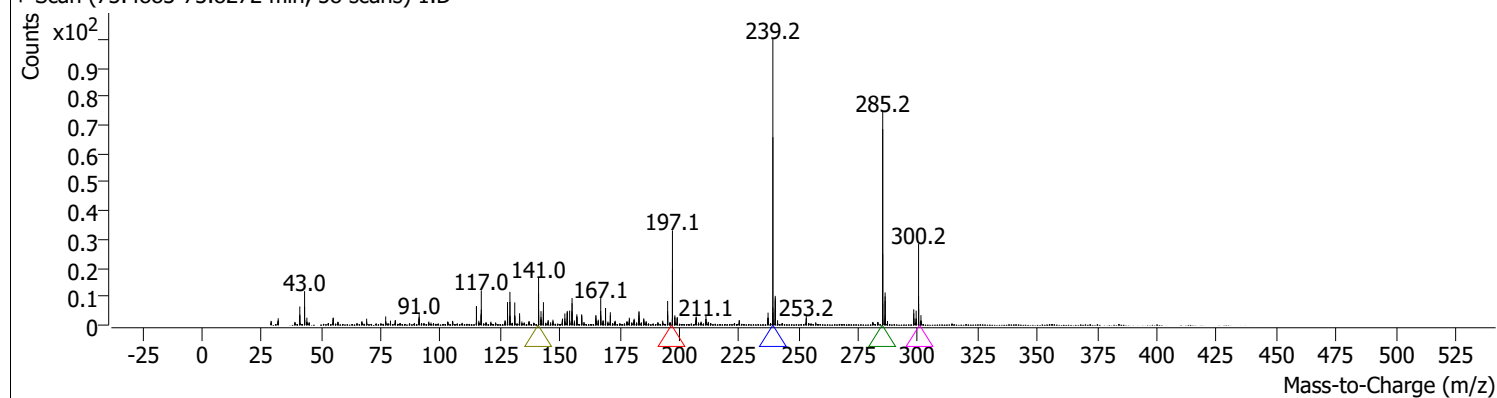
Component RT: 73.6236



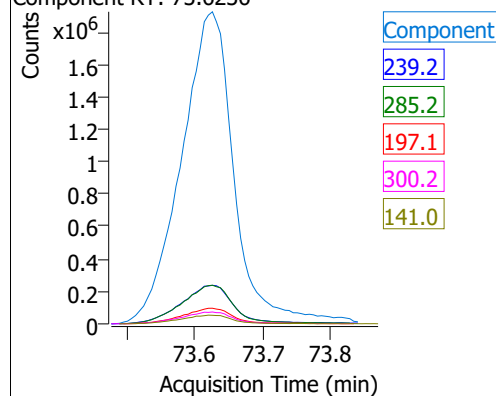
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]- (NIST20.L)



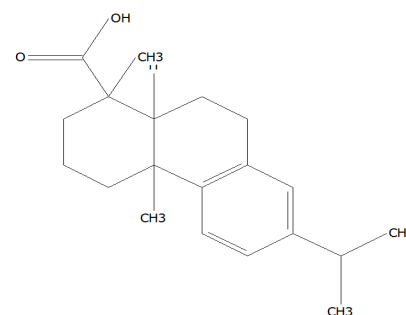
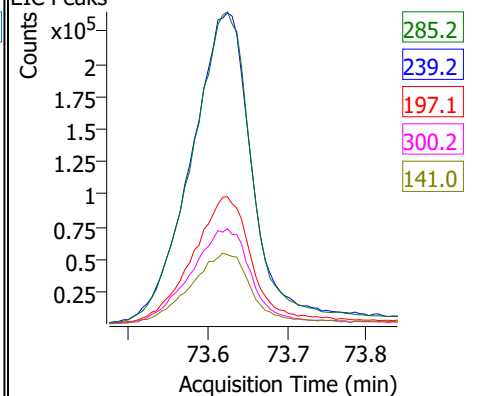
+ Scan (73.4883-73.8272 min, 58 scans) 1.D



Component RT: 73.6236



EIC Peaks



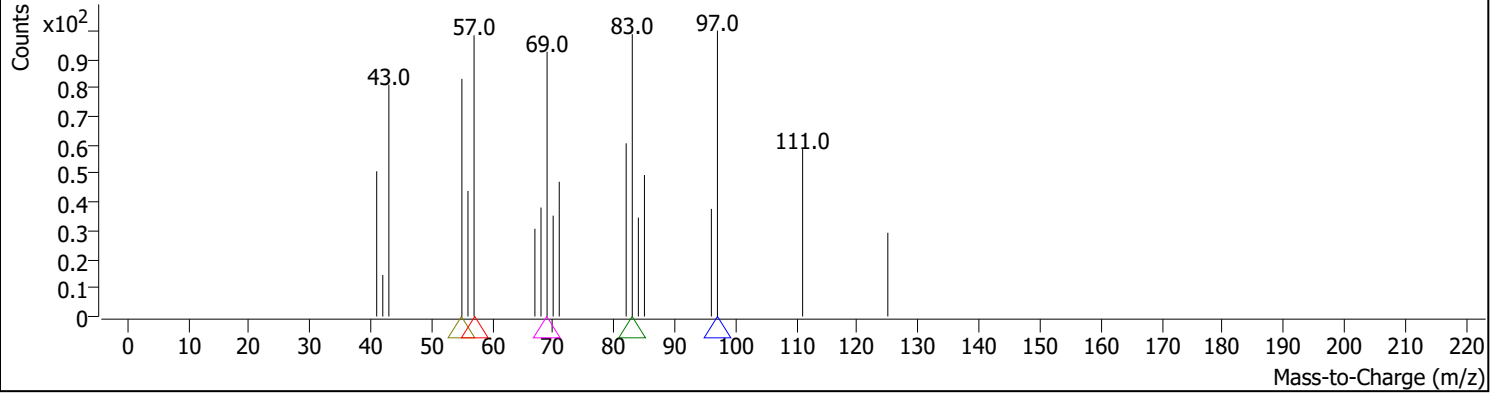
## Library Search Results - NonTarget Hits with Details



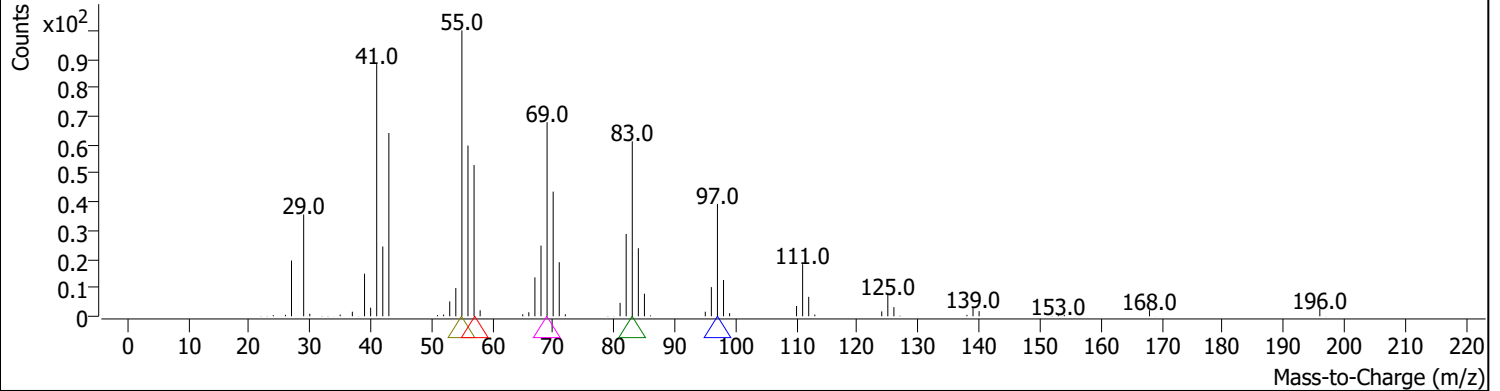
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
75.3528	Cyclotetradecane	268574.4	84.5	295-17-0	C <sub>14</sub> H <sub>28</sub>	

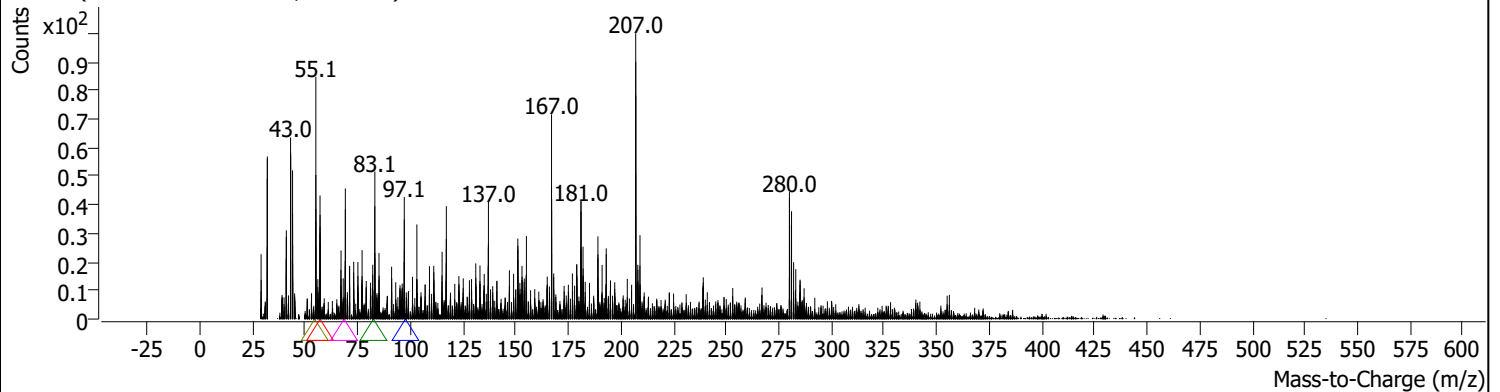
Component RT: 75.3528



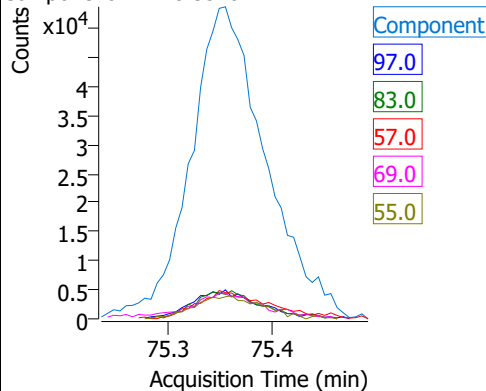
Cyclotetradecane (NIST20.L)



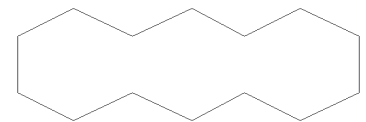
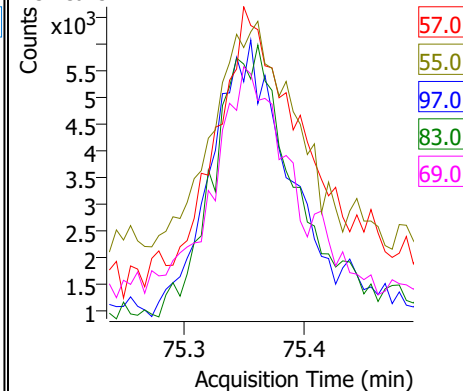
+ Scan (75.2743-75.4743 min, 34 scans) 1.D



Component RT: 75.3528



EIC Peaks



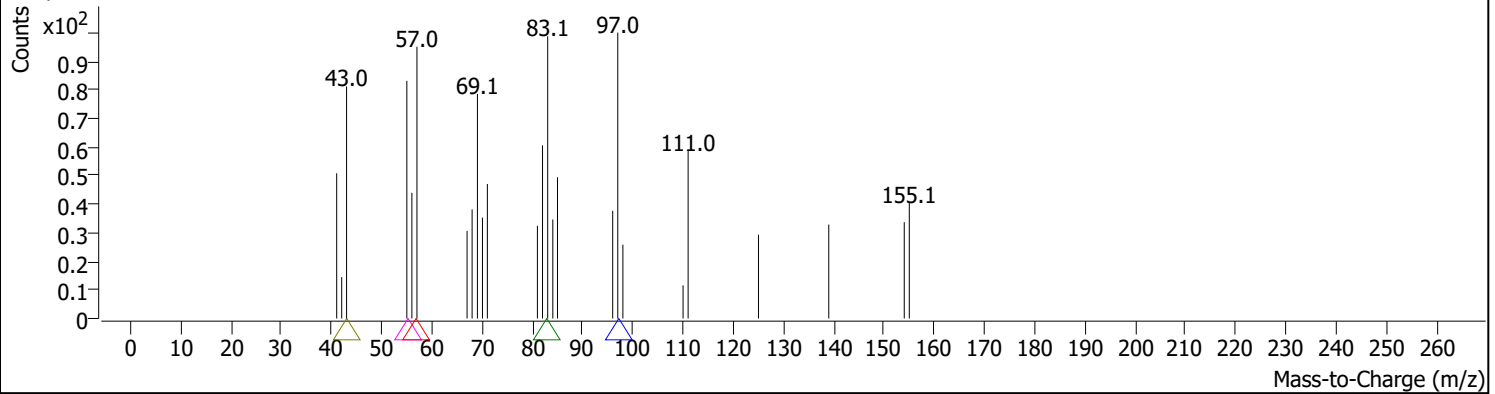
## Library Search Results - NonTarget Hits with Details



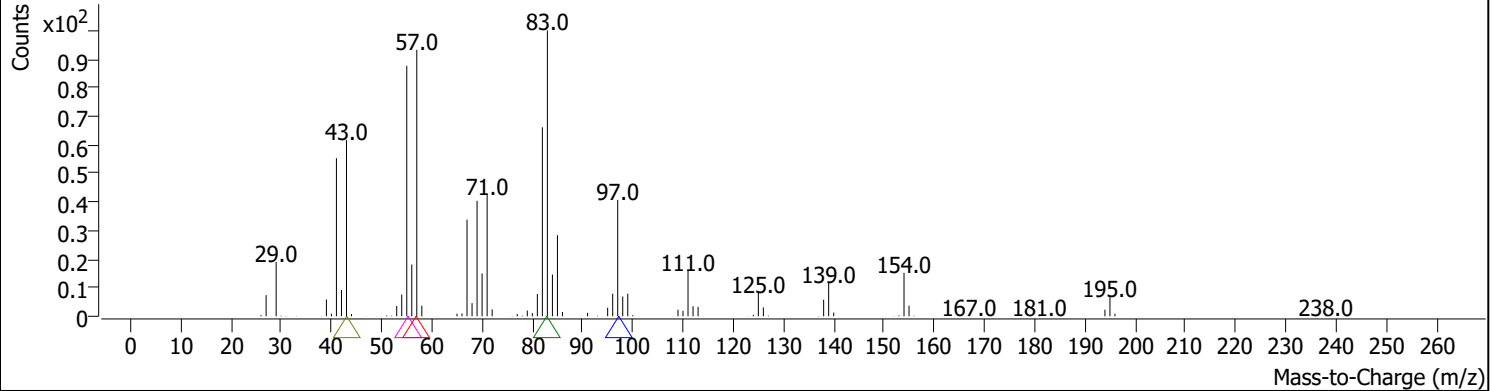
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
75.3538	Undecane, 4-cyclohexyl-	316799.7	84.8	13151-79-6	C <sub>17</sub> H <sub>34</sub>	

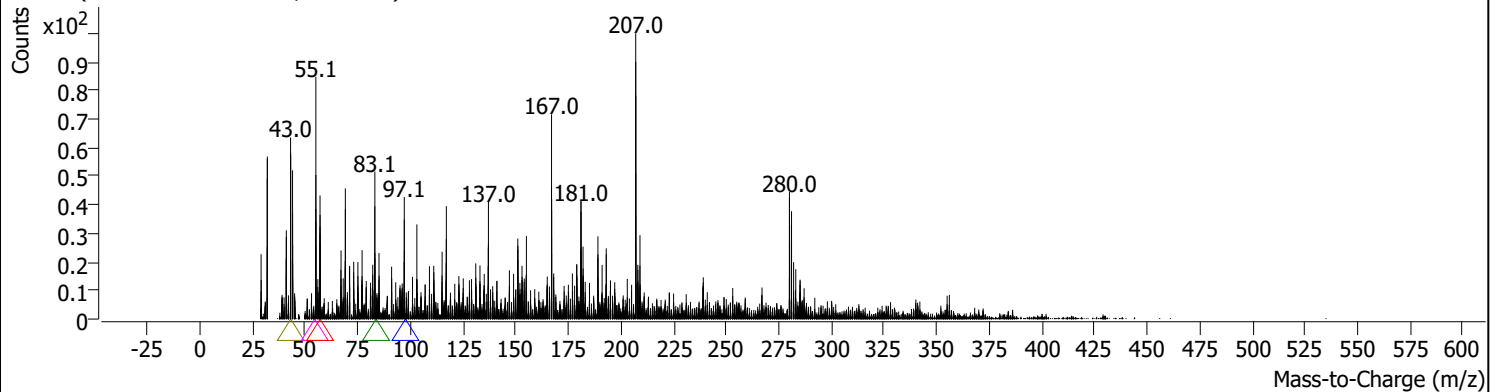
Component RT: 75.3538



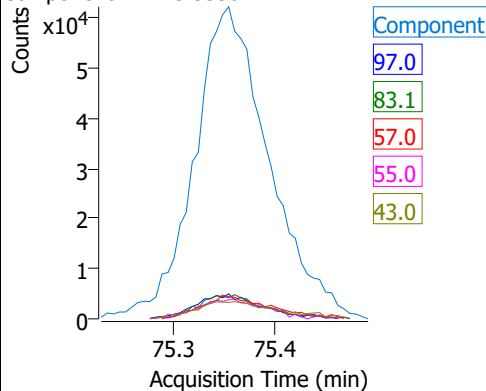
Undecane, 4-cyclohexyl- (NIST20.L)



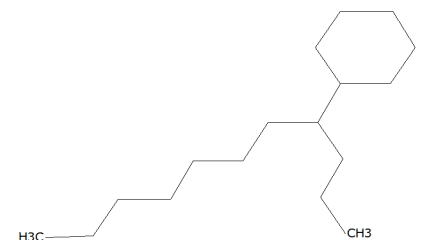
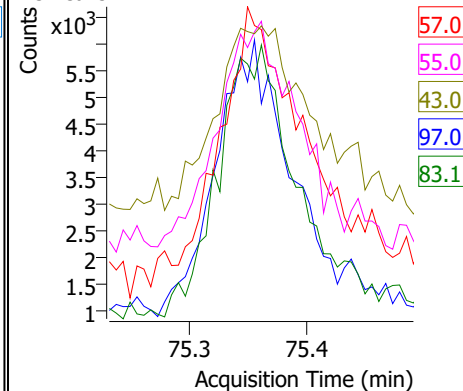
+ Scan (75.2743-75.4743 min, 34 scans) 1.D



Component RT: 75.3538



EIC Peaks



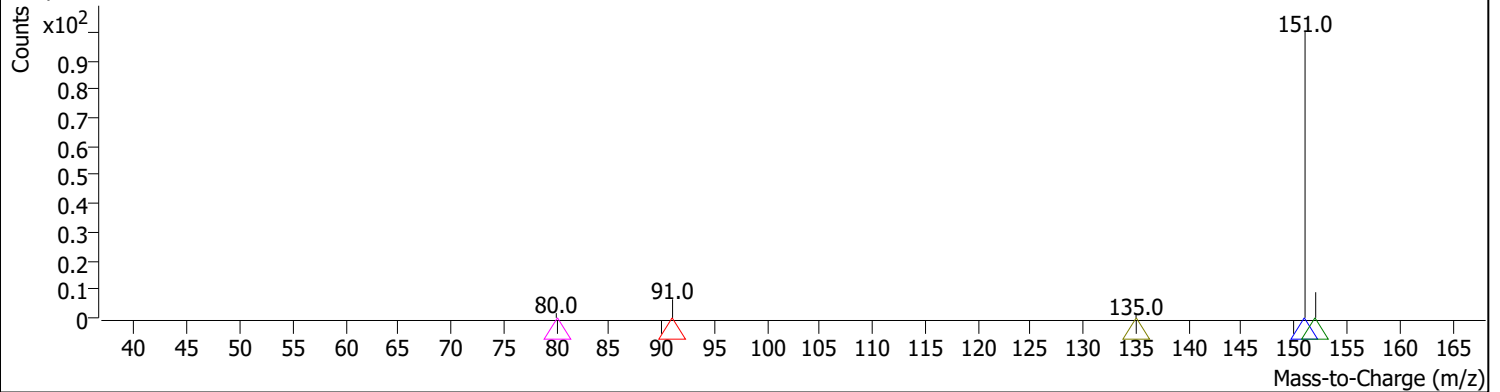
## Library Search Results - NonTarget Hits with Details



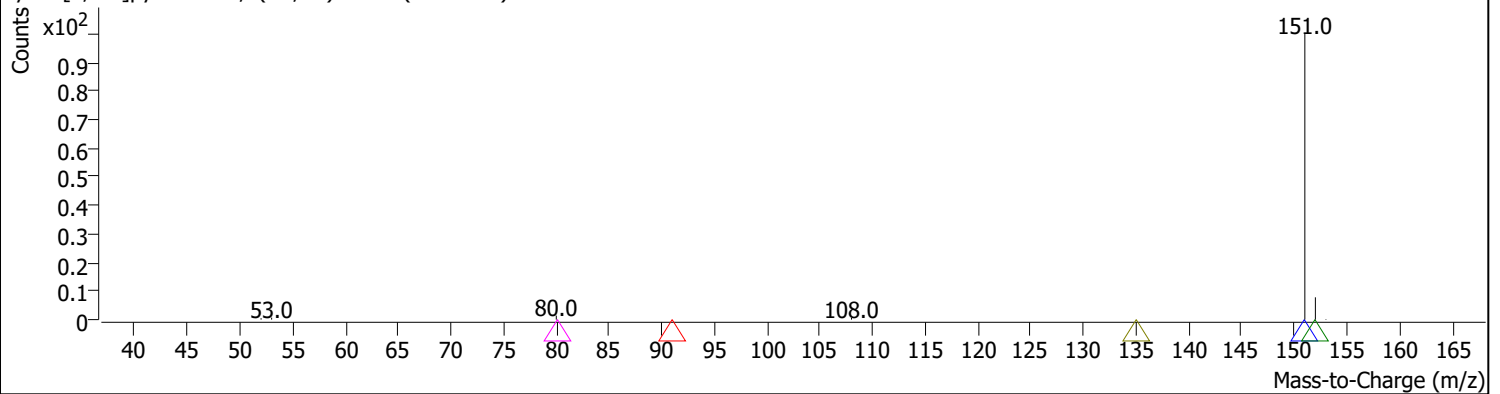
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
75.8826	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	771065.1	92.0	65996-50-1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	

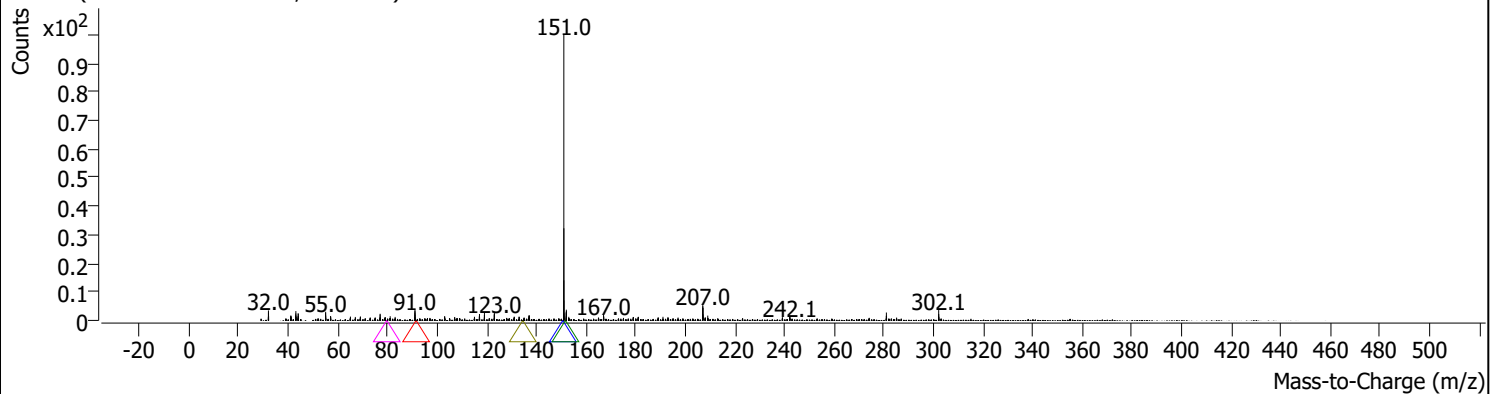
Component RT: 75.8826



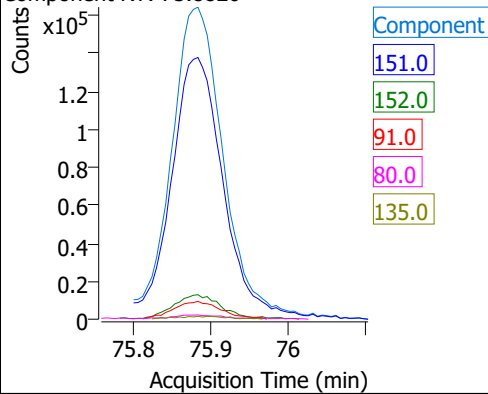
Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)



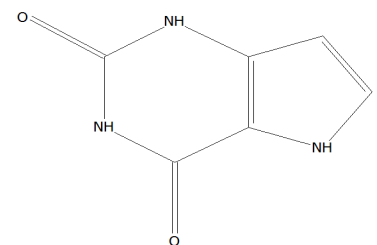
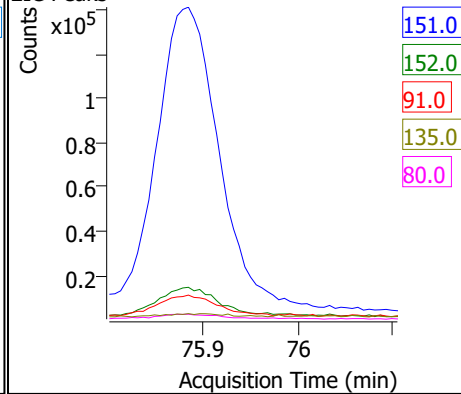
+ Scan (75.8013-76.1046 min, 52 scans) 1.D



Component RT: 75.8826



EIC Peaks



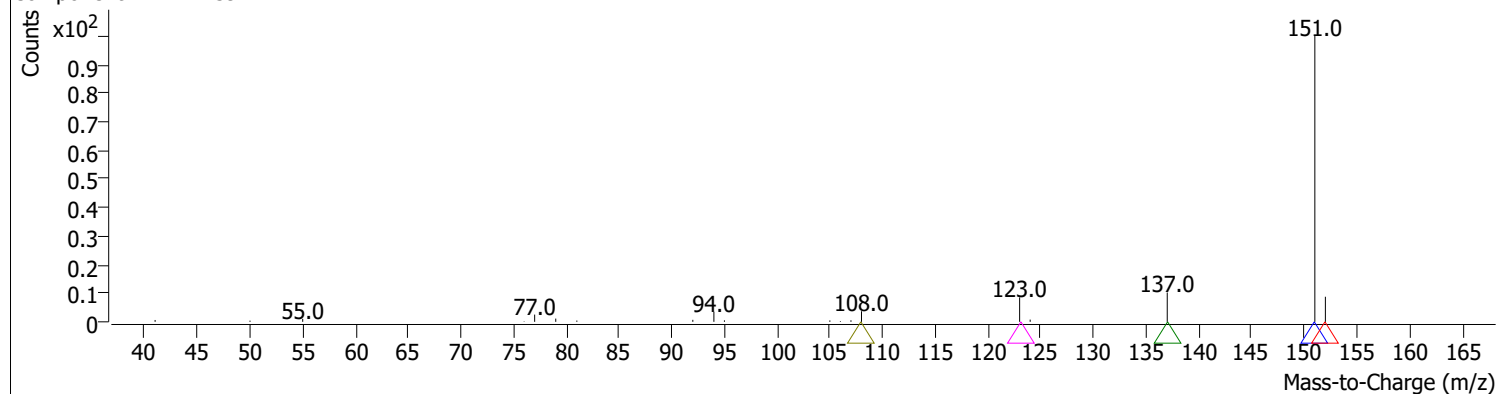
## Library Search Results - NonTarget Hits with Details



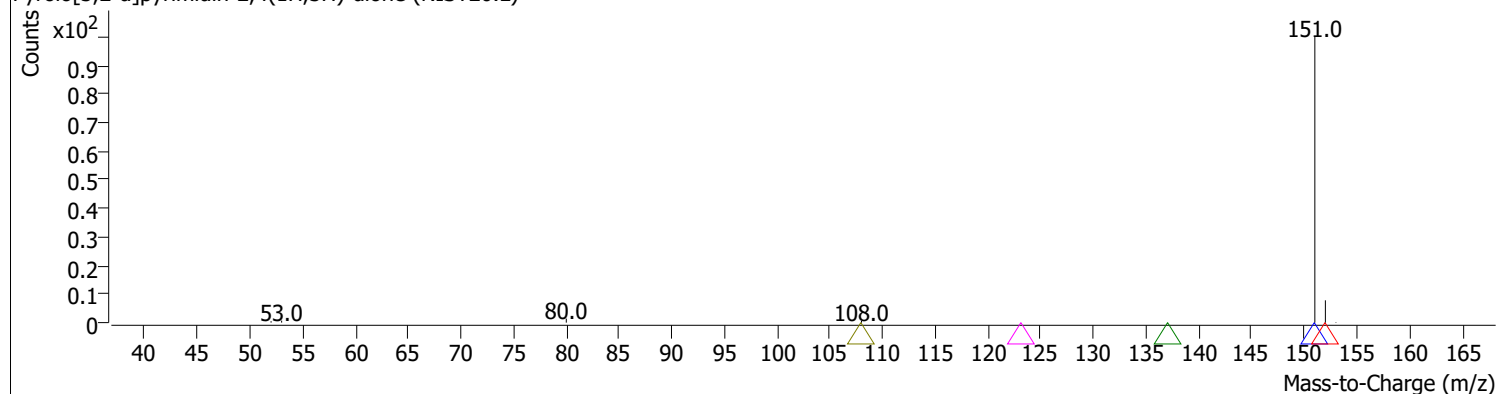
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
77.2394	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	2195585.6	76.2	65996-50-1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	

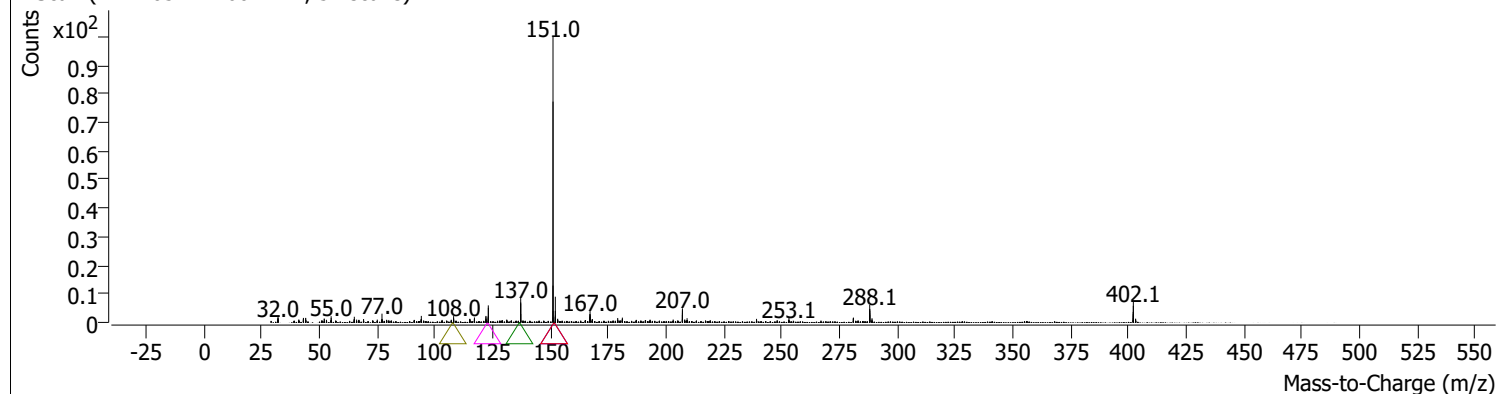
Component RT: 77.2394



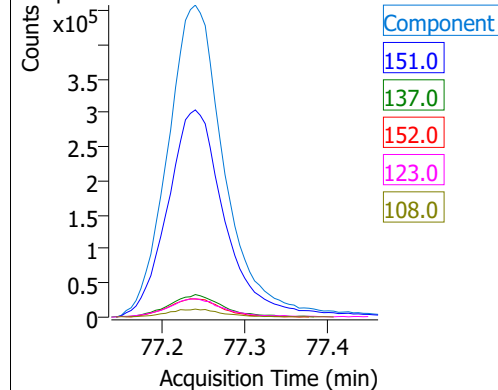
Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)



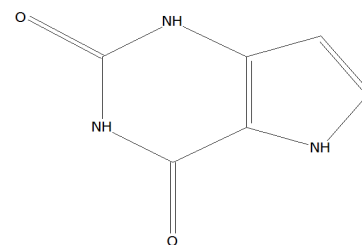
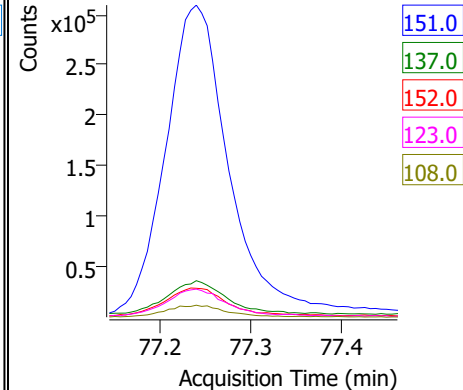
+ Scan (77.1405-77.4602 min, 54 scans) 1.D



Component RT: 77.2394



EIC Peaks





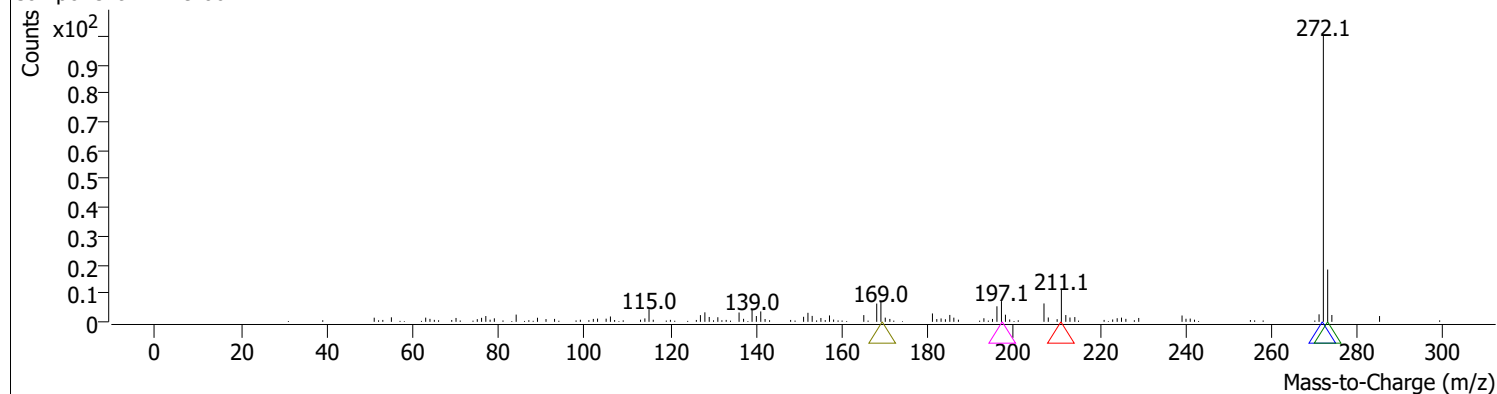
## Library Search Results - NonTarget Hits with Details



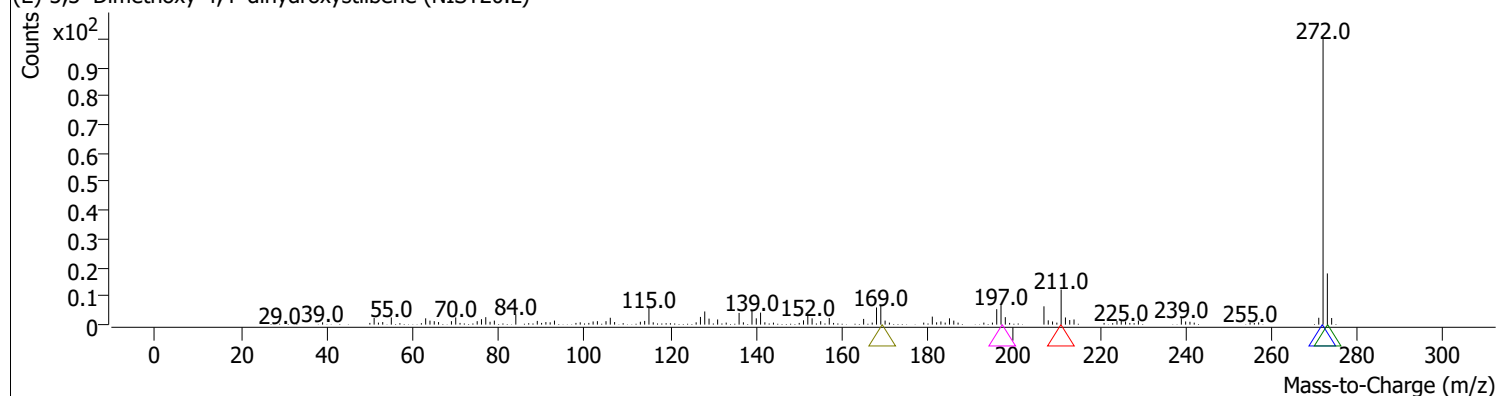
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
79.0627	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	4958162.3	92.6	7329-69-3	C <sub>16</sub> H <sub>16</sub> O <sub>4</sub>	

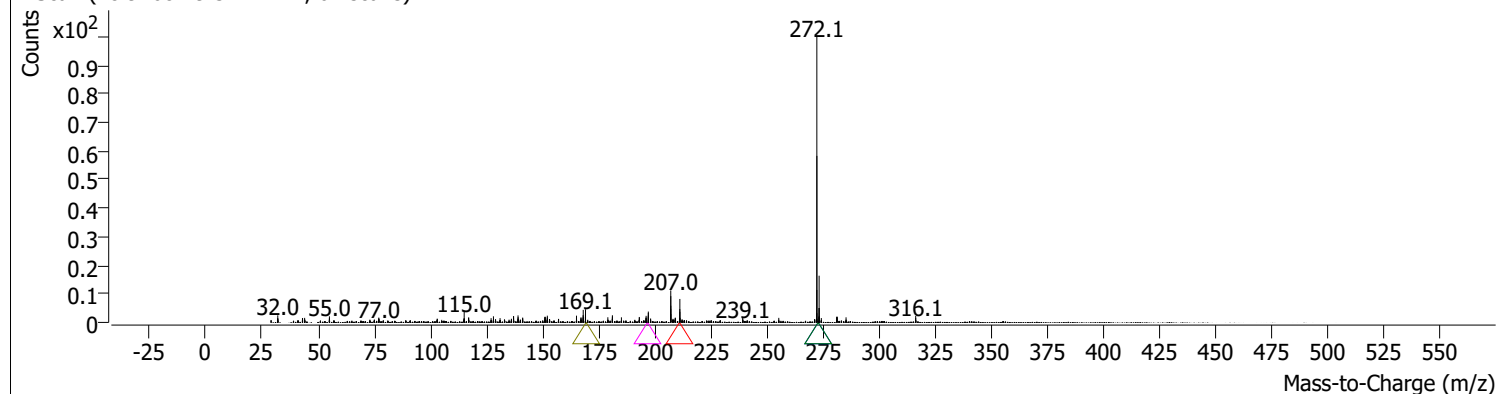
Component RT: 79.0627



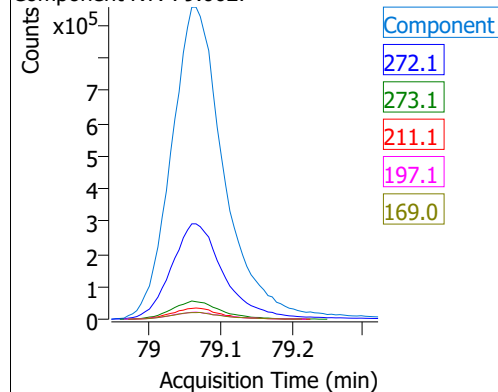
(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene (NIST20.L)



+ Scan (78.9468-79.3214 min, 64 scans) 1.D



Component RT: 79.0627



EIC Peaks

