

## Library Search Results - NonTarget Hits with Details



Trusted Answers

Batch Path	D:\MassHunter\GCMS\1\data\RBEL\240501 scan		
Analysis File Name	240502 data.uaf		
Analyst Name	admin	Analysis Time	5/2/2024 11:31:09 AM
File Name	4.D	Path Name	D:\MassHunter\GCMS\1\data\RBEL\240501 scan
Sample Name	4	Sample Type	Sample
Acq. Method File	240501 scan	Acq. Method Path	D:\MassHunter\GCMS\1\methods\RBEL\
Acq. Date-Time	5/1/2024 6:09:15 PM	Acq. Operator	
Instrument Name	GCMSD	Dil.	1

Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
7.3141	1,3-Propanediol	504-63-2	C3H8O2	1202732.8	94.8	
11.6071	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	528254.6	82.0	
12.3681	Butyrolactone	96-48-0	C4H6O2	10540151.4	96.8	
12.8058	Methyltartronic acid	595-98-2	C4H6O5	1691916.6	94.9	
13.2899	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	532351.4	78.3	
16.4719	2,2-Dimethyl-2-sila-1,3-dioxacyclohexane	14879-83-5	C5H12O2Si	309458.3	77.2	
17.4362	Silane, diethoxydimethyl-	78-62-6	C6H16O2Si	544676.0	75.3	
18.6543	Diisoamyl ether	544-01-4	C10H22O	4244738.5	98.2	
19.7524	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	167867.0	85.4	
20.0568	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	658804.5	95.3	
21.1424	1,3,5-Trioxane	110-88-3	C3H6O3	4088997.3	81.6	
23.0353	1-Octanol	111-87-5	C8H18O	3434766.0	98.7	
23.5037	Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	2002503.1	92.6	
23.5626	Phenol, 2-methoxy-	90-05-1	C7H8O2	5846632.4	97.9	
23.7721	2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-	21835-00-7	C7H10O2	319272.0	78.5	
24.6648	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	2725027.1	91.7	
27.7300	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	521798.4	82.1	
28.7452	Naphthalene	91-20-3	C10H8	774394.9	97.5	
29.1709	Creosol	93-51-6	C8H10O2	734304.1	96.7	
30.4742	1,3-Dioxane	505-22-6	C4H8O2	454800.7	79.1	
30.7369	Catechol	120-80-9	C6H6O2	876657.4	93.0	
31.5746	5-Hydroxymethylfurfural	67-47-0	C6H6O3	360007.4	82.3	
32.5004	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	520439.7	95.2	
33.3356	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	2515777.9	97.4	
34.9749	2,3-dihydroxypropyl isobutyrate	1010458-45-6	C7H14O4	12232779.8	78.5	
35.0843	Phenol, 5-ethenyl-2-methoxy-	621-58-9	C9H10O2	202572.3	82.6	
35.3154	Butanoic acid, 2-methylpropyl ester	539-90-2	C8H16O2	11843195.3	78.6	
35.3163	Butanoic acid, anhydride	106-31-0	C8H14O3	11248701.5	79.7	
36.1877	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	2781061.4	82.1	
36.7974	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	12715578.1	99.1	
37.3896	Ethylamine, 2-((p-bromo-.alpha.-methyl-.alpha.-phenylbenzyl)oxy)-N,N-dimethyl-	3565-72-8	C18H22BrNO	1629293.7	75.7	
37.4168	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	394237.8	78.1	
37.7057	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	475586.9	78.5	
38.9935	Vanillin	121-33-5	C8H8O3	5678104.3	98.5	
40.8895	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	847530.0	93.6	
42.6159	Apocynin	498-02-2	C9H10O3	4014973.2	99.2	
44.0555	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	1629043.1	97.5	
44.2950	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	5445870.8	94.2	
44.3330	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6342821.8	95.2	
45.6451	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	3757-32-2	C9H16O3	435378.6	81.3	
46.0653	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	936058.2	92.6	
46.2195	Oxazolidin-2-one	497-25-6	C3H5NO2	634933.3	80.5	
46.2202	3-Pentanol, 2,2,4,4-tetramethyl-	14609-79-1	C9H20O	744700.7	78.0	
46.4841	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	210231.0	81.4	
46.6461	Butyrovanillone	64142-23-0	C11H14O3	8738295.8	89.8	
47.0820	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	306538.1	76.4	
47.3540	Homosyringaldehyde	87345-52-6	C10H12O4	224103.1	82.6	
48.9895	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	5515590.4	96.4	
49.3613	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	2047327.7	96.5	
49.4171	7-Methoxy-1-naphthol	67247-13-6	C11H10O2	307367.8	84.8	
49.4533	2,6-Dimethoxyhydroquinone	15233-65-5	C8H10O4	449347.7	82.9	
50.4244	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	321466.5	91.8	
51.7398	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-	4899-74-5	C10H12O4	212350.2	89.7	
52.0014	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	5359990.6	98.5	
53.2410	Syringylacetone	19037-58-2	C11H14O4	4823009.2	97.3	
53.6141	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	276859.3	75.6	
54.9715	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	530-57-4	C9H10O5	733657.1	88.0	
55.2057	Butylsyringone	69271-91-6	C12H16O4	4574151.5	93.0	
55.6221	Acetyl syringic acid, ethyl ester	1000454-70-9	C13H16O6	700159.4	89.0	
56.0995	2,3-Dimethoxy-5-aminocinnamnitrite	1000214-46-5	C11H12N2O2	712035.6	79.3	
57.4905	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	1812481.3	92.3	
58.8309	Isoelemicin	487-12-7	C12H16O3	404594.3	77.8	
66.3332	(E)-9-Octadecenoic acid ethyl ester	6114-18-7	C20H38O2	421940.8	78.5	

## Library Search Results - NonTarget Hits with Details



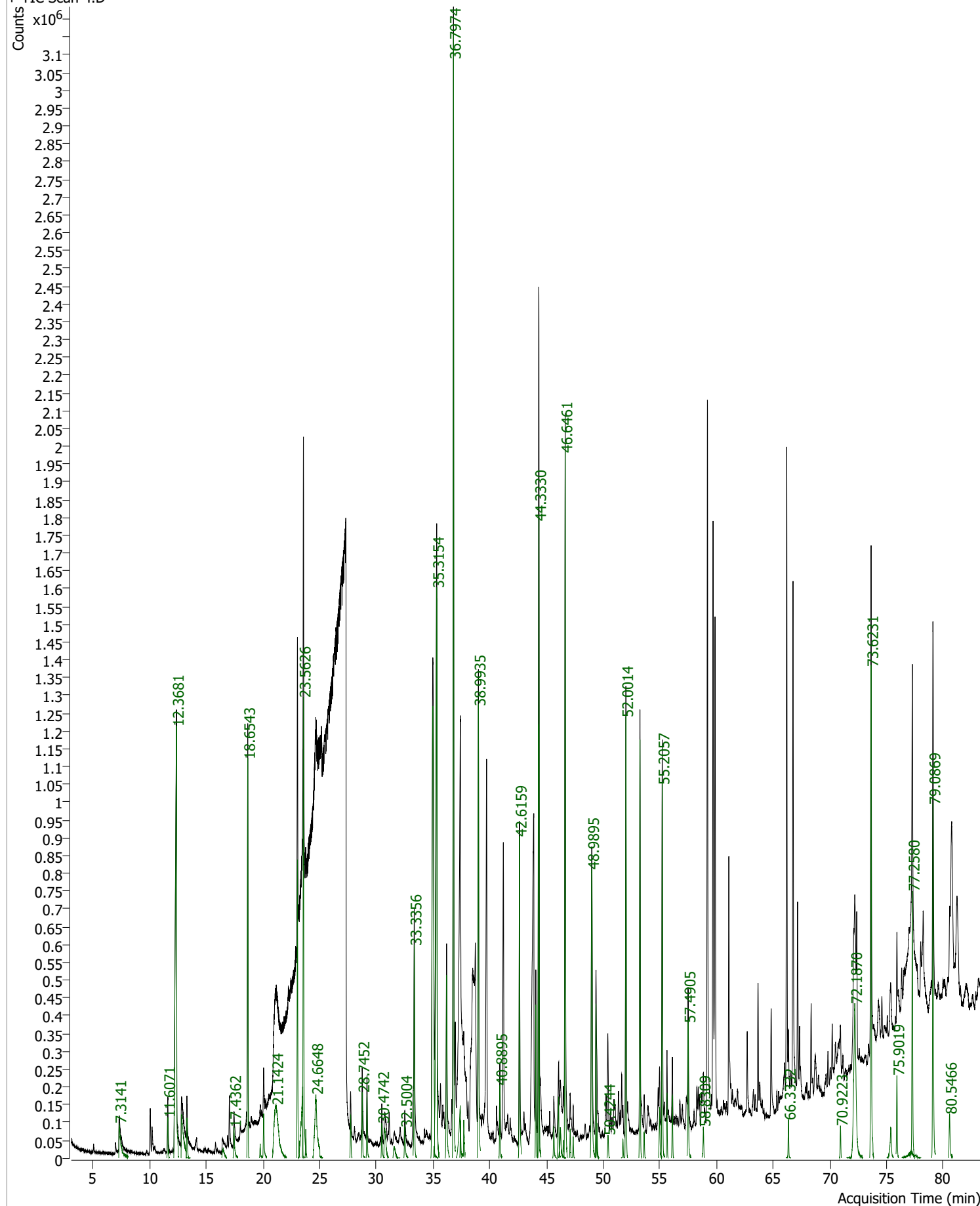
Agilent

Trusted Answers

Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
70.9223	Methyl dehydroabietate	1235-74-1	C21H30O2	359827.9	75.8	
72.1870	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	6222168.8	88.7	
73.6231	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	6817161.6	93.1	
75.3519	Undecane, 4-cyclohexyl-	13151-79-6	C17H34	739647.2	77.0	
75.9019	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether	22318-87-2	C18H22O4	1003347.8	80.1	
77.0919	8-Benzylquinoline	28748-19-8	C16H13N	604940.0	84.3	
77.2580	.alpha.-Amino-3'-hydroxy-4'-methoxyacetophenone	90765-44-9	C9H11NO3	3636759.4	76.5	
79.0869	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	5180261.7	89.1	
80.5466	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	757240.5	83.0	

## Sample Chromatogram

+ TIC Scan 4.D



## Library Search Results - NonTarget Hits with Details

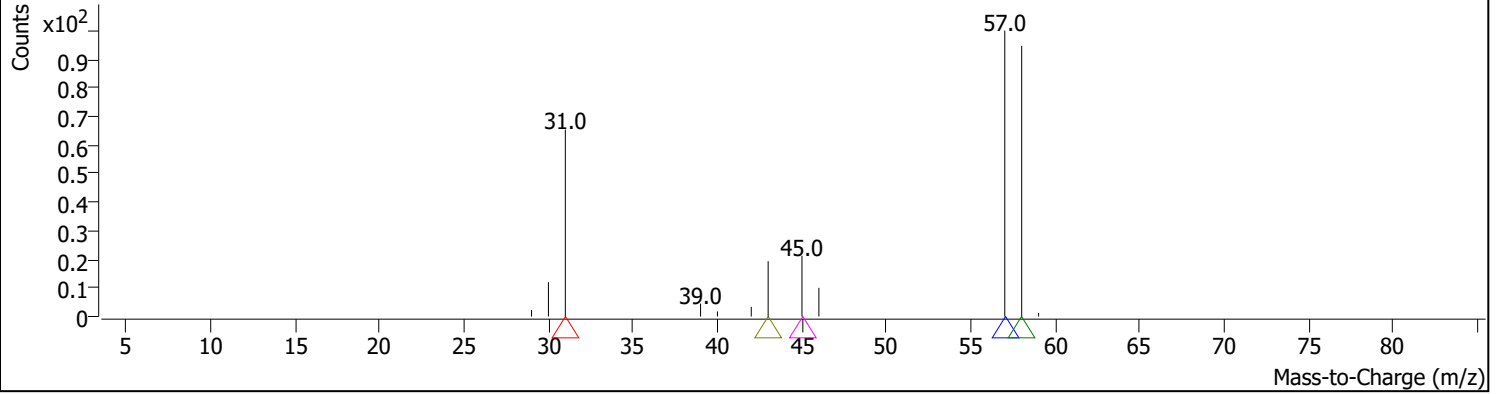


Agilent

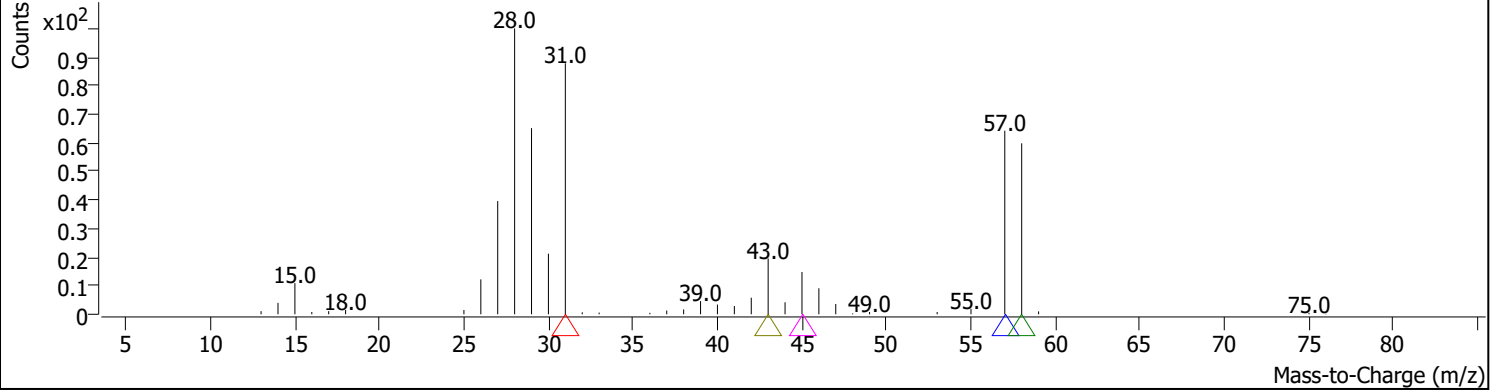
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
7.3141	1,3-Propanediol	1202732.8	94.8	504-63-2	C3H8O2	

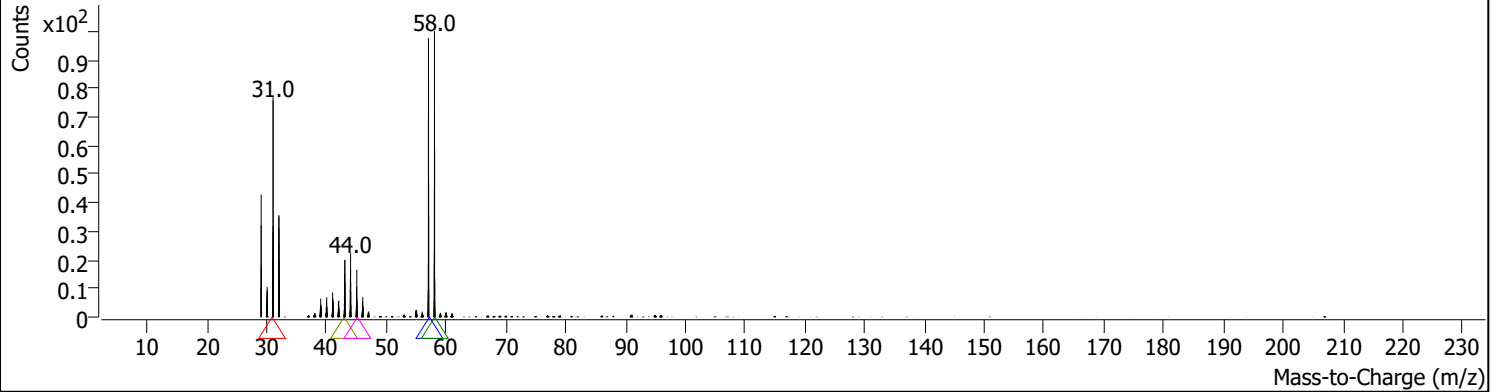
Component RT: 7.3141



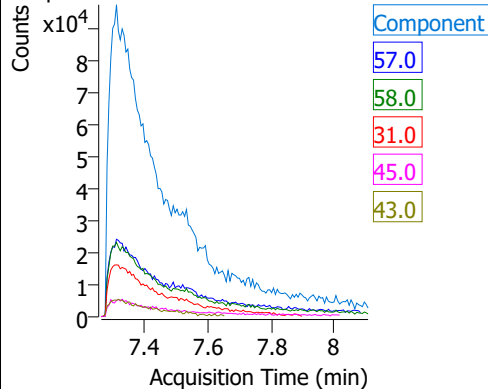
1,3-Propanediol (NIST20.L)



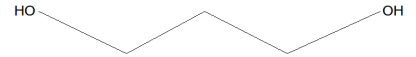
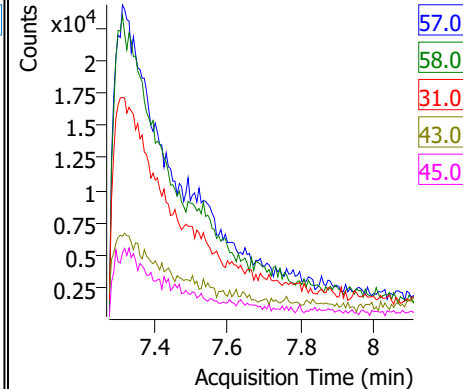
+ Scan (7.2738-8.1054 min, 140 scans) 4.D



Component RT: 7.3141



EIC Peaks



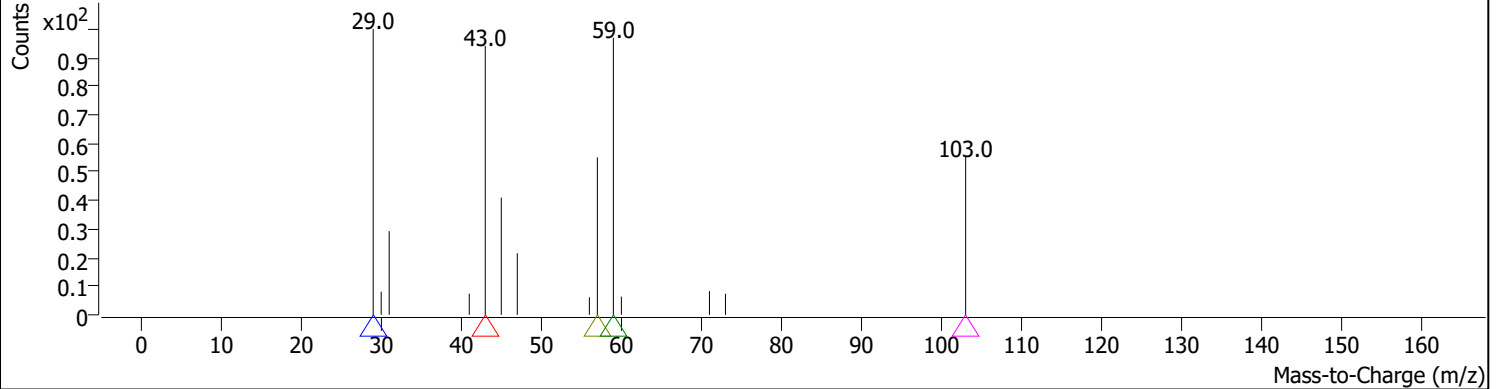
## Library Search Results - NonTarget Hits with Details



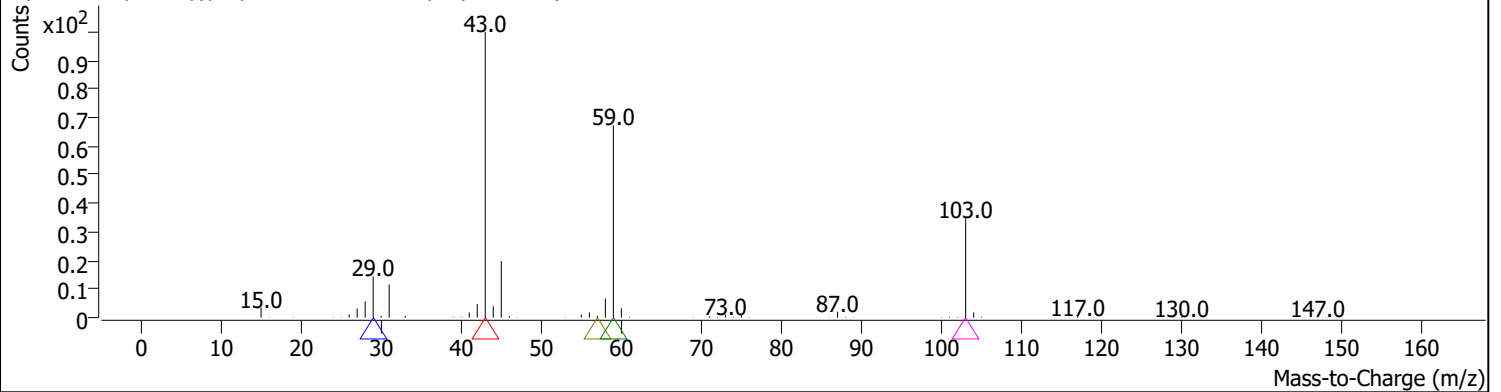
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
11.6071	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	528254.6	82.0	1000506-61-7	C <sub>8</sub> H <sub>14</sub> O <sub>5</sub>	

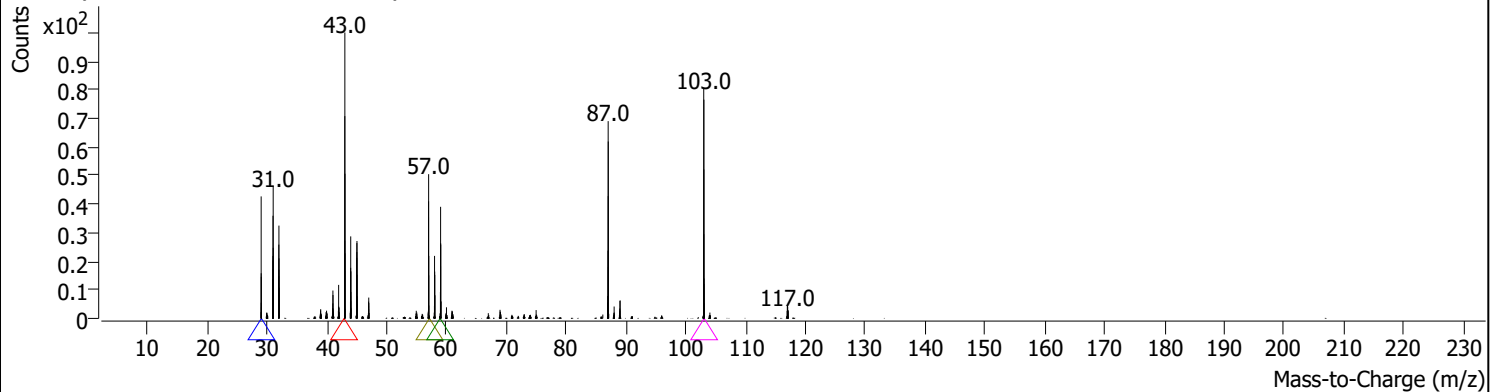
Component RT: 11.6071



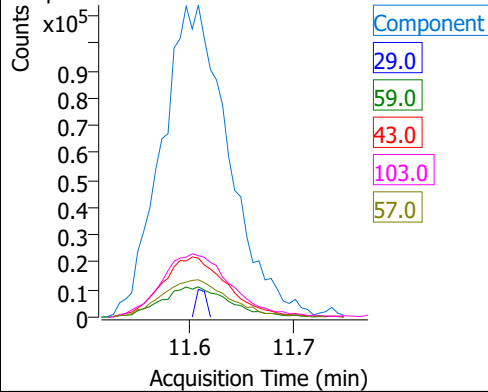
2-(2-methoxyethoxy)propanoic acid, O-acetyl- (NIST20.L)



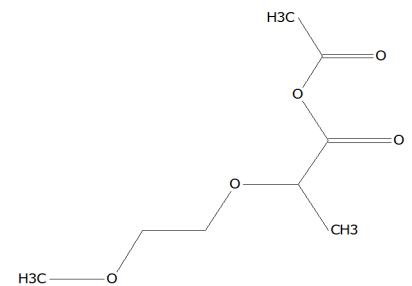
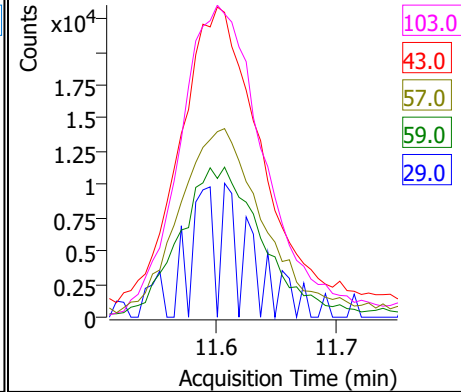
+ Scan (11.5140-11.7503 min, 40 scans) 4.D



Component RT: 11.6071



EIC Peaks



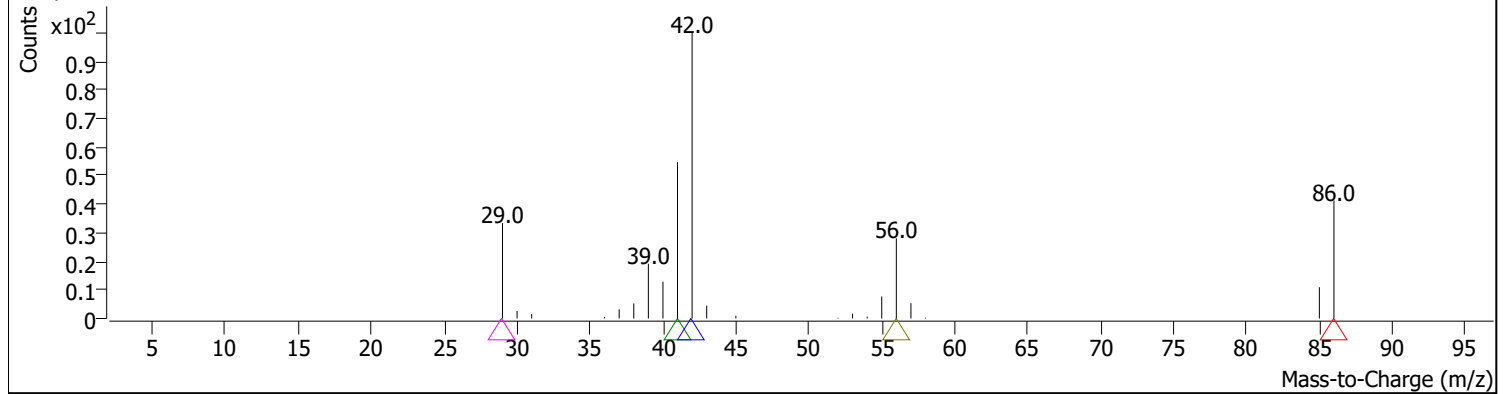
## Library Search Results - NonTarget Hits with Details



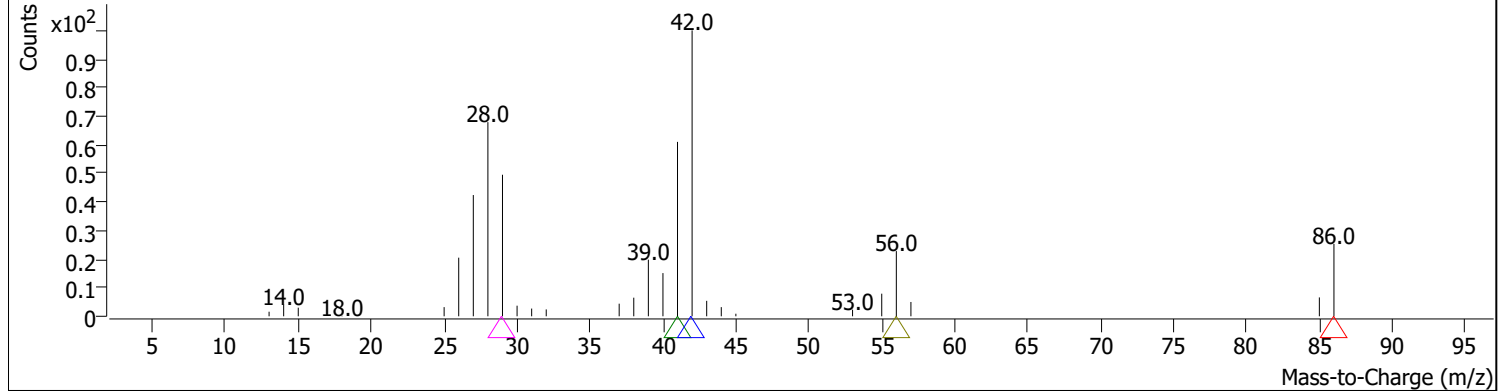
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
12.3681	Butyrolactone	10540151.4	96.8	96-48-0	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	

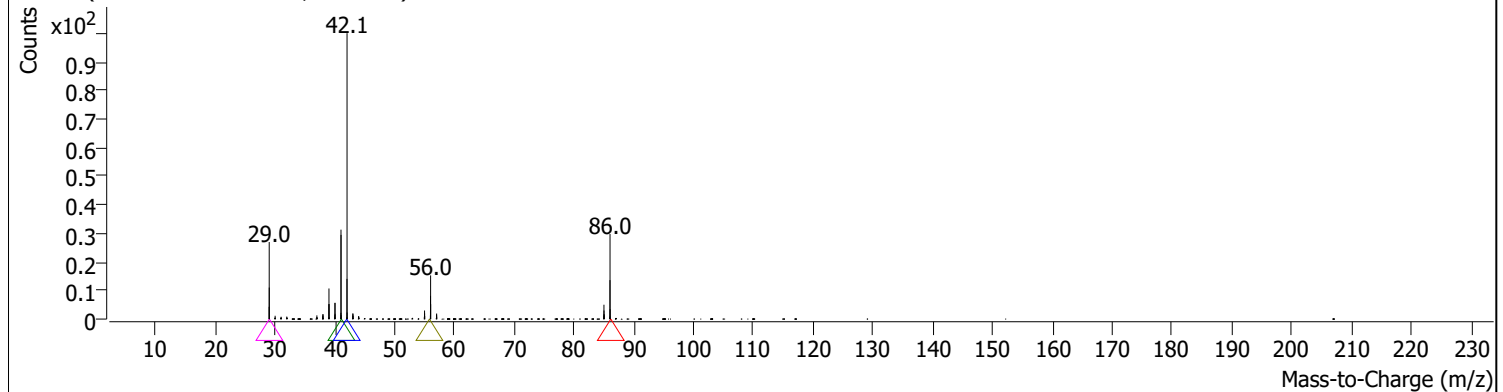
Component RT: 12.3681



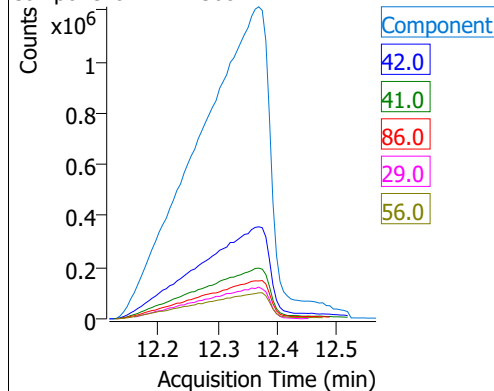
Butyrolactone (NIST20.L)



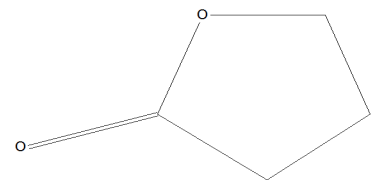
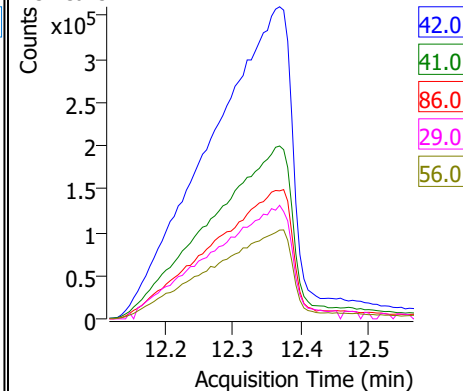
+ Scan (12.1274-12.4877 min, 61 scans) 4.D



Component RT: 12.3681



EIC Peaks



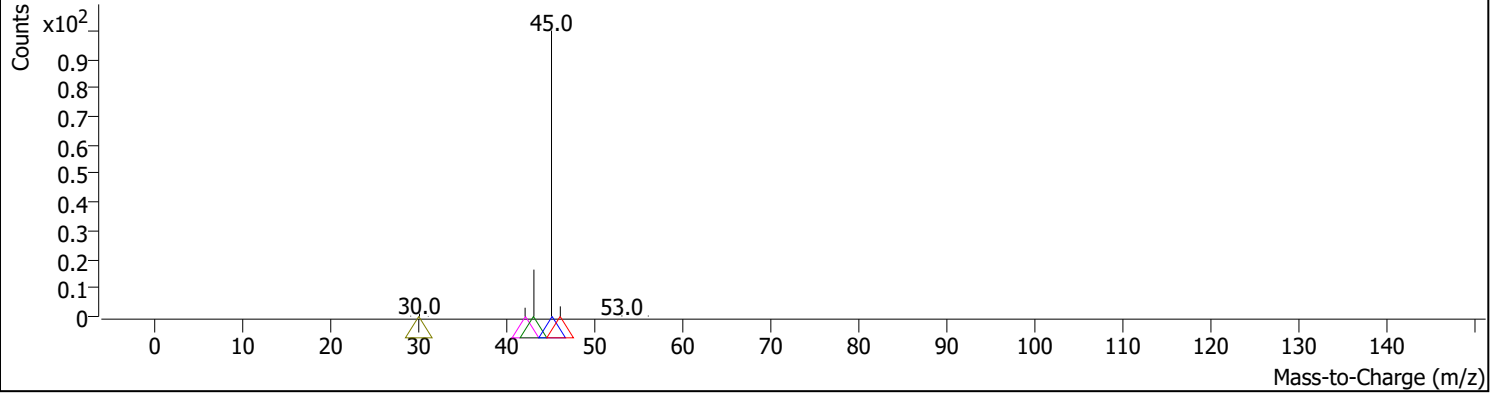
## Library Search Results - NonTarget Hits with Details



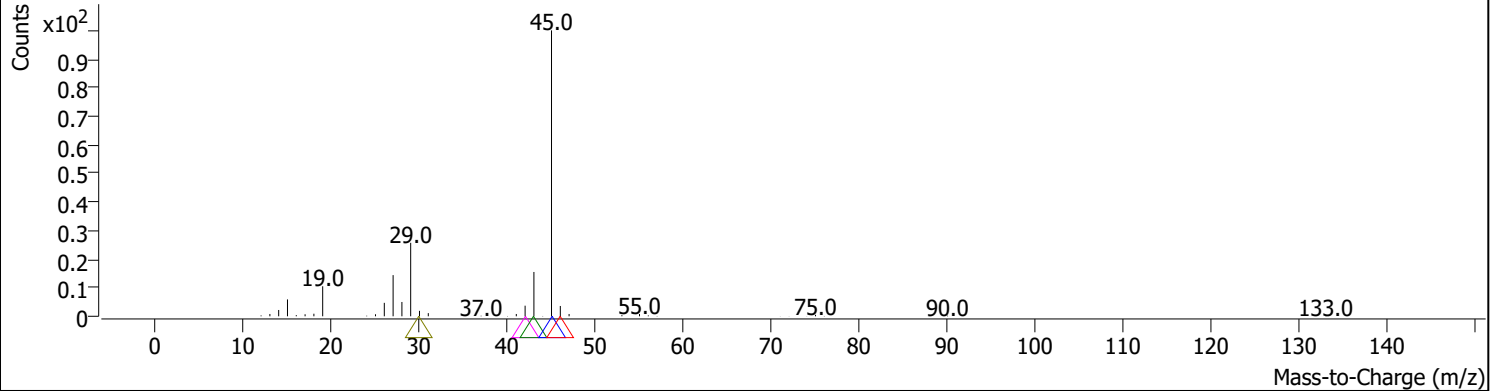
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
12.8058	Methyltartronic acid	1691916.6	94.9	595-98-2	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	

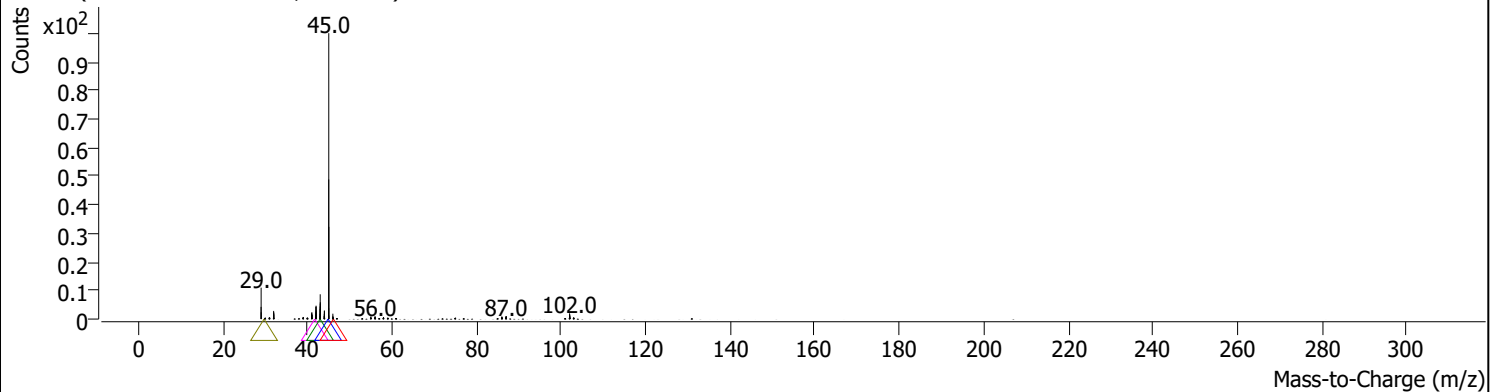
Component RT: 12.8058



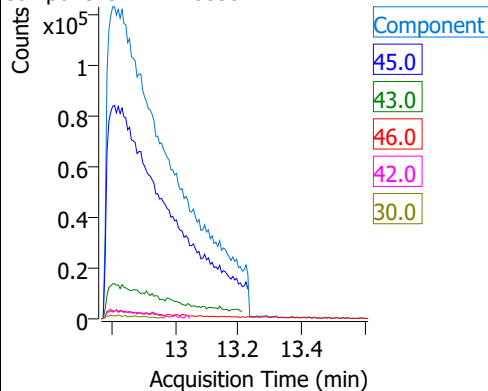
Methyltartronic acid (NIST20.L)



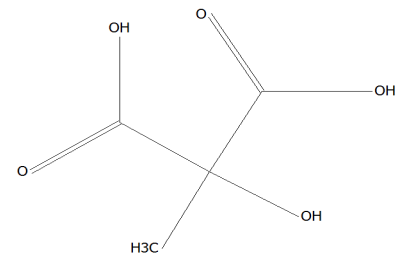
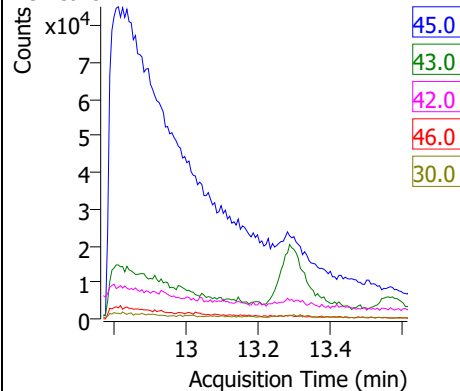
+ Scan (12.7694-13.2309 min, 78 scans) 4.D



Component RT: 12.8058



EIC Peaks



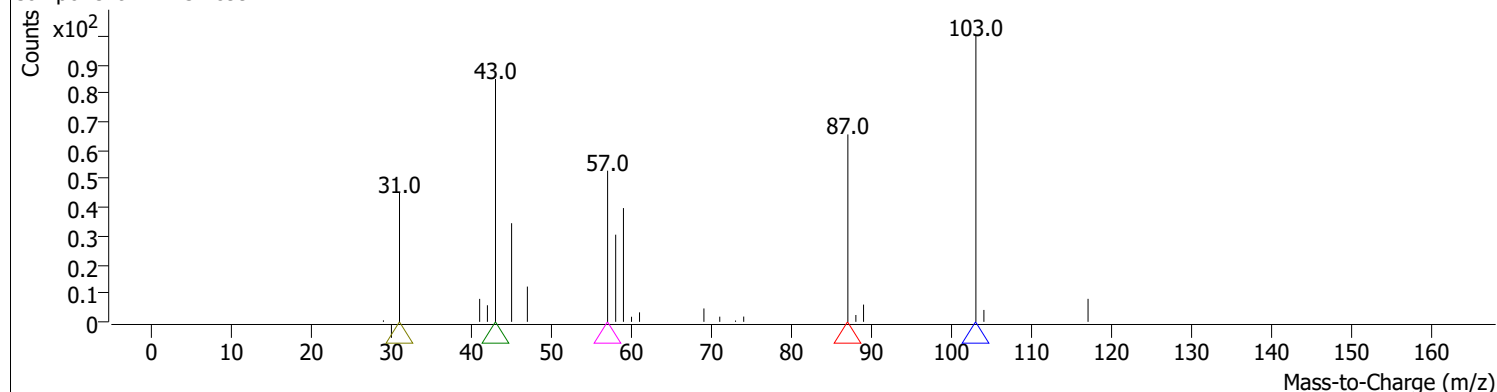
## Library Search Results - NonTarget Hits with Details



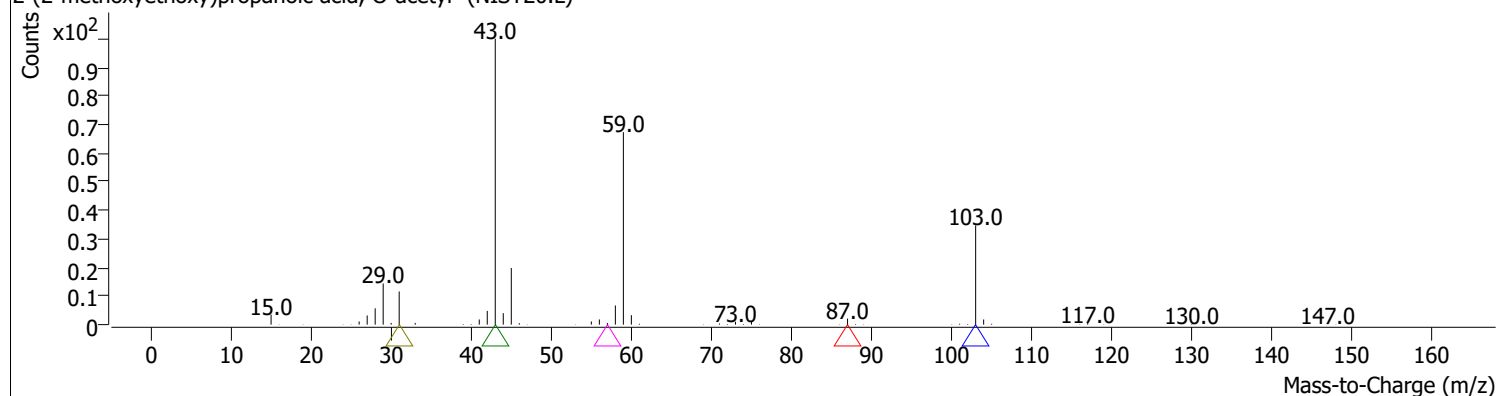
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
13.2899	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	532351.4	78.3	1000506-61-7	C <sub>8</sub> H <sub>14</sub> O <sub>5</sub>	

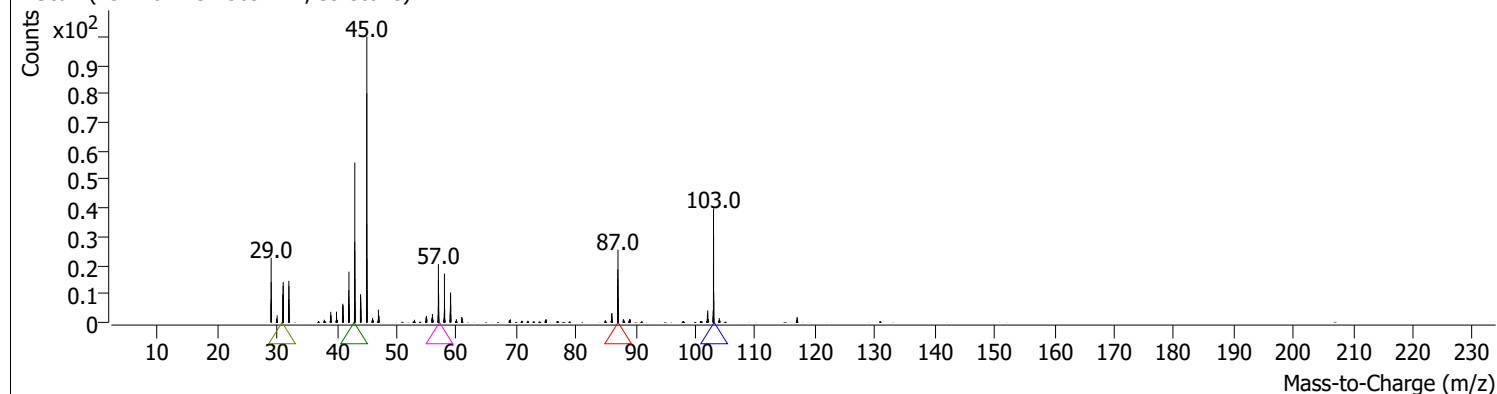
Component RT: 13.2899



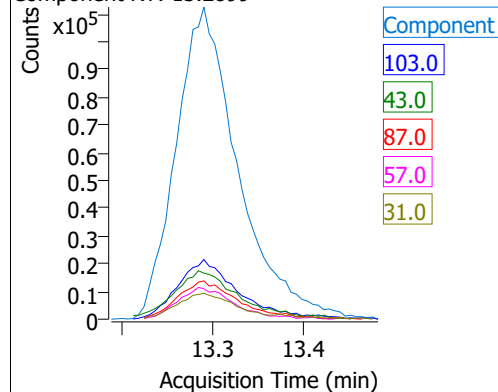
2-(2-methoxyethoxy)propanoic acid, O-acetyl- (NIST20.L)



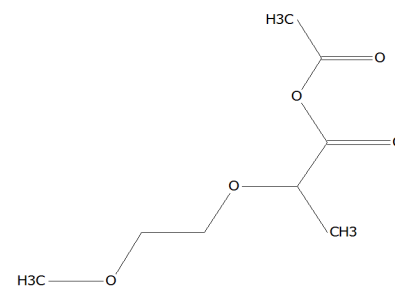
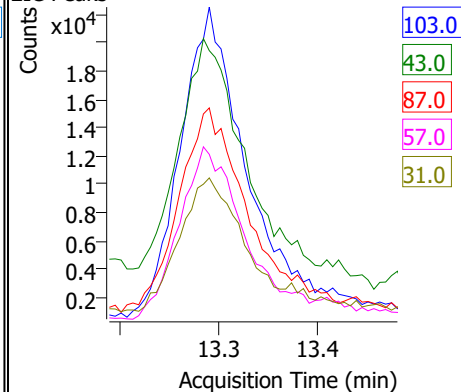
+ Scan (13.2202-13.4509 min, 39 scans) 4.D



Component RT: 13.2899



EIC Peaks





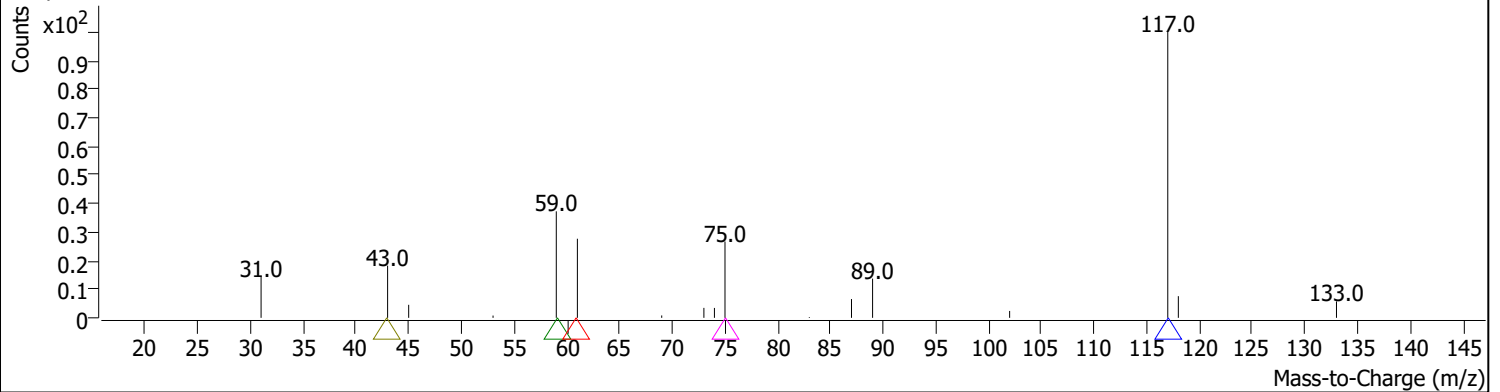
## Library Search Results - NonTarget Hits with Details



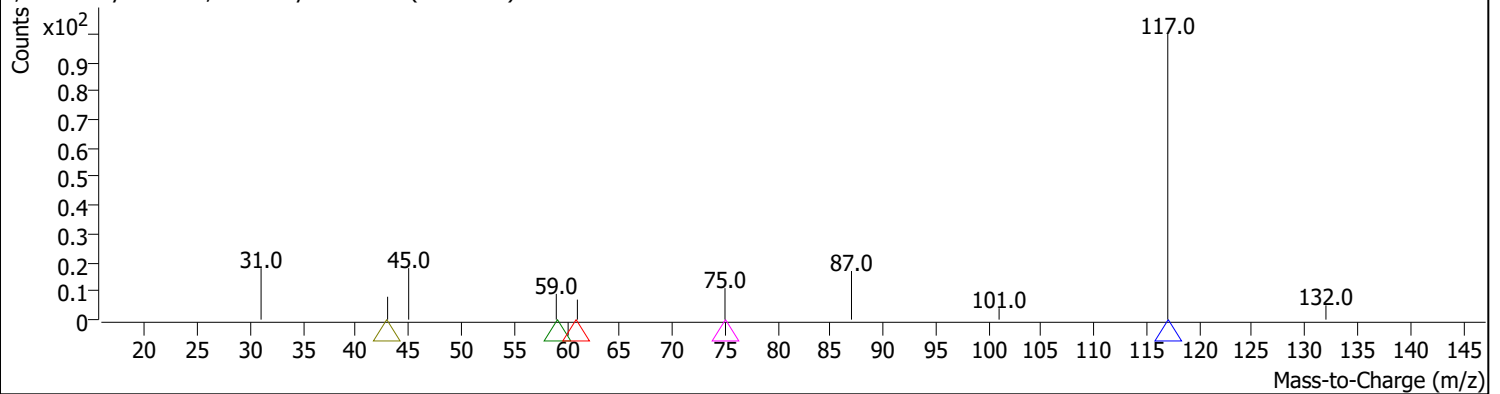
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
16.4719	2,2-Dimethyl-2-sila-1,3-dioxacyclohexane	309458.3	77.2	14879-83-5	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub> Si	

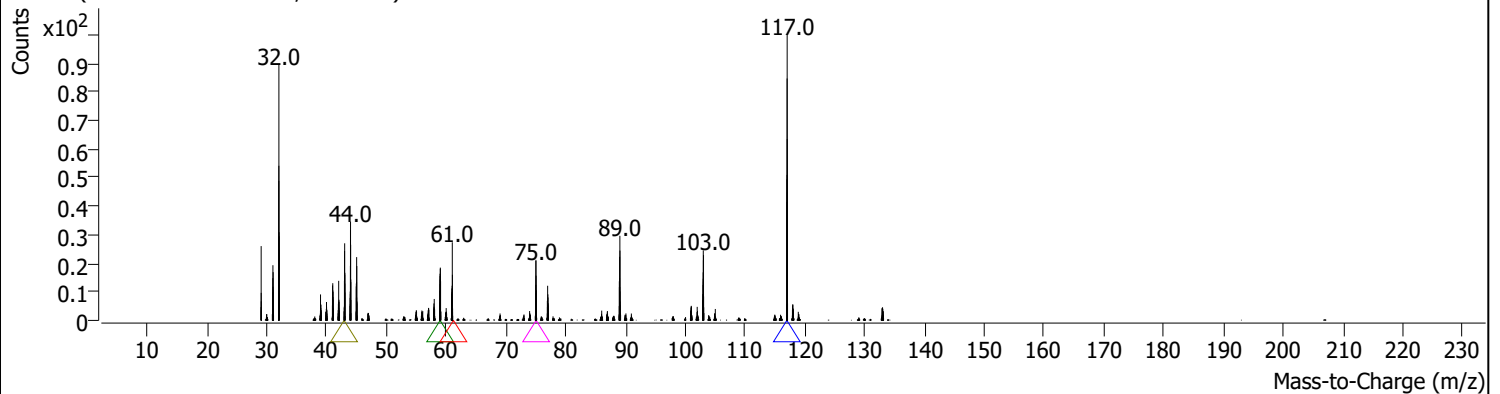
Component RT: 16.4719



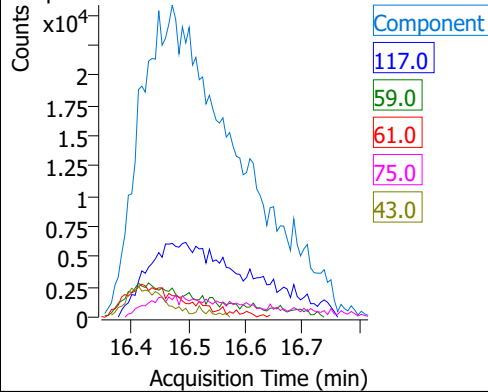
2,2-Dimethyl-2-sila-1,3-dioxacyclohexane (NIST20.L)



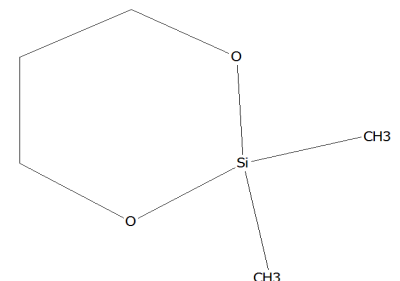
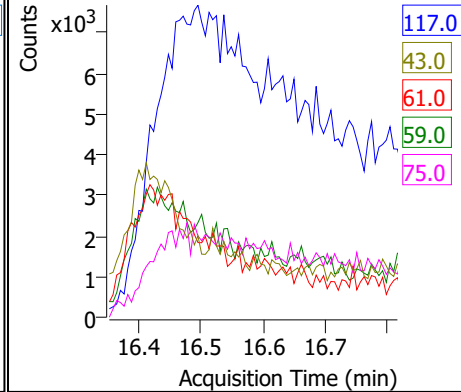
+ Scan (16.3883-16.8164 min, 73 scans) 4.D



Component RT: 16.4719



EIC Peaks



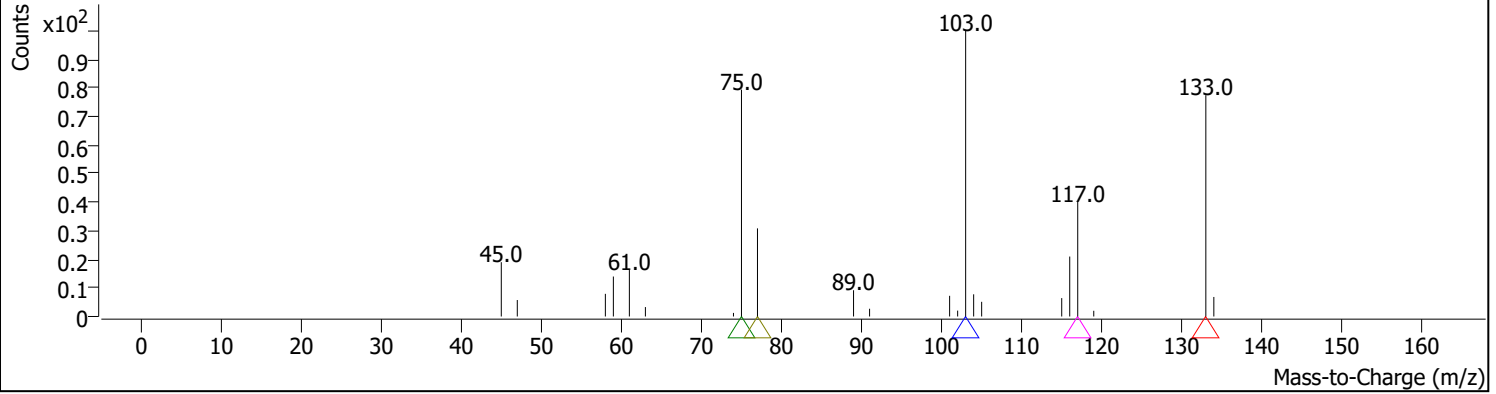
# Library Search Results - NonTarget Hits with Details



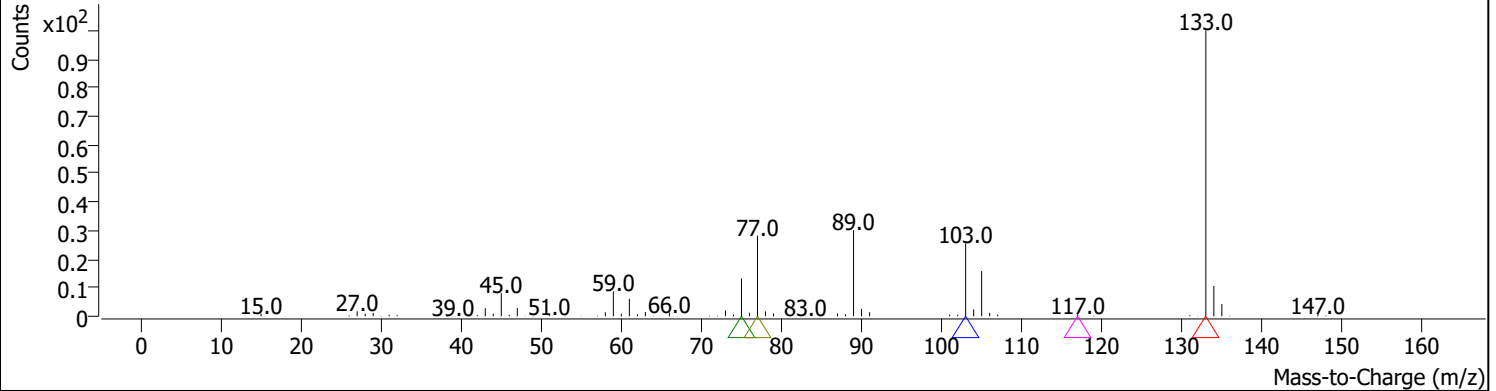
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
17.4362	Silane, diethoxydimethyl-	544676.0	75.3	78-62-6	C <sub>6</sub> H <sub>16</sub> O <sub>2</sub> Si	

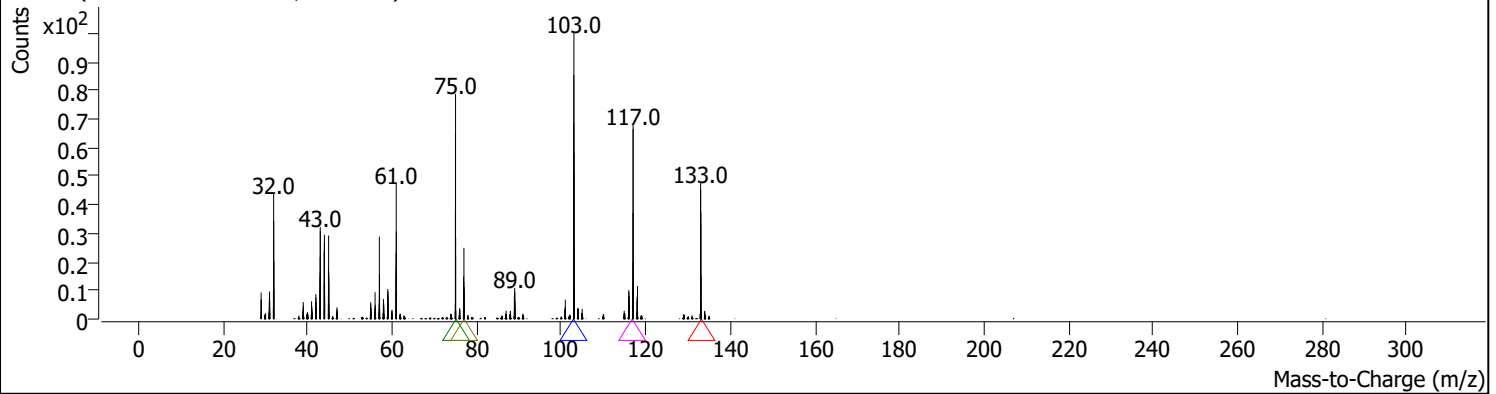
Component RT: 17.4362



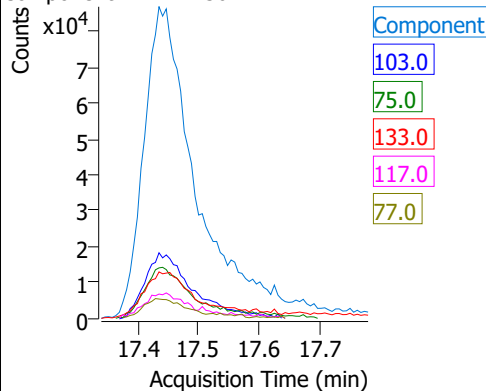
Silane, diethoxydimethyl- (NIST20.L)



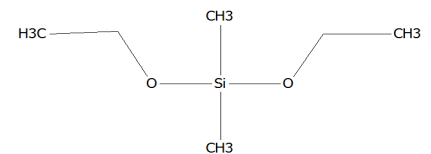
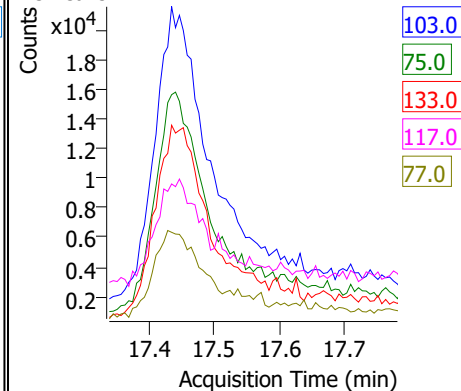
+ Scan (17.3634-17.6964 min, 57 scans) 4.D



Component RT: 17.4362



EIC Peaks



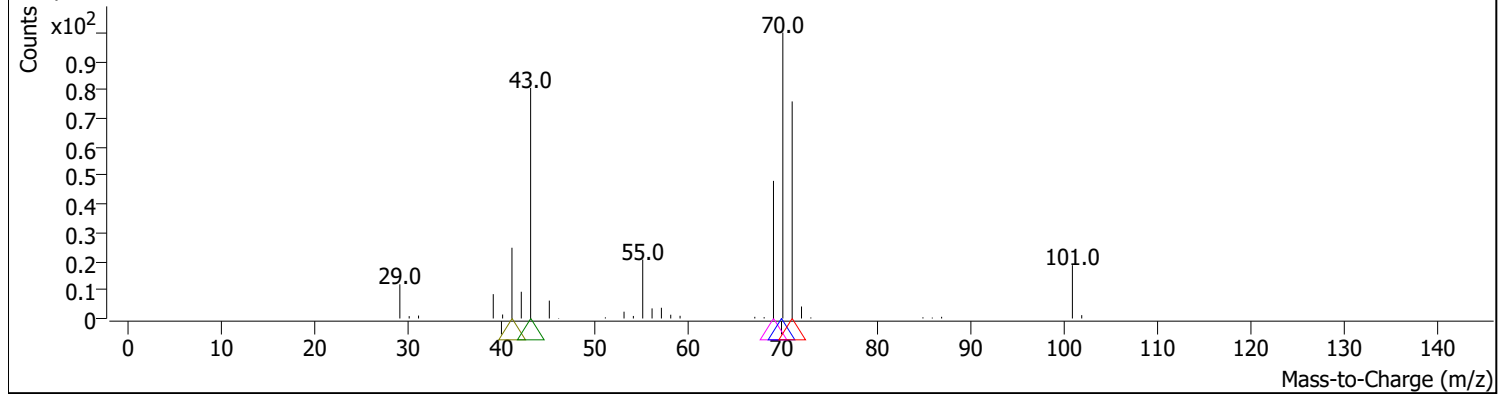
## Library Search Results - NonTarget Hits with Details



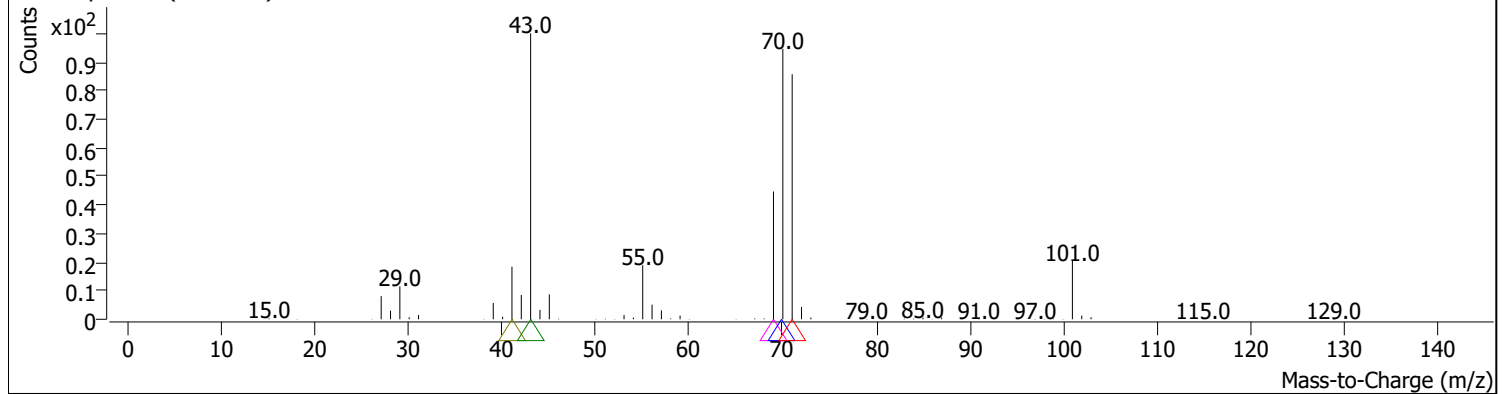
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
18.6543	Diisoamyl ether	4244738.5	98.2	544-01-4	C <sub>10</sub> H <sub>22</sub> O	

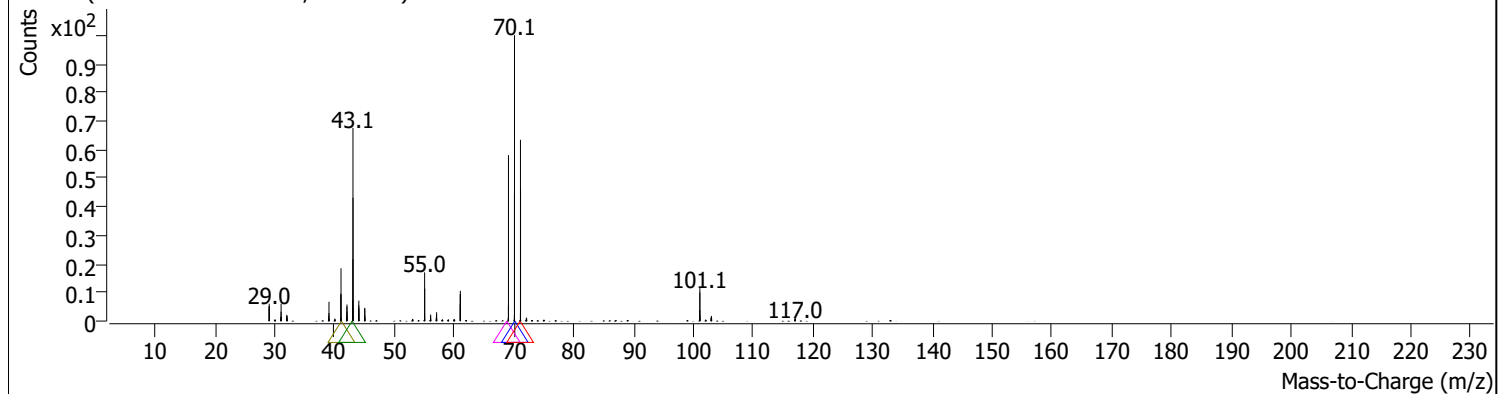
Component RT: 18.6543



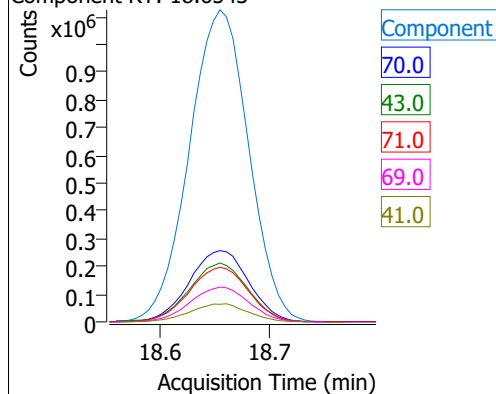
Diisoamyl ether (NIST20.L)



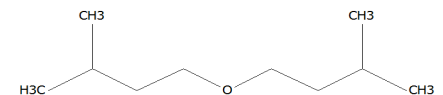
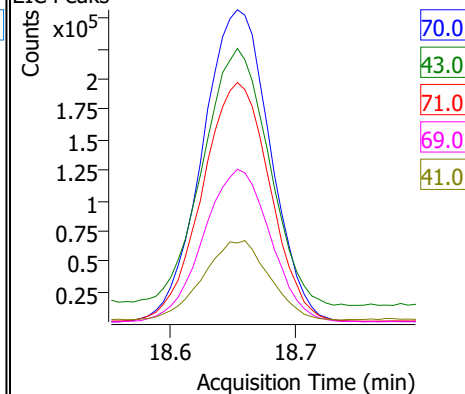
+ Scan (18.5526-18.7964 min, 42 scans) 4.D



Component RT: 18.6543



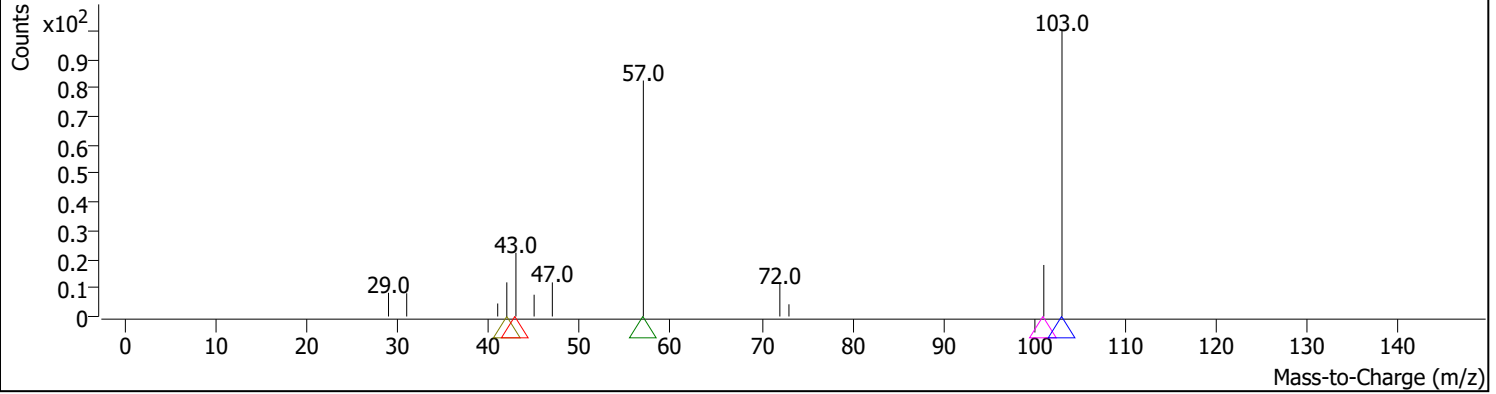
EIC Peaks



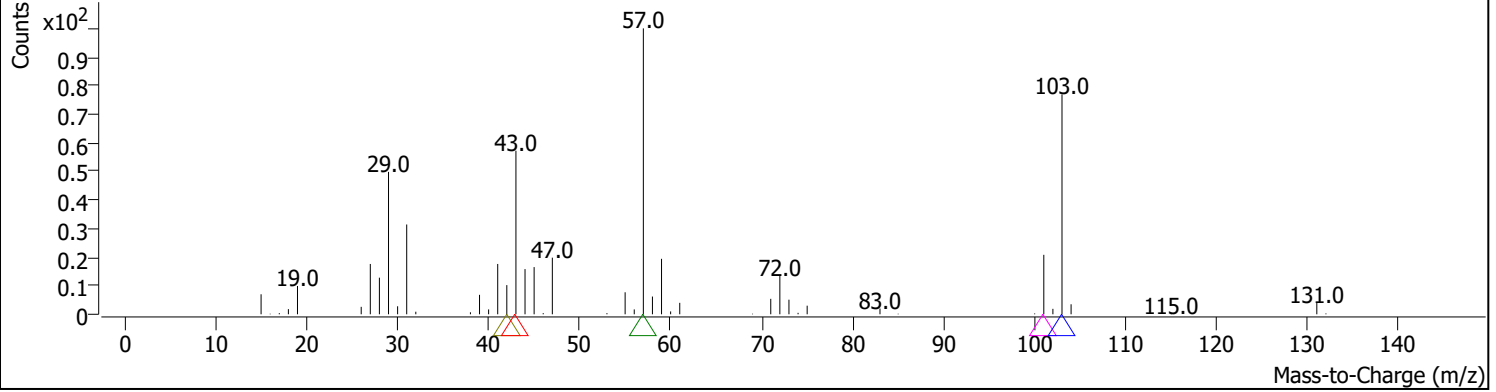
# Library Search Results - NonTarget Hits with Details

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
19.7524	1,3-Dioxolane-4-methanol, 2-ethyl-	167867.0	85.4	53951-44-3	C6H12O3	

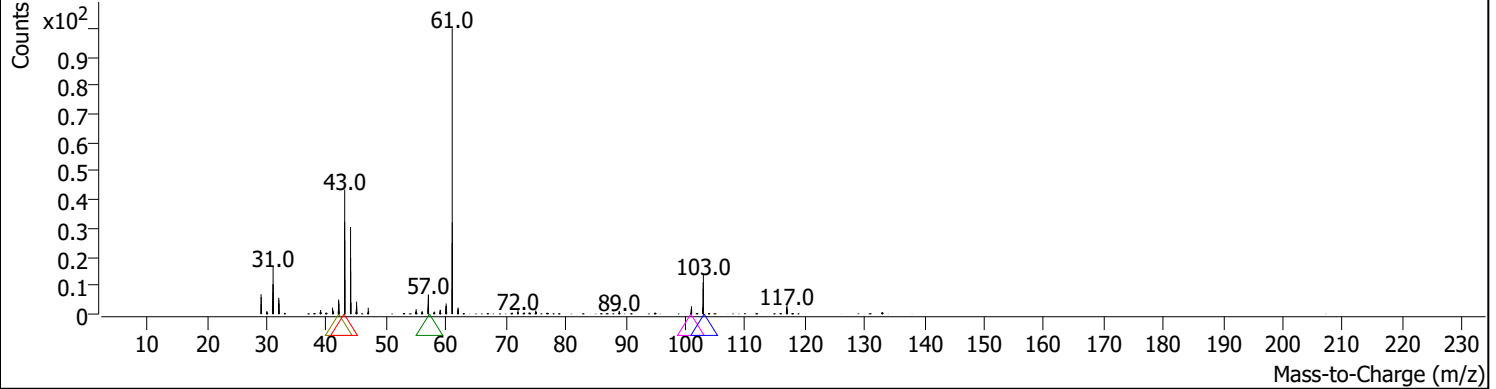
Component RT: 19.7524



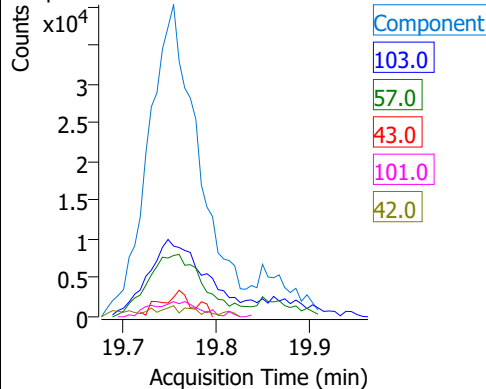
1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L)



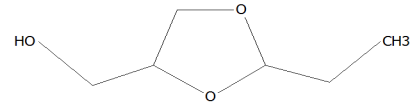
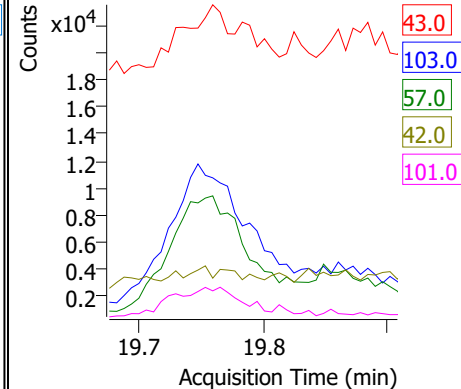
+ Scan (19.6943-19.8072 min, 20 scans) 4.D



Component RT: 19.7524



EIC Peaks



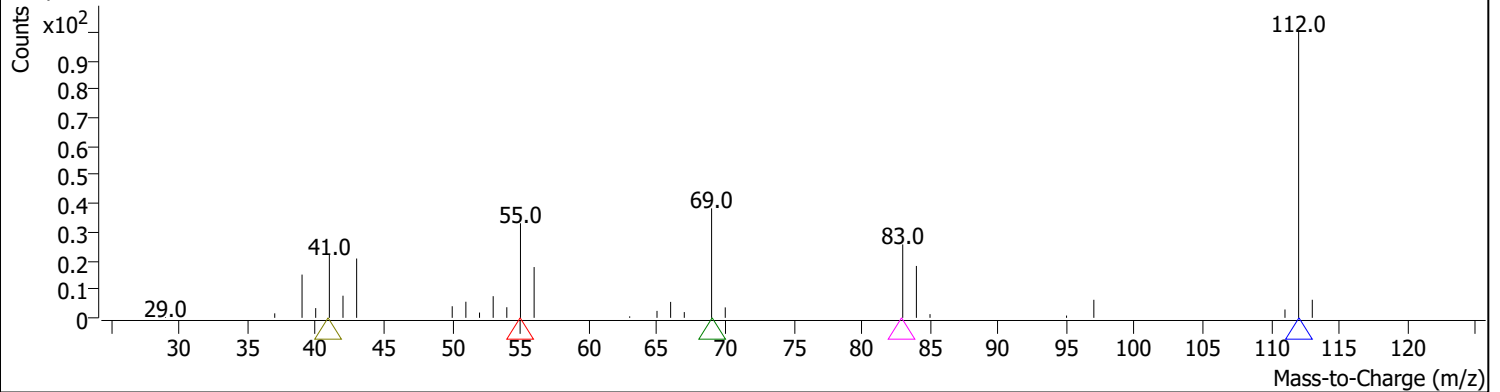
## Library Search Results - NonTarget Hits with Details



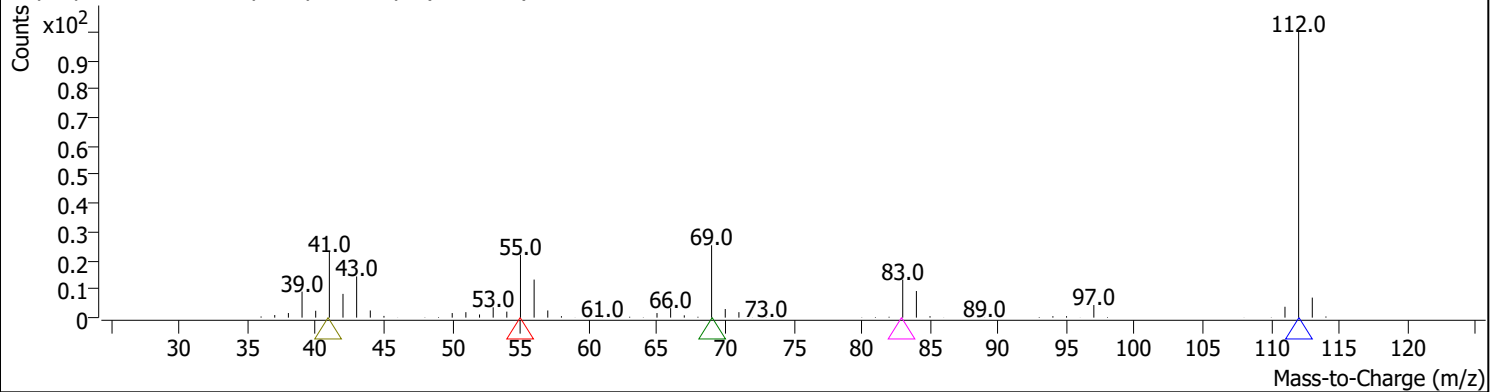
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
20.0568	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	658804.5	95.3	80-71-7	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	

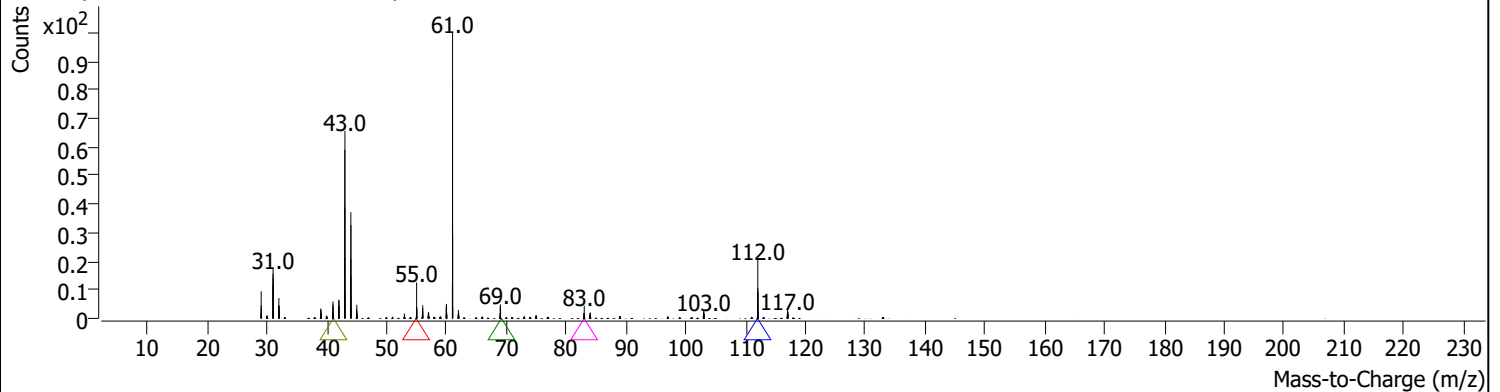
Component RT: 20.0568



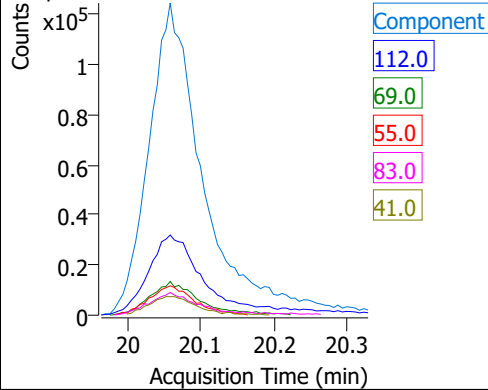
2-Cyclopenten-1-one, 2-hydroxy-3-methyl- (NIST20.L)



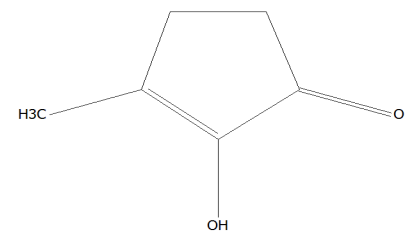
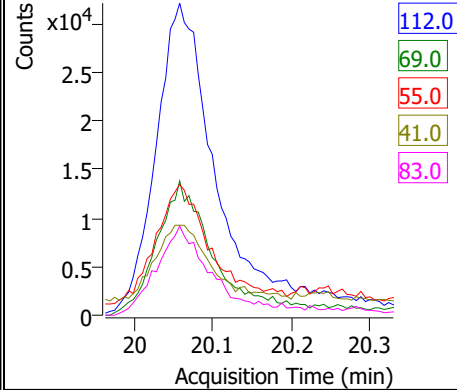
+ Scan (19.9579-20.3305 min, 63 scans) 4.D



Component RT: 20.0568



EIC Peaks



## Library Search Results - NonTarget Hits with Details

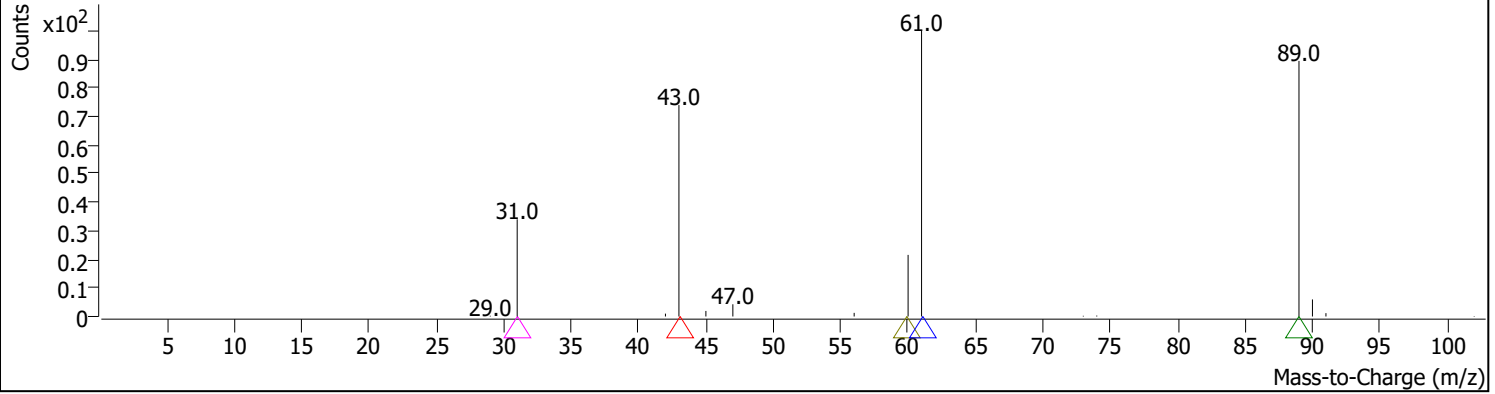


Agilent

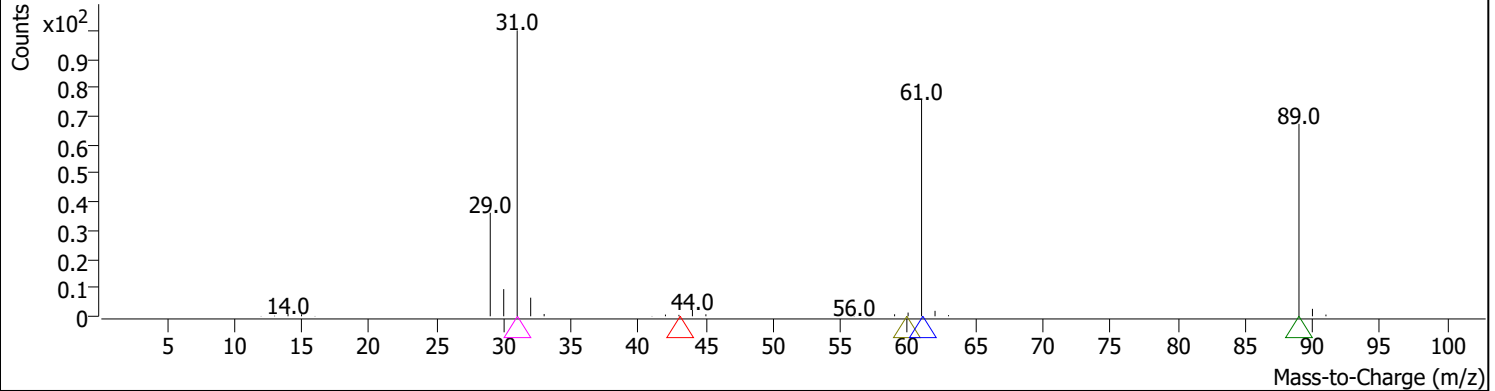
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
21.1424	1,3,5-Trioxane	4088997.3	81.6	110-88-3	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	

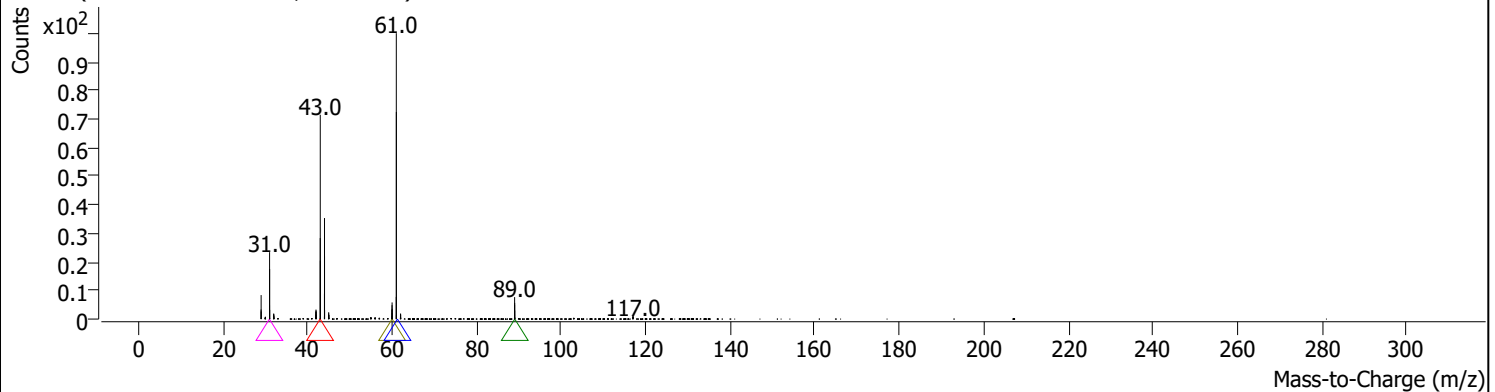
Component RT: 21.1424



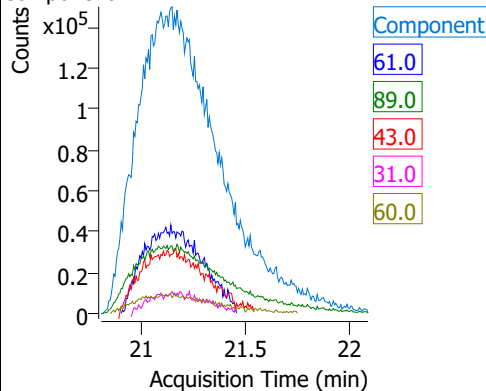
1,3,5-Trioxane (NIST20.L)



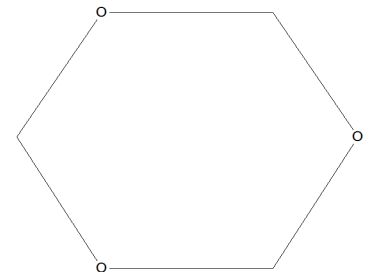
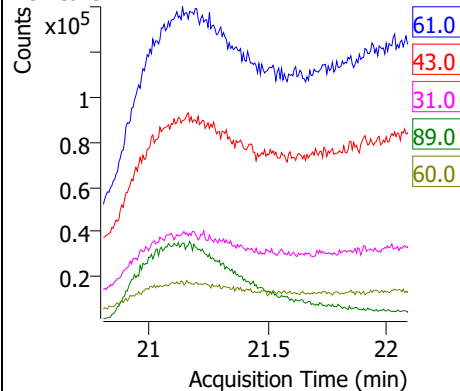
+ Scan (20.8120-22.0846 min, 215 scans) 4.D



Component RT: 21.1424



EIC Peaks



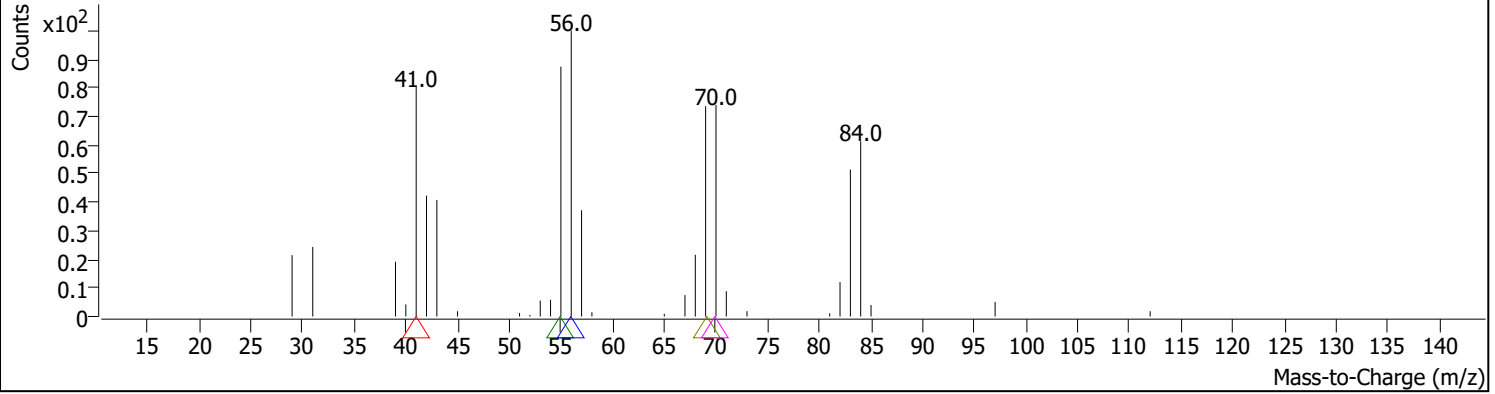
## Library Search Results - NonTarget Hits with Details



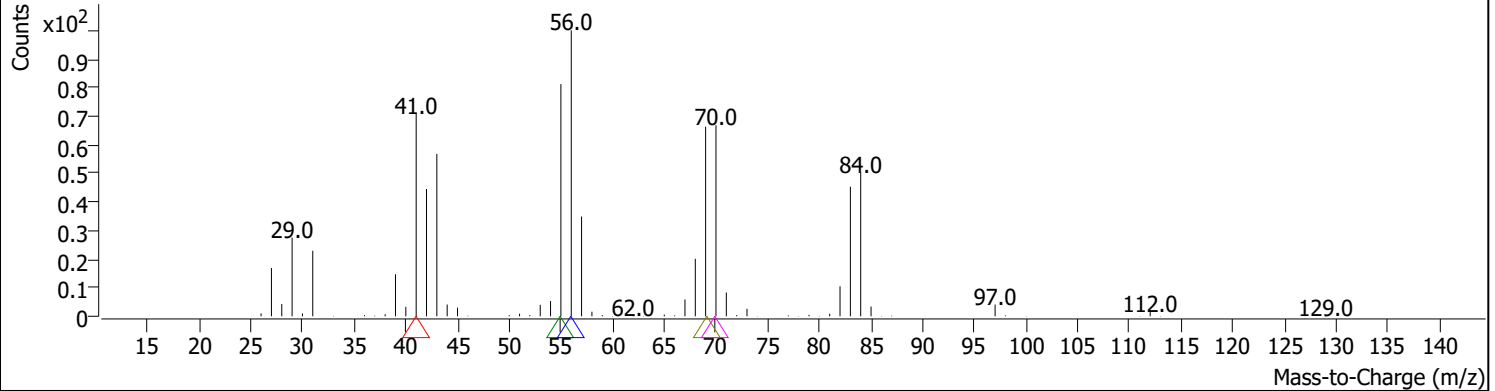
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
23.0353	1-Octanol	3434766.0	98.7	111-87-5	C <sub>8</sub> H <sub>18</sub> O	

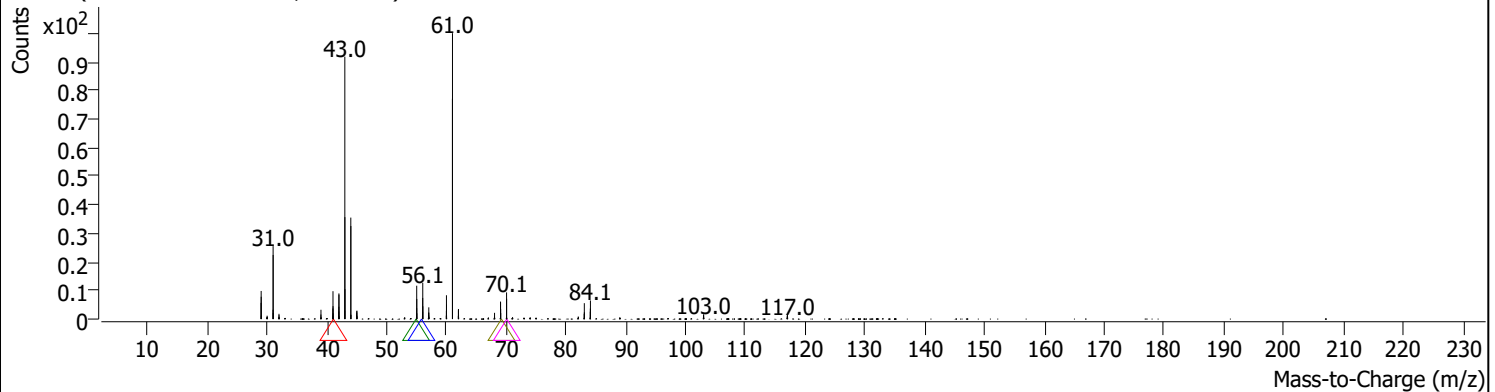
Component RT: 23.0353



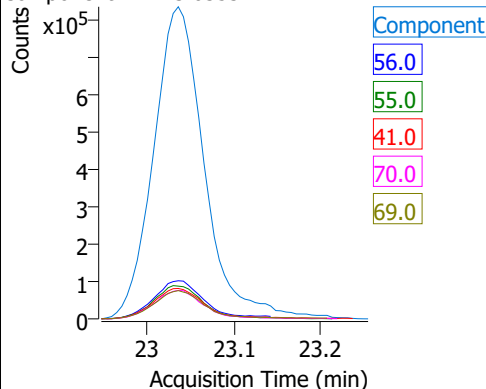
1-Octanol (NIST20.L)



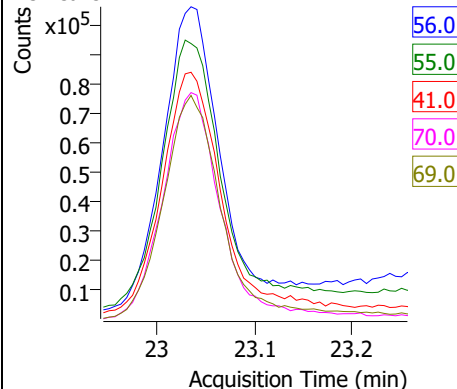
+ Scan (22.9530-23.2262 min, 46 scans) 4.D



Component RT: 23.0353



EIC Peaks



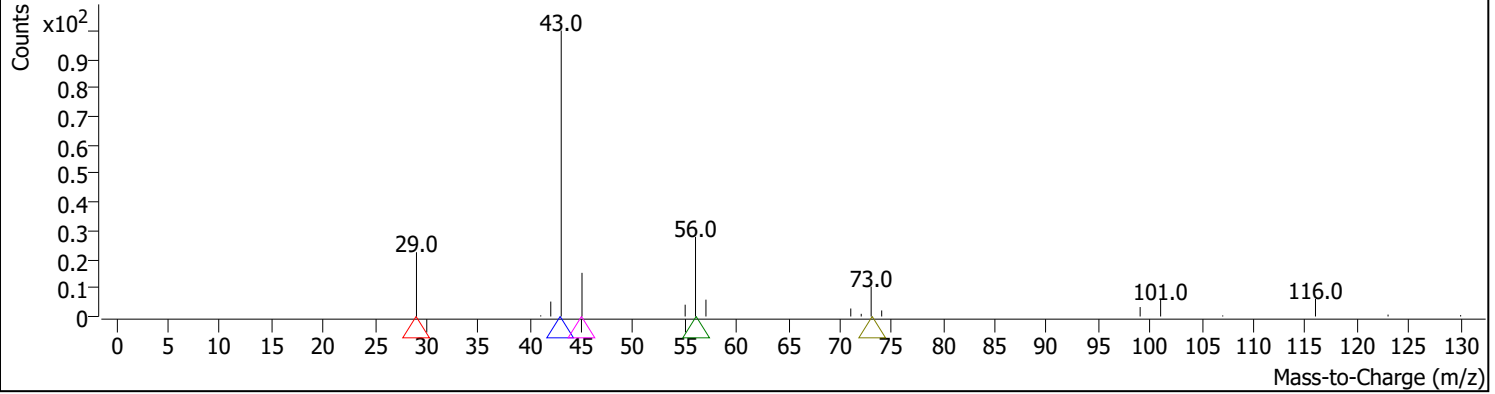
## Library Search Results - NonTarget Hits with Details



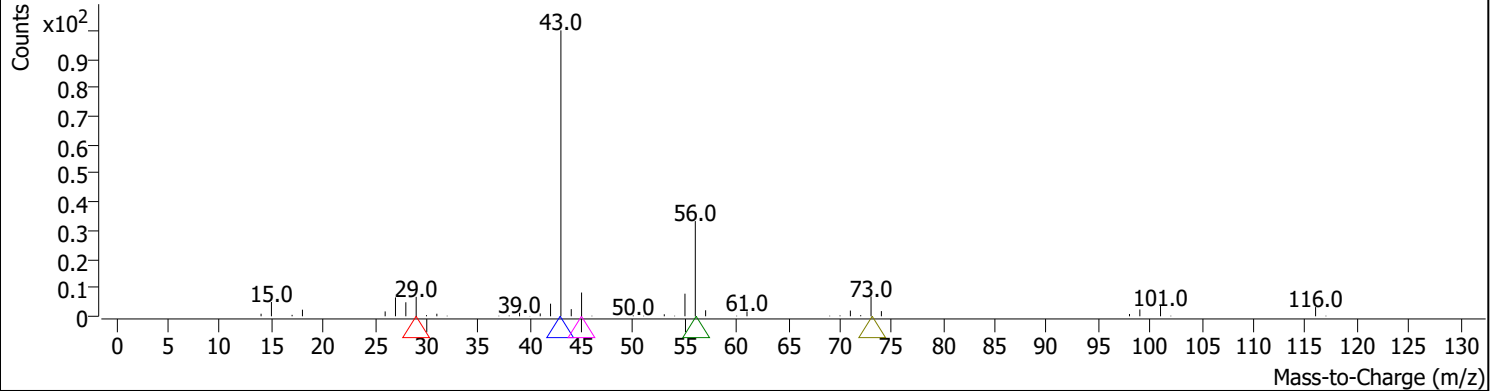
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
23.5037	Pentanoic acid, 4-oxo-	2002503.1	92.6	123-76-2	C5H8O3	

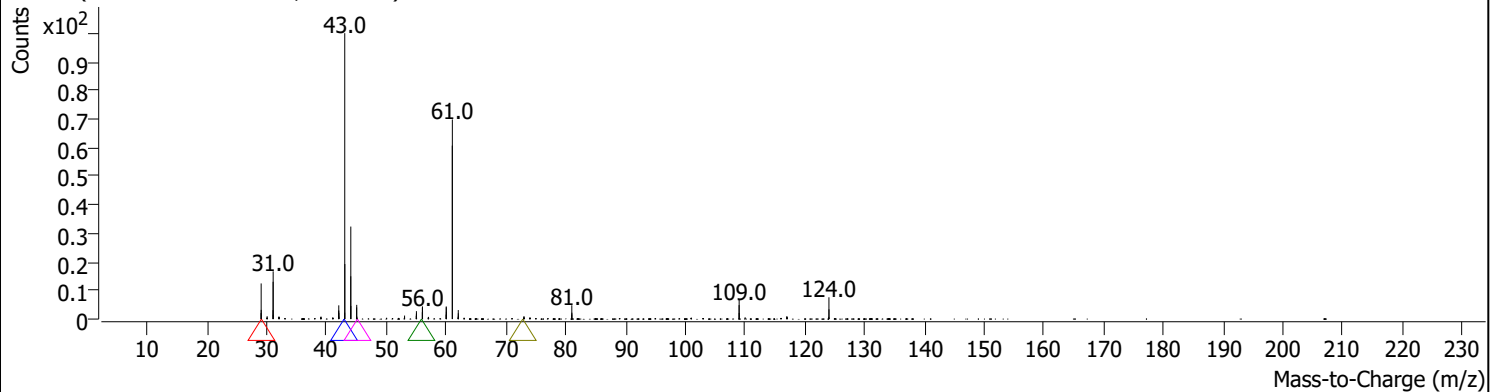
Component RT: 23.5037



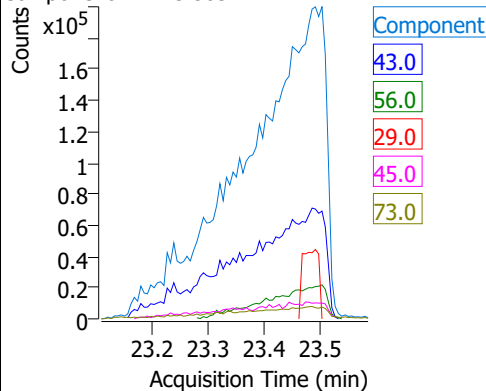
Pentanoic acid, 4-oxo- (NIST20.L)



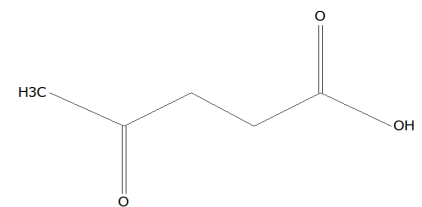
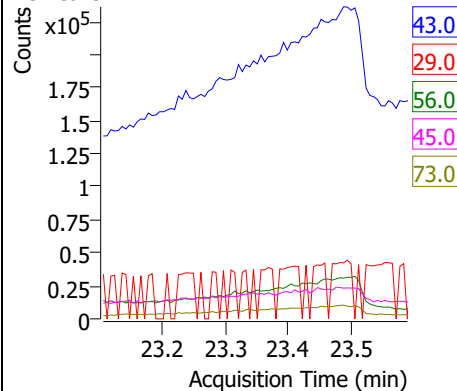
+ Scan (23.2767-23.5413 min, 45 scans) 4.D



Component RT: 23.5037



EIC Peaks





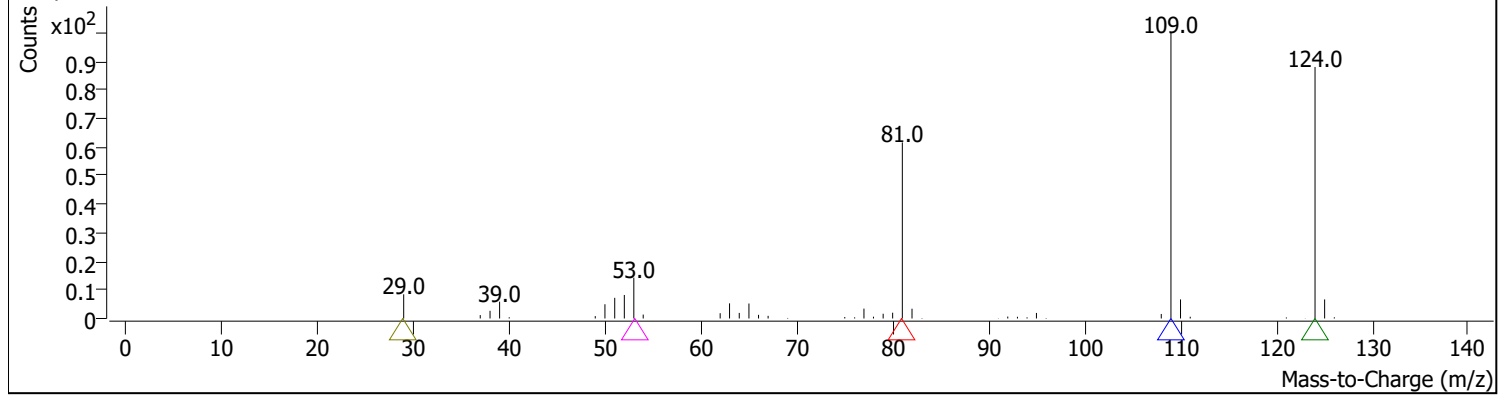
## Library Search Results - NonTarget Hits with Details



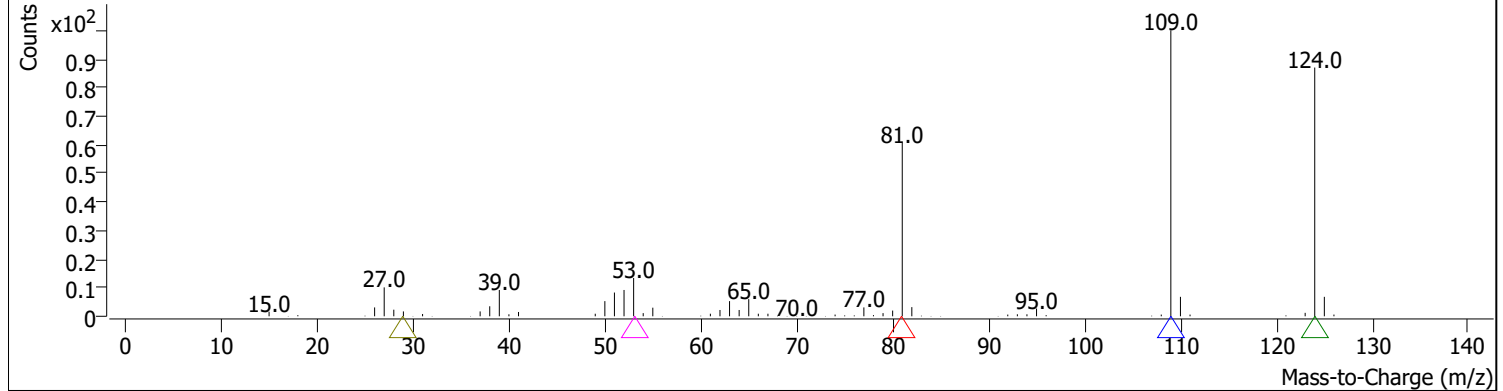
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
23.5626	Phenol, 2-methoxy-	5846632.4	97.9	90-05-1	C7H8O2	

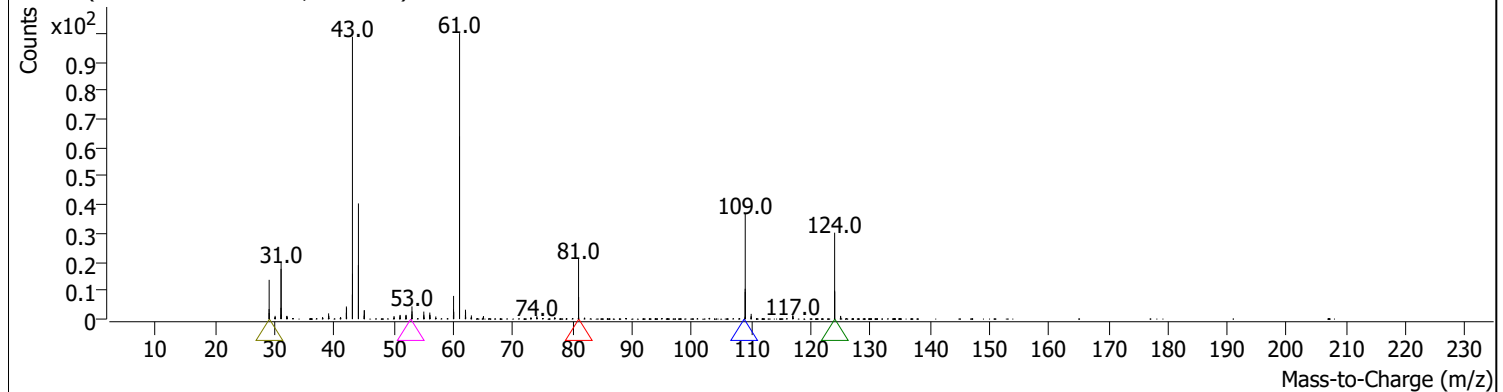
Component RT: 23.5626



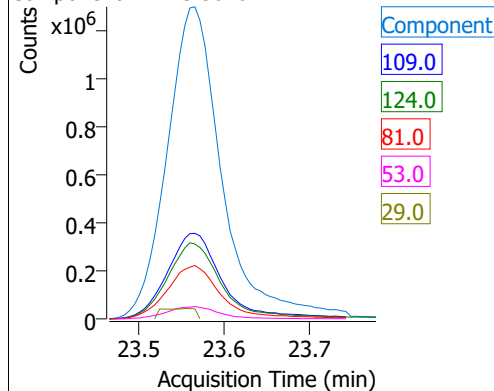
Phenol, 2-methoxy- (NIST20.L)



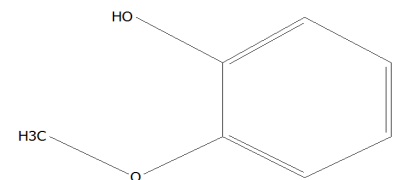
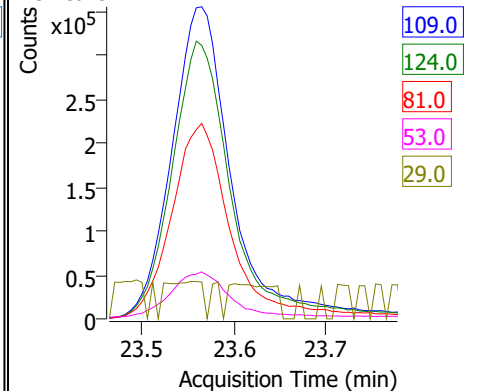
+ Scan (23.4640-23.7792 min, 54 scans) 4.D



Component RT: 23.5626



EIC Peaks



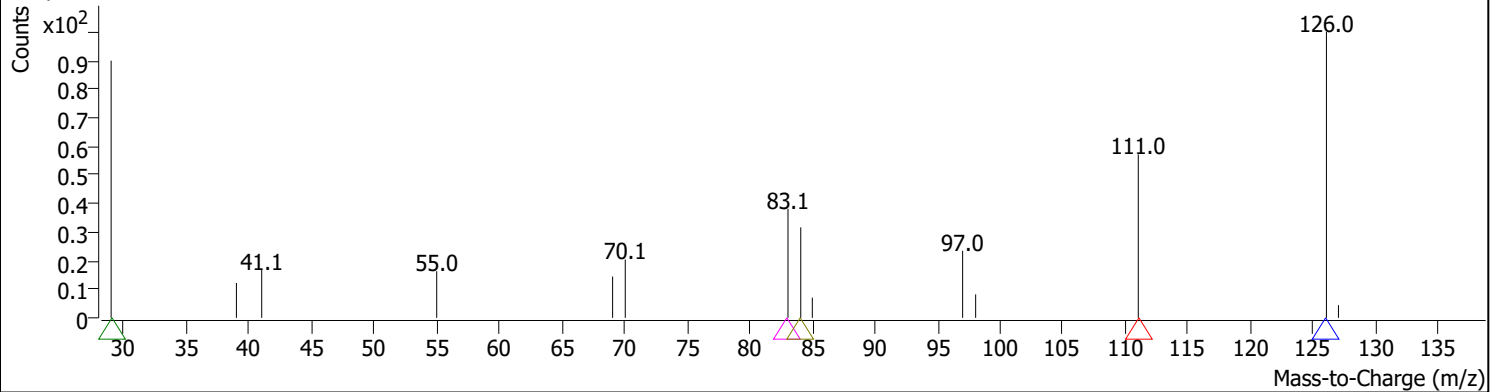
## Library Search Results - NonTarget Hits with Details



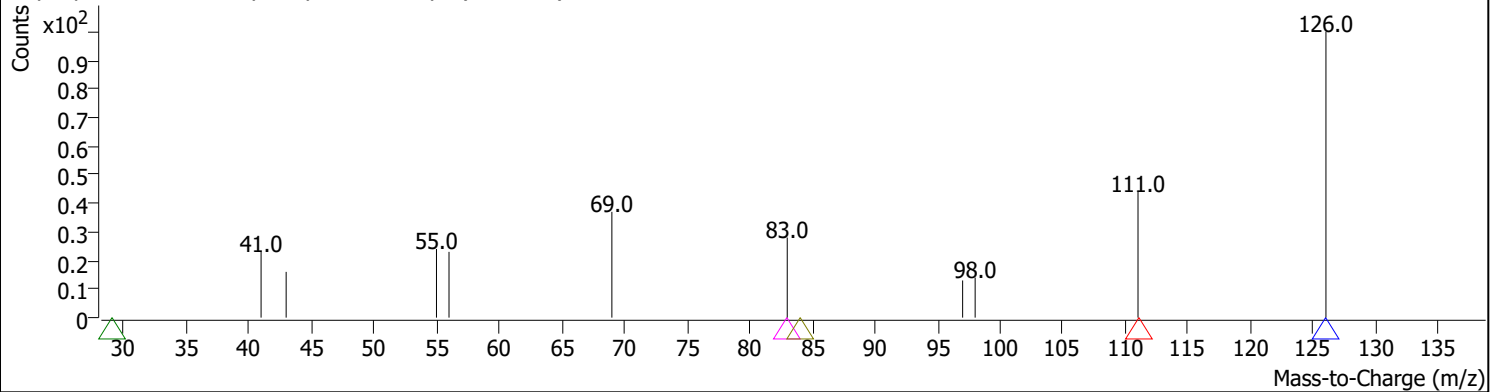
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
23.7721	2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-	319272.0	78.5	21835-00-7	C7H10O2	

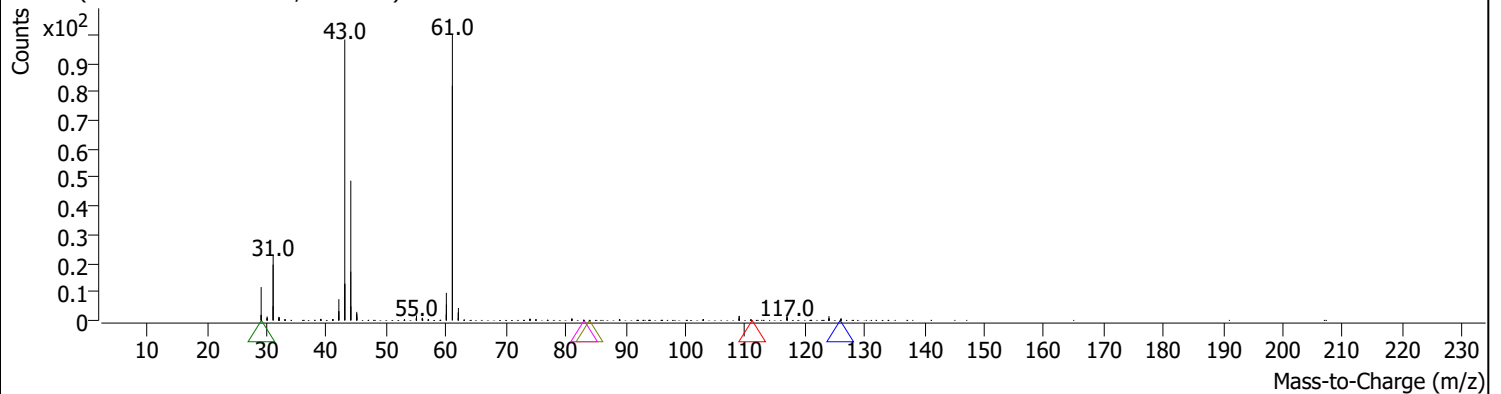
Component RT: 23.7721



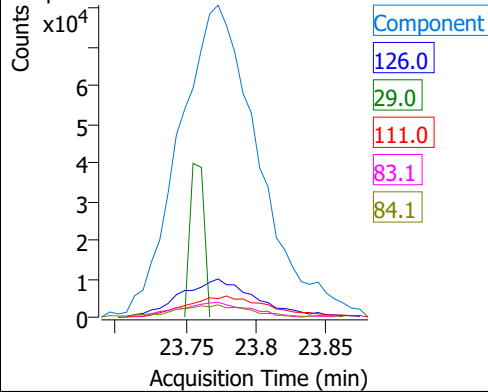
2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl- (NIST20.L)



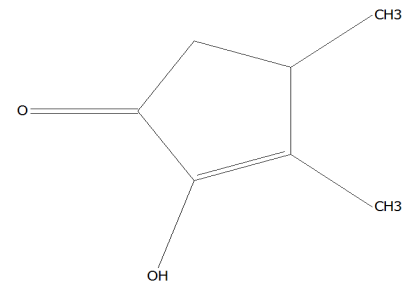
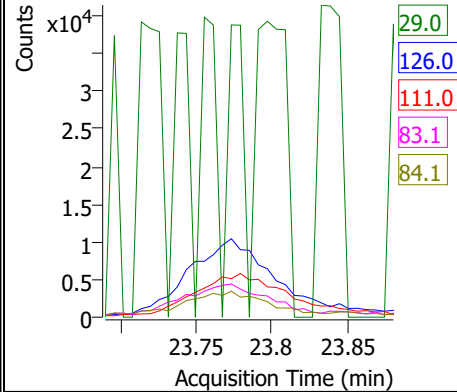
+ Scan (23.7050-23.8743 min, 29 scans) 4.D



Component RT: 23.7721



EIC Peaks



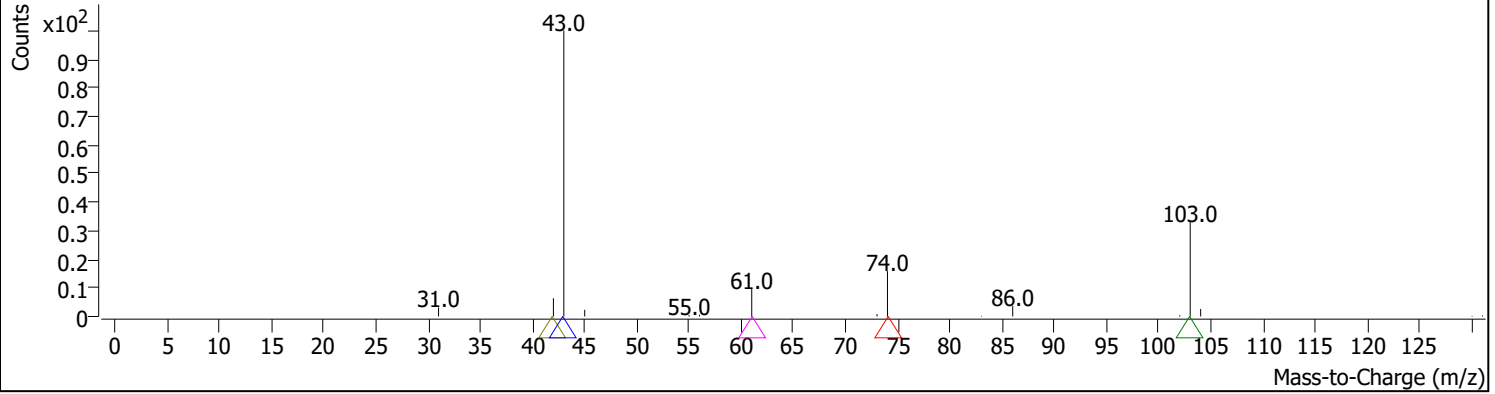
## Library Search Results - NonTarget Hits with Details



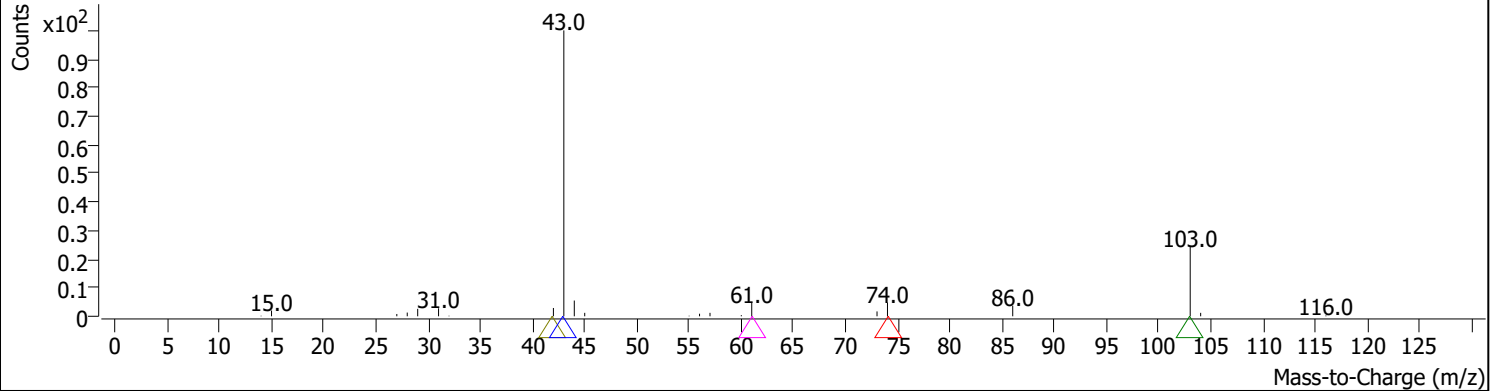
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
24.6648	1,2,3-Propanetriol, 1-acetate	2725027.1	91.7	106-61-6	C5H10O4	

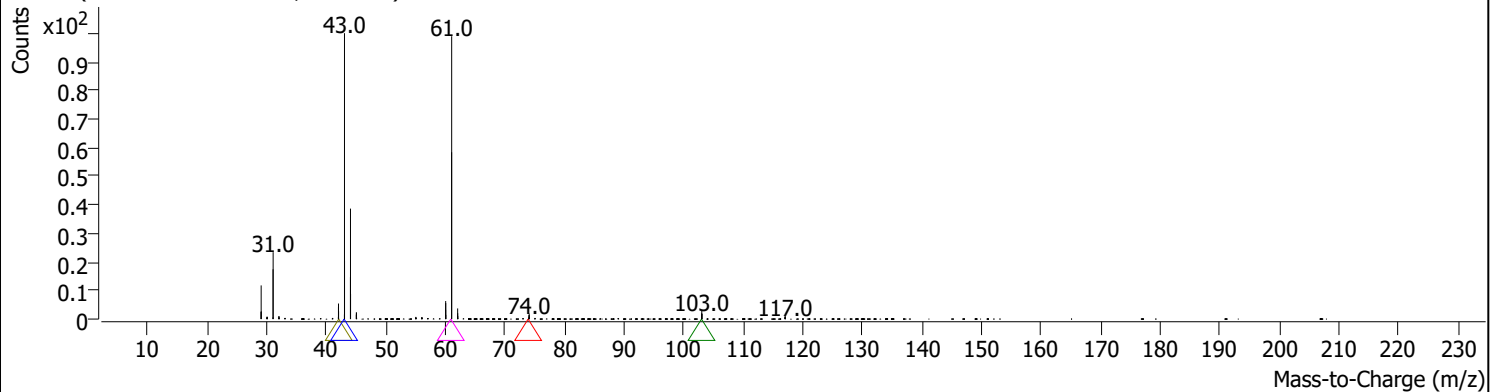
Component RT: 24.6648



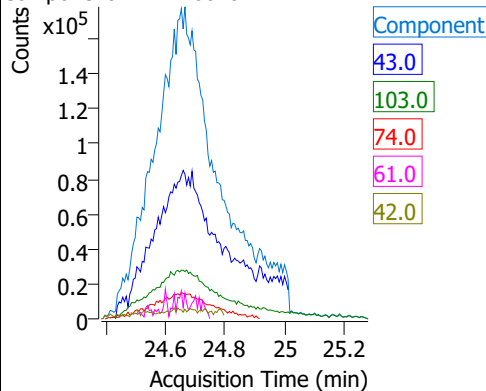
1,2,3-Propanetriol, 1-acetate (NIST20.L)



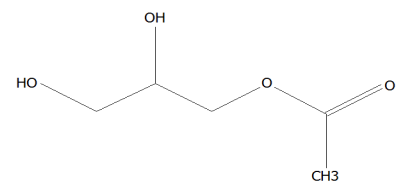
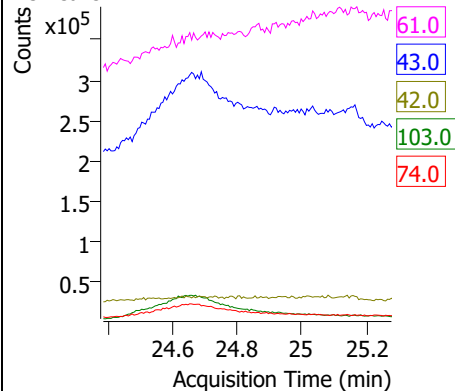
+ Scan (24.3857-24.7960 min, 70 scans) 4.D



Component RT: 24.6648



EIC Peaks



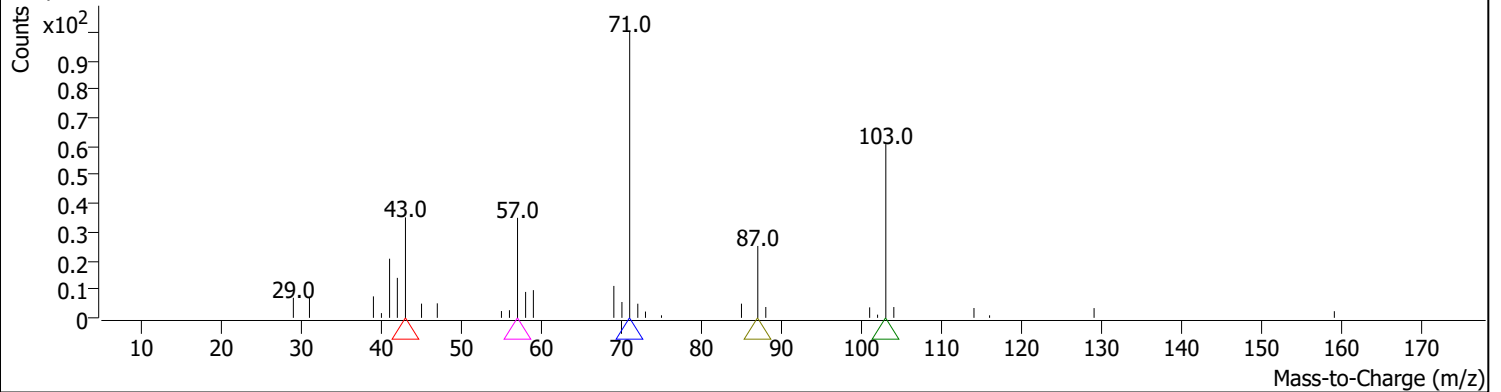
## Library Search Results - NonTarget Hits with Details



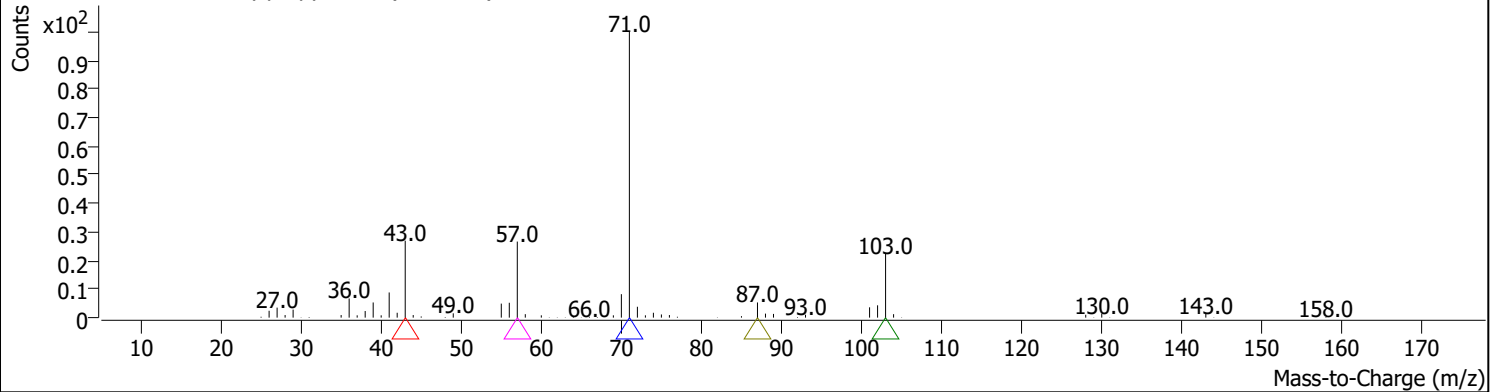
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
27.7300	Butanoic acid, 2,2-dimethylpropyl ester	521798.4	82.1	23361-69-5	C9H18O2	

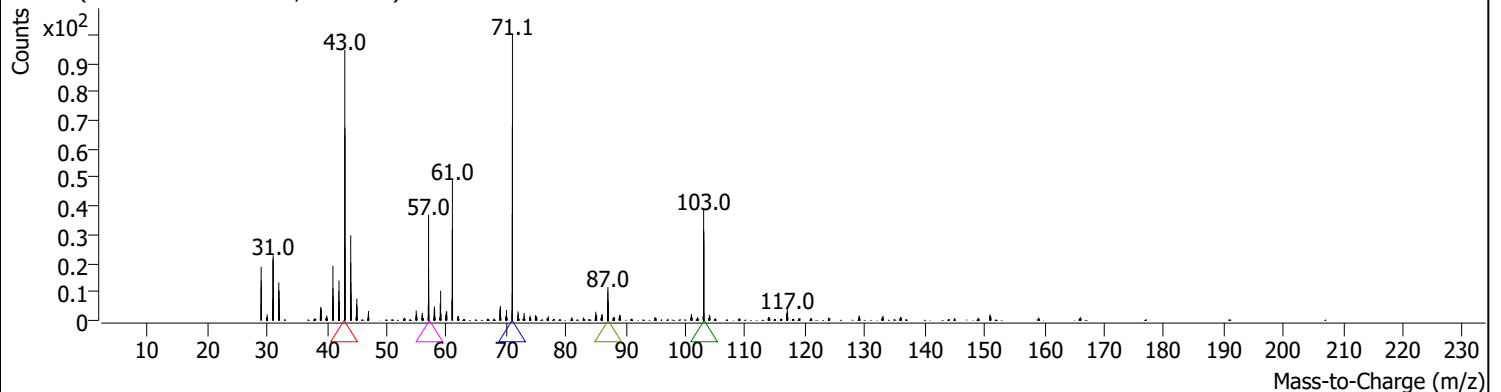
Component RT: 27.7300



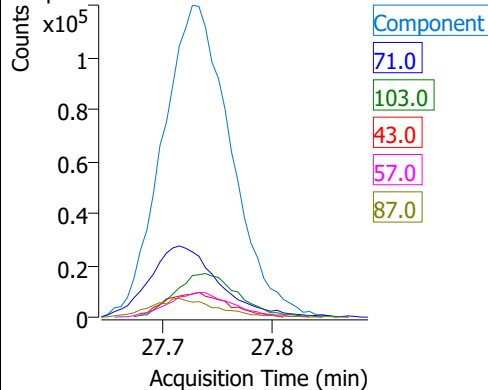
Butanoic acid, 2,2-dimethylpropyl ester (NIST20.L)



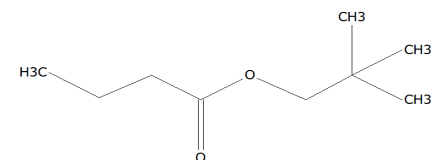
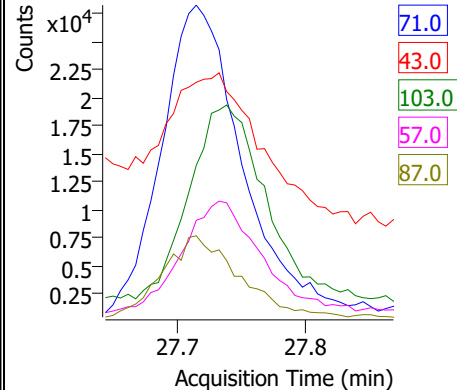
+ Scan (27.6512-27.7809 min, 22 scans) 4.D



Component RT: 27.7300



EIC Peaks



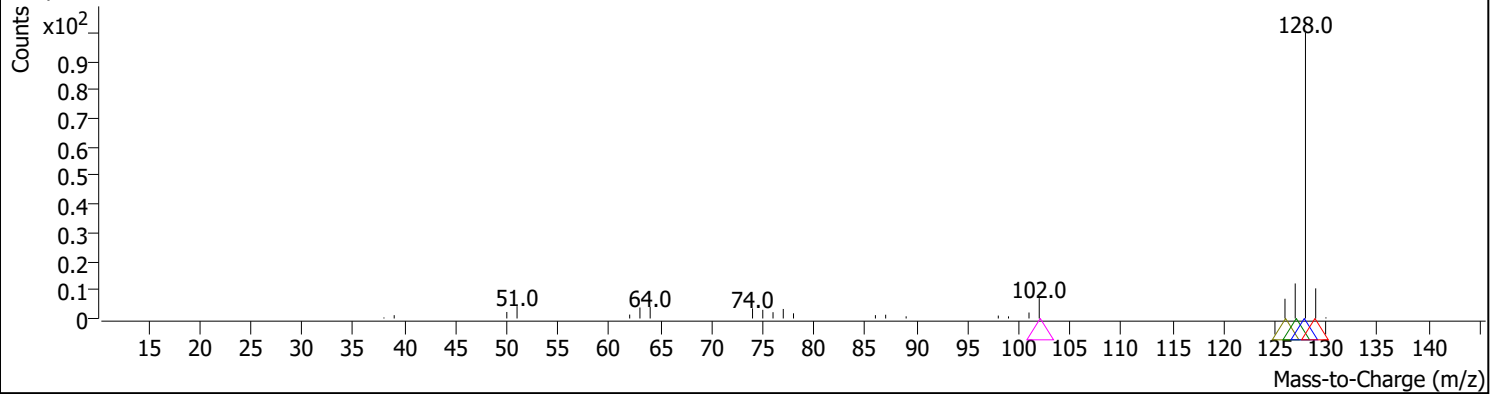
## Library Search Results - NonTarget Hits with Details



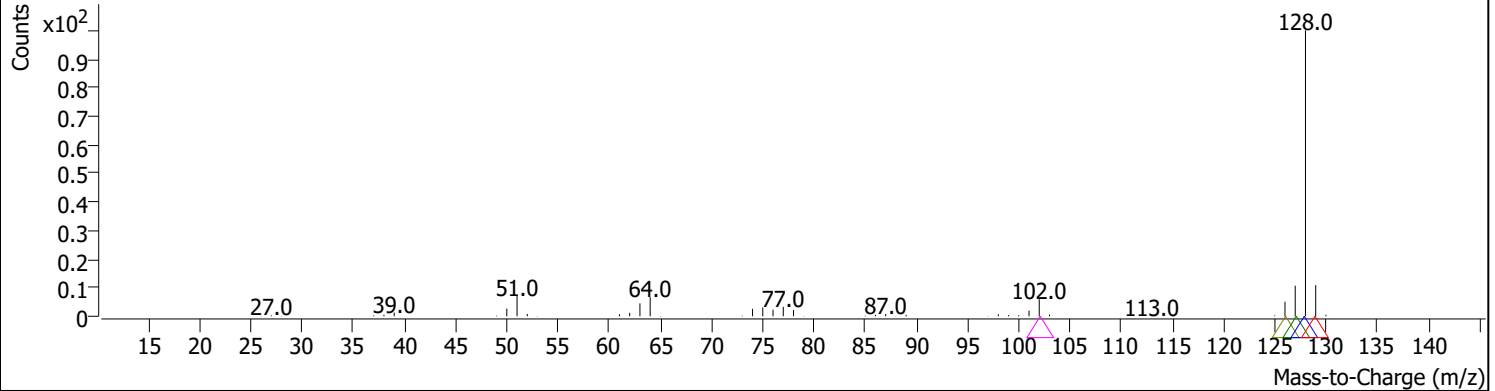
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
28.7452	Naphthalene	774394.9	97.5	91-20-3	C <sub>10</sub> H <sub>8</sub>	

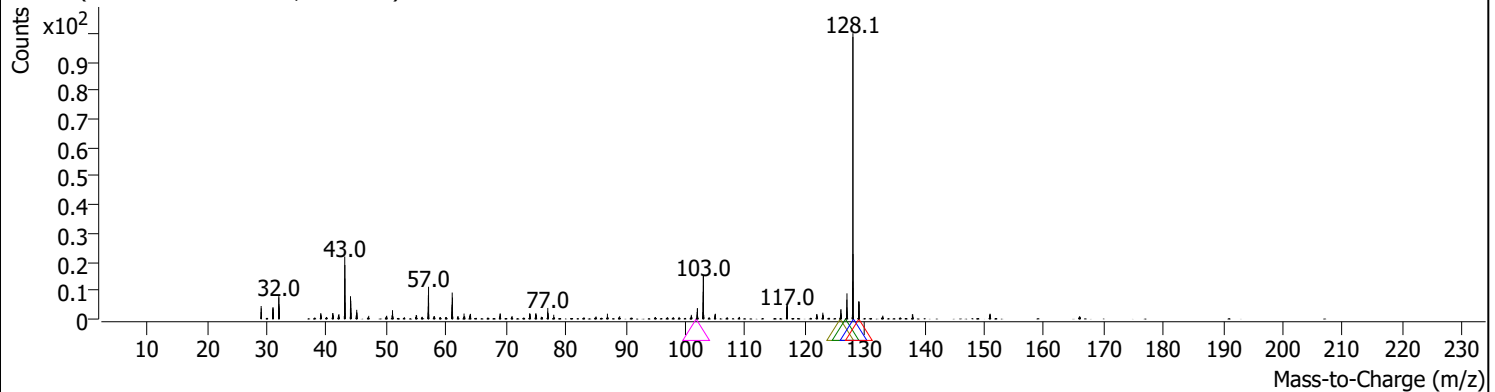
Component RT: 28.7452



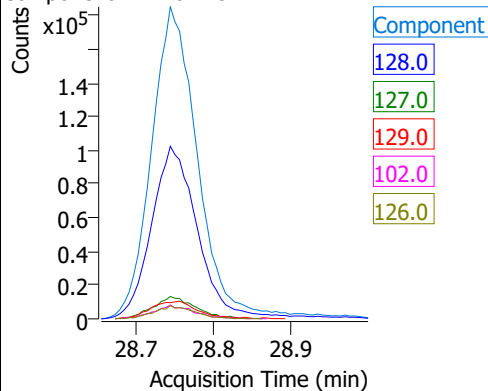
Naphthalene (NIST20.L)



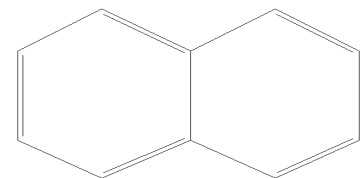
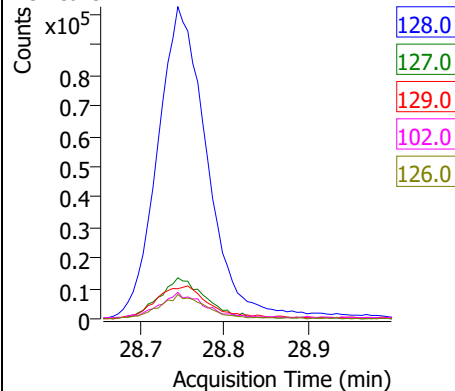
+ Scan (28.6549-28.9998 min, 59 scans) 4.D



Component RT: 28.7452



EIC Peaks



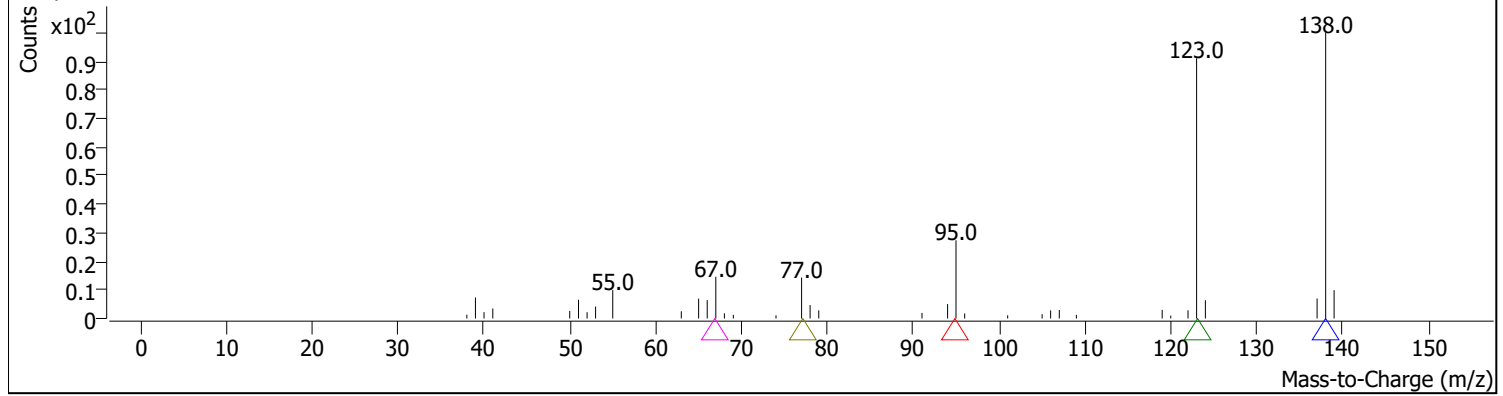
## Library Search Results - NonTarget Hits with Details



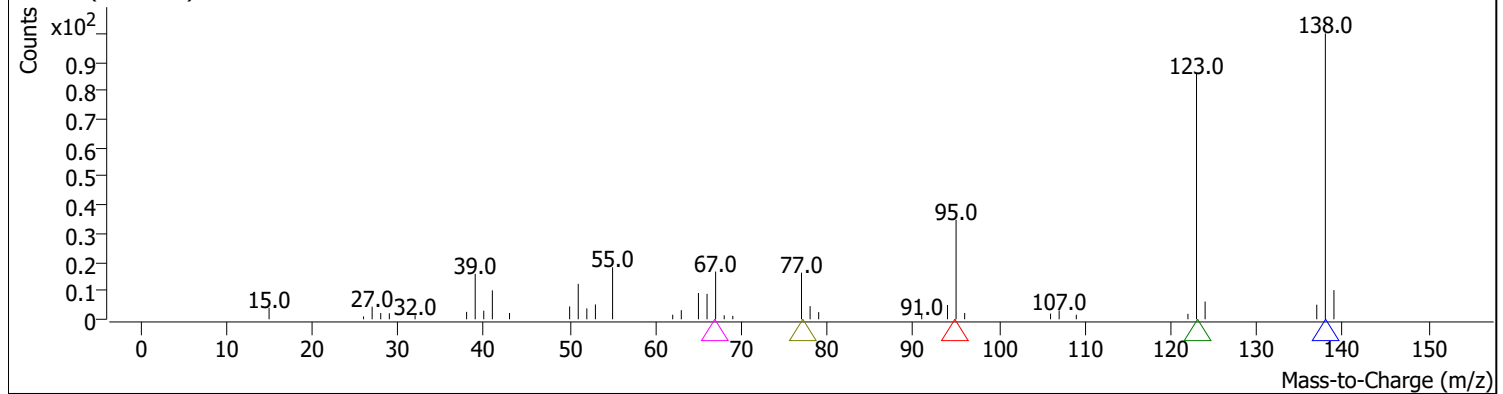
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
29.1709	Creosol	734304.1	96.7	93-51-6	C8H10O2	

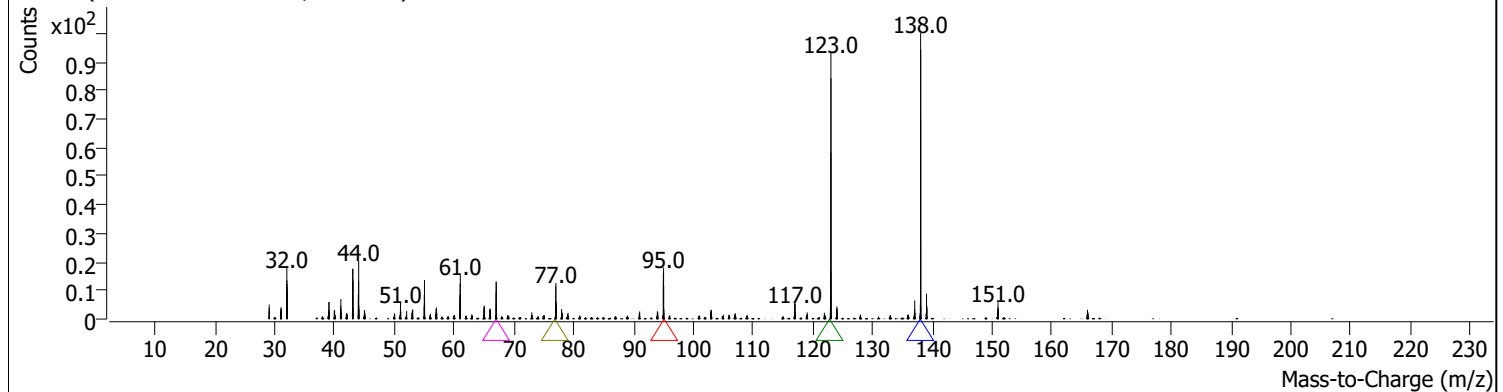
Component RT: 29.1709



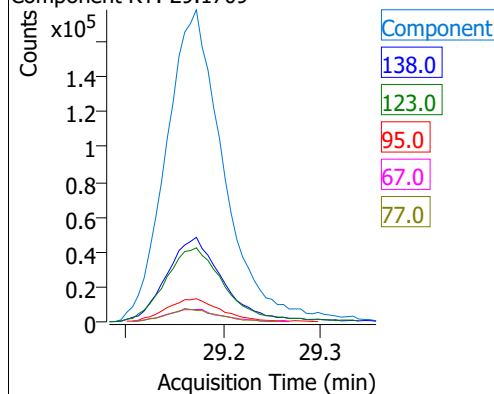
Creosol (NIST20.L)



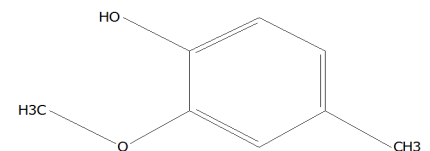
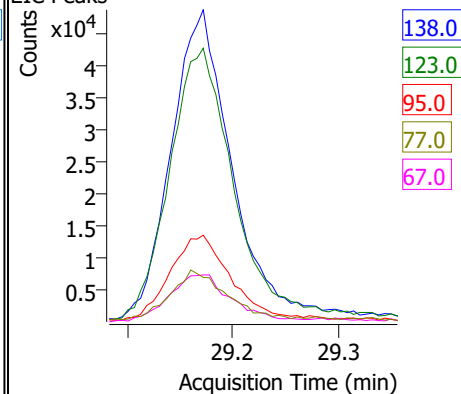
+ Scan (29.0890-29.3566 min, 46 scans) 4.D



Component RT: 29.1709



EIC Peaks



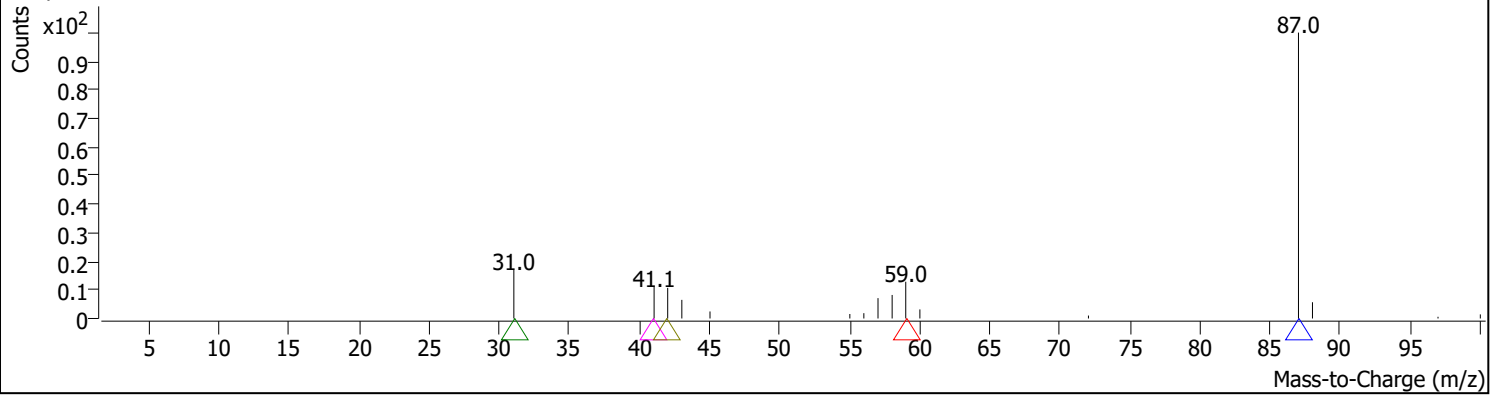
## Library Search Results - NonTarget Hits with Details



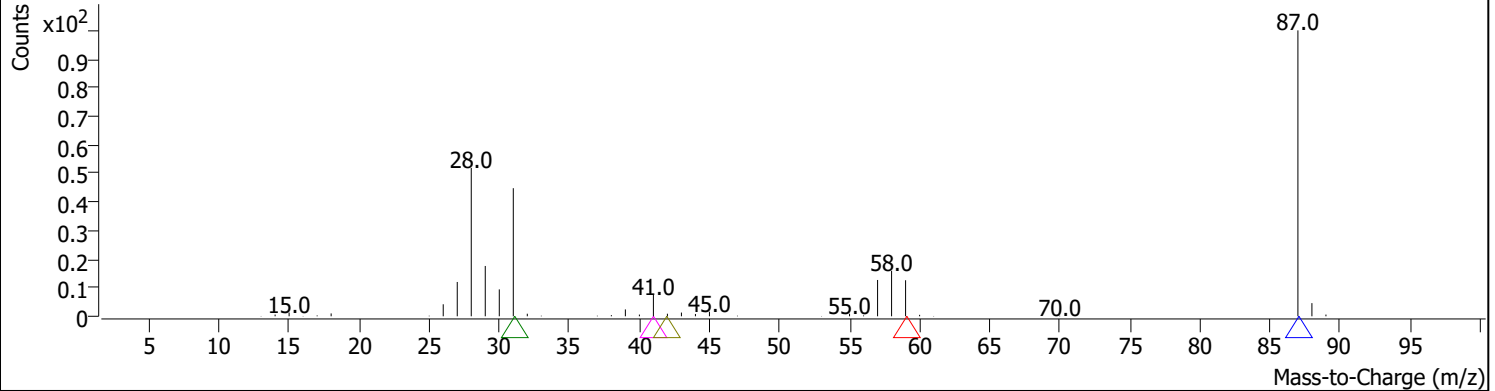
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
30.4742	1,3-Dioxane	454800.7	79.1	505-22-6	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	

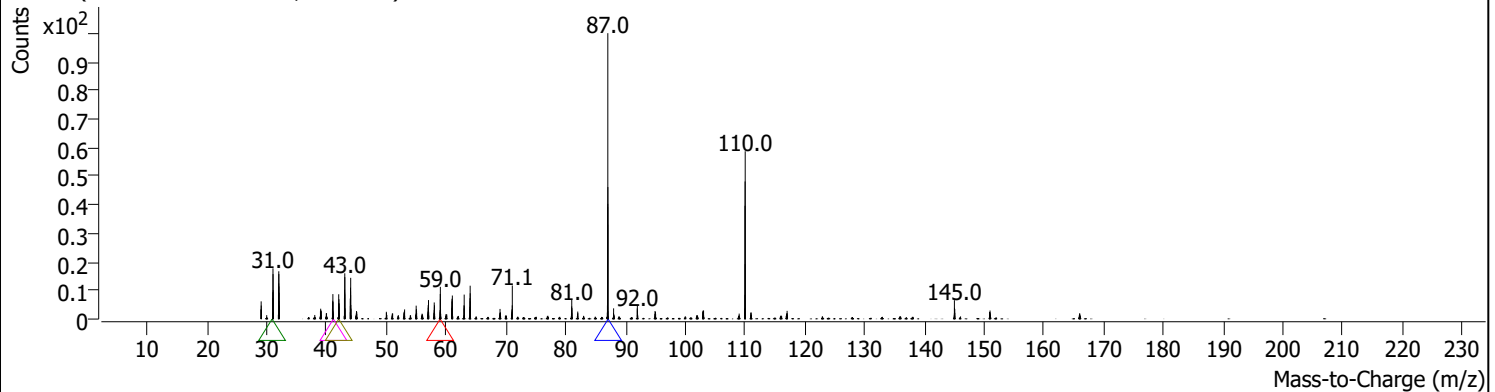
Component RT: 30.4742



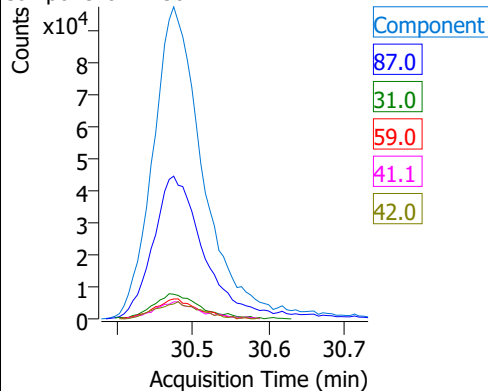
1,3-Dioxane (NIST20.L)



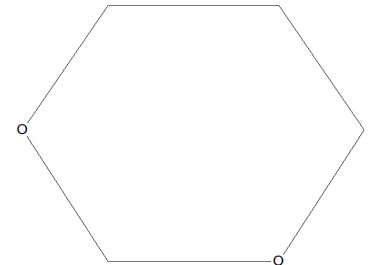
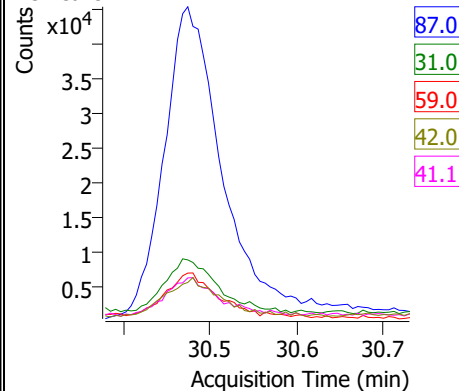
+ Scan (30.3795-30.7301 min, 59 scans) 4.D



Component RT: 30.4742



EIC Peaks



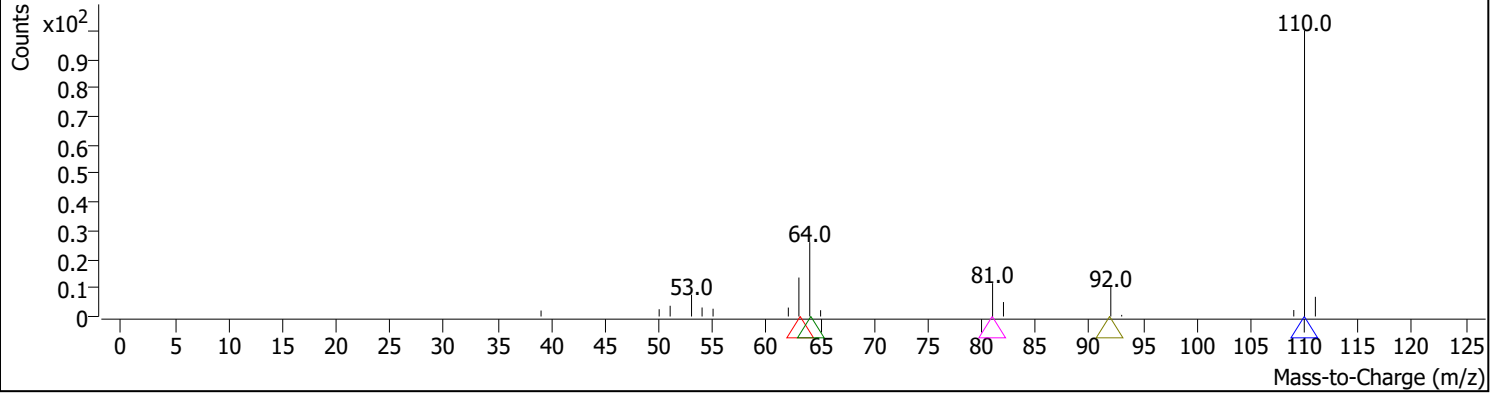
## Library Search Results - NonTarget Hits with Details



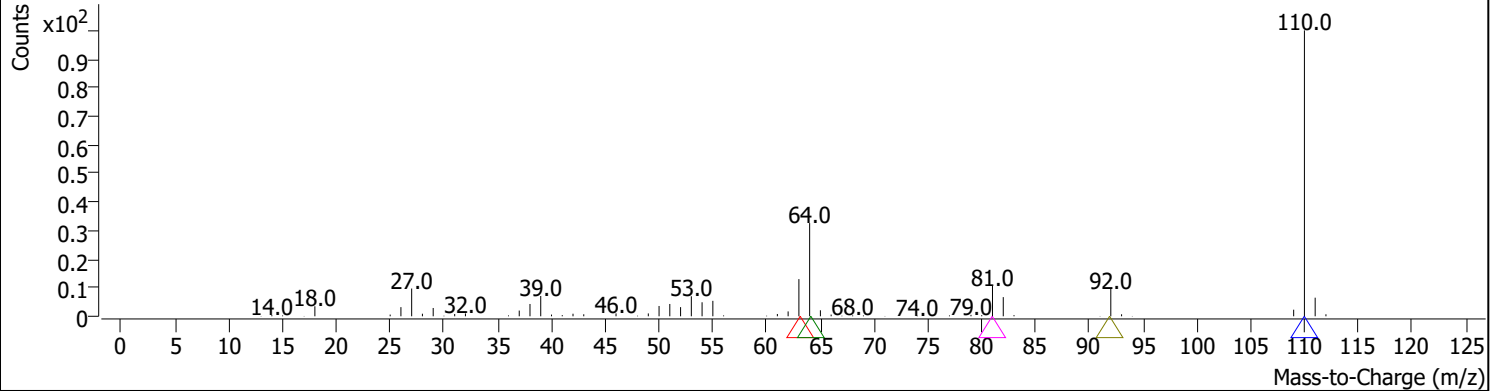
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
30.7369	Catechol	876657.4	93.0	120-80-9	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	

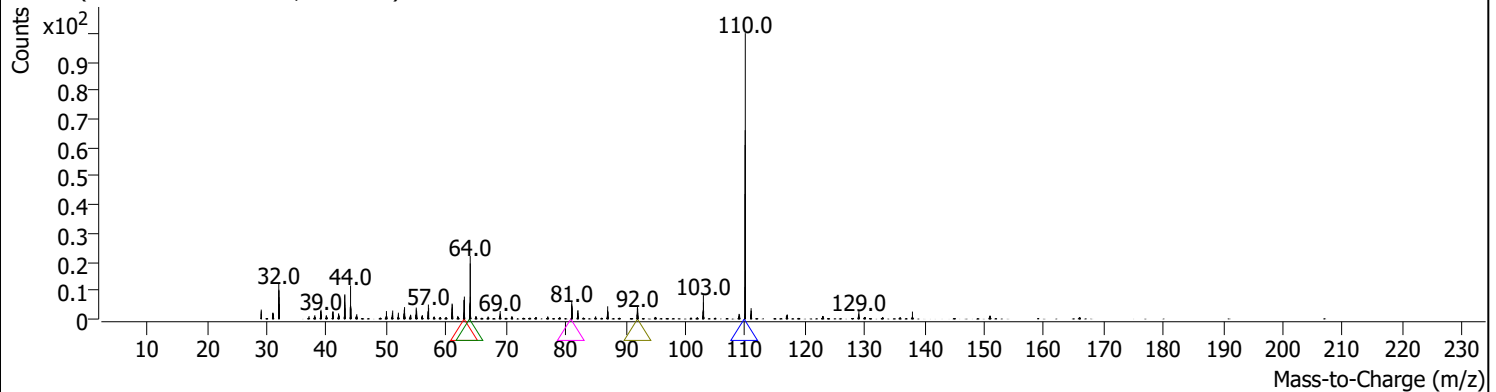
Component RT: 30.7369



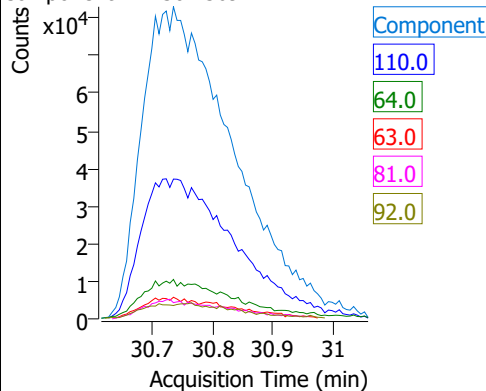
Catechol (NIST20.L)



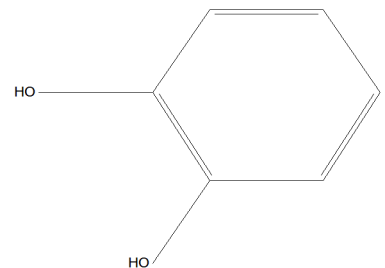
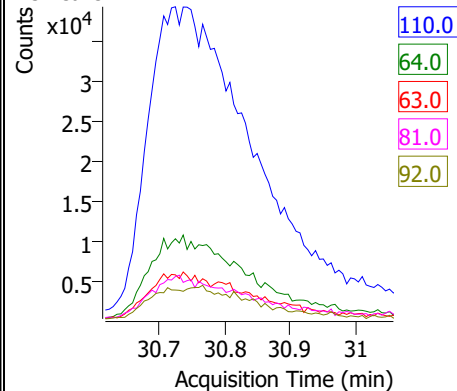
+ Scan (30.6237-31.0571 min, 73 scans) 4.D



Component RT: 30.7369



EIC Peaks





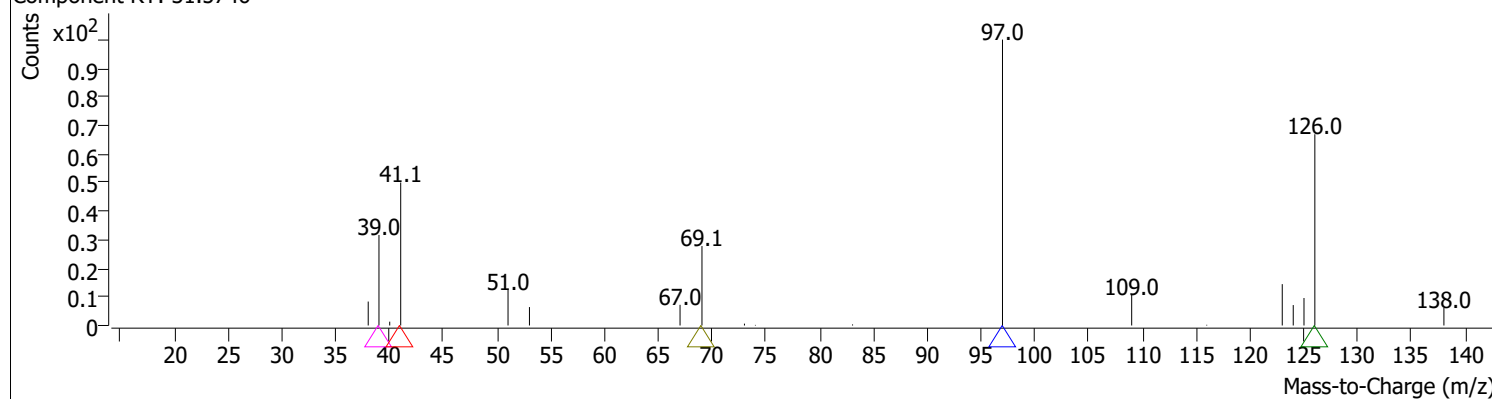
## Library Search Results - NonTarget Hits with Details



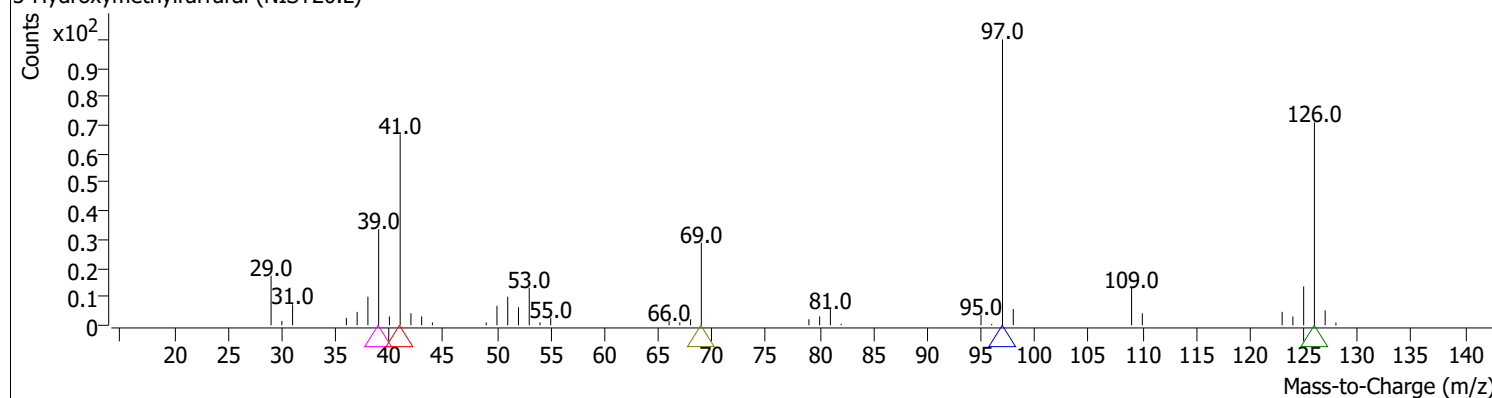
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
31.5746	5-Hydroxymethylfurfural	360007.4	82.3	67-47-0	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	

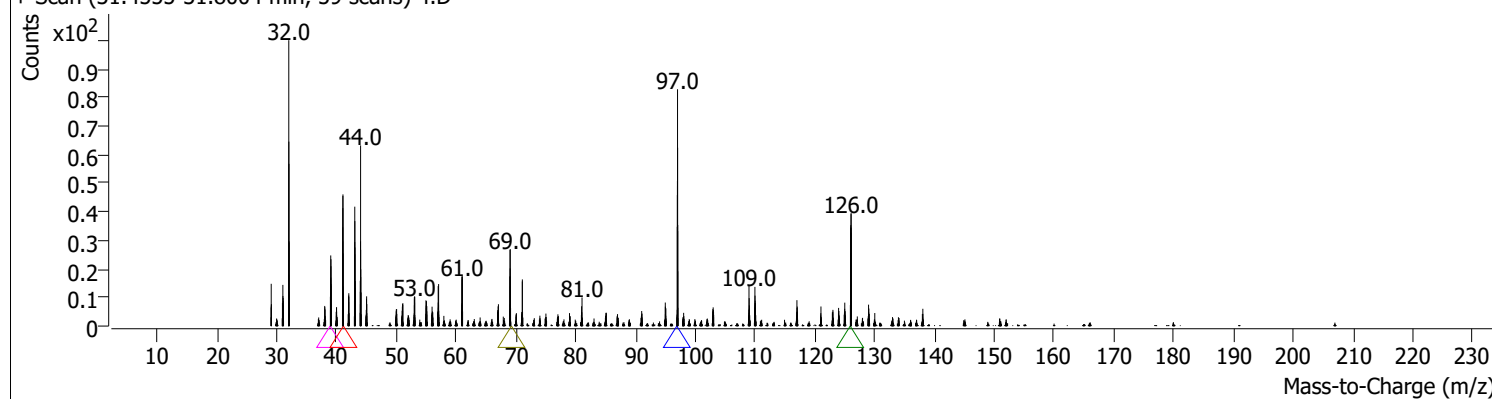
Component RT: 31.5746



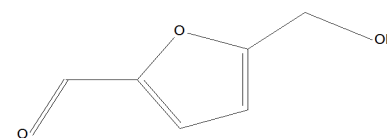
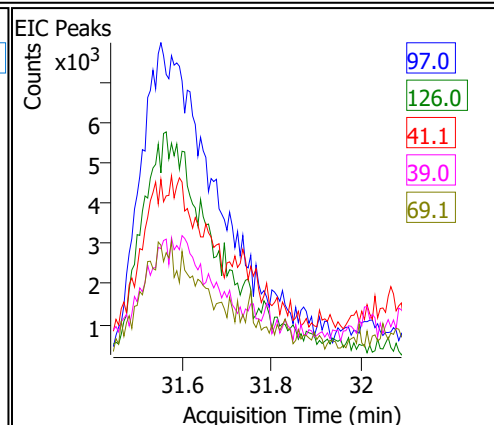
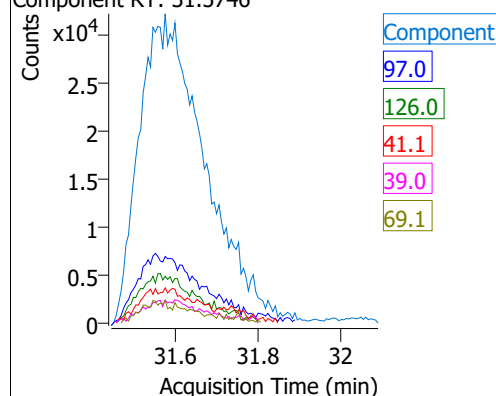
5-Hydroxymethylfurfural (NIST20.L)



+ Scan (31.4555-31.8004 min, 59 scans) 4.D



Component RT: 31.5746



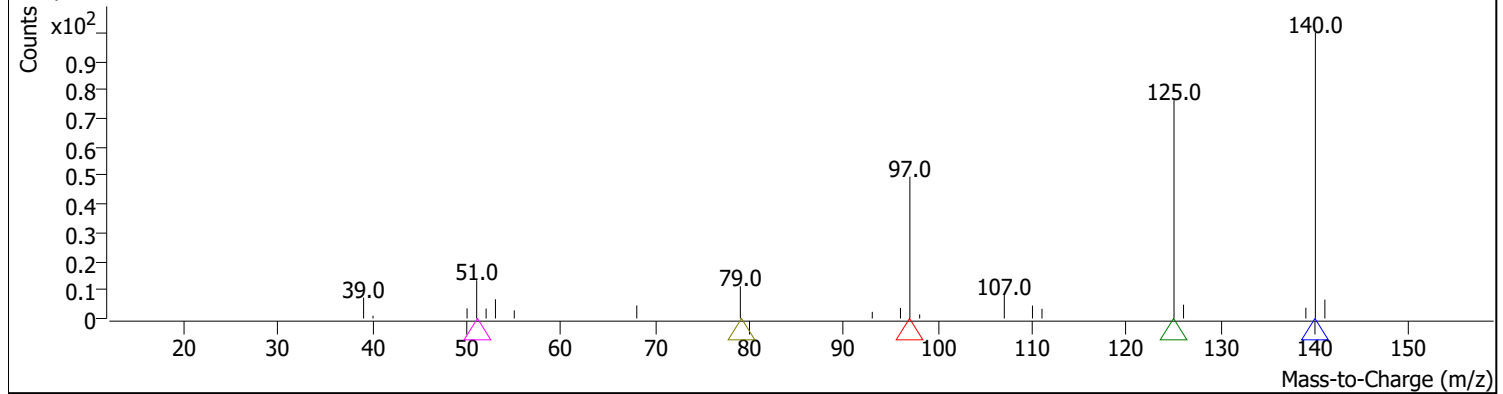
## Library Search Results - NonTarget Hits with Details



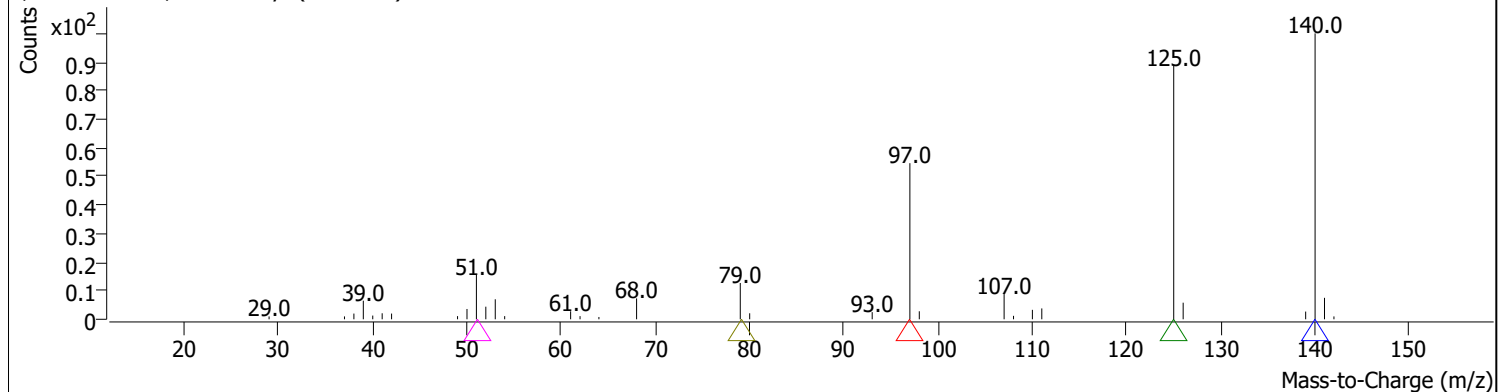
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
32.5004	1,2-Benzenediol, 3-methoxy-	520439.7	95.2	934-00-9	C7H8O3	

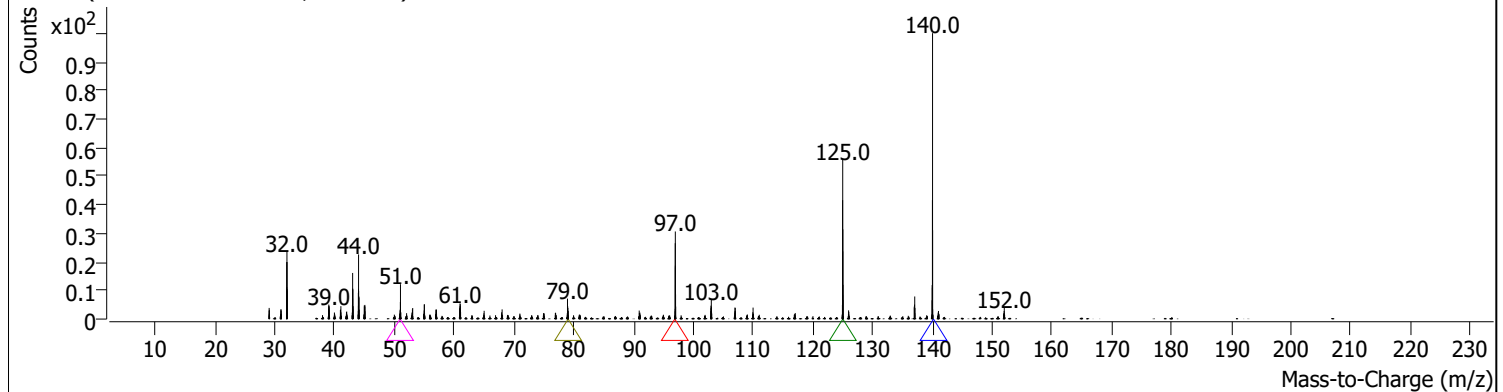
Component RT: 32.5004



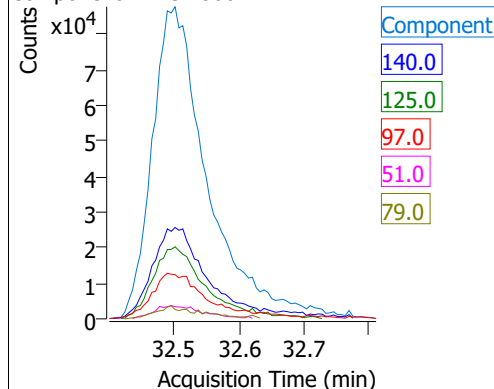
1,2-Benzenediol, 3-methoxy- (NIST20.L)



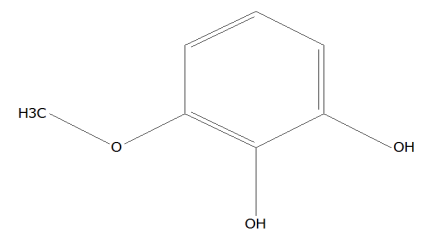
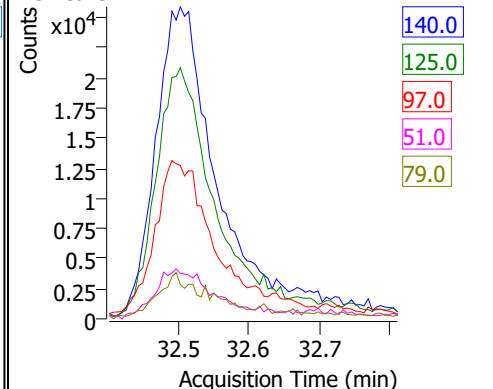
+ Scan (32.4069-32.7755 min, 62 scans) 4.D



Component RT: 32.5004



EIC Peaks



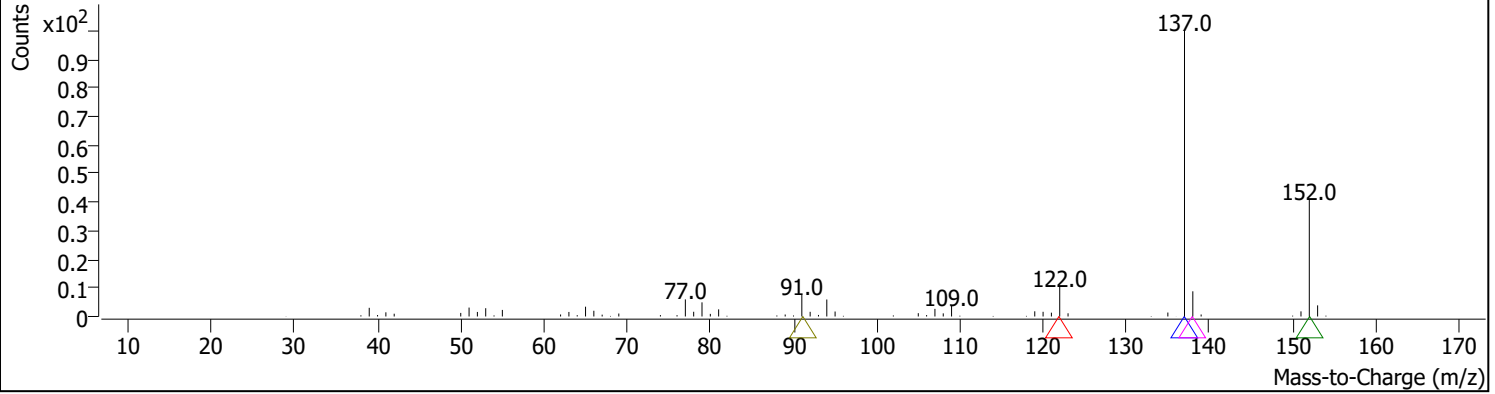
## Library Search Results - NonTarget Hits with Details



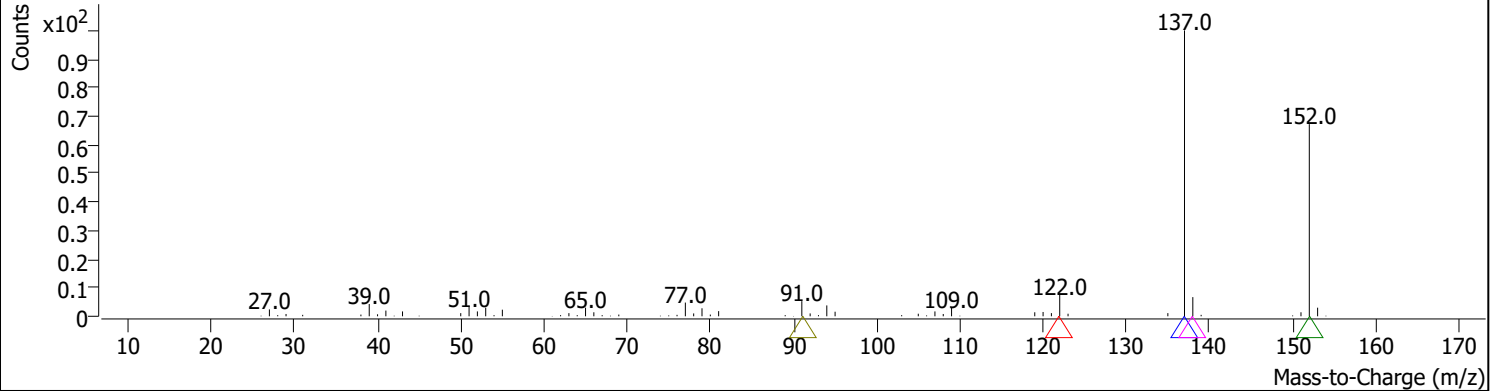
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
33.3356	Phenol, 4-ethyl-2-methoxy-	2515777.9	97.4	2785-89-9	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	

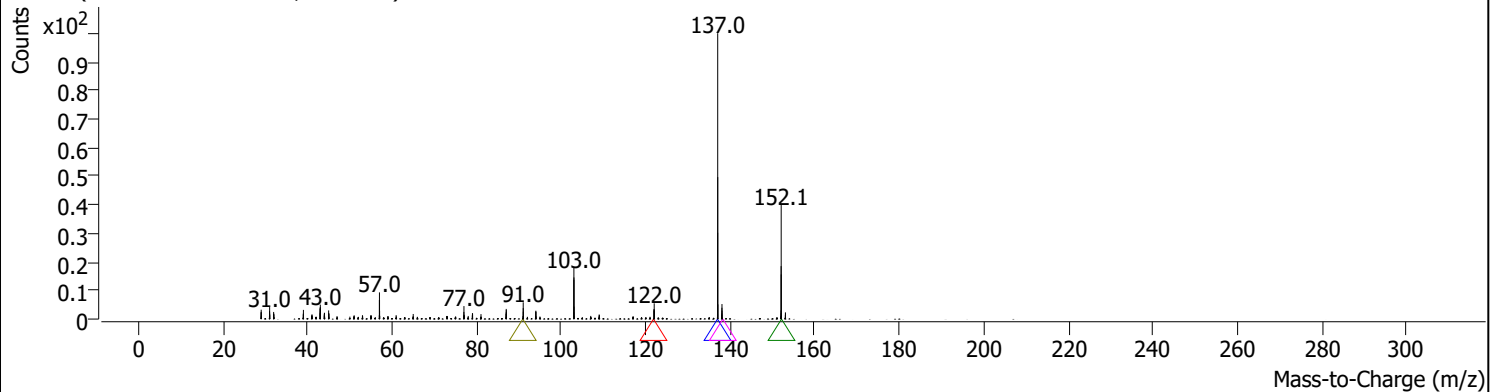
Component RT: 33.3356



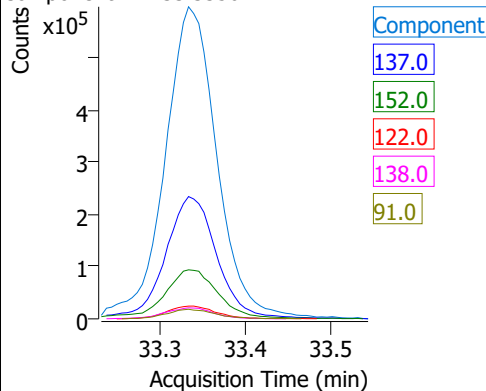
Phenol, 4-ethyl-2-methoxy- (NIST20.L)



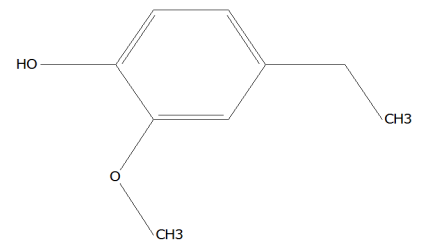
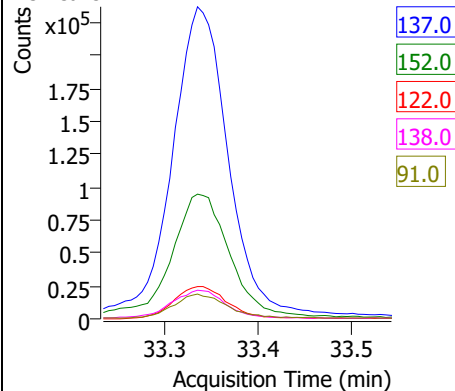
+ Scan (33.2334-33.5366 min, 52 scans) 4.D



Component RT: 33.3356



EIC Peaks



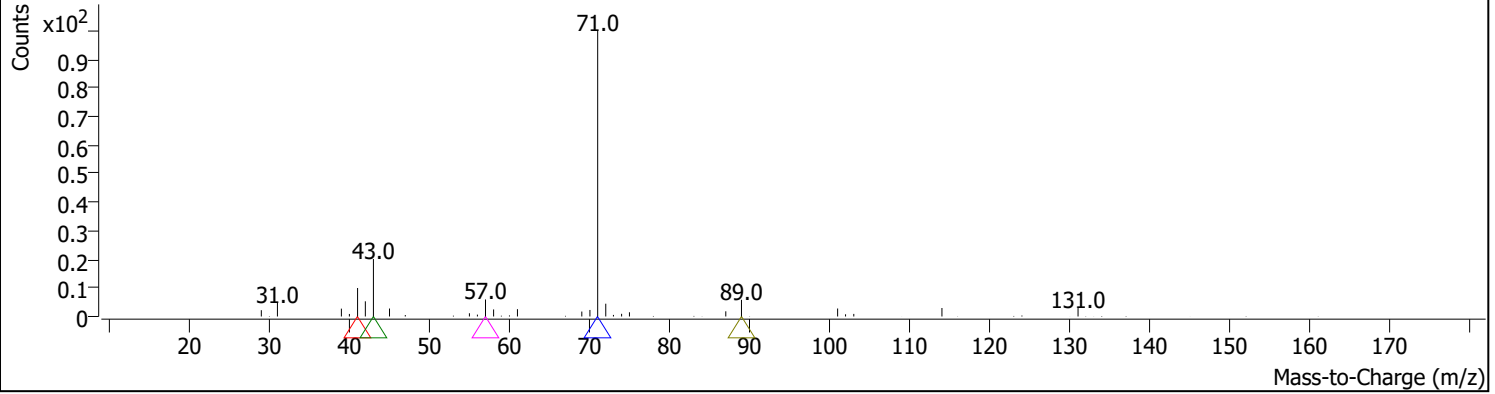
## Library Search Results - NonTarget Hits with Details



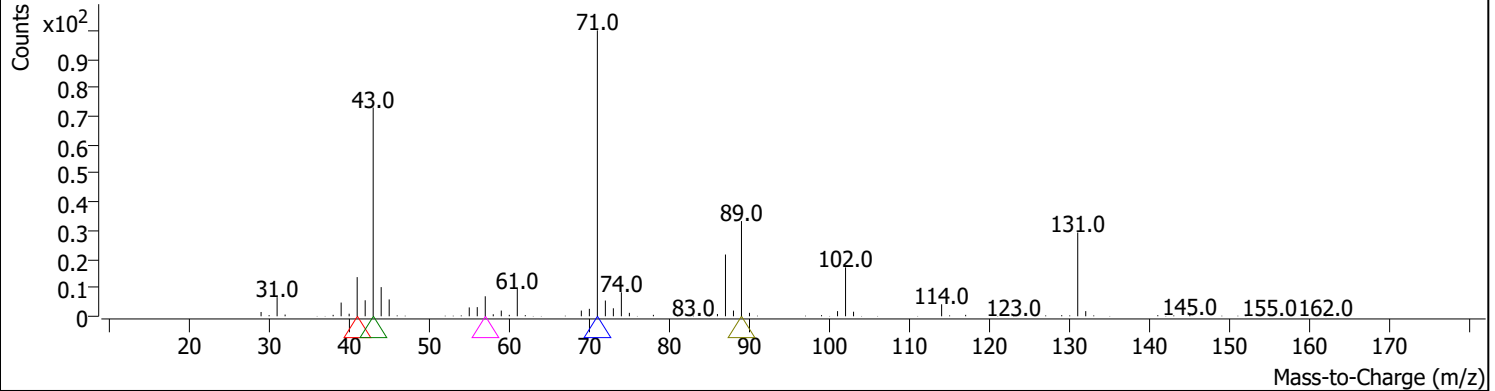
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
34.9749	2,3-dihydroxypropyl isobutyrate	12232779.8	78.5	1010458-45-6	C7H14O4	

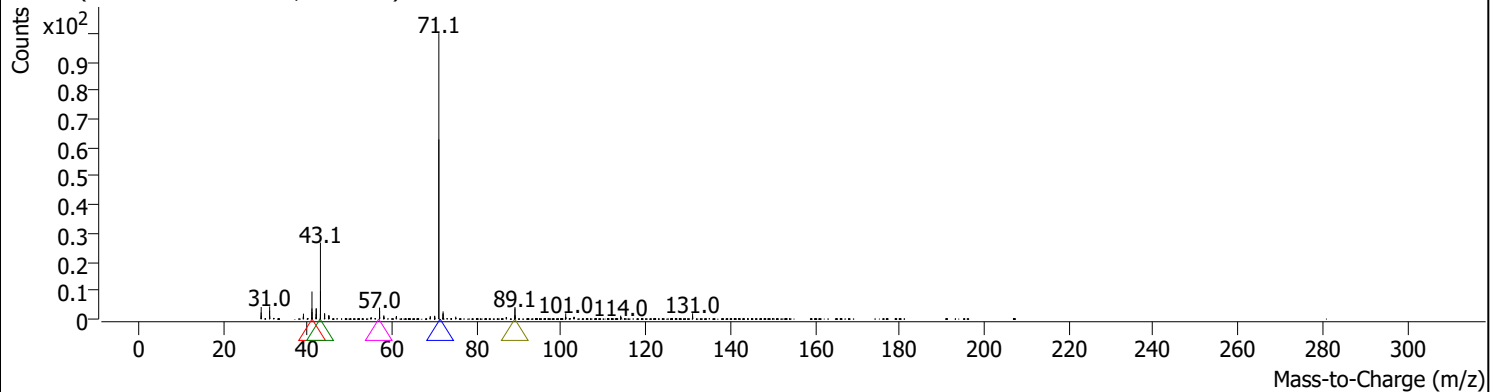
Component RT: 34.9749



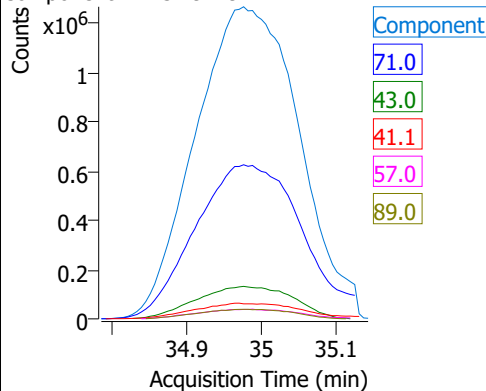
2,3-dihydroxypropyl isobutyrate (NIST20.L)



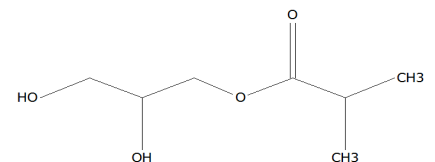
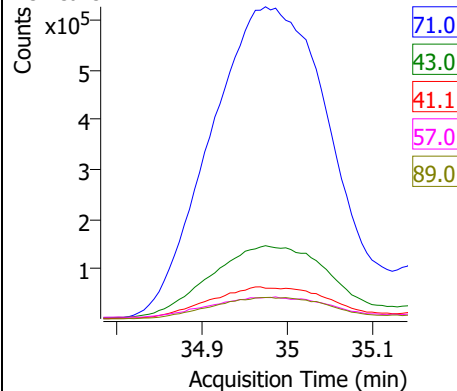
+ Scan (34.7853-35.1242 min, 58 scans) 4.D



Component RT: 34.9749



EIC Peaks



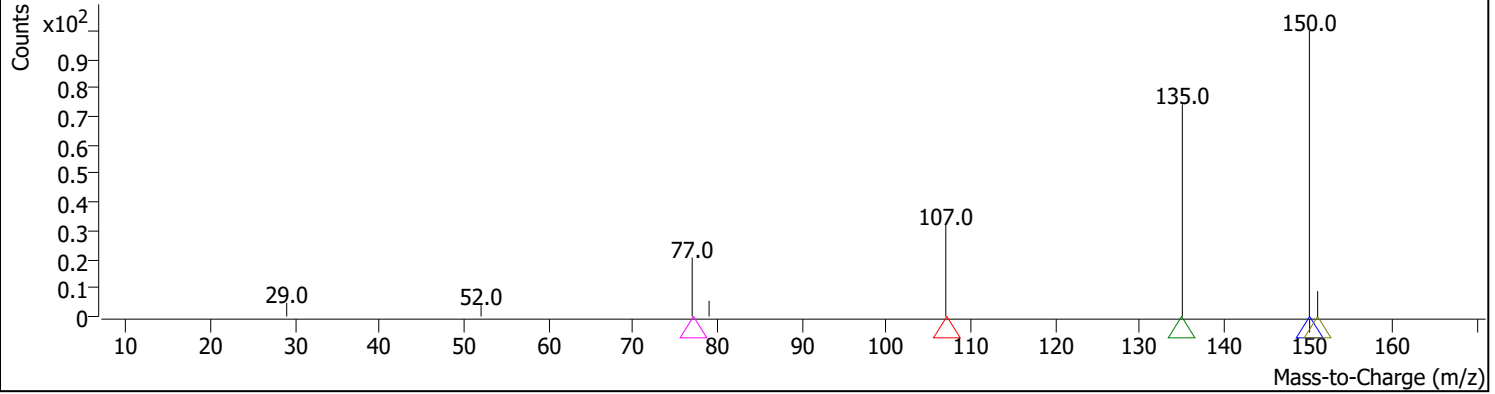
## Library Search Results - NonTarget Hits with Details



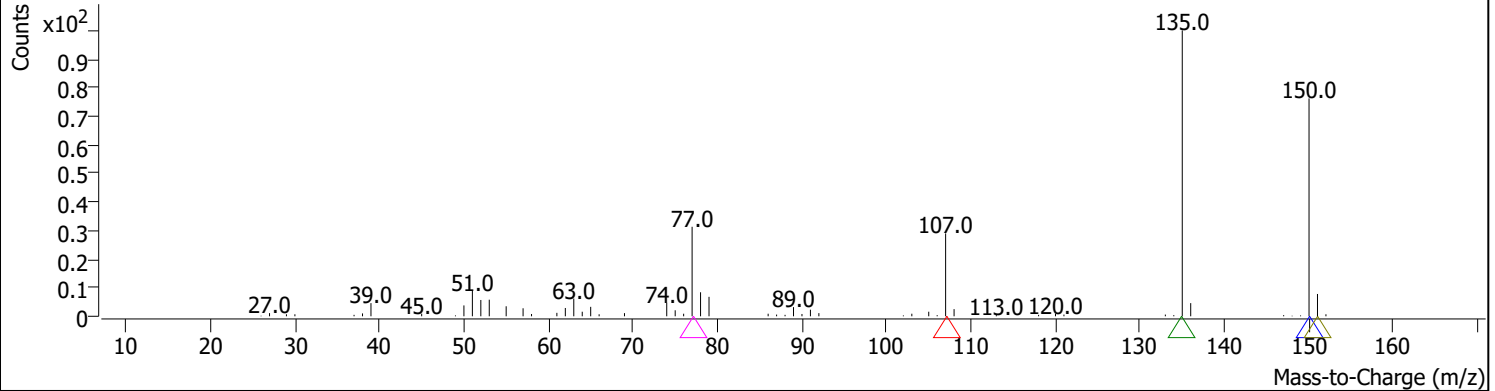
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
35.0843	Phenol, 5-ethenyl-2-methoxy-	202572.3	82.6	621-58-9	C9H10O2	

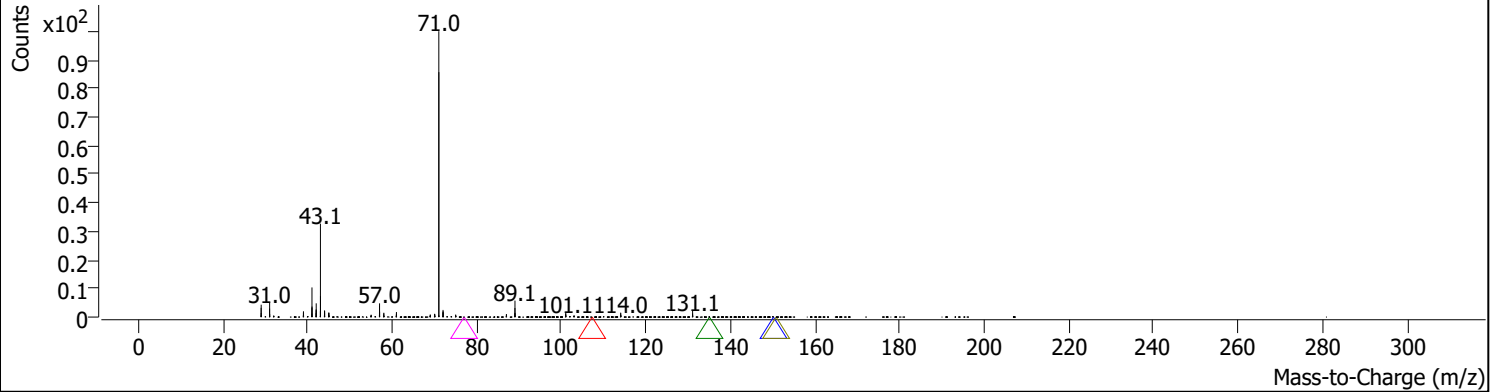
Component RT: 35.0843



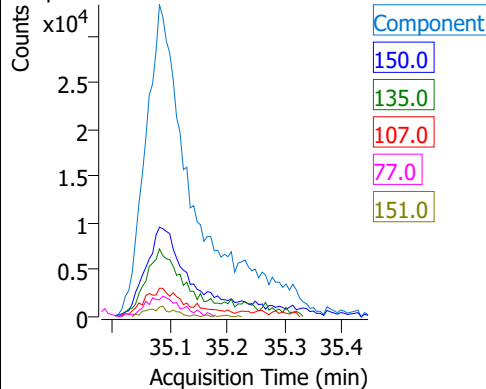
Phenol, 5-ethenyl-2-methoxy- (NIST20.L)



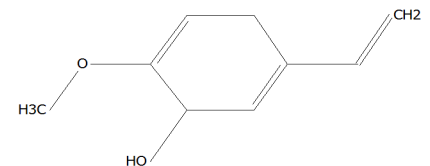
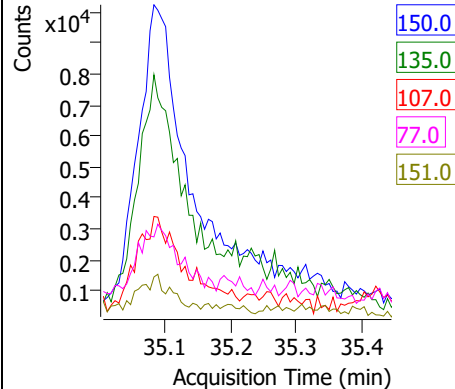
+ Scan (35.0053-35.4453 min, 75 scans) 4.D



Component RT: 35.0843



EIC Peaks



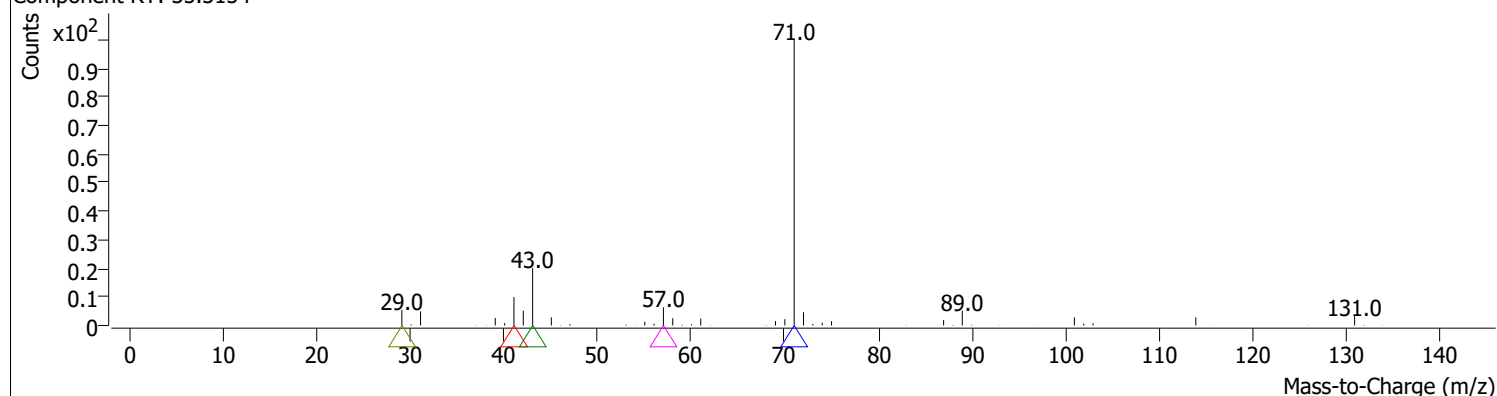
## Library Search Results - NonTarget Hits with Details



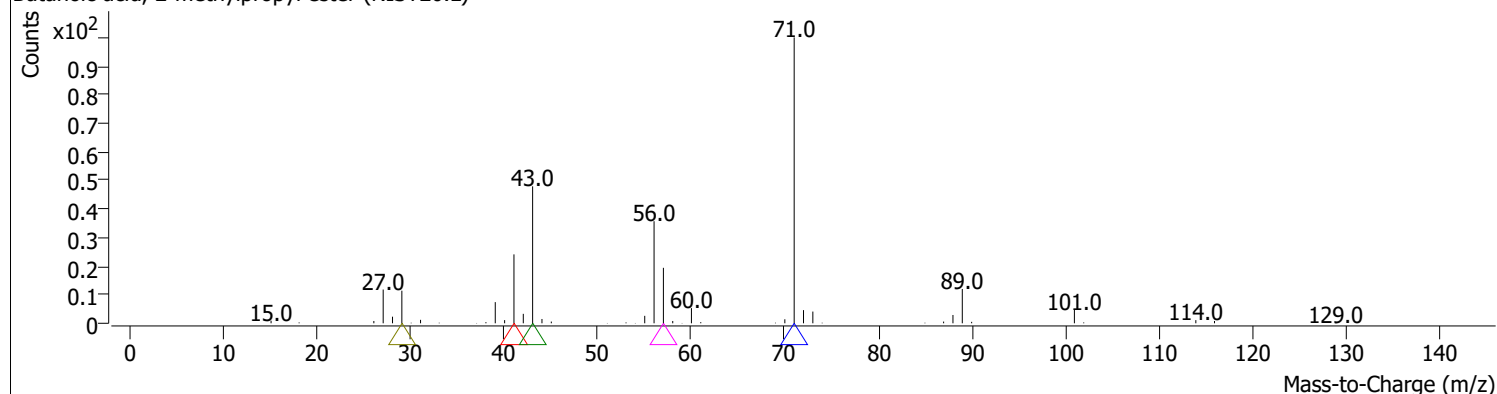
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
35.3154	Butanoic acid, 2-methylpropyl ester	11843195.3	78.6	539-90-2	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	

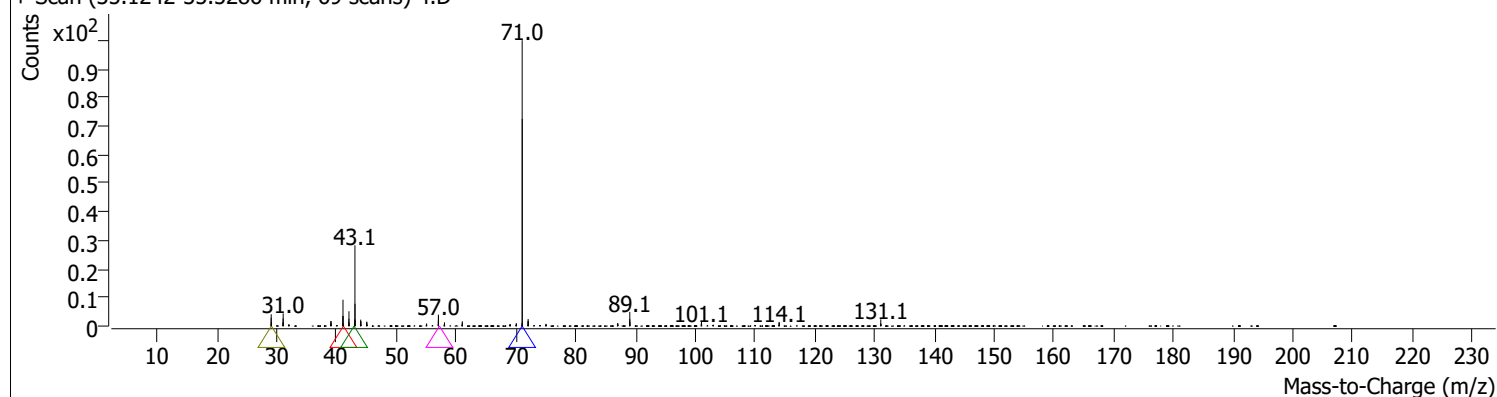
Component RT: 35.3154



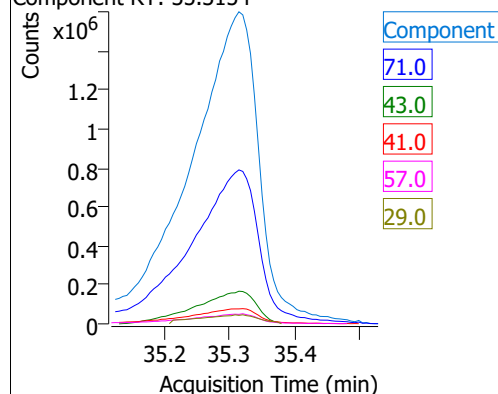
Butanoic acid, 2-methylpropyl ester (NIST20.L)



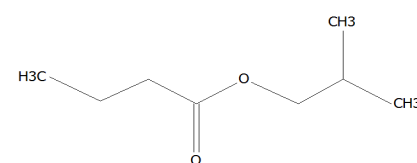
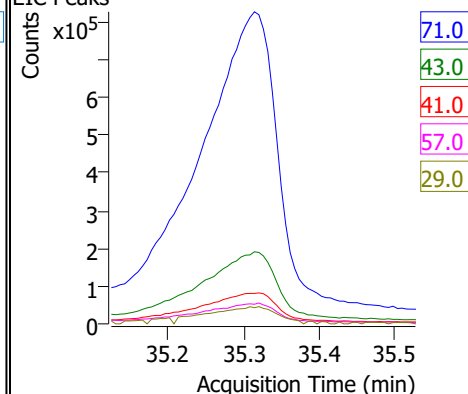
+ Scan (35.1242-35.5286 min, 69 scans) 4.D



Component RT: 35.3154



EIC Peaks



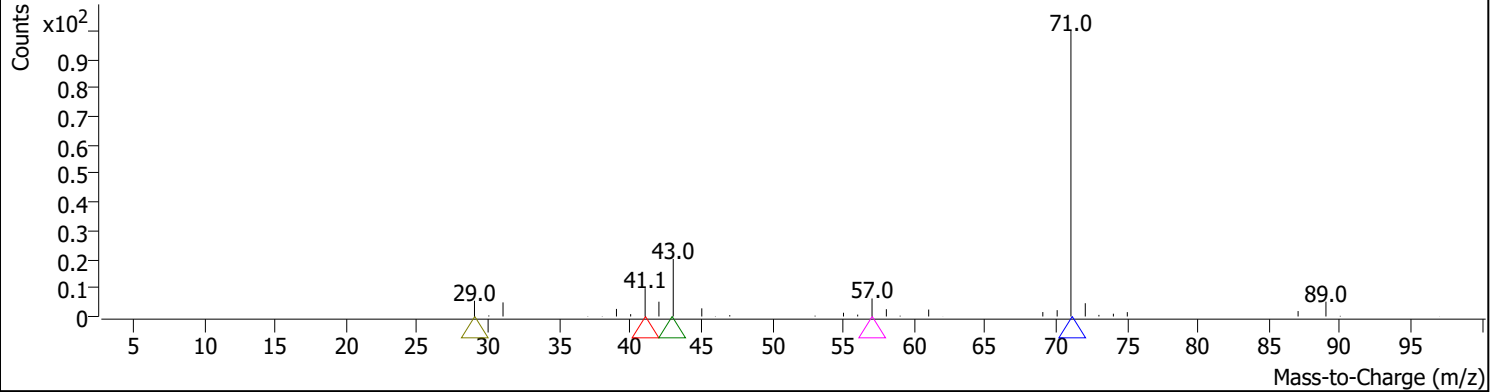
## Library Search Results - NonTarget Hits with Details



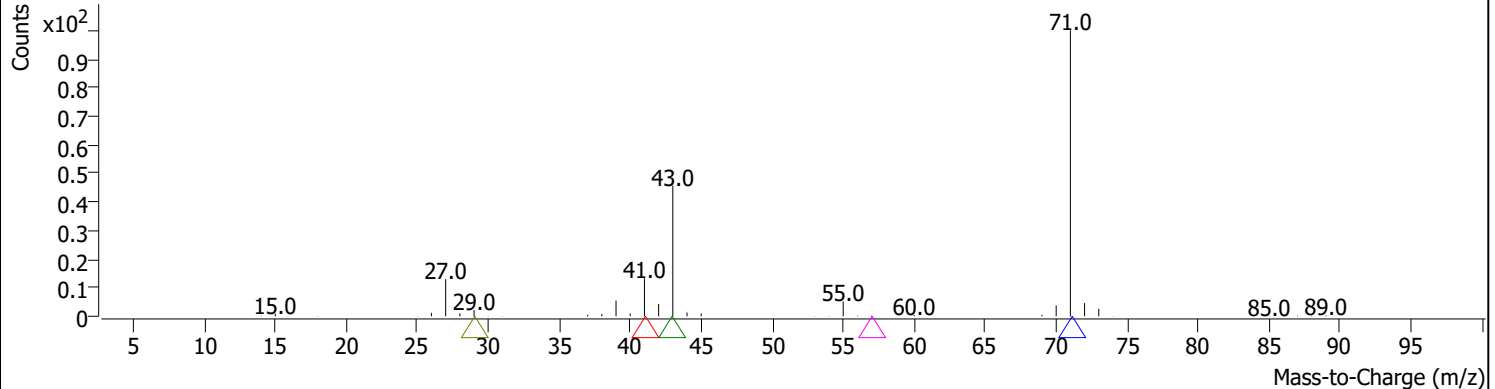
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
35.3163	Butanoic acid, anhydride	11248701.5	79.7	106-31-0	C <sub>8</sub> H <sub>14</sub> O <sub>3</sub>	

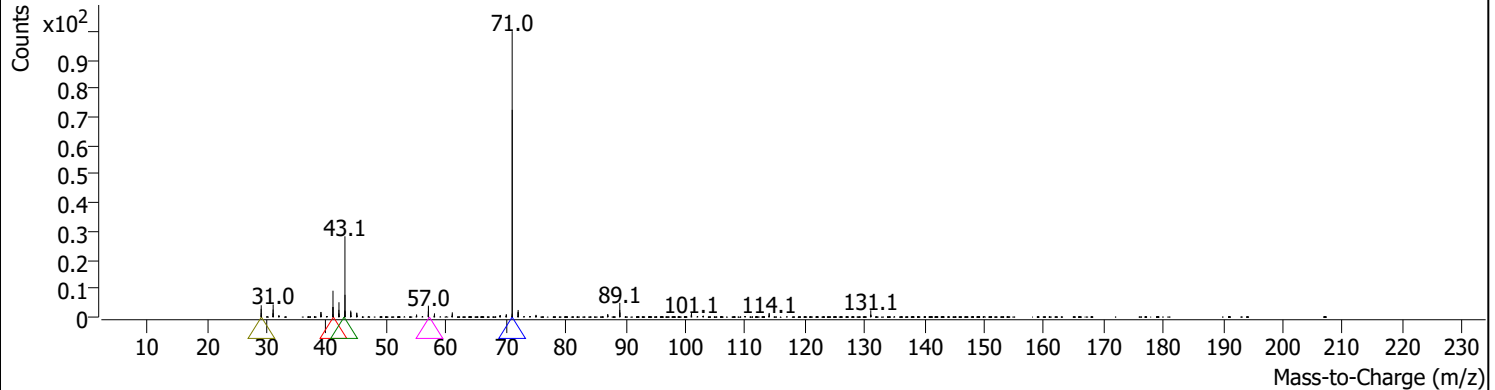
Component RT: 35.3163



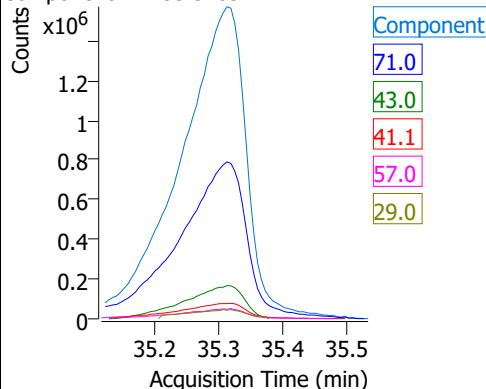
Butanoic acid, anhydride (NIST20.L)



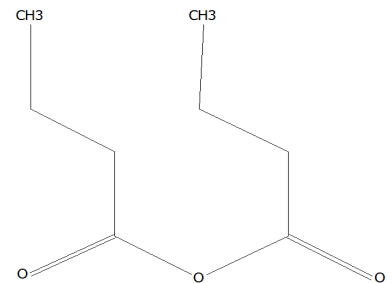
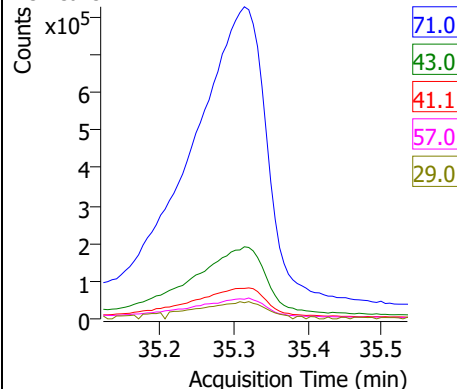
+ Scan (35.1242-35.5286 min, 69 scans) 4.D



Component RT: 35.3163



EIC Peaks



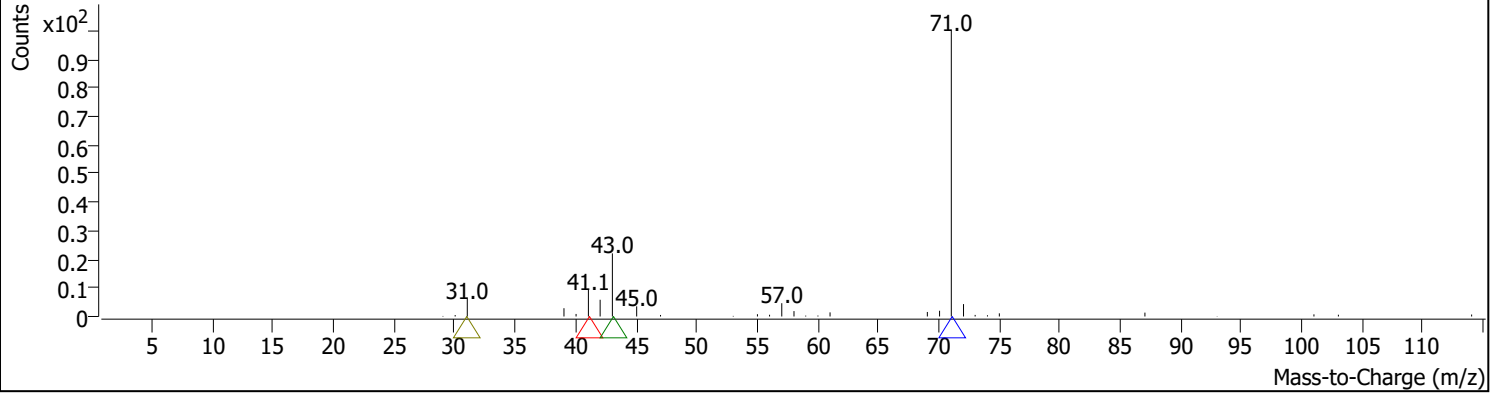
## Library Search Results - NonTarget Hits with Details



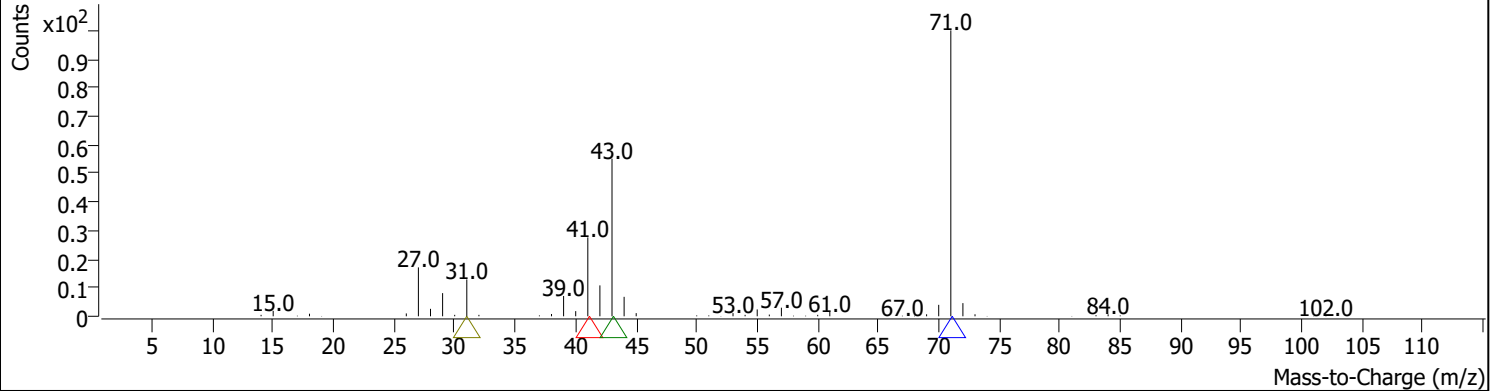
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
36.1877	2-Furanmethanol, tetrahydro-	2781061.4	82.1	97-99-4	C5H10O2	

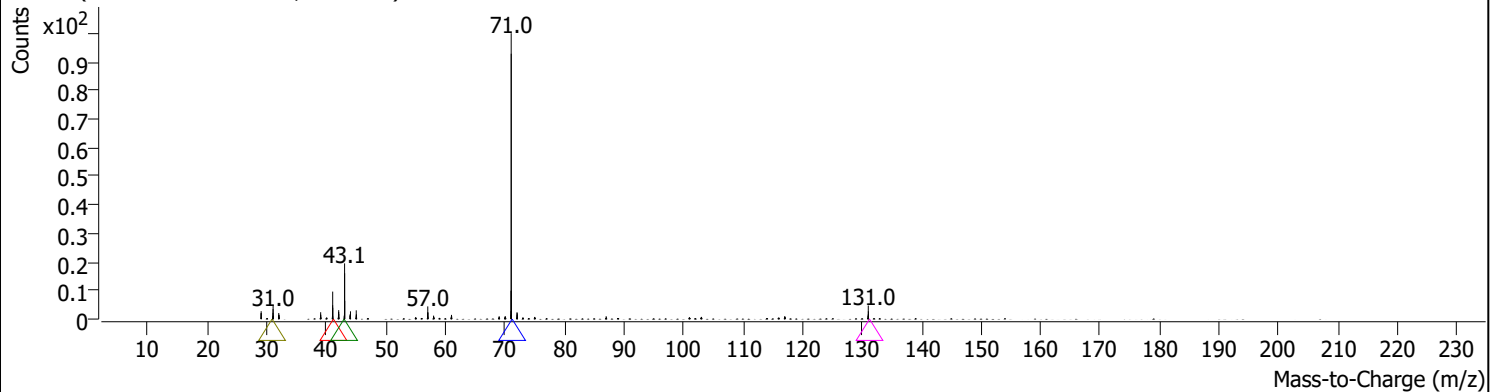
Component RT: 36.1877



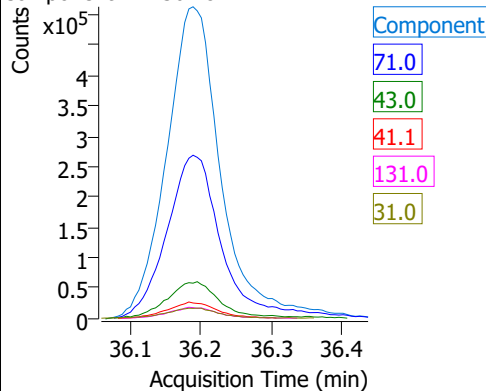
2-Furanmethanol, tetrahydro- (NIST20.L)



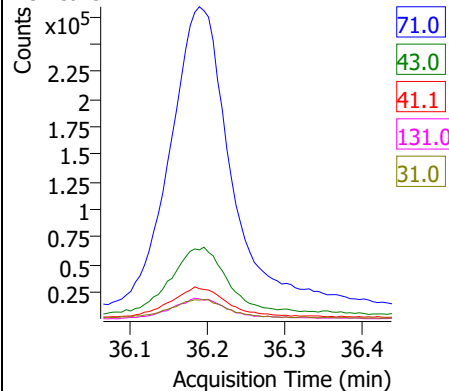
+ Scan (36.0721-36.4383 min, 62 scans) 4.D



Component RT: 36.1877



EIC Peaks





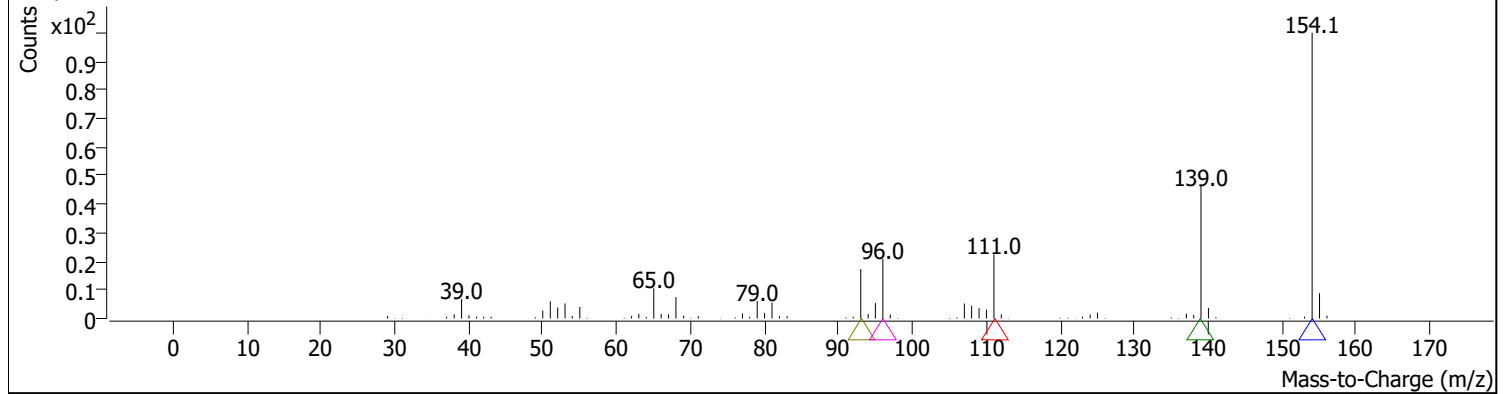
## Library Search Results - NonTarget Hits with Details



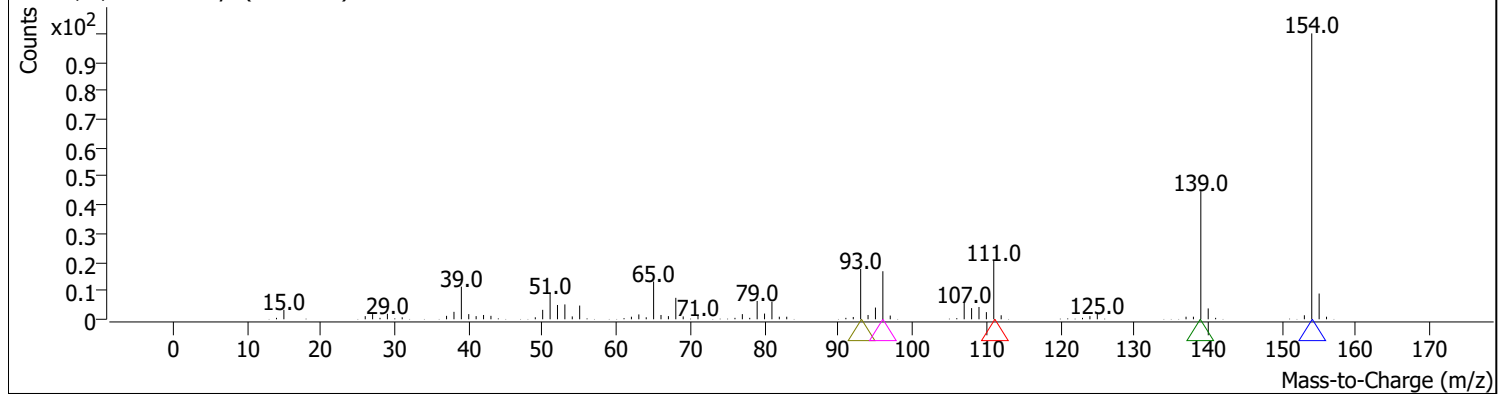
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
36.7974	Phenol, 2,6-dimethoxy-	12715578.1	99.1	91-10-1	C8H10O3	

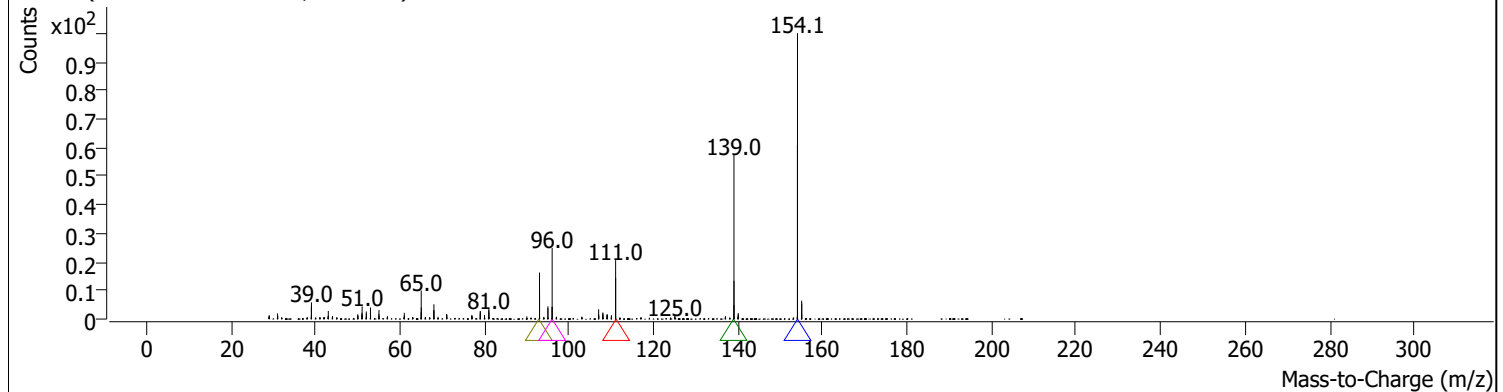
Component RT: 36.7974



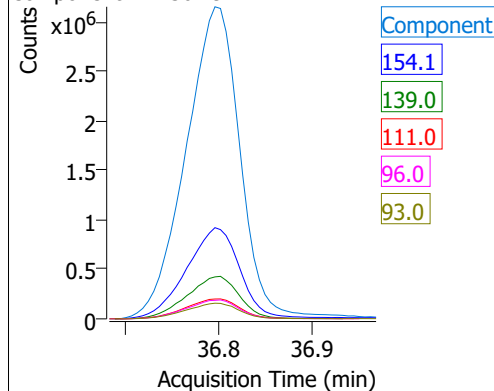
Phenol, 2,6-dimethoxy- (NIST20.L)



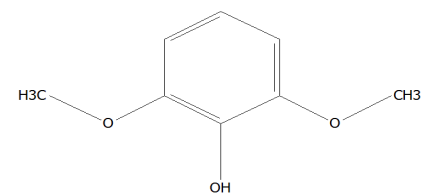
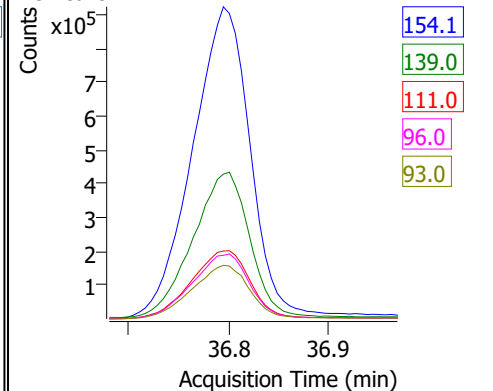
+ Scan (36.6880-36.9675 min, 48 scans) 4.D



Component RT: 36.7974



EIC Peaks



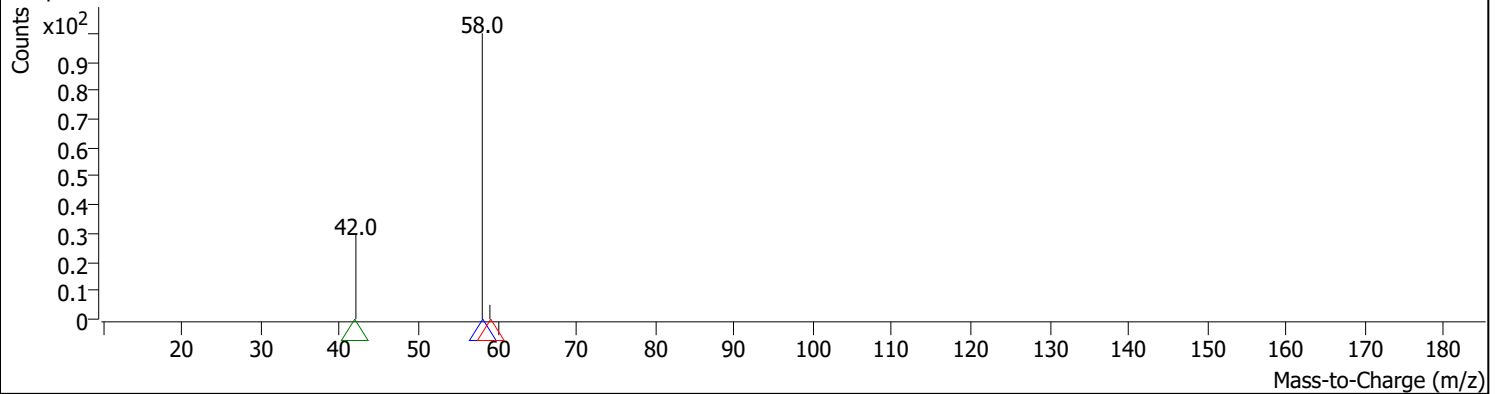
## Library Search Results - NonTarget Hits with Details



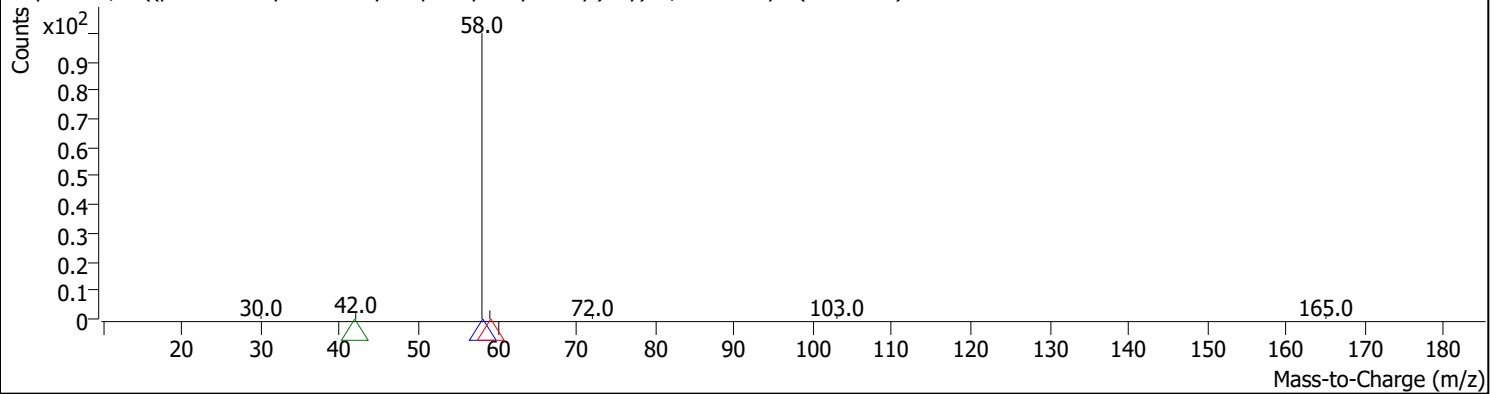
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
37.3896	Ethylamine, 2-((p-bromo-.alpha.-methyl-.alpha.-phenylbenzyl)oxy)-N,N-dimethyl-	1629293.7	75.7	3565-72-8	C <sub>18</sub> H <sub>22</sub> BrNO	

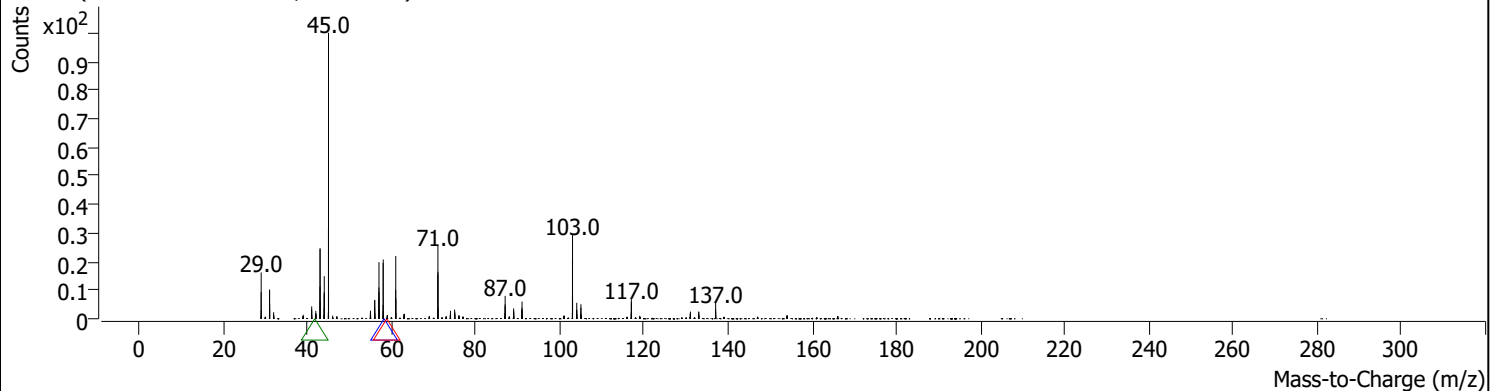
Component RT: 37.3896



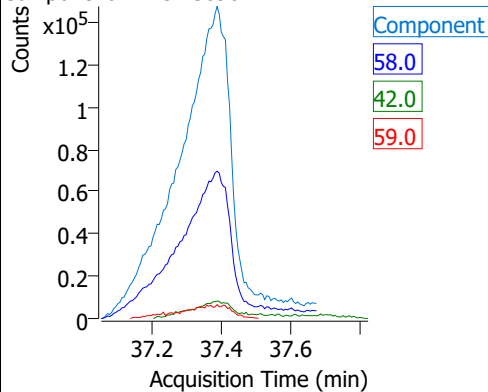
Ethylamine, 2-((p-bromo-.alpha.-methyl-.alpha.-phenylbenzyl)oxy)-N,N-dimethyl- (NIST20.L)



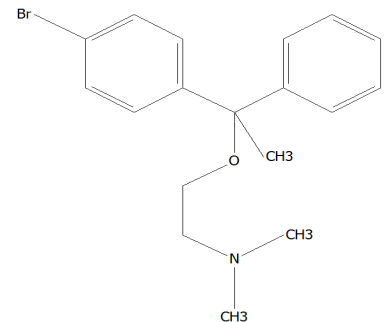
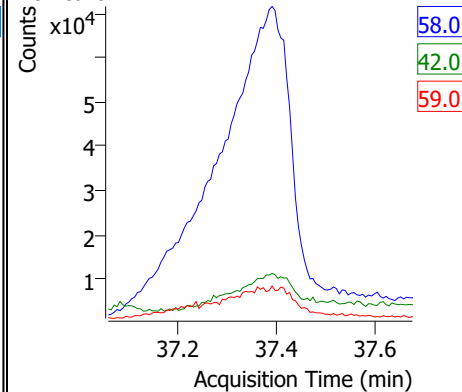
+ Scan (37.0511-37.6751 min, 105 scans) 4.D



Component RT: 37.3896



EIC Peaks



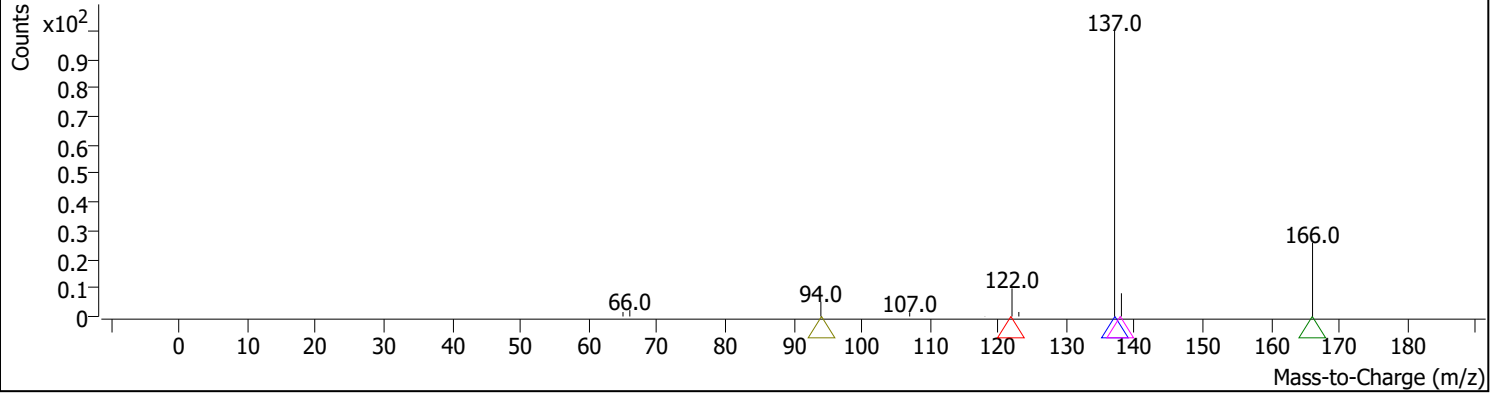
## Library Search Results - NonTarget Hits with Details



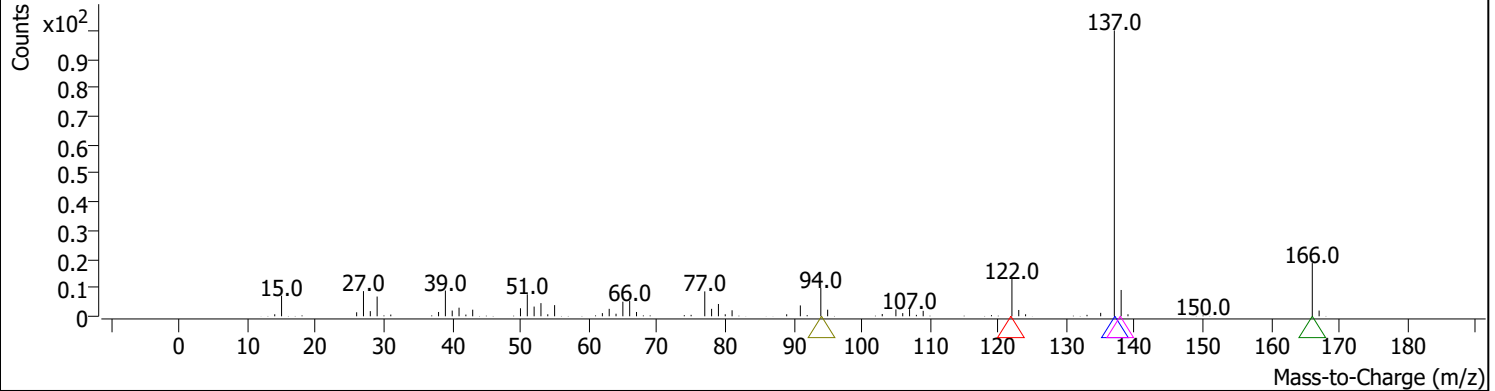
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
37.4168	Phenol, 2-methoxy-4-propyl-	394237.8	78.1	2785-87-7	C10H14O2	

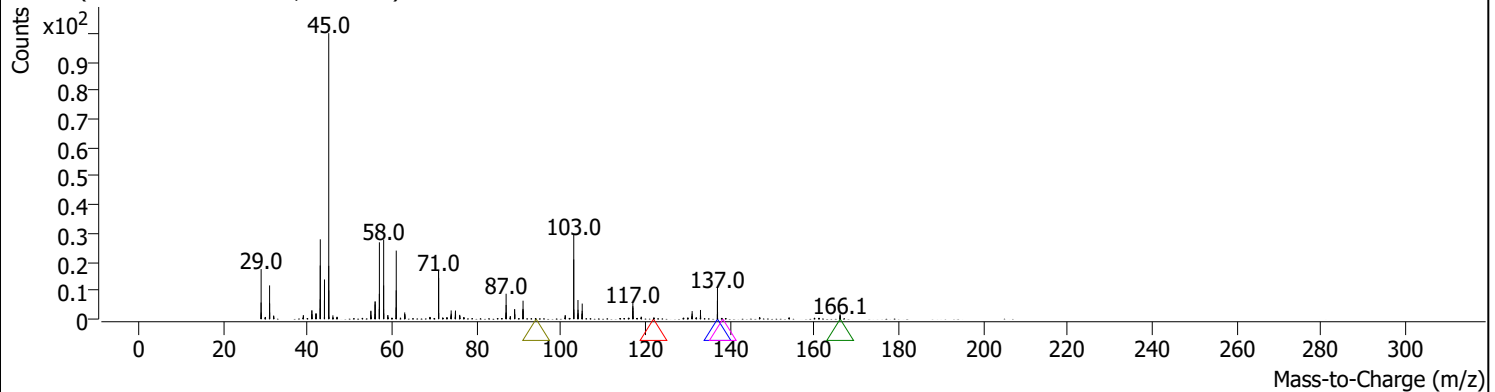
Component RT: 37.4168



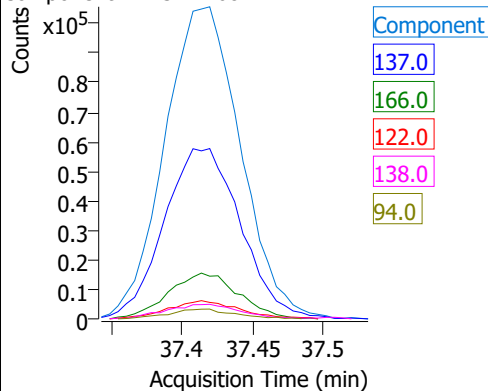
Phenol, 2-methoxy-4-propyl- (NIST20.L)



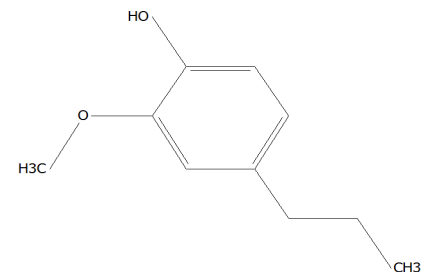
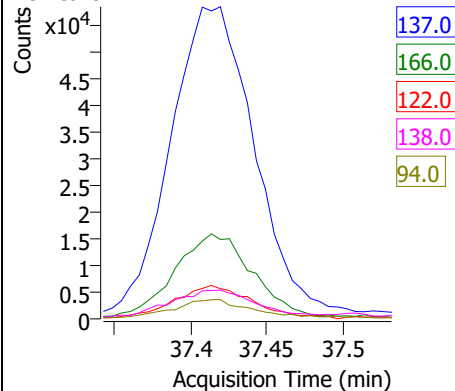
+ Scan (37.3481-37.4967 min, 26 scans) 4.D



Component RT: 37.4168



EIC Peaks



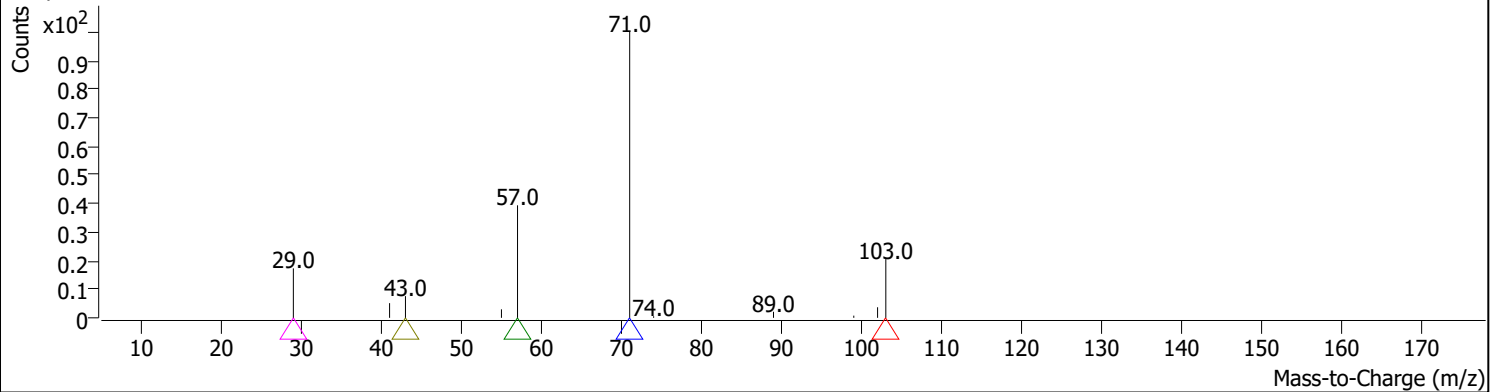
## Library Search Results - NonTarget Hits with Details



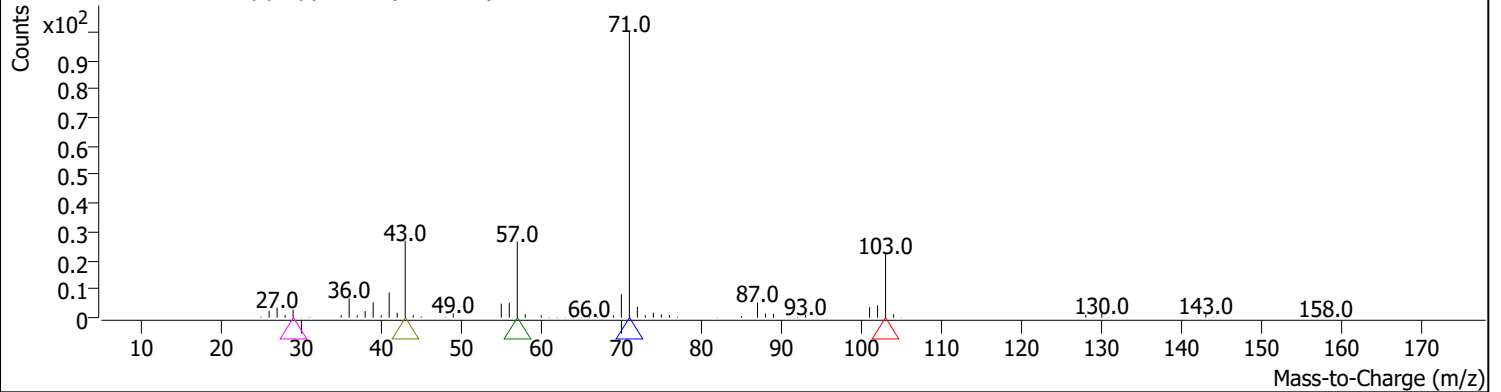
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
37.7057	Butanoic acid, 2,2-dimethylpropyl ester	475586.9	78.5	23361-69-5	C9H18O2	

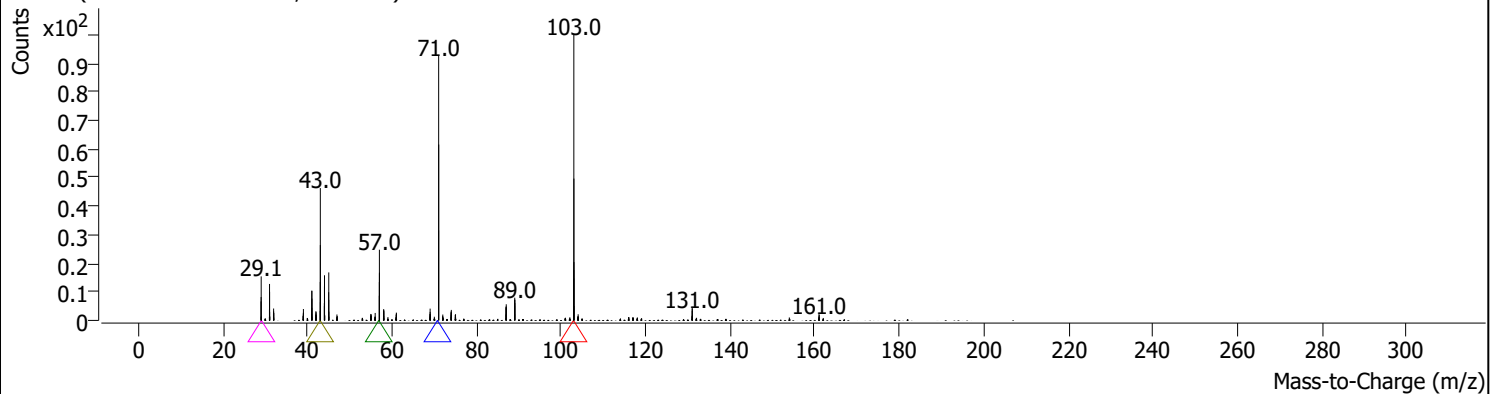
Component RT: 37.7057



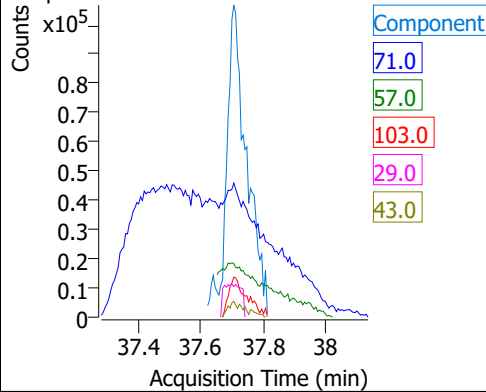
Butanoic acid, 2,2-dimethylpropyl ester (NIST20.L)



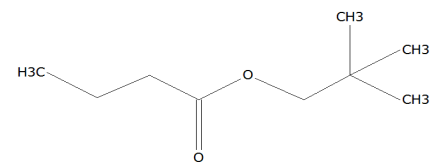
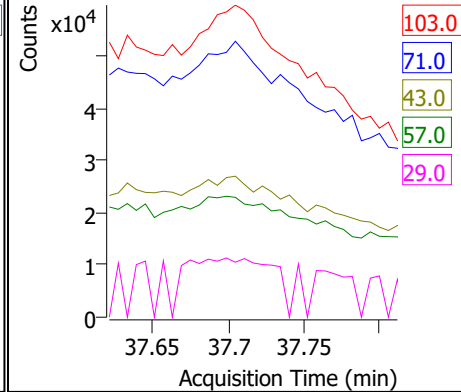
+ Scan (37.6275-37.8000 min, 30 scans) 4.D



Component RT: 37.7057



EIC Peaks



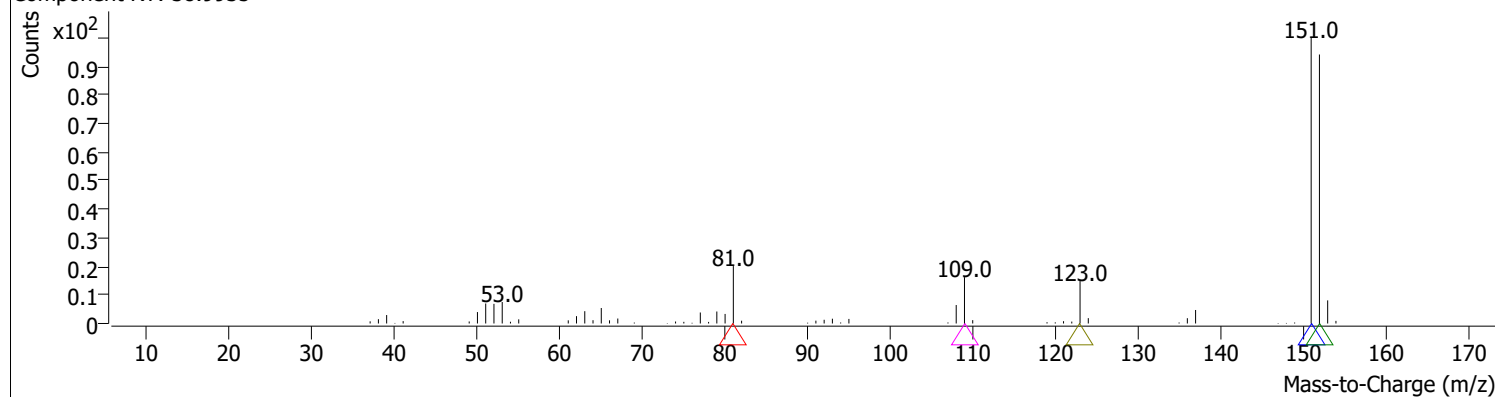
## Library Search Results - NonTarget Hits with Details



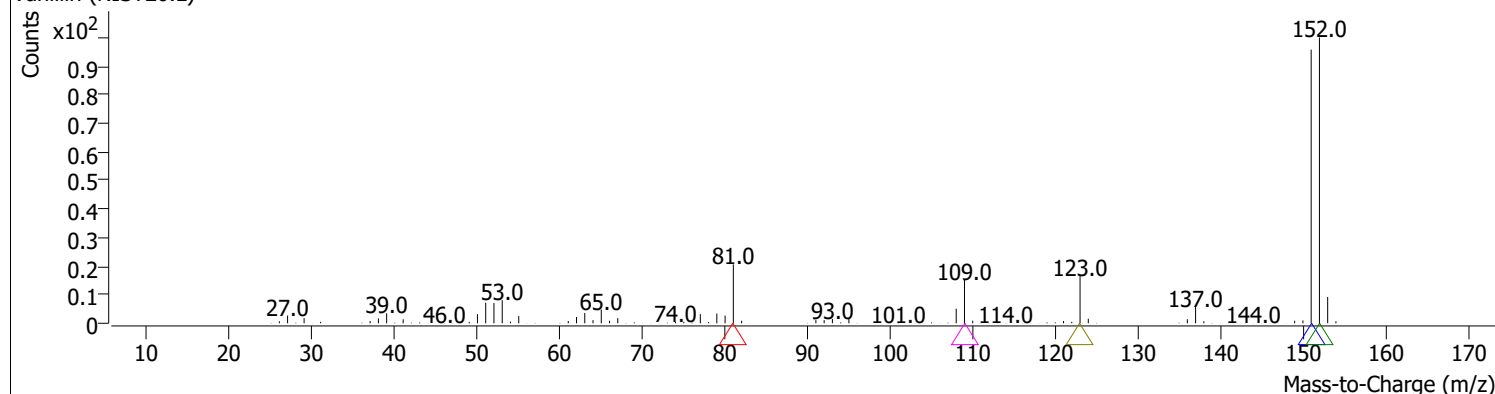
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
38.9935	Vanillin	5678104.3	98.5	121-33-5	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	

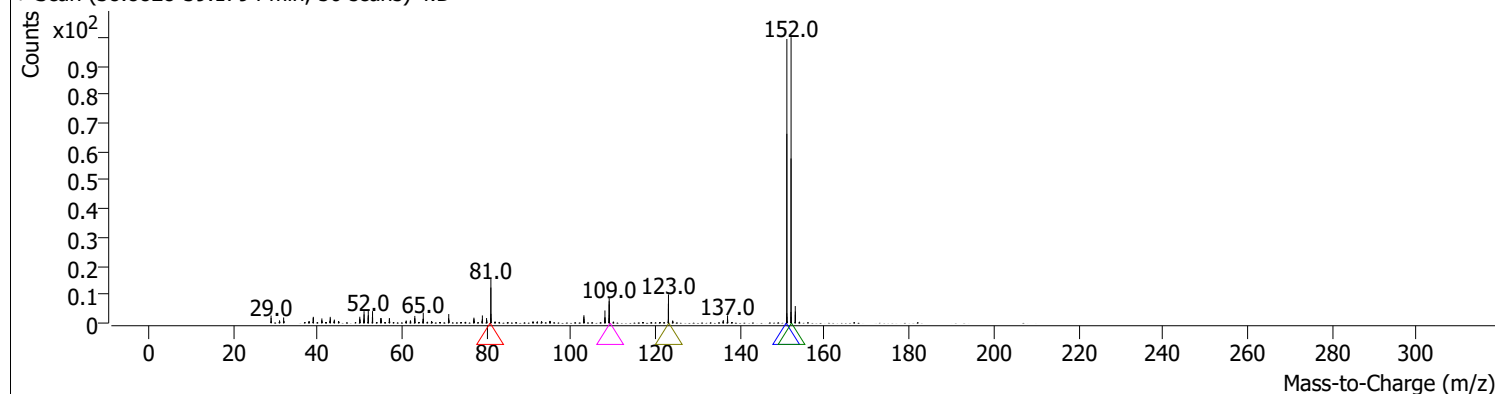
Component RT: 38.9935



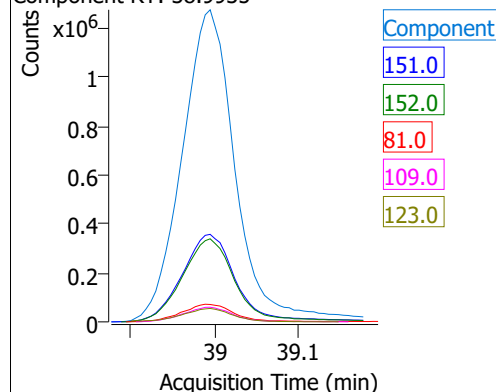
Vanillin (NIST20.L)



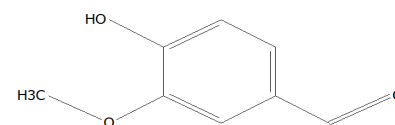
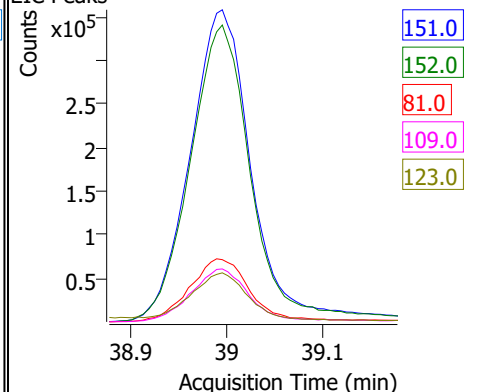
+ Scan (38.8828-39.1794 min, 50 scans) 4.D



Component RT: 38.9935



EIC Peaks



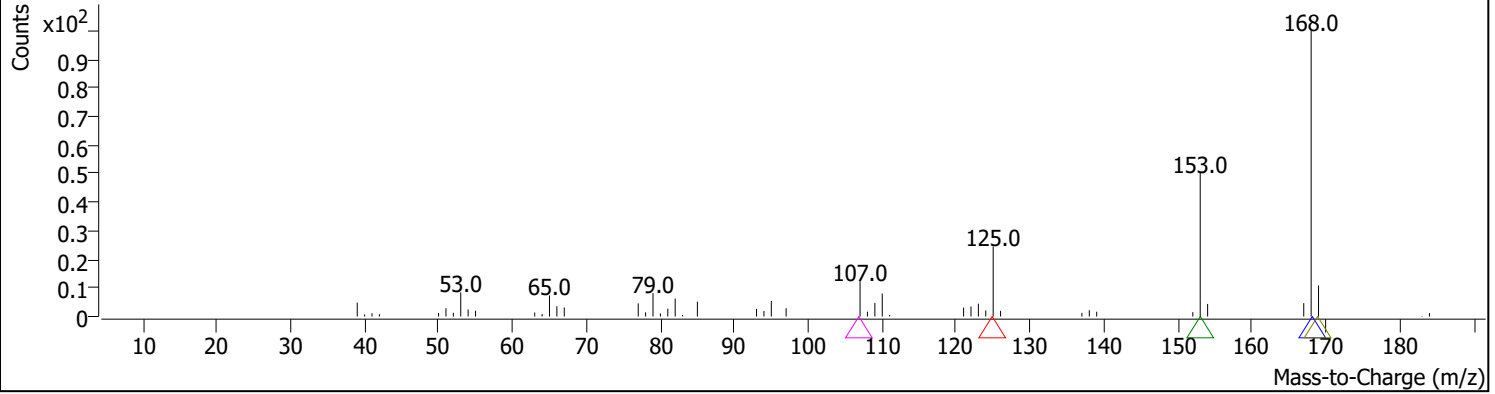
## Library Search Results - NonTarget Hits with Details



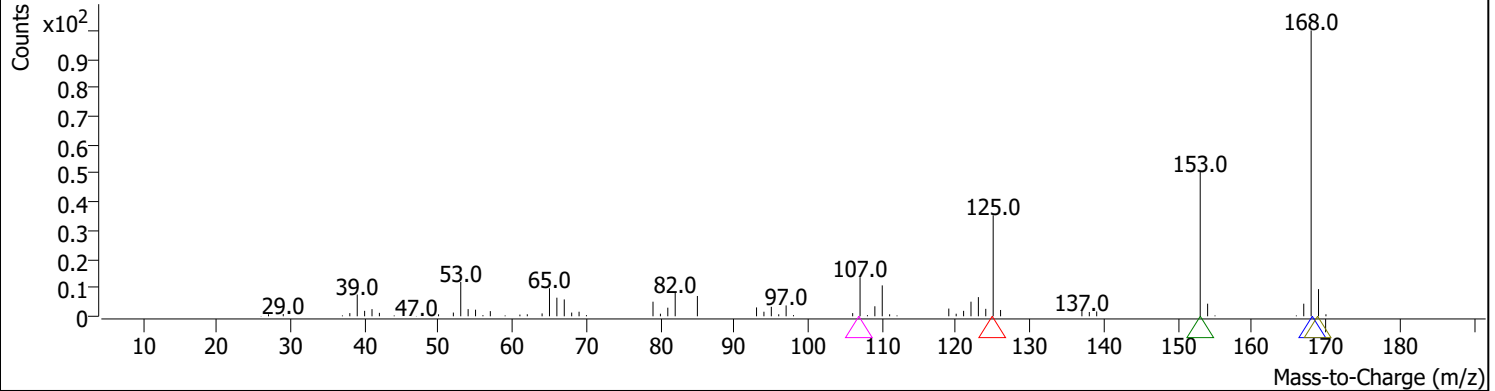
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
40.8895	3,5-Dimethoxy-4-hydroxytoluene	847530.0	93.6	6638-05-7	C <sub>9</sub> H <sub>12</sub> O <sub>3</sub>	

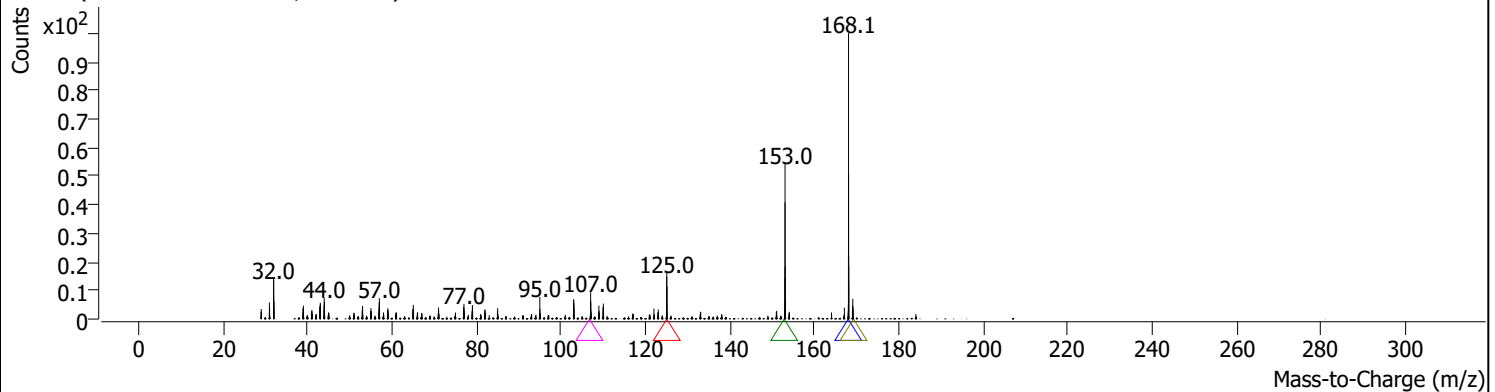
Component RT: 40.8895



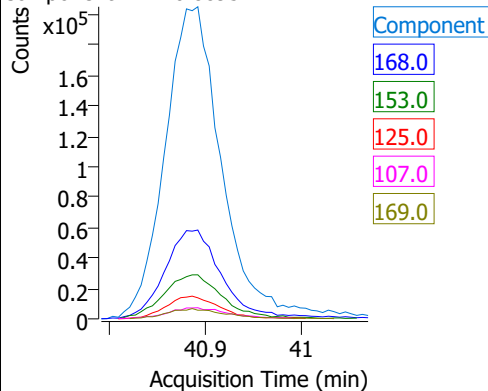
3,5-Dimethoxy-4-hydroxytoluene (NIST20.L)



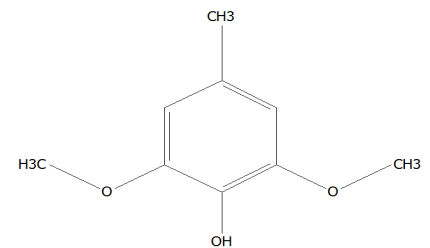
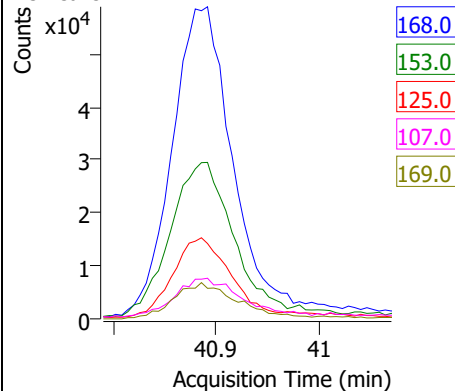
+ Scan (40.7954-41.0703 min, 47 scans) 4.D



Component RT: 40.8895



EIC Peaks



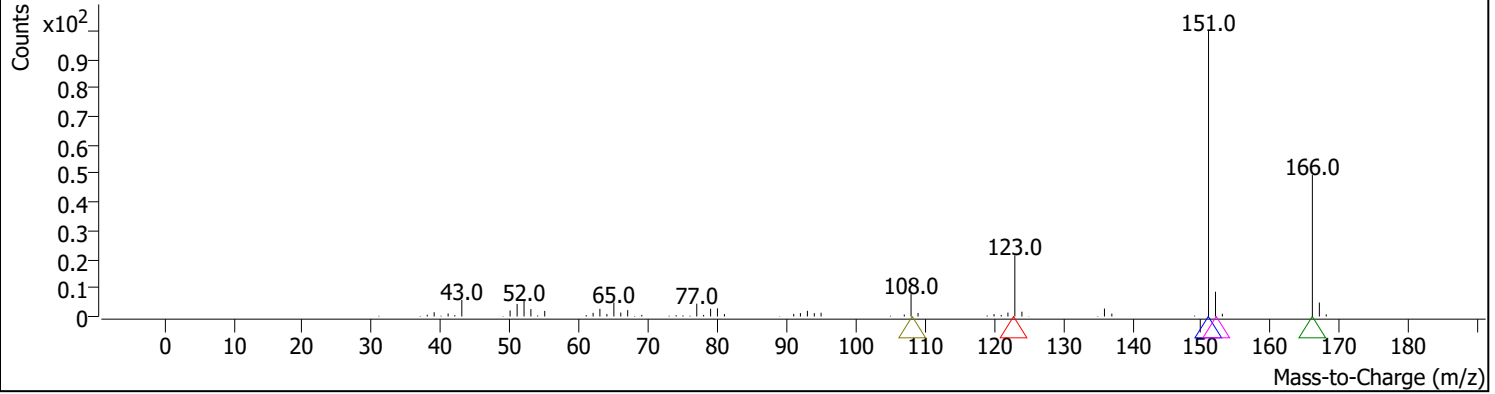
## Library Search Results - NonTarget Hits with Details



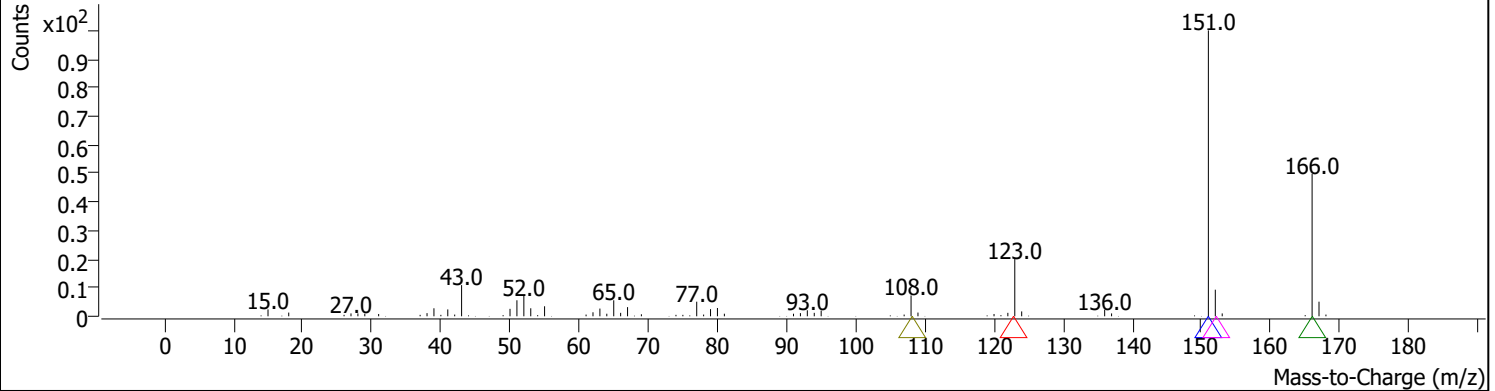
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
42.6159	Apocynin	4014973.2	99.2	498-02-2	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	

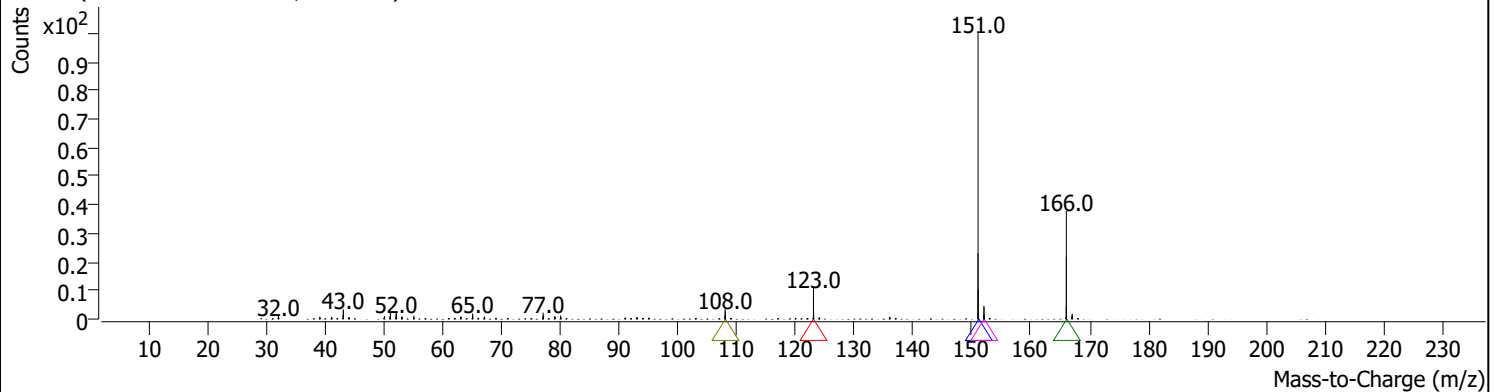
Component RT: 42.6159



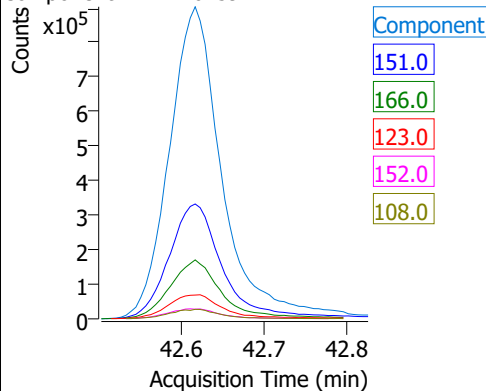
Apocynin (NIST20.L)



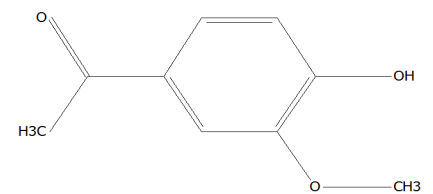
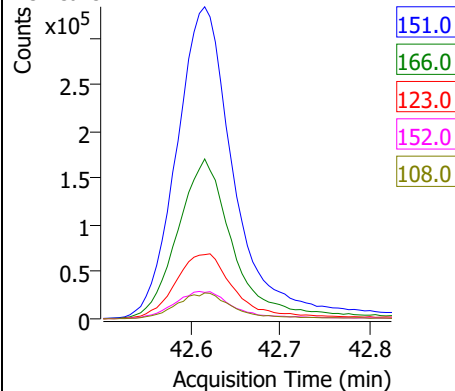
+ Scan (42.5033-42.7946 min, 50 scans) 4.D



Component RT: 42.6159



EIC Peaks



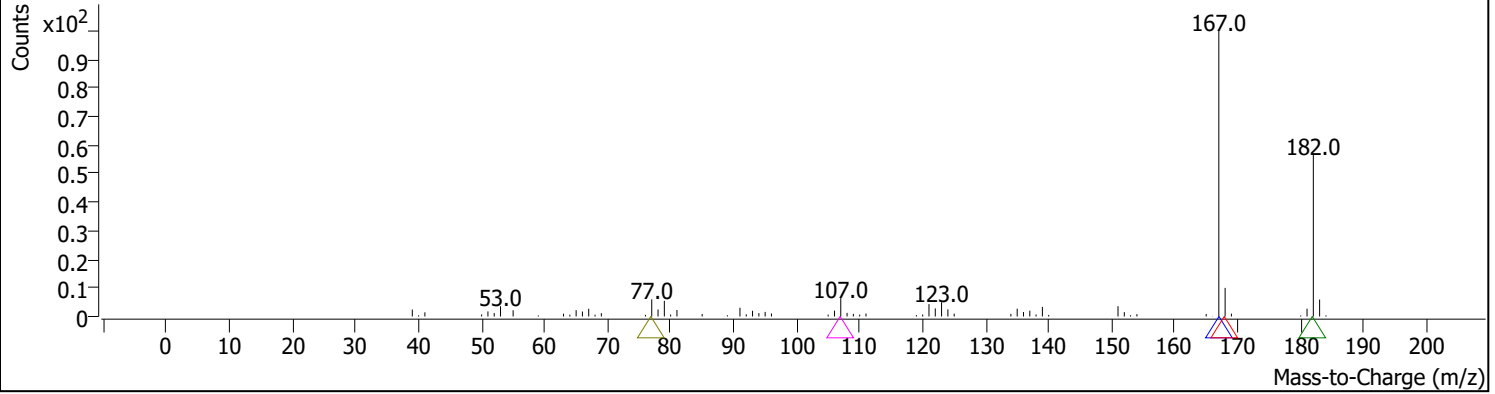
## Library Search Results - NonTarget Hits with Details



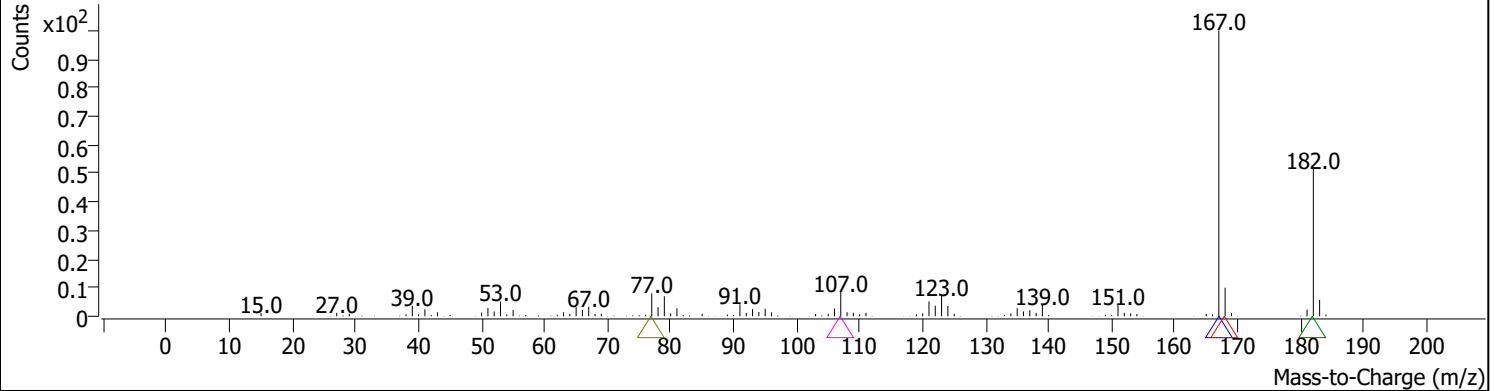
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
44.0555	4-Ethyl-2,6-dimethoxyphenol	1629043.1	97.5	14059-92-8	C <sub>10</sub> H <sub>14</sub> O <sub>3</sub>	

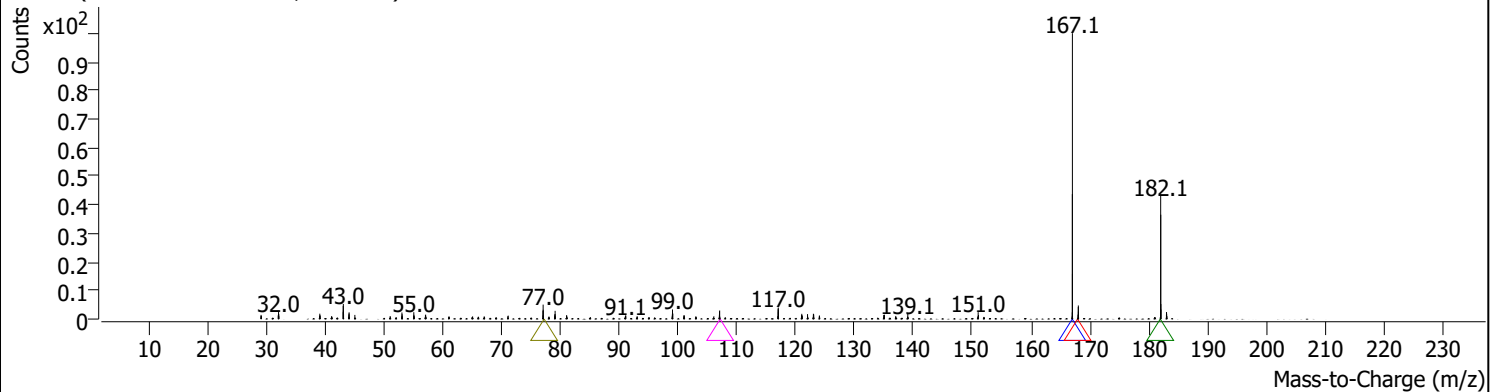
Component RT: 44.0555



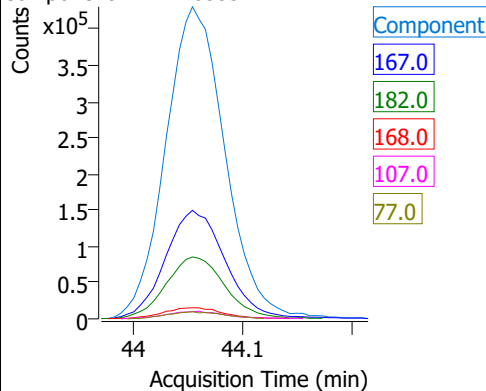
4-Ethyl-2,6-dimethoxyphenol (NIST20.L)



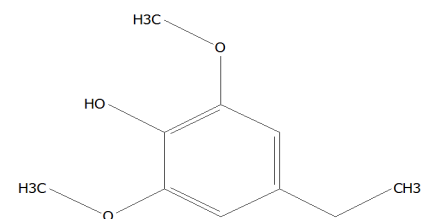
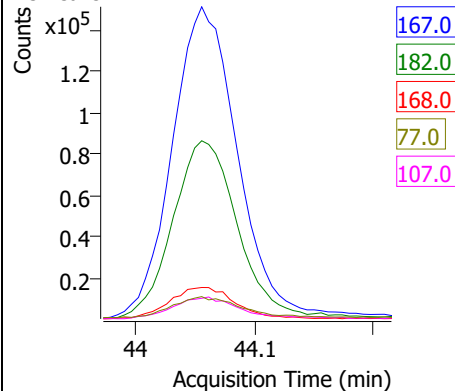
+ Scan (43.9664-44.1799 min, 35 scans) 4.D



Component RT: 44.0555



EIC Peaks





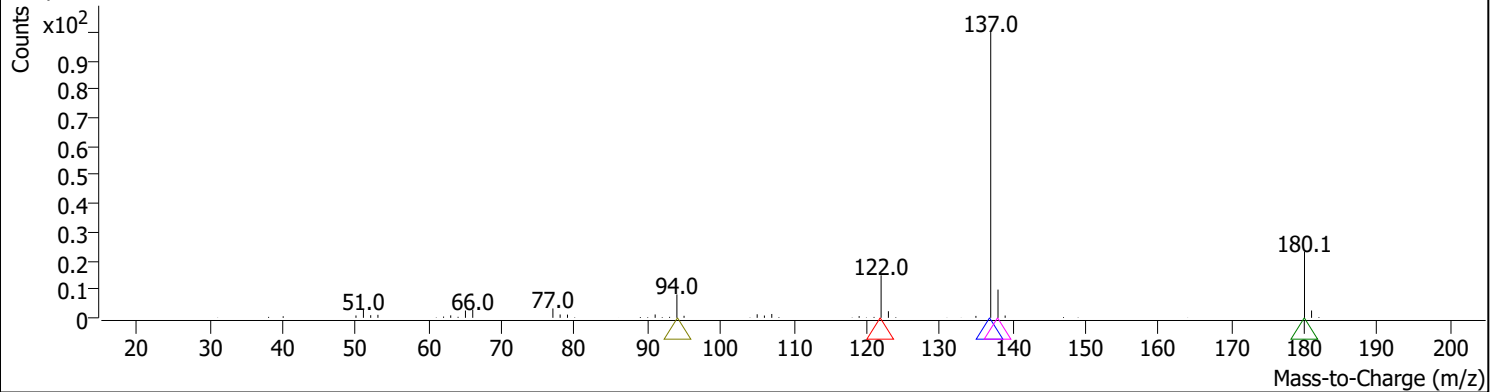
## Library Search Results - NonTarget Hits with Details



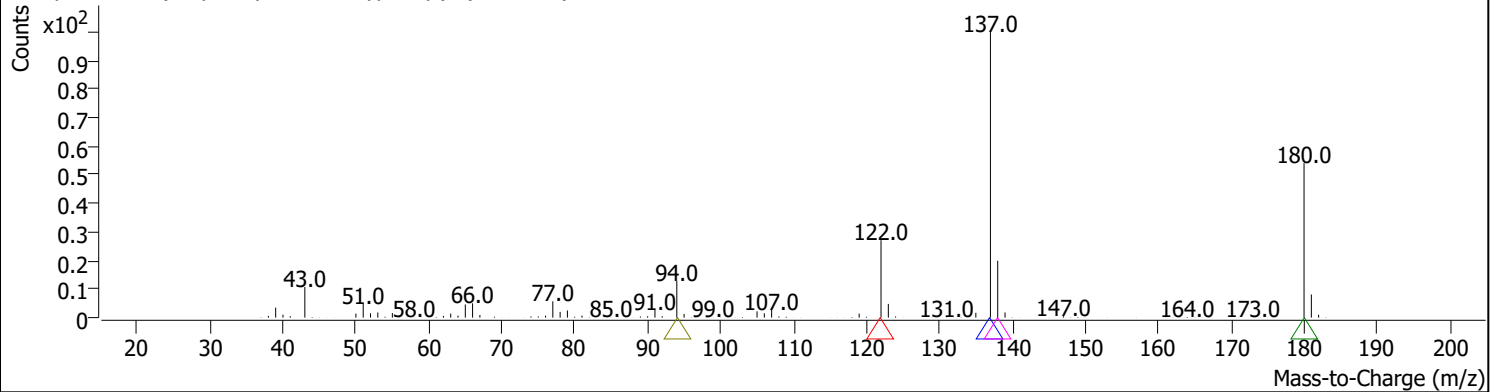
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
44.2950	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	5445870.8	94.2	2503-46-0	C10H12O3	

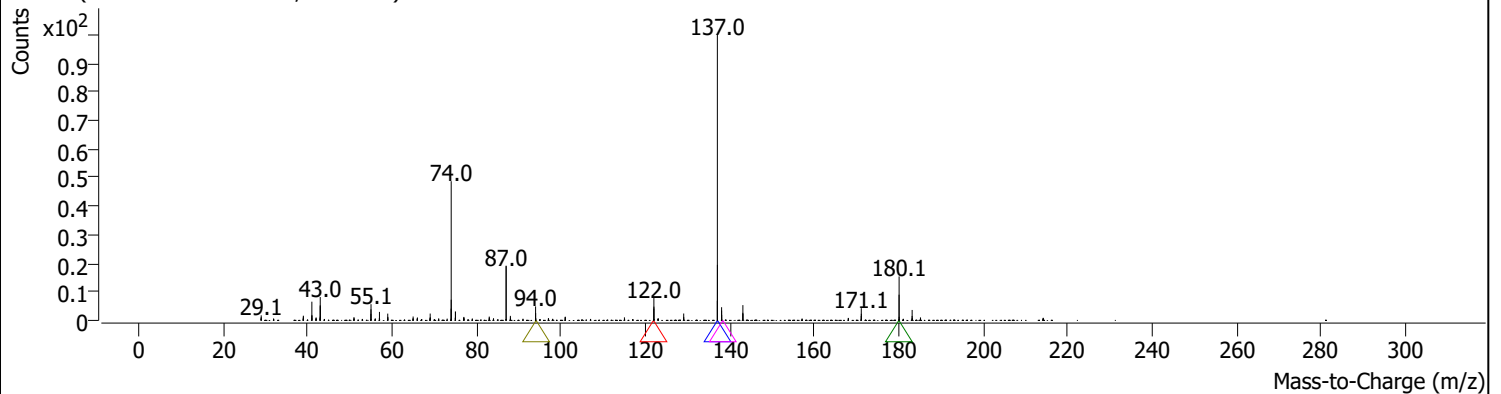
Component RT: 44.2950



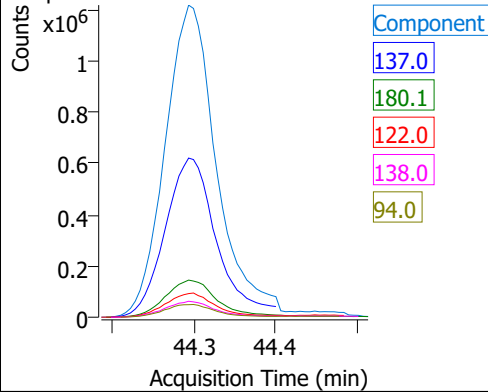
2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L)



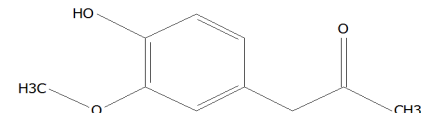
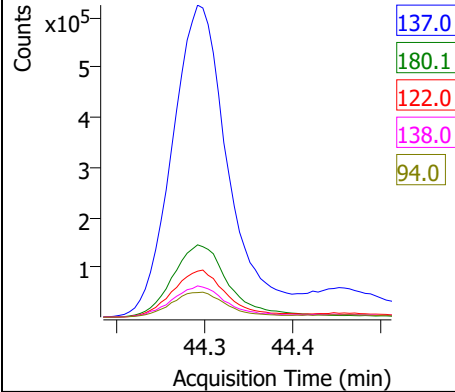
+ Scan (44.1919-44.5130 min, 55 scans) 4.D



Component RT: 44.2950



EIC Peaks



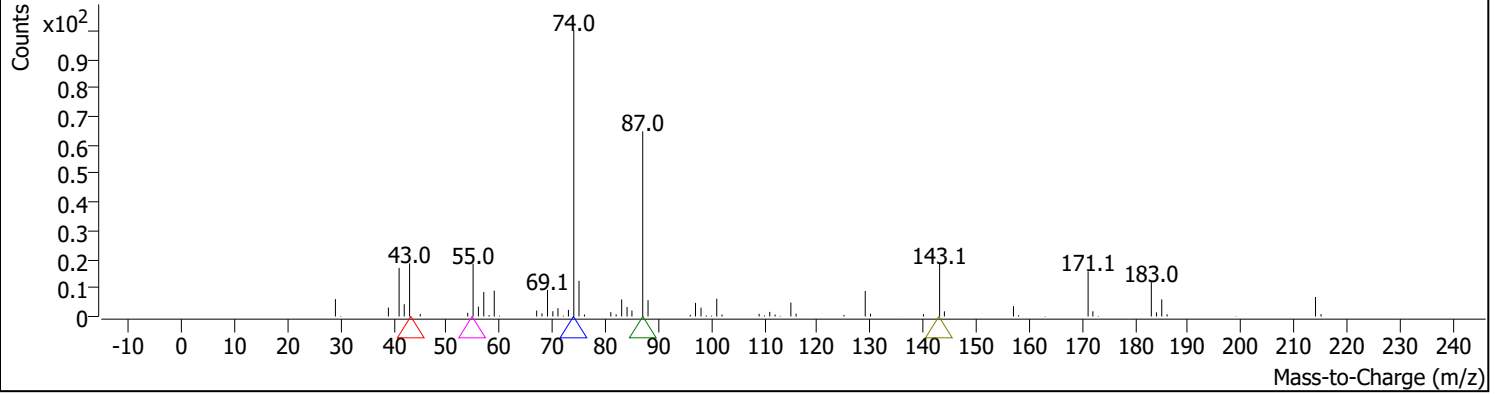
## Library Search Results - NonTarget Hits with Details



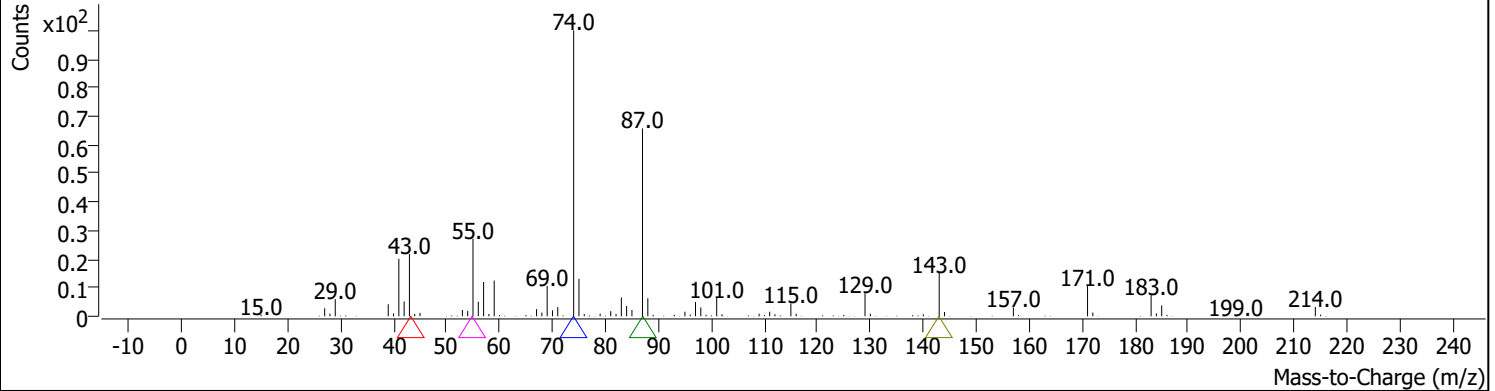
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
44.3330	Dodecanoic acid, methyl ester	6342821.8	95.2	111-82-0	C13H26O2	

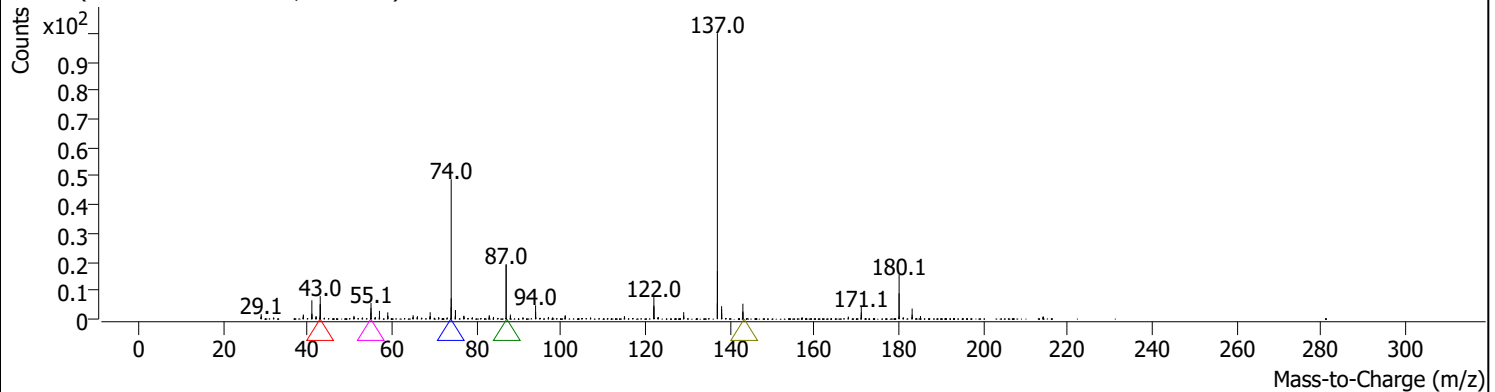
Component RT: 44.3330



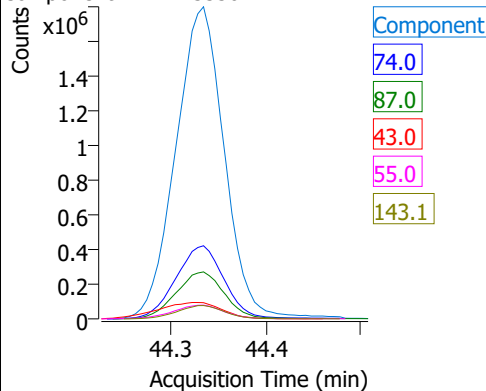
Dodecanoic acid, methyl ester (NIST20.L)



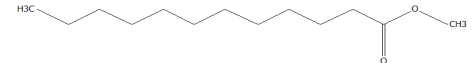
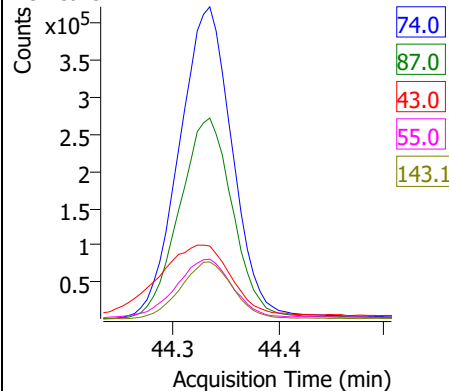
+ Scan (44.2336-44.4774 min, 42 scans) 4.D



Component RT: 44.3330



EIC Peaks



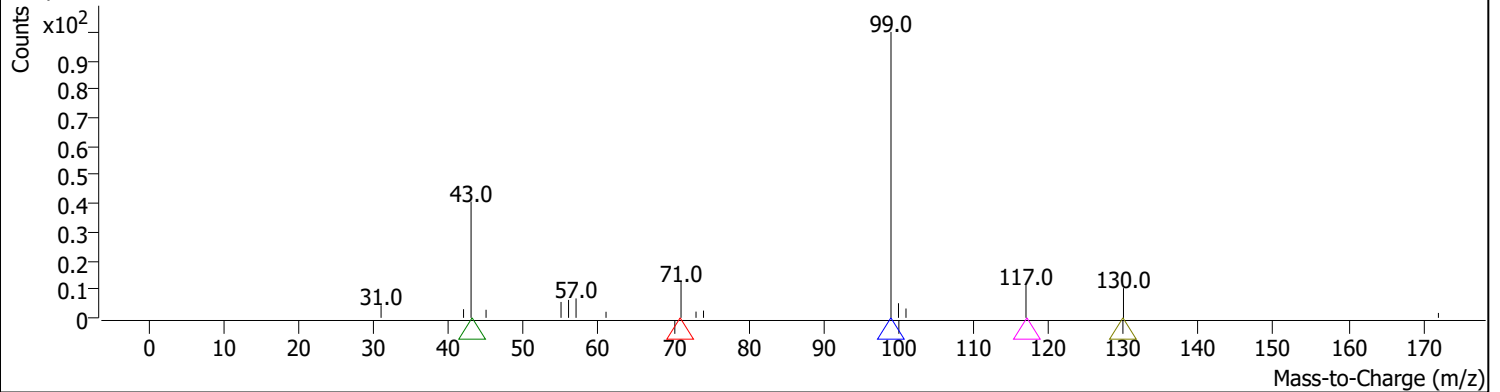
## Library Search Results - NonTarget Hits with Details



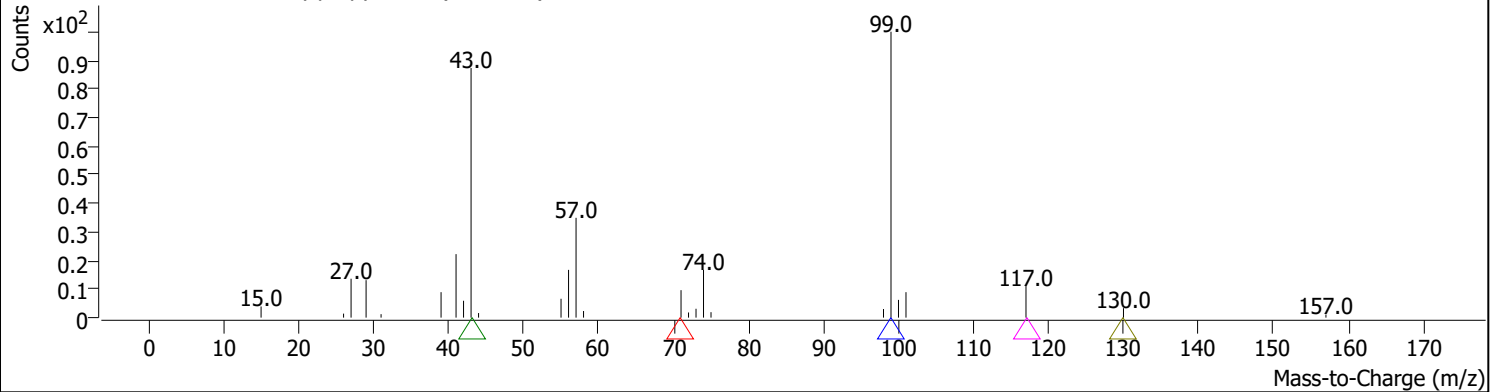
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
45.6451	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	435378.6	81.3	3757-32-2	C9H16O3	

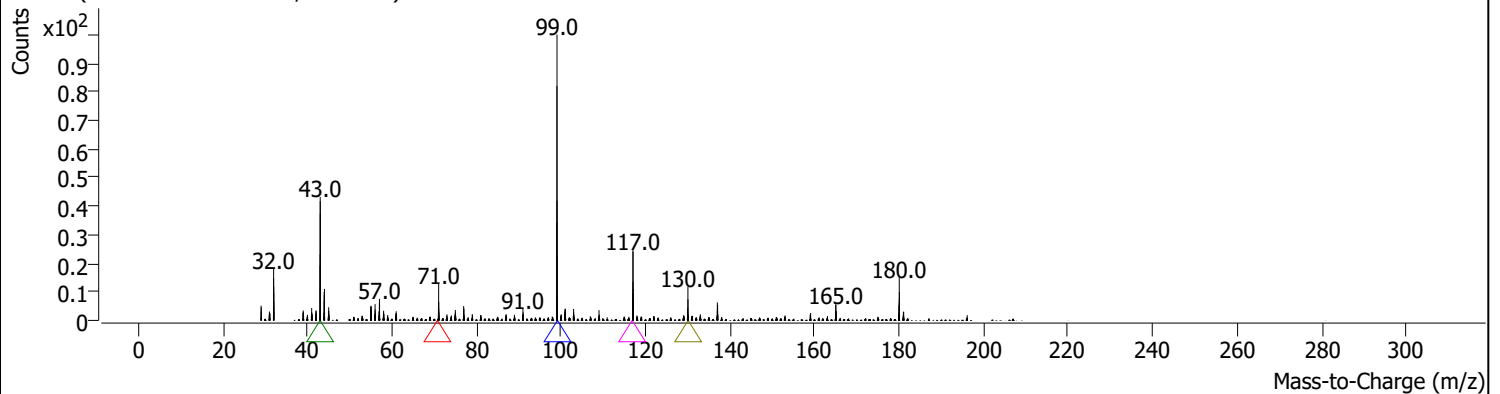
Component RT: 45.6451



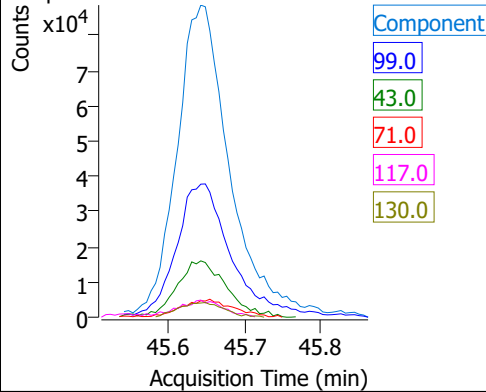
Pentanoic acid, 4-oxo-, 2-methylpropyl ester (NIST20.L)



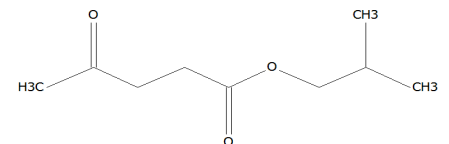
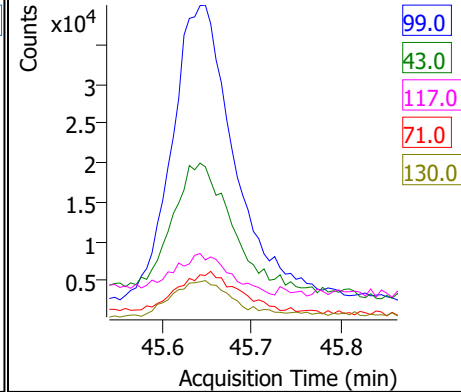
+ Scan (45.5417-45.8628 min, 55 scans) 4.D



Component RT: 45.6451



EIC Peaks



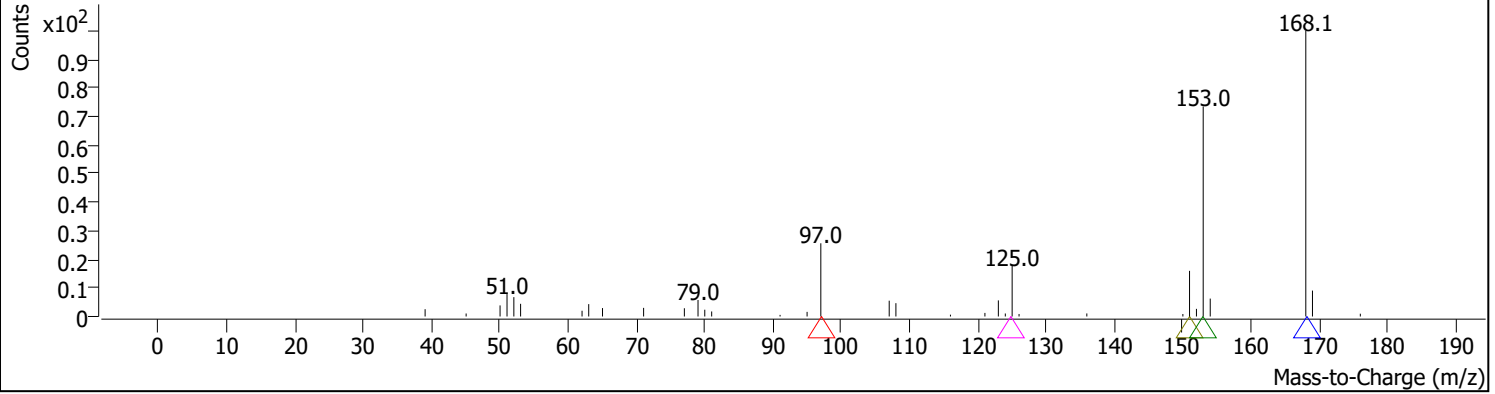
## Library Search Results - NonTarget Hits with Details



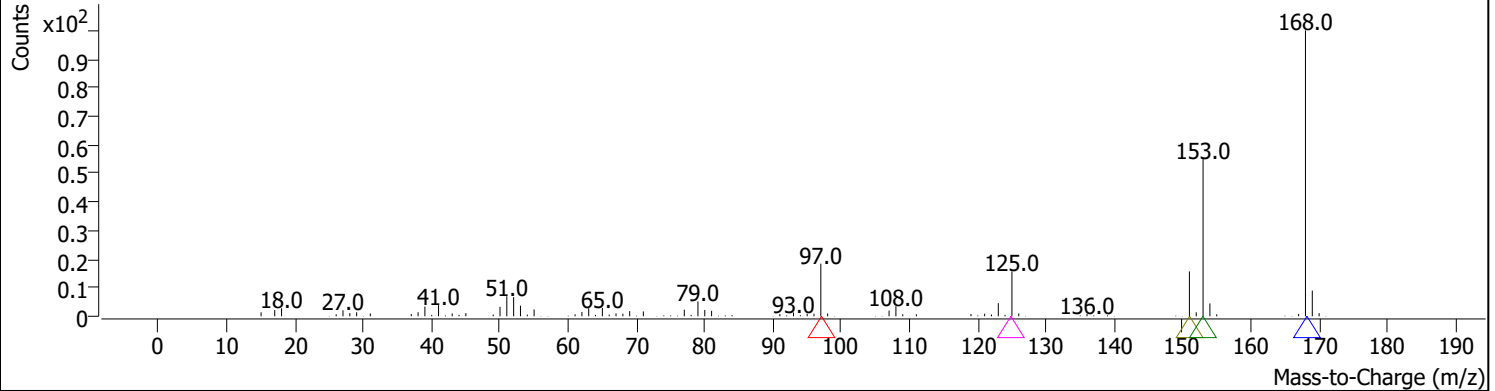
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.0653	3-Hydroxy-4-methoxybenzoic acid	936058.2	92.6	645-08-9	C <sub>8</sub> H <sub>8</sub> O <sub>4</sub>	

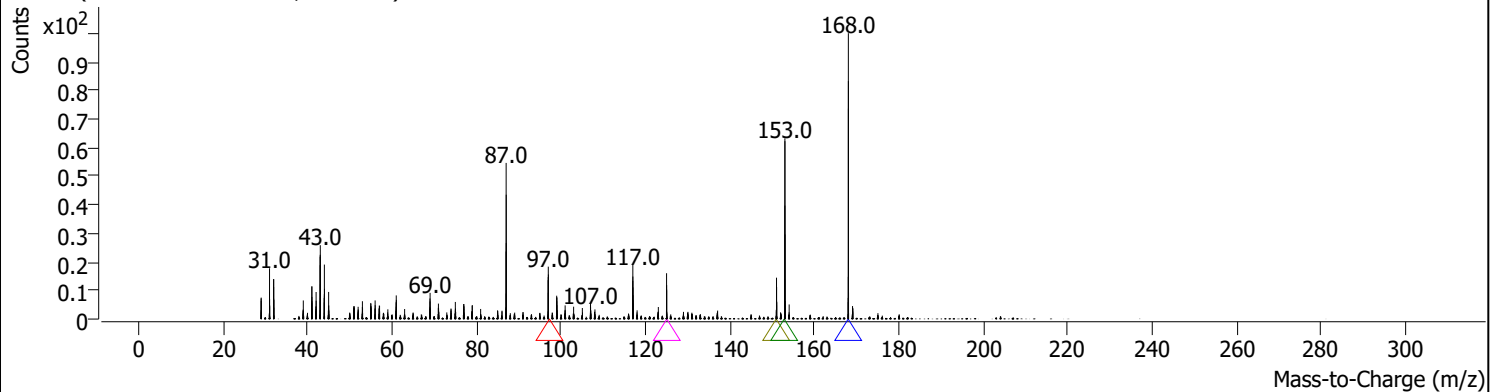
Component RT: 46.0653



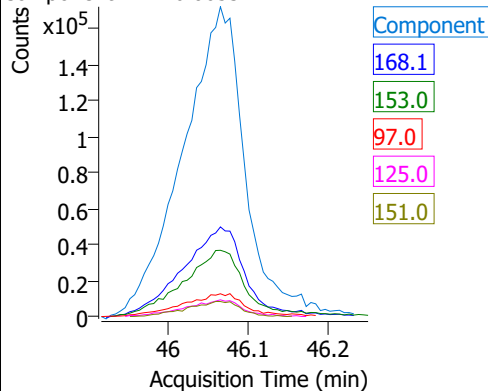
3-Hydroxy-4-methoxybenzoic acid (NIST20.L)



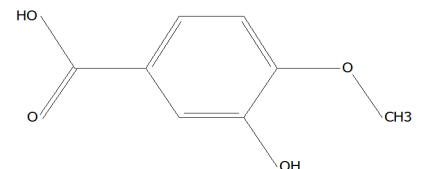
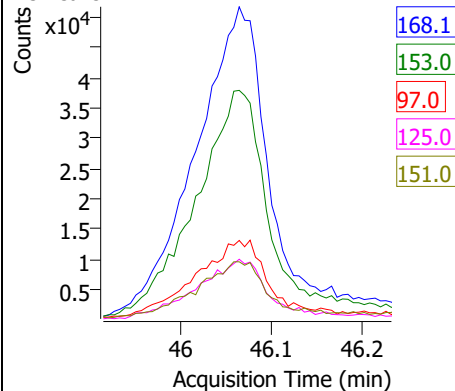
+ Scan (45.9275-46.2374 min, 52 scans) 4.D



Component RT: 46.0653



EIC Peaks



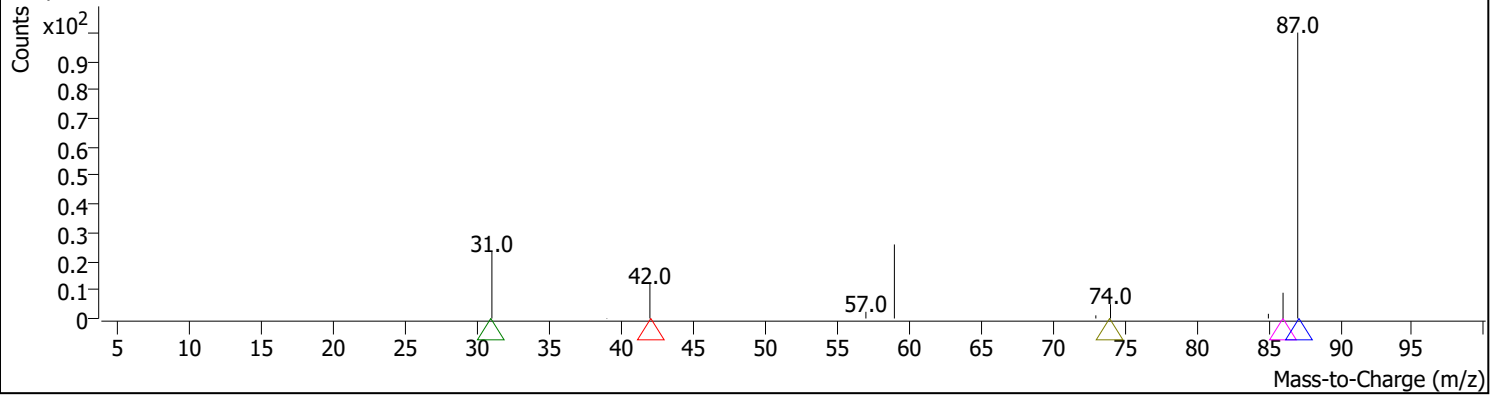
## Library Search Results - NonTarget Hits with Details



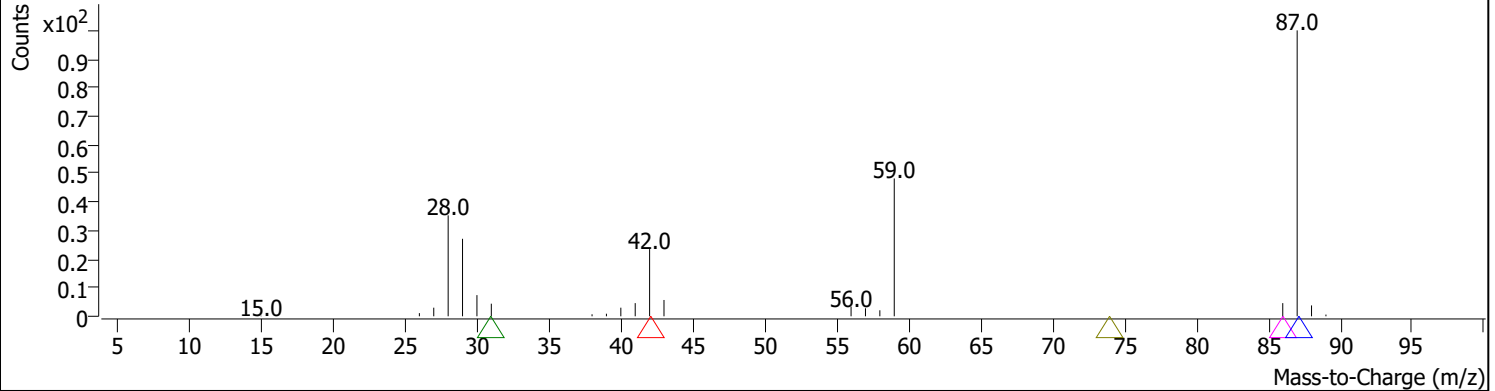
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.2195	Oxazolidin-2-one	634933.3	80.5	497-25-6	C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub>	

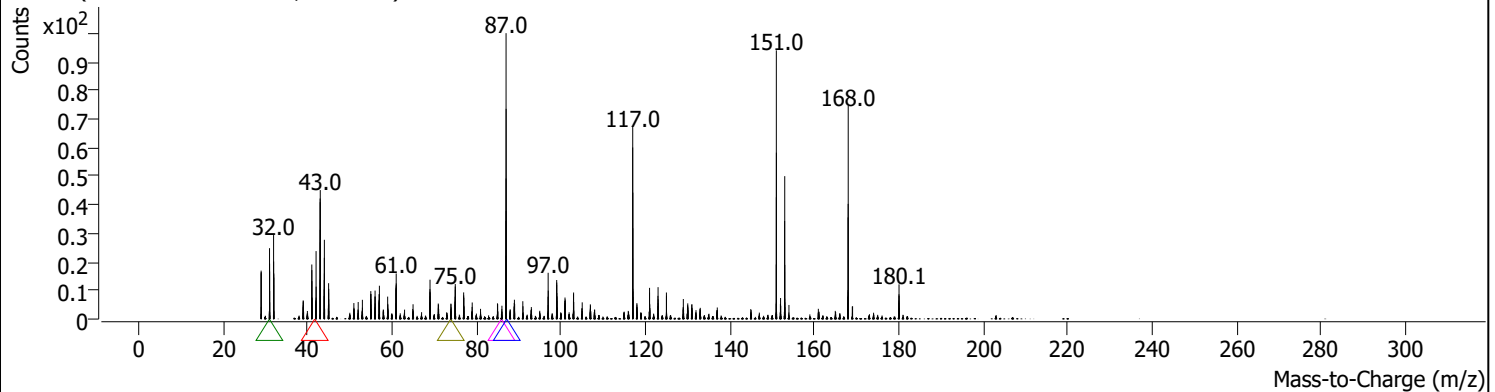
Component RT: 46.2195



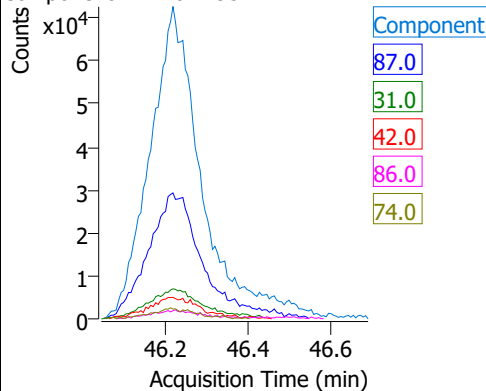
Oxazolidin-2-one (NIST20.L)



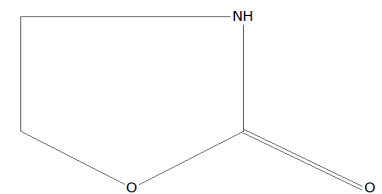
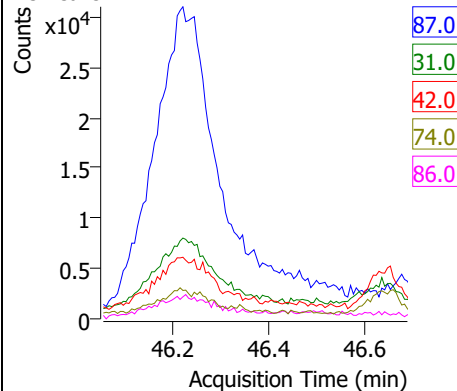
+ Scan (46.0590-46.5466 min, 83 scans) 4.D



Component RT: 46.2195



EIC Peaks



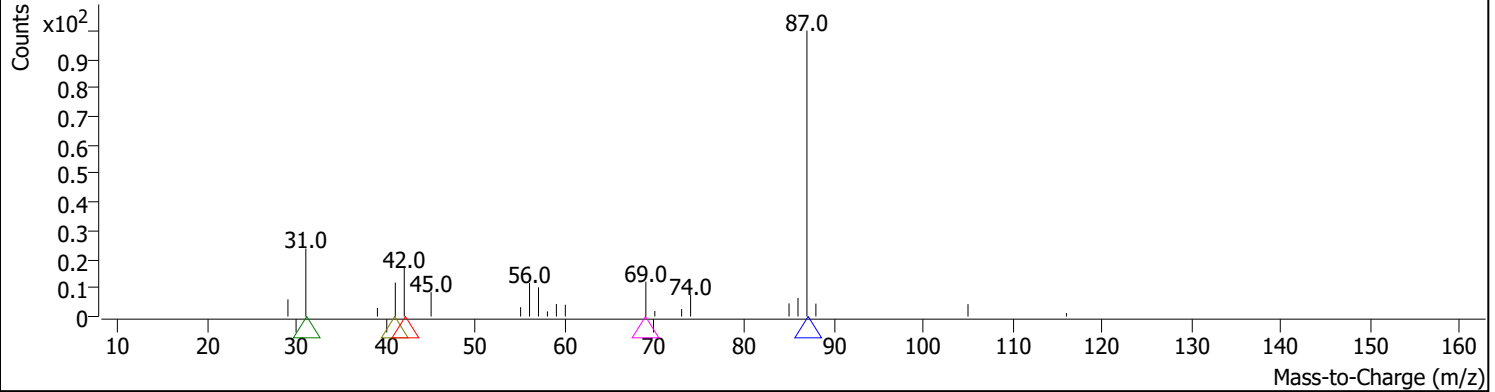
## Library Search Results - NonTarget Hits with Details



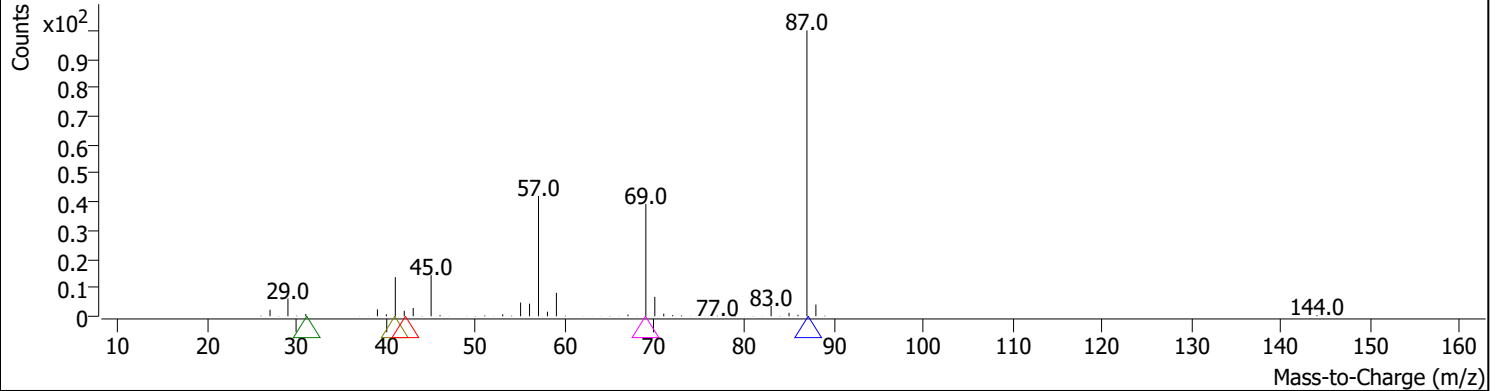
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.2202	3-Pentanol, 2,2,4,4-tetramethyl-	744700.7	78.0	14609-79-1	C <sub>9</sub> H <sub>20</sub> O	

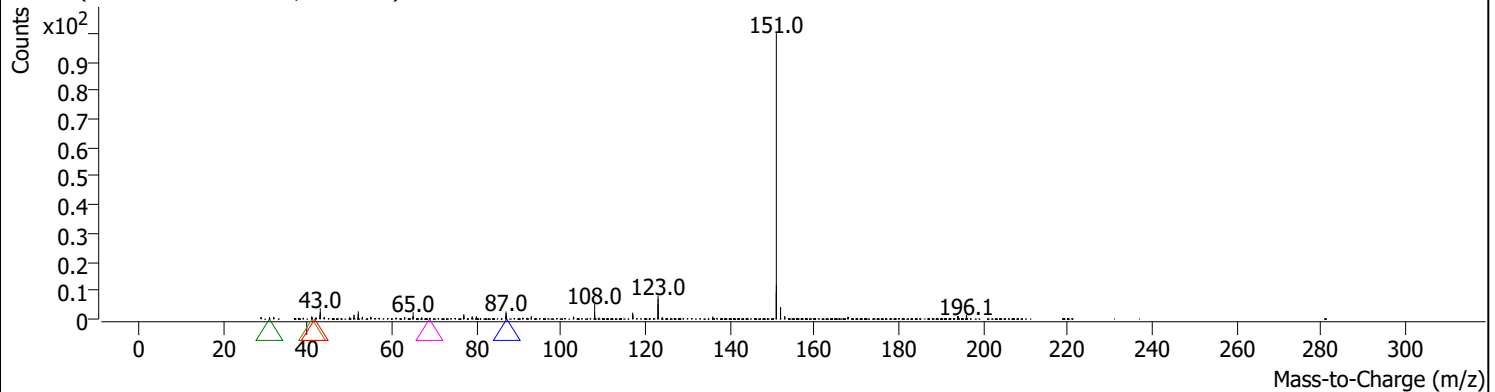
Component RT: 46.2202



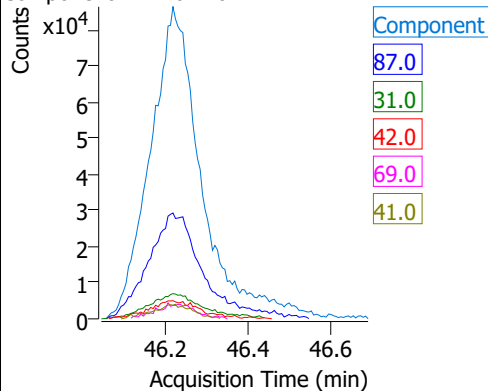
3-Pentanol, 2,2,4,4-tetramethyl- (NIST20.L)



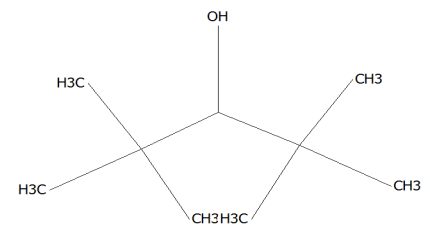
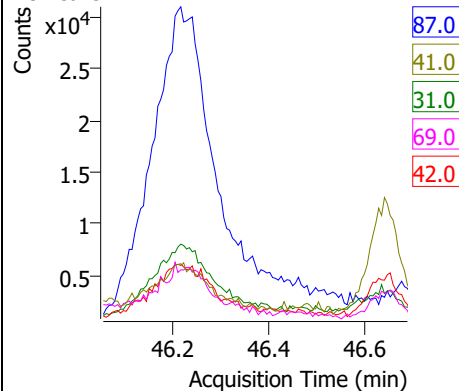
+ Scan (46.1185-46.6893 min, 97 scans) 4.D



Component RT: 46.2202



EIC Peaks



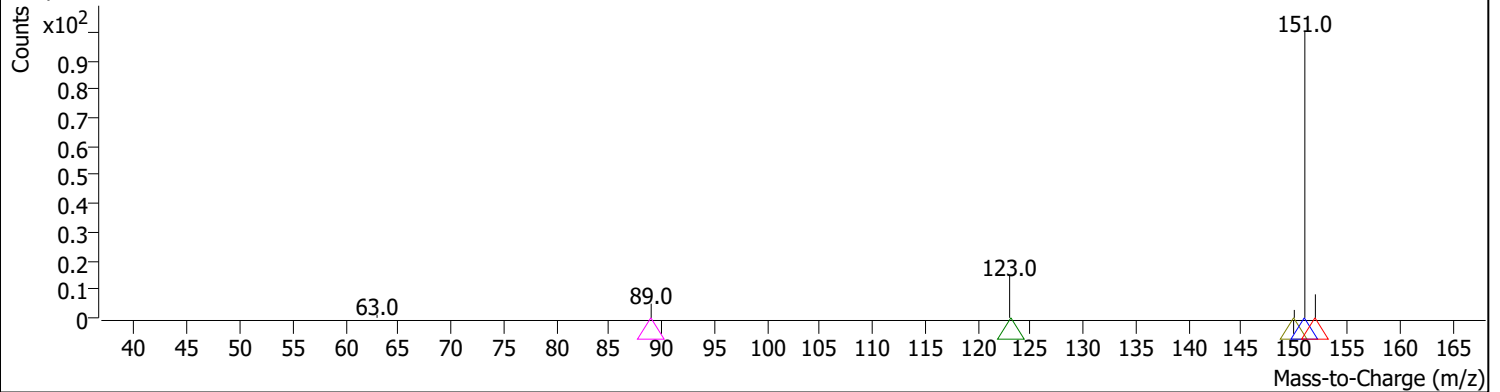
## Library Search Results - NonTarget Hits with Details



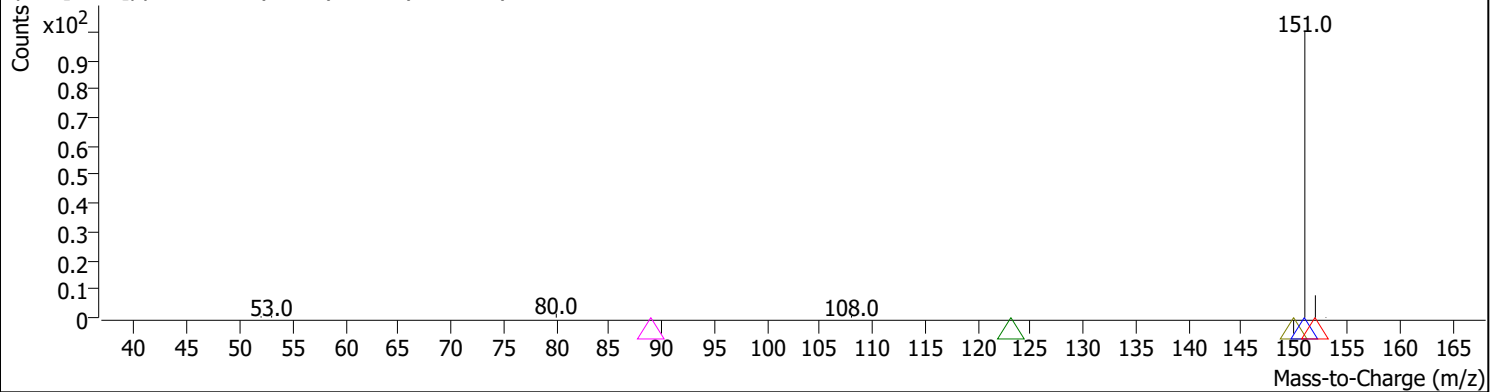
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.4841	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	210231.0	81.4	65996-50-1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	

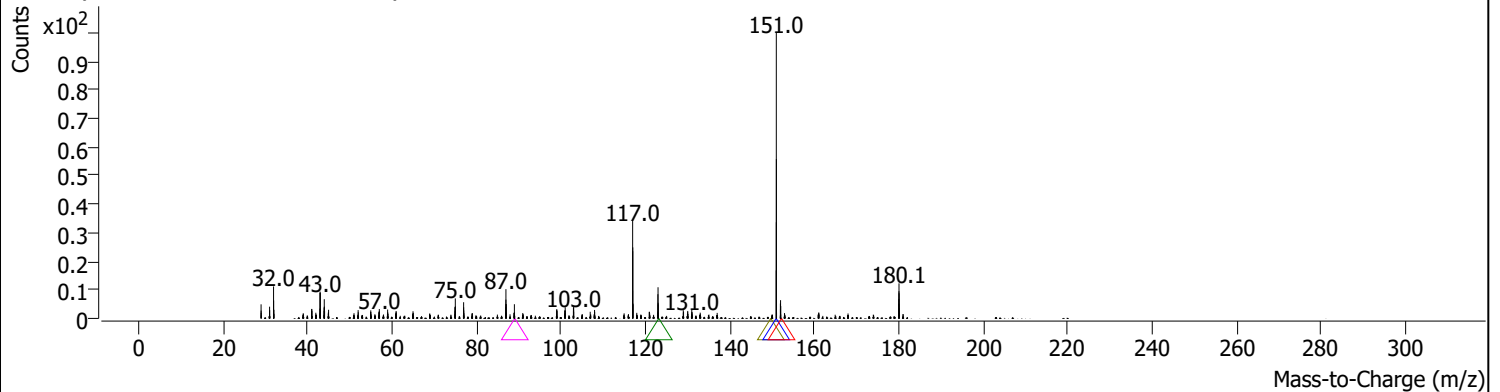
Component RT: 46.4841



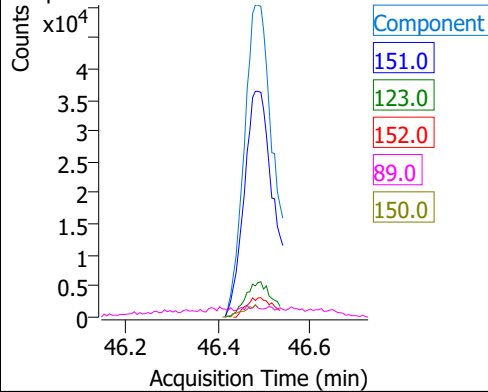
Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)



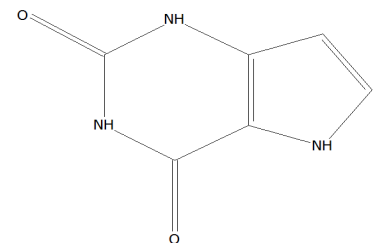
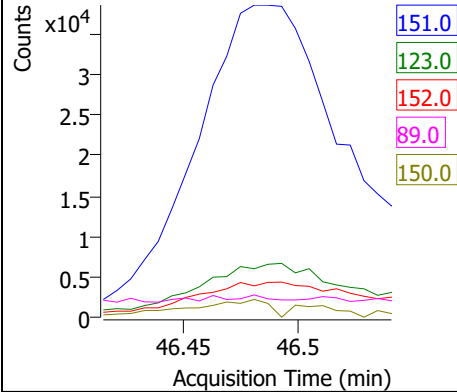
+ Scan (46.4111-46.5406 min, 22 scans) 4.D



Component RT: 46.4841



EIC Peaks



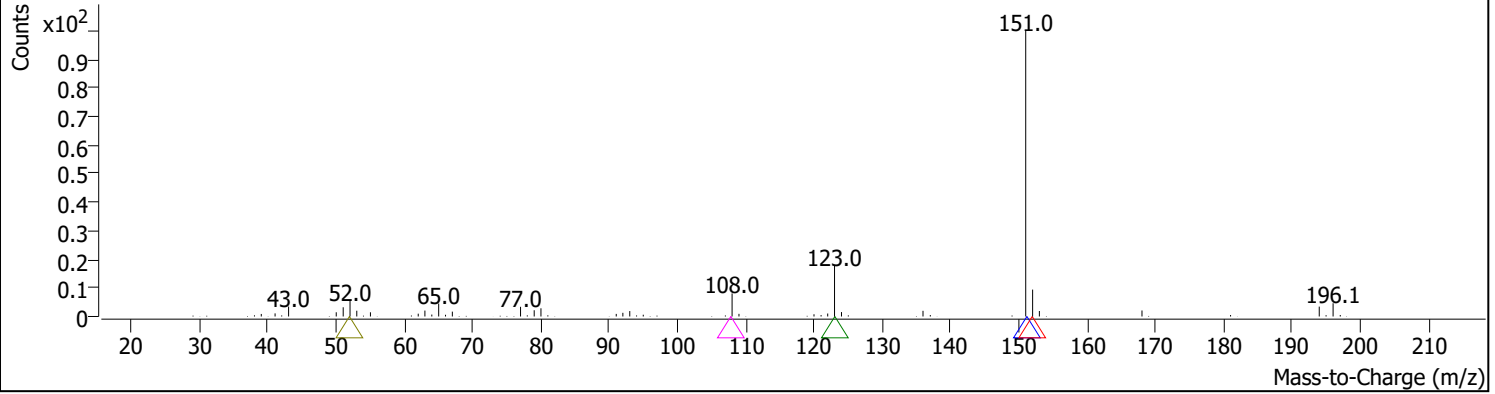
## Library Search Results - NonTarget Hits with Details



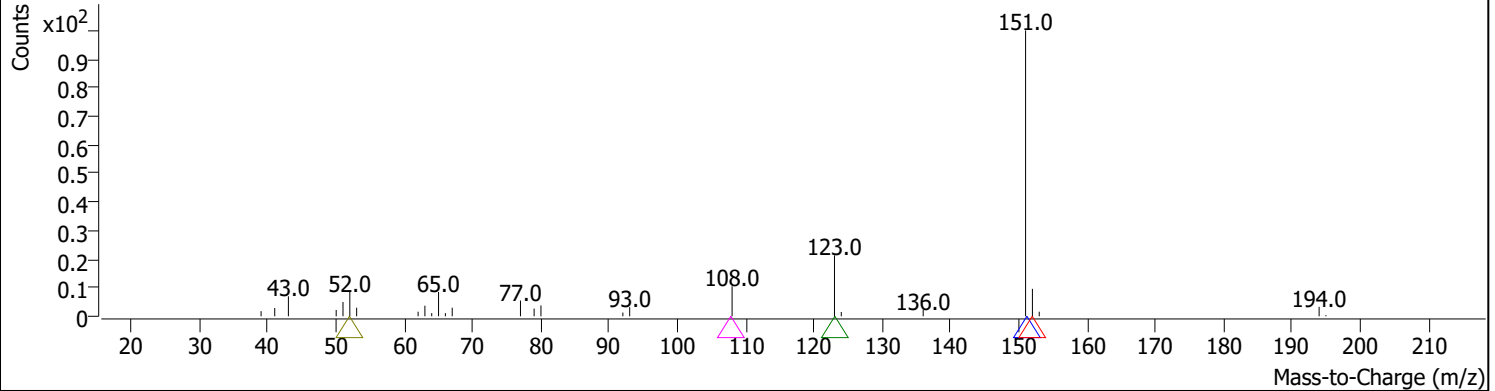
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
46.6461	Butyrovanihone	8738295.8	89.8	64142-23-0	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	

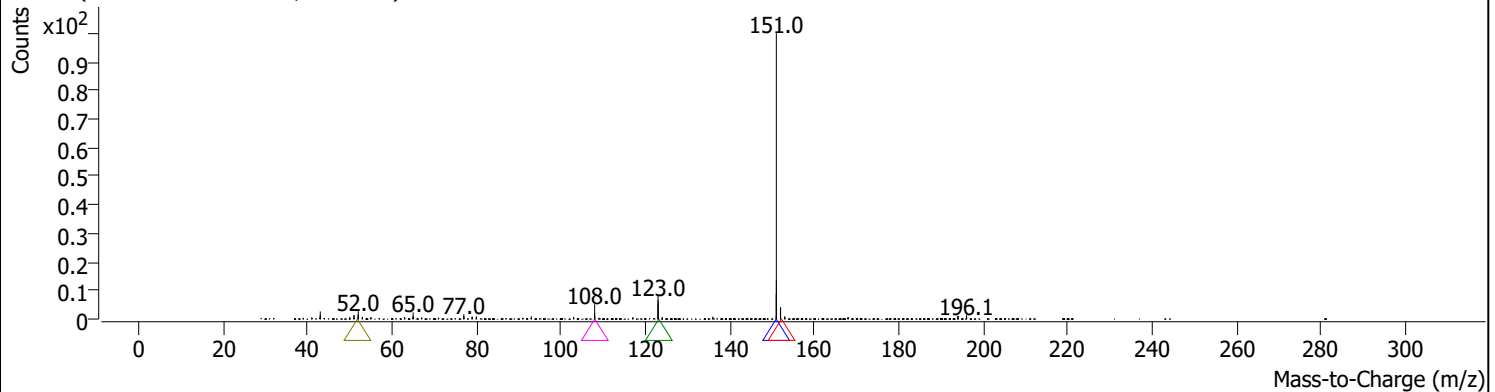
Component RT: 46.6461



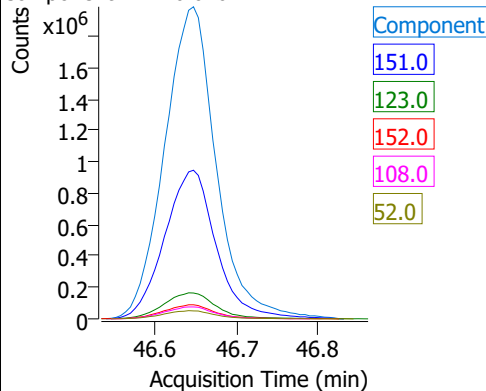
Butyrovanihone (NIST20.L)



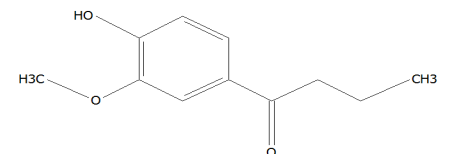
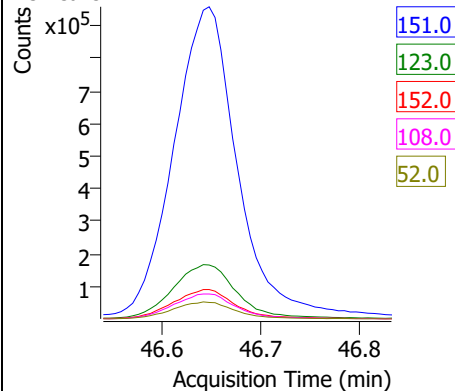
+ Scan (46.5406-46.8320 min, 50 scans) 4.D



Component RT: 46.6461



EIC Peaks





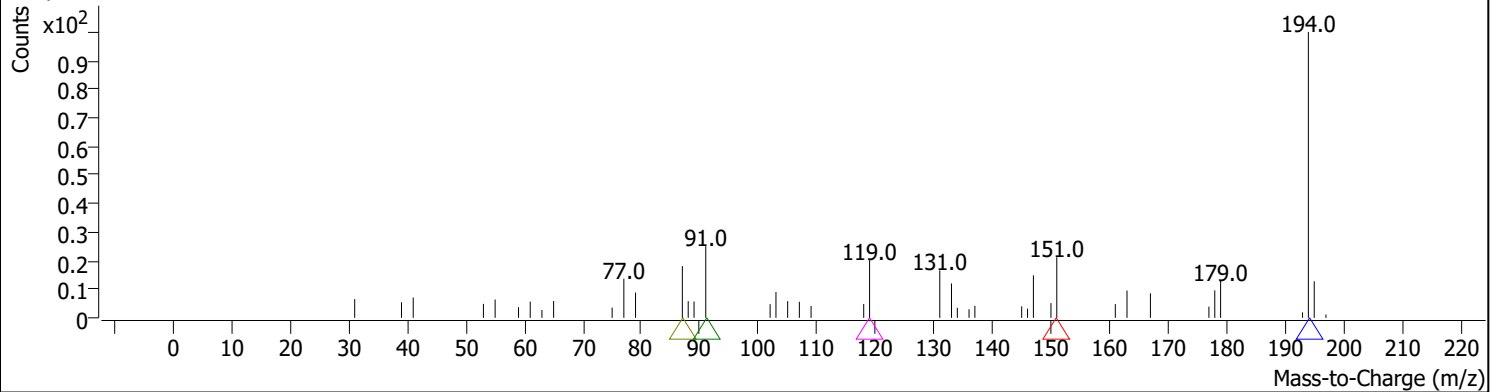
## Library Search Results - NonTarget Hits with Details



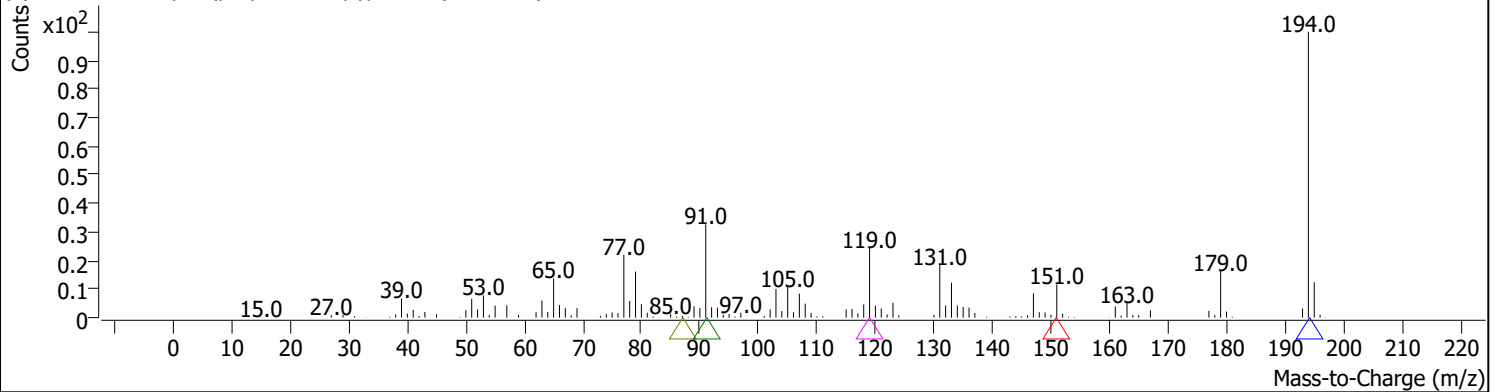
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
47.0820	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	306538.1	76.4	20675-95-0	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	

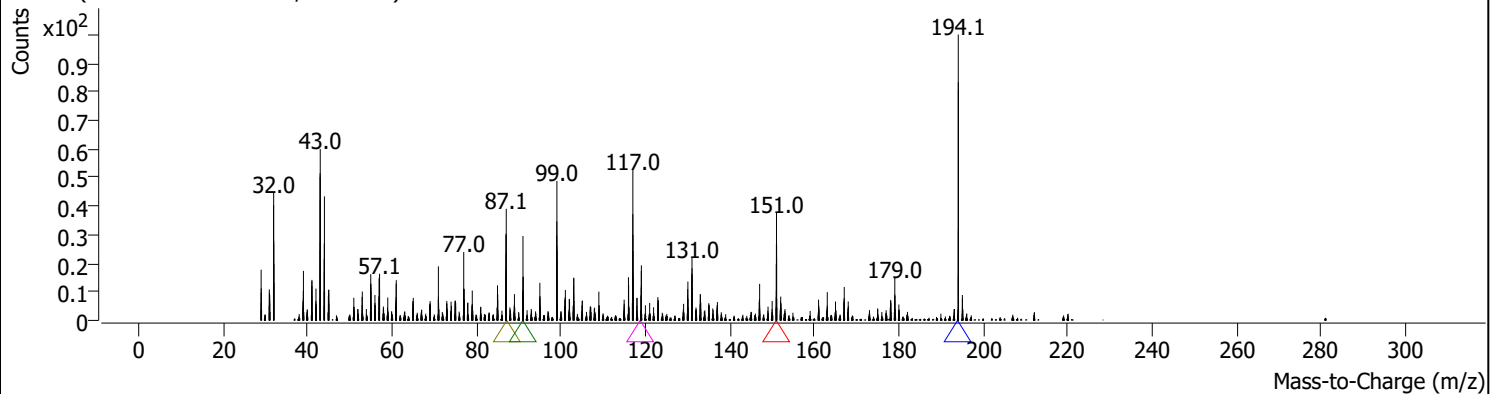
Component RT: 47.0820



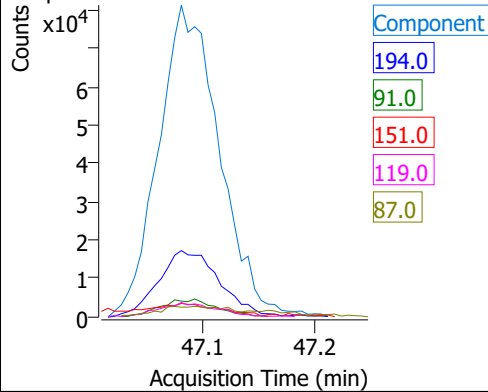
(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L)



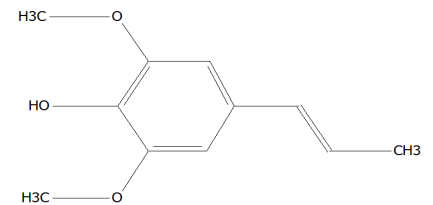
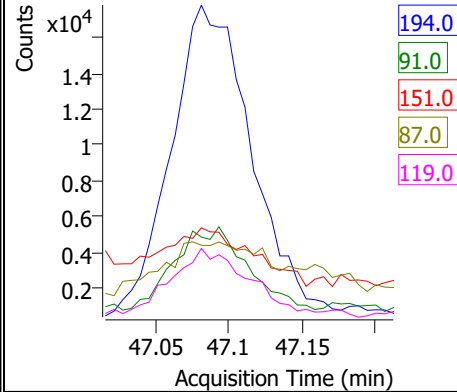
+ Scan (47.0189-47.2148 min, 33 scans) 4.D



Component RT: 47.0820



EIC Peaks



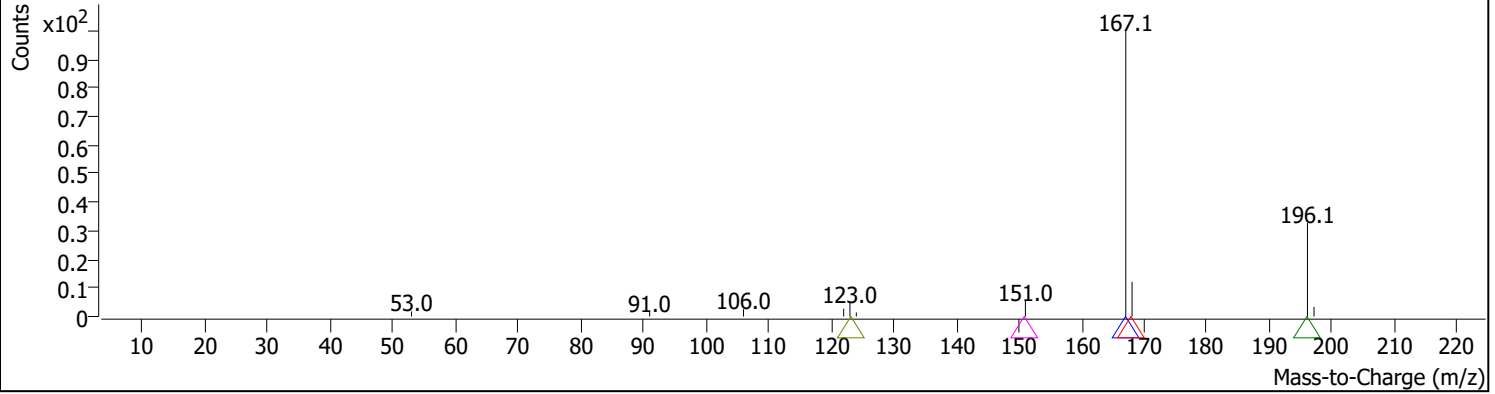
# Library Search Results - NonTarget Hits with Details



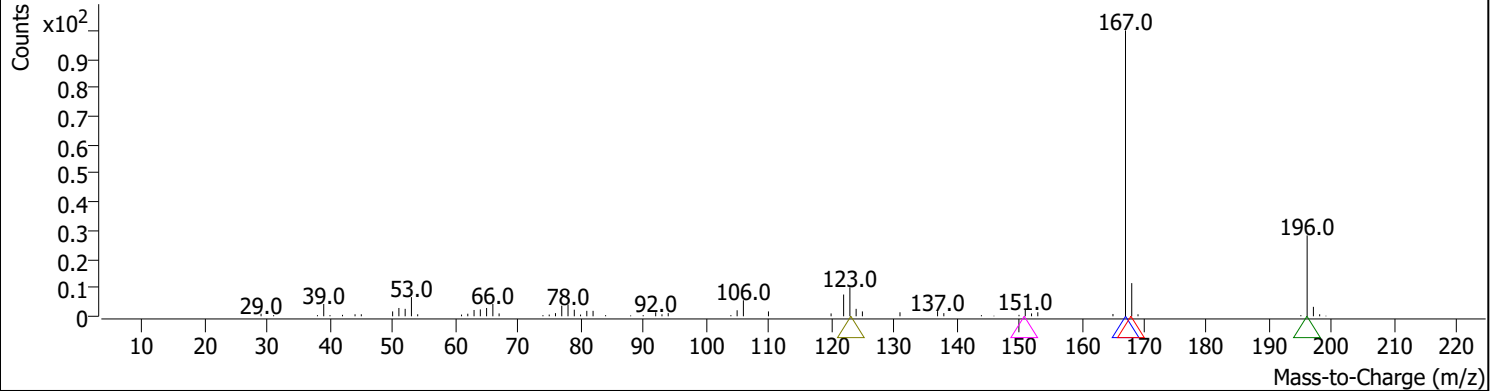
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
47.3540	Homosyringaldehyde	224103.1	82.6	87345-52-6	C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>	

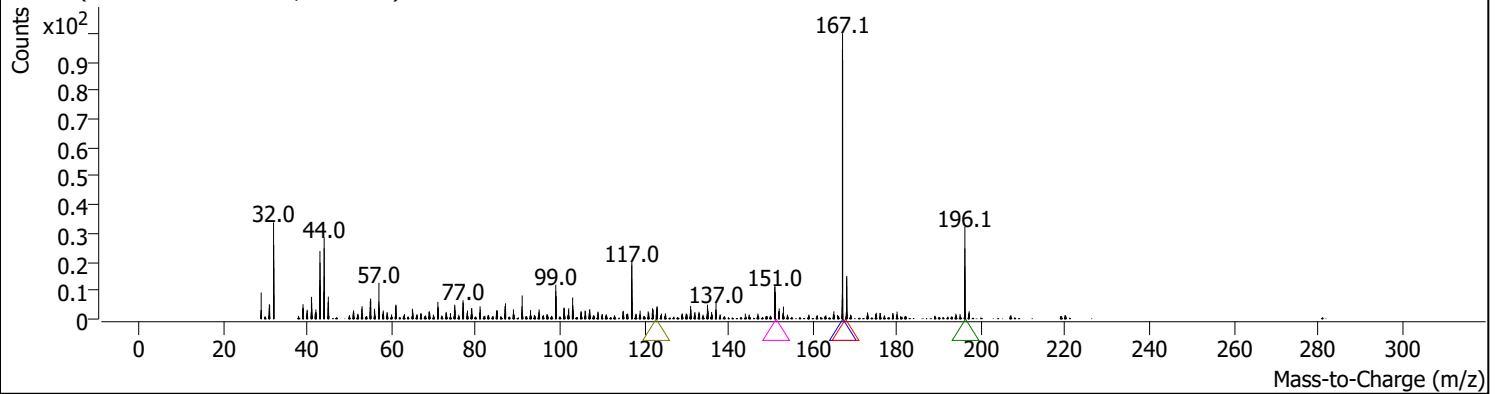
Component RT: 47.3540



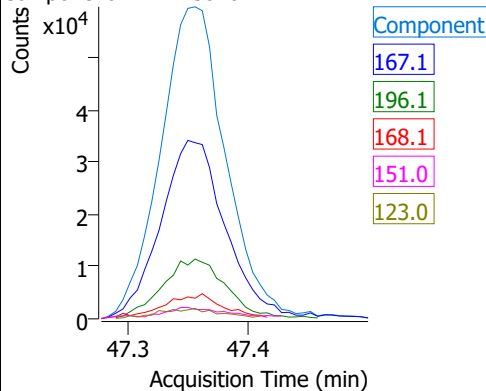
Homosyringaldehyde (NIST20.L)



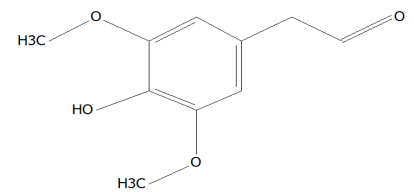
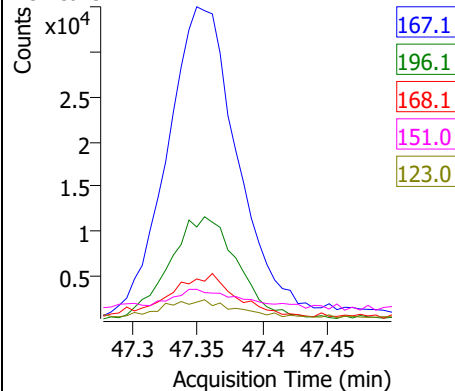
+ Scan (47.2783-47.4979 min, 37 scans) 4.D



Component RT: 47.3540



EIC Peaks



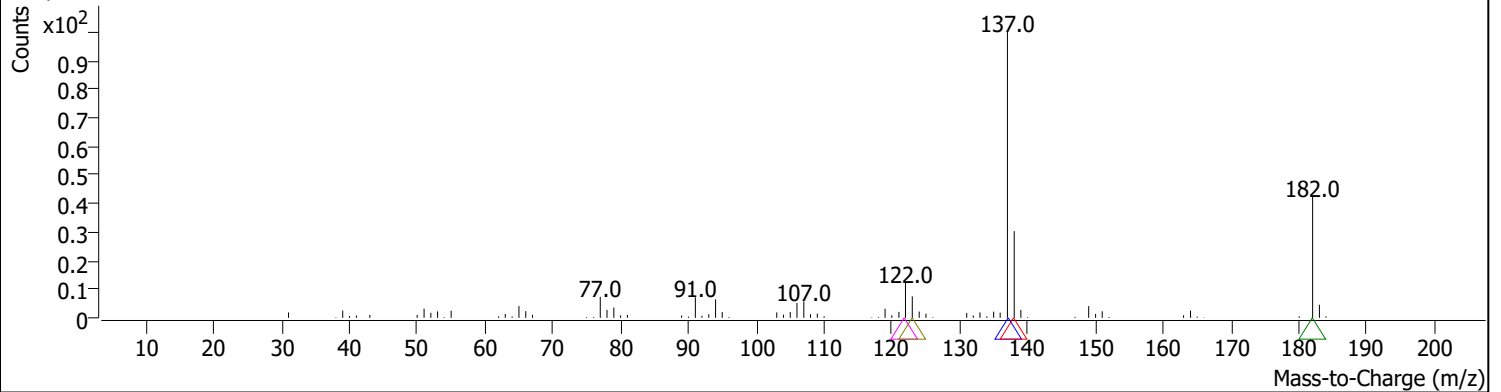
## Library Search Results - NonTarget Hits with Details



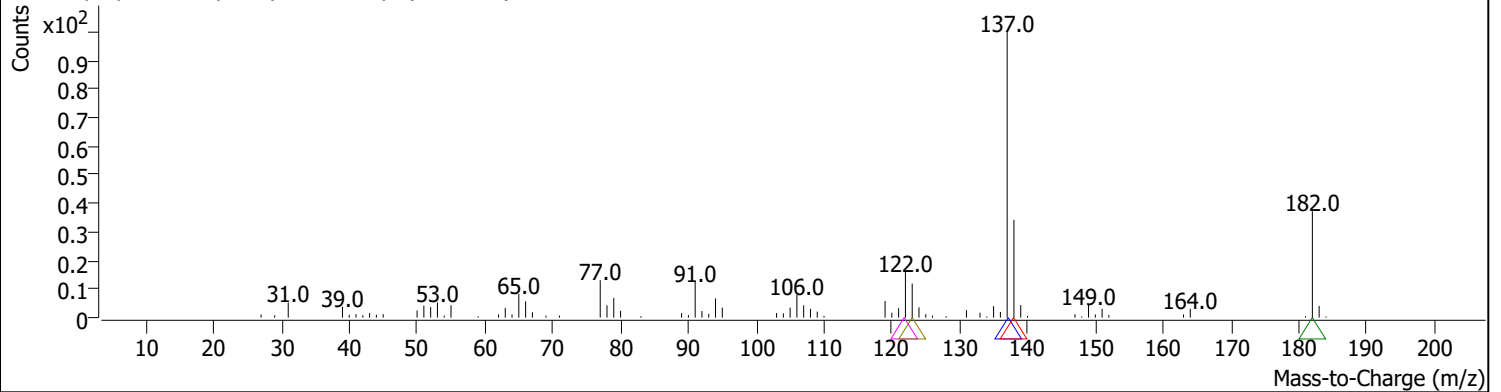
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
48.9895	Benzenepropanol, 4-hydroxy-3-methoxy-	5515590.4	96.4	2305-13-7	C10H14O3	

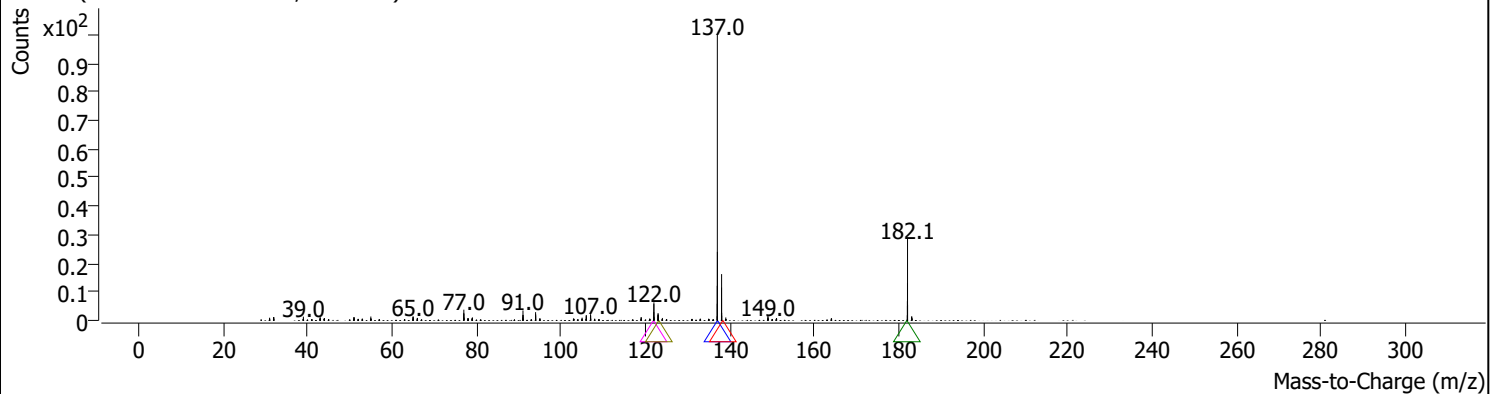
Component RT: 48.9895



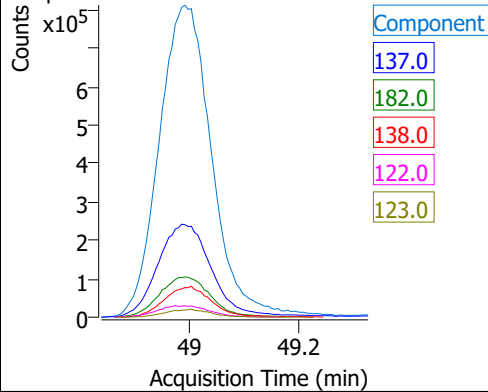
Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L)



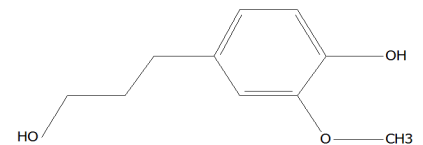
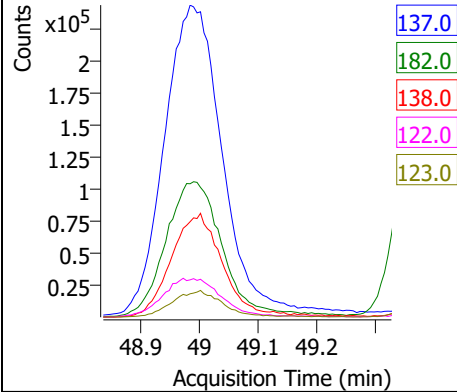
+ Scan (48.8550-49.2340 min, 63 scans) 4.D



Component RT: 48.9895



EIC Peaks



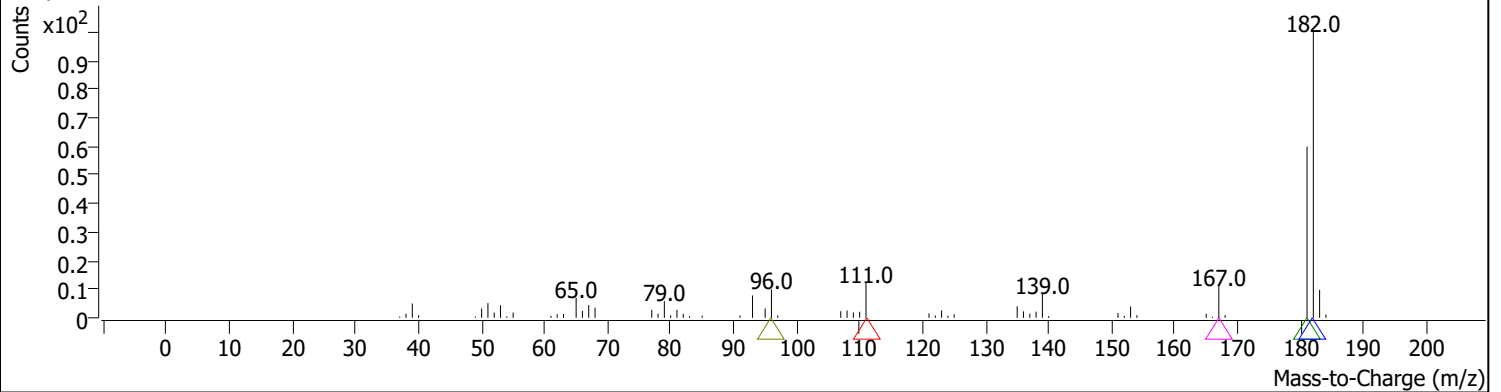
## Library Search Results - NonTarget Hits with Details



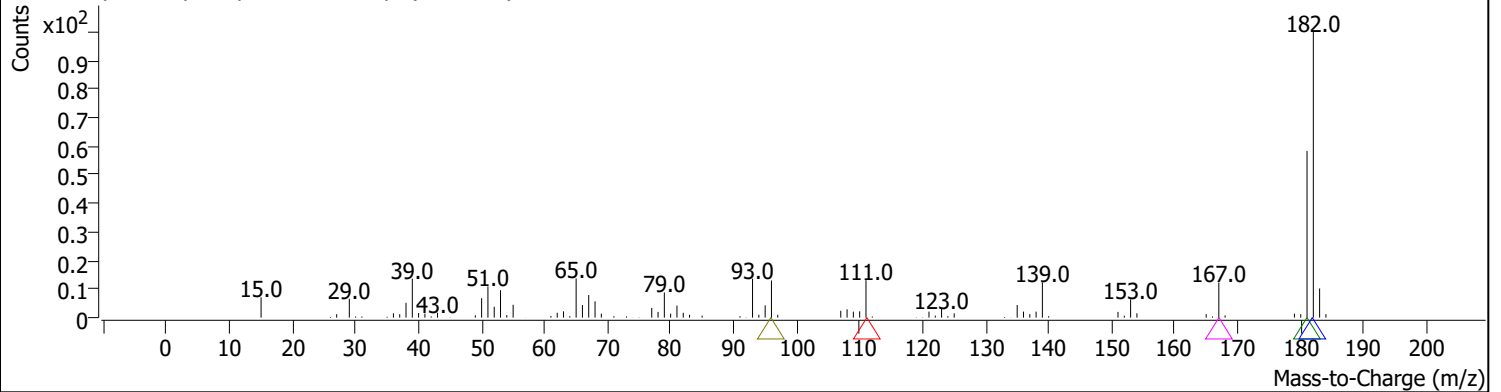
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
49.3613	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	2047327.7	96.5	134-96-3	C9H10O4	

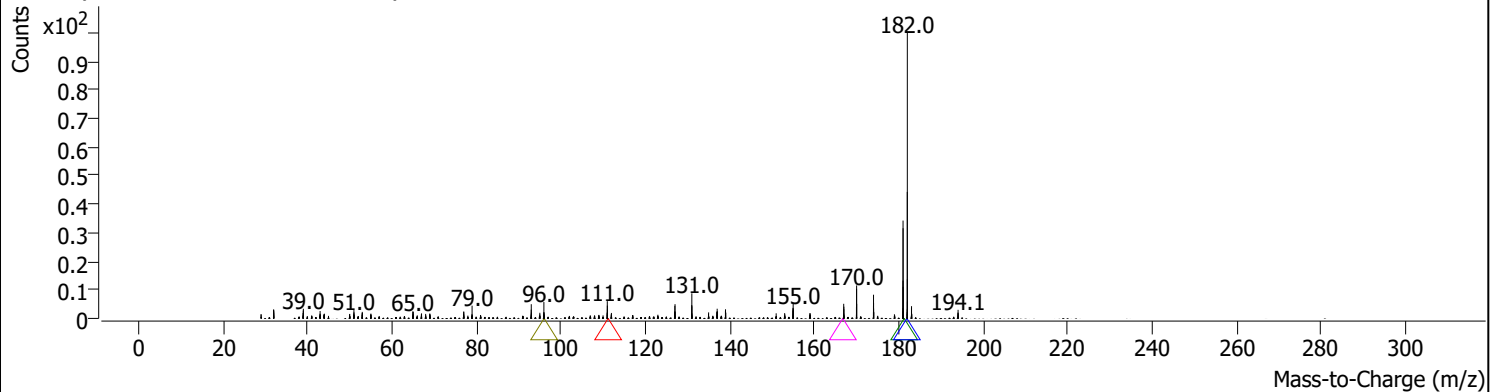
Component RT: 49.3613



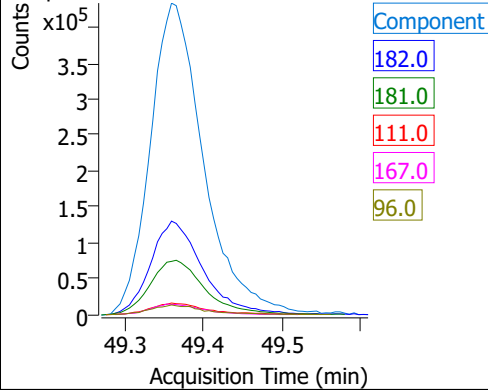
Benzaldehyde, 4-hydroxy-3,5-dimethoxy- (NIST20.L)



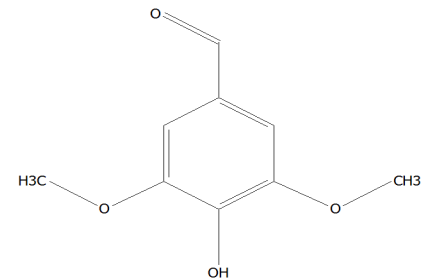
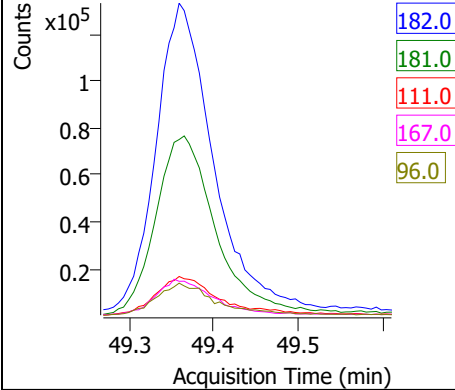
+ Scan (49.2786-49.6141 min, 56 scans) 4.D



Component RT: 49.3613



EIC Peaks



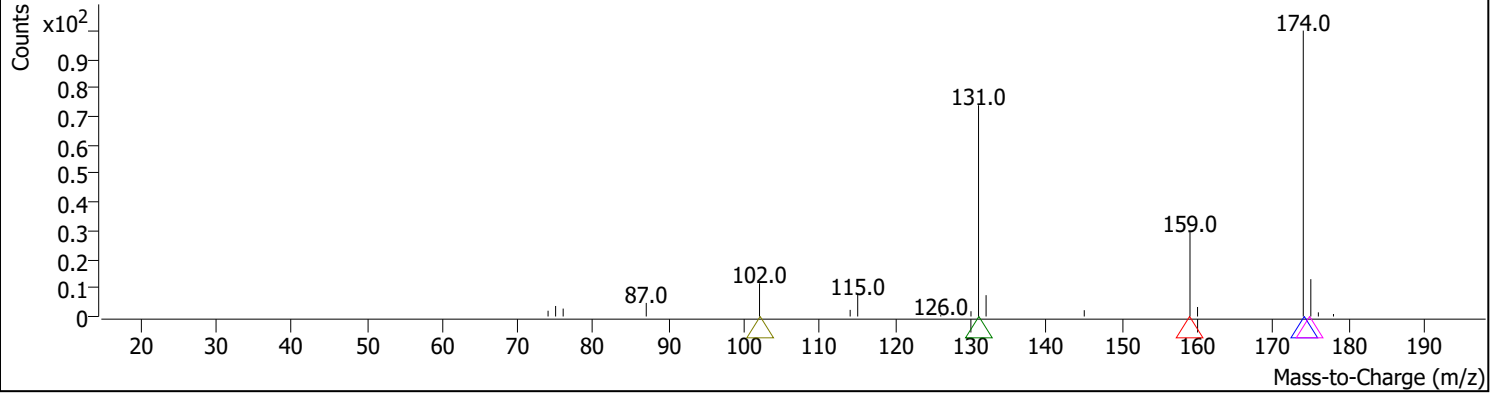
## Library Search Results - NonTarget Hits with Details



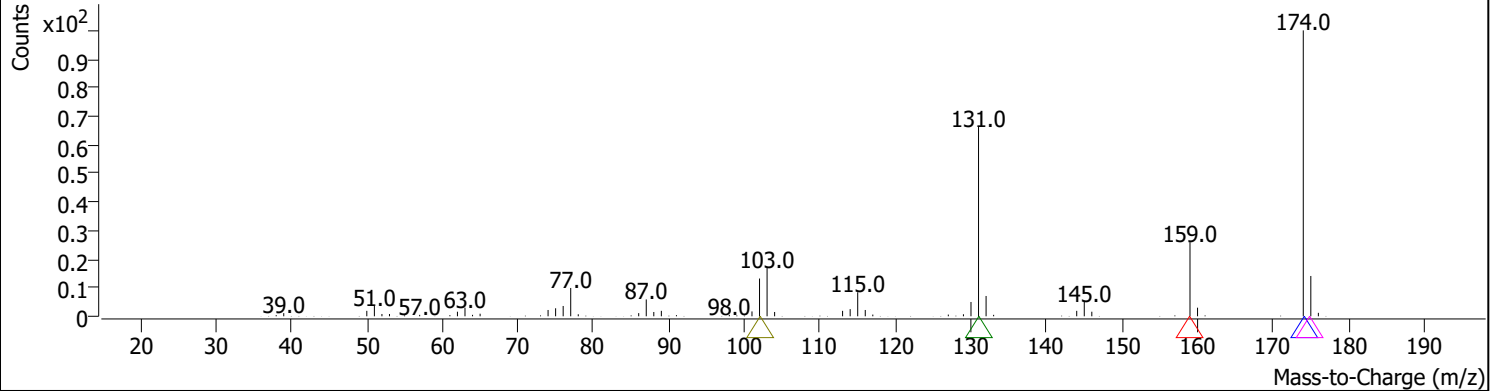
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
49.4171	7-Methoxy-1-naphthol	307367.8	84.8	67247-13-6	C <sub>11</sub> H <sub>10</sub> O <sub>2</sub>	

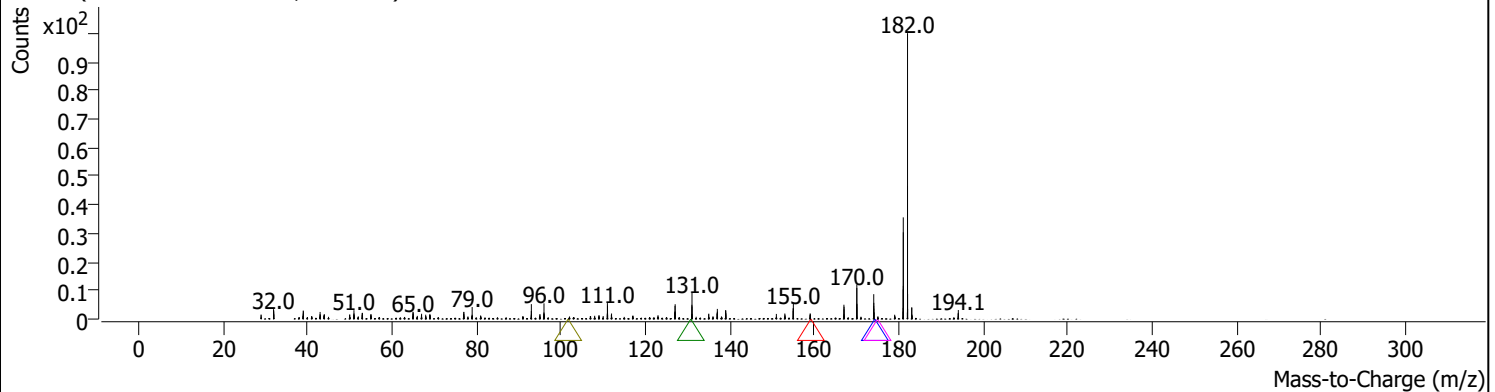
Component RT: 49.4171



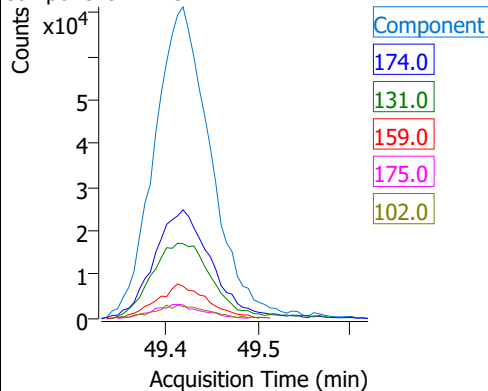
7-Methoxy-1-naphthol (NIST20.L)



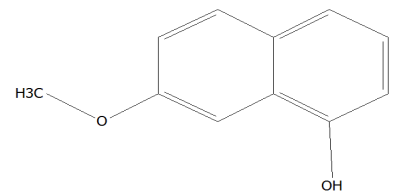
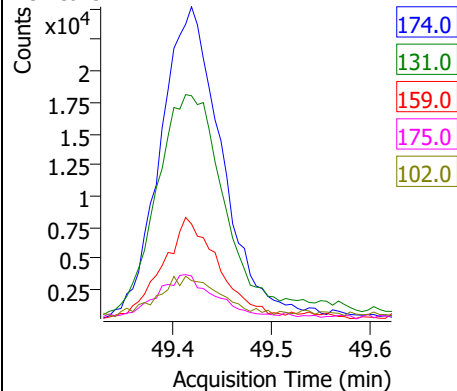
+ Scan (49.3261-49.6207 min, 50 scans) 4.D



Component RT: 49.4171



EIC Peaks



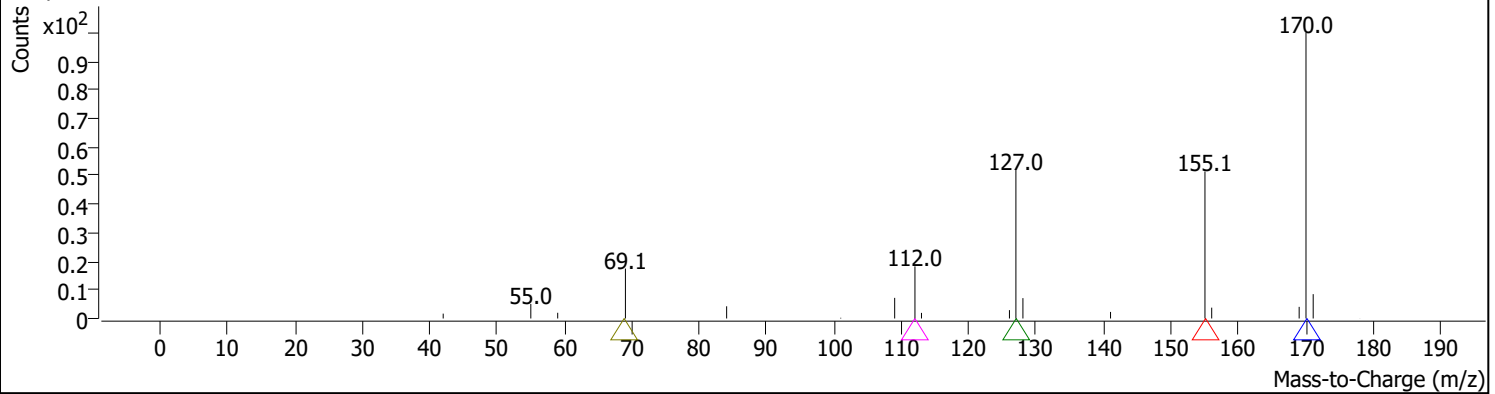
## Library Search Results - NonTarget Hits with Details



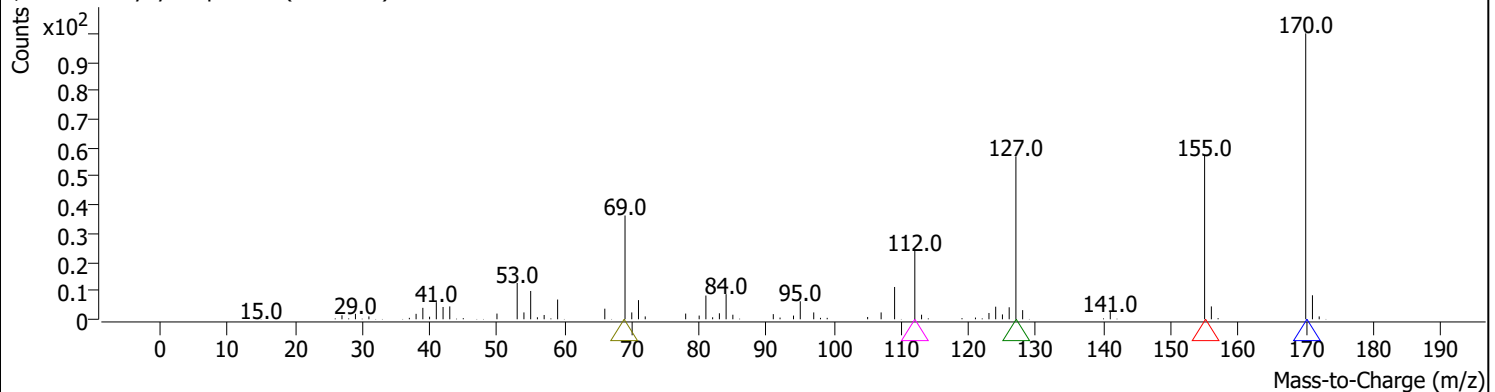
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
49.4533	2,6-Dimethoxyhydroquinone	449347.7	82.9	15233-65-5	C <sub>8</sub> H <sub>10</sub> O <sub>4</sub>	

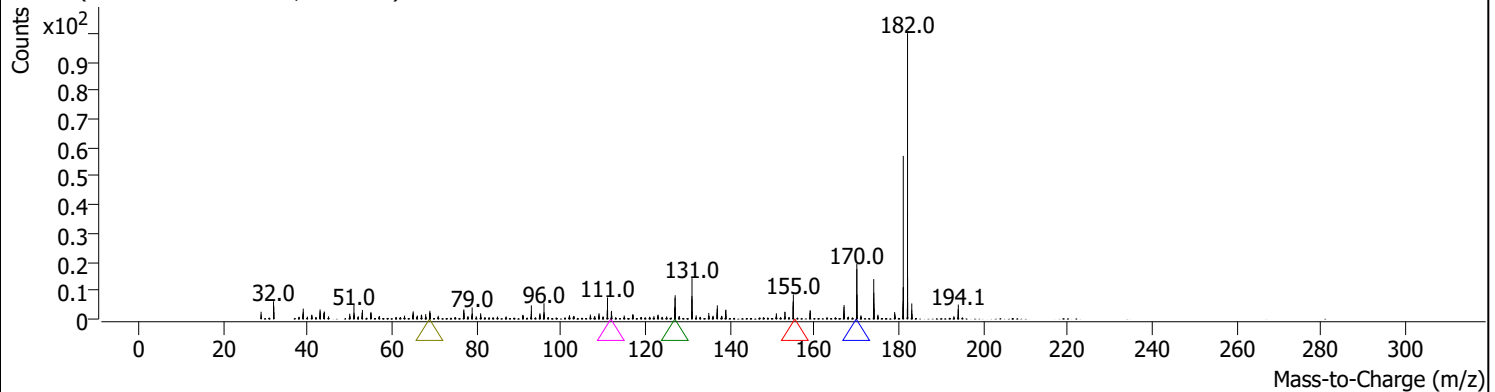
Component RT: 49.4533



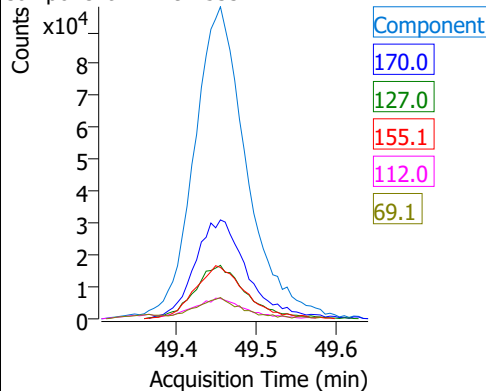
2,6-Dimethoxyhydroquinone (NIST20.L)



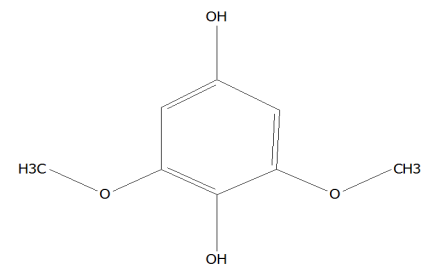
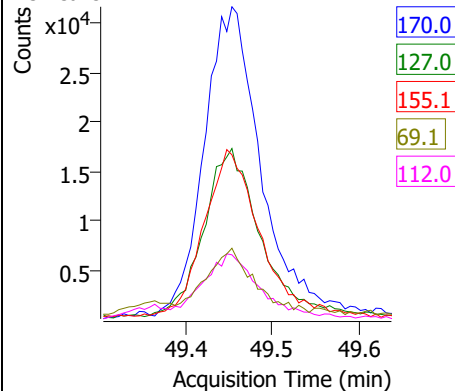
+ Scan (49.3650-49.6385 min, 47 scans) 4.D



Component RT: 49.4533



EIC Peaks



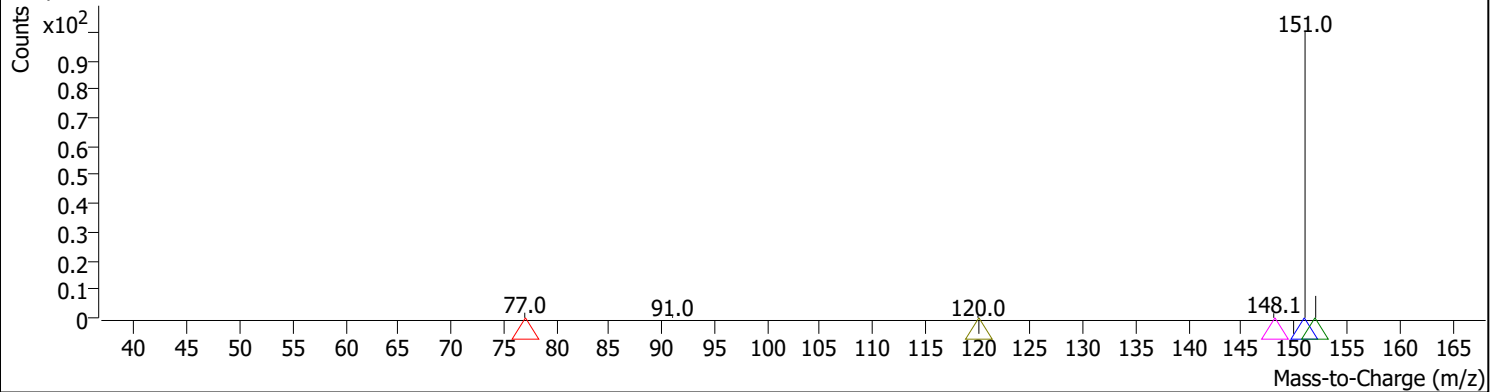
## Library Search Results - NonTarget Hits with Details



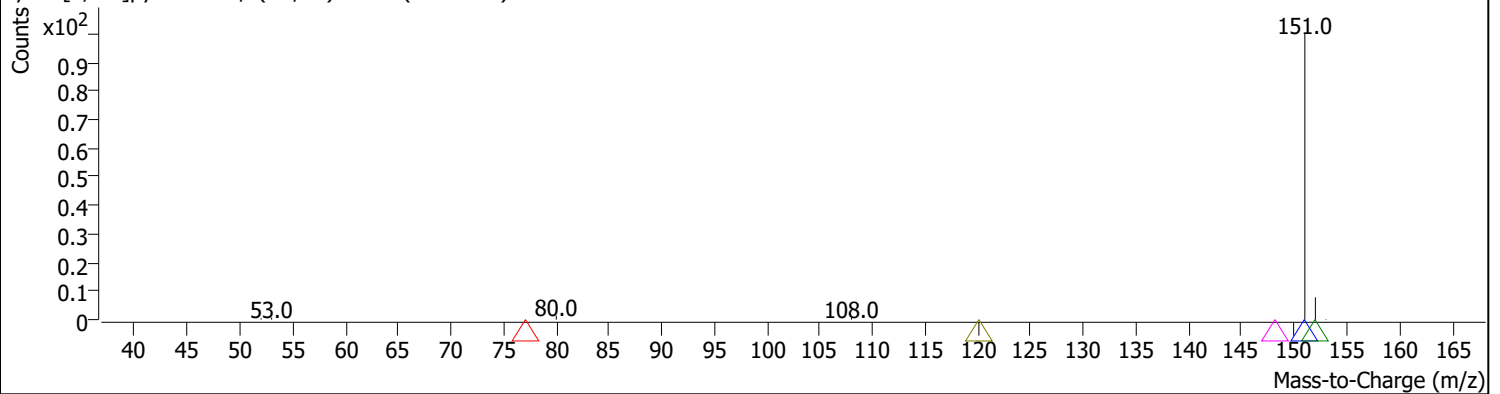
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
50.4244	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	321466.5	91.8	65996-50-1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	

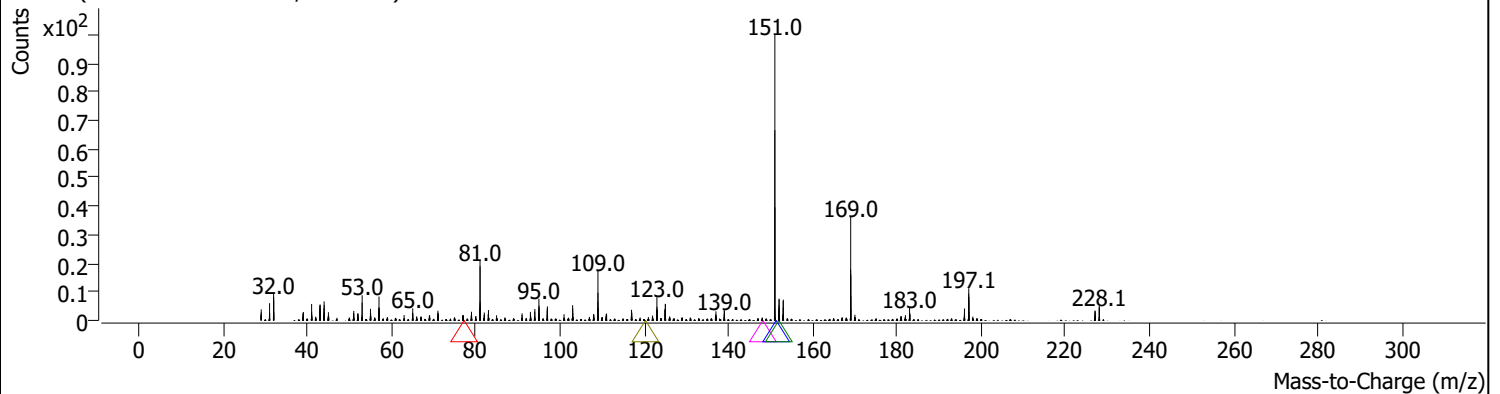
Component RT: 50.4244



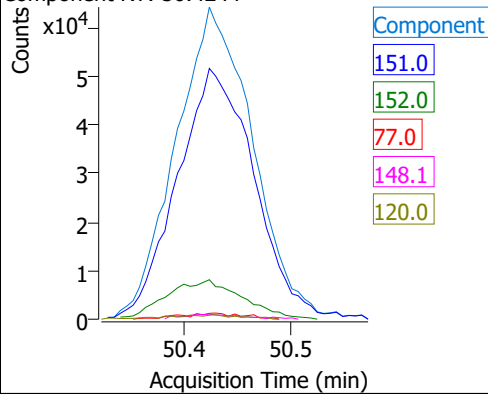
Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)



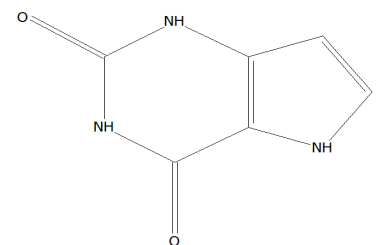
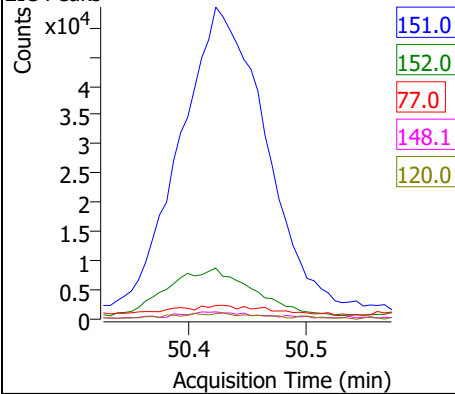
+ Scan (50.3227-50.5721 min, 42 scans) 4.D



Component RT: 50.4244



EIC Peaks



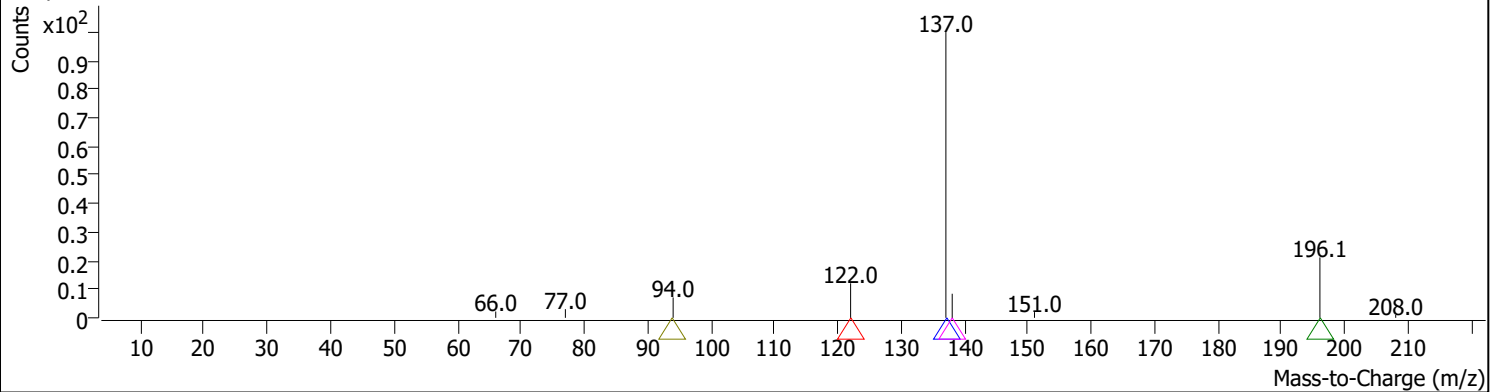
## Library Search Results - NonTarget Hits with Details



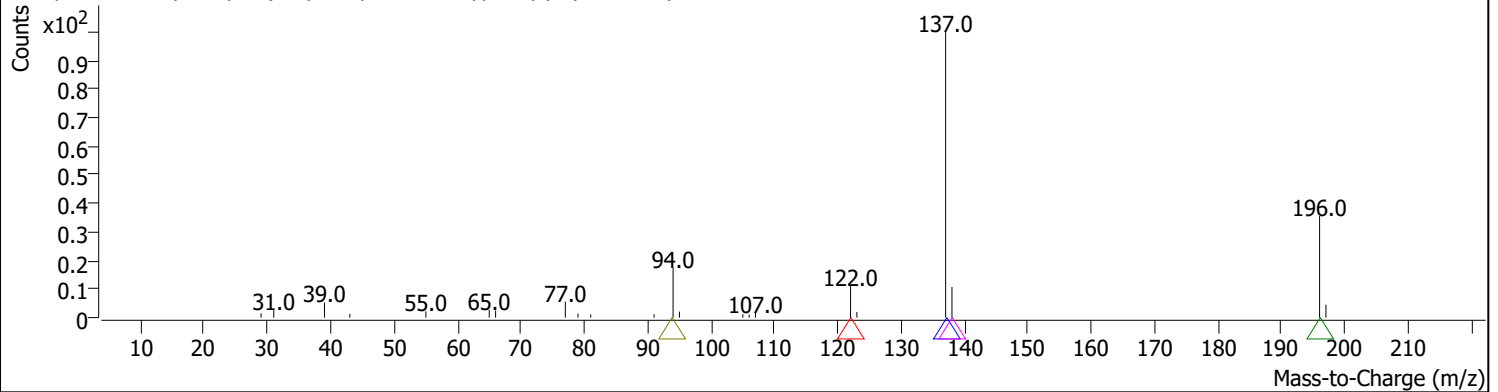
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
51.7398	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-	212350.2	89.7	4899-74-5	C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>	

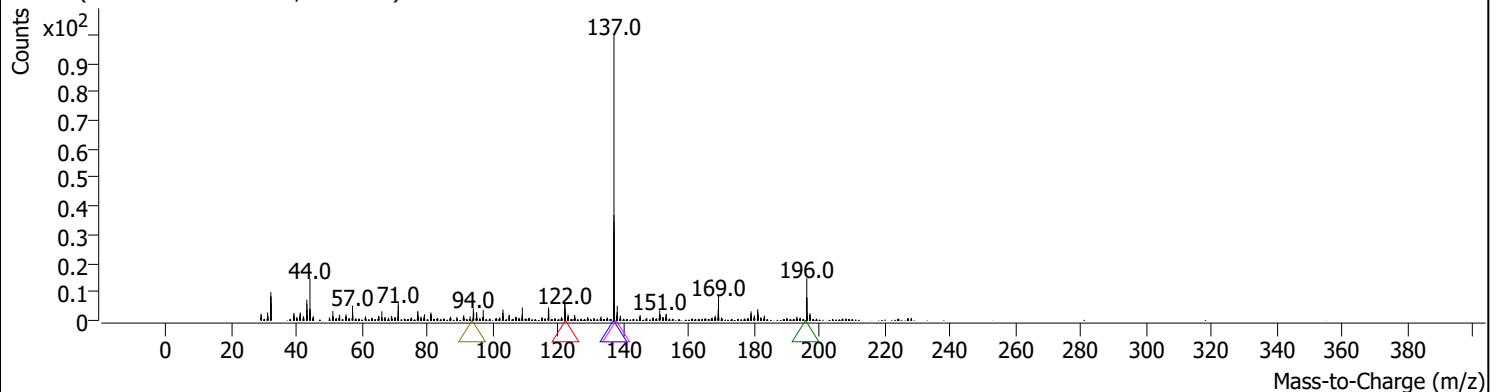
Component RT: 51.7398



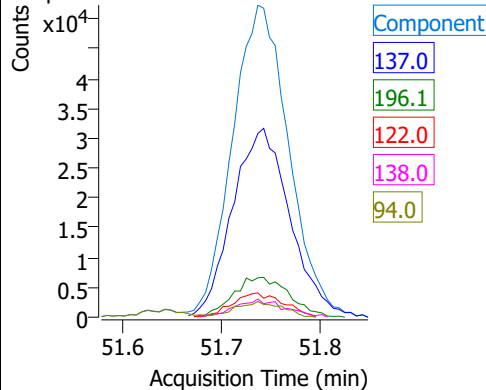
2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)- (NIST20.L)



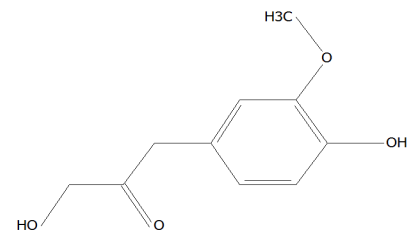
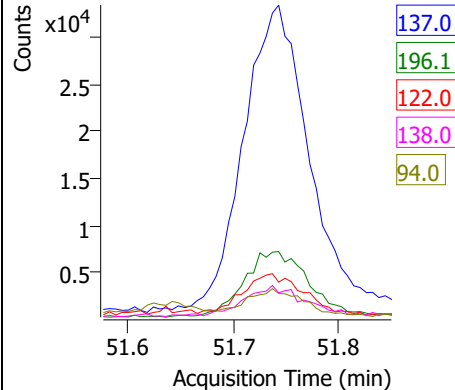
+ Scan (51.6671-51.8304 min, 27 scans) 4.D



Component RT: 51.7398



EIC Peaks





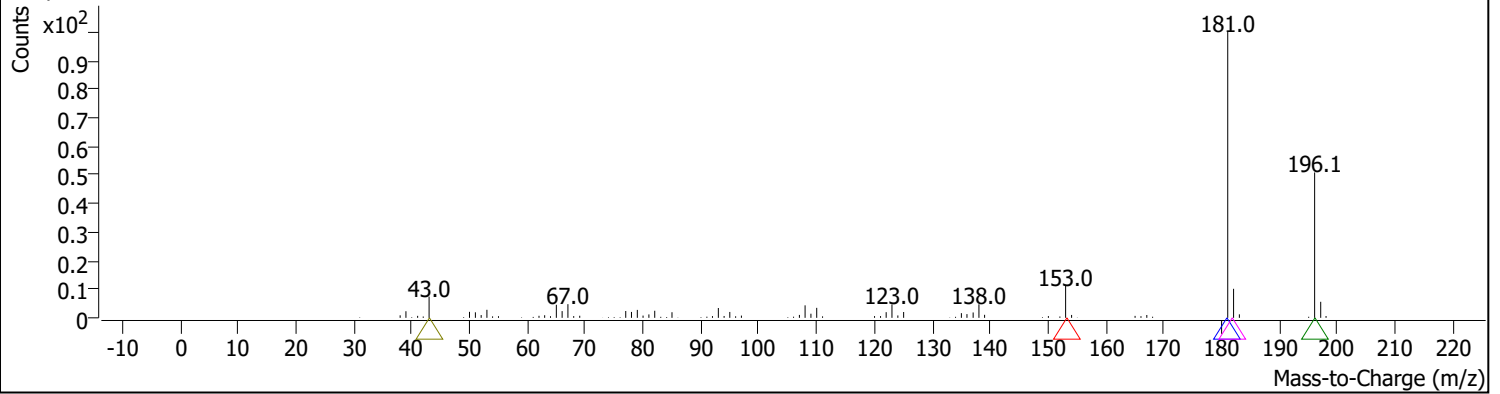
## Library Search Results - NonTarget Hits with Details



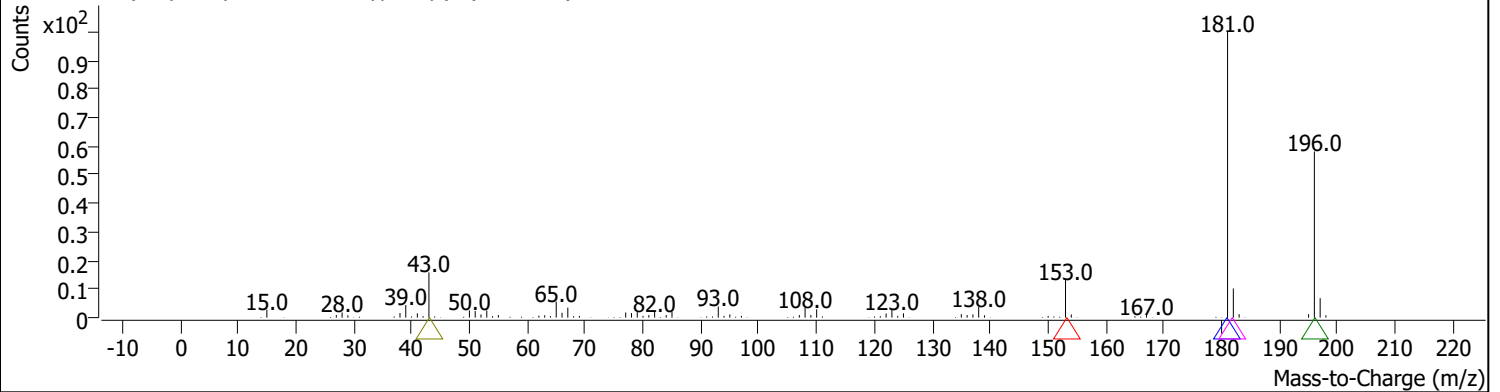
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
52.0014	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	5359990.6	98.5	2478-38-8	C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>	

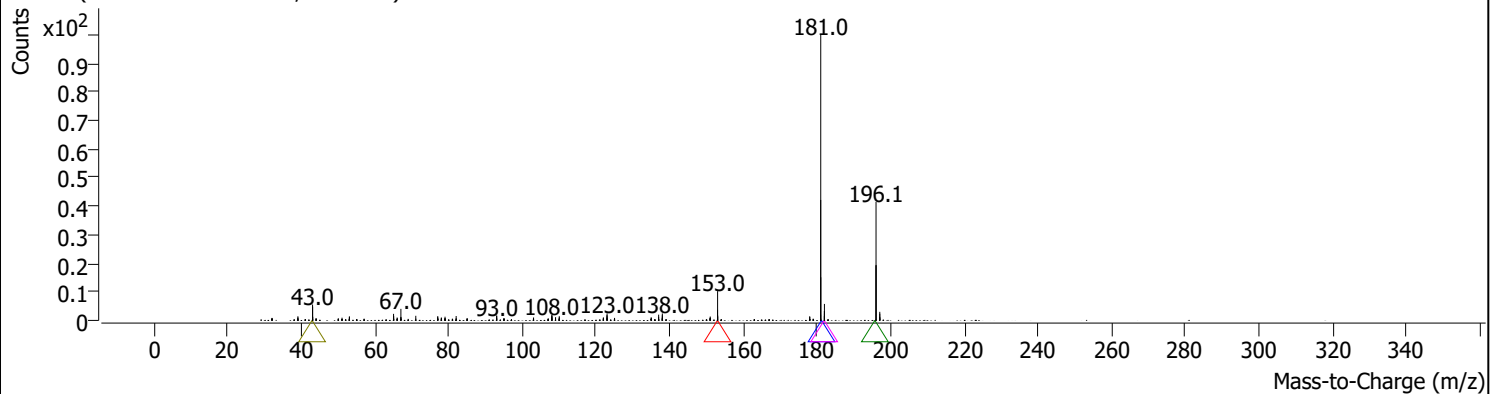
Component RT: 52.0014



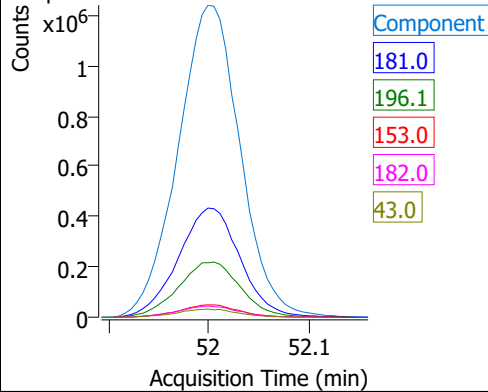
Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)- (NIST20.L)



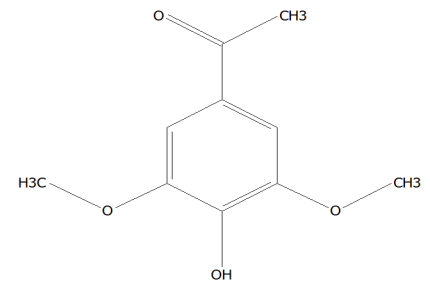
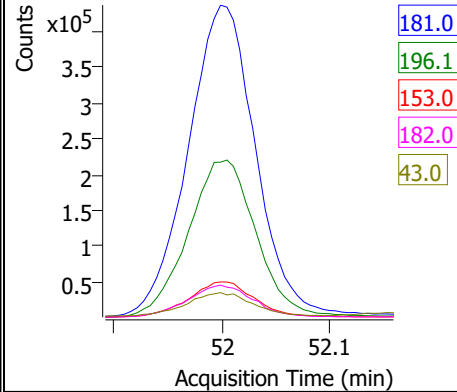
+ Scan (51.8921-52.1533 min, 44 scans) 4.D



Component RT: 52.0014



EIC Peaks



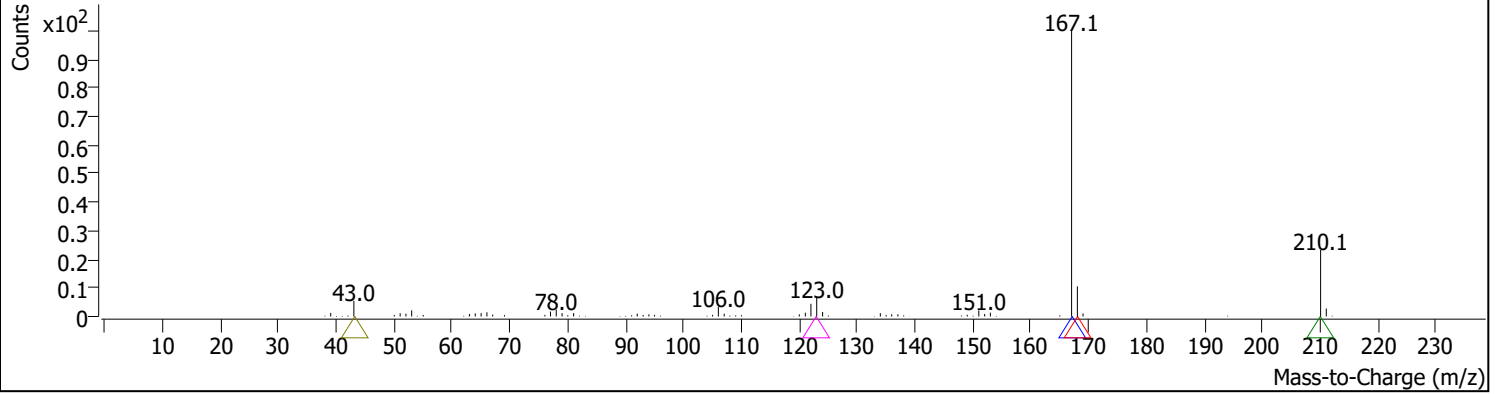
## Library Search Results - NonTarget Hits with Details



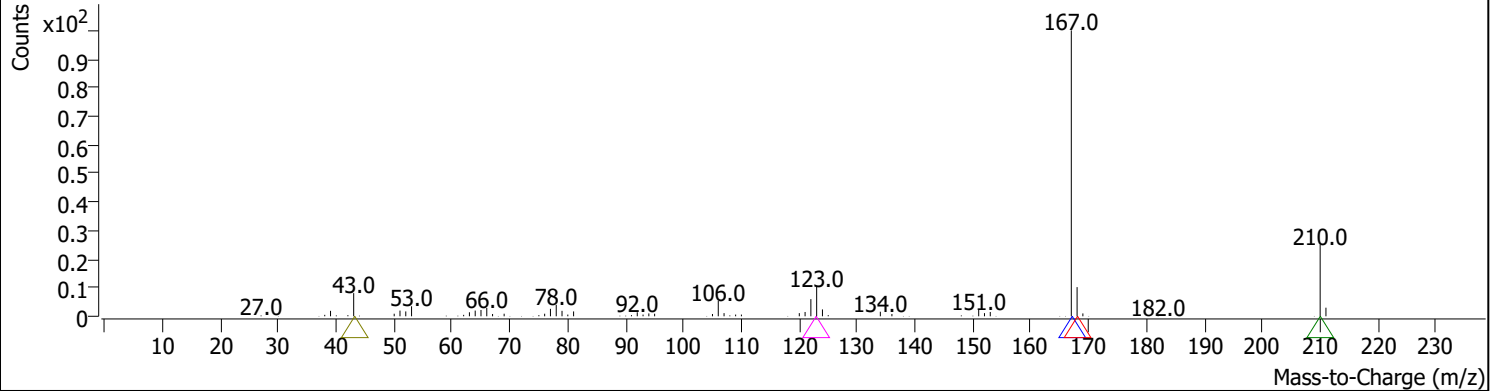
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
53.2410	Syringylacetone	4823009.2	97.3	19037-58-2	C <sub>11</sub> H <sub>14</sub> O <sub>4</sub>	

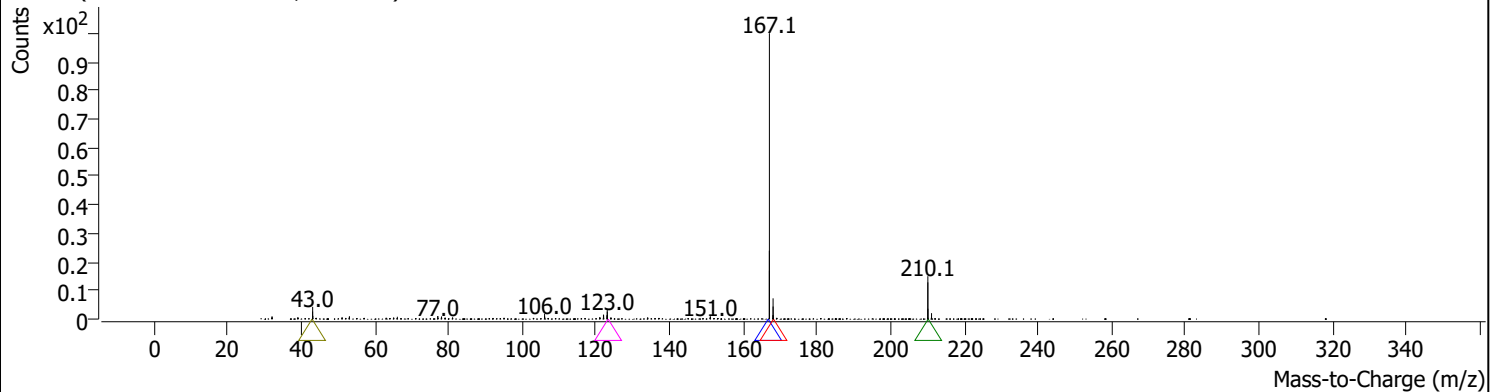
Component RT: 53.2410



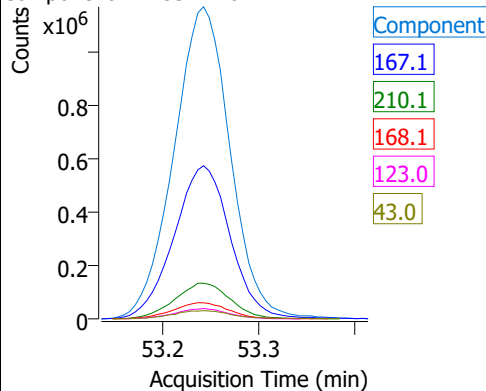
Syringylacetone (NIST20.L)



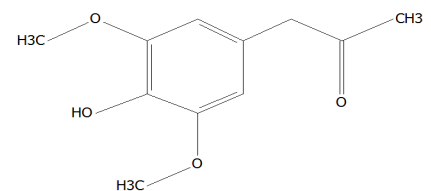
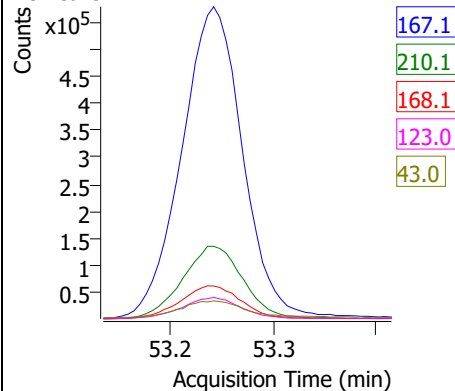
+ Scan (53.1348-53.4143 min, 48 scans) 4.D



Component RT: 53.2410



EIC Peaks



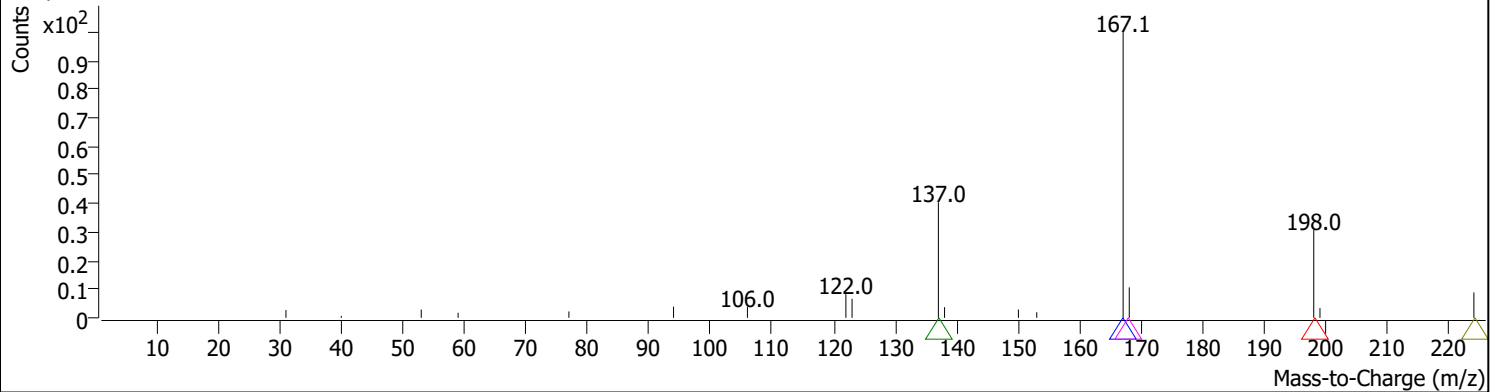
## Library Search Results - NonTarget Hits with Details



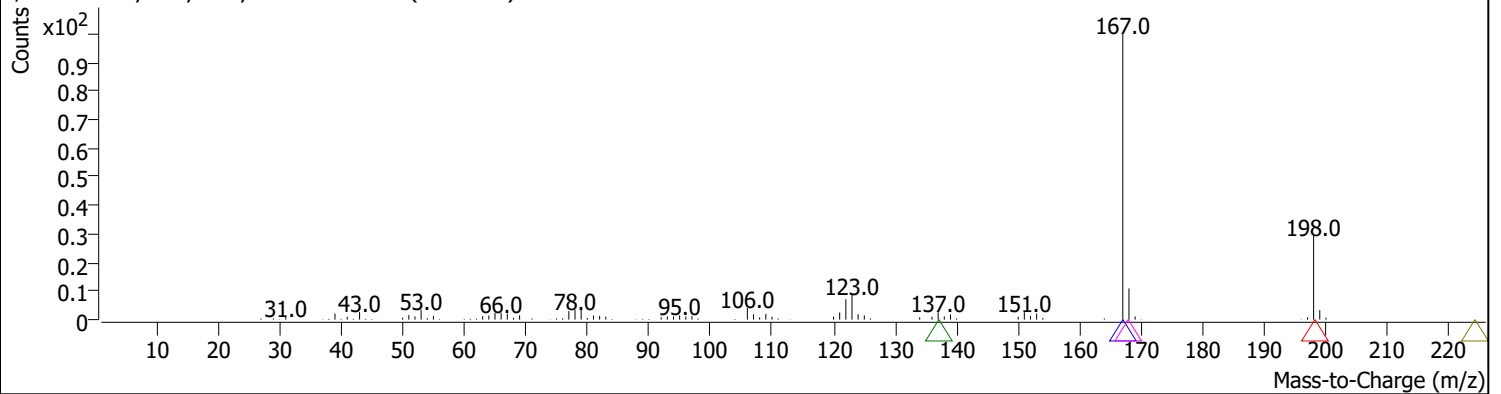
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
53.6141	3,5-Dimethoxy-4-hydroxybenzeneethanol	276859.3	75.6	20824-45-7	C10H14O4	

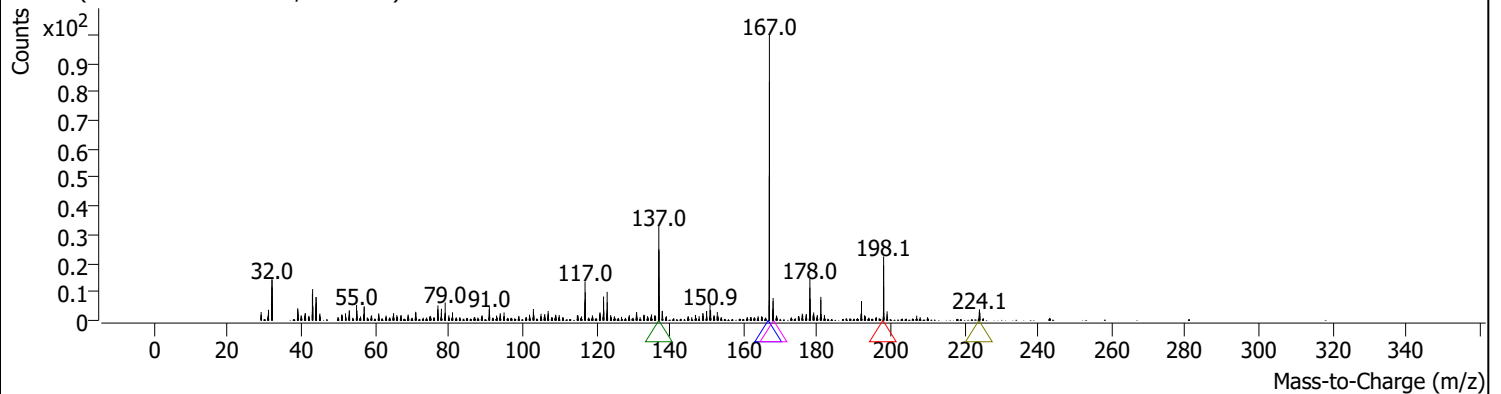
Component RT: 53.6141



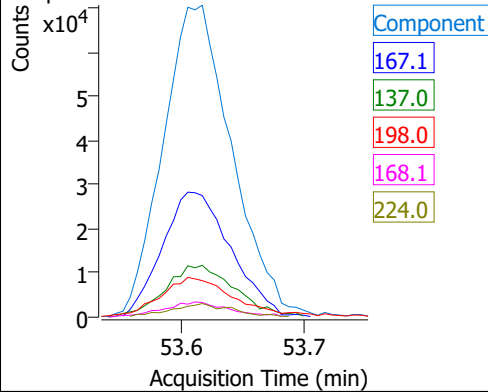
3,5-Dimethoxy-4-hydroxybenzeneethanol (NIST20.L)



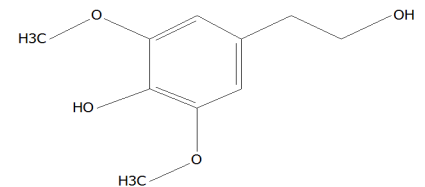
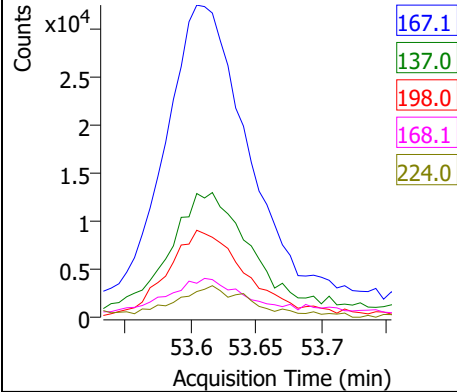
+ Scan (53.5479-53.7099 min, 27 scans) 4.D



Component RT: 53.6141



EIC Peaks



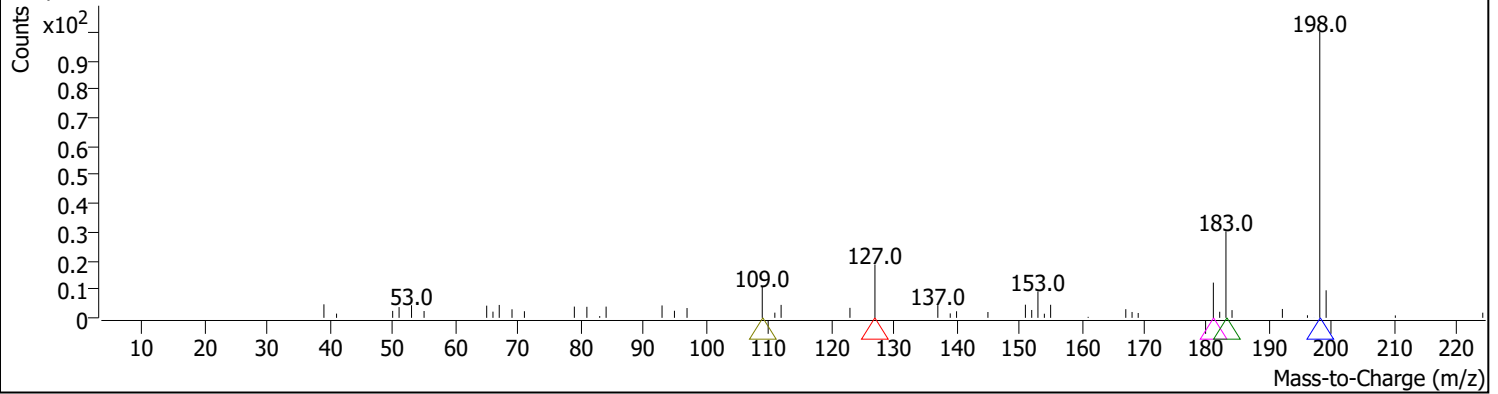
## Library Search Results - NonTarget Hits with Details



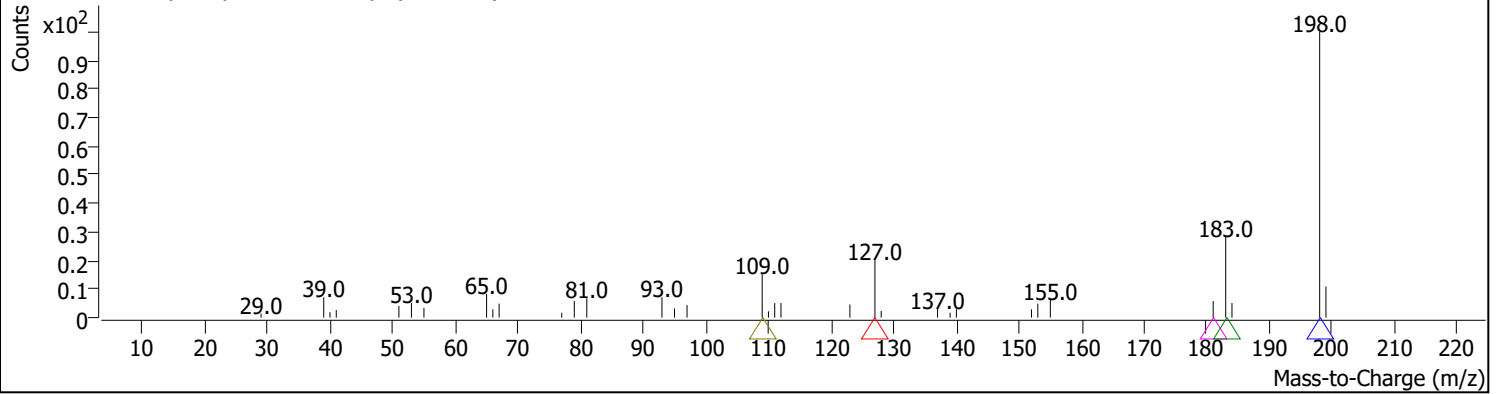
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
54.9715	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	733657.1	88.0	530-57-4	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	

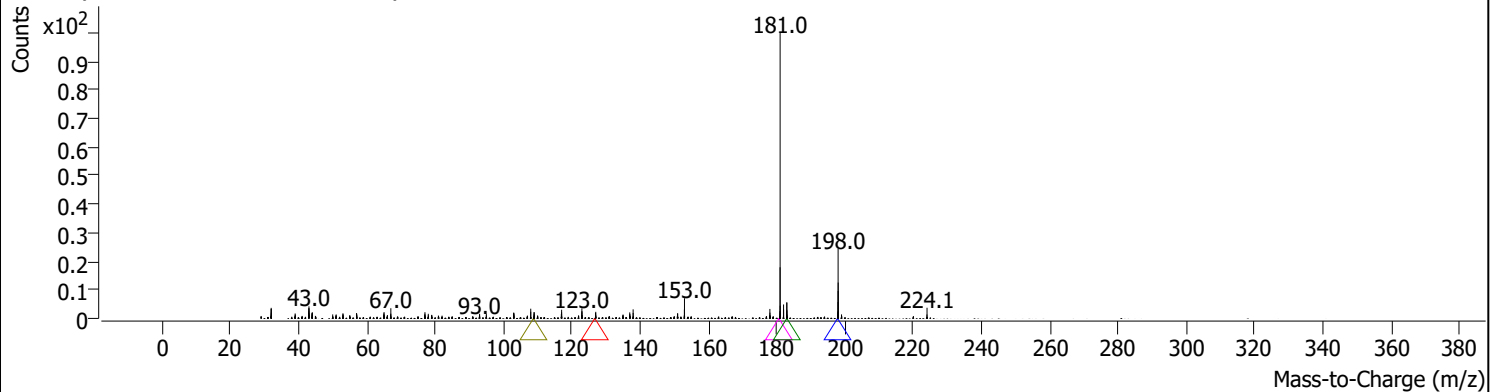
Component RT: 54.9715



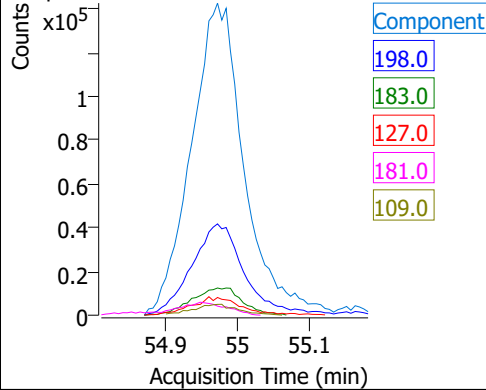
Benzoic acid, 4-hydroxy-3,5-dimethoxy- (NIST20.L)



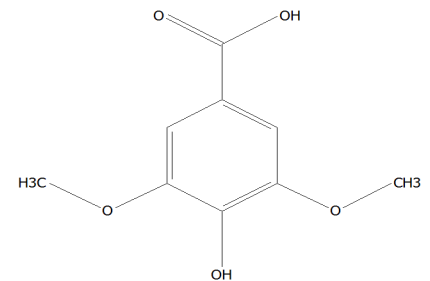
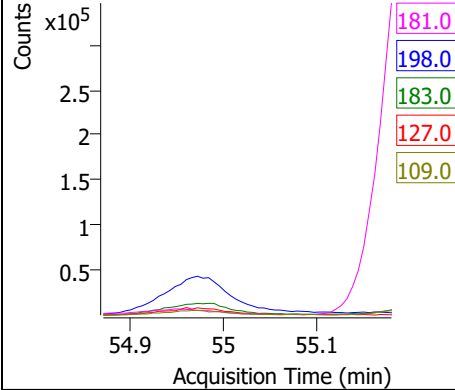
+ Scan (54.8657-55.1802 min, 53 scans) 4.D



Component RT: 54.9715



EIC Peaks



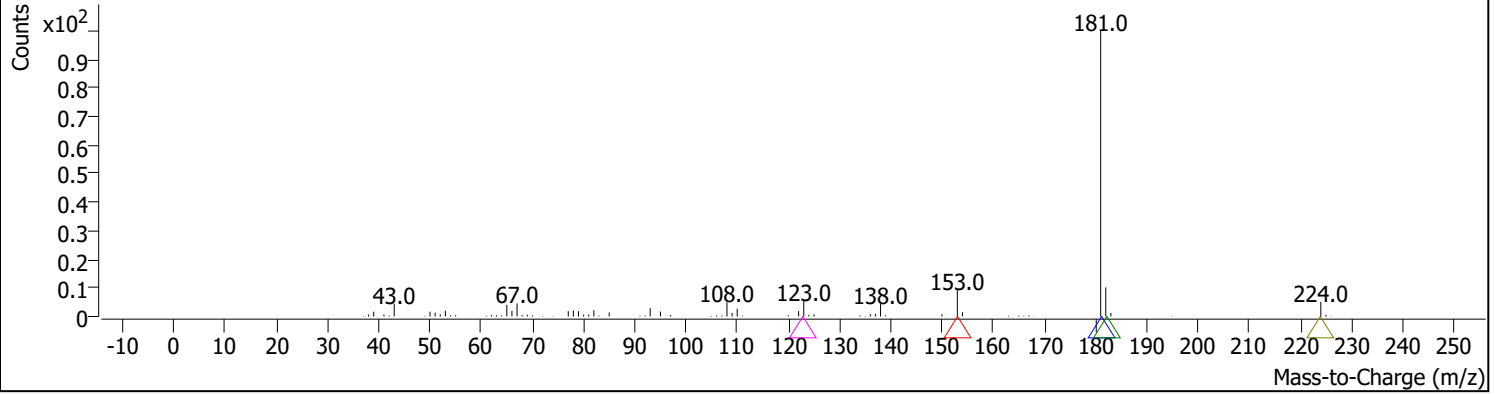
## Library Search Results - NonTarget Hits with Details



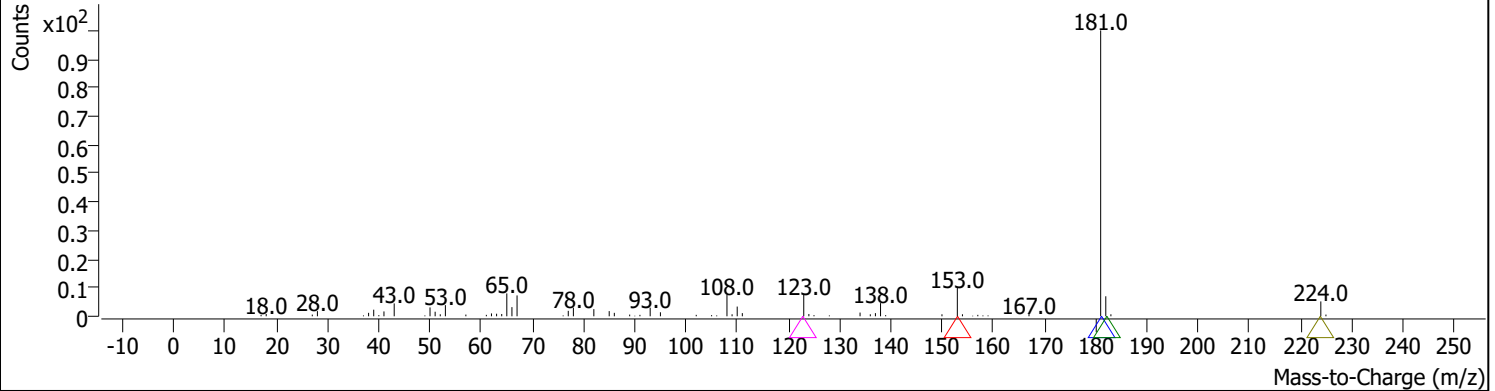
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
55.2057	Butylsyringone	4574151.5	93.0	69271-91-6	C <sub>12</sub> H <sub>16</sub> O <sub>4</sub>	

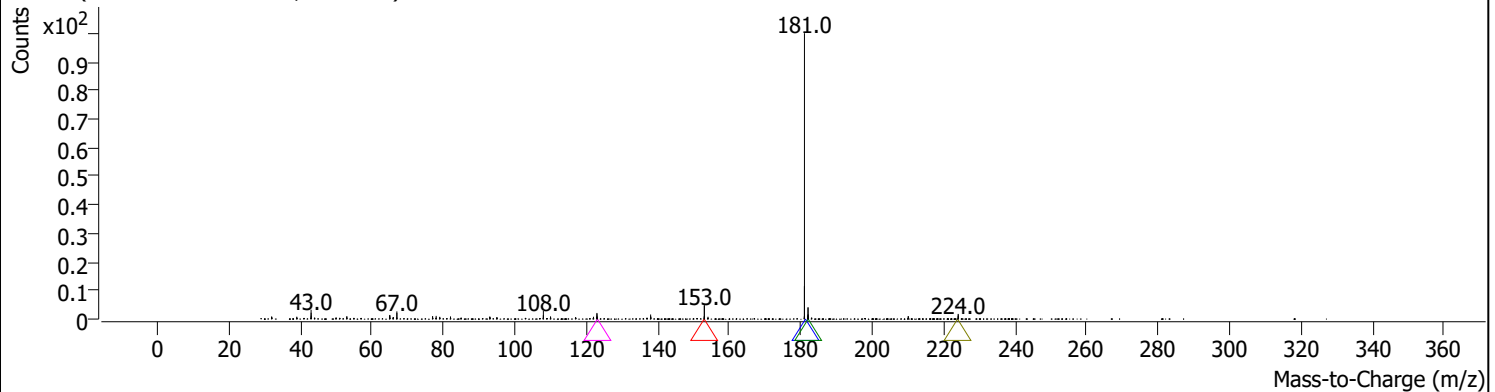
Component RT: 55.2057



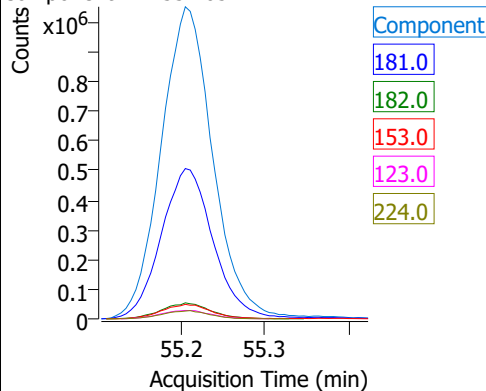
Butylsyringone (NIST20.L)



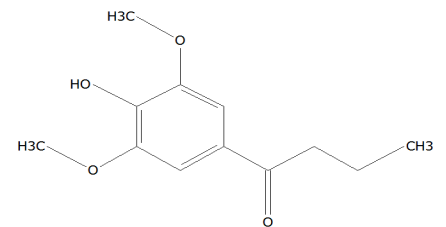
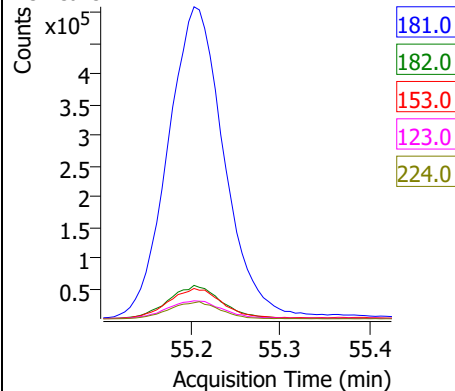
+ Scan (55.1029-55.4240 min, 55 scans) 4.D



Component RT: 55.2057



EIC Peaks



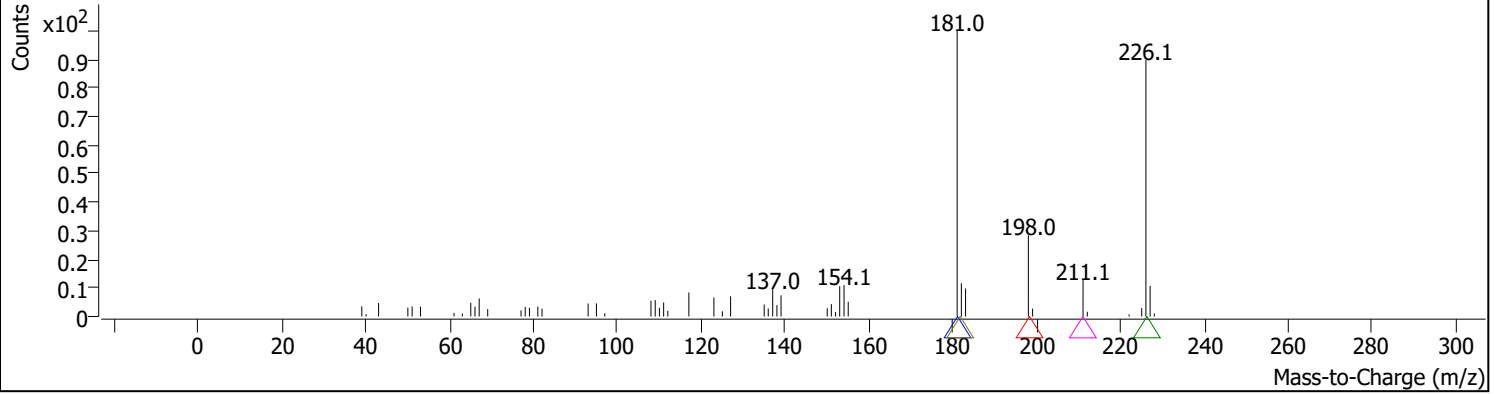
## Library Search Results - NonTarget Hits with Details



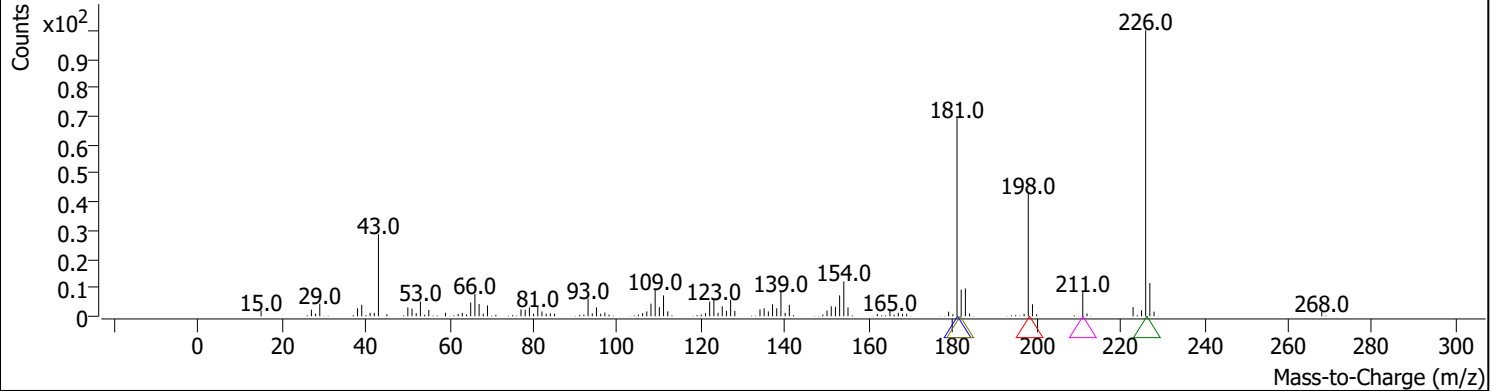
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
55.6221	Acetyl syringic acid, ethyl ester	700159.4	89.0	1000454-70-9	C <sub>13</sub> H <sub>16</sub> O <sub>6</sub>	

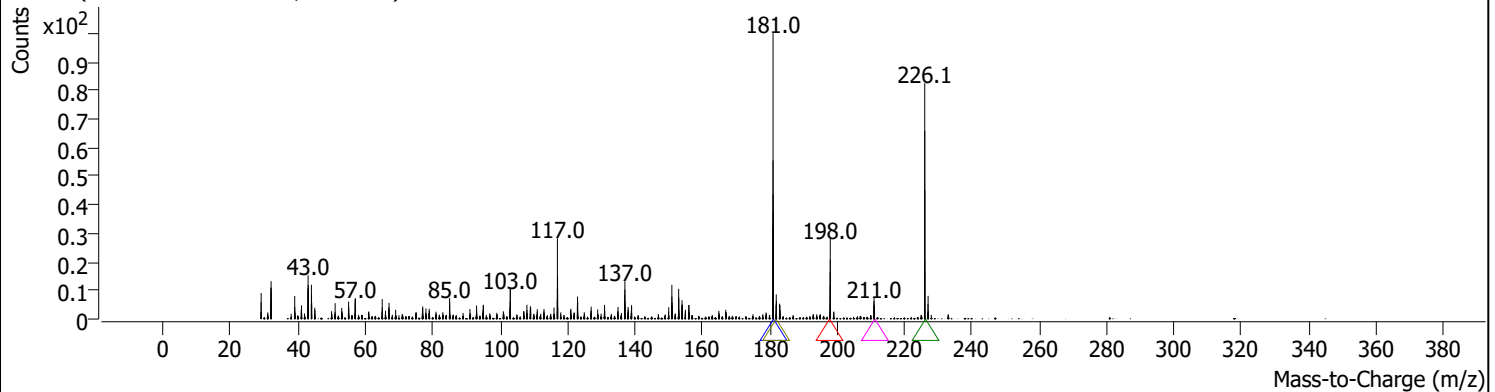
Component RT: 55.6221



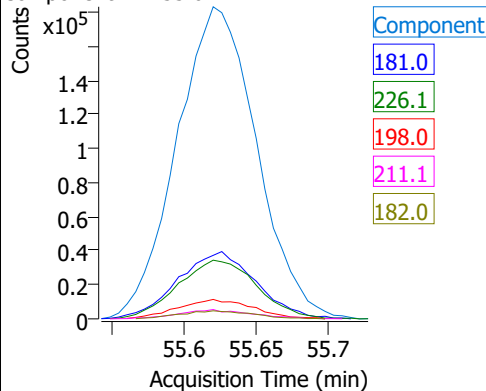
Acetyl syringic acid, ethyl ester (NIST20.L)



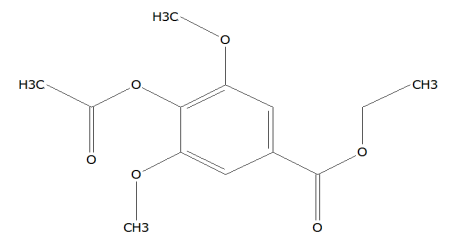
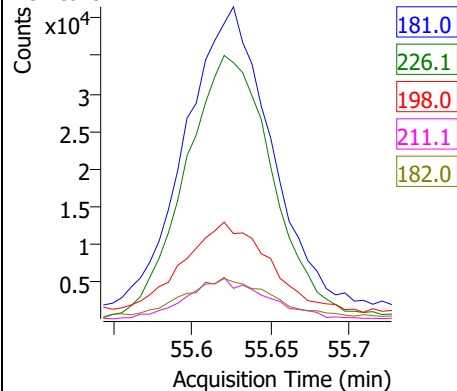
+ Scan (55.5440-55.7313 min, 31 scans) 4.D



Component RT: 55.6221



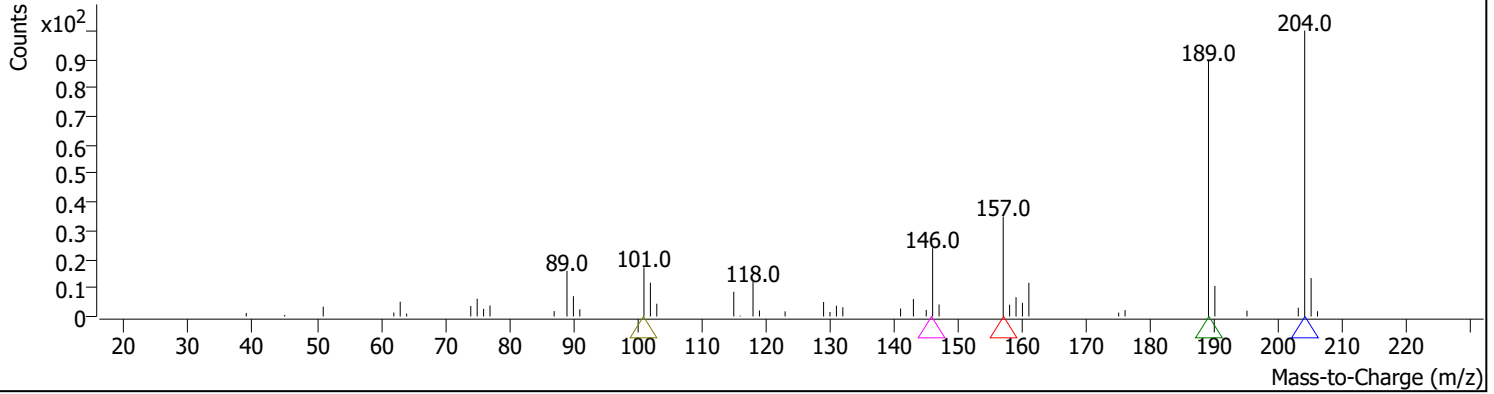
EIC Peaks



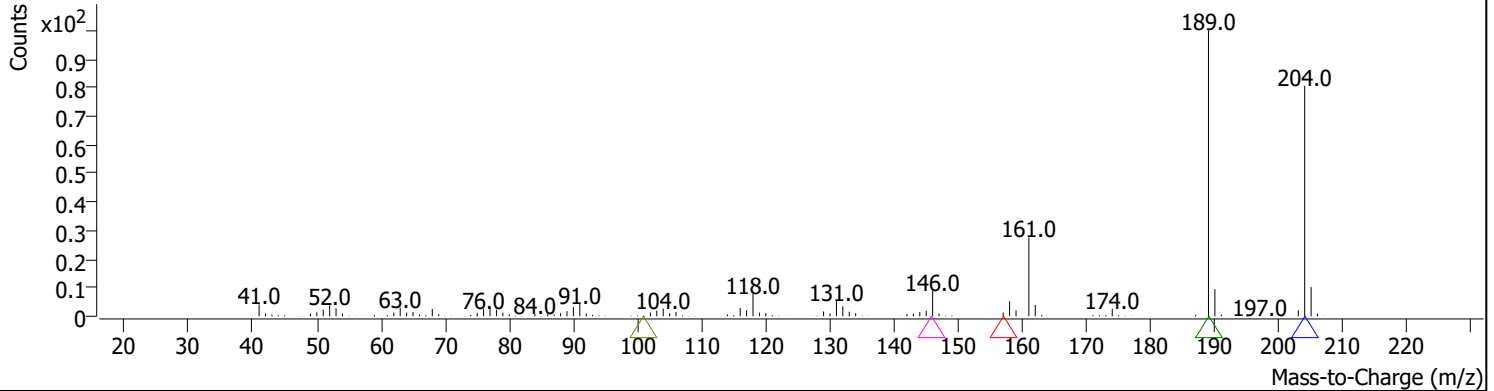
# Library Search Results - NonTarget Hits with Details

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
56.0995	2,3-Dimethoxy-5-aminocinnamionitrile	712035.6	79.3	1000214-46-5	C11H12N2O2	

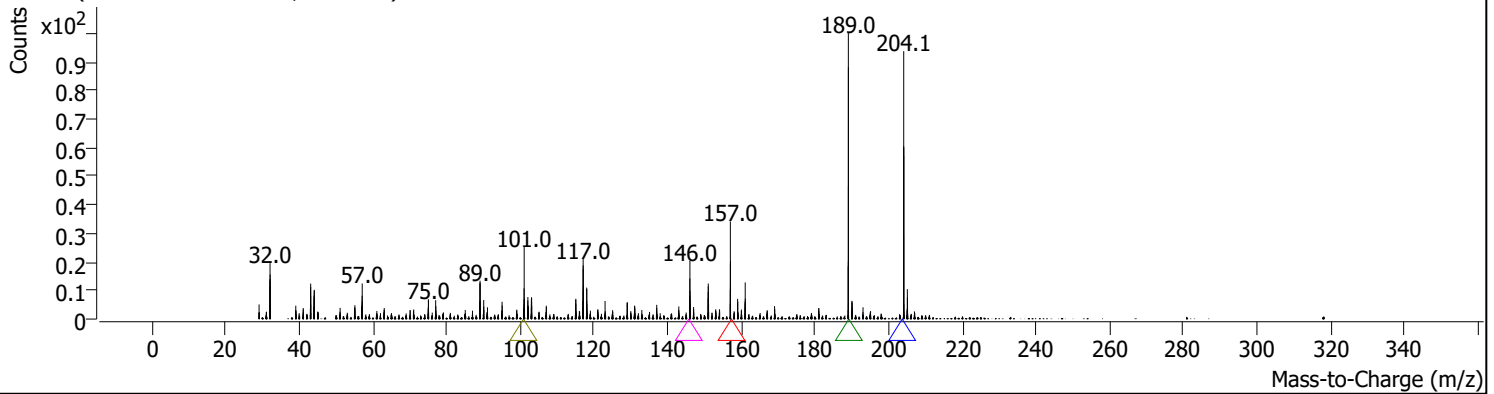
Component RT: 56.0995



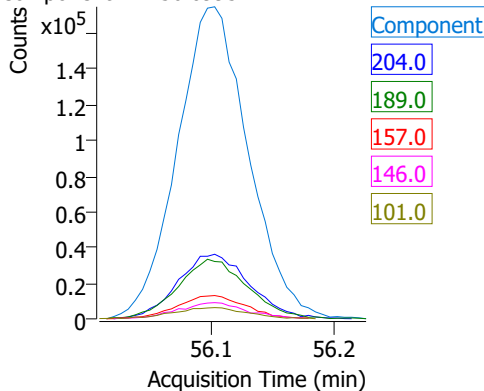
2,3-Dimethoxy-5-aminocinnamionitrile (NIST20.L)



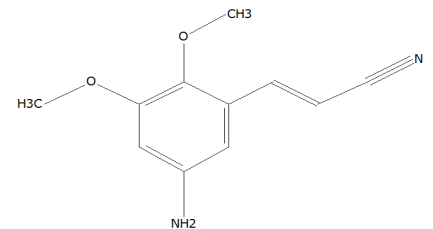
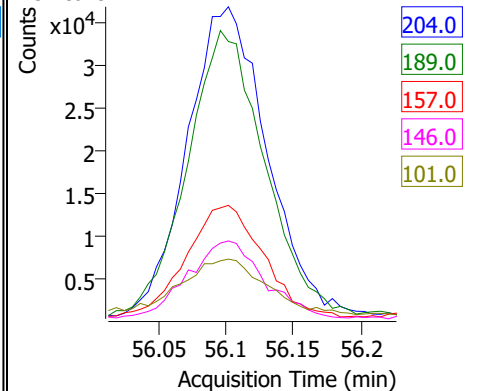
+ Scan (56.0186-56.2148 min, 34 scans) 4.D



Component RT: 56.0995



EIC Peaks



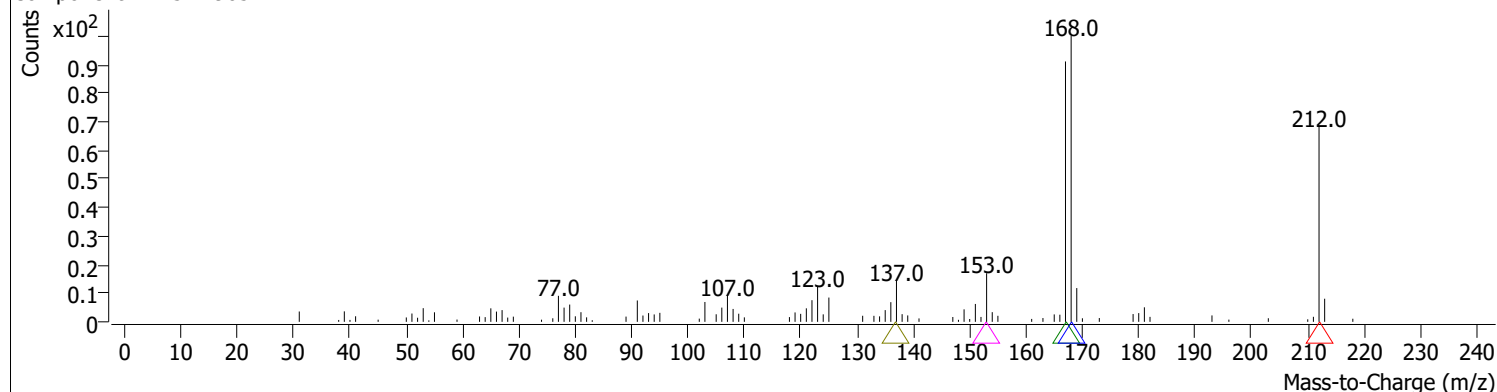
## Library Search Results - NonTarget Hits with Details



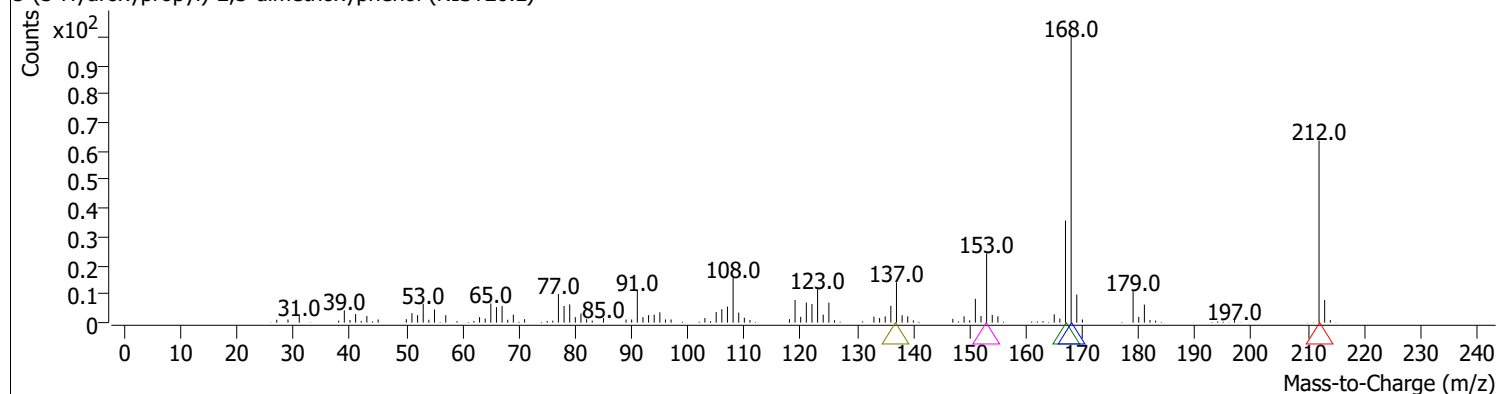
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
57.4905	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	1812481.3	92.3	63543-12-4	C <sub>11</sub> H <sub>16</sub> O <sub>4</sub>	

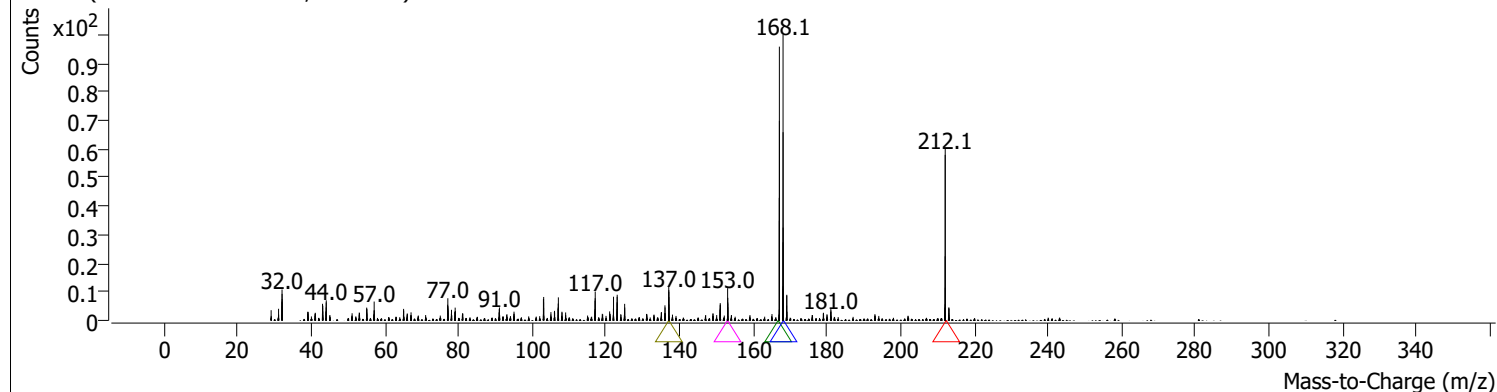
Component RT: 57.4905



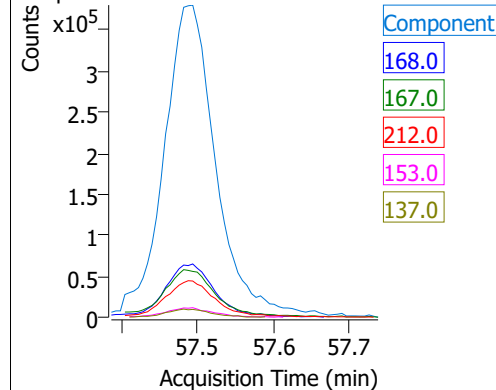
5-(3-Hydroxypropyl)-2,3-dimethoxyphenol (NIST20.L)



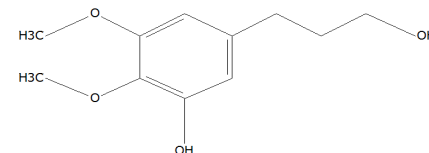
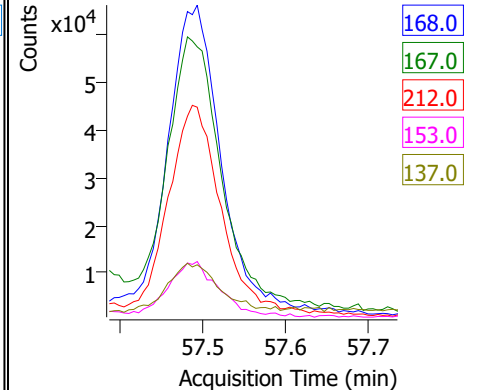
+ Scan (57.3862-57.6657 min, 48 scans) 4.D



Component RT: 57.4905



EIC Peaks





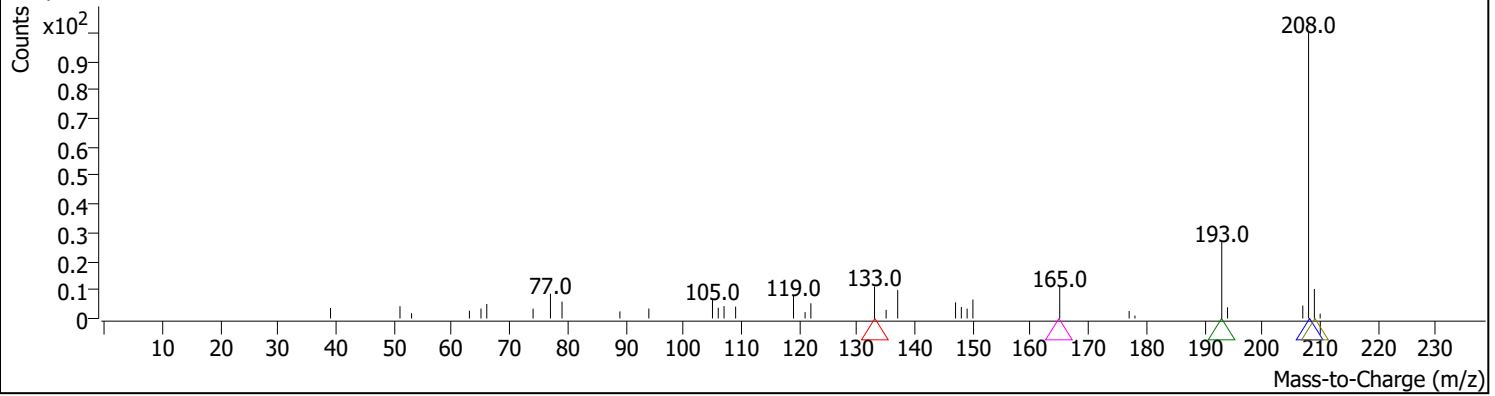
## Library Search Results - NonTarget Hits with Details



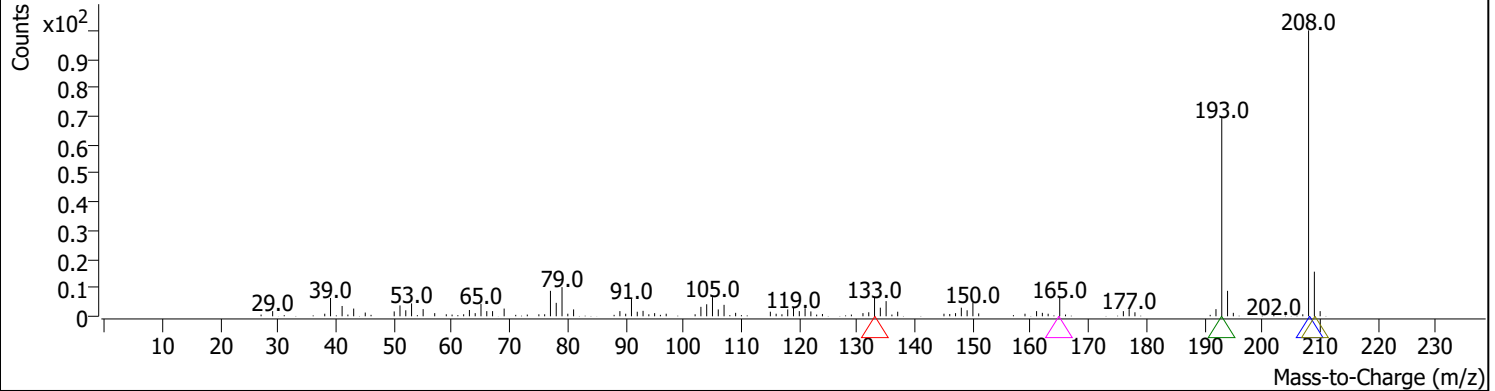
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
58.8309	Isoelemicin	404594.3	77.8	487-12-7	C <sub>12</sub> H <sub>16</sub> O <sub>3</sub>	

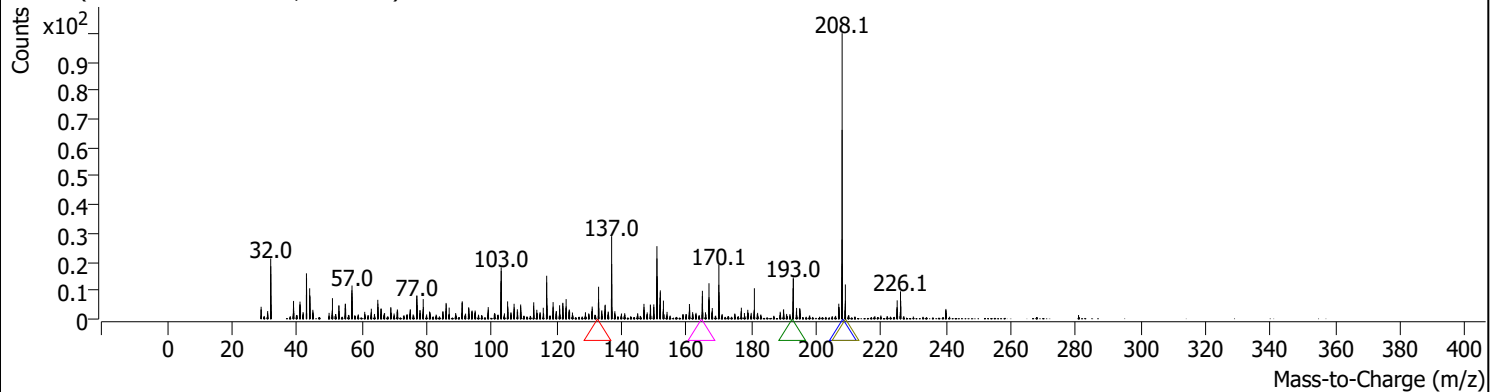
Component RT: 58.8309



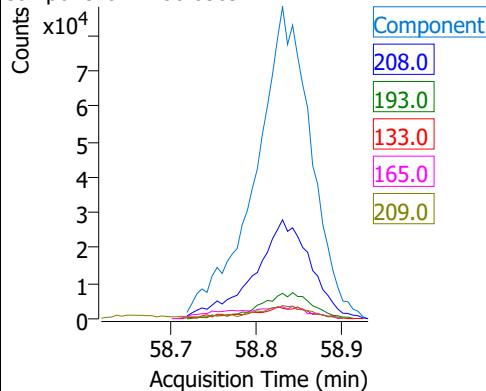
Isoelemicin (NIST20.L)



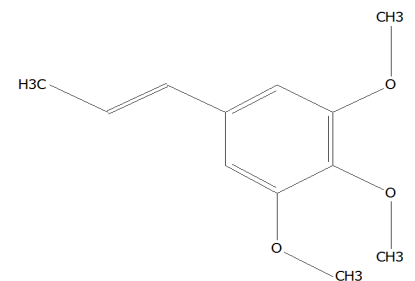
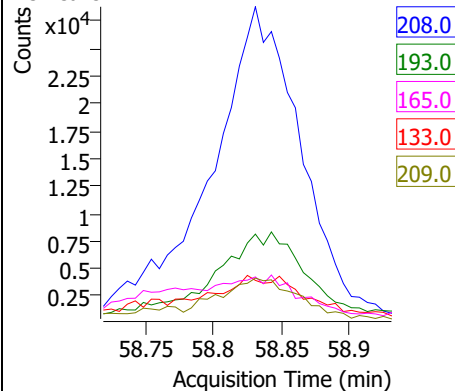
+ Scan (58.7181-58.9322 min, 37 scans) 4.D



Component RT: 58.8309



EIC Peaks



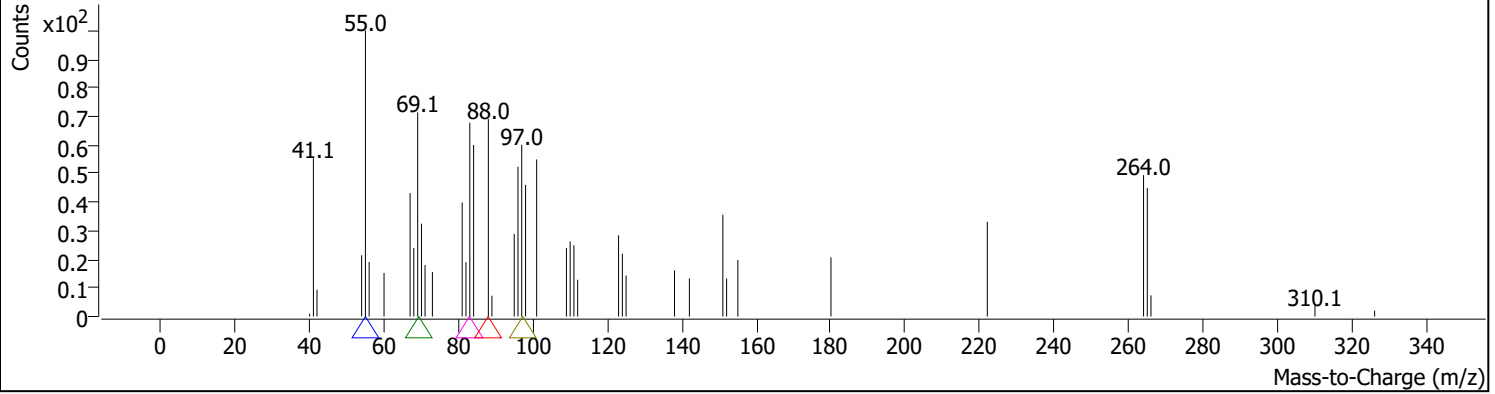
## Library Search Results - NonTarget Hits with Details



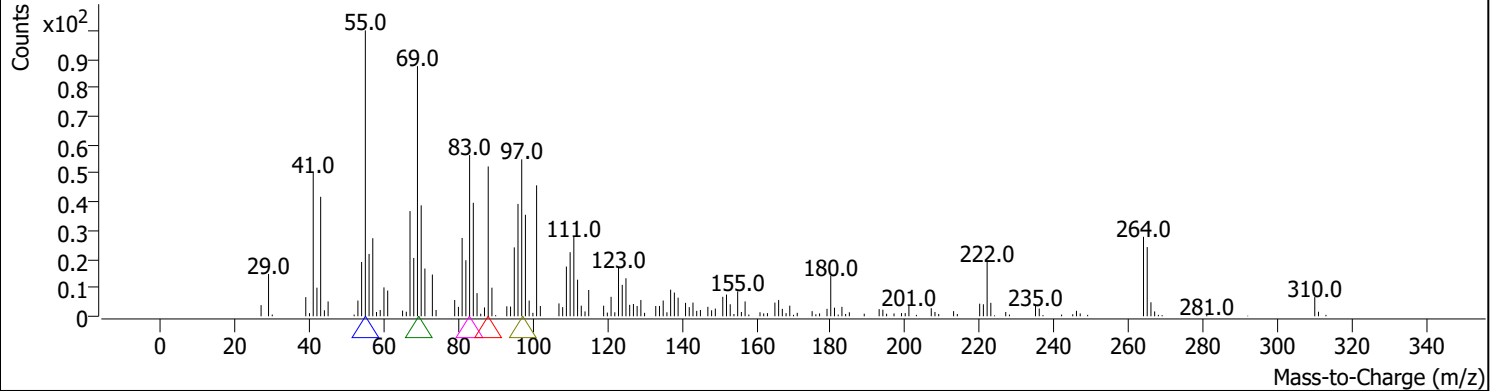
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
66.3332	(E)-9-Octadecenoic acid ethyl ester	421940.8	78.5	6114-18-7	C20H38O2	

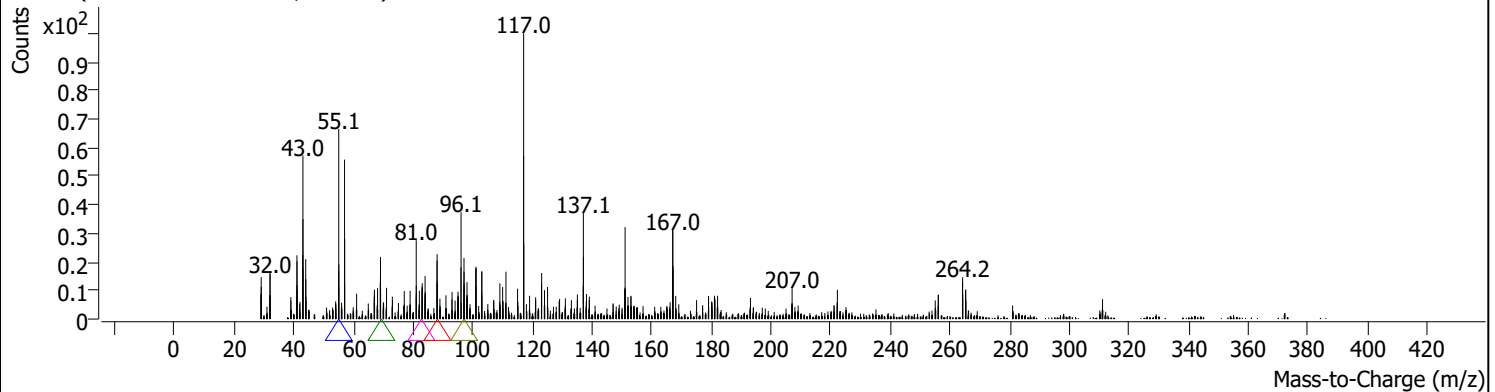
Component RT: 66.3332



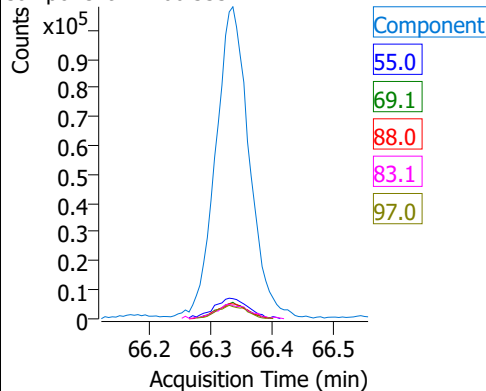
(E)-9-Octadecenoic acid ethyl ester (NIST20.L)



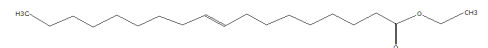
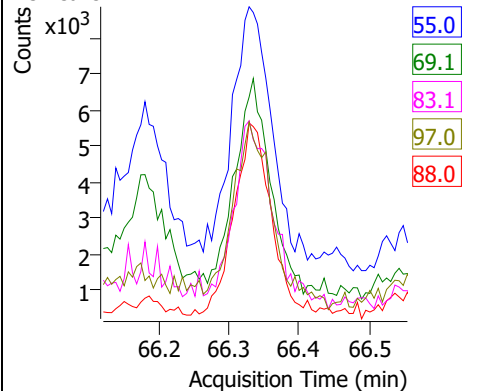
+ Scan (66.3252-66.3695 min, 7 scans) 4.D



Component RT: 66.3332



EIC Peaks



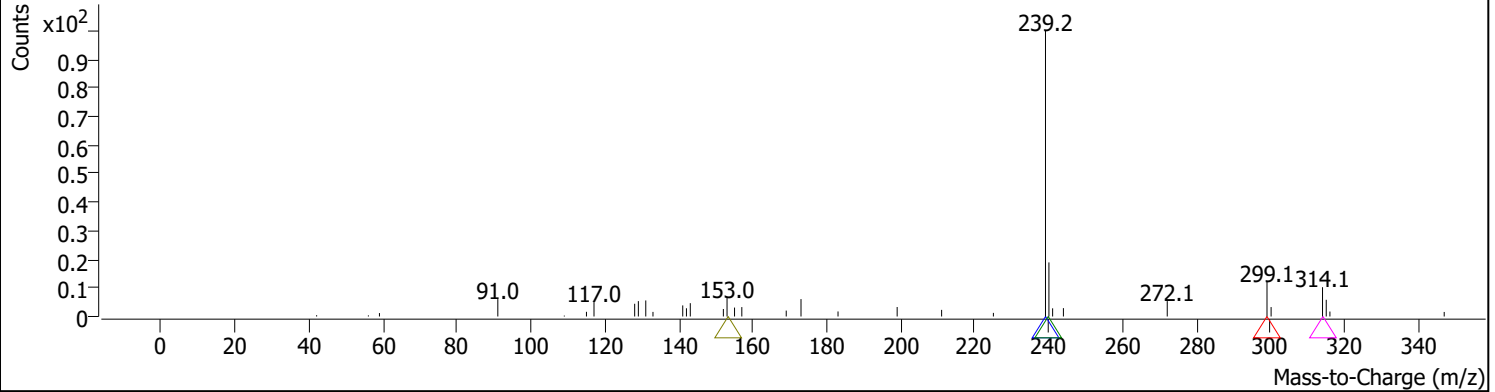
## Library Search Results - NonTarget Hits with Details



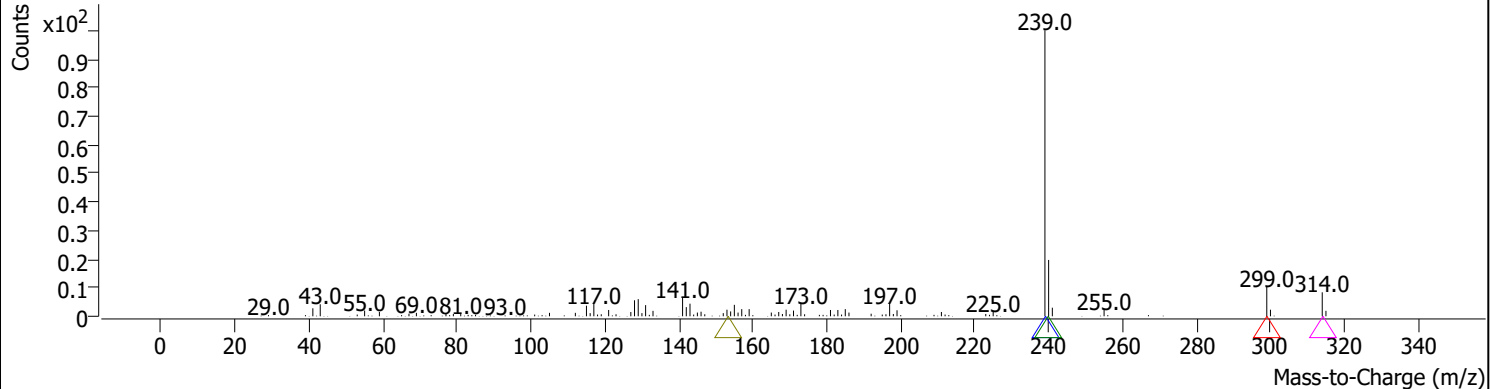
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
70.9223	Methyl dehydroabietate	359827.9	75.8	1235-74-1	C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>	

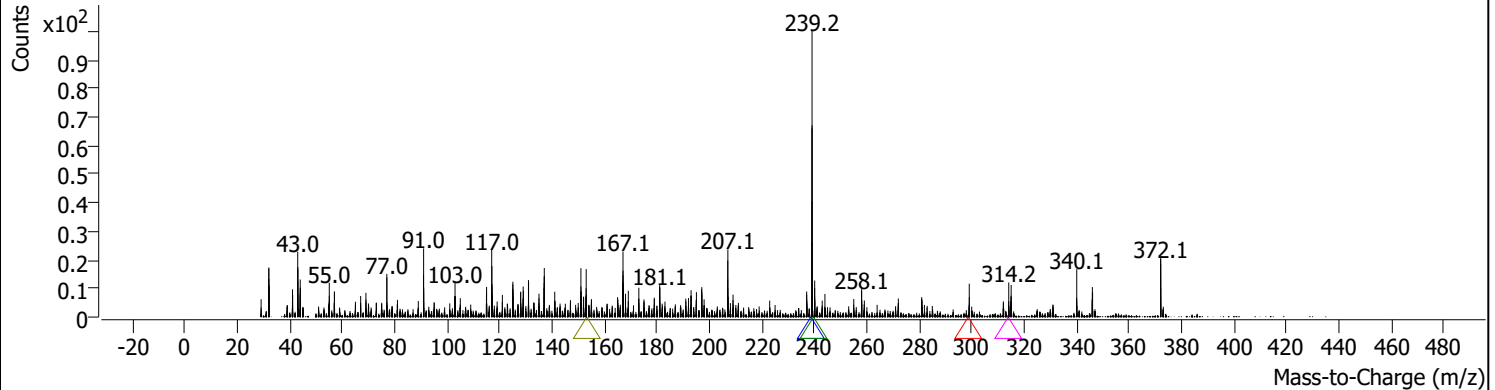
Component RT: 70.9223



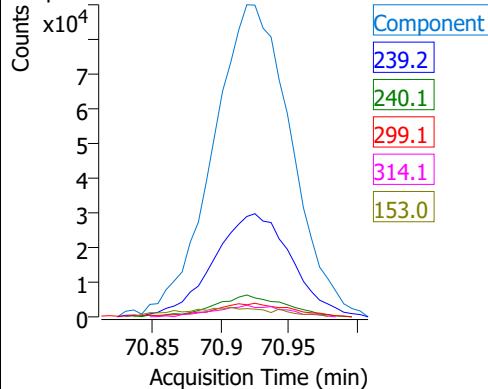
Methyl dehydroabietate (NIST20.L)



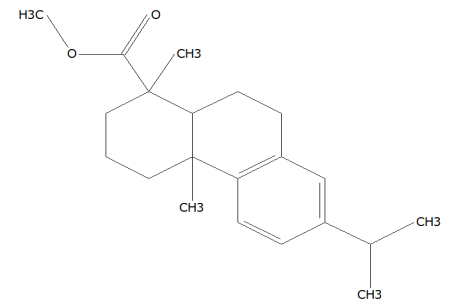
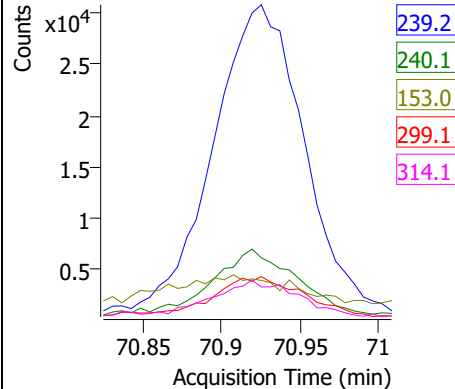
+ Scan (70.8243-71.0086 min, 31 scans) 4.D



Component RT: 70.9223



EIC Peaks



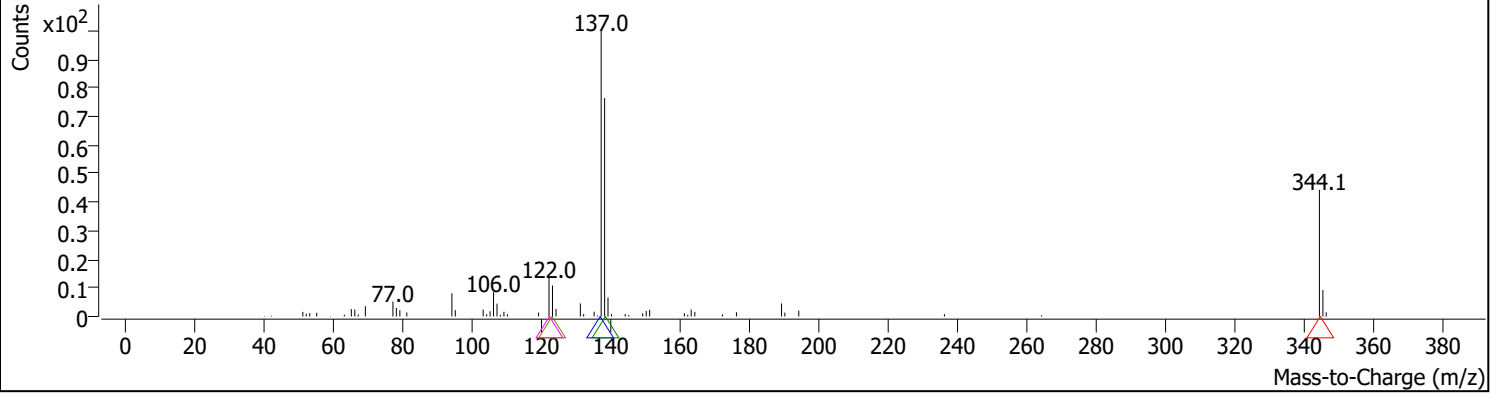
## Library Search Results - NonTarget Hits with Details



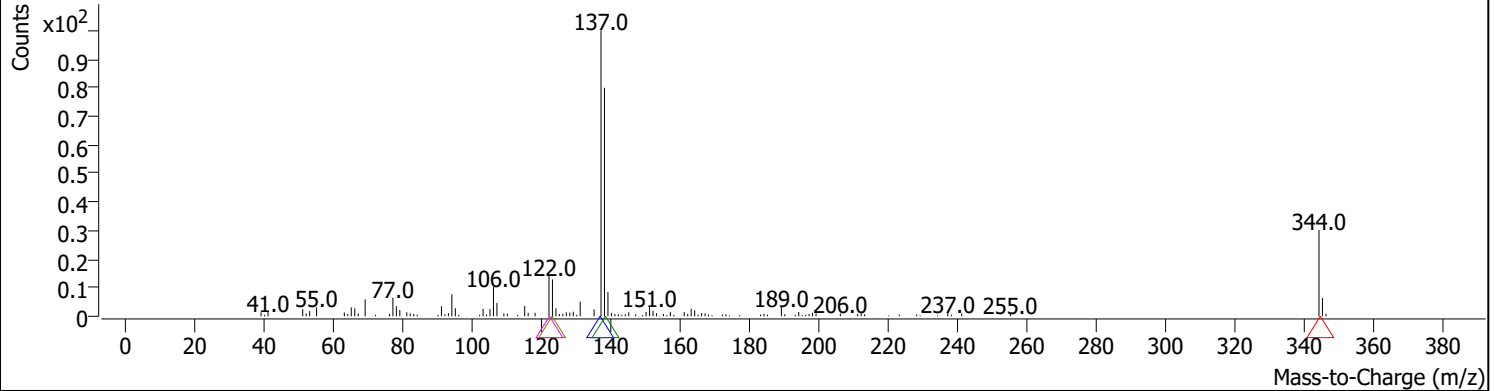
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
72.1870	3,4-Divanillyltetrahydrofuran	6222168.8	88.7	34730-78-4	C <sub>20</sub> H <sub>24</sub> O <sub>5</sub>	

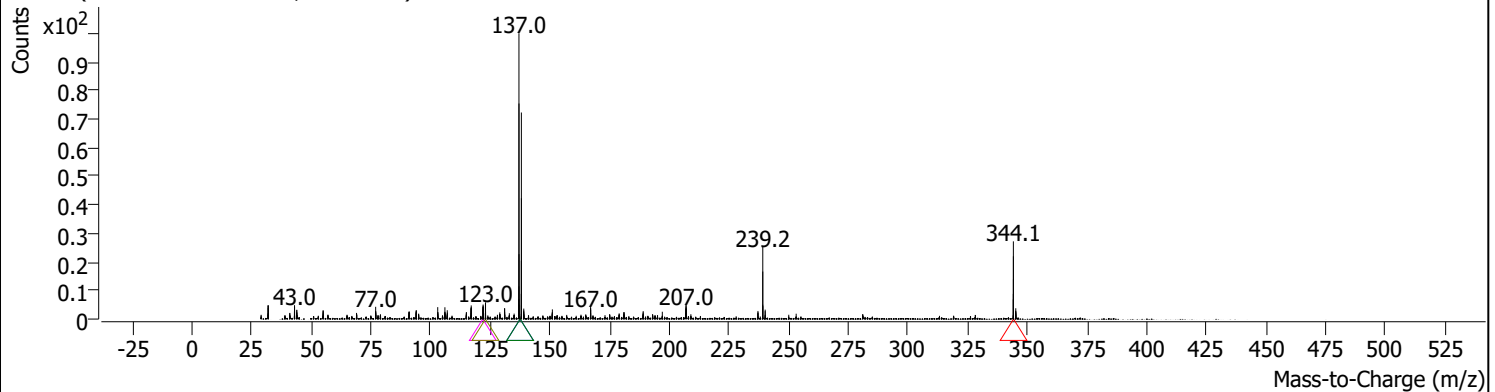
Component RT: 72.1870



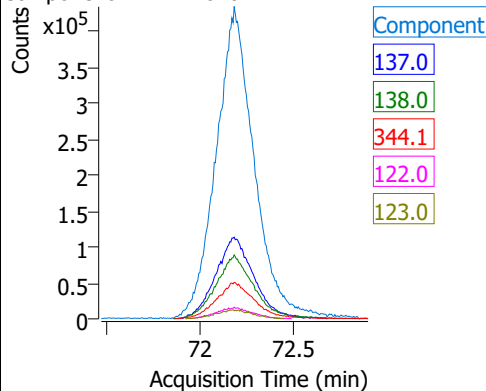
3,4-Divanillyltetrahydrofuran (NIST20.L)



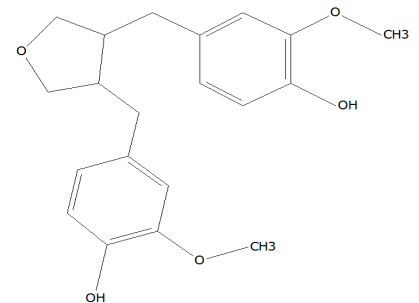
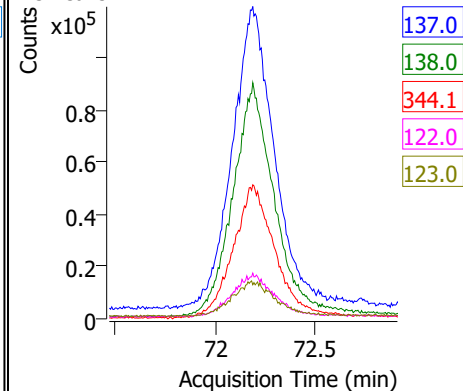
+ Scan (71.8589-72.8519 min, 168 scans) 4.D



Component RT: 72.1870



EIC Peaks



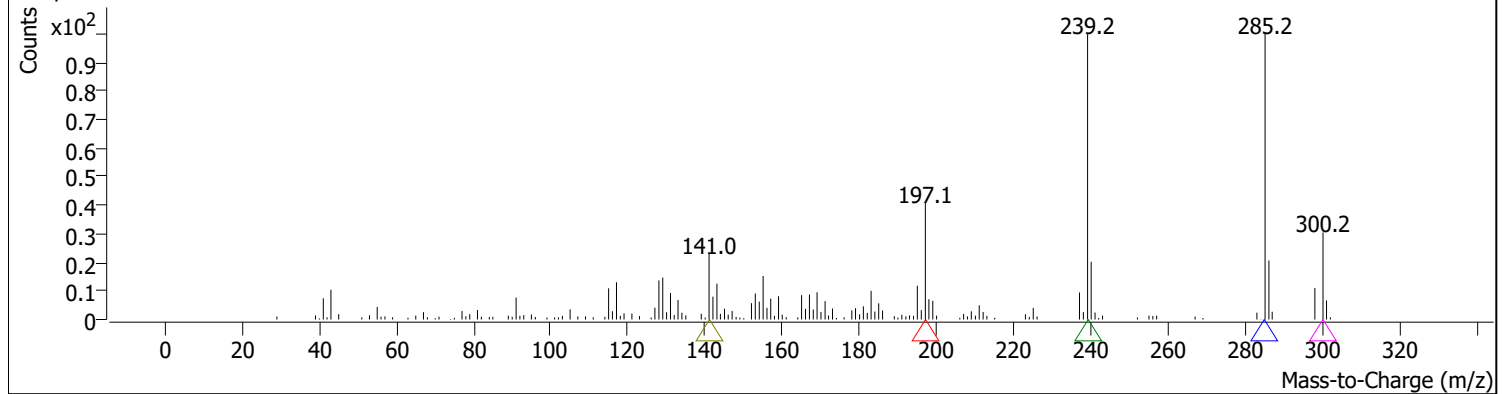
## Library Search Results - NonTarget Hits with Details



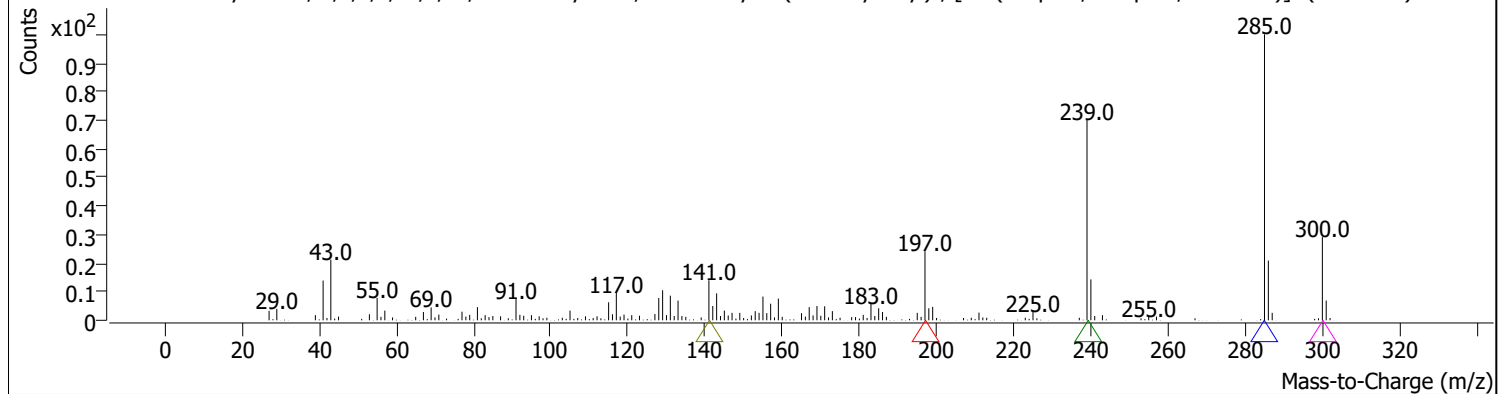
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
73.6231	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.)]-	6817161.6	93.1	5155-70-4	C20H28O2	

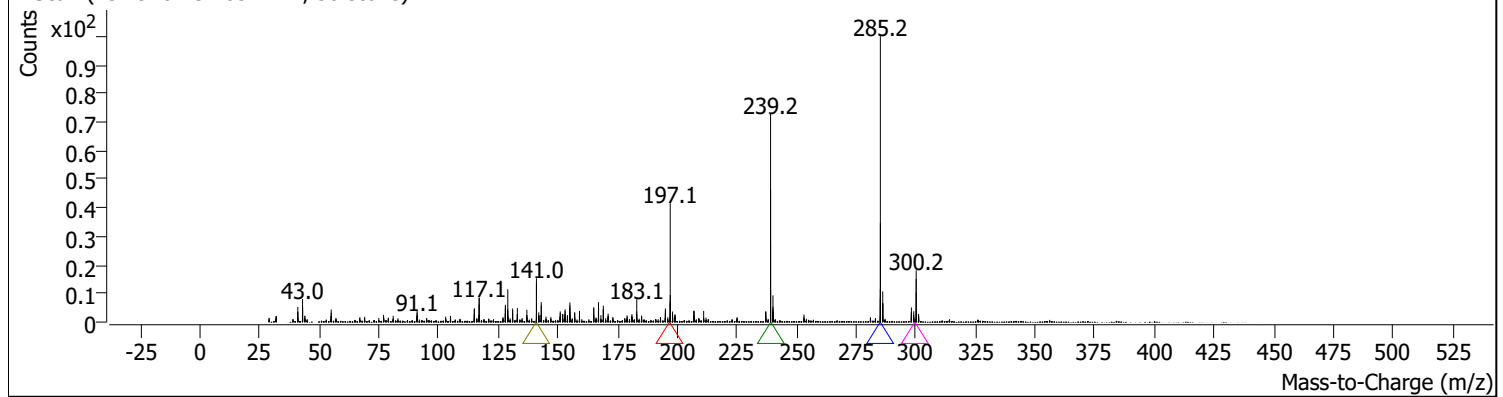
Component RT: 73.6231



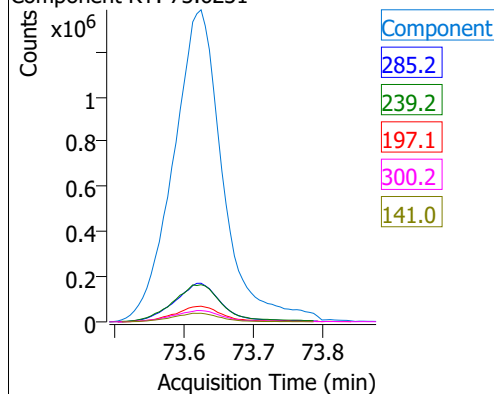
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]- (NIST20.L)



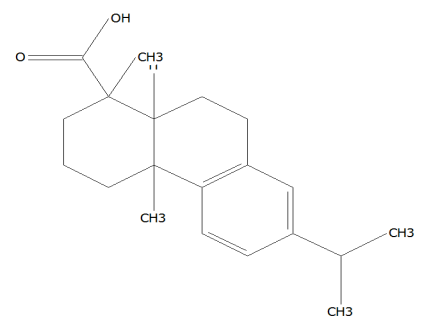
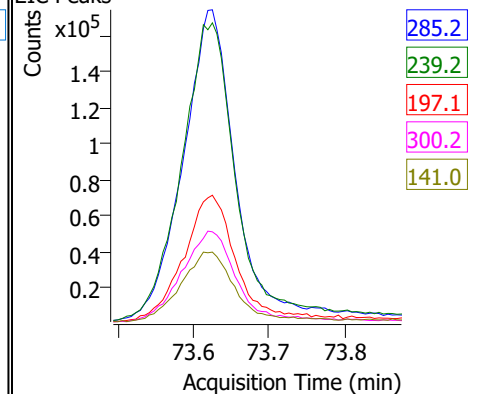
+ Scan (73.4940-73.7854 min, 50 scans) 4.D



Component RT: 73.6231



EIC Peaks



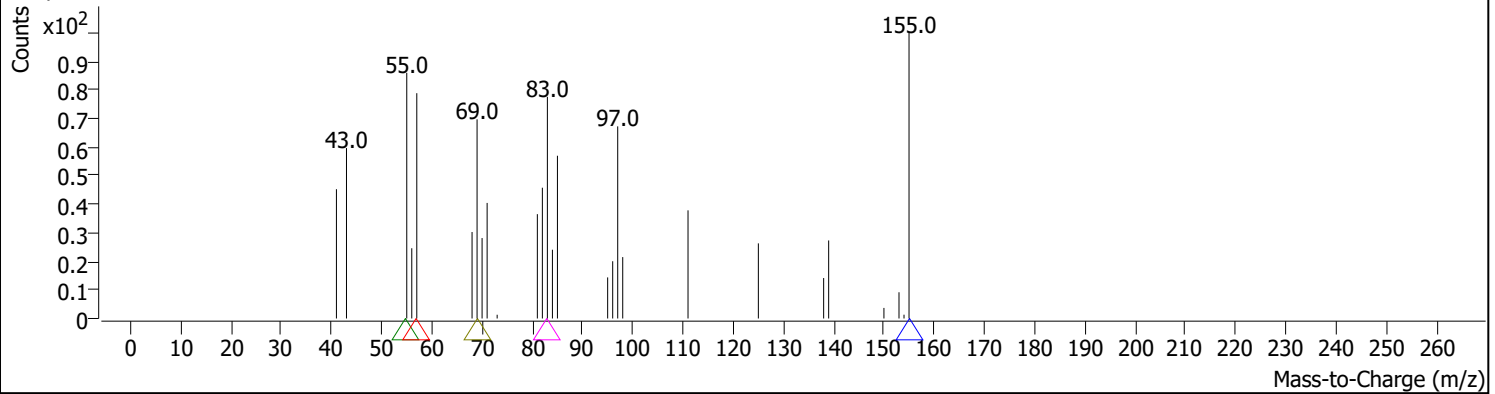
## Library Search Results - NonTarget Hits with Details



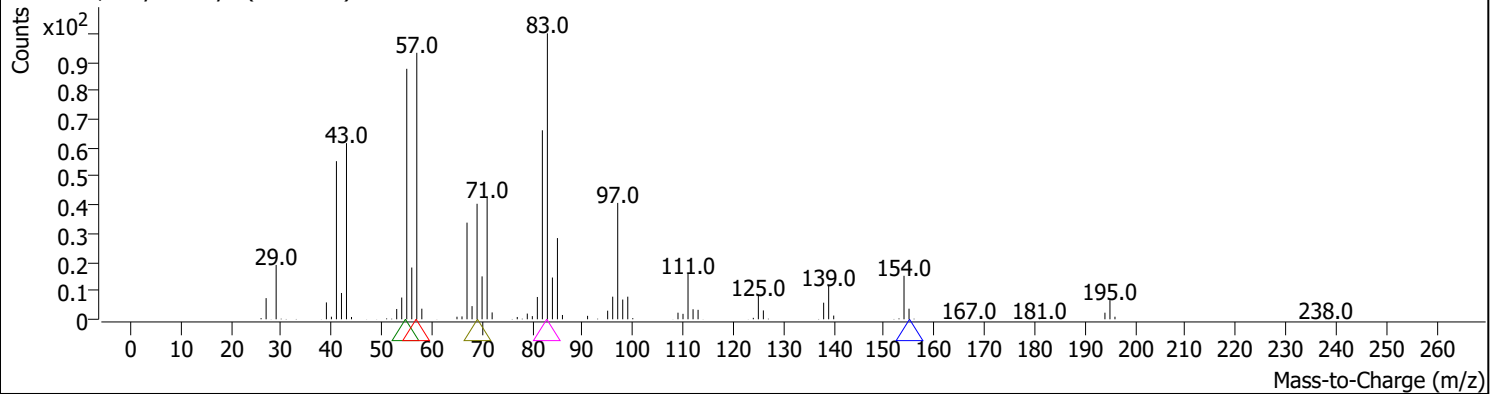
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
75.3519	Undecane, 4-cyclohexyl-	739647.2	77.0	13151-79-6	C17H34	

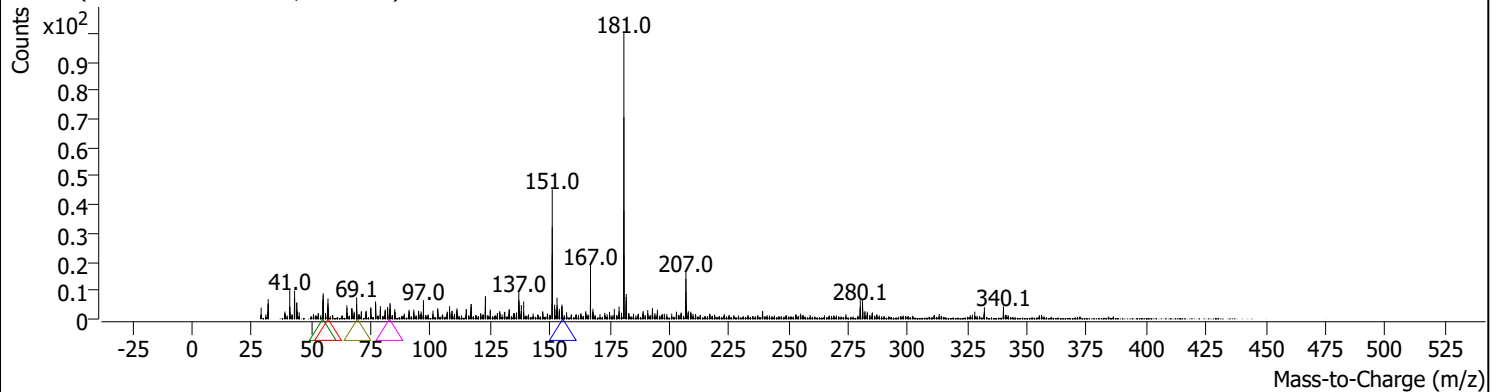
Component RT: 75.3519



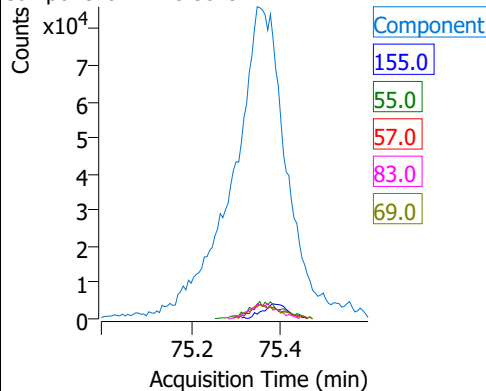
Undecane, 4-cyclohexyl- (NIST20.L)



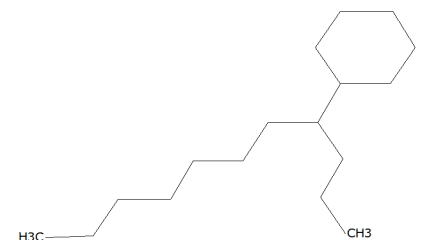
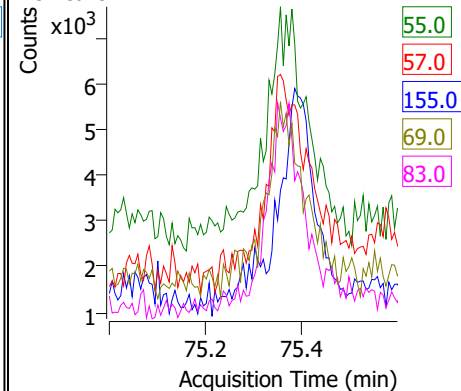
+ Scan (75.2879-75.4443 min, 27 scans) 4.D



Component RT: 75.3519



EIC Peaks



## Library Search Results - NonTarget Hits with Details

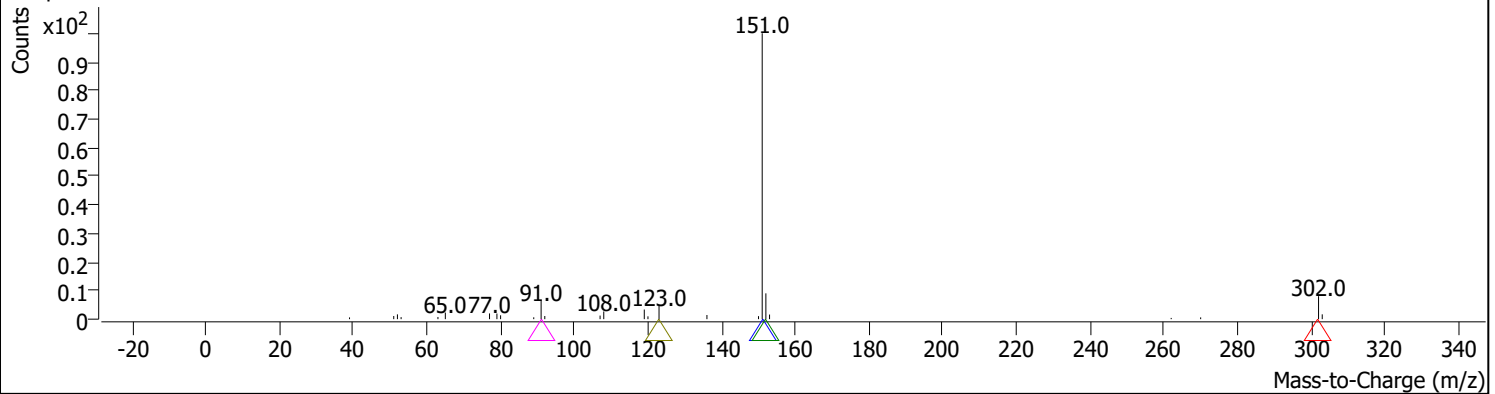


Agilent

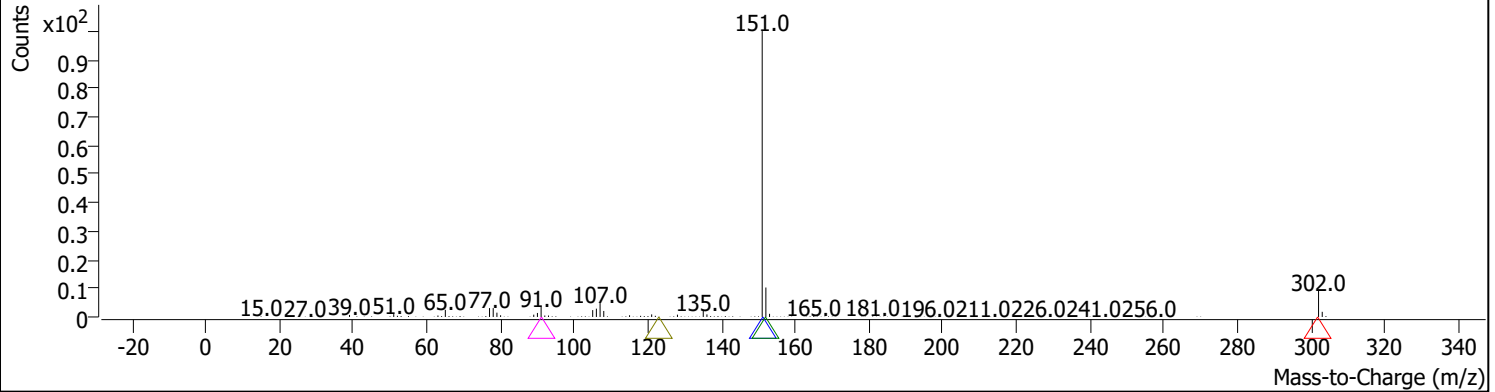
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
75.9019	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether	1003347.8	80.1	22318-87-2	C <sub>18</sub> H <sub>22</sub> O <sub>4</sub>	

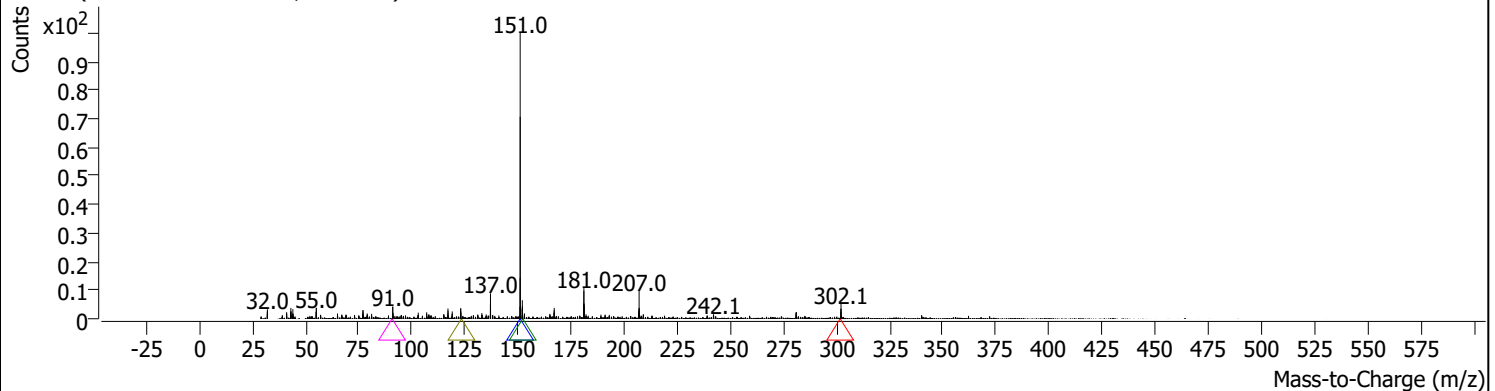
Component RT: 75.9019



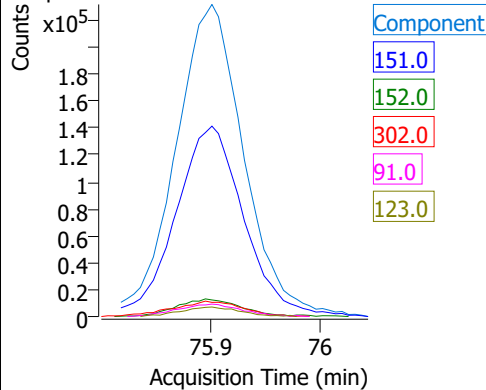
5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether (NIST20.L)



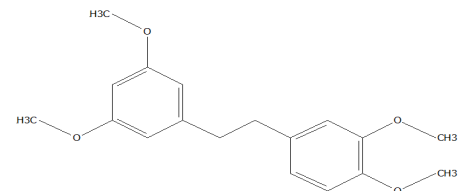
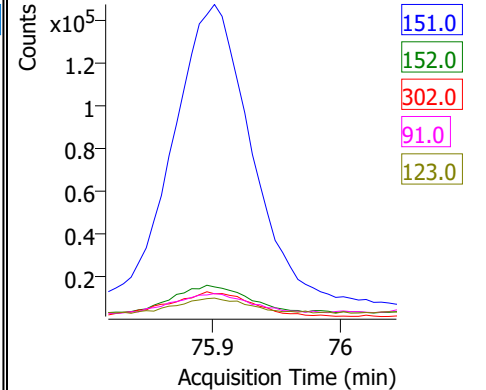
+ Scan (75.8189-76.0449 min, 39 scans) 4.D



Component RT: 75.9019



EIC Peaks



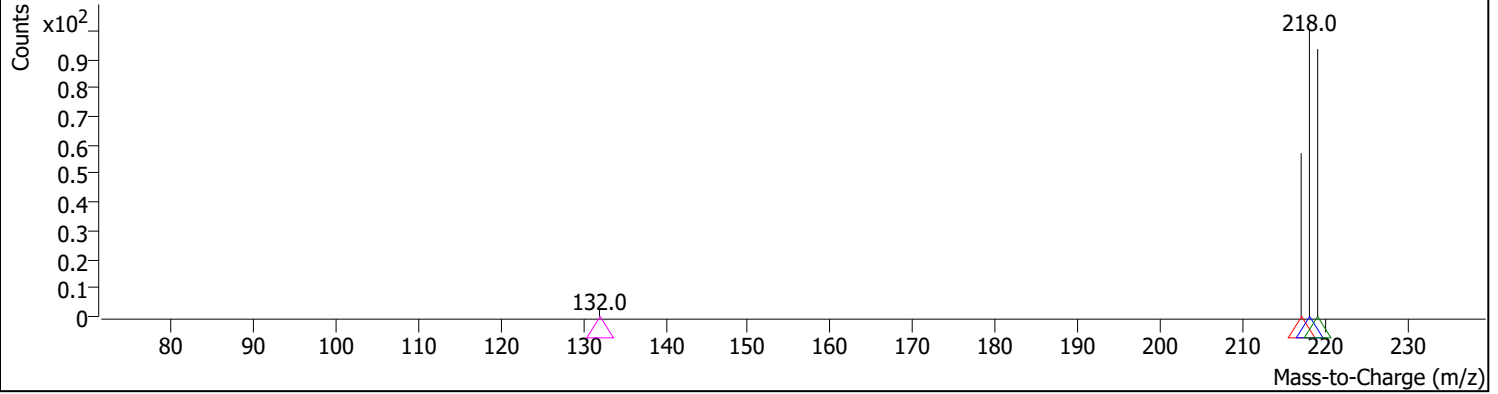
## Library Search Results - NonTarget Hits with Details



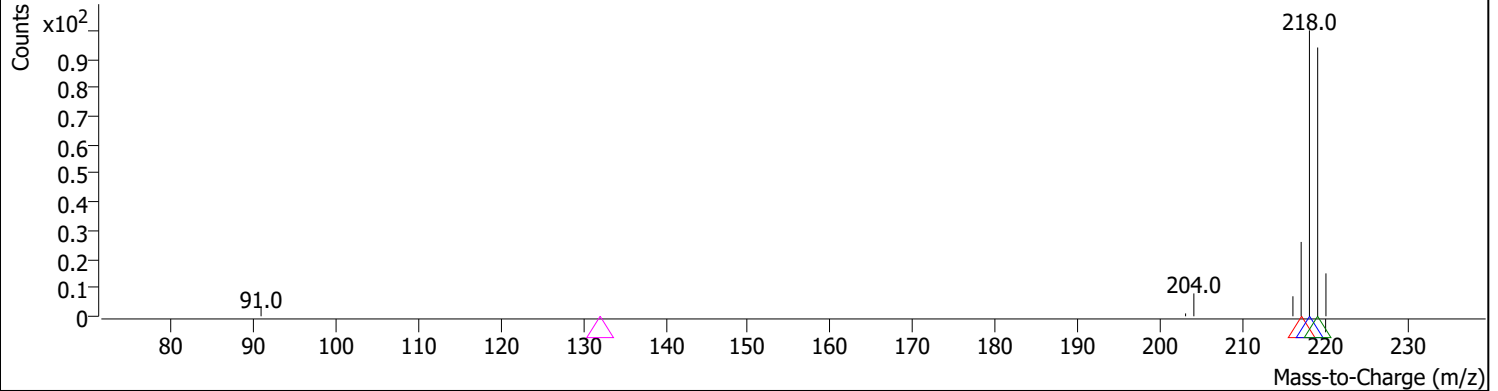
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
77.0919	8-Benzylquinoline	604940.0	84.3	28748-19-8	C <sub>16</sub> H <sub>13</sub> N	

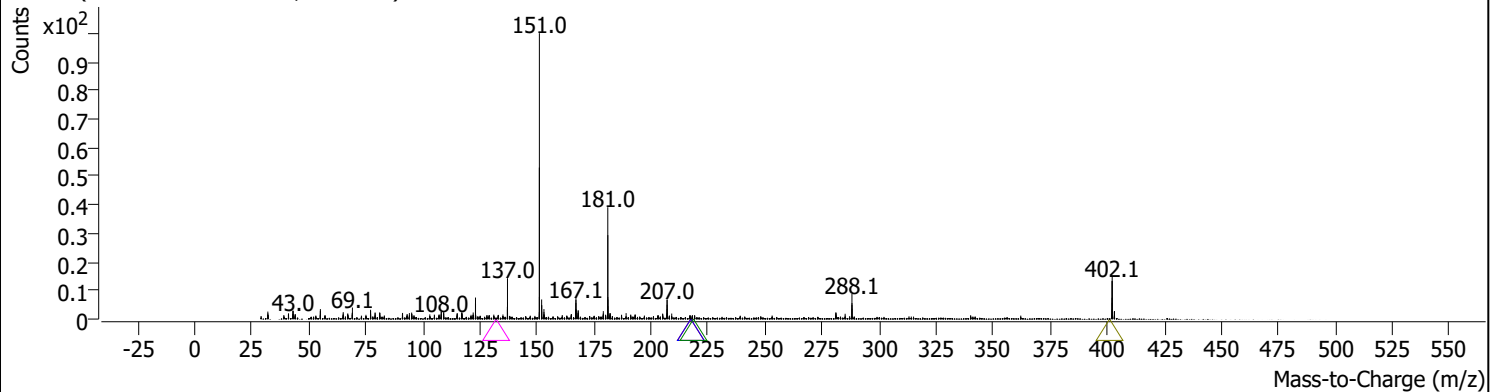
Component RT: 77.0919



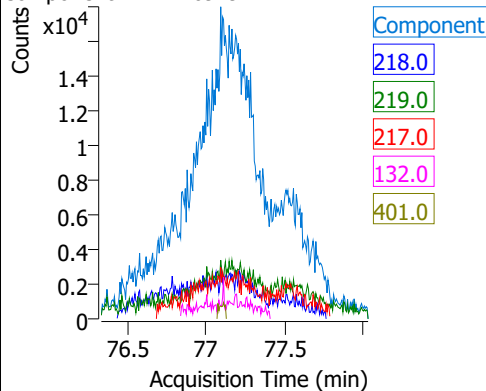
8-Benzylquinoline (NIST20.L)



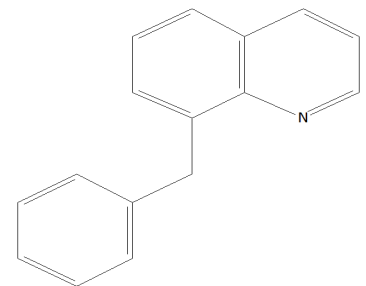
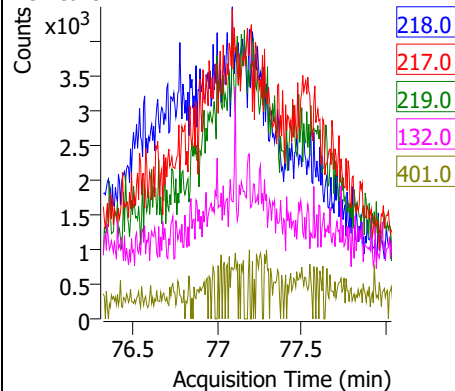
+ Scan (76.8357-77.4065 min, 97 scans) 4.D



Component RT: 77.0919



EIC Peaks





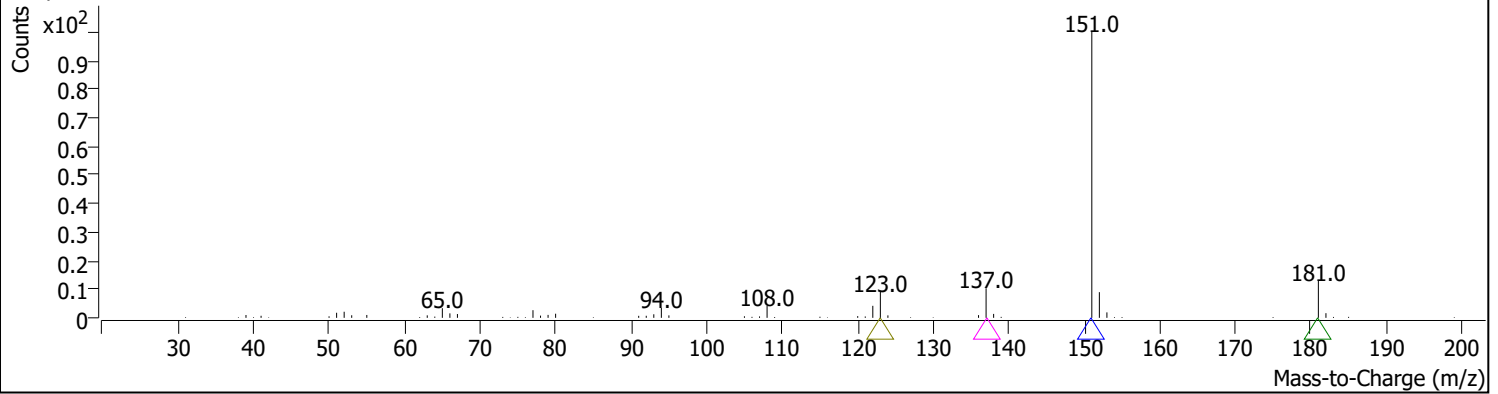
## Library Search Results - NonTarget Hits with Details



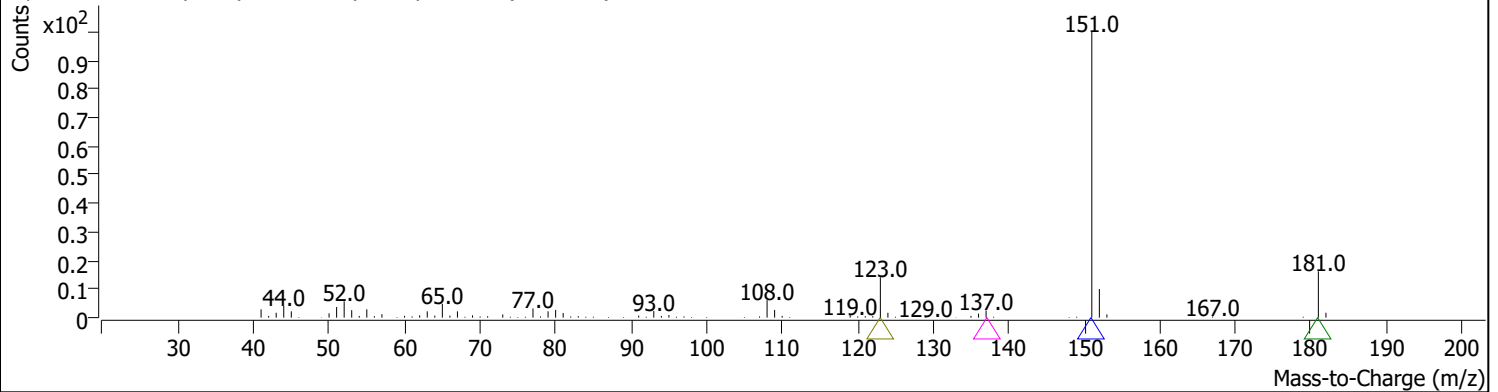
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
77.2580	.alpha.-Amino-3'-hydroxy-4'-methoxyacetophenone	3636759.4	76.5	90765-44-9	C9H11NO3	

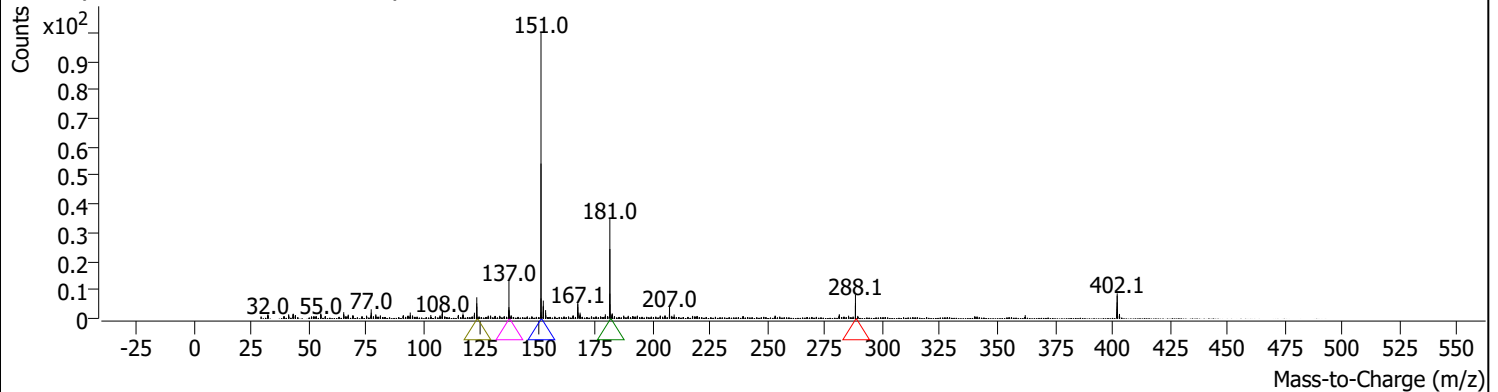
Component RT: 77.2580



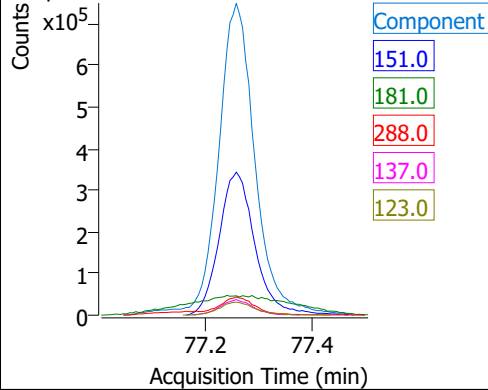
.alpha.-Amino-3'-hydroxy-4'-methoxyacetophenone (NIST20.L)



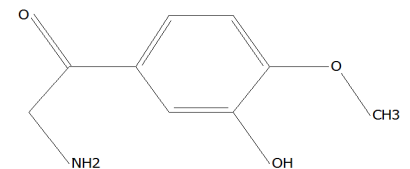
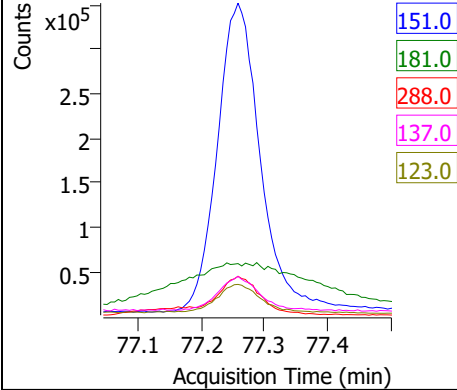
+ Scan (77.1580-77.4719 min, 53 scans) 4.D



Component RT: 77.2580



EIC Peaks



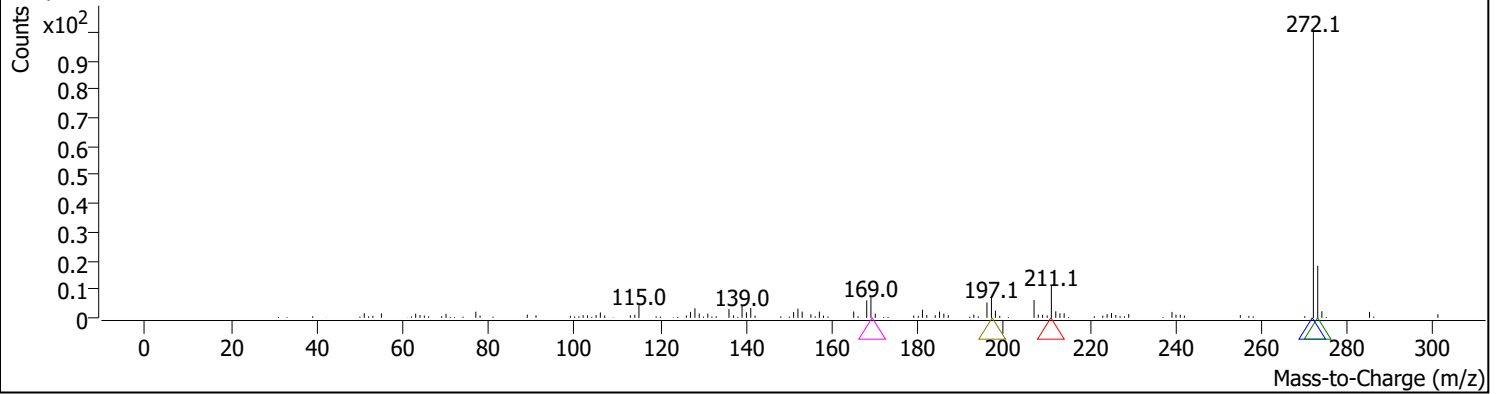
## Library Search Results - NonTarget Hits with Details



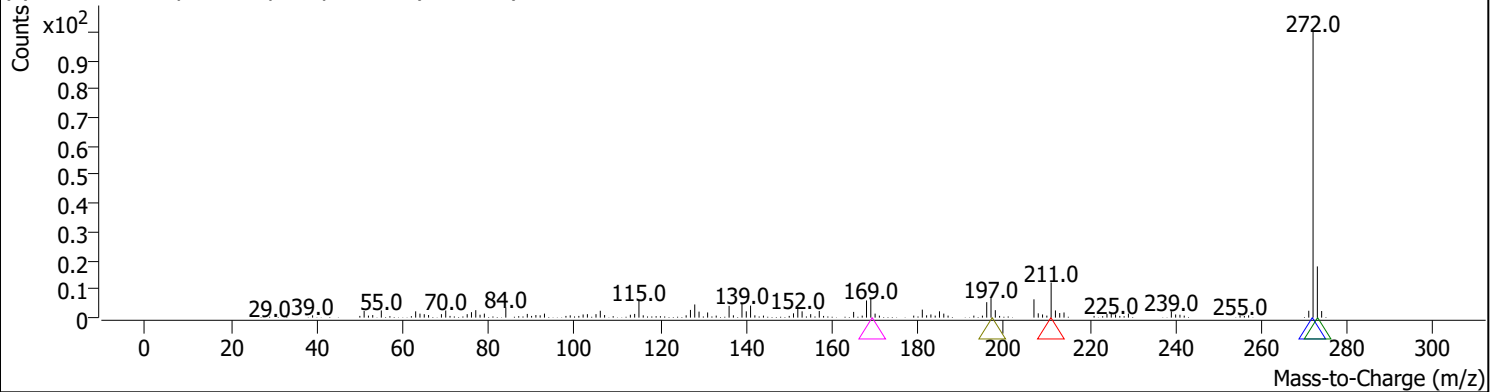
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
79.0869	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	5180261.7	89.1	7329-69-3	C <sub>16</sub> H <sub>16</sub> O <sub>4</sub>	

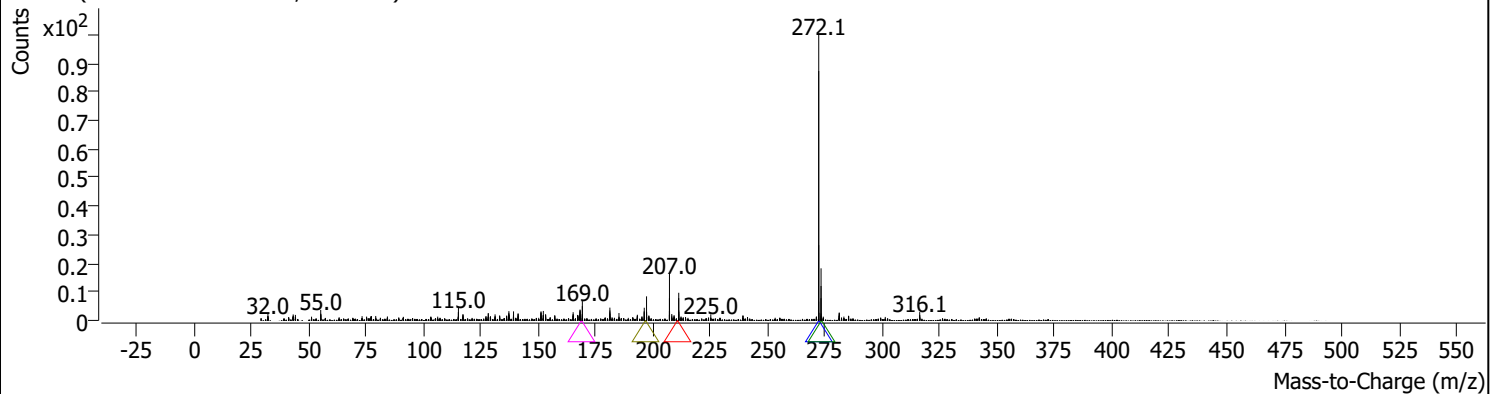
Component RT: 79.0869



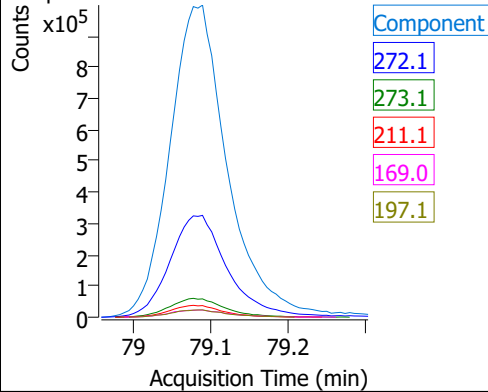
(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene (NIST20.L)



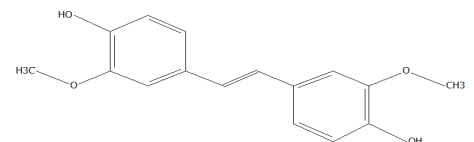
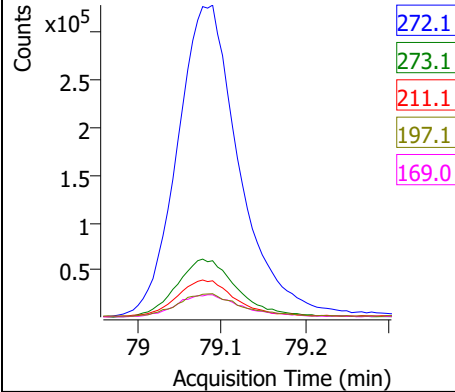
+ Scan (78.9585-79.3033 min, 59 scans) 4.D



Component RT: 79.0869



EIC Peaks



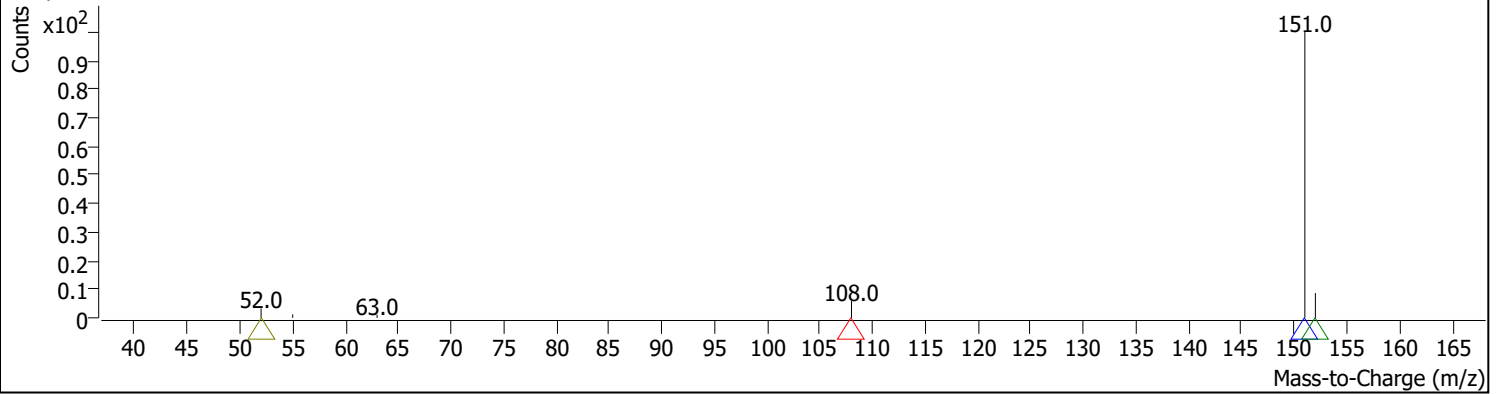
## Library Search Results - NonTarget Hits with Details



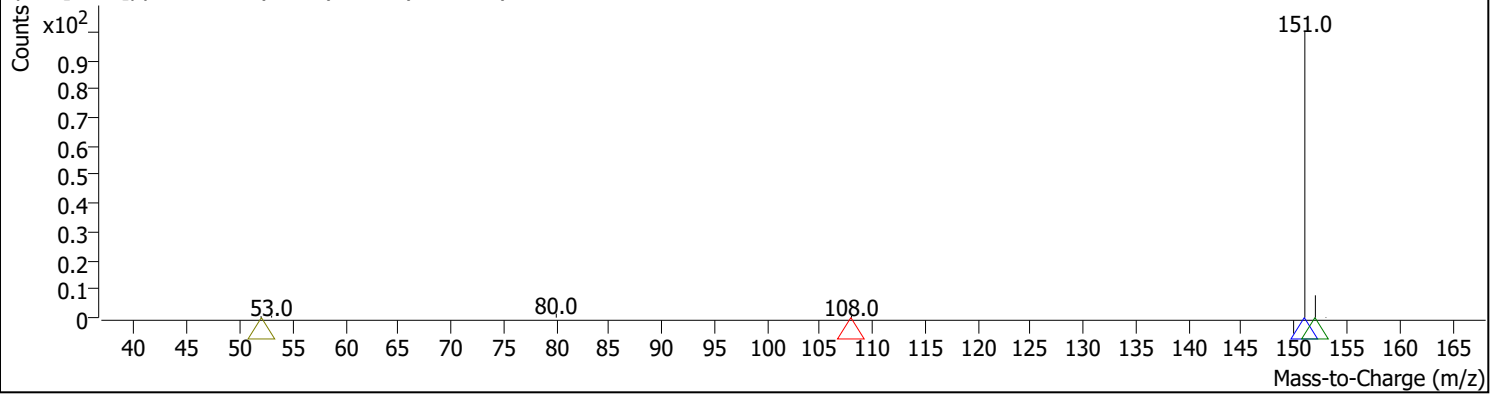
Trusted Answers

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
80.5466	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	757240.5	83.0	65996-50-1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	

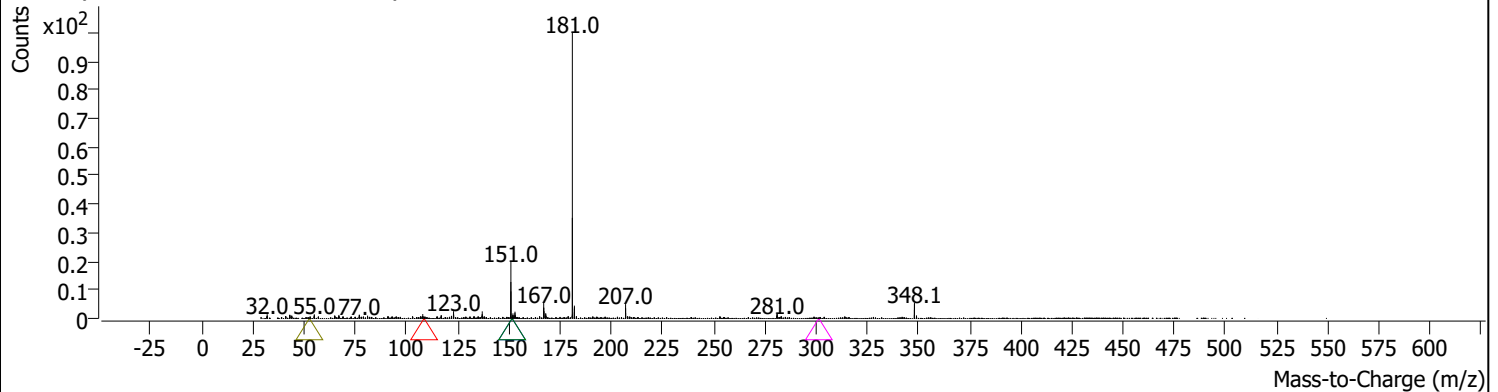
Component RT: 80.5466



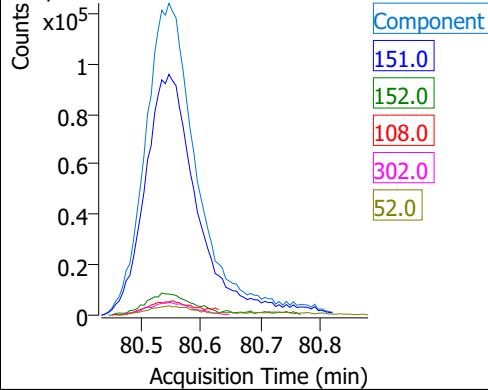
Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)



+ Scan (80.4331-80.8196 min, 66 scans) 4.D



Component RT: 80.5466



EIC Peaks

