

Supporting Information II

Comparison of Trace Organic Chemical Removal Efficiencies between Aerobic and Anaerobic Membrane Bioreactors Treating Municipal Wastewater

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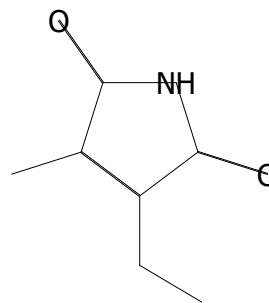
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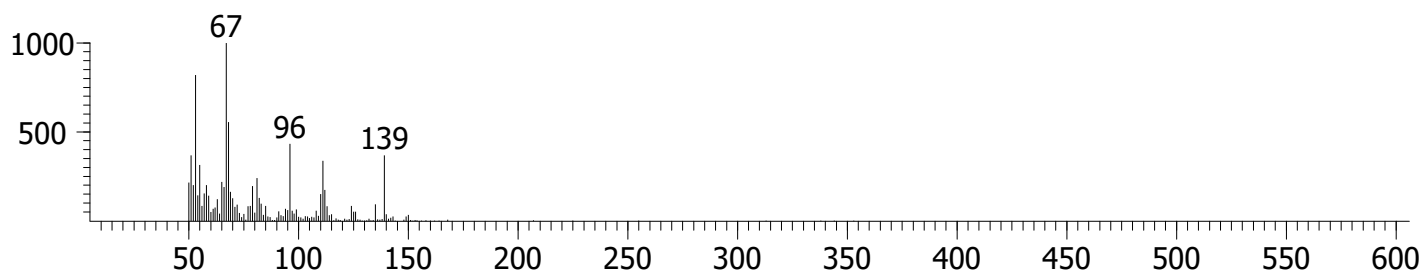
Mass spectra of the 351 tentatively identified compounds S3-S354

1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-

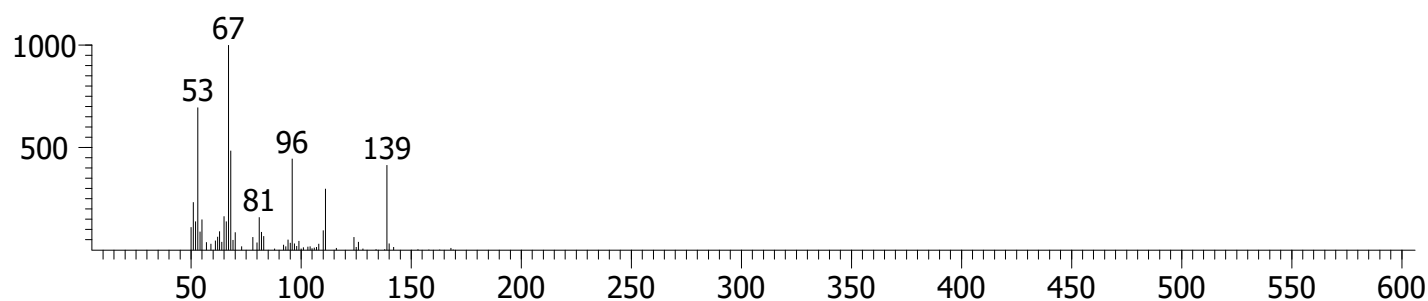
1st Dimension R.T. = 1008.2
2nd Dimension R.T. = 2.072
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Area = 103392
Height = 11179
Similarity = 750



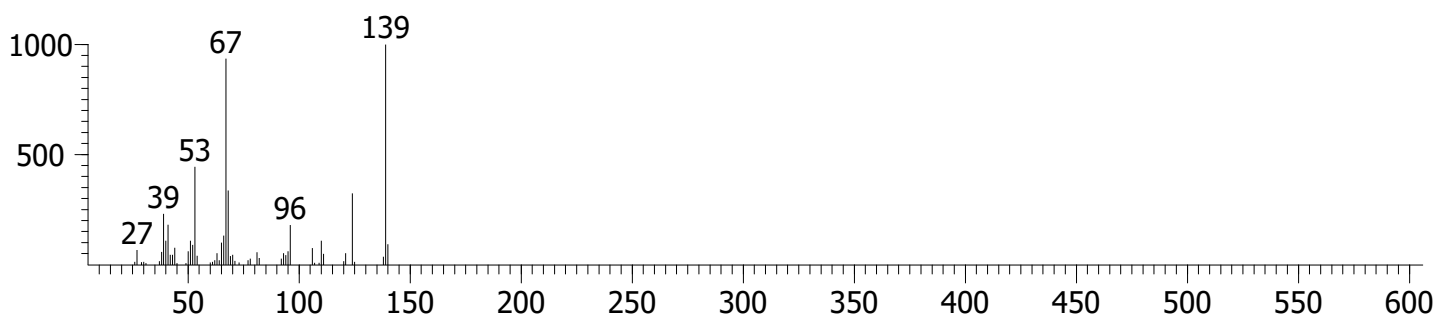
Peak Apex - sample "AnBxr B (20191121):1", peak 2097, at 1008.2 , 2.072 sec , sec (Spec # 80344)



Peak True - sample "AnBxr B (20191121):1", peak 2097, at 1008.2 , 2.072 sec , sec (Spec # 80344)



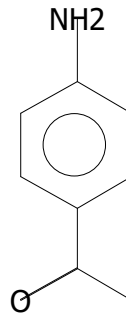
Library Hit - similarity 750, "1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-"



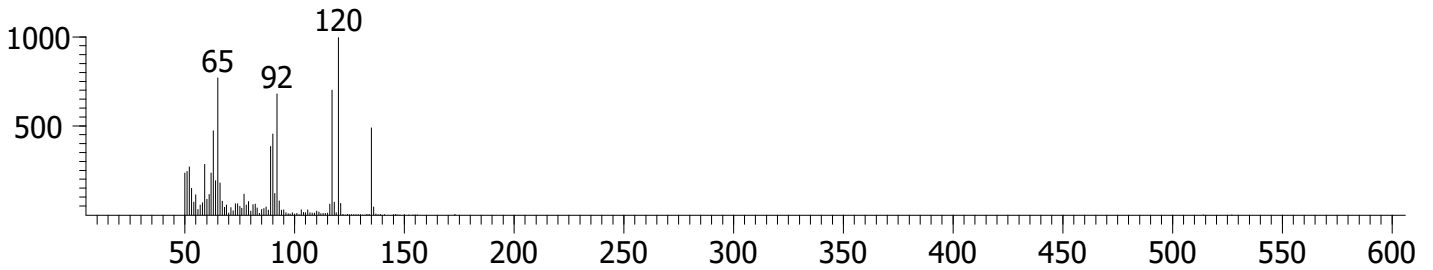
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	750	5051	20189-42-8	mainlib	C7H9NO2	139
2	Piperidine, 1-methyl,4-methylene-	690	896	13669-28-8	mainlib	C7H13N	111
3	2-Cyclopenten-1-one, 2-methyl-	680	2313	1120-73-6	replib	C6H8O	96
4	2,5-Methano-2H-furo[3,2-b]pyrrole, hexahydro-4-methyl-	669	381	38225-15-9	mainlib	C8H13NO	139
5	4-Cyclopropyl-4-methylpyrrolidin-2-one	666	337	0-00-0	mainlib	C8H13NO	139

Acetophenone, 4'-amino-

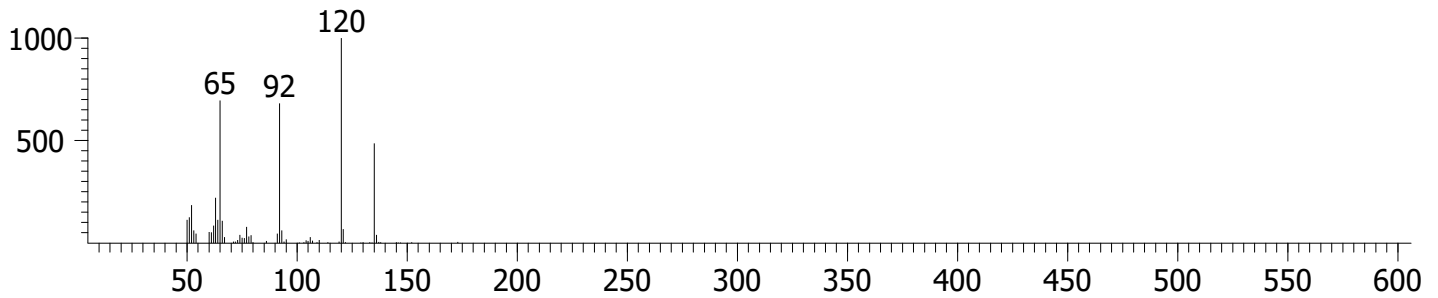
1st Dimension R.T. = 1018.69
2nd Dimension R.T. = 2.165
Quant Mass(es) = 120
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Height = 42506
Similarity = 936



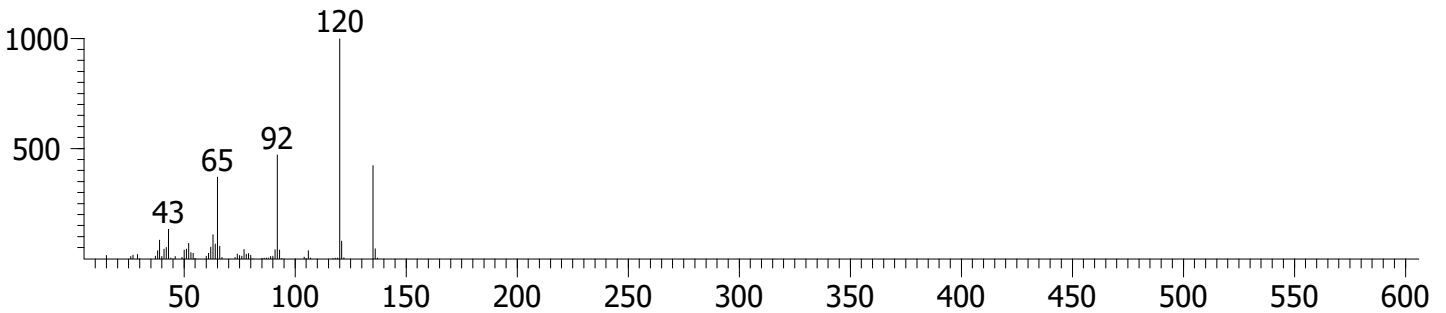
Peak Apex - sample "AnBxr B (20191121):1", peak 2161, at 1018.69 , 2.165 sec , sec (Spec # 81948)



Peak True - sample "AnBxr B (20191121):1", peak 2161, at 1018.69 , 2.165 sec , sec (Spec # 81948)



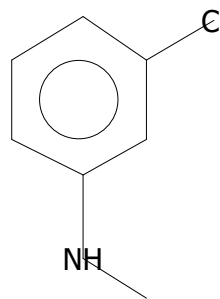
Library Hit - similarity 936, "Acetophenone, 4'-amino-"



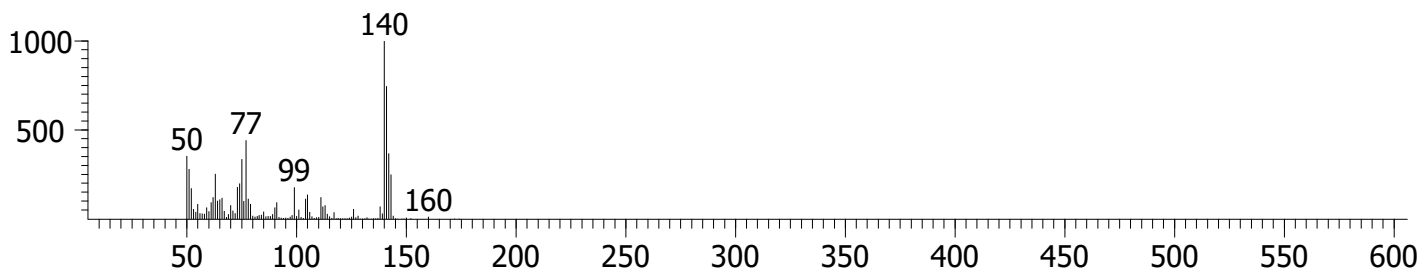
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Acetophenone, 4'-amino-	936	7127	99-92-3	replib	C8H9NO	135
2	Acetophenone, 4'-amino-	922	3853	99-92-3	mainlib	C8H9NO	135
3	Ethanone, 1-(2-aminophenyl)-	921	3703	551-93-9	mainlib	C8H9NO	135
4	Ethanone, 1-(2-aminophenyl)-	910	2135	551-93-9	replib	C8H9NO	135
5	Acetophenone, 4'-amino-	907	7127	99-92-3	replib	C8H9NO	135

Benzenamine, 3-chloro-N-methyl-

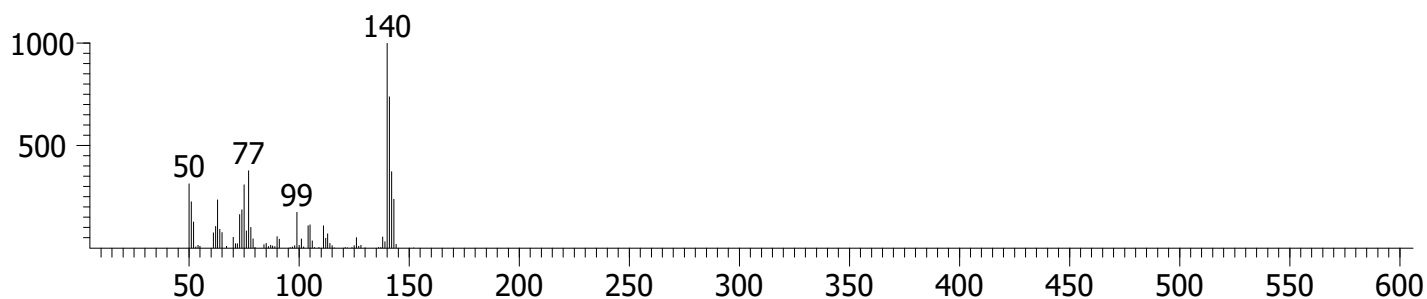
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Quant Mass(es) = 140
S/N = 5731.3
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Similarity = 906



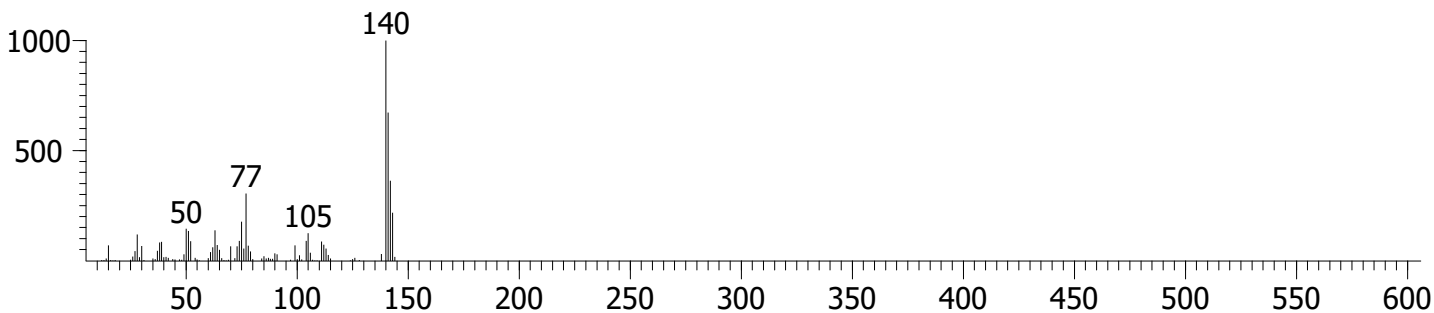
Peak Apex - sample "AnMbr B (20191120):1", peak 1632, at 1001.2 , 1.973 sec , sec (Spec # 79269)



Peak True - sample "AnMbr B (20191120):1", peak 1632, at 1001.2 , 1.973 sec , sec (Spec # 79269)



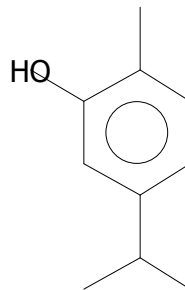
Library Hit - similarity 906, "Benzenamine, 3-chloro-N-methyl-"



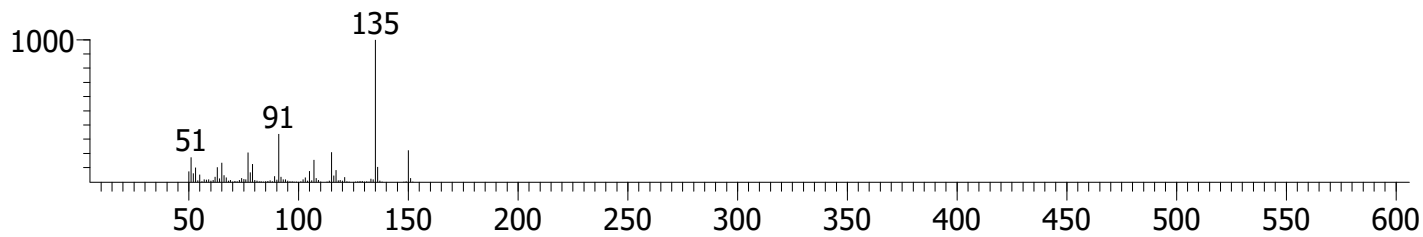
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenamine, 3-chloro-N-methyl-	906	5234	7006-52-2	mainlib	C7H8ClN	141
2	Benzenamine, 2-chloro-N-methyl-	891	3172	932-32-1	mainlib	C7H8ClN	141
3	Benzenamine, 4-chloro-N-methyl-	871	1444	932-96-7	mainlib	C7H8ClN	141
4	Urea, 1-(3-chlorophenyl)-1-methyl-3-phenyl-	736	54	67309-72-2	mainlib	C14H13ClN2O	260
5	Benzenamine, 3-chloro-4-methyl-	707	15	95-74-9	mainlib	C7H8ClN	141

Phenol, 2-methyl-5-(1-methylethyl)-

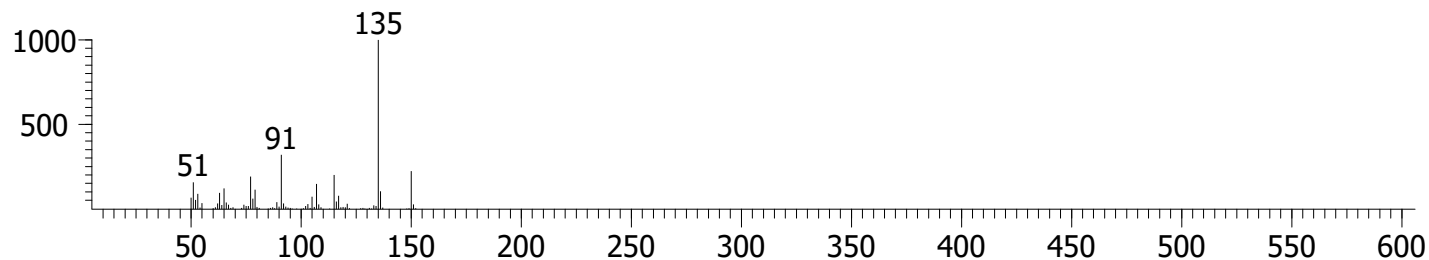
1st Dimension R.T. = 994.206
2nd Dimension R.T. = 1.676
Quant Mass(es) = 135
S/N = 22046
Area = 5886671
Height = 807393
Similarity = 918



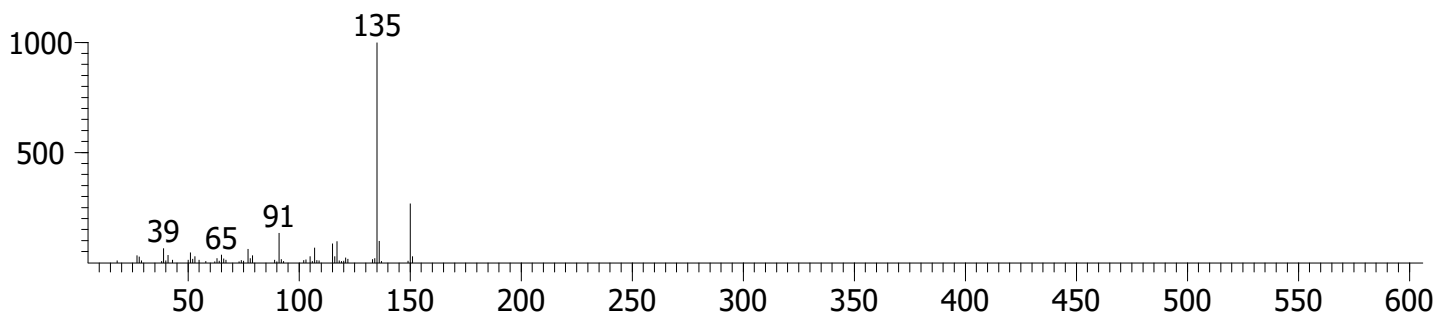
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 1799, at 994.206 , 1.676 sec , sec (Spec # 78164)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 1799, at 994.206 , 1.676 sec , sec (Spec # 78164)



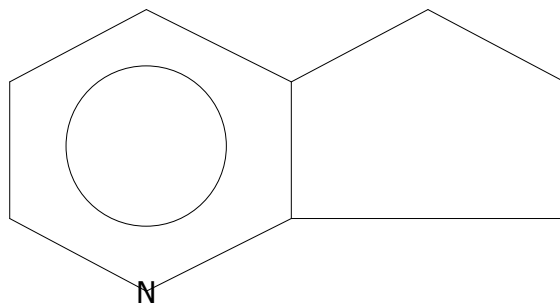
Library Hit - similarity 918, "Phenol, 2-methyl-5-(1-methylethyl)-"



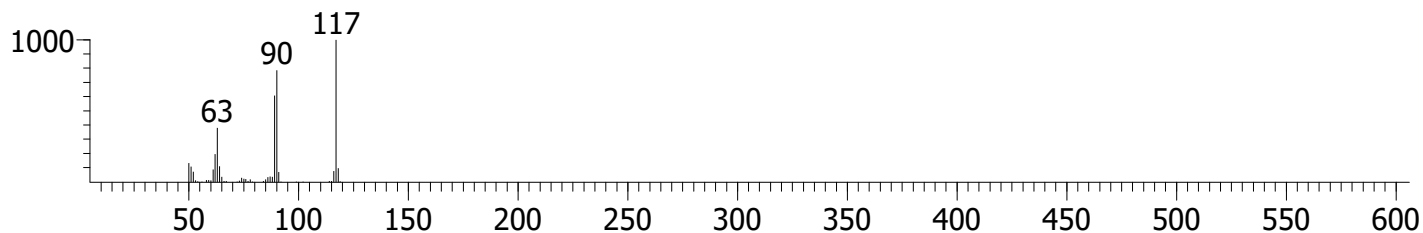
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 2-methyl-5-(1-methylethyl)-	918	3729	499-75-2	mainlib	C ₁₀ H ₁₄ O	150
2	Thymol	916	3439	89-83-8	mainlib	C ₁₀ H ₁₄ O	150
3	3-Methyl-4-isopropylphenol	873	758	3228-02-2	mainlib	C ₁₀ H ₁₄ O	150
4	Benzenemethanol, 2,4,6-trimethyl-	864	550	1197-01-9	mainlib	C ₁₀ H ₁₄ O	150
5	Phenol, 2-ethyl-4,5-dimethyl-	860	465	2219-78-5	mainlib	C ₁₀ H ₁₄ O	150

5H-1-Pyridine

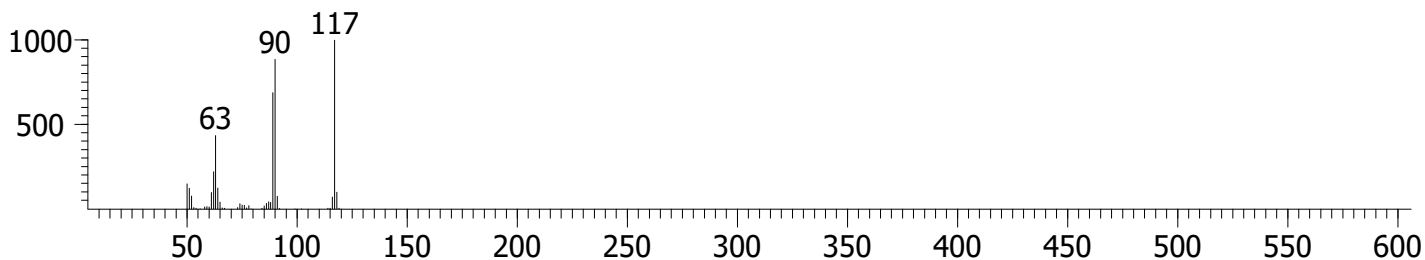
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2nd Dimension R.T. = 2.284
Quant Mass(es) = 117
S/N = 128960
Area = 98201869
Height = 6455334
Similarity = 926



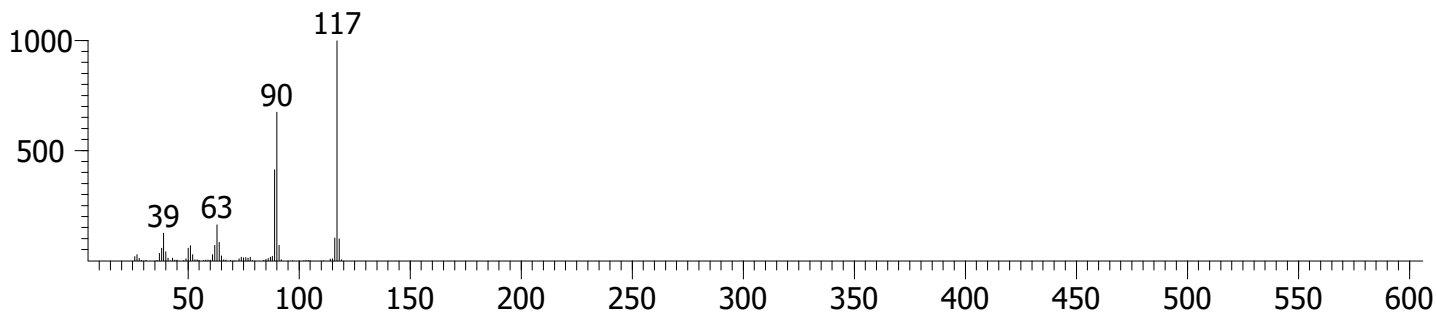
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 1883, at 1011.7 , 2.284 sec , sec (Spec # 80906)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 1883, at 1011.7 , 2.284 sec , sec (Spec # 80906)



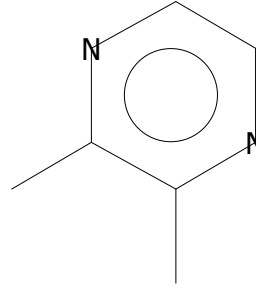
Library Hit - similarity 926, "5H-1-Pyridine"



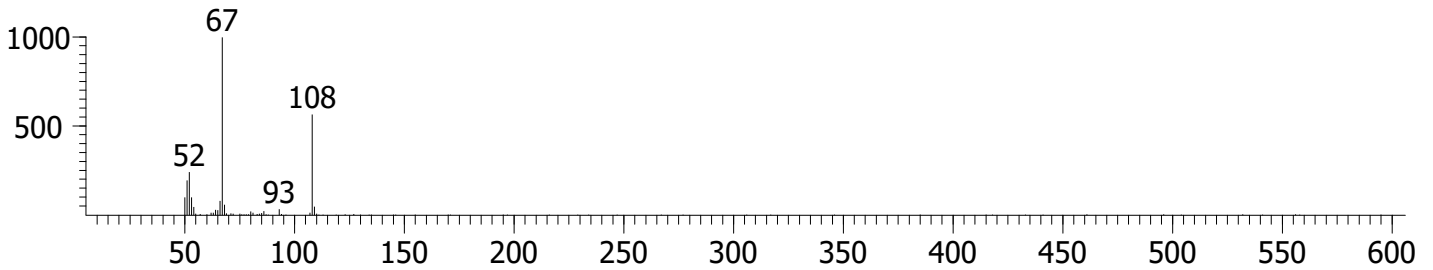
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5H-1-Pyridine	926	6374	270-91-7	mainlib	C8H7N	117
2	Indolizine	903	2327	274-40-8	mainlib	C8H7N	117
3	Indole	875	672	120-72-9	mainlib	C8H7N	117
4	N-Acetylindole	828	140	576-15-8	mainlib	C10H9NO	159
5	4-Ethynylaniline	826	129	14235-81-5	mainlib	C8H7N	117

Pyrazine, 2,3-dimethyl-

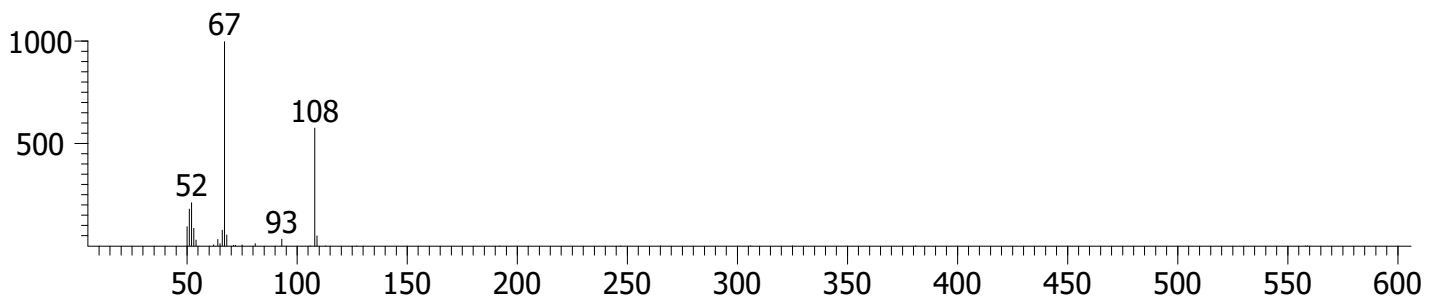
1st Dimension R.T. = 483.498
2nd Dimension R.T. = 1.465
Quant Mass(es) = 108
S/N = 521.17
Area = 105236
Height = 12195
Similarity = 904



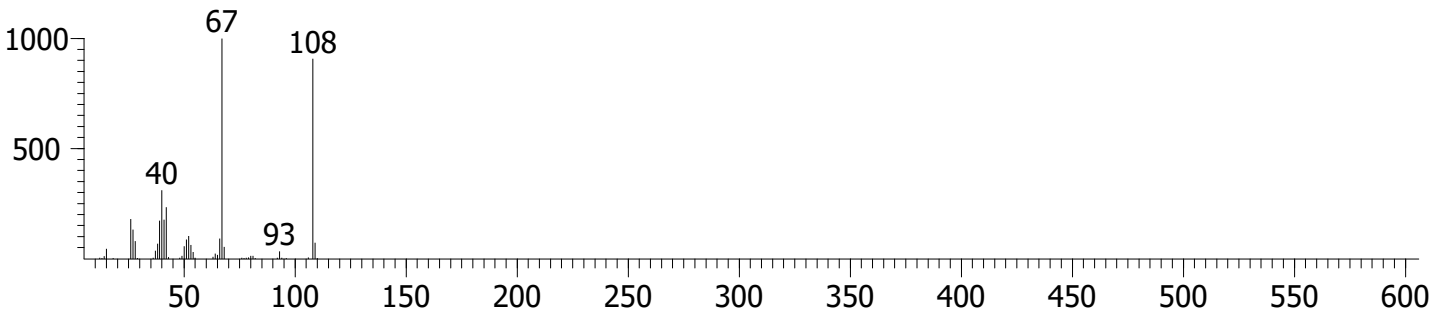
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 7, at 483.498 , 1.465 sec , sec (Spec # 752)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 7, at 483.498 , 1.465 sec , sec (Spec # 752)



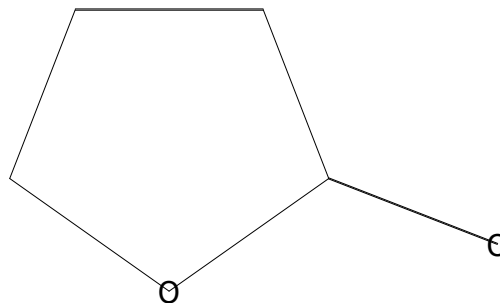
Library Hit - similarity 904, "Pyrazine, 2,3-dimethyl-"



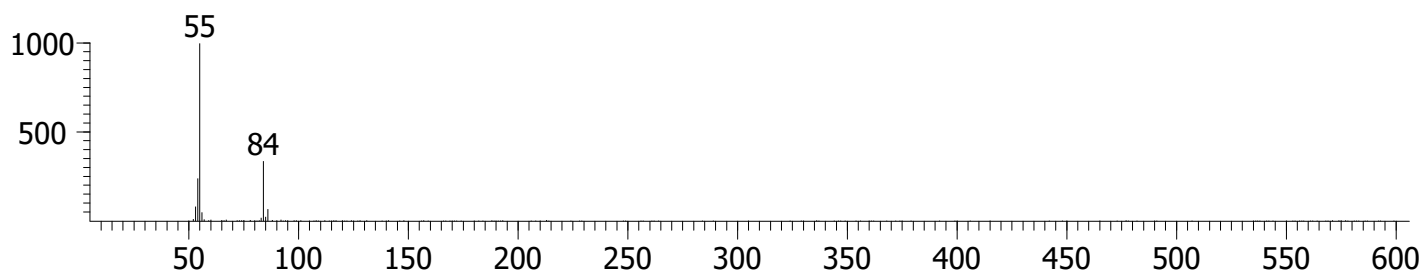
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pyrazine, 2,3-dimethyl-	904	9676	5910-89-4	mainlib	C6H8N2	108
2	Pyrimidine, 2,4-dimethyl-	752	263	14331-54-5	mainlib	C6H8N2	108
3	Pyridine, 2-ethoxy-	643	17	14529-53-4	mainlib	C7H9NO	123
4	Ethanone, 1-[1-(3-methyl-4-furoxanyl)-5-methyl-1,2,3-triazol-4-yl]-	630	11	296892-75-6	mainlib	C8H9N5O3	223
5	2-(Cyclopenten-1-yl)acetic acid	623	8	13668-61-6	mainlib	C7H10O2	126

2(5H)-Furanone

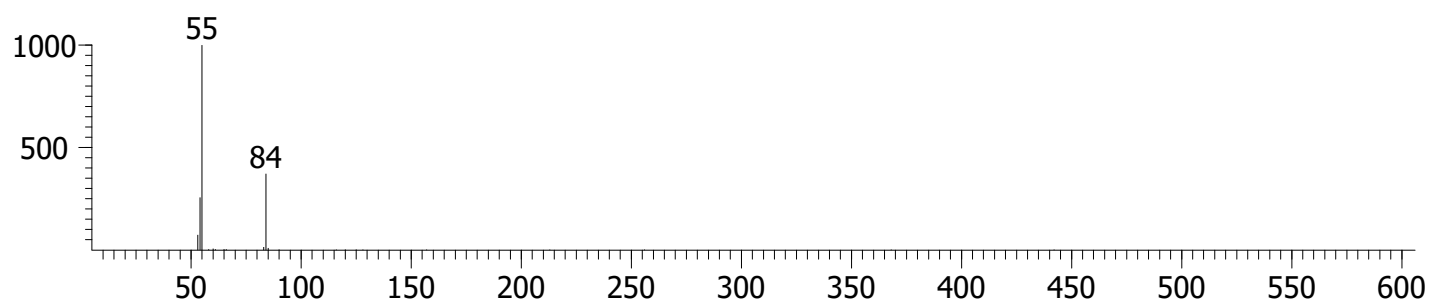
1st Dimension R.T. = 483.498
2nd Dimension R.T. = 1.987
Quant Mass(es) = 84
S/N = 254.06
Area = 101745
Height = 10426
Similarity = 898



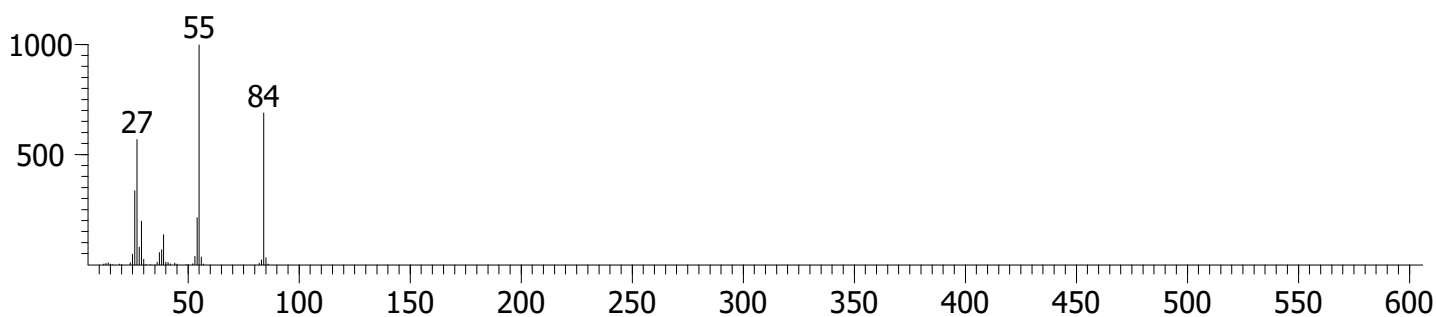
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 10, at 483.498 , 1.987 sec , sec (Spec # 831)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 10, at 483.498 , 1.987 sec , sec (Spec # 831)

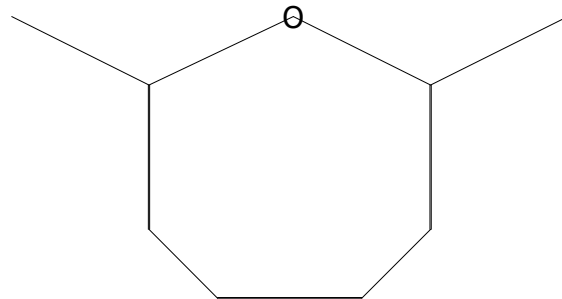


Library Hit - similarity 898, "2(5H)-Furanone"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2(5H)-Furanone	898	7559	497-23-4	mainlib	C4H4O2	84
2	2(3H)-Furanone	863	1897	20825-71-2	mainlib	C4H4O2	84
3	Borane, diethylmethyl-	805	349	1115-07-7	mainlib	C5H13B	84
4	Borane, ethyldimethyl-	775	97	1113-22-0	mainlib	C4H11B	70
5	4,8-Dioxaspiro[2.5]oct-1-ene, 6,6-dimethyl-	726	19	60935-22-0	mainlib	C8H12O2	140

Oxepine, 2,7-dimethyl-



1st Dimension R.T. = 500.988

2nd Dimension R.T. = 1.287

Quant Mass(es) = 122

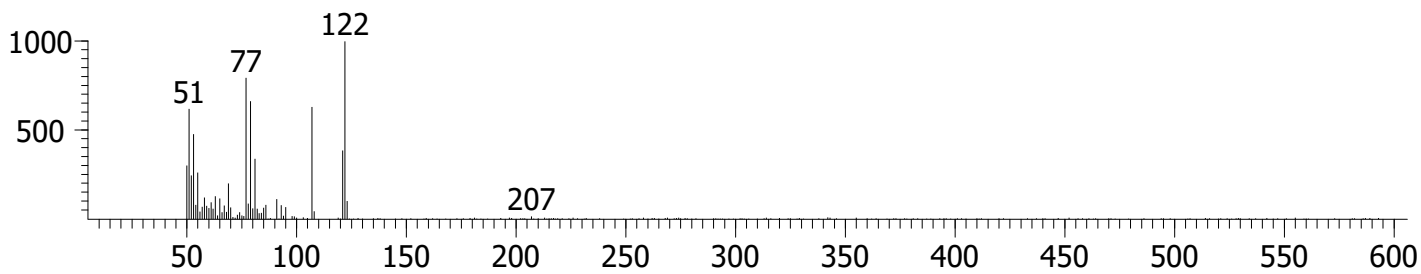
S/N = 323.78

Area = 36523

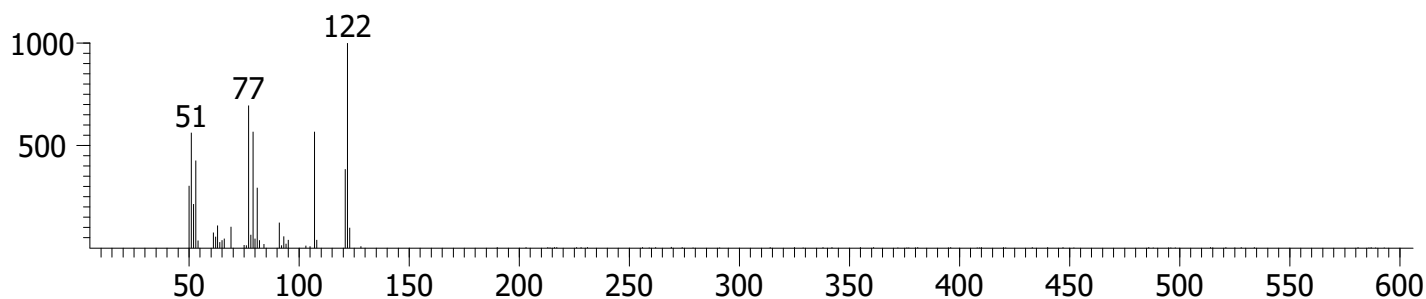
Height = 4423.9

Similarity = 799

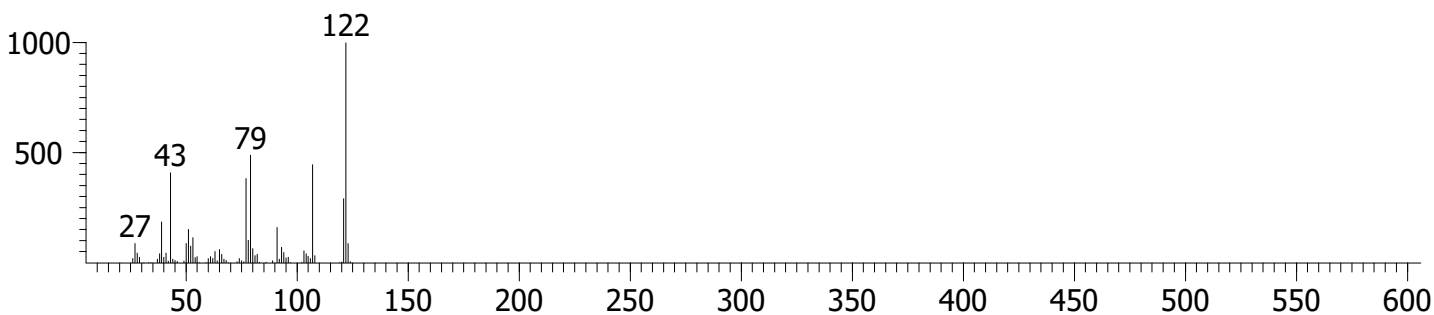
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 43, at 500.988 , 1.287 sec , sec (Spec # 3375)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 43, at 500.988 , 1.287 sec , sec (Spec # 3375)



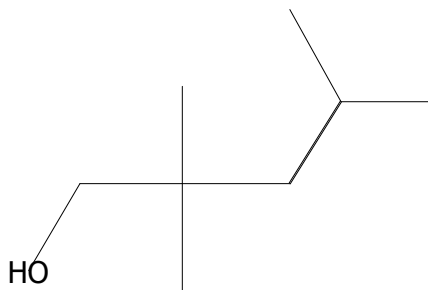
Library Hit - similarity 799, "Oxepine, 2,7-dimethyl-"



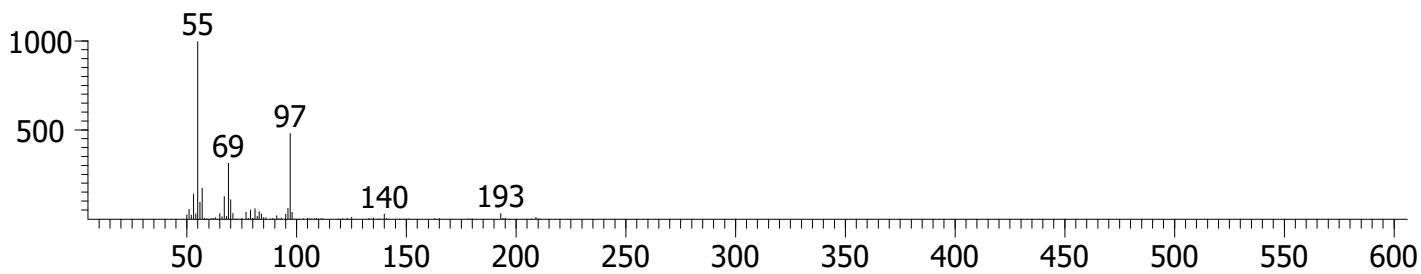
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Oxepine, 2,7-dimethyl-	799	3932	1487-99-6	mainlib	C8H10O	122
2	Phenol, 2,4-dimethyl-	771	1135	105-67-9	mainlib	C8H10O	122
3	Benzene, 1-methoxy-2-methyl-	752	551	578-58-5	mainlib	C8H10O	122
4	1,3,5-Cycloheptatriene, 1-methoxy-	751	530	1728-32-1	mainlib	C8H10O	122
5	Phenol, 2,5-dimethyl-	751	530	95-87-4	mainlib	C8H10O	122

3-Penten-1-ol, 2,2,4-trimethyl-

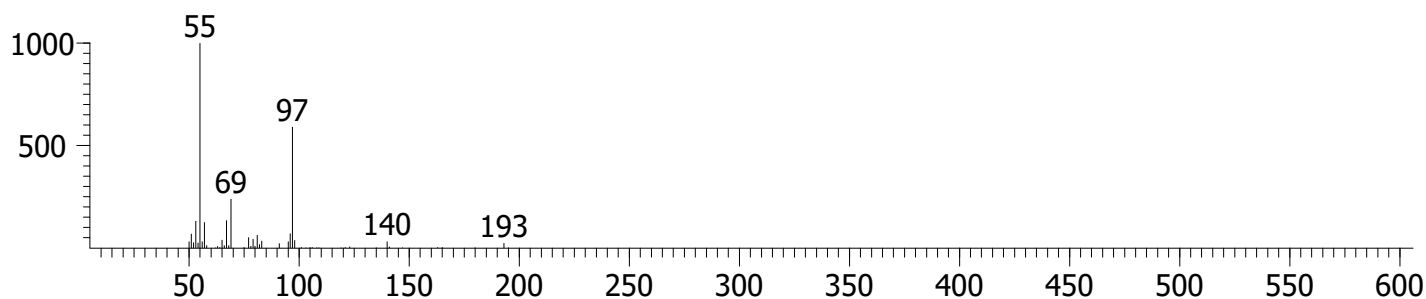
1st Dimension R.T. = 518.478
2nd Dimension R.T. = 1.076
Quant Mass(es) = 97
S/N = 833.06
Area = 184433
Height = 24032
Similarity = 858



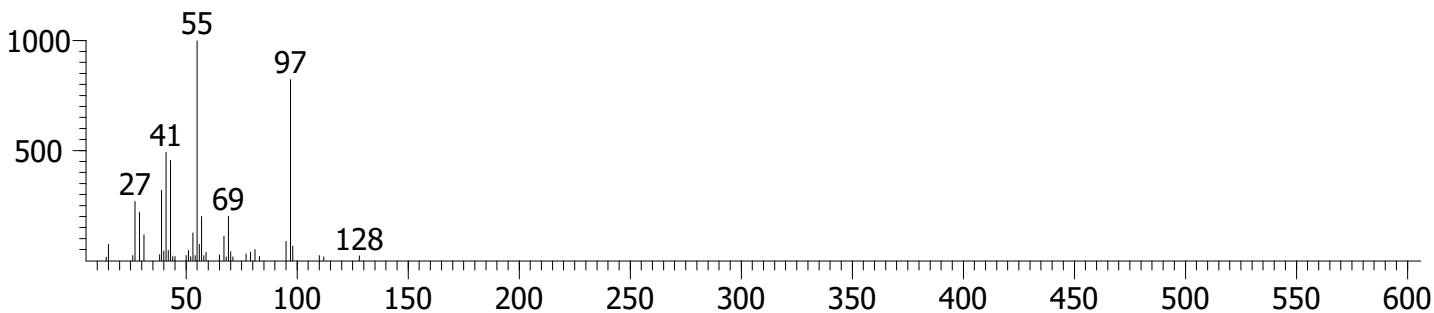
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 81, at 518.478 , 1.076 sec , sec (Spec # 5993)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 81, at 518.478 , 1.076 sec , sec (Spec # 5993)

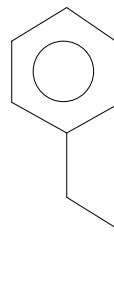


Library Hit - similarity 858, "3-Penten-1-ol, 2,2,4-trimethyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Penten-1-ol, 2,2,4-trimethyl-	858	4666	5842-53-5	mainlib	C8H16O	128
2	3-Isopropyl-4-methyl-1-pentyn-3-ol	839	2265	5333-87-9	mainlib	C9H16O	140
3	2-Pentene, 1-bromo-3,4-dimethyl-	806	593	922-99-6	mainlib	C7H13Br	176
4	Cyclohexane, 1-ethyl-2-methyl-, cis-	790	341	4923-77-7	mainlib	C9H18	126
5	Cyclopropane, 3-chloro-1,1,2,2-tetramethyl-	787	301	14123-41-2	mainlib	C7H13Cl	132

Benzene, propyl-



1st Dimension R.T. = 528.972

2nd Dimension R.T. = 1.307

Quant Mass(es) = 91

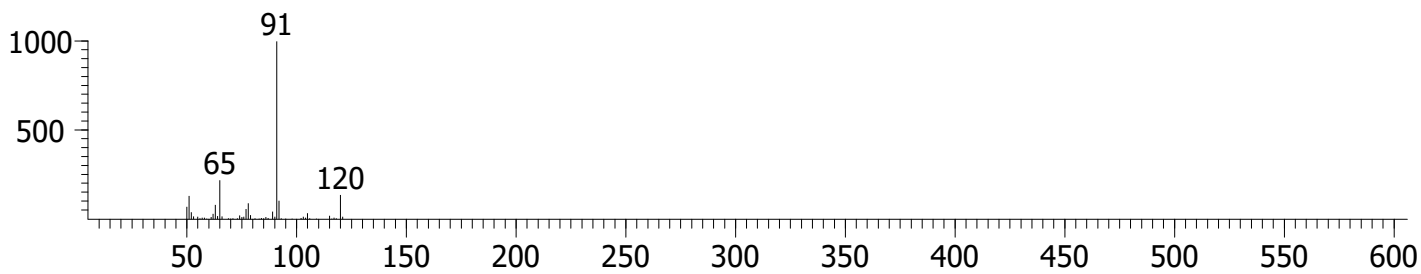
S/N = 2744.6

Area = 819438

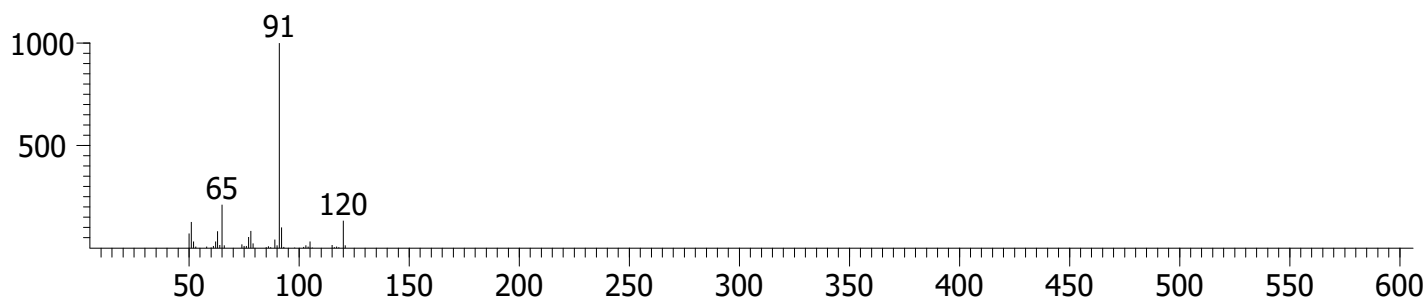
Height = 104231

Similarity = 894

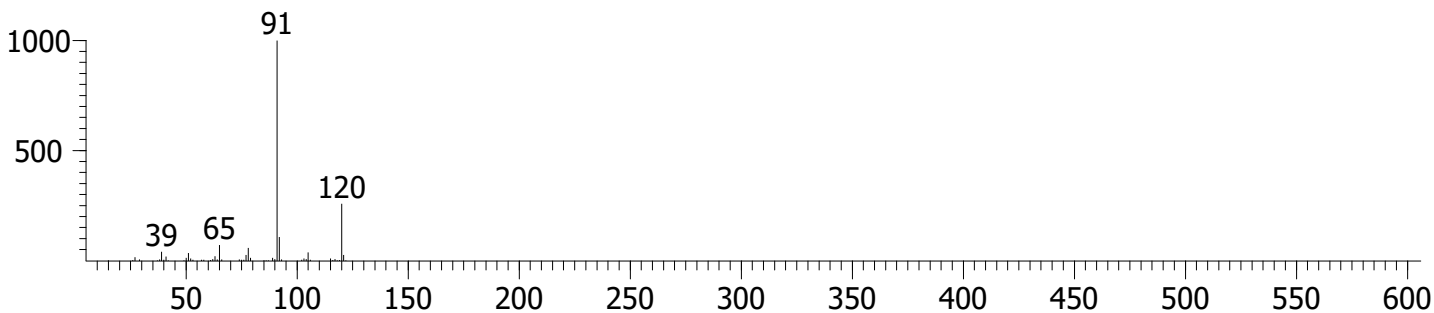
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 101, at 528.972 , 1.307 sec , sec (Spec # 7618)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 101, at 528.972 , 1.307 sec , sec (Spec # 7618)



Library Hit - similarity 894, "Benzene, propyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, propyl-	894	2357	103-65-1	mainlib	C9H12	120
2	Propanedinitrile, (1-methyl-3-phenylpropylidene)-	866	680	69564-94-9	mainlib	C13H12N2	196
3	1,3,5-Cycloheptatriene, 7-ethyl-	866	680	17634-51-4	mainlib	C9H12	120
4	Acetamide, 2-(4-benzyloxyphenoxy]-N-(3-tolyl)-	862	575	0-00-0	mainlib	C22H21NO3	347
5	[4-(Benzyloxy)phenyl]methanamine	859	508	22171-15-9	mainlib	C14H15NO	213

3-Hexene-2,5-dione

1st Dimension R.T. = 528.972

2nd Dimension R.T. = 1.676

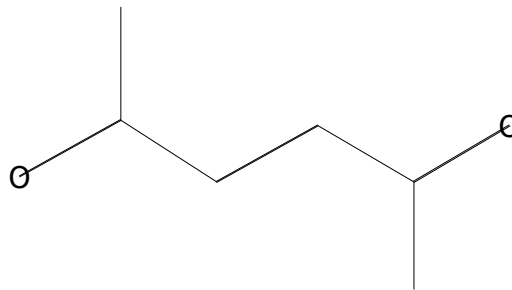
Quant Mass(es) = 97

S/N = 8442.1

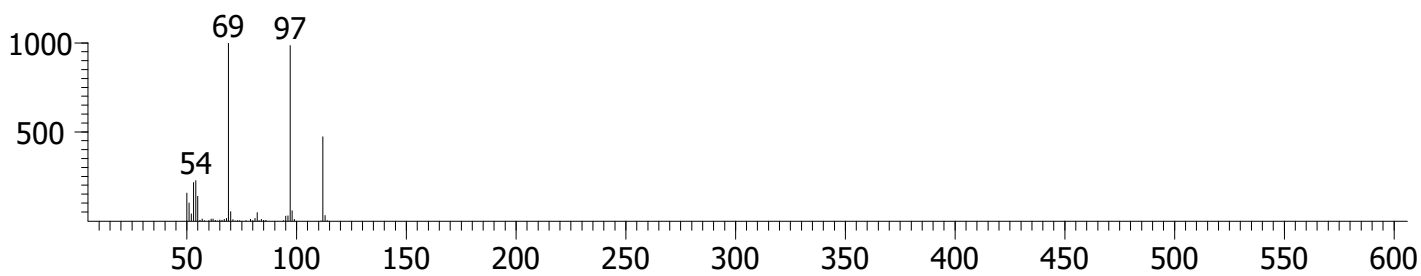
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Height = 292015

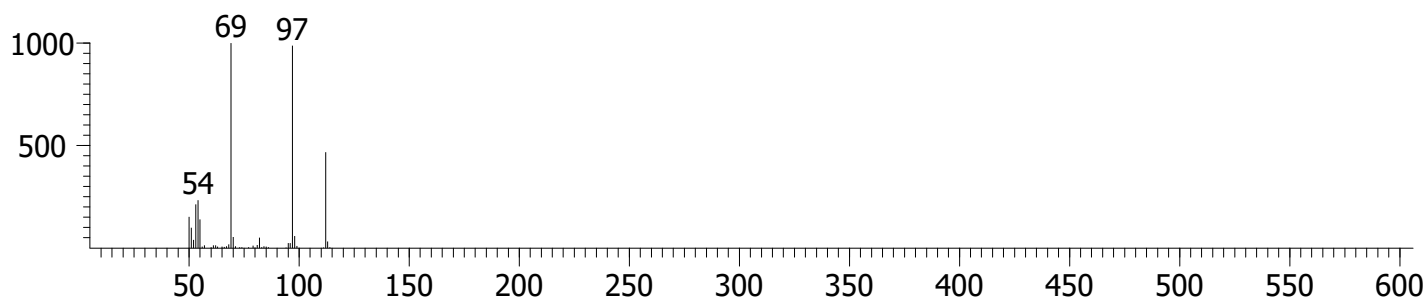
Similarity = 871



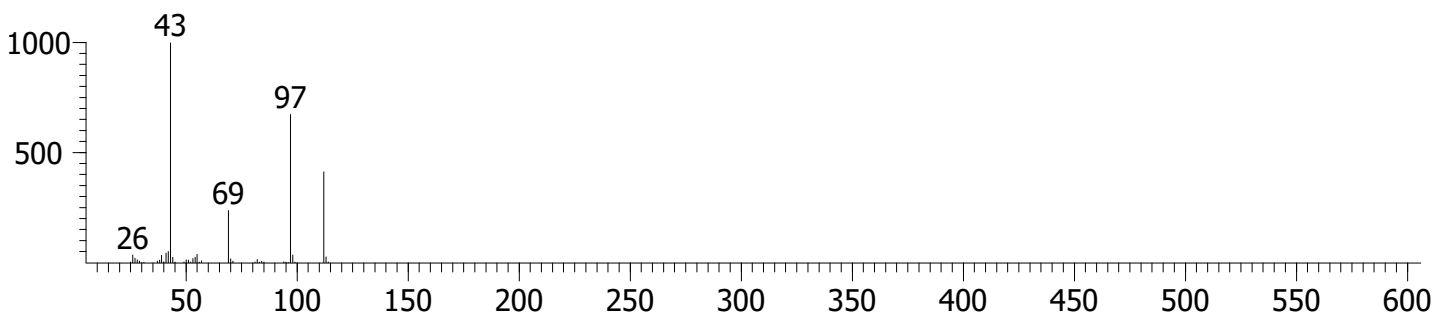
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 106, at 528.972 , 1.676 sec , sec (Spec # 7674)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 106, at 528.972 , 1.676 sec , sec (Spec # 7674)



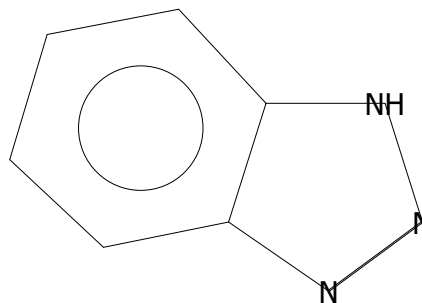
Library Hit - similarity 871, "3-Hexene-2,5-dione"



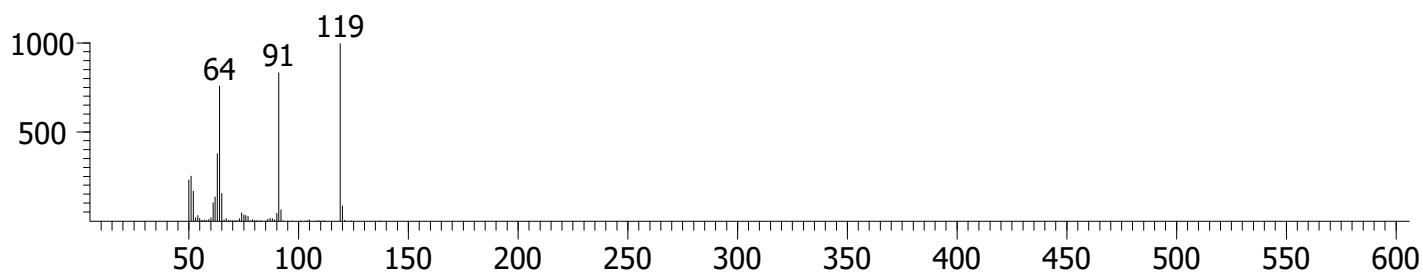
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Hexene-2,5-dione	871	5650	4436-75-3	mainlib	C6H8O2	112
2	2(5H)-Furanone, 5,5-dimethyl-	850	2403	20019-64-1	mainlib	C6H8O2	112
3	3-Hexen-2-one, 3-methyl-	825	733	1187-80-0	mainlib	C7H12O	112
4	Cyclopentanecarboxylic acid, 2-fluorophenyl ester	807	378	0-00-0	mainlib	C12H13FO2	208
5	Cyclopentanecarboxylic acid, 3-fluorophenyl ester	807	378	0-00-0	mainlib	C12H13FO2	208

1H-Benzotriazole

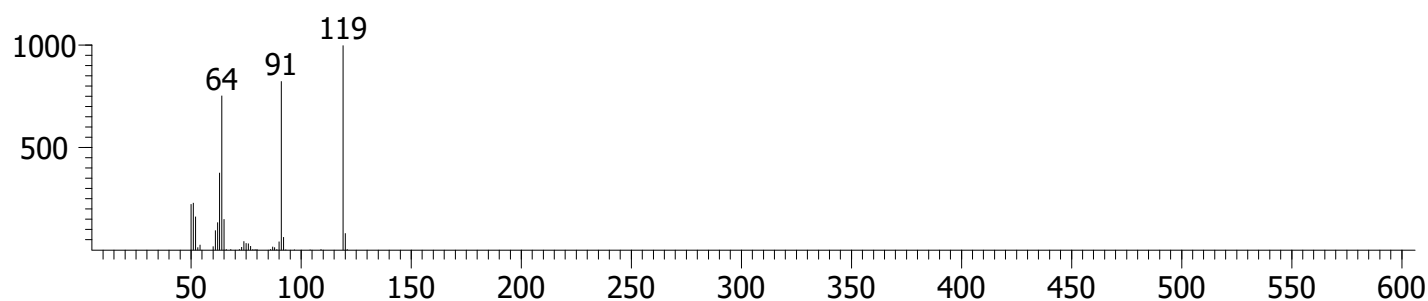
1st Dimension R.T. = 535.968
2nd Dimension R.T. = 1.406
Quant Mass(es) = 119
S/N = 3061.5
Area = 386216
Height = 62101
Similarity = 922



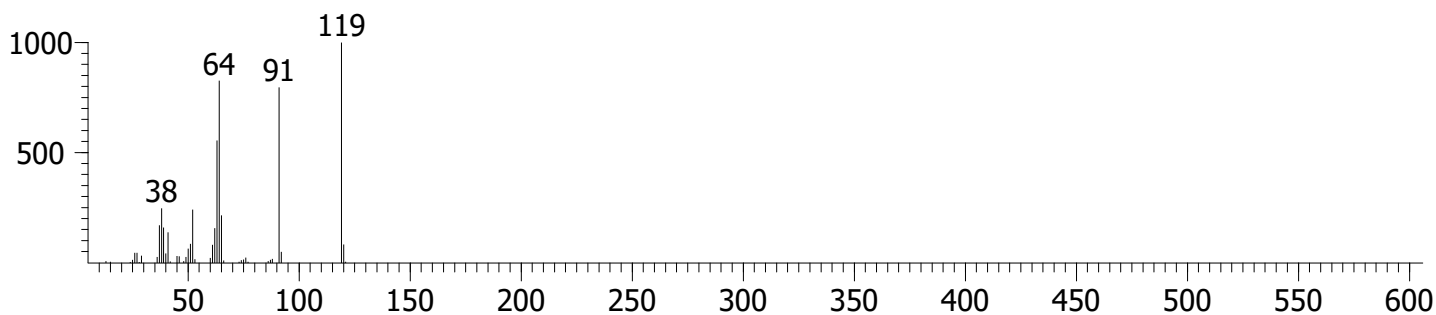
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 117, at 535.968 , 1.406 sec , sec (Spec # 8693)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 117, at 535.968 , 1.406 sec , sec (Spec # 8693)



Library Hit - similarity 922, "1H-Benzotriazole"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Proximpam	964	4827	2828-42-4	mainlib	C10H12N2O2	192
2	Carbamoyl chloride, phenyl-	947	2634	2040-76-8	mainlib	C7H6ClNO	155
3	1H-Benzotriazole	922	803	95-14-7	mainlib	C6H5N3	119
4	1H-Benzotriazole-1-carboxaldehyde	899	293	72773-04-7	mainlib	C7H5N3O	147
5	Benzene, isocyanato-	898	282	103-71-9	mainlib	C7H5NO	119

3-Ethylcyclopentanone

1st Dimension R.T. = 535.968

2nd Dimension R.T. = 1.459

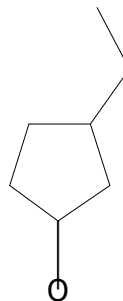
Quant Mass(es) = 83

S/N = 251.70

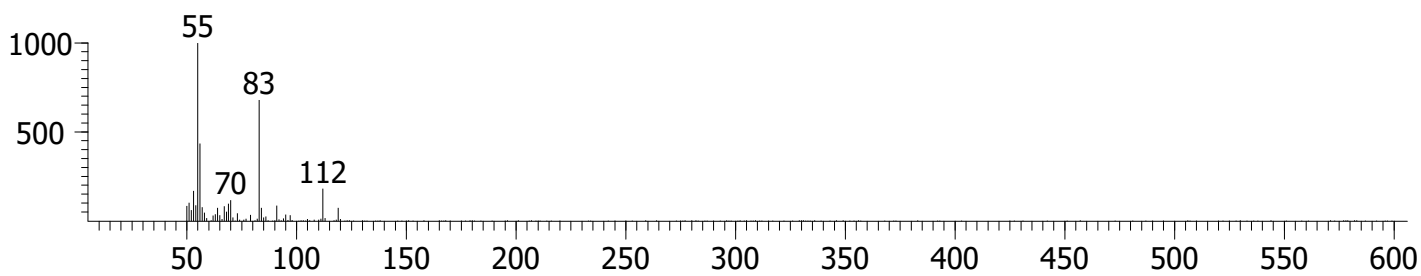
Area = 76991

Height = 9008.9

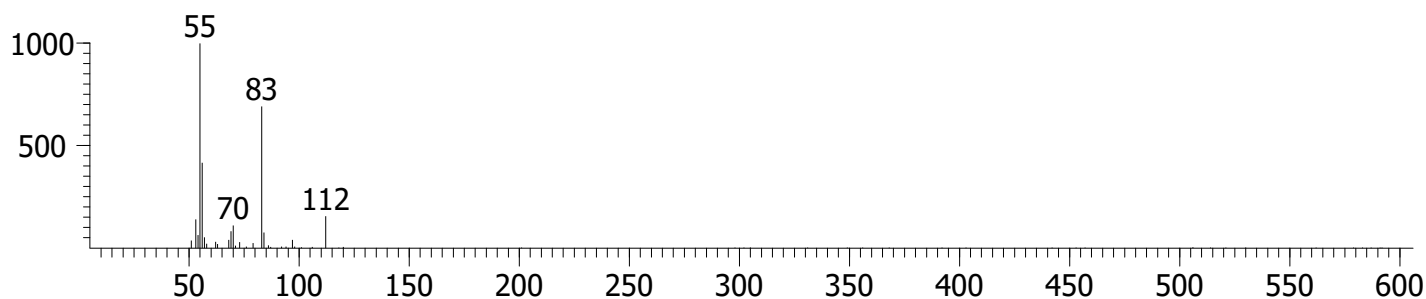
Similarity = 892



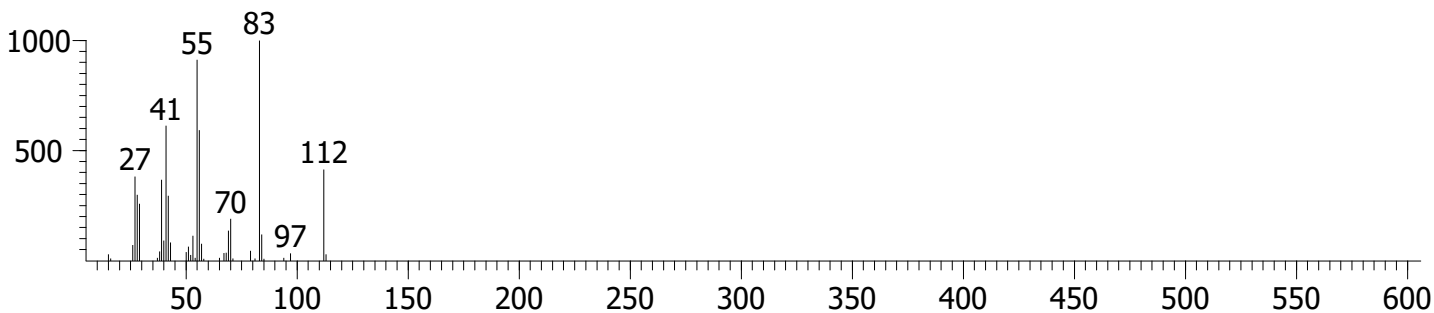
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 118, at 535.968 , 1.459 sec , sec (Spec # 8701)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 118, at 535.968 , 1.459 sec , sec (Spec # 8701)



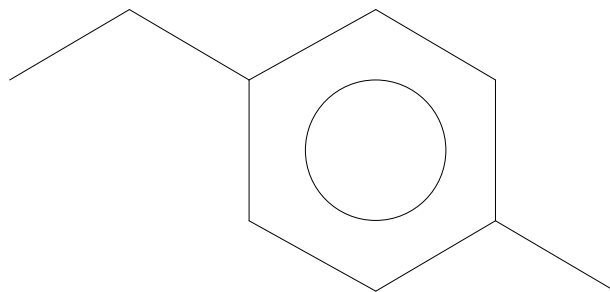
Library Hit - similarity 892, "3-Ethylcyclopentanone"



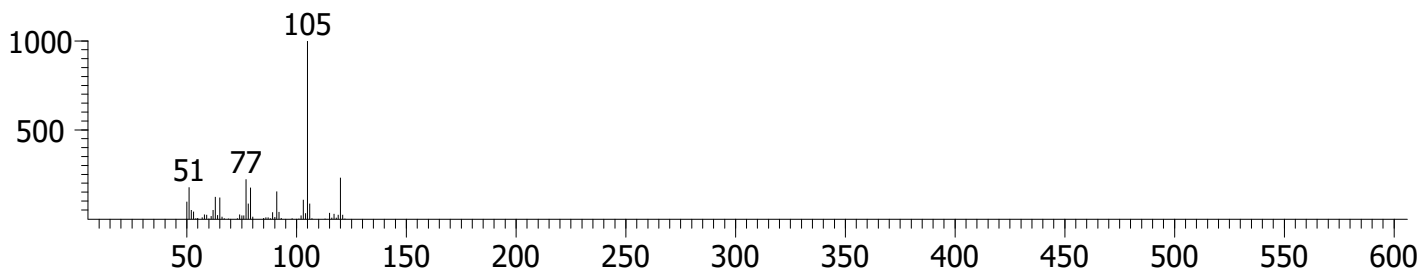
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Ethylcyclopentanone	892	4729	10264-55-8	mainlib	C7H12O	112
2	3-Heptene, 5-methyl-	846	998	13172-91-3	mainlib	C8H16	112
3	2-Hexene, 2,3-dimethyl-	838	744	7145-20-2	mainlib	C8H16	112
4	3-Ethyl-3-hexene	818	339	16789-51-8	mainlib	C8H16	112
5	4-Ethyl-2-hexene	810	253	19780-46-2	mainlib	C8H16	112

Benzene, 1-ethyl-4-methyl-

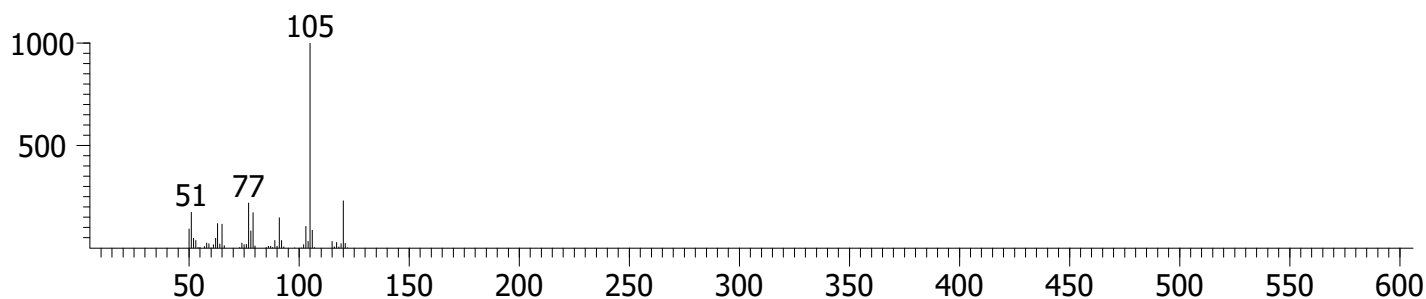
1st Dimension R.T. = 539.466
2nd Dimension R.T. = 1.327
Quant Mass(es) = 105
S/N = 13801
Area = 3567742
Height = 483997
Similarity = 917



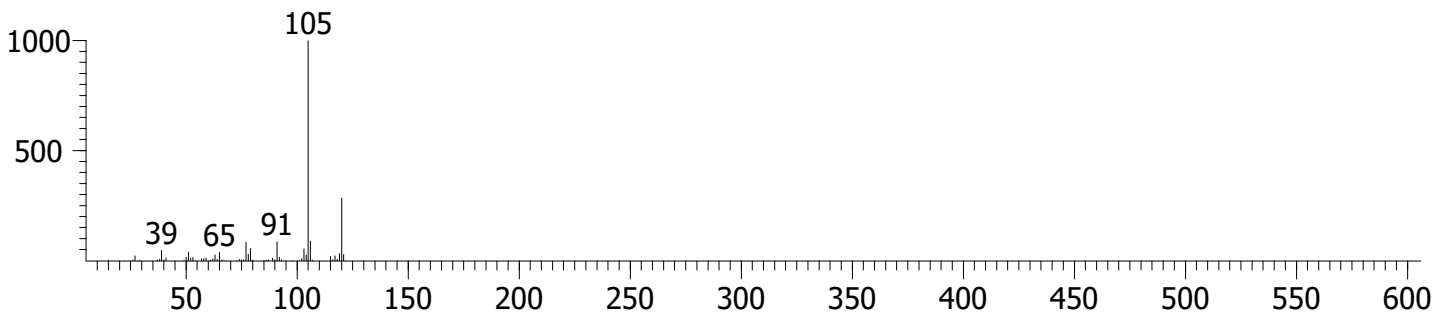
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 121, at 539.466 , 1.327 sec , sec (Spec # 9211)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 121, at 539.466 , 1.327 sec , sec (Spec # 9211)



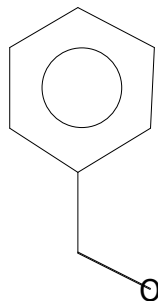
Library Hit - similarity 917, "Benzene, 1-ethyl-4-methyl-"



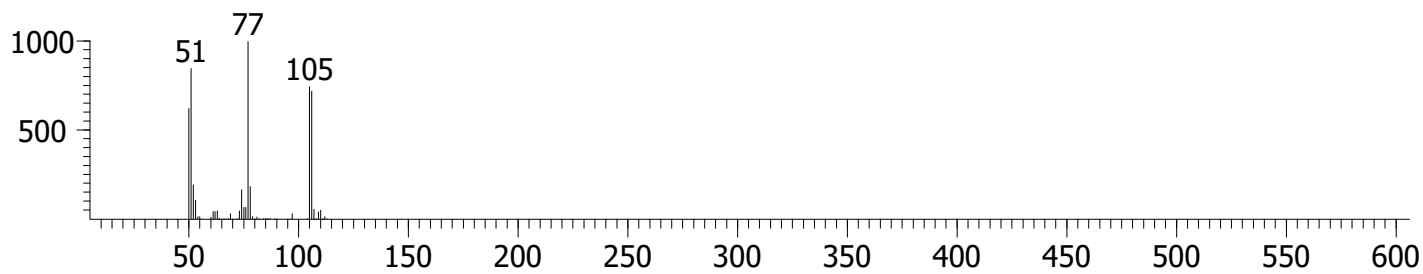
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-ethyl-4-methyl-	917	2035	622-96-8	mainlib	C9H12	120
2	Benzene, 1-ethyl-3-methyl-	915	1877	620-14-4	mainlib	C9H12	120
3	Benzene, 1-ethyl-2-methyl-	912	1658	611-14-3	mainlib	C9H12	120
4	Benzene, (1-methylethyl)-	902	1171	98-82-8	mainlib	C9H12	120
5	Benzene, 1,2,3-trimethyl-	894	873	526-73-8	mainlib	C9H12	120

Benzaldehyde

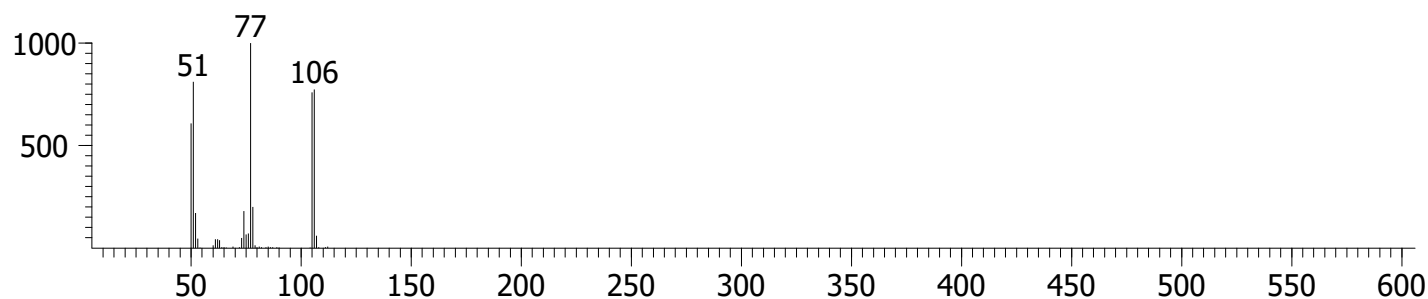
1st Dimension R.T. = 542.964
2nd Dimension R.T. = 1.637
Quant Mass(es) = 106
S/N = 6998.9
Area = 785867
Height = 112419
Similarity = 889



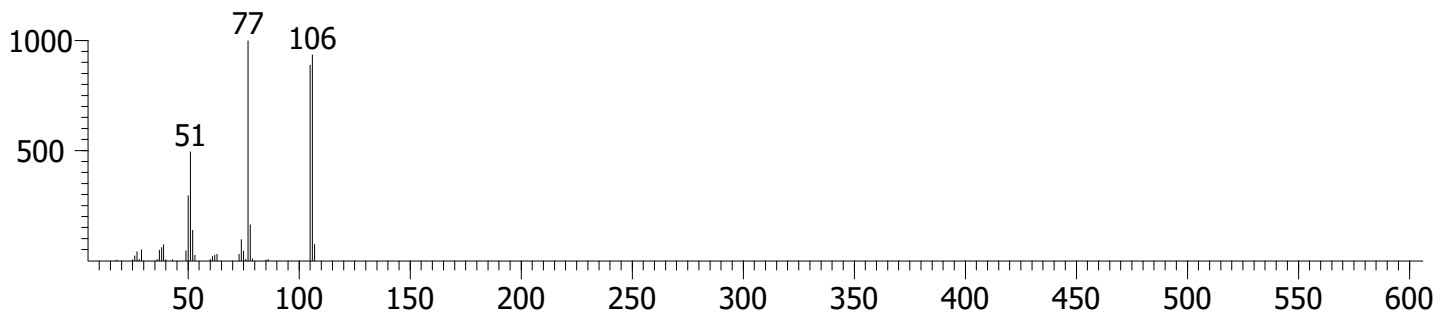
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 124, at 542.964 , 1.637 sec , sec (Spec # 9788)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 124, at 542.964 , 1.637 sec , sec (Spec # 9788)



Library Hit - similarity 889, "Benzaldehyde"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzaldehyde	889	5374	100-52-7	mainlib	C7H6O	106
2	1,2,4-Trioxolane, 3,5-diphenyl-	844	1144	23888-15-5	mainlib	C14H12O3	228
3	Bis[4-acetamidophenylsulfonyl]phenyl methane	840	967	81269-03-6	mainlib	C23H22N2O6S2	486
4	1,2,4-Trioxolane, 3-phenyl-	824	556	23253-30-7	mainlib	C8H8O3	152
5	Ethanone, 2-amino-1-phenyl-	820	470	613-89-8	mainlib	C8H9NO	135

Dimethyl trisulfide

1st Dimension R.T. = 556.956

2nd Dimension R.T. = 1.624

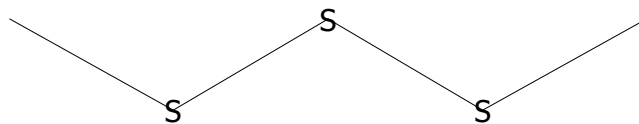
Quant Mass(es) = 126

S/N = 609.80

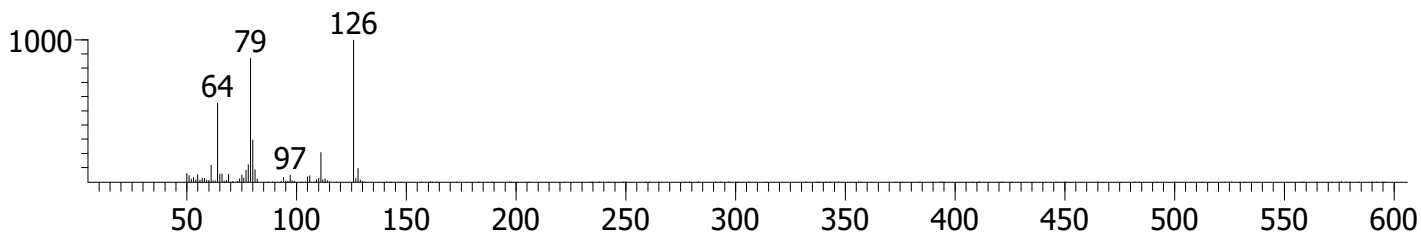
Area = 74036

Height = 10209

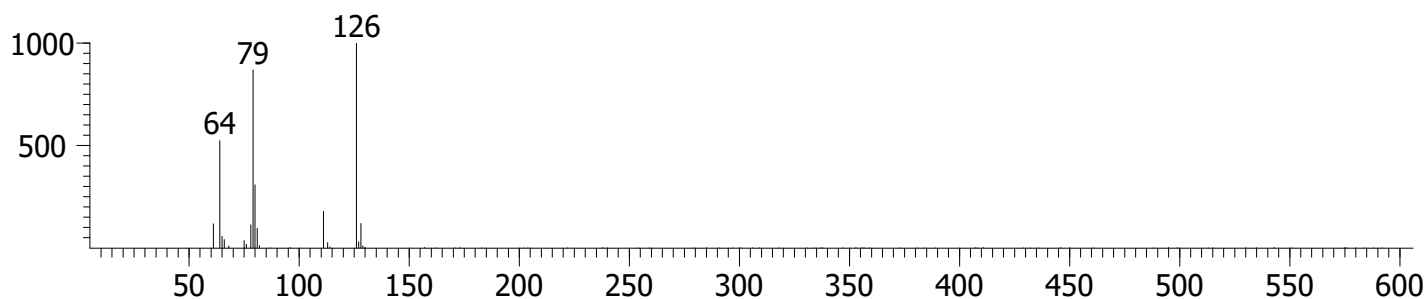
Similarity = 930



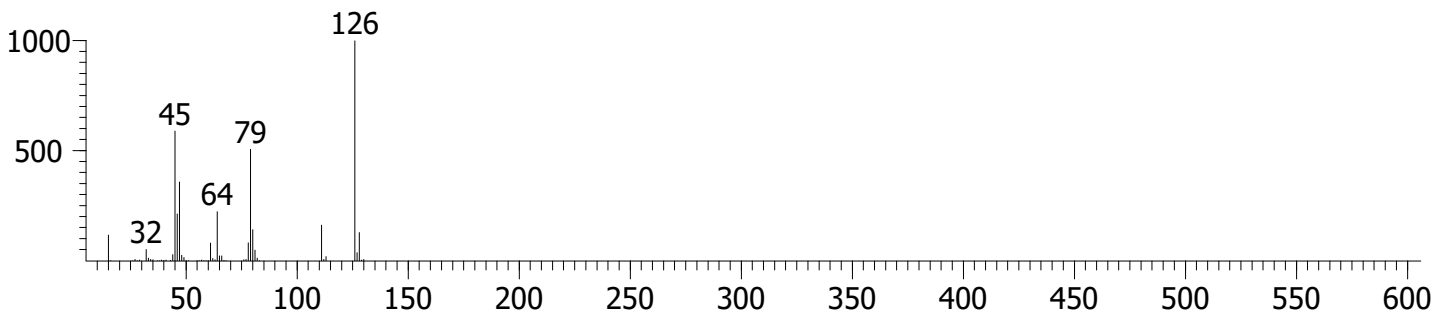
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 148, at 556.956 , 1.624 sec , sec (Spec # 11906)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 148, at 556.956 , 1.624 sec , sec (Spec # 11906)



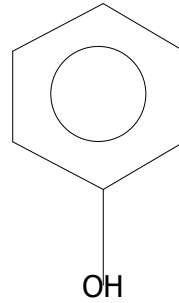
Library Hit - similarity 930, "Dimethyl trisulfide"



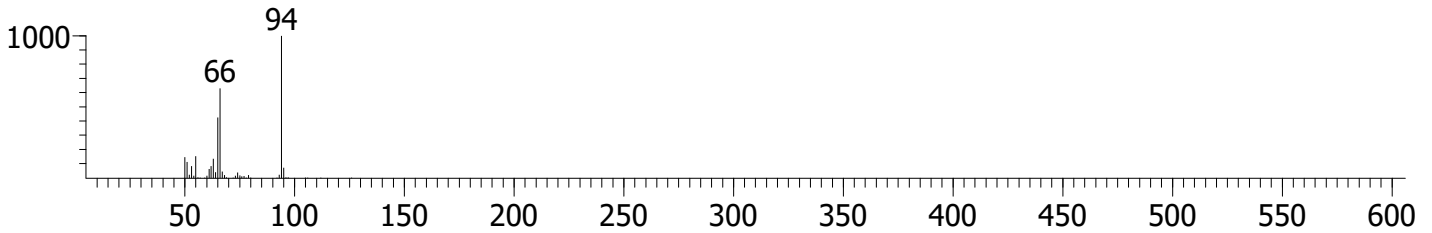
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Dimethyl trisulfide	930	9775	3658-80-8	mainlib	C2H6S3	126
2	Bis-(methylthio)-phosphine	669	97	105414-86-6	mainlib	C2H7PS2	126
3	Thiophosphordiamide, S-methyl ester	661	72	0-00-0	mainlib	CH7N2OPS	126
4	S-Methyl methanethiosulphonate	606	14	2949-92-0	mainlib	C2H6O2S2	126
5	Pentasulfide, dimethyl	604	13	7330-31-6	mainlib	C2H6S5	190

Phenol

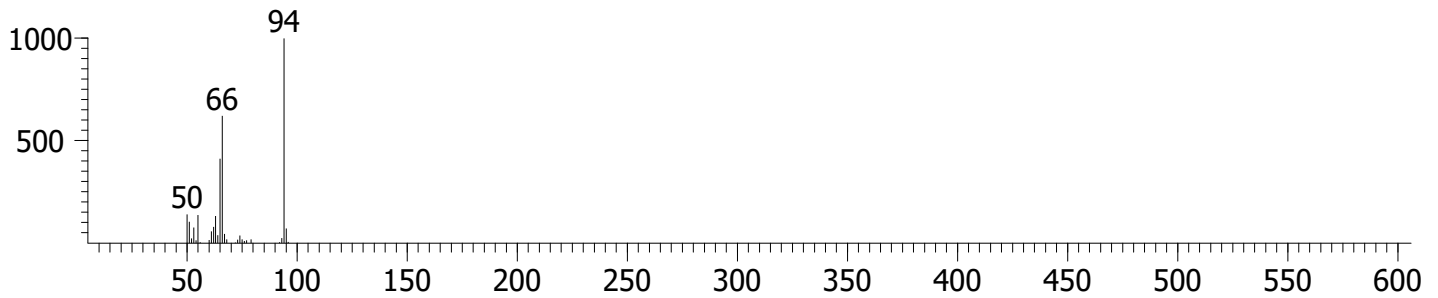
1st Dimension R.T. = 560.454
2nd Dimension R.T. = 1.584
Quant Mass(es) = 94
S/N = 25771
Area = 5949848
Height = 870160
Similarity = 957



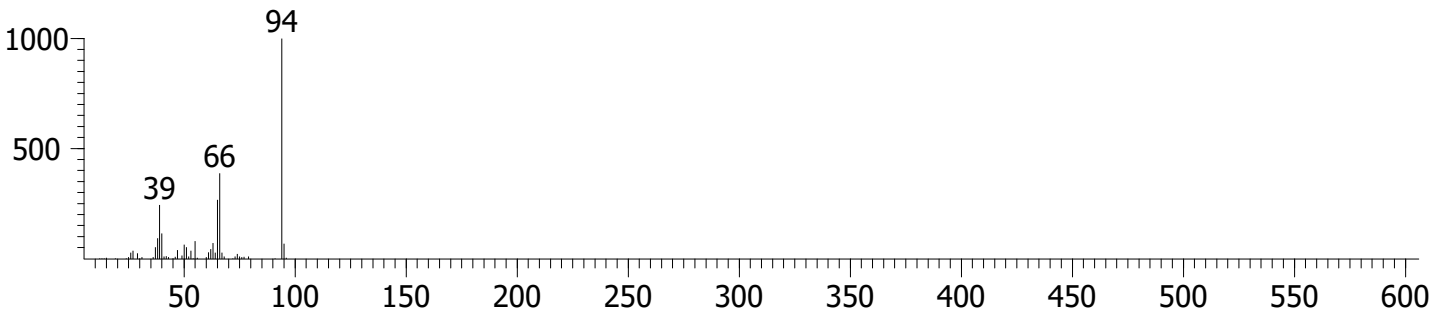
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 158, at 560.454 , 1.584 sec , sec (Spec # 12430)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 158, at 560.454 , 1.584 sec , sec (Spec # 12430)



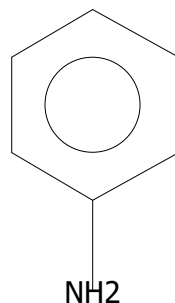
Library Hit - similarity 957, "Phenol"



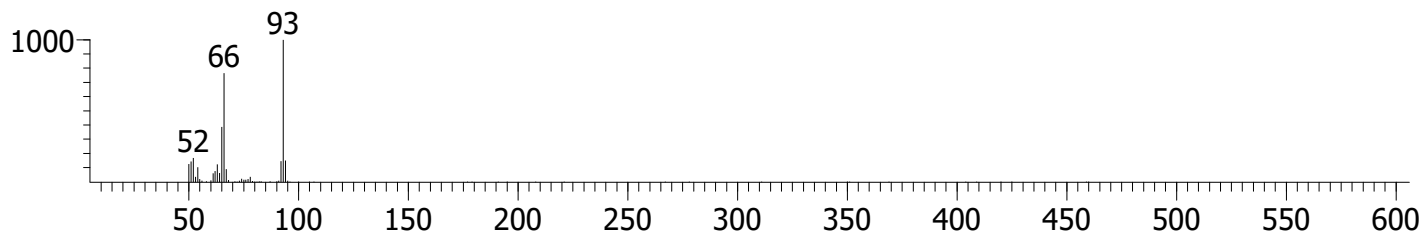
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol	957	4468	108-95-2	mainlib	C6H6O	94
2	Phosphonic acid, (p-hydroxyphenyl)-	946	3065	33795-18-5	mainlib	C6H7O4P	174
3	Carbamic acid, phenyl ester	933	1980	622-46-8	mainlib	C7H7NO2	137
4	2-Vinylfuran	848	178	1487-18-9	mainlib	C6H6O	94
5	Formic acid phenyl ester	846	164	1864-94-4	mainlib	C7H6O2	122

Aniline

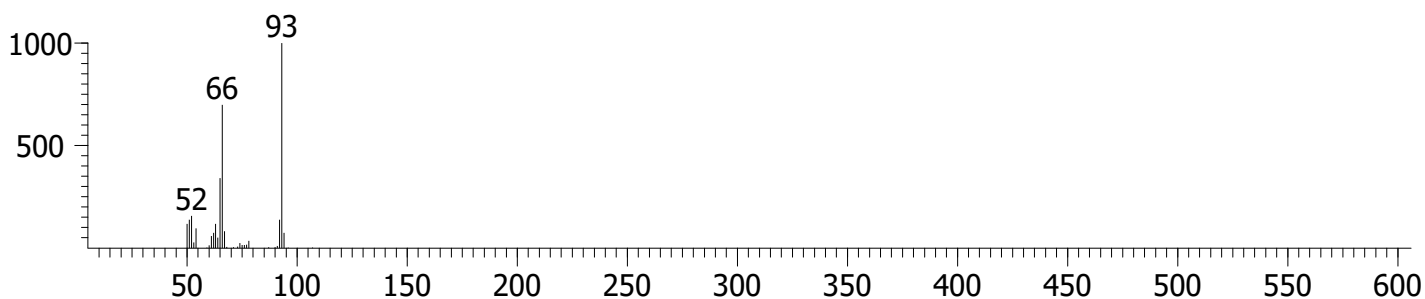
1st Dimension R.T. = 563.952
2nd Dimension R.T. = 1.775
Quant Mass(es) = 93
S/N = 1138.5
Area = 217340
Height = 27616
Similarity = 948



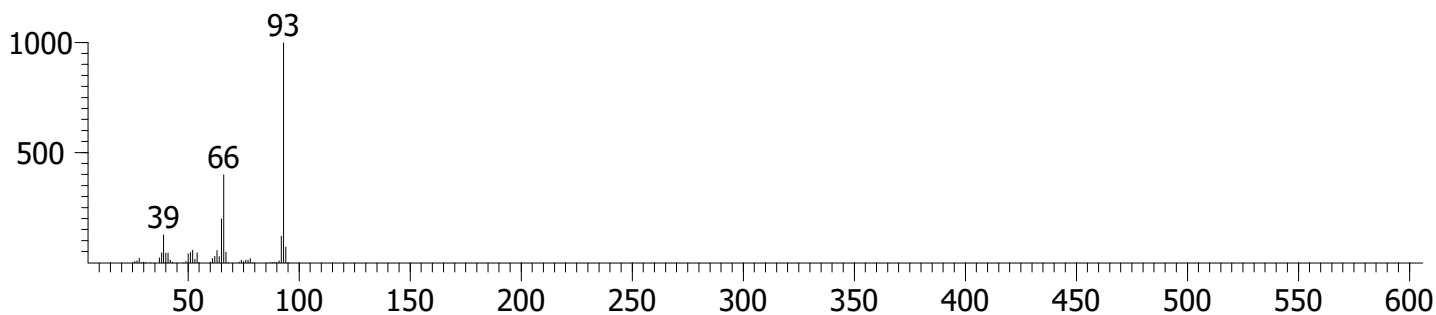
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 168, at 563.952 , 1.775 sec , sec (Spec # 12989)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 168, at 563.952 , 1.775 sec , sec (Spec # 12989)



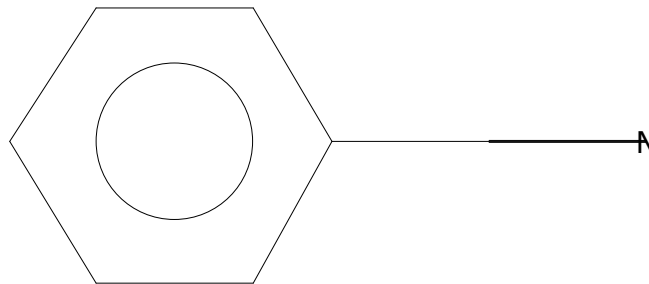
Library Hit - similarity 948, "Aniline"



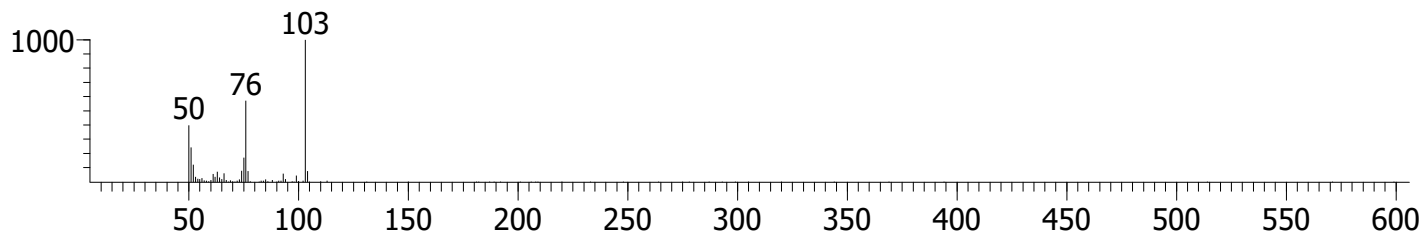
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Aniline	948	5596	62-53-3	mainlib	C6H7N	93
2	Silanediamine, 1,1-dimethyl-N,N'-diphenyl-	931	3054	13435-09-1	mainlib	C14H18N2Si	242
3	Pyridine, 3-methyl-	884	638	108-99-6	mainlib	C6H7N	93
4	Pyridine, 4-methyl-	860	214	108-89-4	mainlib	C6H7N	93
5	2-Pyridineacetic acid	856	180	13115-43-0	mainlib	C7H7NO2	137

Benzonitrile

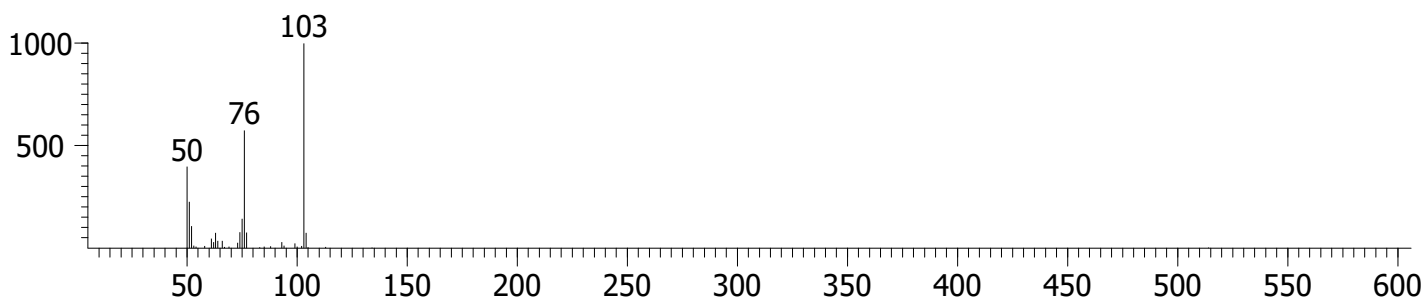
1st Dimension R.T. = 574.446
2nd Dimension R.T. = 1.723
Quant Mass(es) = 103
S/N = 743.24
Area = 107603
Height = 14837
Similarity = 951



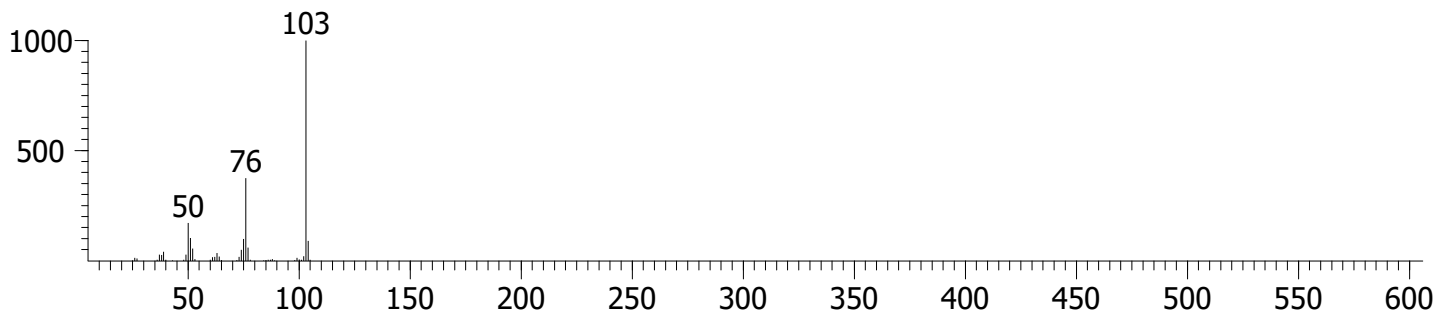
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 197, at 574.446 , 1.723 sec , sec (Spec # 14571)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 197, at 574.446 , 1.723 sec , sec (Spec # 14571)



Library Hit - similarity 951, "Benzonitrile"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzonitrile	951	5002	100-47-0	mainlib	C7H5N	103
2	2-Ethynyl pyridine	942	3631	1945-84-2	mainlib	C7H5N	103
3	Tricyclo[3.1.0.0(2,4)]hex-3-ene-3-carbonitrile	901	828	103495-51-8	mainlib	C7H5N	103
4	Bicyclo[2.2.2]octa-2,5-diene-2-carbonitrile	876	252	39863-23-5	mainlib	C9H9N	131
5	6H-1,2,5-Oxadiazine-6-thione, 4,5-dihydro-3-phenyl-	862	158	33406-07-4	mainlib	C9H8N2OS	192

Pyridine, 2,3,5-trimethyl-

1st Dimension R.T. = 577.944

2nd Dimension R.T. = 1.459

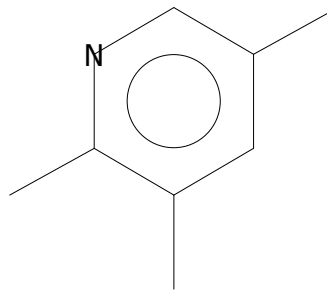
Quant Mass(es) = 121

S/N = 372.38

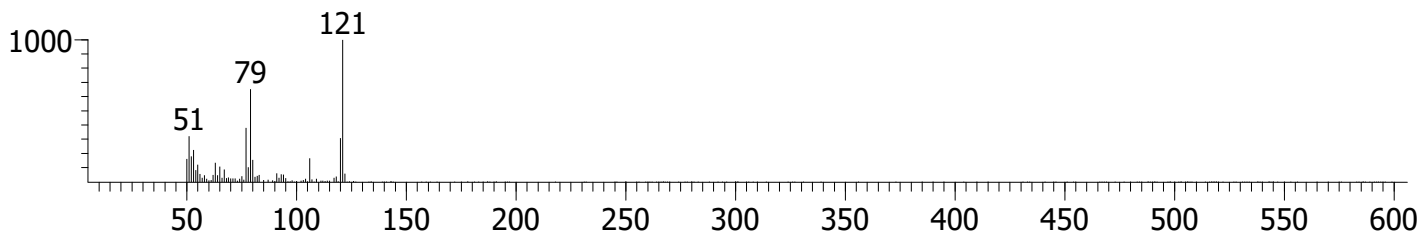
Area = 45204

Height = 5686.5

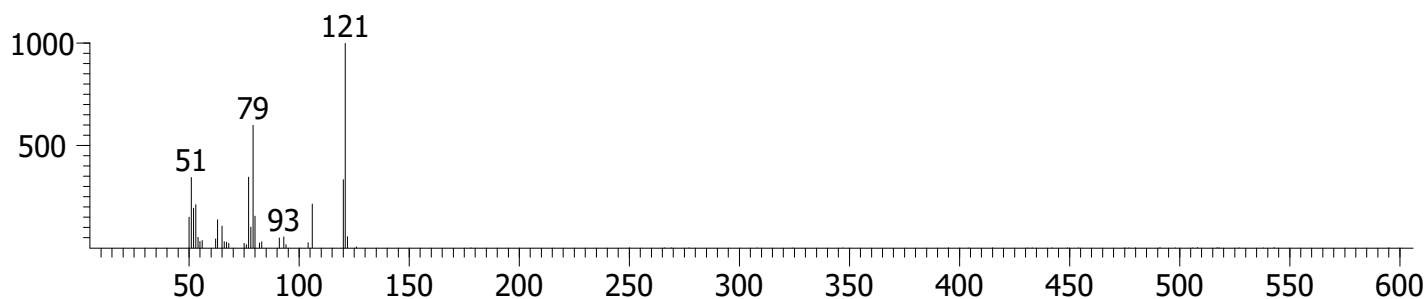
Similarity = 922



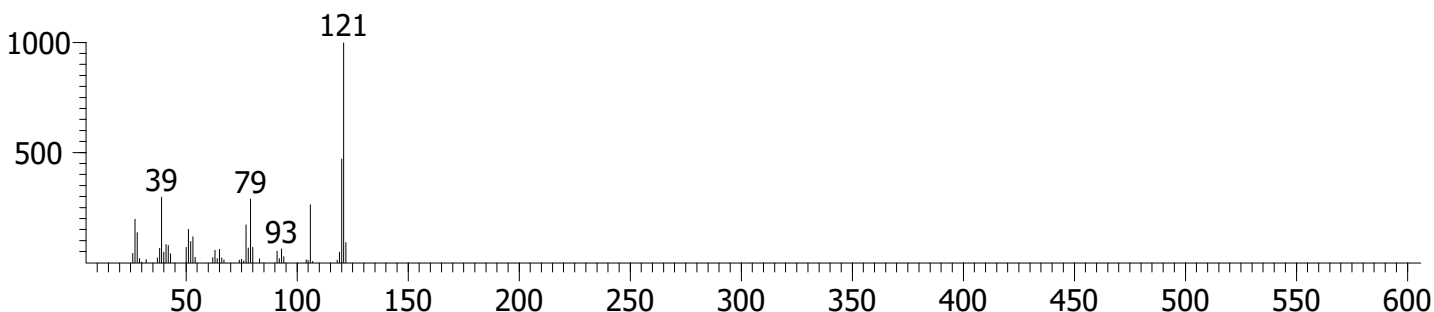
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 201, at 577.944 , 1.459 sec , sec (Spec # 15061)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 201, at 577.944 , 1.459 sec , sec (Spec # 15061)



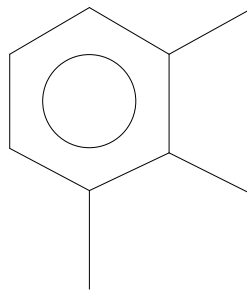
Library Hit - similarity 922, "Pyridine, 2,3,5-trimethyl-"



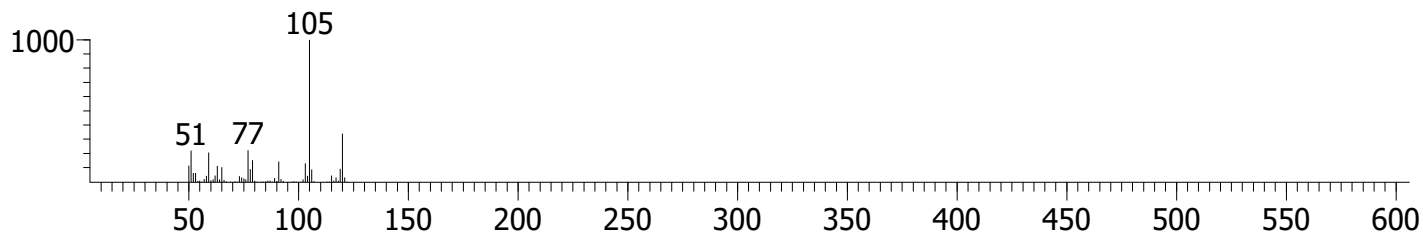
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pyridine, 2,3,5-trimethyl-	922	5787	695-98-7	mainlib	C8H11N	121
2	Pyridine, 2,3,6-trimethyl-	899	2113	1462-84-6	mainlib	C8H11N	121
3	Pyridine, 2,4,6-trimethyl-	888	1450	108-75-8	mainlib	C8H11N	121
4	N-Fluoro-2,4,6-trimethylpyridinium trifluoromethanesulfonate	803	130	107264-00-6	mainlib	C9H11F4NO3S	289
5	Pyridine, 3-ethyl-5-methyl-	795	97	3999-78-8	mainlib	C8H11N	121

Benzene, 1,2,3-trimethyl-

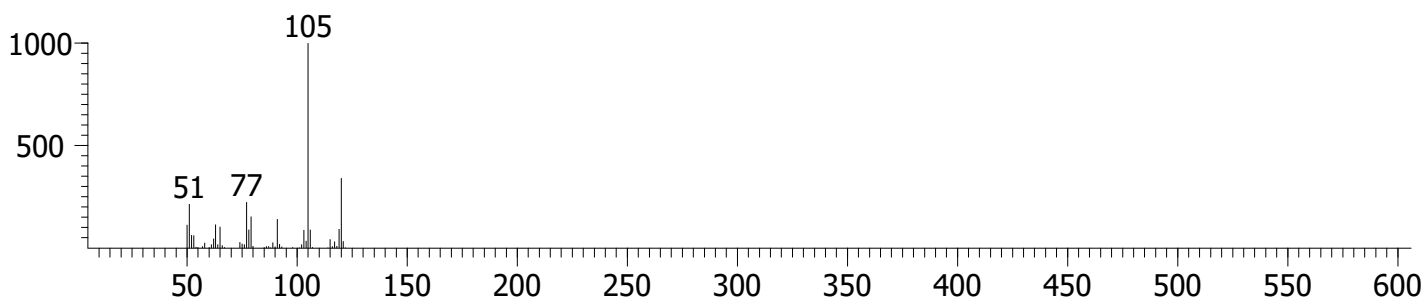
1st Dimension R.T. = 581.442
2nd Dimension R.T. = 1.373
Quant Mass(es) = 105
S/N = 12672
Area = 2460637
Height = 355064
Similarity = 961



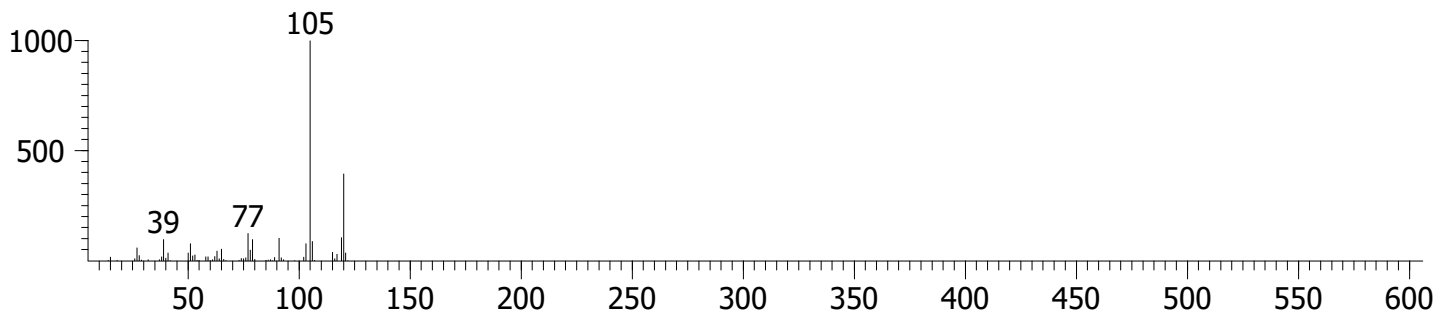
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 205, at 581.442 , 1.373 sec , sec (Spec # 15578)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 205, at 581.442 , 1.373 sec , sec (Spec # 15578)



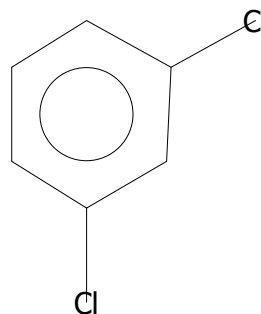
Library Hit - similarity 961, "Benzene, 1,2,3-trimethyl-"



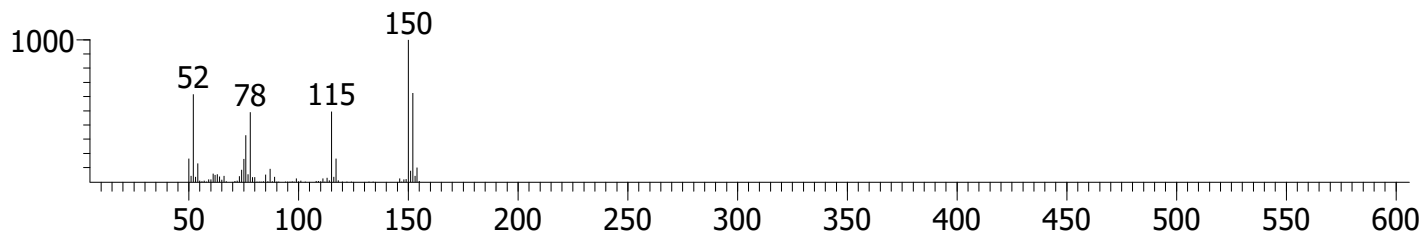
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1,2,3-trimethyl-	961	5796	526-73-8	mainlib	C9H12	120
2	Benzene, 1,2,4-trimethyl-	936	1768	95-63-6	mainlib	C9H12	120
3	2,4-Nonadiyne	912	592	63621-15-8	mainlib	C9H12	120
4	Benzene, 1-ethyl-3-methyl-	900	394	620-14-4	mainlib	C9H12	120
5	Benzene, 1-ethyl-4-methyl-	899	379	622-96-8	mainlib	C9H12	120

Benzene, 1,3-dichloro-

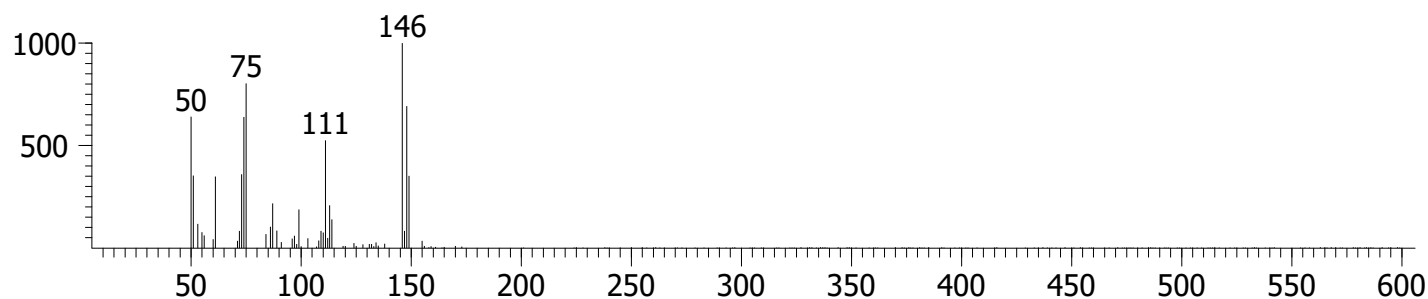
1st Dimension R.T. = 609.426
2nd Dimension R.T. = 1.518
Quant Mass(es) = 146
S/N = 762.55
Area = 87252
Height = 13961
Similarity = 734



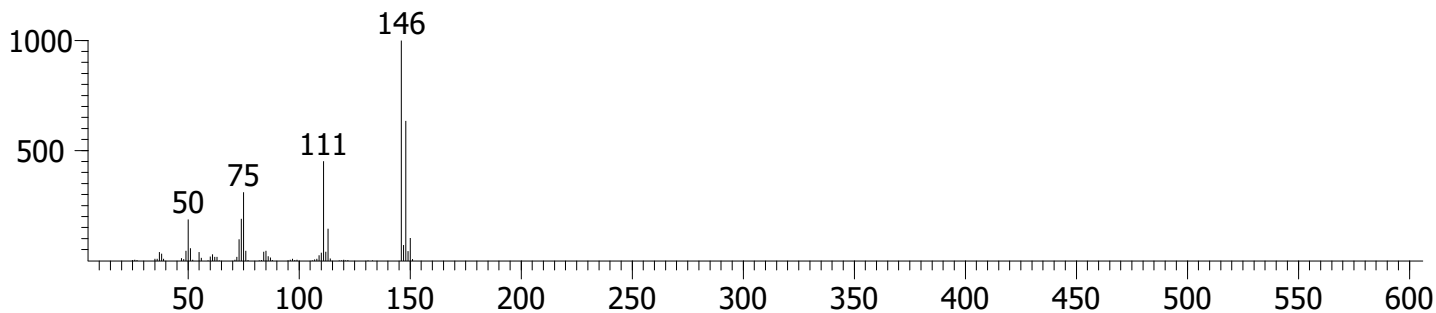
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 263, at 609.426 , 1.518 sec , sec (Spec # 19840)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 263, at 609.426 , 1.518 sec , sec (Spec # 19840)



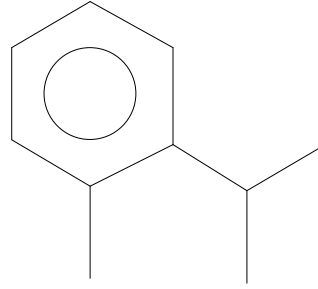
Library Hit - similarity 734, "Benzene, 1,3-dichloro-"



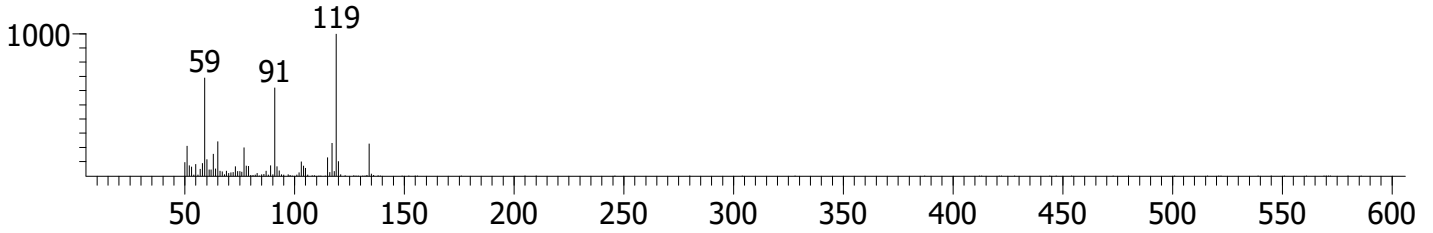
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1,3-dichloro-	734	6867	541-73-1	mainlib	C6H4Cl2	146
2	Benzene, 1,4-dichloro-	709	2094	106-46-7	mainlib	C6H4Cl2	146
3	Benzene, 1,2-dichloro-	688	891	95-50-1	mainlib	C6H4Cl2	146
4	2,5-Dichloro-2,4,6-cycloheptatrien-1-one	592	71	7157-27-9	mainlib	C7H4Cl2O	174
5	2-Chloro-6-fluorophenol, pentyl ether	542	14	0-00-0	mainlib	C11H14ClFO	216

o-Cymene

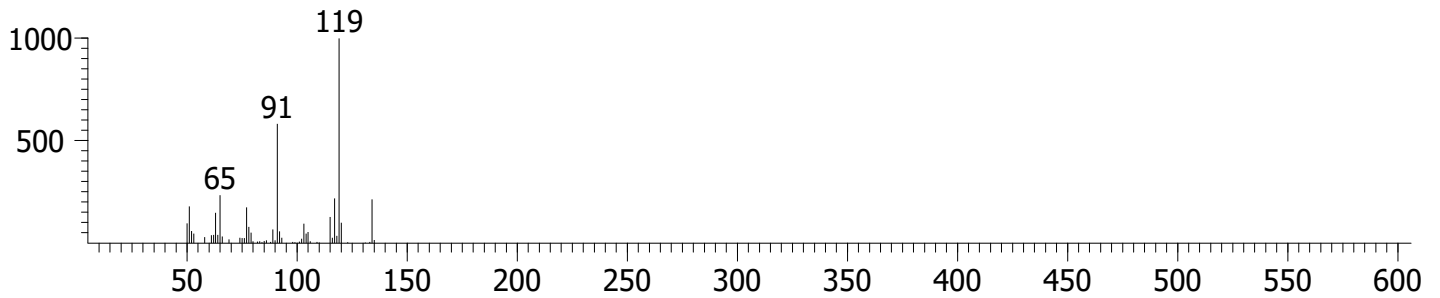
1st Dimension R.T. = 623.418
2nd Dimension R.T. = 1.353
Quant Mass(es) = 119
S/N = 875.78
Area = 97954
Height = 13547
Similarity = 963



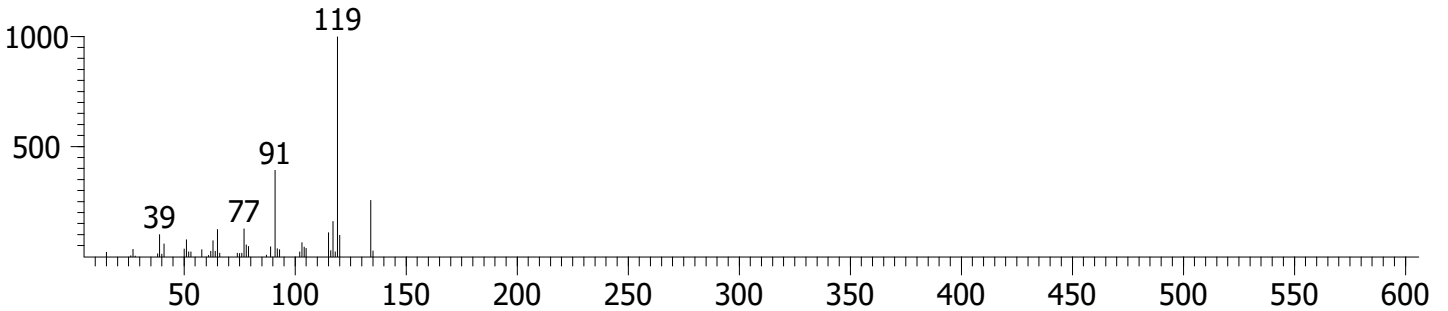
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 296, at 623.418 , 1.353 sec , sec (Spec # 21935)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 296, at 623.418 , 1.353 sec , sec (Spec # 21935)



Library Hit - similarity 963, "o-Cymene"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	o-Cymene	963	6612	527-84-4	mainlib	C10H14	134
2	1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	903	1173	3479-89-8	mainlib	C10H14	134
3	p-Cymene	887	675	99-87-6	mainlib	C10H14	134
4	Benzene, 1-methyl-3-(1-methylethyl)-	876	463	535-77-3	mainlib	C10H14	134
5	Benzene, 2-ethyl-1,3-dimethyl-	829	97	2870-04-4	mainlib	C10H14	134

Eucalyptol

1st Dimension R.T. = 633.912

2nd Dimension R.T. = 1.333

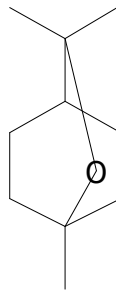
Quant Mass(es) = 108

S/N = 120.19

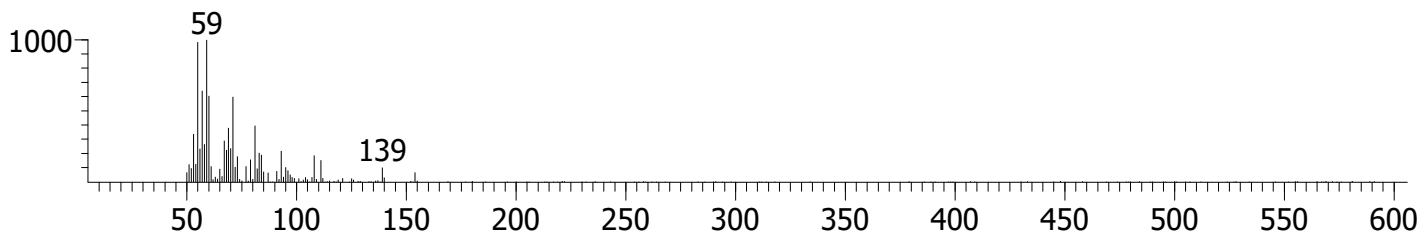
Area = 8095.4

Height = 797.19

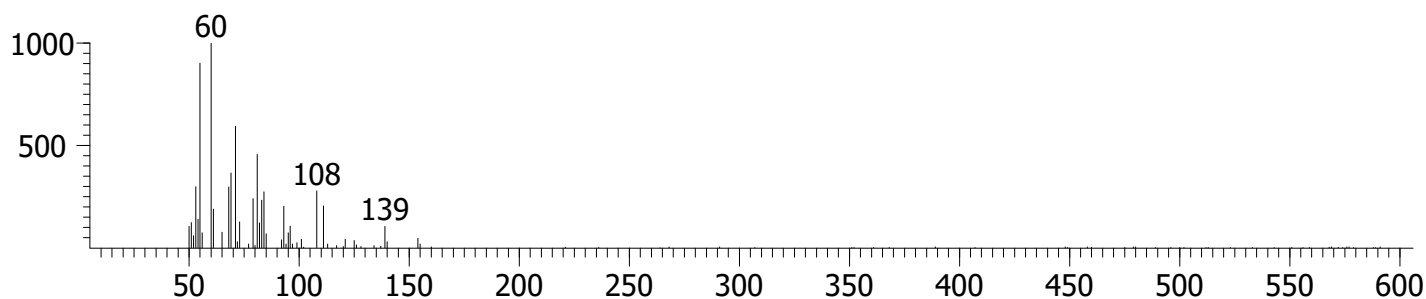
Similarity = 662



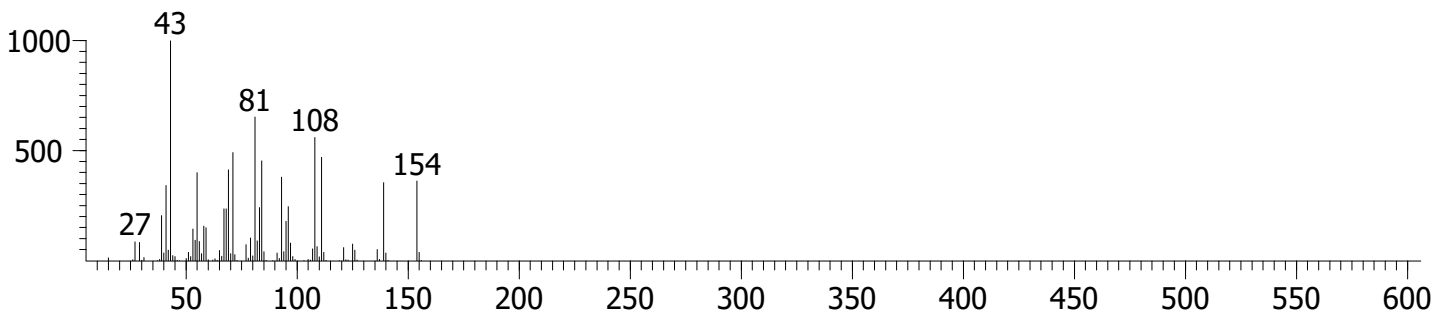
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 322, at 633.912 , 1.333 sec , sec (Spec # 23522)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 322, at 633.912 , 1.333 sec , sec (Spec # 23522)



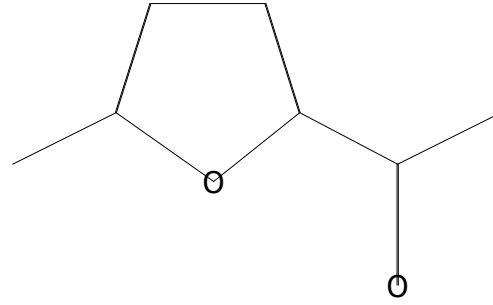
Library Hit - similarity 662, "Eucalyptol"



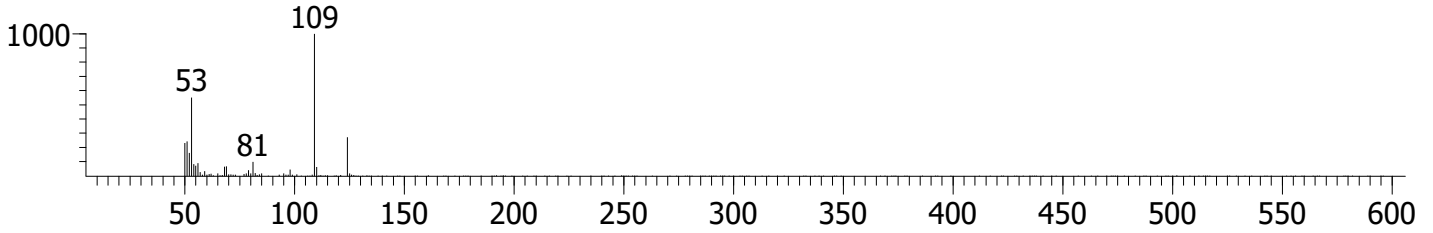
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Eucalyptol	662	2333	470-82-6	mainlib	C10H18O	154
2	1,7-Octadien-3-ol, 2,6-dimethyl-	630	623	22460-59-9	mainlib	C10H18O	154
3	7-Octene-2,6-diol, 2,6-dimethyl-	625	502	29210-77-3	mainlib	C10H20O2	172
4	6,6-Dimethyl-2-(3-oxobutyl)bicyclo[3.1.1]heptan-3-one	619	394	0-00-0	mainlib	C13H20O2	208
5	Cyclohexanebutanoic acid	619	394	4441-63-8	mainlib	C10H18O2	170

2-Acetyl-5-methylfuran

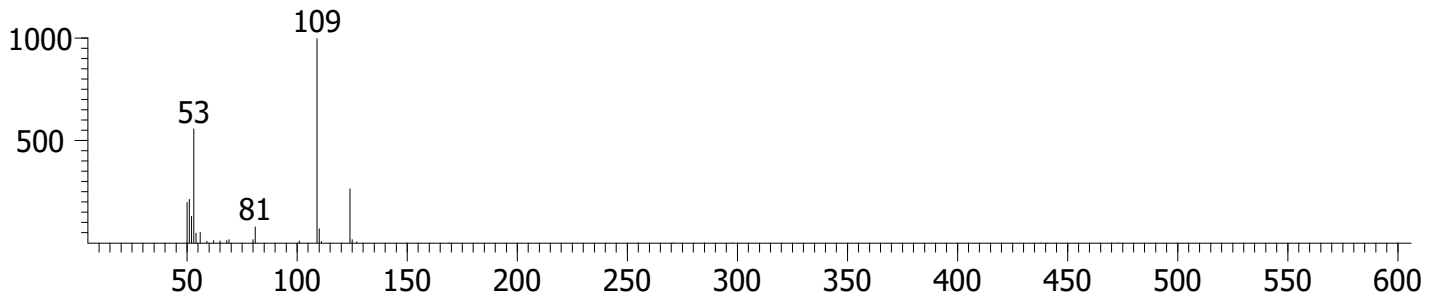
1st Dimension R.T. = 640.908
2nd Dimension R.T. = 1.696
Quant Mass(es) = 109
S/N = 533.42
Area = 84844
Height = 11286
Similarity = 911



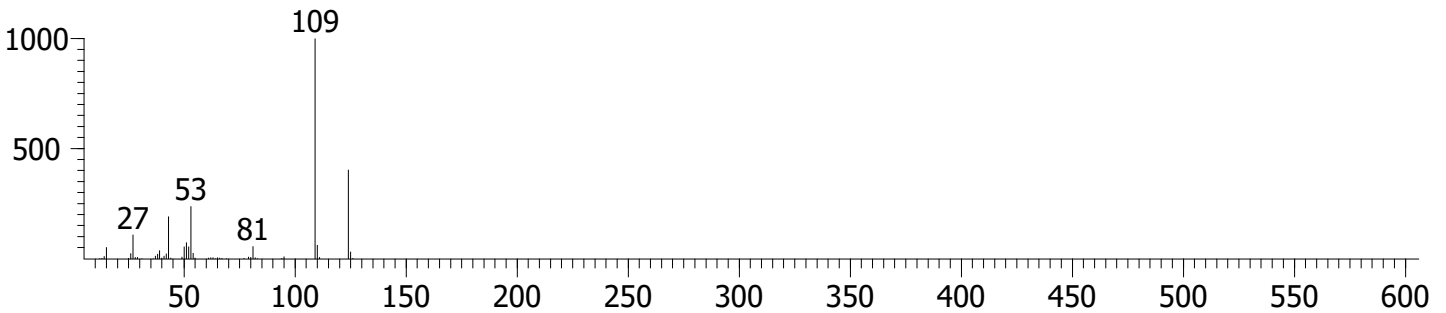
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 335, at 640.908 , 1.696 sec , sec (Spec # 24637)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 335, at 640.908 , 1.696 sec , sec (Spec # 24637)



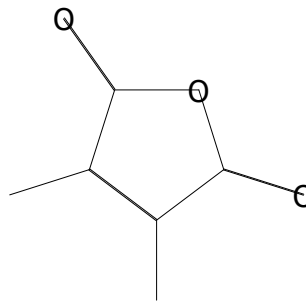
Library Hit - similarity 911, "2-Acetyl-5-methylfuran"



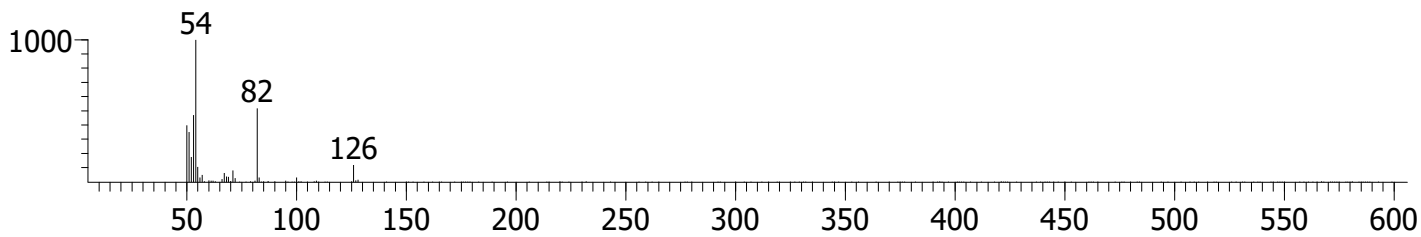
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Acetyl-5-methylfuran	911	7490	1193-79-9	mainlib	C7H8O2	124
2	2-Cyclopenten-1-one, 3,5,5-trimethyl-	842	1113	24156-95-4	mainlib	C8H12O	124
3	Elsholtzia ketone	811	303	488-05-1	mainlib	C10H14O2	166
4	2-Cyclopenten-1-one, 3,4,4-trimethyl-	808	268	30434-65-2	mainlib	C8H12O	124
5	Furane-2-carboxaldehyde, 5-(3,4-dichlorophenoxyethyl)-	800	200	0-00-0	mainlib	C12H8Cl2O3	270

2,5-Furandione, 3,4-dimethyl-

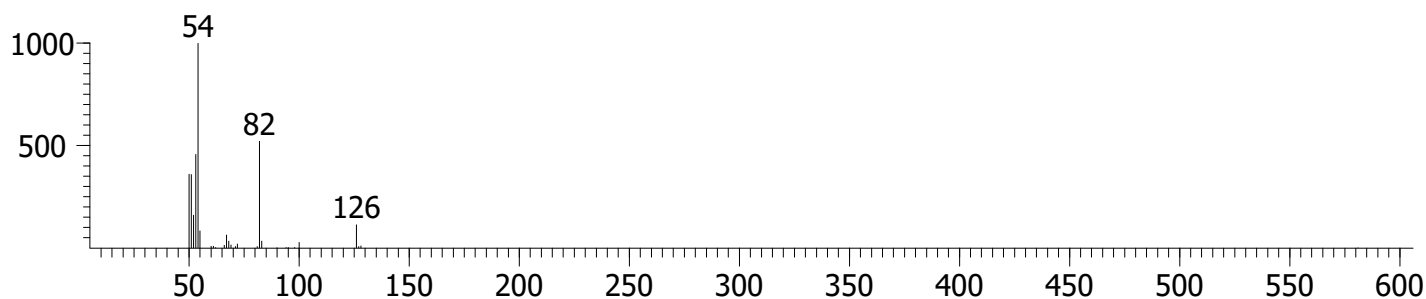
1st Dimension R.T. = 644.406
2nd Dimension R.T. = 1.828
Quant Mass(es) = 54
S/N = 355.23
Area = 126516
Height = 16835
Similarity = 888



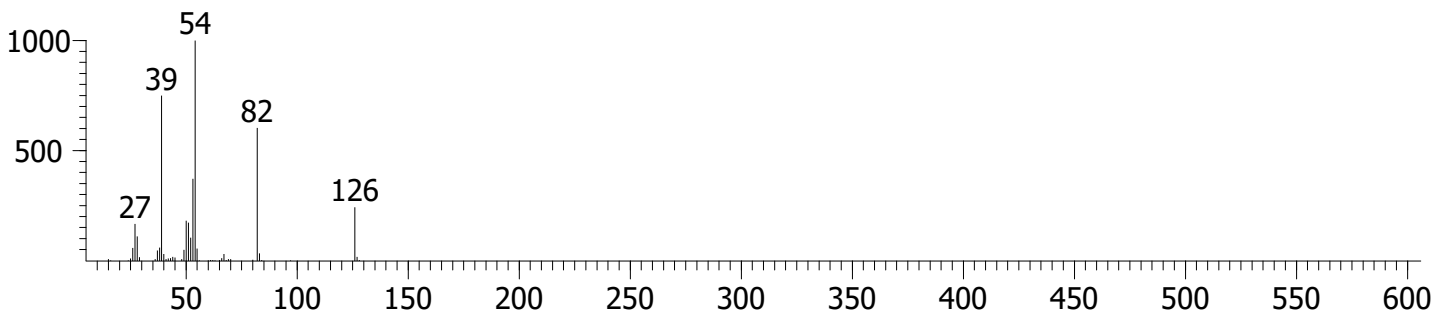
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 342, at 644.406 , 1.828 sec , sec (Spec # 25187)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 342, at 644.406 , 1.828 sec , sec (Spec # 25187)



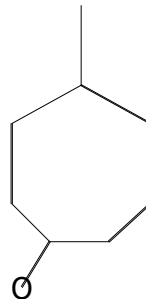
Library Hit - similarity 888, "2,5-Furandione, 3,4-dimethyl-"



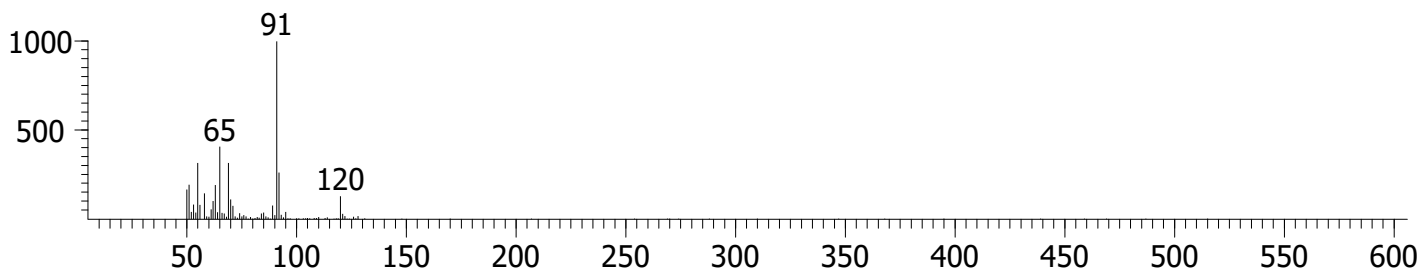
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,5-Furandione, 3,4-dimethyl-	888	7705	766-39-2	mainlib	C6H6O3	126
2	1,2-Butadiene	773	462	590-19-2	mainlib	C4H6	54
3	3-Oxabicyclo[3.2.0]heptane-2,4-dione, cis-	763	326	118554-23-7	mainlib	C6H6O3	126
4	1-Butyne	753	230	107-00-6	mainlib	C4H6	54
5	3-Cyclobutene-1,2-dione, 3,4-dimethyl-	752	221	1121-15-9	mainlib	C6H6O2	110

2,4,6-Cycloheptatrien-1-one, 4-methyl-

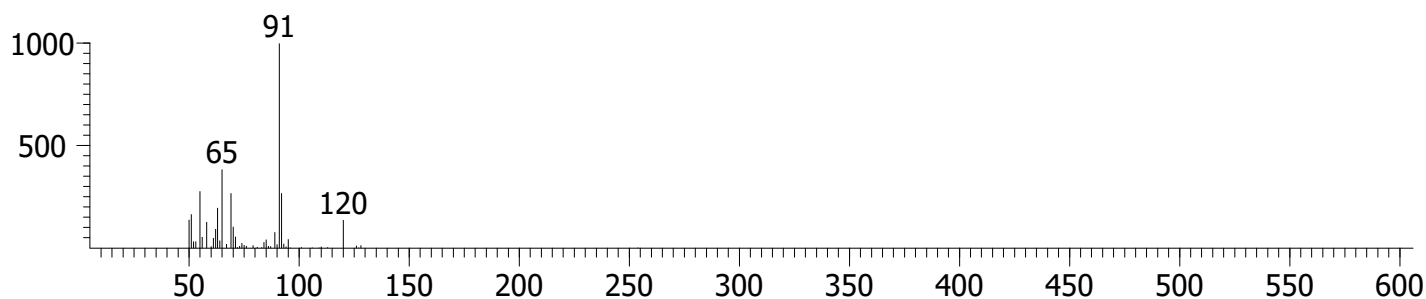
1st Dimension R.T. = 654.9
2nd Dimension R.T. = 1.769
Quant Mass(es) = 91
S/N = 498.38
Area = 178736
Height = 23996
Similarity = 748



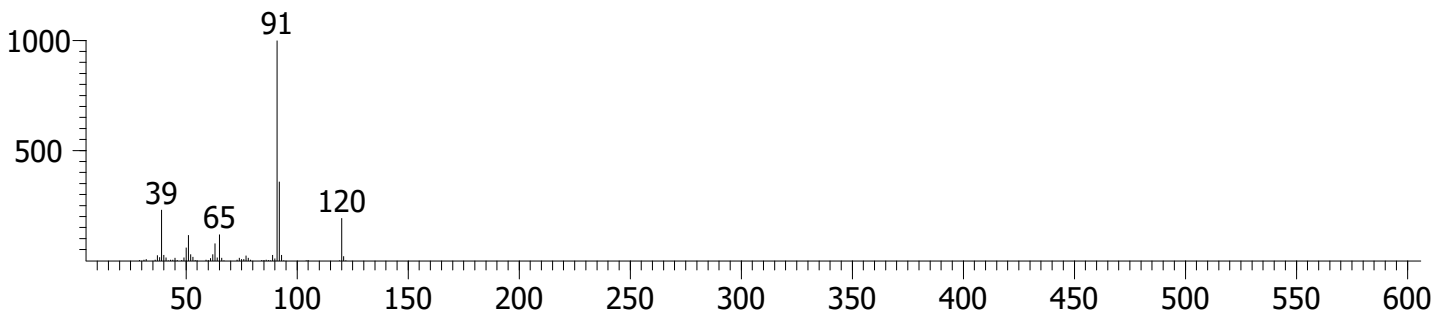
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 367, at 654.9 , 1.769 sec , sec (Spec # 26768)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 367, at 654.9 , 1.769 sec , sec (Spec # 26768)



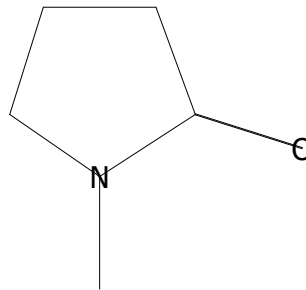
Library Hit - similarity 748, "2,4,6-Cycloheptatrien-1-one, 4-methyl-"



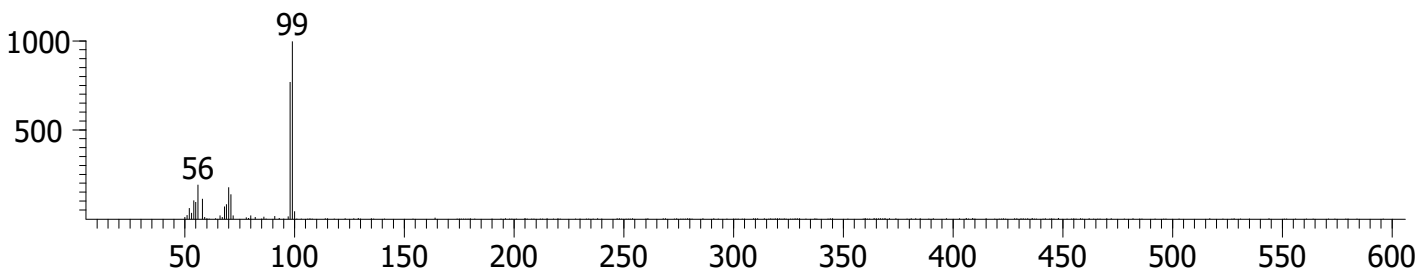
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,4,6-Cycloheptatrien-1-one, 4-methyl-	748	839	0-00-0	mainlib	C8H8O	120
2	Benzeneacetaldehyde	745	742	122-78-1	mainlib	C8H8O	120
3	2-Benzyloxyethylamine	741	627	38336-04-8	mainlib	C9H13NO	151
4	Benzaldehyde, 3-benzyloxy-2-fluoro-4-methoxy-	736	505	0-00-0	mainlib	C15H13FO3	260
5	4-Benzylsulfanyl-6-fluoro-2-trifluoromethyl-pyrimidine-5-carbonitrile	735	485	0-00-0	mainlib	C13H7F4N3S	313

2-Pyrrolidinone, 1-methyl-

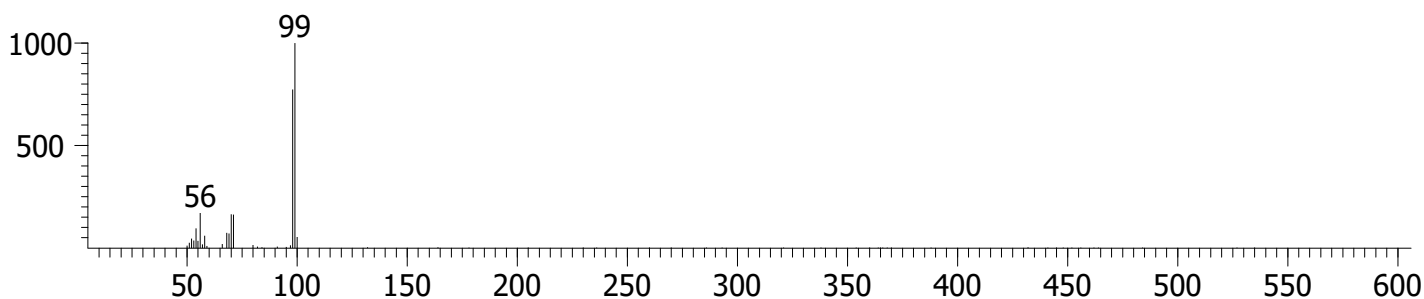
1st Dimension R.T. = 654.9
2nd Dimension R.T. = 1.993
Quant Mass(es) = 99
S/N = 439.95
Area = 113976
Height = 12797
Similarity = 944



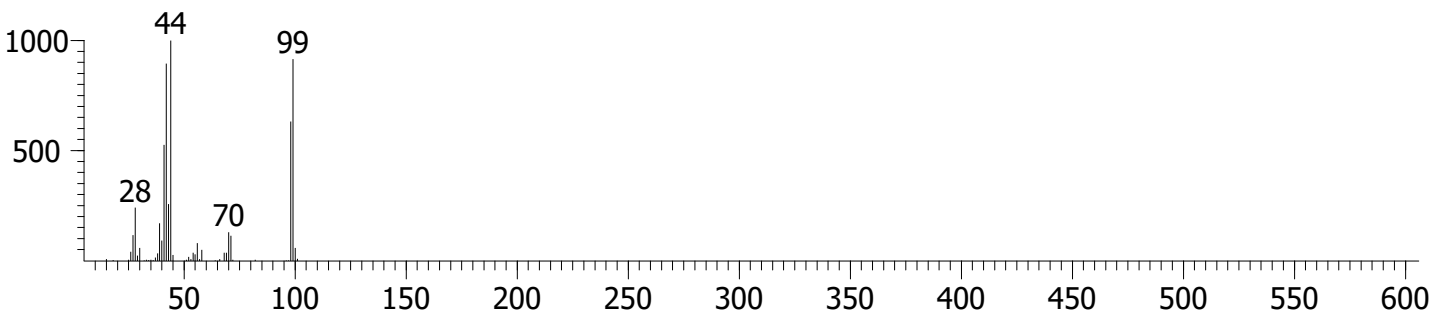
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 370, at 654.9 , 1.993 sec , sec (Spec # 26802)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 370, at 654.9 , 1.993 sec , sec (Spec # 26802)

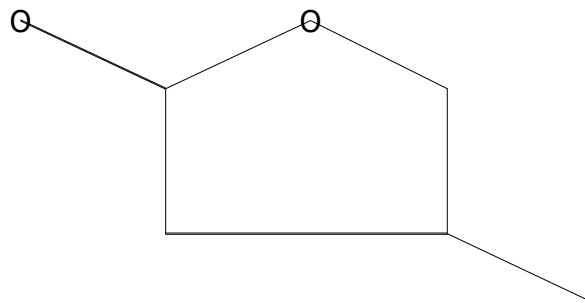


Library Hit - similarity 944, "2-Pyrrolidinone, 1-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Pyrrolidinone, 1-methyl-	944	8234	872-50-4	mainlib	C5H9NO	99
2	4-(Methylamino)butyric acid	881	1380	1119-48-8	mainlib	C5H11NO2	117
3	4,4'-Bi-1,3,2-dioxaborolane, 2,2'-diethyl-, (R*,S*)-	804	168	62337-94-4	mainlib	C8H16B2O4	198
4	2-Pyrrolidinone, 1-(2-aminoethyl)-	783	71	24935-08-8	mainlib	C6H12N2O	128
5	Cyclopropanecarboxamide, N-(4-methyl-1-piperazinyl)-	763	32	0-00-0	mainlib	C9H17N3O	183

4-Methyl-5H-furan-2-one



1st Dimension R.T. = 658.398

2nd Dimension R.T. = 2.138

Quant Mass(es) = 69

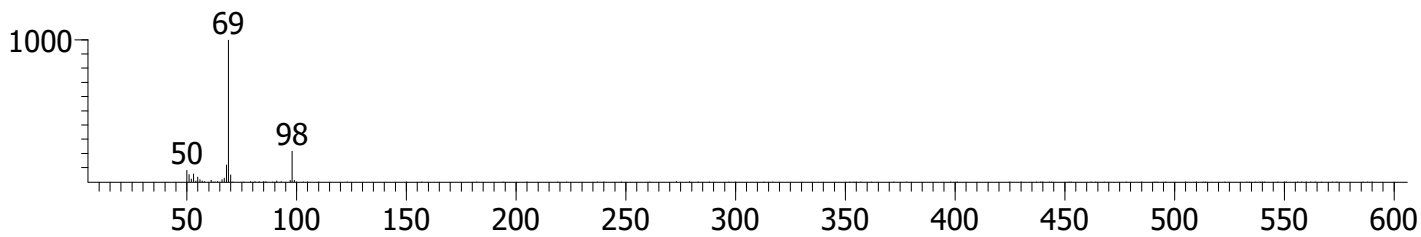
S/N = 219.27

Area = 111840

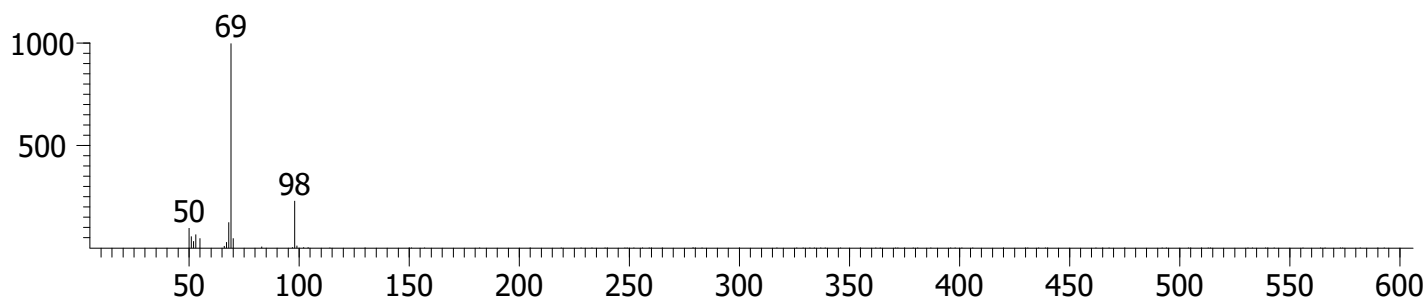
Height = 12860

Similarity = 928

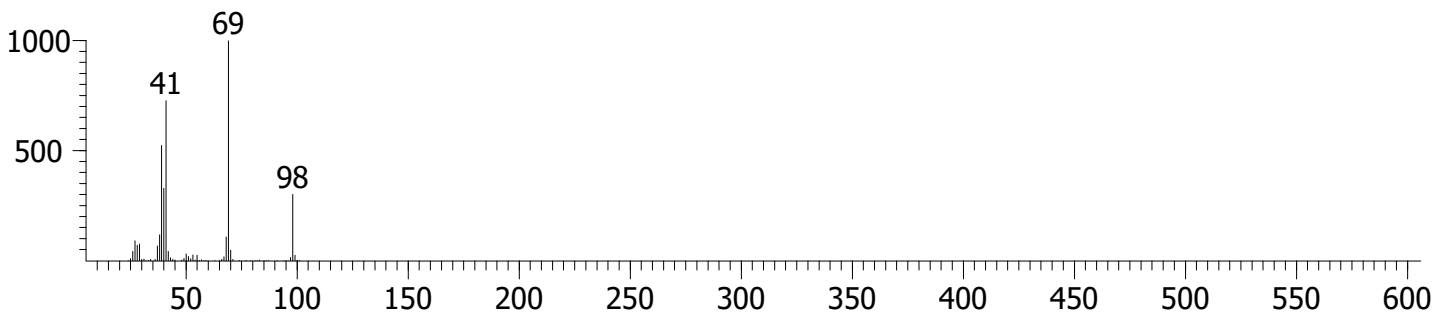
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 380, at 658.398 , 2.138 sec , sec (Spec # 27354)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 380, at 658.398 , 2.138 sec , sec (Spec # 27354)



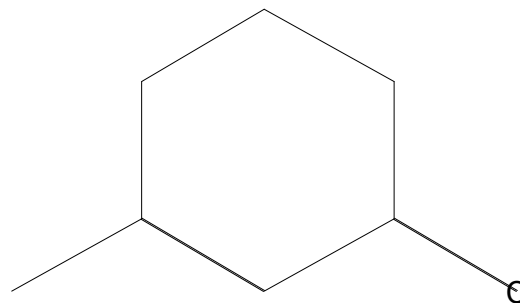
Library Hit - similarity 928, "4-Methyl-5H-furan-2-one"



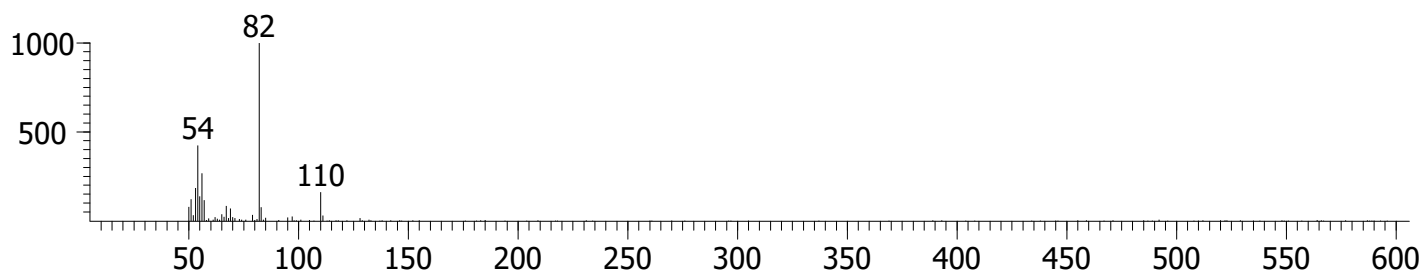
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Methyl-5H-furan-2-one	928	8221	6124-79-4	mainlib	C5H6O2	98
2	1-Propanone, 1-cyclopropyl-	855	1119	6704-19-4	mainlib	C6H10O	98
3	4-Hexen-3-one	814	255	2497-21-4	mainlib	C6H10O	98
4	2(5H)-Furanone, 3-methyl-	810	215	22122-36-7	mainlib	C5H6O2	98
5	Di(1-methylcyclobutyl) ether	774	53	86301-90-8	mainlib	C10H18O	154

2-Cyclohexen-1-one, 3-methyl-

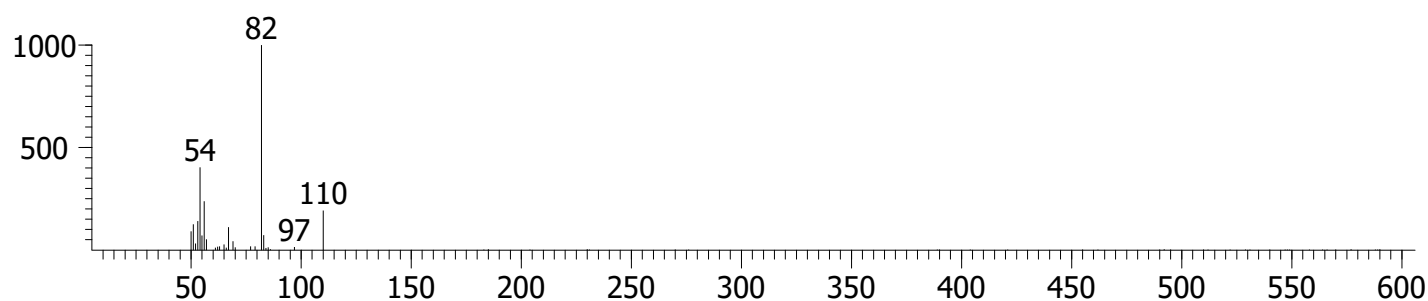
1st Dimension R.T. = 672.39
2nd Dimension R.T. = 1.795
Quant Mass(es) = 82
S/N = 239.41
Area = 36846
Height = 4337.4
Similarity = 808



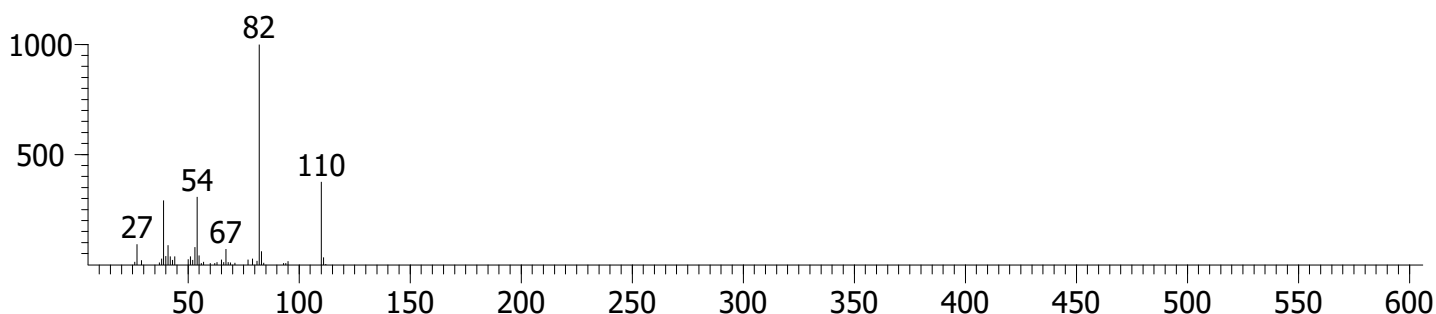
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 406, at 672.39 , 1.795 sec , sec (Spec # 29422)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 406, at 672.39 , 1.795 sec , sec (Spec # 29422)



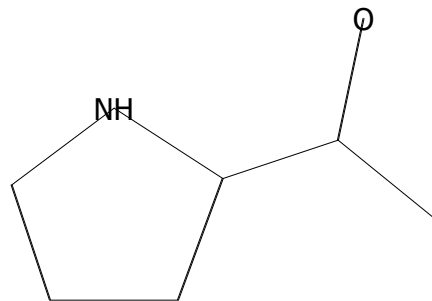
Library Hit - similarity 808, "2-Cyclohexen-1-one, 3-methyl-"



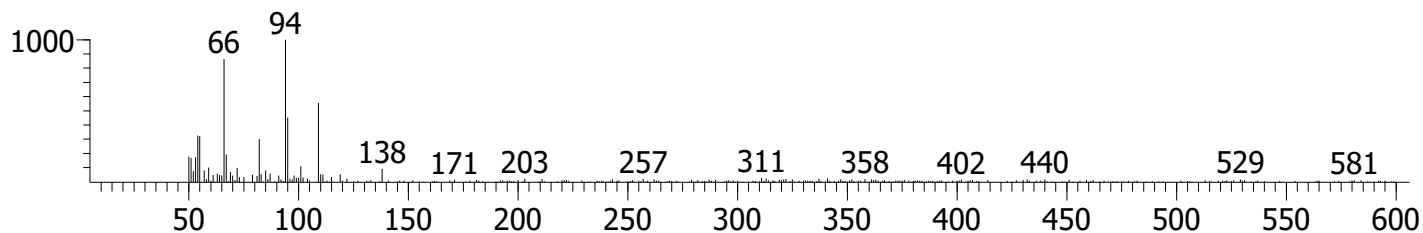
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Cyclohexen-1-one, 3-methyl-	808	4087	1193-18-6	mainlib	C7H10O	110
2	2-Cyclohexen-1-one, 2-methyl-	807	3928	1121-18-2	mainlib	C7H10O	110
3	2-Cyclohexen-1-one, 6-(1-hydroxy-1-methylethyl)-3-methyl-	764	866	87791-00-2	mainlib	C10H16O2	168
4	Pyrazole-3-propanoic acid, á-(trans-2-hydroxycyclohexylamino)-	722	194	0-00-0	mainlib	C12H19N3O3	253
5	2-Cyclohexen-1-one, 3,5-dimethyl-	721	186	1123-09-7	mainlib	C8H12O	124

Ethanone, 1-(1H-pyrrol-2-yl)-

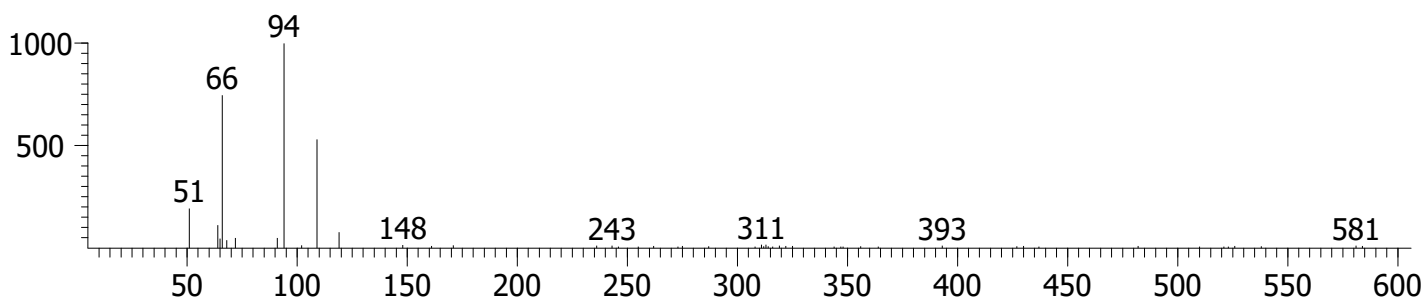
1st Dimension R.T. = 675.888
2nd Dimension R.T. = 1.848
Quant Mass(es) = 94
S/N = 74.829
Area = 8804.7
Height = 1062.1
Similarity = 813



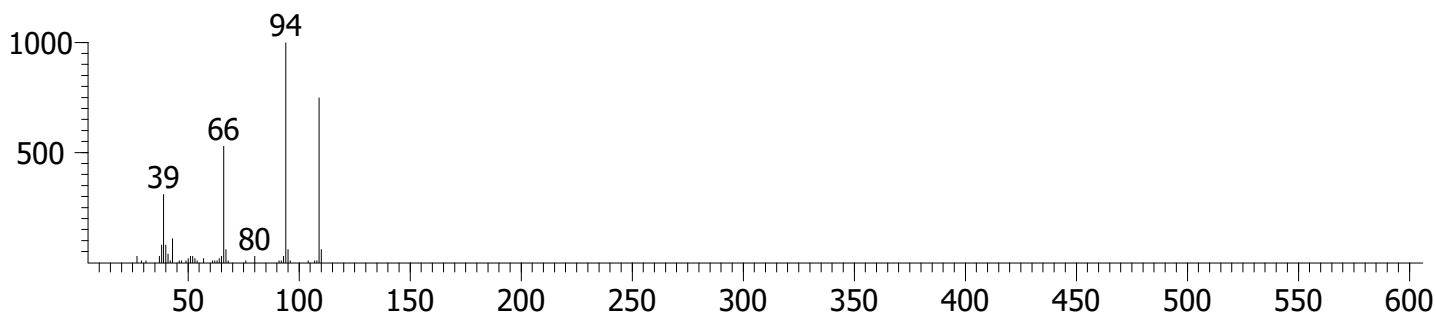
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 413, at 675.888 , 1.848 sec , sec (Spec # 29960)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 413, at 675.888 , 1.848 sec , sec (Spec # 29960)



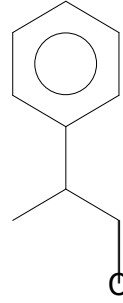
Library Hit - similarity 813, "Ethanone, 1-(1H-pyrrol-2-yl)-"



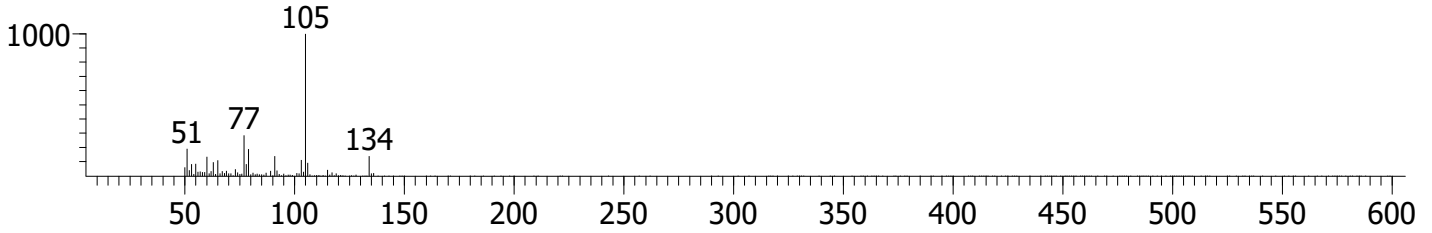
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanone, 1-(1H-pyrrol-2-yl)-	813	8178	1072-83-9	mainlib	C6H7NO	109
2	3-Acetyl-1H-pyrroline	761	1633	1072-82-8	mainlib	C6H7NO	109
3	Pyrrole, 4-ethyl-2-methyl-	632	68	5690-96-0	mainlib	C7H11N	109
4	Pyrimidine, 5-methyl-	623	50	2036-41-1	mainlib	C5H6N2	94
5	3-Aminopyridine	605	25	462-08-8	mainlib	C5H6N2	94

Benzeneacetaldehyde, à-methyl-

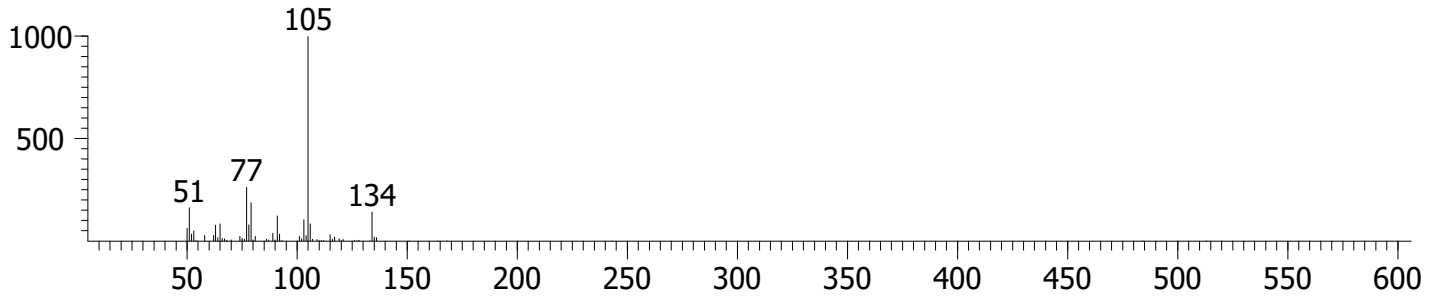
1st Dimension R.T. = 682.884
2nd Dimension R.T. = 1.419
Quant Mass(es) = 105
S/N = 648.82
Area = 106601
Height = 15159
Similarity = 913



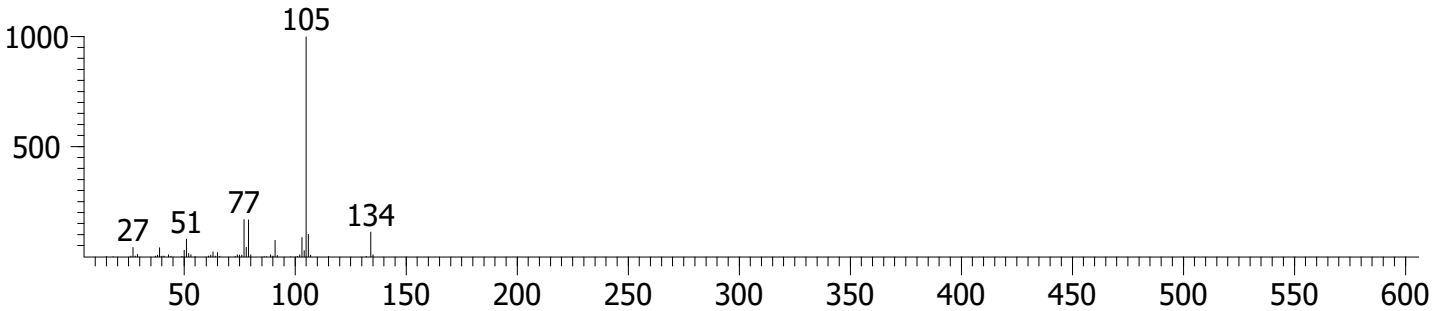
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 422, at 682.884 , 1.419 sec , sec (Spec # 30955)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 422, at 682.884 , 1.419 sec , sec (Spec # 30955)



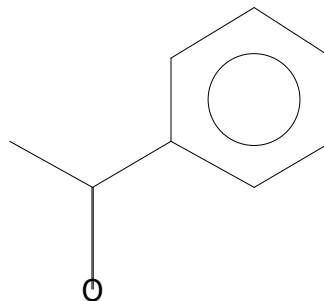
Library Hit - similarity 913, "Benzeneacetaldehyde, à-methyl-"



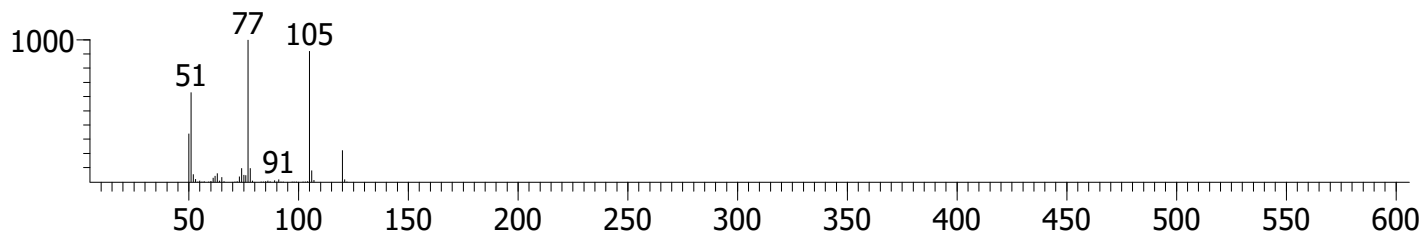
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzeneacetaldehyde, à-methyl-	913	2048	93-53-8	mainlib	C9H10O	134
2	Benzeneacetaldehyde, 4-methyl-	901	1364	104-09-6	mainlib	C9H10O	134
3	Hydratropaldehyde	896	1099	34713-70-7	mainlib	C9H10O	134
4	Benzene, 1-methyl-2-propyl-	891	886	1074-17-5	mainlib	C10H14	134
5	Benzene, (1-methylpropyl)-	889	817	135-98-8	mainlib	C10H14	134

Acetophenone

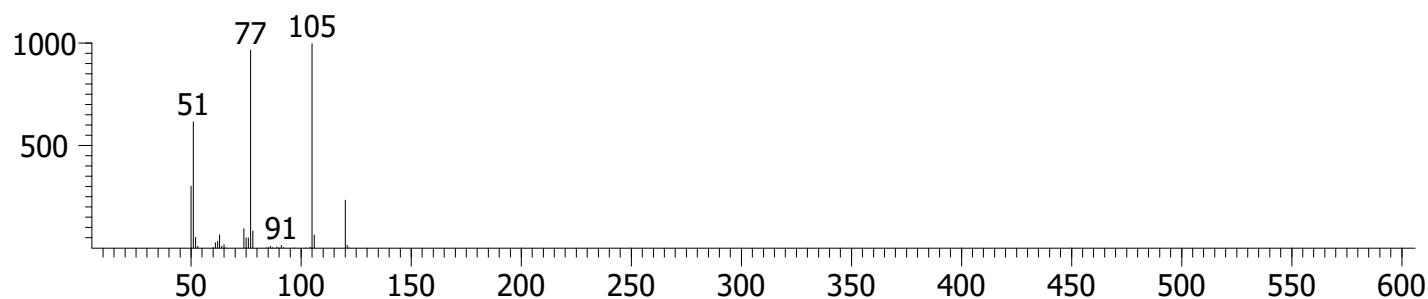
1st Dimension R.T. = 686.382
2nd Dimension R.T. = 1.775
Quant Mass(es) = 105
S/N = 4308.2
Area = 751101
Height = 99588
Similarity = 952



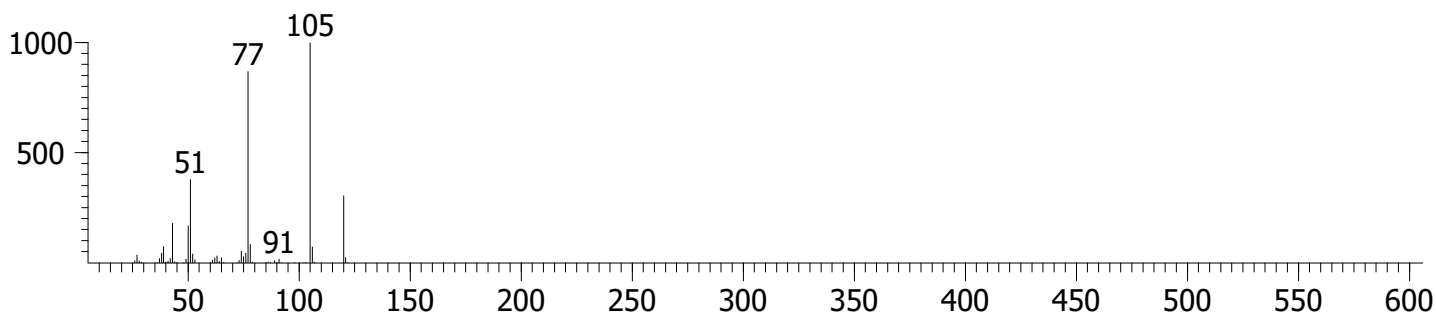
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 431, at 686.382 , 1.775 sec , sec (Spec # 31539)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 431, at 686.382 , 1.775 sec , sec (Spec # 31539)



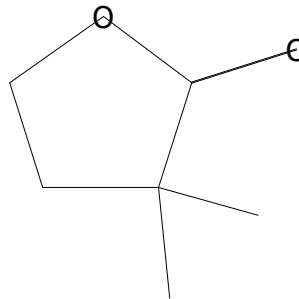
Library Hit - similarity 952, "Acetophenone"



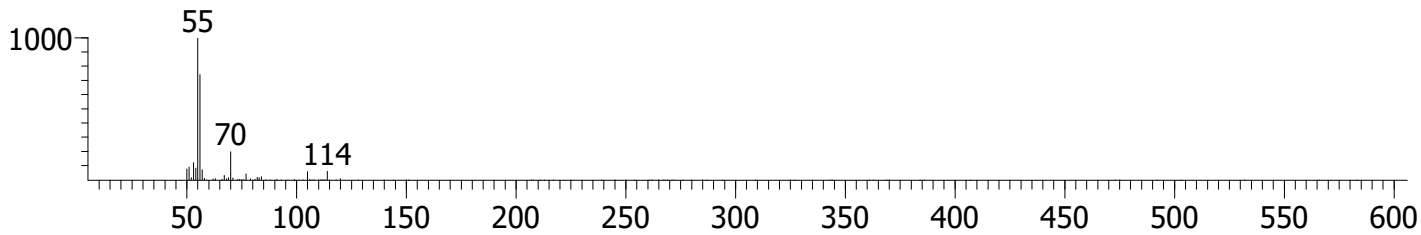
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Acetophenone	952	4931	98-86-2	mainlib	C8H8O	120
2	5-Benzoylpentanoic acid	909	1087	4144-62-1	mainlib	C12H14O3	206
3	ç-Chlorobutyrophenone	898	746	939-52-6	mainlib	C10H11ClO	182
4	N-(5-Ethyl-1,3,4-thiadiazol-2-yl)benzamide	871	219	36231-88-6	mainlib	C11H11N3OS	233
5	1-Pentanone, 1-phenyl-	871	219	1009-14-9	mainlib	C11H14O	162

2(3H)-Furanone, dihydro-3,3-dimethyl-

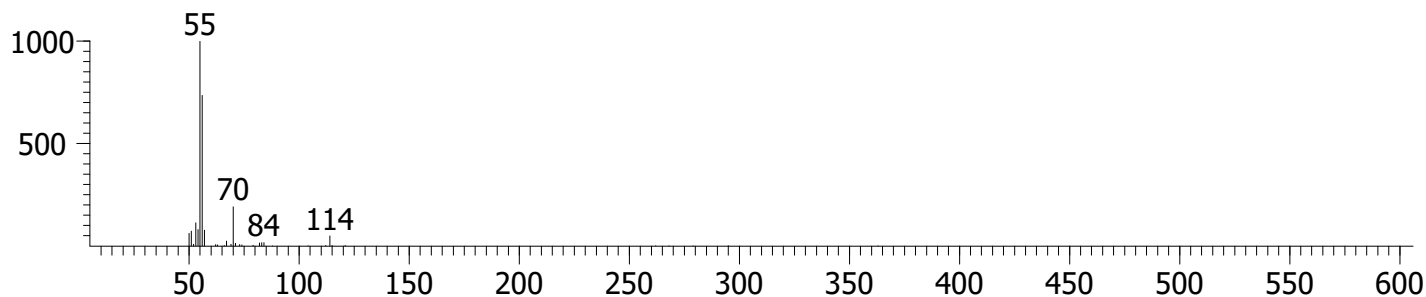
1st Dimension R.T. = 686.382
2nd Dimension R.T. = 1.940
Quant Mass(es) = 56
S/N = 243.42
Area = 119254
Height = 14556
Similarity = 857



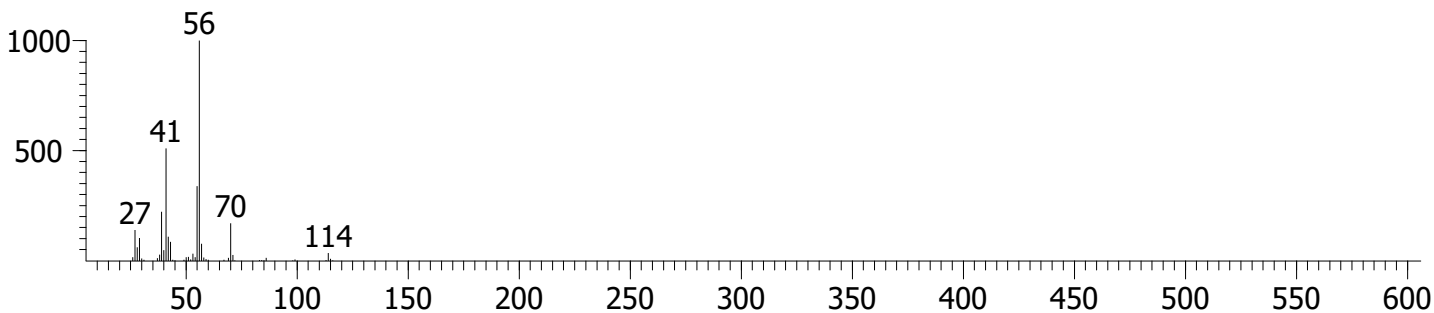
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 433, at 686.382 , 1.940 sec , sec (Spec # 31564)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 433, at 686.382 , 1.940 sec , sec (Spec # 31564)



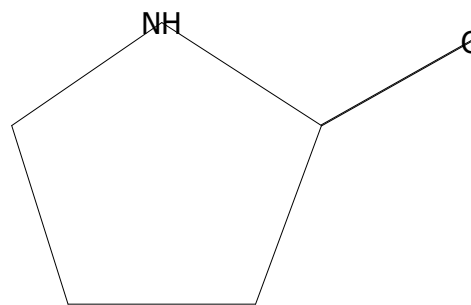
Library Hit - similarity 857, "2(3H)-Furanone, dihydro-3,3-dimethyl-"



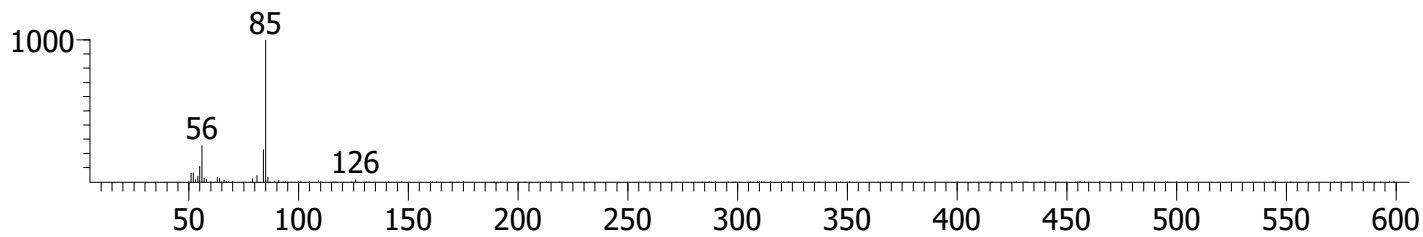
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2(3H)-Furanone, dihydro-3,3-dimethyl-	857	3384	3709-08-8	mainlib	C6H10O2	114
2	1-Pentene, 3,4-dimethyl-	804	669	7385-78-6	mainlib	C7H14	98
3	2-Butene, (Z)-	802	617	590-18-1	mainlib	C4H8	56
4	Cyclopropane, butyl-	799	545	930-57-4	mainlib	C7H14	98
5	1-Butene	796	482	106-98-9	mainlib	C4H8	56

2-Pyrrolidinone

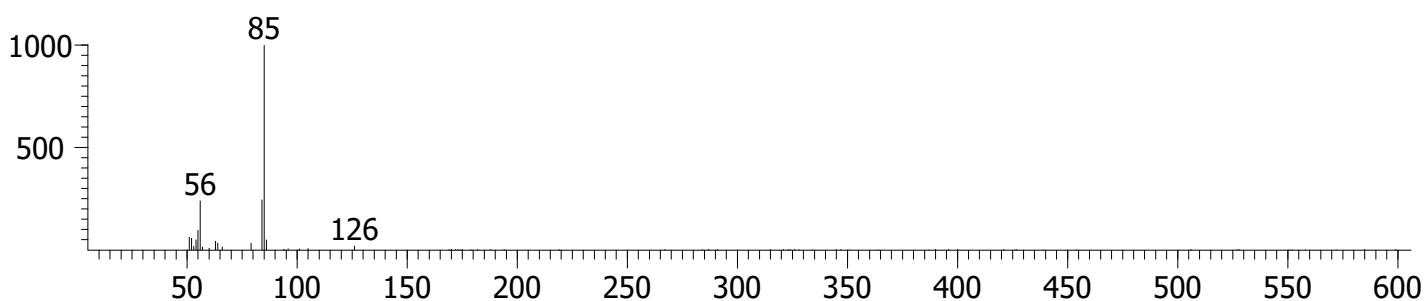
1st Dimension R.T. = 696.876
2nd Dimension R.T. = 2.211
Quant Mass(es) = 85
S/N = 191.55
Area = 141134
Height = 13334
Similarity = 908



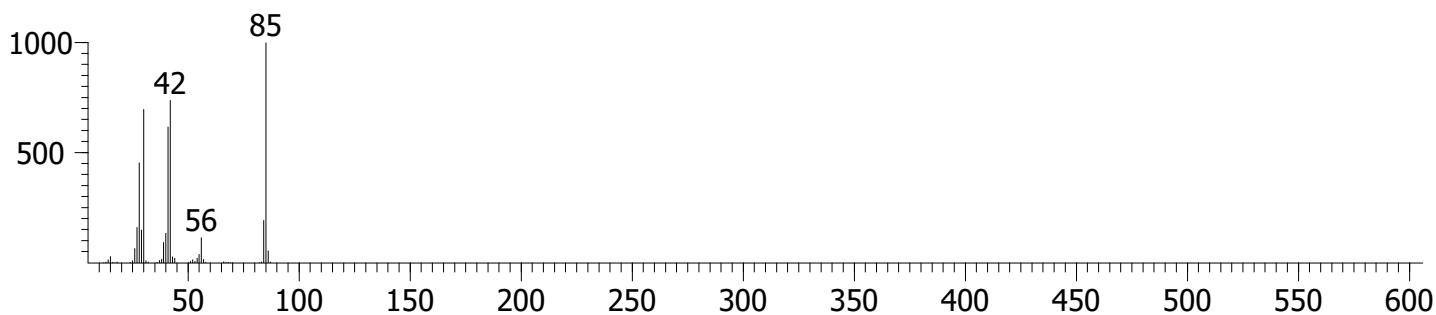
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 457, at 696.876 , 2.211 sec , sec (Spec # 33195)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 457, at 696.876 , 2.211 sec , sec (Spec # 33195)



Library Hit - similarity 908, "2-Pyrrolidinone"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Pyrrolidinone	908	7210	616-45-5	mainlib	C4H7NO	85
2	5-Methyl-2-(2-methyl-2-tetrahydrofuryl)tetrahydrofuran	846	1232	0-00-0	mainlib	C10H18O2	170
3	Pyrrolidine, 3-methyl-	808	295	34375-89-8	mainlib	C5H11N	85
4	Cyclobutene-3,4-dione, 1-dimethylamino-2-hydroxy-	801	226	182881-06-7	mainlib	C6H7NO3	141
5	Succinic acid, di(2-methylpent-3-yl) ester	796	182	0-00-0	mainlib	C16H30O4	286

Undecane, 5,7-dimethyl-

1st Dimension R.T. = 710.868

2nd Dimension R.T. = 1.102

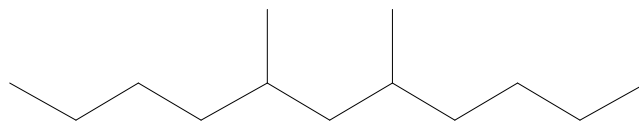
Quant Mass(es) = 71

S/N = 1025.2

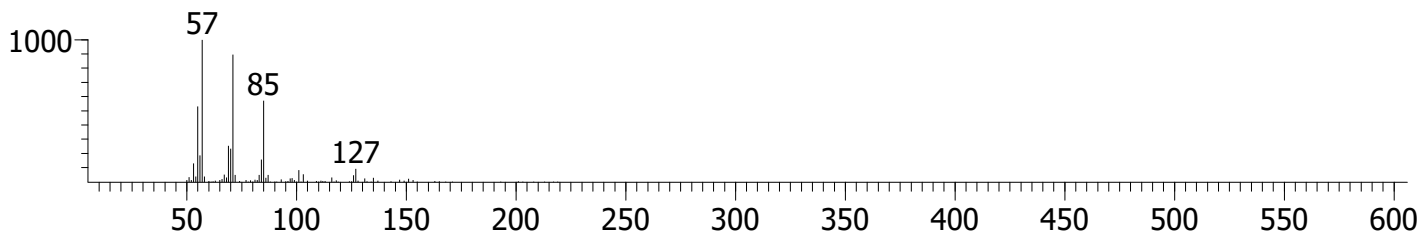
Area = 176331

Height = 23102

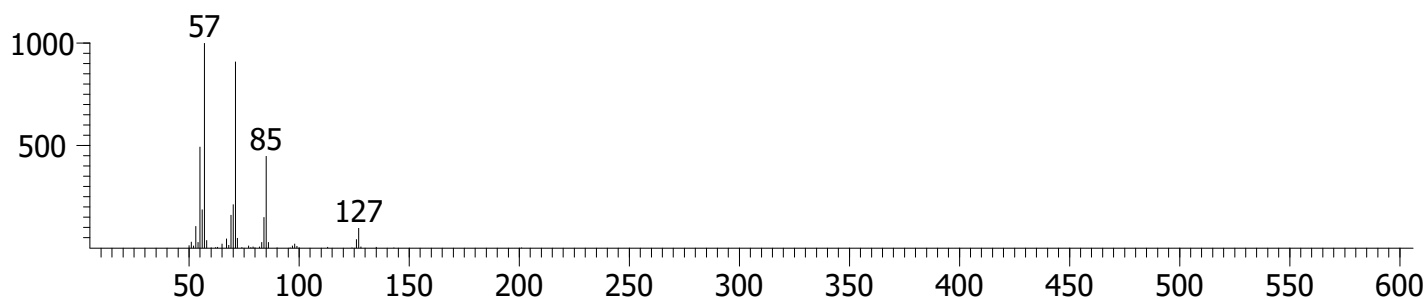
Similarity = 889



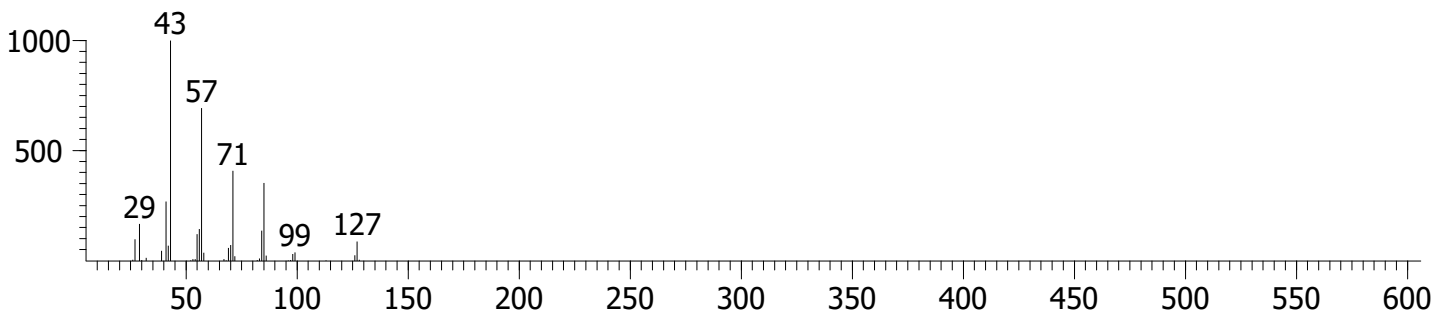
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 482, at 710.868 , 1.102 sec , sec (Spec # 35147)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 482, at 710.868 , 1.102 sec , sec (Spec # 35147)



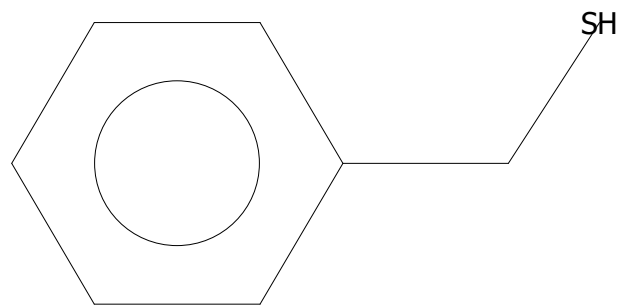
Library Hit - similarity 889, "Undecane, 5,7-dimethyl-"



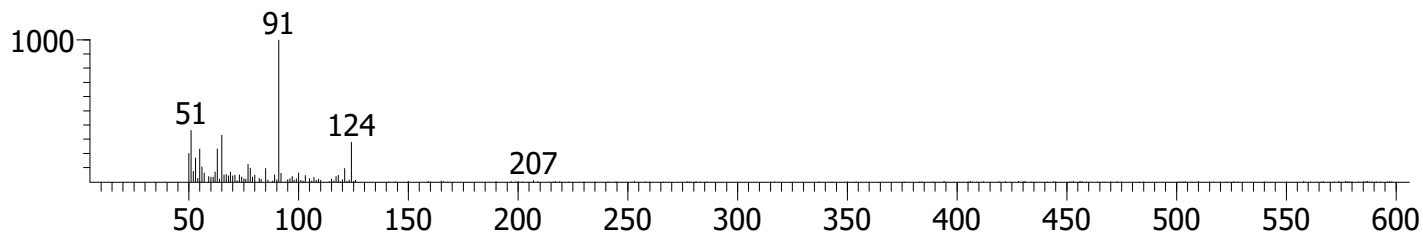
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Undecane, 5,7-dimethyl-	889	1781	17312-83-3	mainlib	C13H28	184
2	Undecane, 3,7-dimethyl-	877	1186	17301-29-0	mainlib	C13H28	184
3	Octane, 2,3,6,7-tetramethyl-	869	885	52670-34-5	mainlib	C12H26	170
4	Undecane, 4,7-dimethyl-	858	607	17301-32-5	mainlib	C13H28	184
5	Oxalic acid, isohexyl neopentyl ester	855	536	0-00-0	mainlib	C13H24O4	244

Benzenemethanethiol

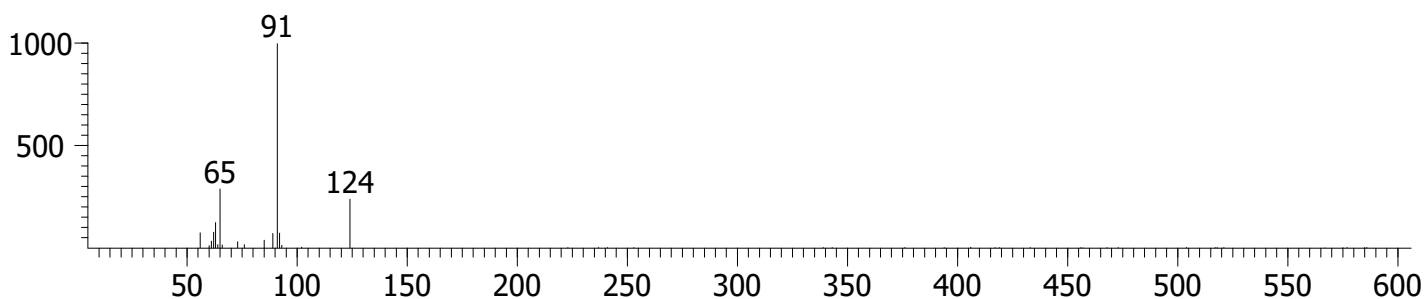
1st Dimension R.T. = 710.868
2nd Dimension R.T. = 1.782
Quant Mass(es) = 91
S/N = 72.462
Area = 23731
Height = 2729.5
Similarity = 912



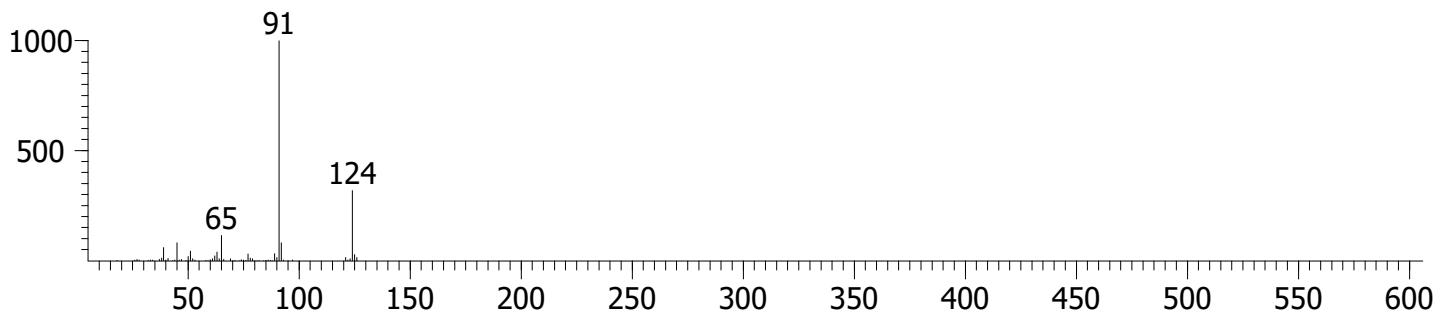
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 489, at 710.868 , 1.782 sec , sec (Spec # 35250)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 489, at 710.868 , 1.782 sec , sec (Spec # 35250)



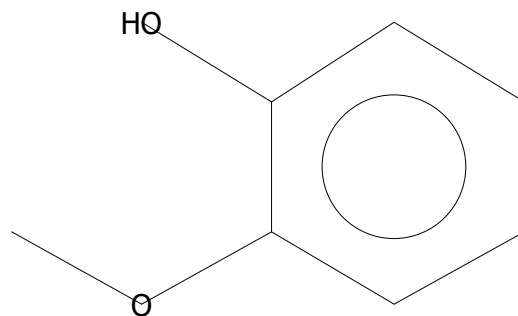
Library Hit - similarity 912, "Benzenemethanethiol"



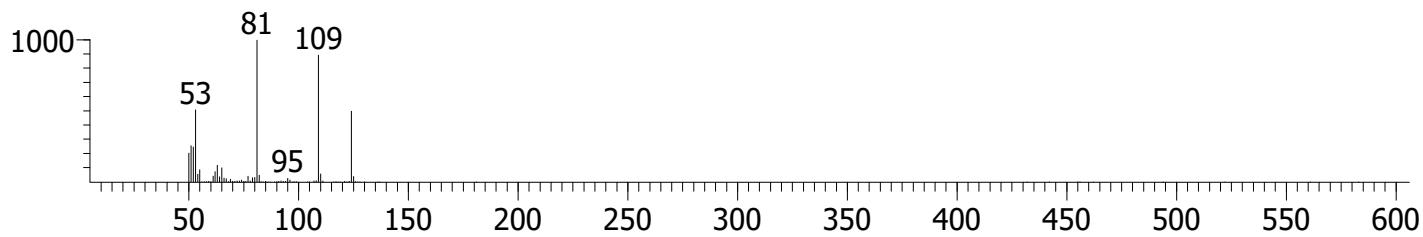
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenemethanethiol	912	4368	100-53-8	mainlib	C7H8S	124
2	(2-Chloro-4-nitrophenyl)thiocarbamic acid, S-benzyl ester	852	775	0-00-0	mainlib	C14H11ClN2O3S	322
3	Benzonitrile, 2-chloro-6-(phenylmethoxy)-	848	655	92161-40-5	mainlib	C14H10ClNO	243
4	Phenylmethanesulfonylacetic acid	832	377	0-00-0	mainlib	C9H10O4S	214
5	Benzenemethanesulfonamide	829	333	4563-33-1	mainlib	C7H9NO2S	171

Phenol, 2-methoxy-

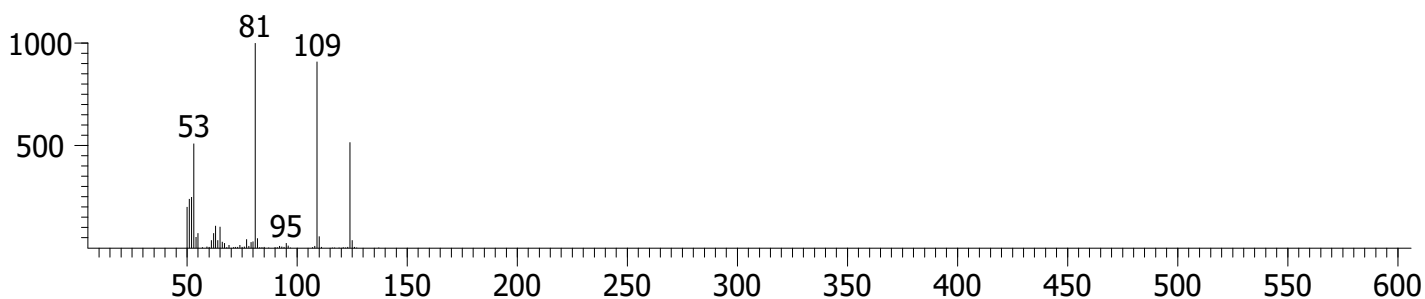
1st Dimension R.T. = 717.864
2nd Dimension R.T. = 1.756
Quant Mass(es) = 109
S/N = 1565.0
Area = 251575
Height = 33177
Similarity = 923



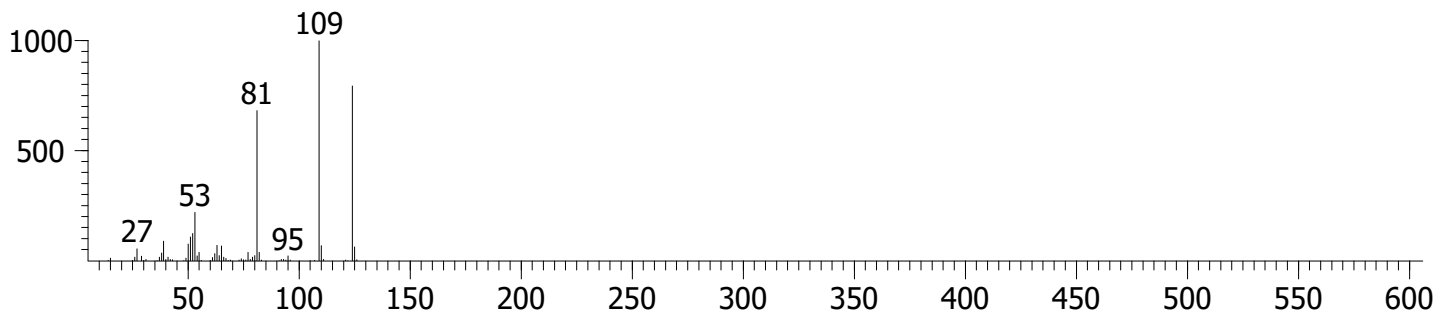
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 506, at 717.864 , 1.756 sec , sec (Spec # 36306)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 506, at 717.864 , 1.756 sec , sec (Spec # 36306)



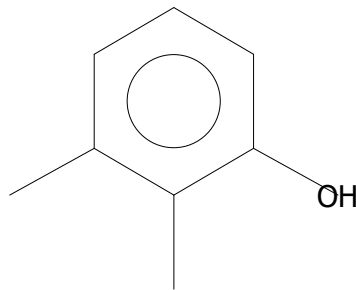
Library Hit - similarity 923, "Phenol, 2-methoxy-"



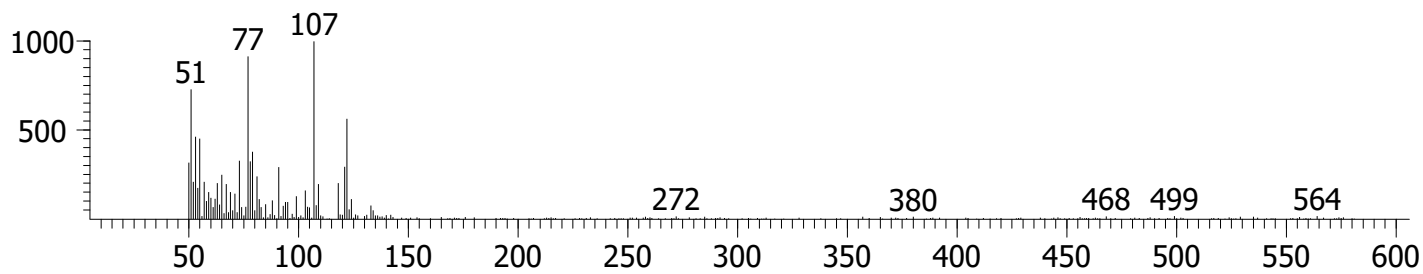
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 2-methoxy-	923	7518	90-05-1	mainlib	C7H8O2	124
2	Mequinol	885	1801	150-76-5	mainlib	C7H8O2	124
3	Formic acid, 2-methoxyphenyl ester	839	380	0-00-0	mainlib	C8H8O3	152
4	2-Acetyl-5-methylfuran	790	78	1193-79-9	mainlib	C7H8O2	124
5	Ethanone, 1-(1-cyclohexen-1-yl)-	778	52	932-66-1	mainlib	C8H12O	124

Phenol, 2,3-dimethyl-

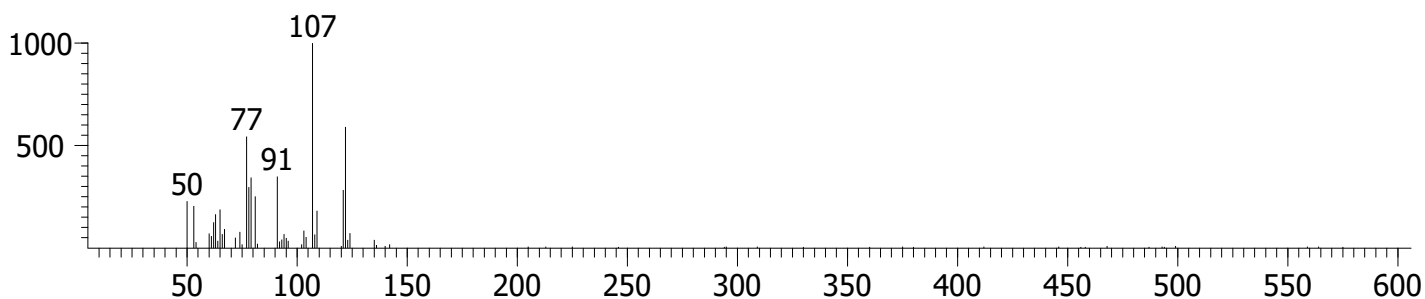
1st Dimension R.T. = 742.35
2nd Dimension R.T. = 1.683
Quant Mass(es) = 107
S/N = 91.487
Area = 9677.0
Height = 1391.5
Similarity = 781



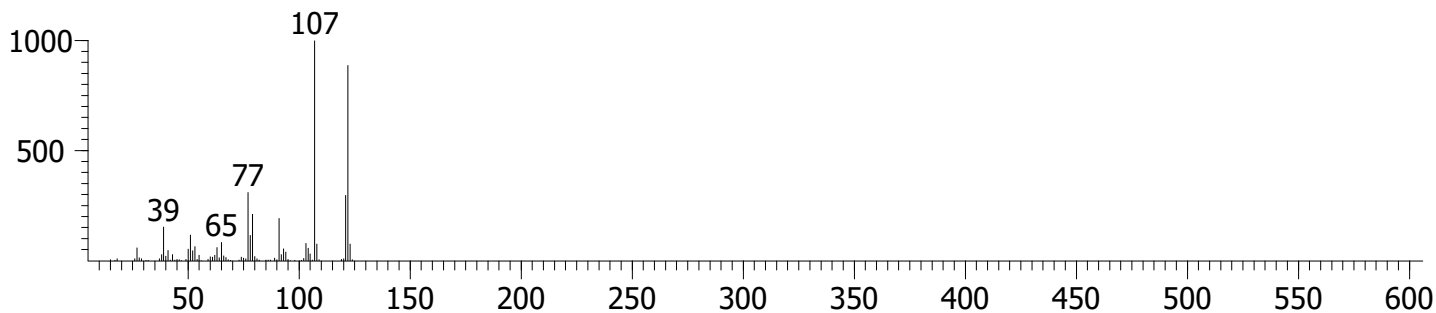
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 548, at 742.35 , 1.683 sec , sec (Spec # 40005)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 548, at 742.35 , 1.683 sec , sec (Spec # 40005)



Library Hit - similarity 781, "Phenol, 2,3-dimethyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 2,3-dimethyl-	781	2426	526-75-0	mainlib	C ₈ H ₁₀ O	122
2	Oxepine, 2,7-dimethyl-	773	1809	1487-99-6	mainlib	C ₈ H ₁₀ O	122
3	Phenol, 2,6-dimethyl-	766	1386	576-26-1	mainlib	C ₈ H ₁₀ O	122
4	Phenol, 2,5-dimethyl-	754	923	95-87-4	mainlib	C ₈ H ₁₀ O	122
5	Phenol, 2,4-dimethyl-	740	578	105-67-9	mainlib	C ₈ H ₁₀ O	122

1H-Pyrazole

4,5-dihydro-5,5-dimethyl-4-isopropylidene-

1st Dimension R.T. = 763.338

2nd Dimension R.T. = 1.643

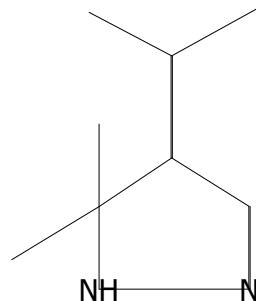
Quant Mass(es) = 82

S/N = 303.28

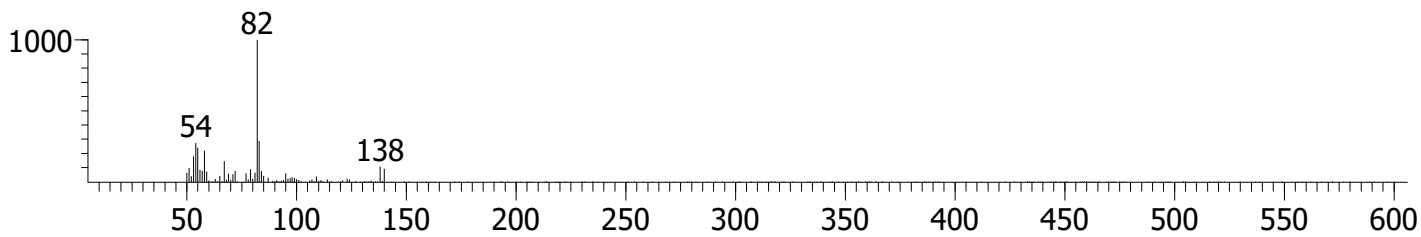
Area = 65231

Height = 7425.3

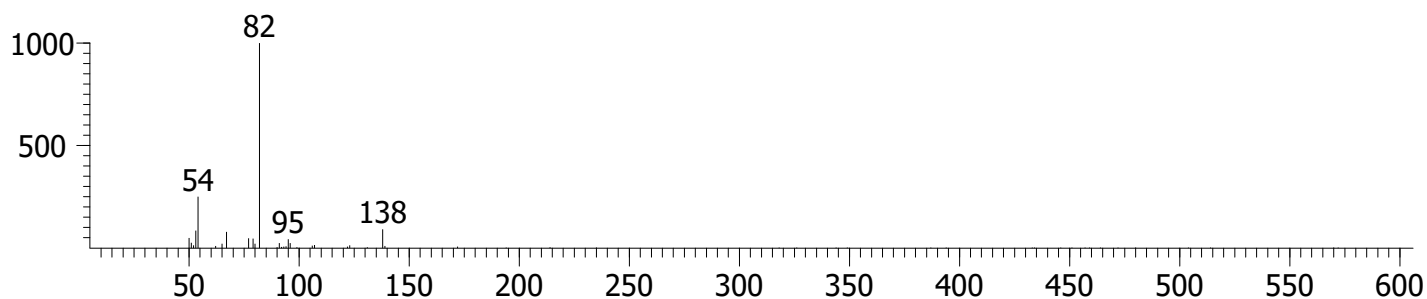
Similarity = 907



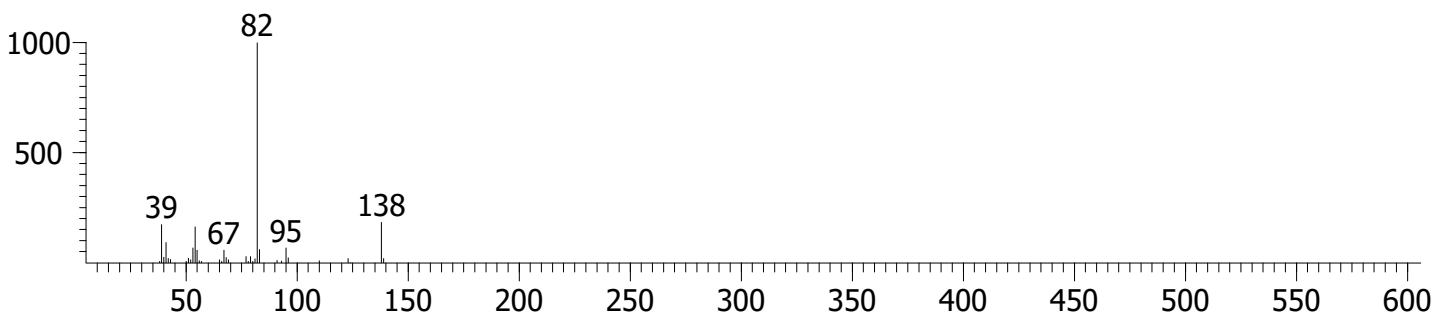
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 589, at 763.338 , 1.643 sec , sec (Spec # 43179)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 589, at 763.338 , 1.643 sec , sec (Spec # 43179)



Library Hit - similarity 907, "1H-Pyrazole, 4,5-dihydro-5,5-dimethyl-4-isopropylidene-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Pyrazole, 4,5-dihydro-5,5-dimethyl-4-isopropylidene-	907	6165	106251-09-6	mainlib	C8H14N2	138
2	Isophorone	890	3365	78-59-1	mainlib	C9H14O	138
3	2-Cyclohexen-1-one, 3,5-dimethyl-	757	132	1123-09-7	mainlib	C8H12O	124
4	1,2,4,5-Tetrazine	749	98	290-96-0	mainlib	C2H2N4	82
5	2-Cyclohexen-1-one, 3-methyl-	742	75	1193-18-6	mainlib	C7H10O	110

Benzaldehyde, 4-chloro-

1st Dimension R.T. = 766.836

2nd Dimension R.T. = 1.808

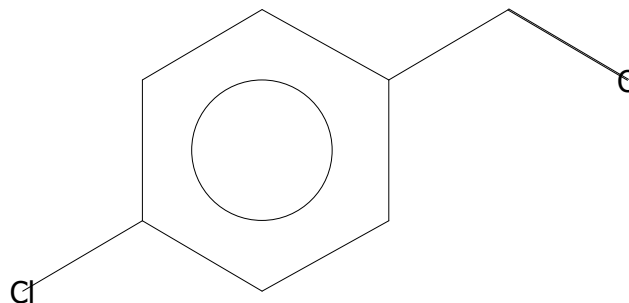
Quant Mass(es) = 139

S/N = 1178.1

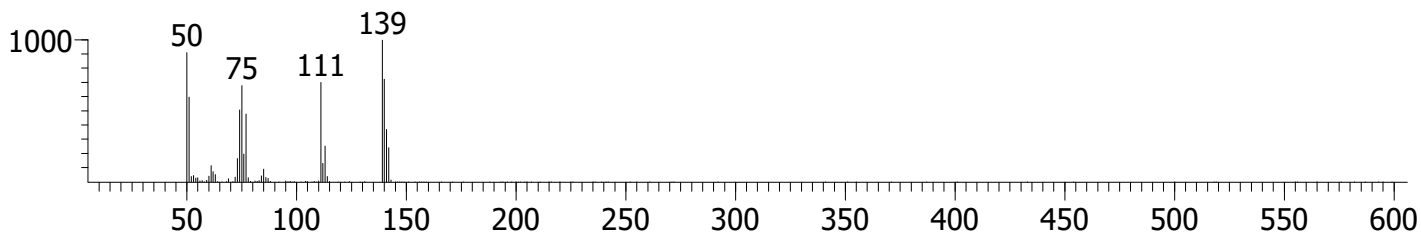
Area = 143822

Height = 19073

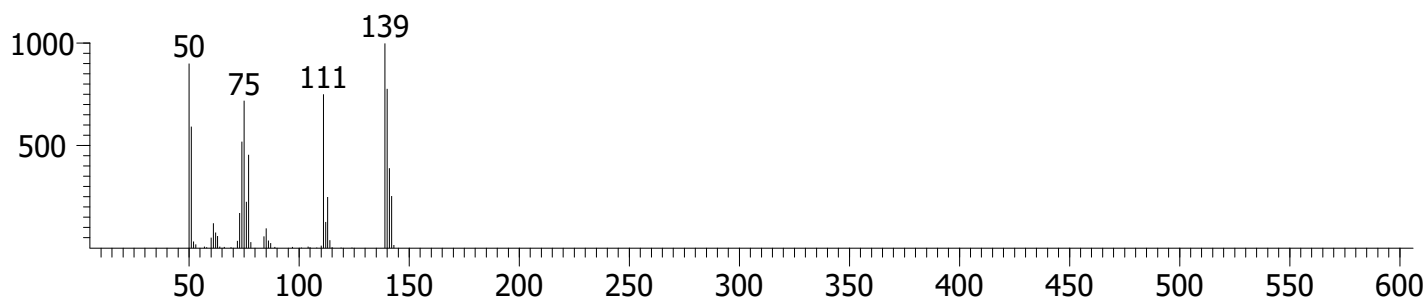
Similarity = 955



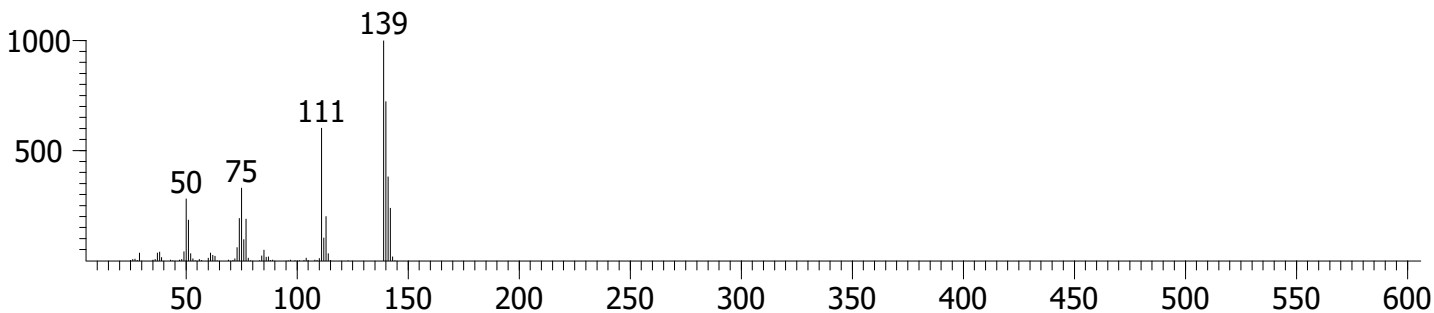
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 595, at 766.836 , 1.808 sec , sec (Spec # 43734)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 595, at 766.836 , 1.808 sec , sec (Spec # 43734)



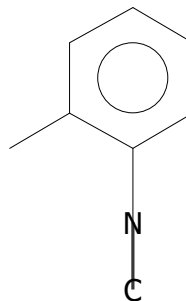
Library Hit - similarity 955, "Benzaldehyde, 4-chloro-"



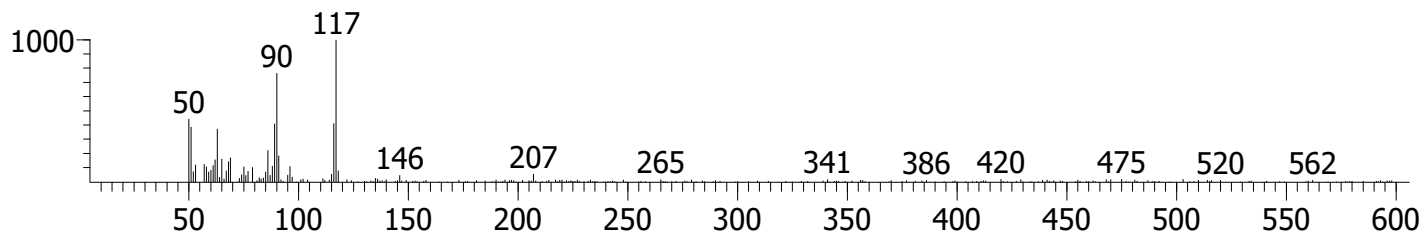
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzaldehyde, 4-chloro-	955	6283	104-88-1	mainlib	C7H5ClO	140
2	Benzaldehyde, 2-chloro-	931	2105	89-98-5	mainlib	C7H5ClO	140
3	Benzaldehyde, 3-chloro-	917	1318	587-04-2	mainlib	C7H5ClO	140
4	1-Ethanone, 2-amino-1-(4-chlorophenyl)-	771	39	0-00-0	mainlib	C8H8ClNO	169
5	Benzoyl chloride, 2-(4-chlorobenzoyloxy)-	762	28	0-00-0	mainlib	C14H8Cl2O3	294

Benzene, 1-isocyano-2-methyl-

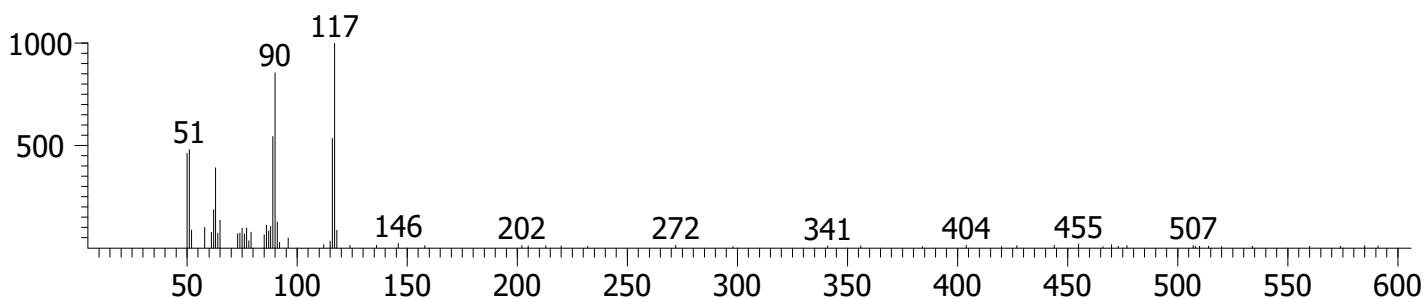
1st Dimension R.T. = 787.824
2nd Dimension R.T. = 2.033
Quant Mass(es) = 90
S/N = 62.511
Area = 4945.1
Height = 626.02
Similarity = 860



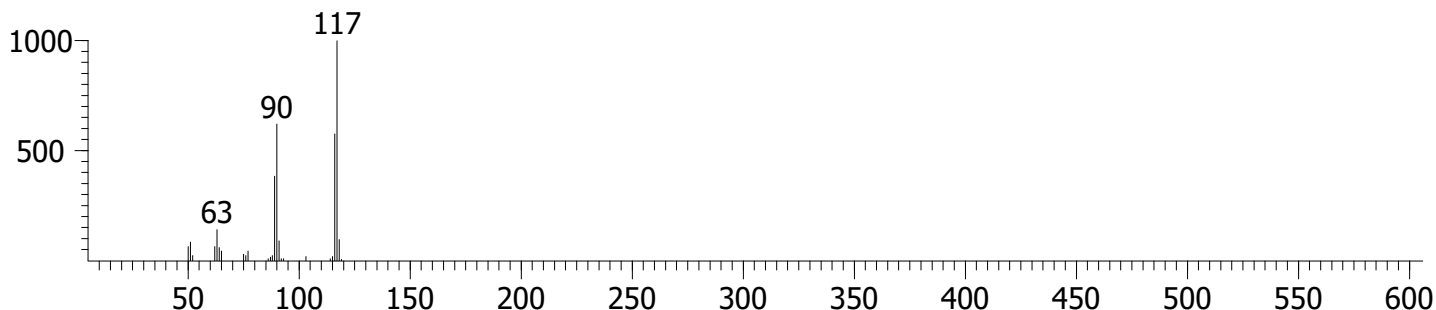
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 638, at 787.824 , 2.033 sec , sec (Spec # 46948)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 638, at 787.824 , 2.033 sec , sec (Spec # 46948)



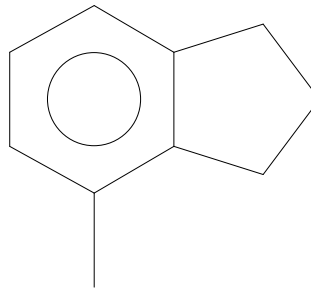
Library Hit - similarity 860, "Benzene, 1-isocyano-2-methyl-"



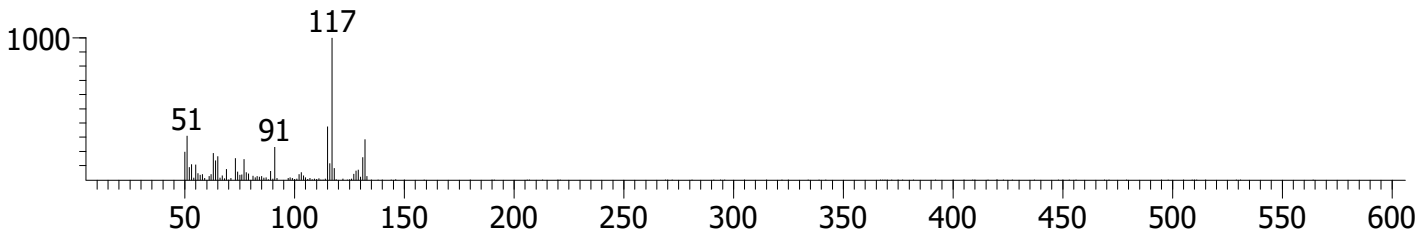
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-isocyano-2-methyl-	860	2226	10468-64-1	mainlib	C8H7N	117
2	Benzonitrile, 3-methyl-	848	1482	620-22-4	mainlib	C8H7N	117
3	Benzenepropanoic acid, à-(hydroxyimino)-	846	1367	3682-17-5	mainlib	C9H9NO3	179
4	Benzonitrile, 2-methyl-	838	1020	529-19-1	mainlib	C8H7N	117
5	Benzyl nitrile	837	980	140-29-4	mainlib	C8H7N	117

1H-Indene, 2,3-dihydro-4-methyl-

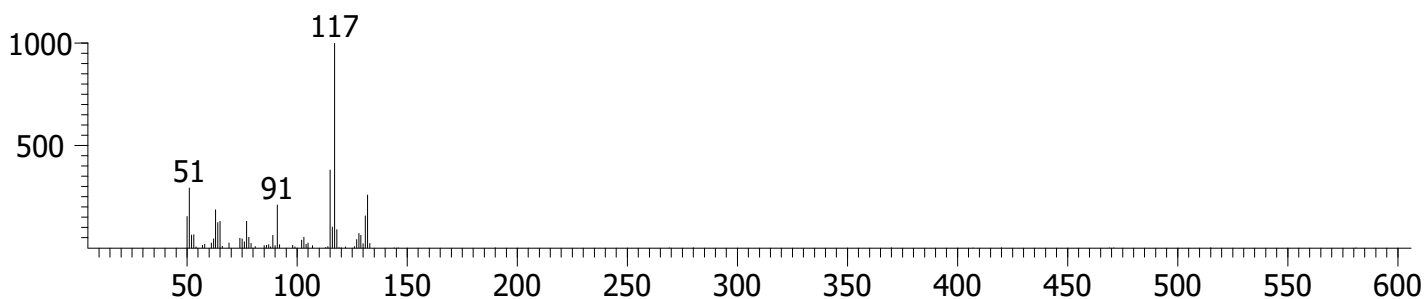
1st Dimension R.T. = 791.322
2nd Dimension R.T. = 1.571
Quant Mass(es) = 117
S/N = 548.67
Area = 66856
Height = 10215
Similarity = 925



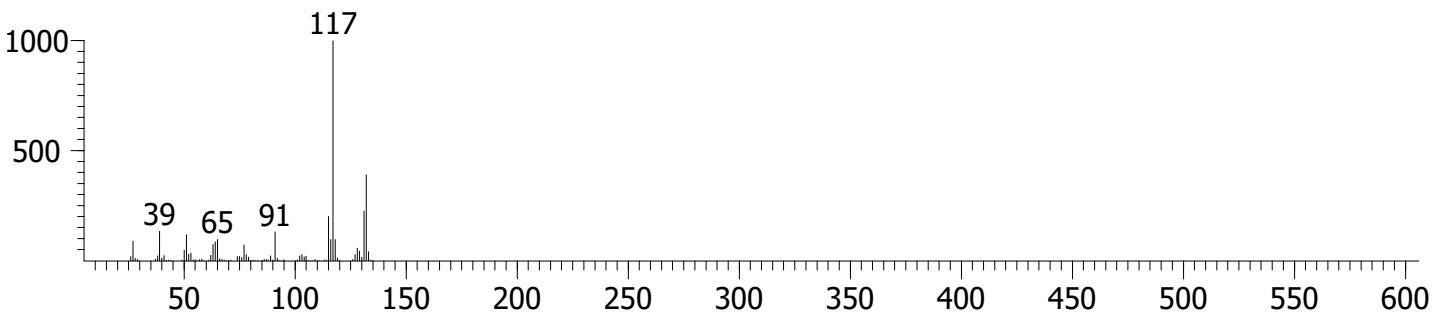
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 642, at 791.322 , 1.571 sec , sec (Spec # 47408)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 642, at 791.322 , 1.571 sec , sec (Spec # 47408)



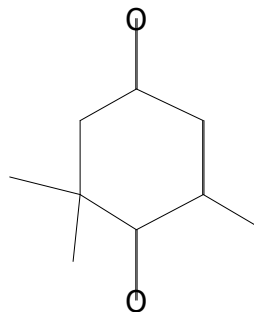
Library Hit - similarity 925, "1H-Indene, 2,3-dihydro-4-methyl-"



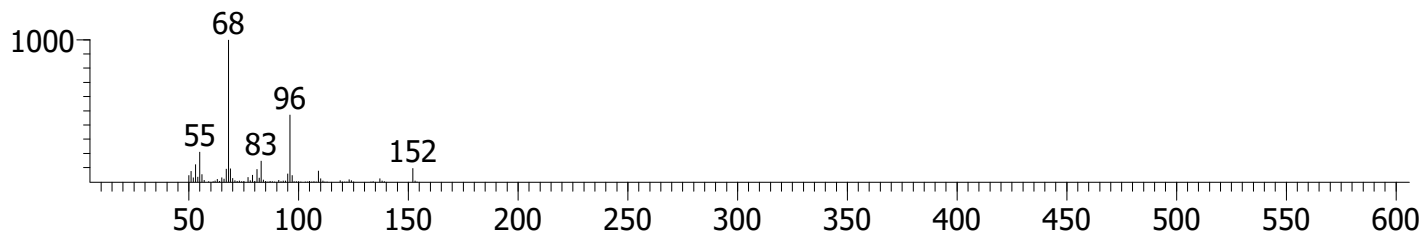
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Indene, 2,3-dihydro-4-methyl-	925	2024	824-22-6	mainlib	C10H12	132
2	1H-Indene, 2,3-dihydro-5-methyl-	919	1590	874-35-1	mainlib	C10H12	132
3	(E)-1-Phenyl-1-butene	914	1282	1005-64-7	mainlib	C10H12	132
4	Indan, 1-methyl-	897	699	767-58-8	mainlib	C10H12	132
5	Benzene, 1-ethenyl-3-ethyl-	891	550	7525-62-4	mainlib	C10H12	132

2,6,6-Trimethyl-2-cyclohexene-1,4-dione

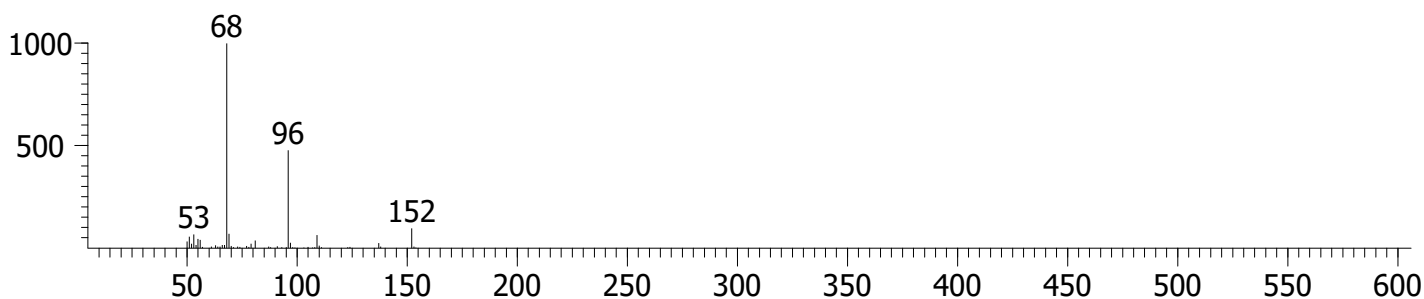
1st Dimension R.T. = 791.322
2nd Dimension R.T. = 1.762
Quant Mass(es) = 68
S/N = 2163.9
Area = 707342
Height = 85765
Similarity = 901



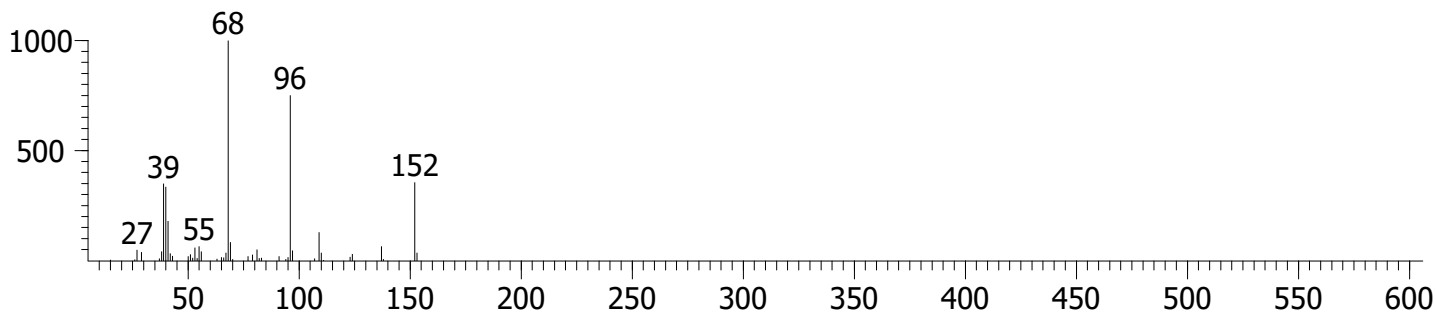
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 646, at 791.322 , 1.762 sec , sec (Spec # 47437)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 646, at 791.322 , 1.762 sec , sec (Spec # 47437)



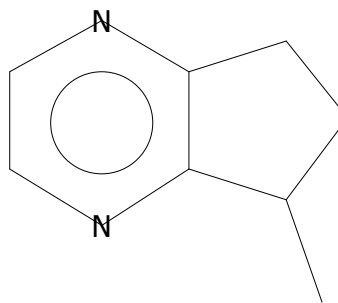
Library Hit - similarity 901, "2,6,6-Trimethyl-2-cyclohexene-1,4-dione"



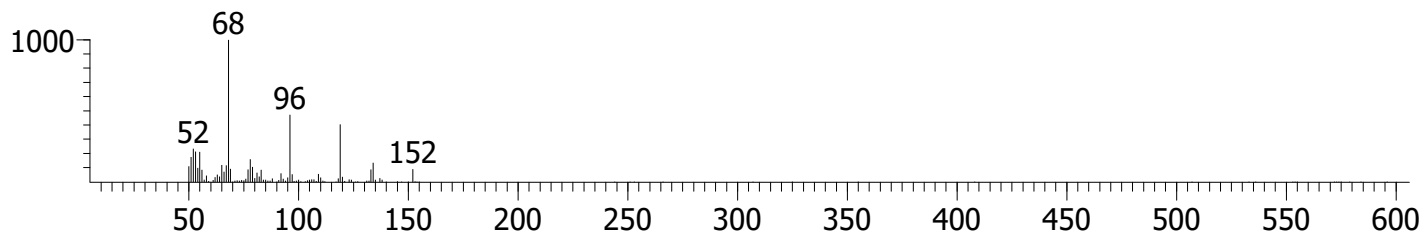
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	901	8186	1125-21-9	mainlib	C9H12O2	152
2	2-Cyclohexen-1-one	843	1507	930-68-7	mainlib	C6H8O	96
3	But-1-ene-3-yne, 1-ethoxy-	752	127	2806-41-9	mainlib	C6H8O	96
4	4(1H)-Pyrimidinone	735	69	4562-27-0	mainlib	C4H4N2O	96
5	1-Cyclohexene-1-carboxaldehyde, 5,5-dimethyl-3-oxo-	734	66	56621-35-3	mainlib	C9H12O2	152

5H-5-Methyl-6,7-dihydrocyclopentapyrazine

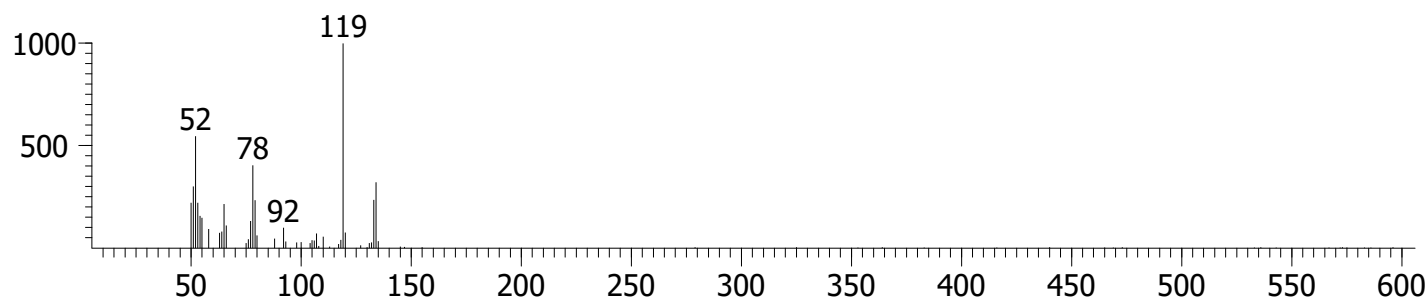
1st Dimension R.T. = 791.322
2nd Dimension R.T. = 1.802
Quant Mass(es) = 119
S/N = 248.37
Area = 28668
Height = 3592.2
Similarity = 788



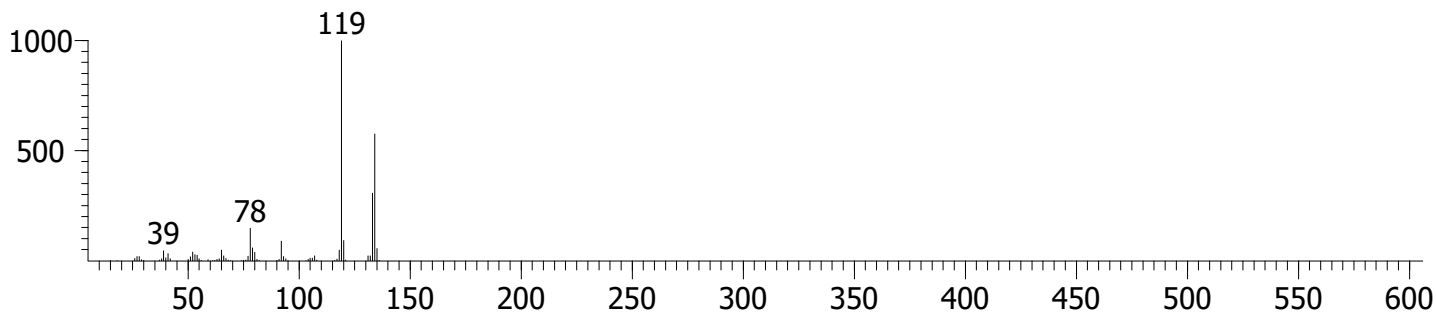
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 647, at 791.322 , 1.802 sec , sec (Spec # 47443)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 647, at 791.322 , 1.802 sec , sec (Spec # 47443)

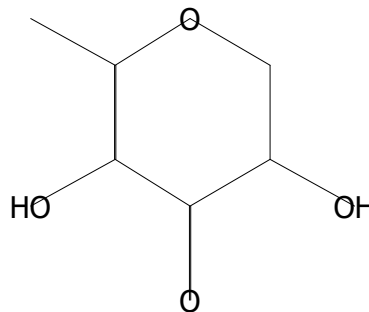


Library Hit - similarity 788, "5H-5-Methyl-6,7-dihydrocyclopentapyrazine"



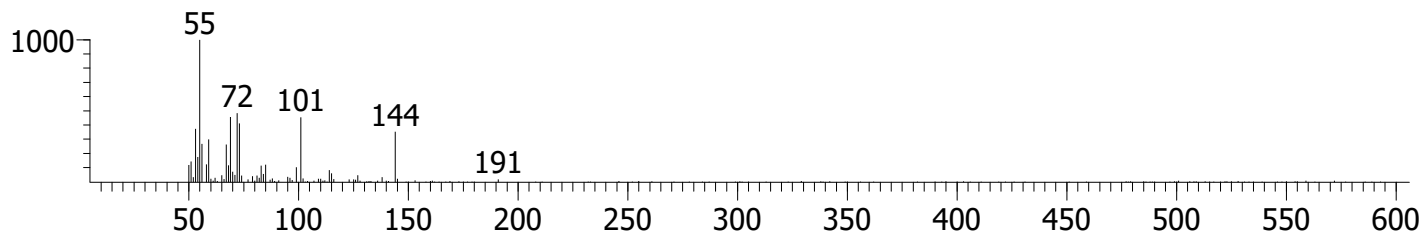
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5H-5-Methyl-6,7-dihydrocyclopentapyrazine	788	3829	23747-48-0	mainlib	C8H10N2	134
2	Pyridine, 2-(4-methyl-5-trans-phenyl-1,3-oxazolidin-2-yl)-	774	2397	0-00-0	mainlib	C15H16N2O	240
3	Pyrazine, 2-methyl-3-(1-propenyl)-, (Z)-	755	1164	55138-65-3	mainlib	C8H10N2	134
4	Pyridine, 2-(4-methyl-5-cis-phenyl-1,3-oxazolidin-2-yl)-	742	752	0-00-0	mainlib	C15H16N2O	240
5	Propanedinitrile, (1,2-dimethylpropylidene)-	735	576	13017-52-2	mainlib	C8H10N2	134

4H-Pyran-4-one,
2,3-dihydro-3,5-dihydroxy-6-methyl-

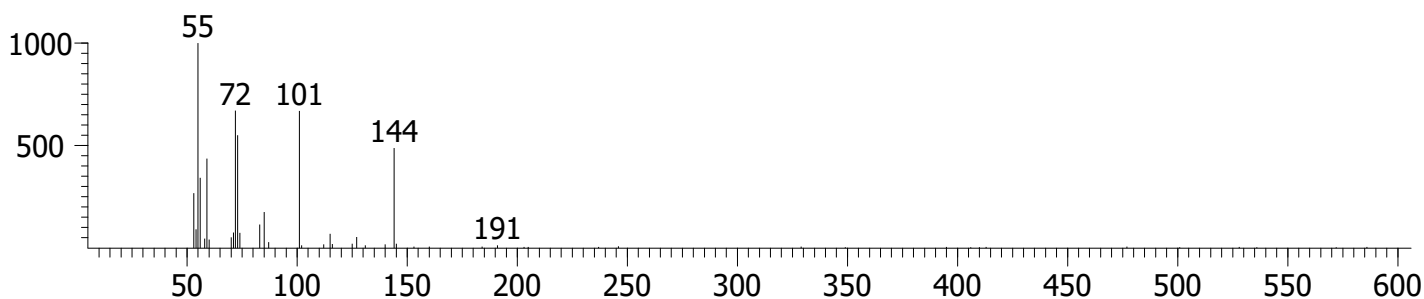


1st Dimension R.T. = 798.318
2nd Dimension R.T. = 1.822
Quant Mass(es) = 144
S/N = 100.83
Area = 10179
Height = 1302.5
Similarity = 777

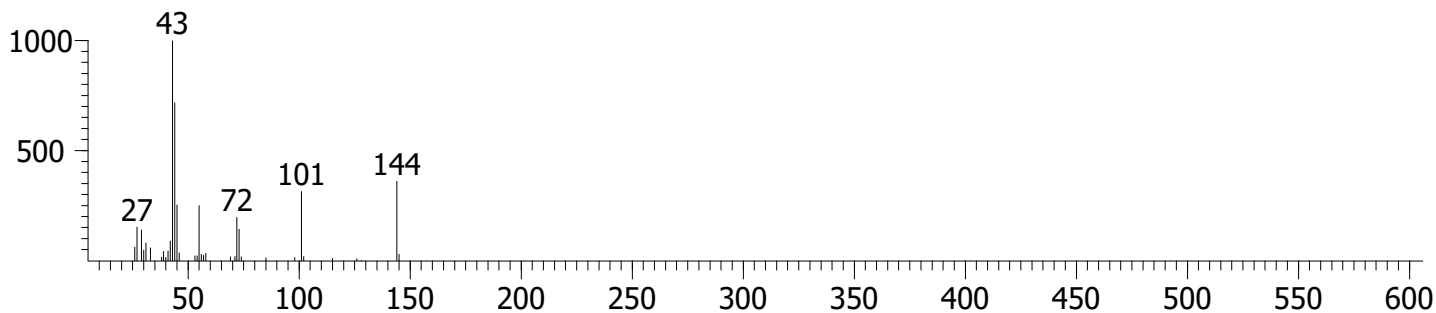
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 663, at 798.318 , 1.822 sec , sec (Spec # 48506)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 663, at 798.318 , 1.822 sec , sec (Spec # 48506)

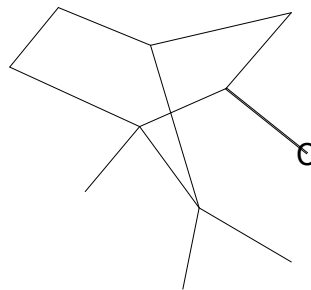


Library Hit - similarity 777, "4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	777	8420	28564-83-2	mainlib	C ₆ H ₈ O ₄	144
2	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one	596	148	10230-62-3	mainlib	C ₆ H ₈ O ₄	144
3	cis-3-Methyl-2-n-propylthiophane	592	125	118068-76-1	mainlib	C ₈ H ₁₆ S	144
4	trans-3-Methyl-2-n-propylthiophane	588	105	118068-75-0	mainlib	C ₈ H ₁₆ S	144
5	1,3-Dioxane, 2,4-dimethyl-	587	101	766-20-1	mainlib	C ₆ H ₁₂ O ₂	116

Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-



1st Dimension R.T. = 801.816

2nd Dimension R.T. = 1.630

Quant Mass(es) = 95

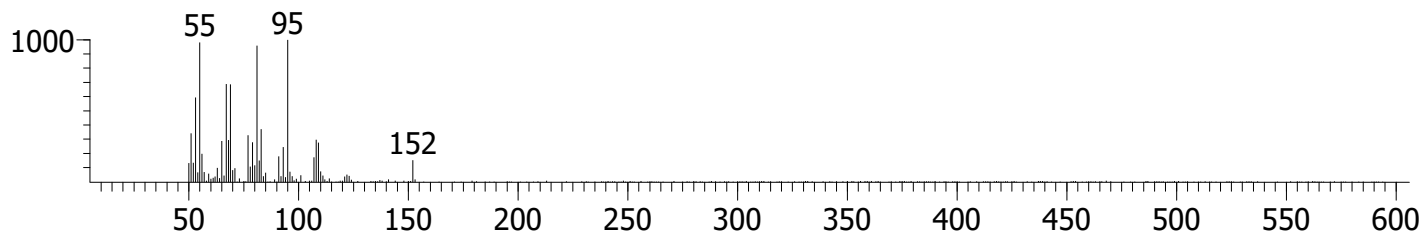
S/N = 163.91

Area = 31212

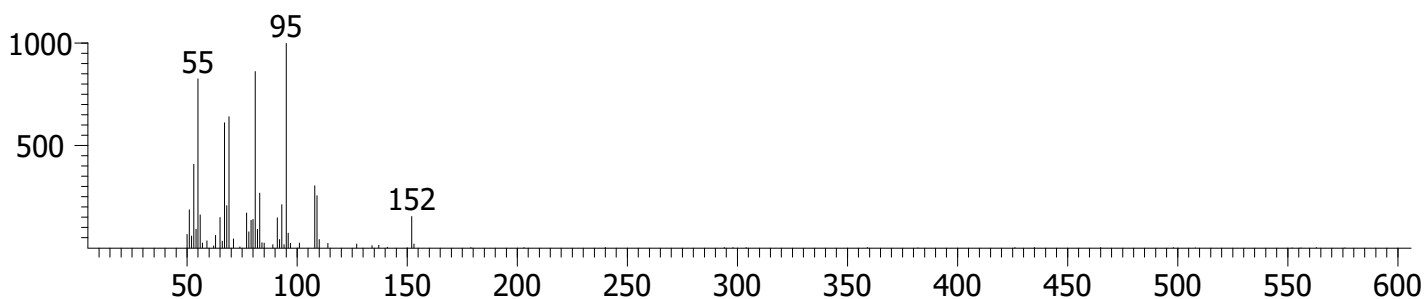
Height = 3115.2

Similarity = 882

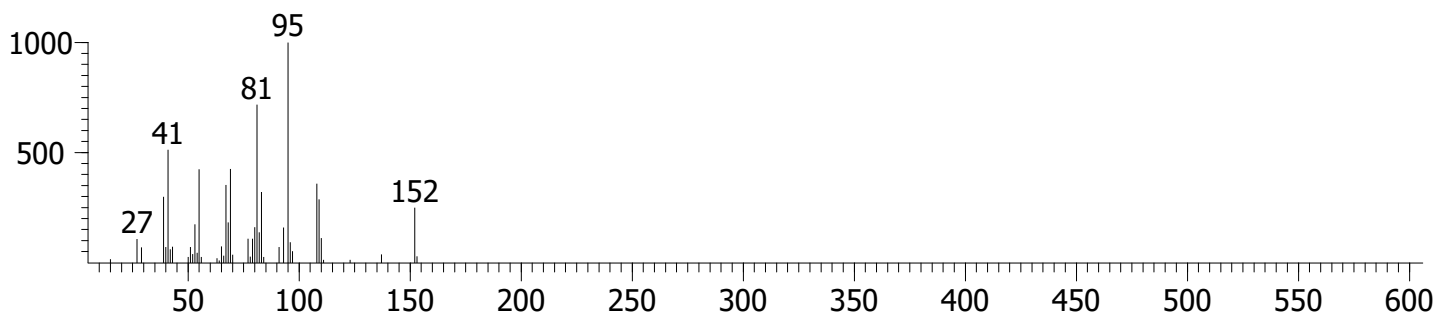
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 668, at 801.816 , 1.630 sec , sec (Spec # 49007)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 668, at 801.816 , 1.630 sec , sec (Spec # 49007)



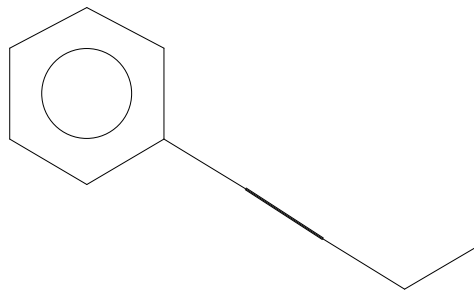
Library Hit - similarity 882, "Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-"



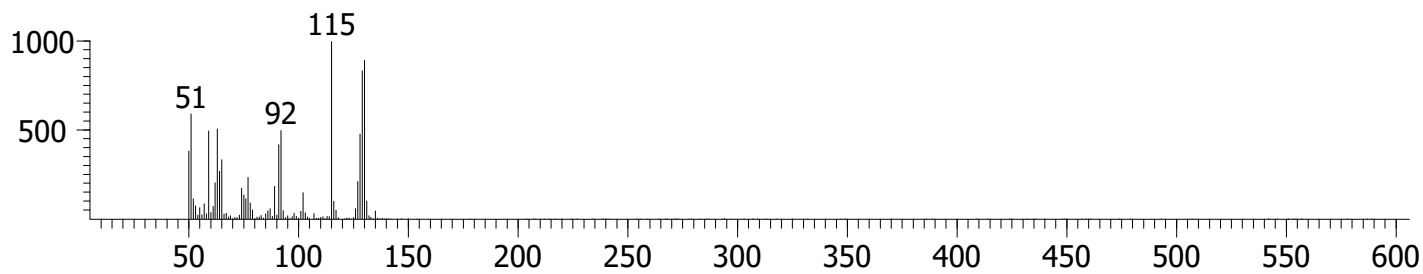
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	882	6647	464-48-2	mainlib	C10H16O	152
2	Camphor	852	1847	76-22-2	mainlib	C10H16O	152
3	(+)-2-Bornanone	818	473	464-49-3	mainlib	C10H16O	152
4	Spirobicyclo[2.2.1]heptane-2,2'-(1',3'-dioxo-2'-oxocyclohex-5'-ene), 1,6',7,7-tetramethyl-	803	287	0-00-0	mainlib	C14H20O3	236
5	4-Methyl-1,4-heptadiene	784	139	13857-55-1	mainlib	C8H14	110

Benzene, 1-butynyl-

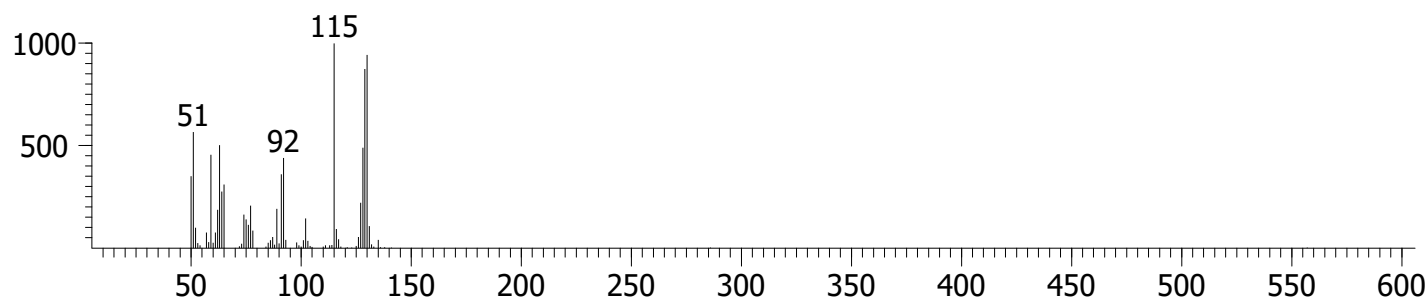
1st Dimension R.T. = 812.31
2nd Dimension R.T. = 1.650
Quant Mass(es) = 92
S/N = 1423.1
Area = 75526
Height = 9957.2
Similarity = 861



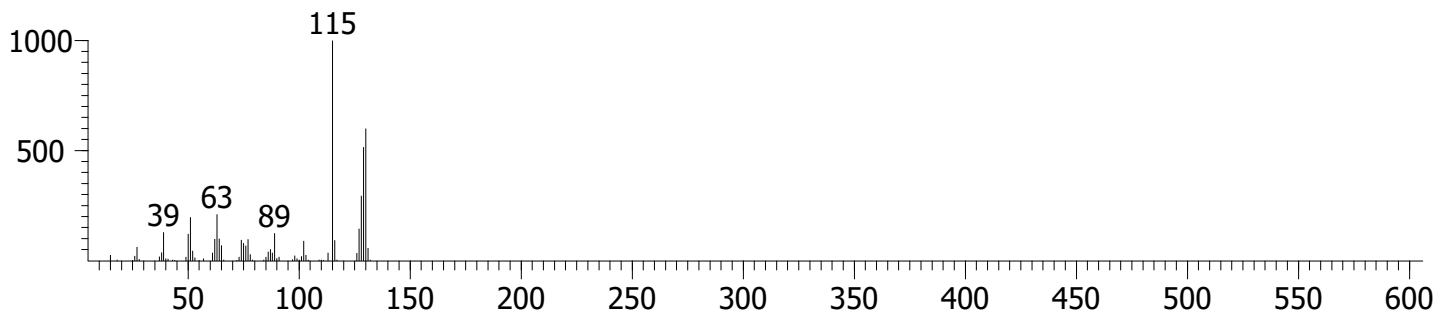
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 694, at 812.31 , 1.650 sec , sec (Spec # 50600)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 694, at 812.31 , 1.650 sec , sec (Spec # 50600)



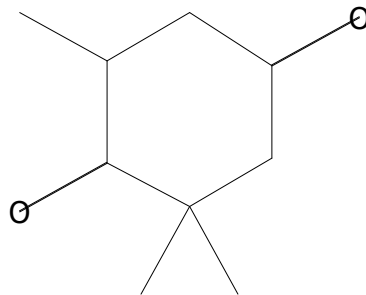
Library Hit - similarity 861, "Benzene, 1-butynyl-"



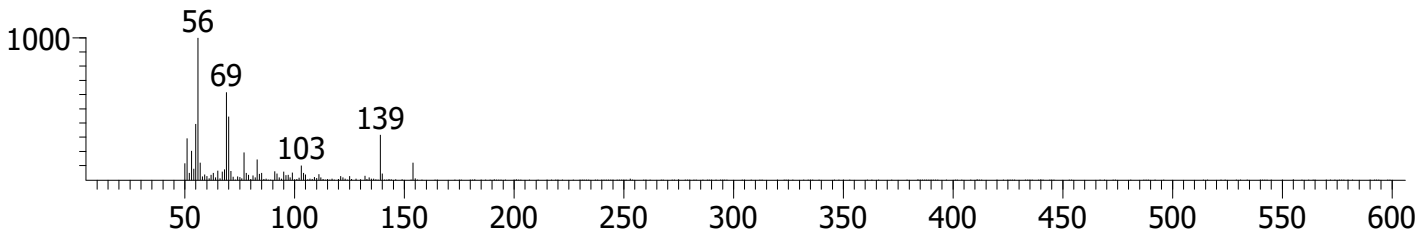
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-butynyl-	861	1761	622-76-4	mainlib	C10H10	130
2	1H-Indene, 3-methyl-	849	1172	767-60-2	mainlib	C10H10	130
3	2-Methylindene	846	1036	2177-47-1	mainlib	C10H10	130
4	Benzene, 1,3-butadienyl-	841	835	1515-78-2	mainlib	C10H10	130
5	Benzene, (1-methylene-2-propenyl)-	840	802	2288-18-8	mainlib	C10H10	130

1,4-Cyclohexanedione, 2,2,6-trimethyl-

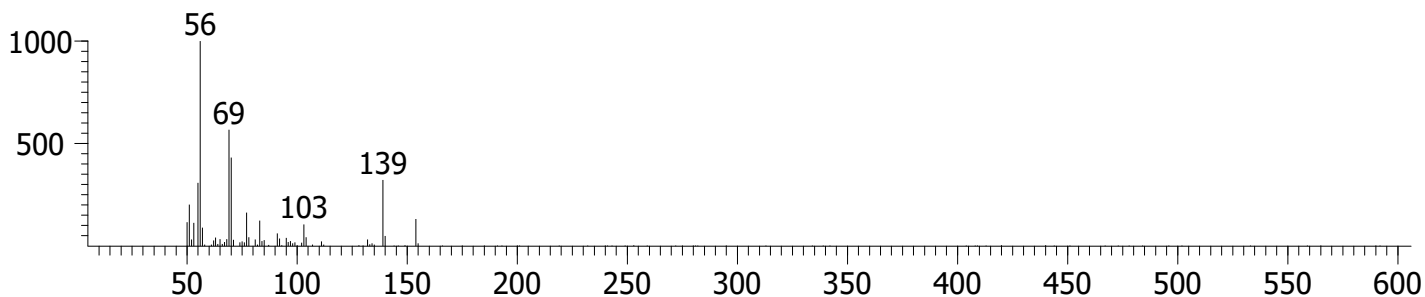
1st Dimension R.T. = 826.302
2nd Dimension R.T. = 1.855
Quant Mass(es) = 139
S/N = 229.00
Area = 23789
Height = 2824.7
Similarity = 721



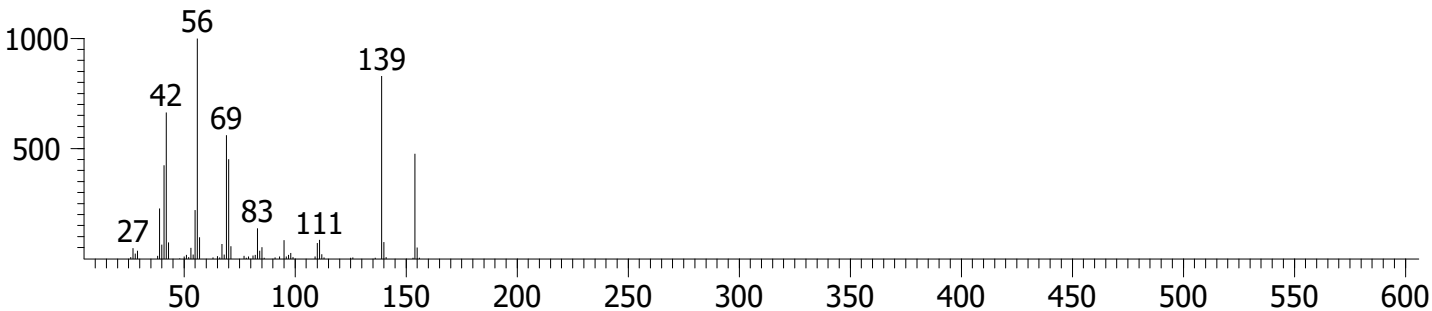
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 736, at 826.302 , 1.855 sec , sec (Spec # 52751)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 736, at 826.302 , 1.855 sec , sec (Spec # 52751)



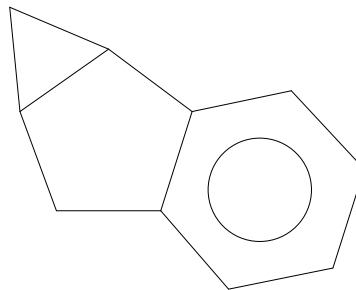
Library Hit - similarity 721, "1,4-Cyclohexanedione, 2,2,6-trimethyl-"



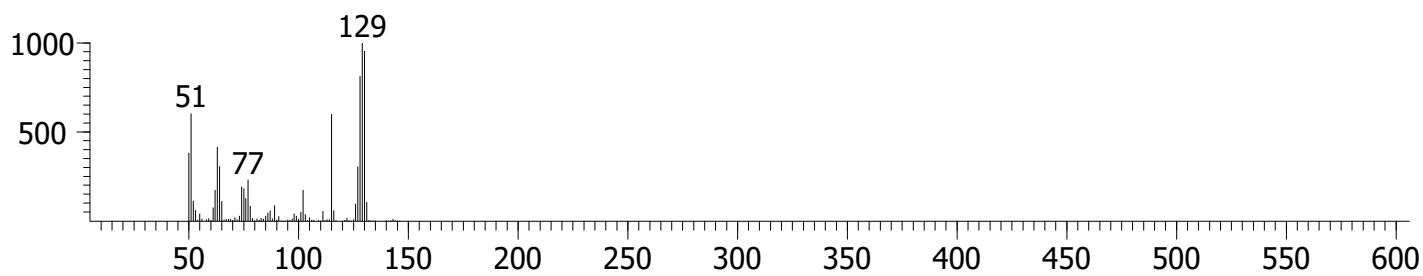
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,4-Cyclohexanedione, 2,2,6-trimethyl-	721	4134	20547-99-3	mainlib	C9H14O2	154
2	2-Methyl-2-hexyl methylphosphonofluoridate	663	761	0-00-0	mainlib	C8H18FO2P	196
3	1-Propene, 1-(2-propenyloxy)-, (E)-	656	583	61142-13-0	mainlib	C6H10O	98
4	Cyclohexane, 1,1-dimethyl-2-propyl-	636	265	81983-71-3	mainlib	C11H22	154
5	1,4-Dioxaspiro[2.4]heptan-5-one, 6-methyl-	635	255	0-00-0	mainlib	C6H8O3	128

Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-

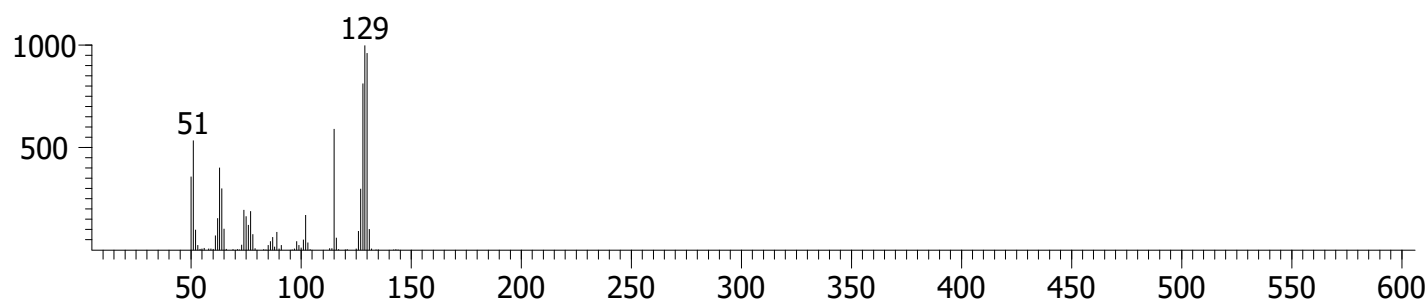
1st Dimension R.T. = 829.8
2nd Dimension R.T. = 1.742
Quant Mass(es) = 130
S/N = 4121.4
Area = 302317
Height = 43119
Similarity = 934



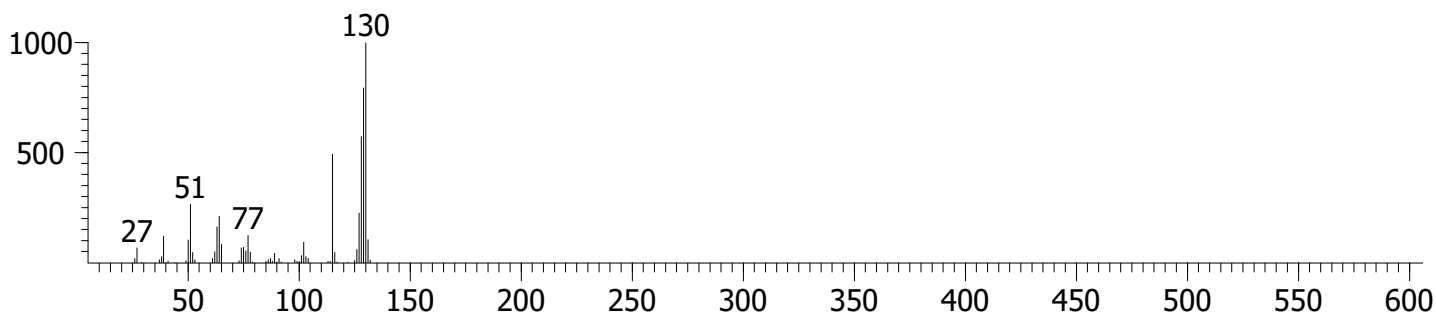
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 744, at 829.8 , 1.742 sec , sec (Spec # 53264)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 744, at 829.8 , 1.742 sec , sec (Spec # 53264)

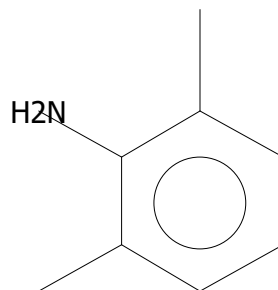


Library Hit - similarity 934, "Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-"



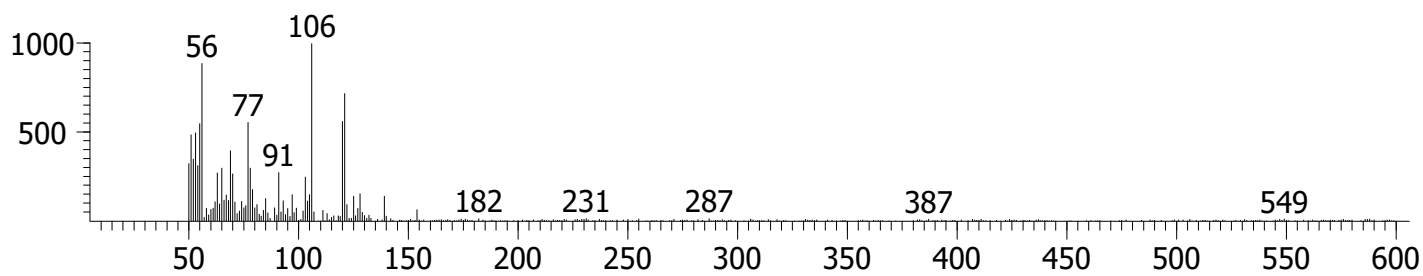
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-	934	4121	15677-15-3	mainlib	C10H10	130
2	1,4-Dihydronaphthalene	915	2001	612-17-9	mainlib	C10H10	130
3	1H-Indene, 3-methyl-	884	545	767-60-2	mainlib	C10H10	130
4	1,4-Methanonaphthalen-9-one, 1,2,3,4-tetrahydro-	881	482	6165-88-4	mainlib	C11H10O	158
5	Benzene, 1-butynyl-	880	463	622-76-4	mainlib	C10H10	130

2,6-Xylidine

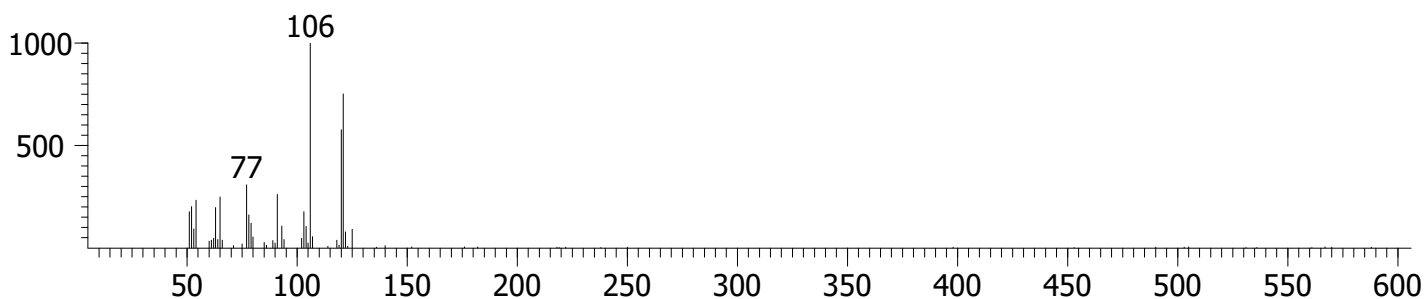


1st Dimension R.T. = 829.8
2nd Dimension R.T. = 1.868
Quant Mass(es) = 106
S/N = 161.29
Area = 15424
Height = 1825.1
Similarity = 908

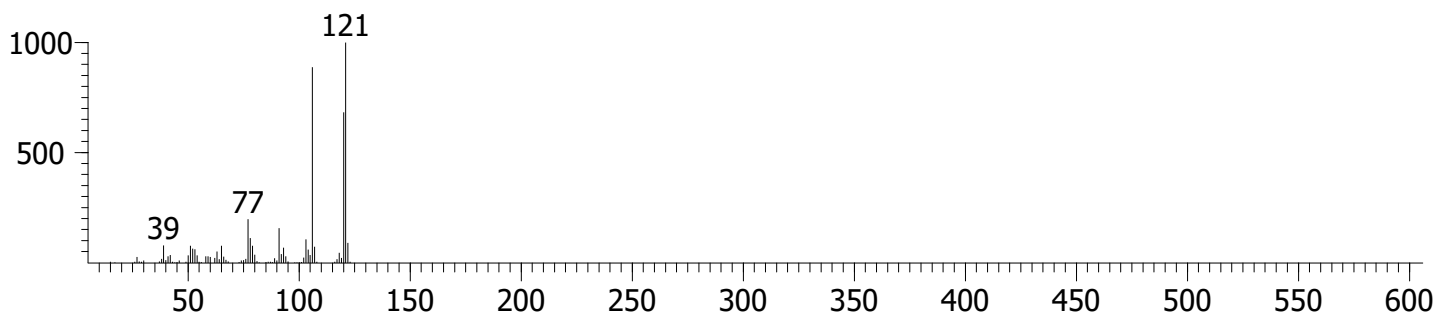
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 747, at 829.8 , 1.868 sec , sec (Spec # 53283)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 747, at 829.8 , 1.868 sec , sec (Spec # 53283)



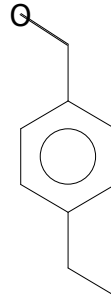
Library Hit - similarity 908, "2,6-Xylidine"



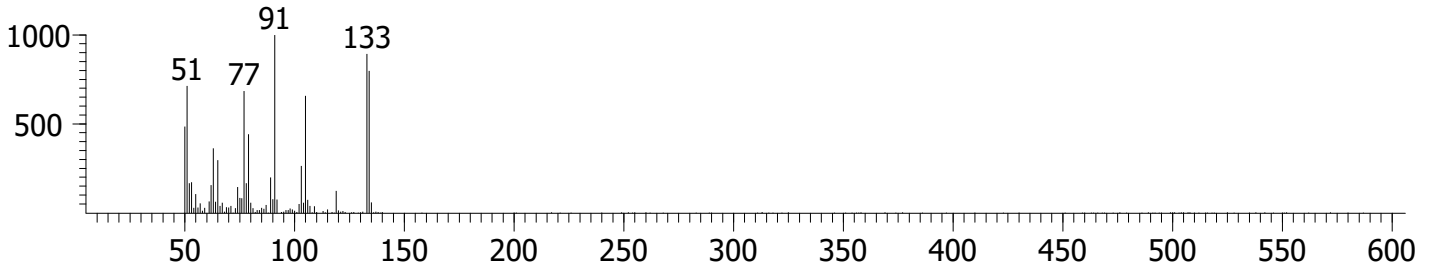
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,6-Xylidine	908	4288	87-62-7	mainlib	C8H11N	121
2	Benzenamine, 2,3-dimethyl-	897	2941	87-59-2	mainlib	C8H11N	121
3	Benzenamine, 2,5-dimethyl-	872	897	95-78-3	mainlib	C8H11N	121
4	4-Nitro-N-(2,6-xylyl)benzenesulfonamide	857	543	109508-84-1	mainlib	C14H14N2O4S	306
5	Benzenamine, 3,4-dimethyl-	851	427	95-64-7	mainlib	C8H11N	121

Benzaldehyde, 4-ethyl-

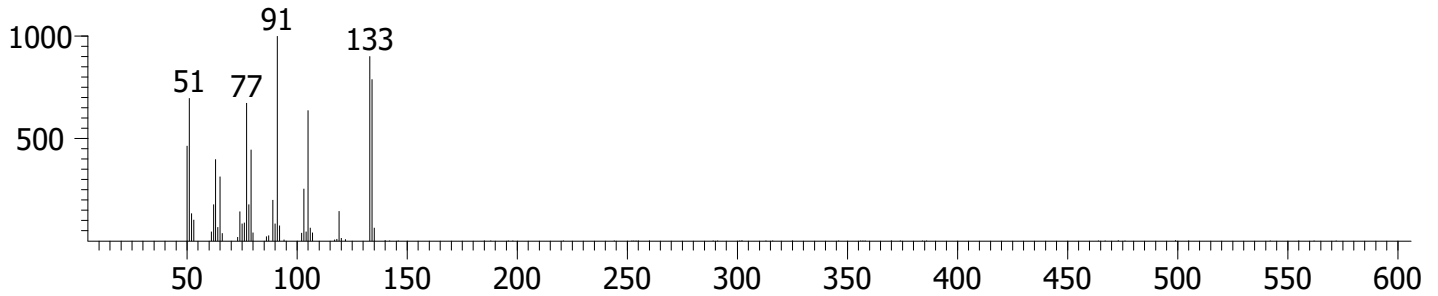
1st Dimension R.T. = 847.29
2nd Dimension R.T. = 1.729
Quant Mass(es) = 134
S/N = 495.33
Area = 59628
Height = 8005.7
Similarity = 893



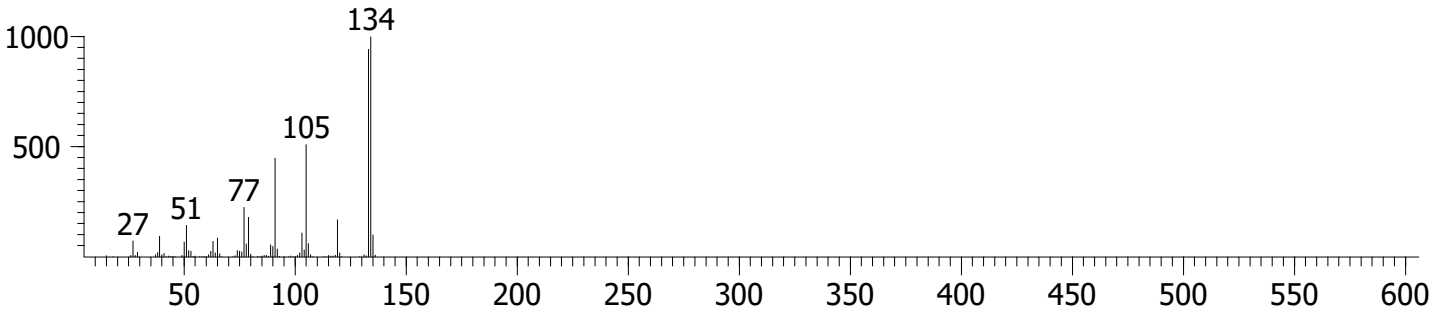
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 770, at 847.29 , 1.729 sec , sec (Spec # 55912)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 770, at 847.29 , 1.729 sec , sec (Spec # 55912)



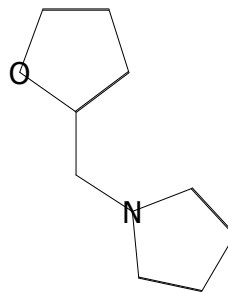
Library Hit - similarity 893, "Benzaldehyde, 4-ethyl-"



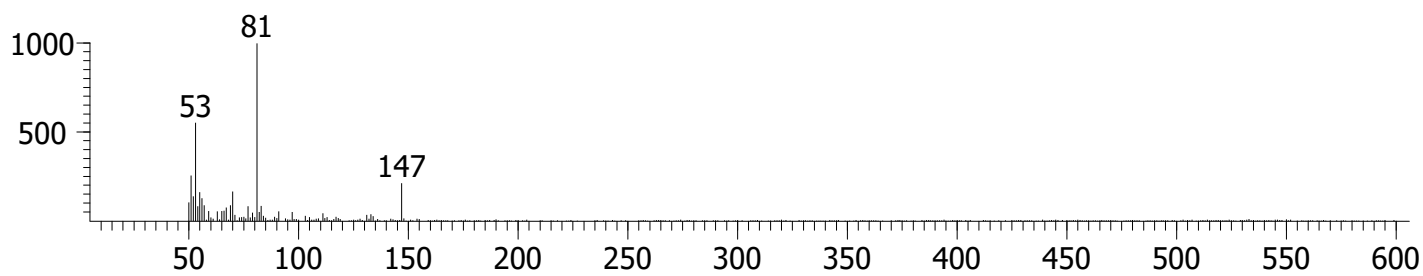
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzaldehyde, 4-ethyl-	893	4838	4748-78-1	mainlib	C9H10O	134
2	2,6-Dimethylbenzaldehyde	829	794	1123-56-4	mainlib	C9H10O	134
3	Benzaldehyde, 3,5-dimethyl-	829	794	5779-95-3	mainlib	C9H10O	134
4	6-APDB	816	513	1281872-58-9	mainlib	C11H15NO	177
5	Benzaldehyde, 3,4-dimethyl-	815	493	5973-71-7	mainlib	C9H10O	134

1H-Pyrrole, 1-(2-furanylmethyl)-

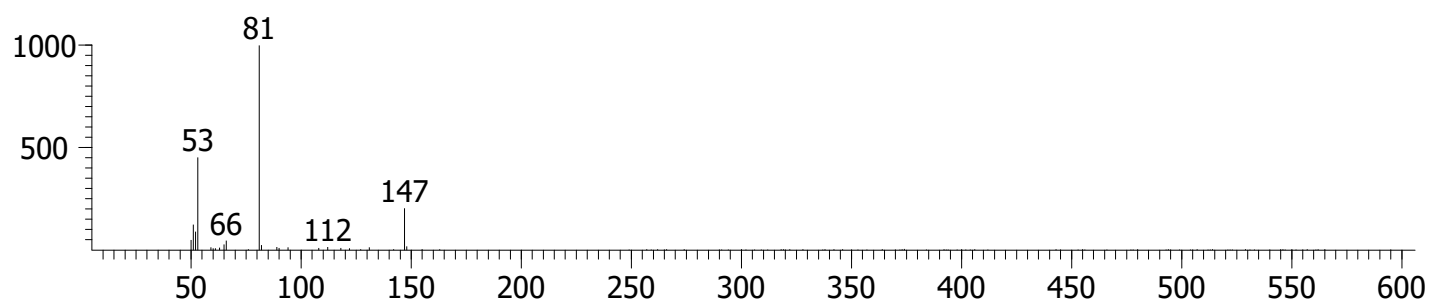
1st Dimension R.T. = 847.29
2nd Dimension R.T. = 1.841
Quant Mass(es) = 81
S/N = 163.80
Area = 31421
Height = 3997.0
Similarity = 863



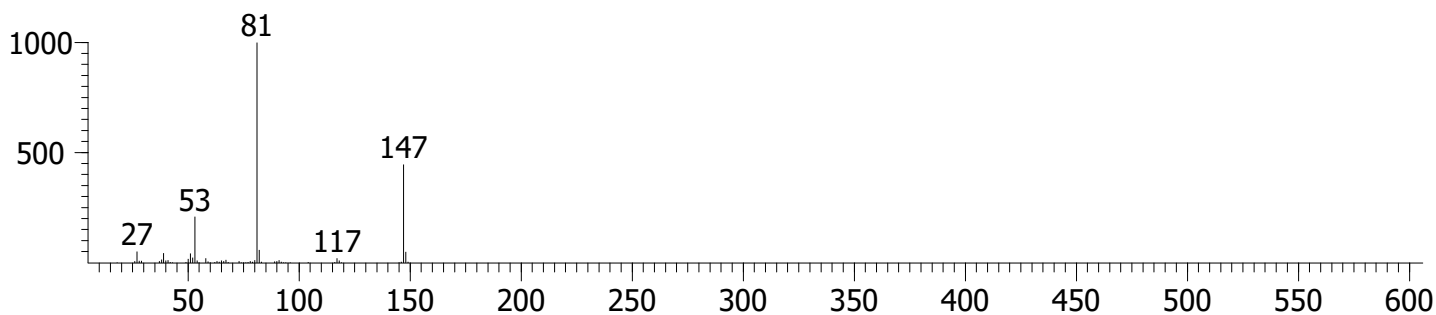
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 771, at 847.29 , 1.841 sec , sec (Spec # 55929)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 771, at 847.29 , 1.841 sec , sec (Spec # 55929)



Library Hit - similarity 863, "1H-Pyrrole, 1-(2-furanylmethyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Pyrrole, 1-(2-furanylmethyl)-	863	6638	1438-94-4	mainlib	C9H9NO	147
2	2,4-Pentadienoic acid, 1-cyclopenten-3-on-1-yl ester	816	1388	0-00-0	mainlib	C10H10O3	178
3	Furfuryl isothiocyanate	767	285	4650-60-6	mainlib	C6H5NOS	139
4	4-(2-Chloro-4-fluorophenyl)-1-(furan-2-ylmethyl)-4H,5H,7H-pyrazolo[3,4-b]pyridin-6-one	766	274	0-00-0	mainlib	C17H13ClFNO2	345
5	Cyclohexane, 1-chloro-2-nitroso-	763	242	16580-31-7	mainlib	C6H10ClNO	147

4-Phenylbut-3-ene-1-yne

1st Dimension R.T. = 861.282

2nd Dimension R.T. = 1.841

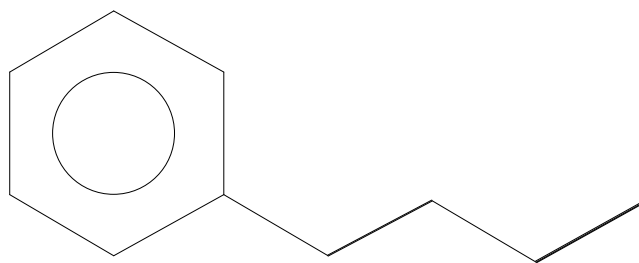
Quant Mass(es) = 128

S/N = 13173

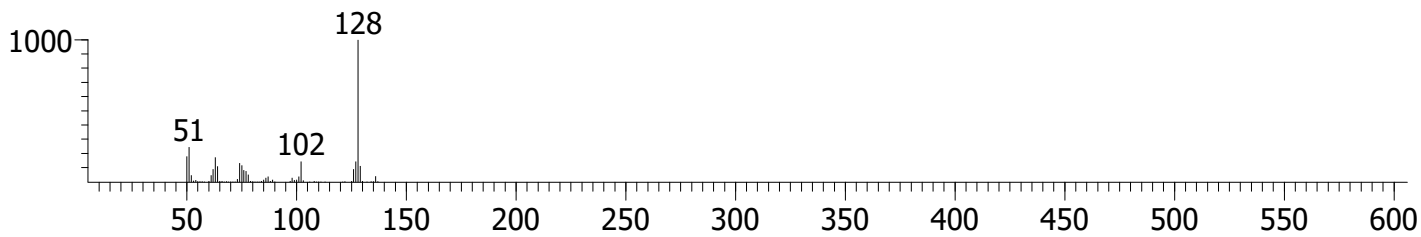
Area = 1659504

Height = 222761

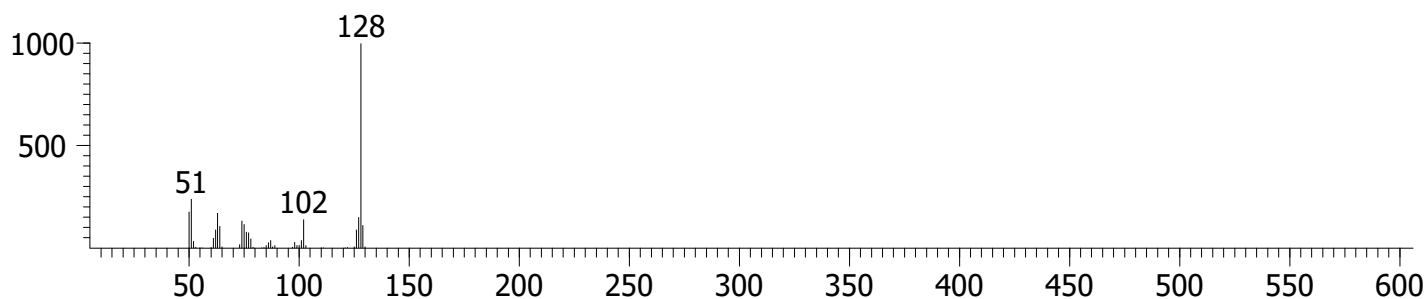
Similarity = 923



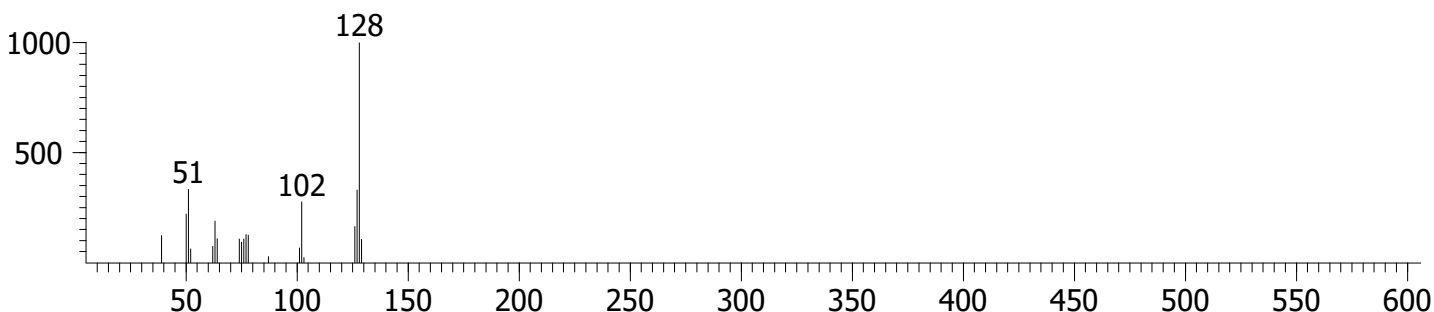
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 797, at 861.282 , 1.841 sec , sec (Spec # 58049)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 797, at 861.282 , 1.841 sec , sec (Spec # 58049)



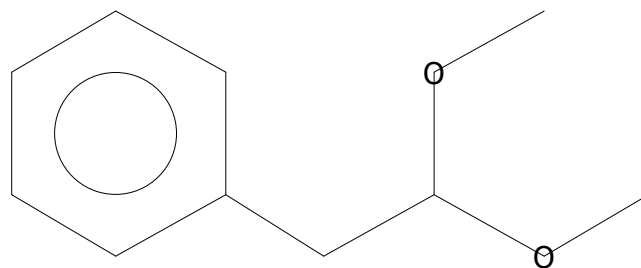
Library Hit - similarity 923, "4-Phenylbut-3-ene-1-yne"



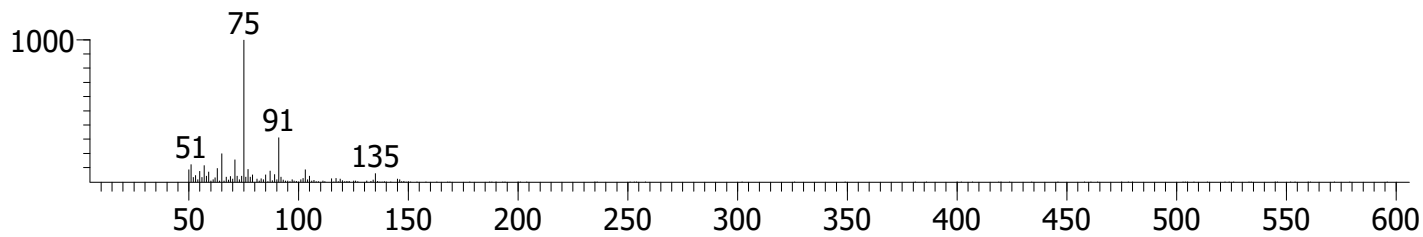
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Phenylbut-3-ene-1-yne	923	3973	0-00-0	mainlib	C10H8	128
2	1H-Indene, 1-methylene-	919	3356	2471-84-3	mainlib	C10H8	128
3	Azulene	891	969	275-51-4	mainlib	C10H8	128
4	Naphthalene	887	818	91-20-3	mainlib	C10H8	128
5	N-Methyl-9-aza-tricyclo[6.2.2.0(2,7)]dodec-2,4,6,11-tetraene-10-one	872	496	13131-19-6	mainlib	C12H11NO	185

Benzene, (2,2-dimethoxyethyl)-

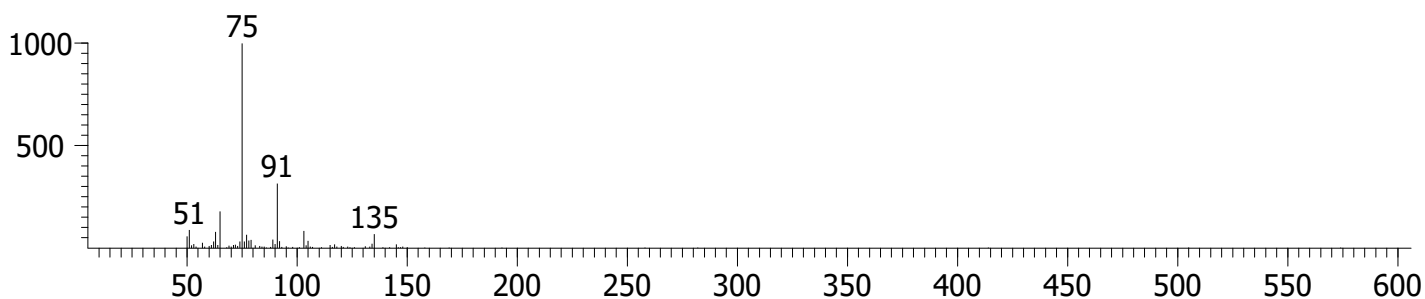
1st Dimension R.T. = 896.262
2nd Dimension R.T. = 1.670
Quant Mass(es) = 75
S/N = 680.39
Area = 129984
Height = 17644
Similarity = 898



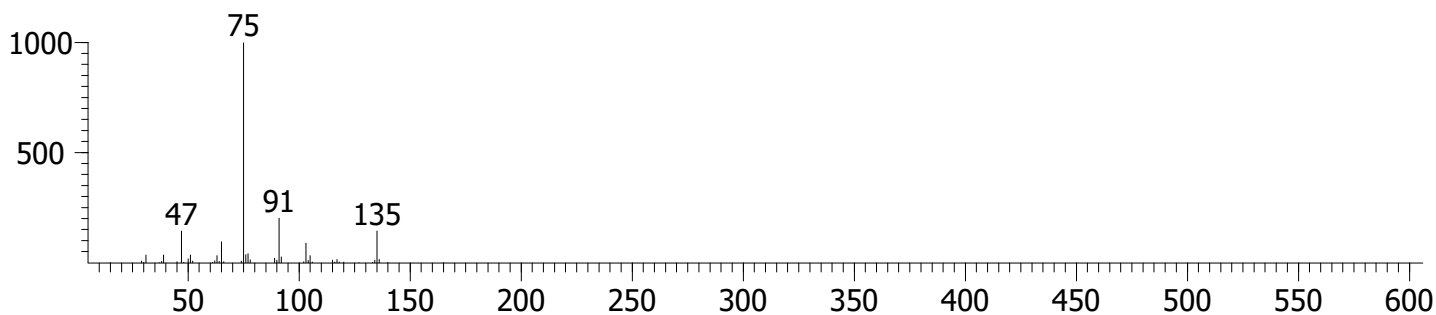
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 853, at 896.262 , 1.670 sec , sec (Spec # 63323)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 853, at 896.262 , 1.670 sec , sec (Spec # 63323)



Library Hit - similarity 898, "Benzene, (2,2-dimethoxyethyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, (2,2-dimethoxyethyl)-	898	9702	101-48-4	mainlib	C10H14O2	166
2	Benzoyloxyacetaldehyde dimethyl acetal	723	194	127657-97-0	mainlib	C11H16O3	196
3	N-Benzylaminoacetaldehyde diethyl acetal	670	38	61190-10-1	mainlib	C13H21NO2	223
4	benzenemethanamine, N-(2,2-dimethoxyethyl)-	647	14	0-00-0	mainlib	C11H17NO2	195
5	Benzene, [2-(ethylthio)ethyl]-	644	12	22914-08-5	mainlib	C10H14S	166

Phenol, 4-ethenyl-, acetate

1st Dimension R.T. = 903.258

2nd Dimension R.T. = 1.795

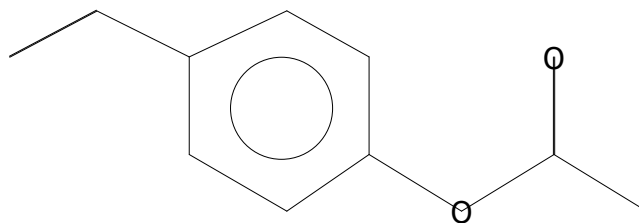
Quant Mass(es) = 120

S/N = 164.32

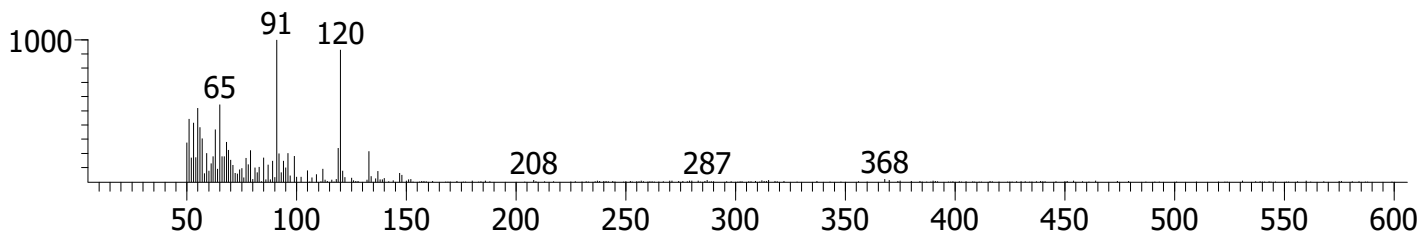
Area = 36968

Height = 4971.0

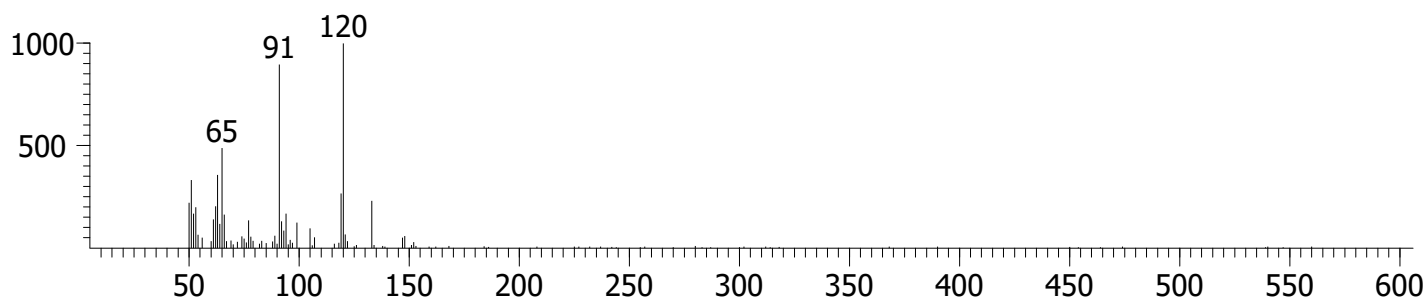
Similarity = 770



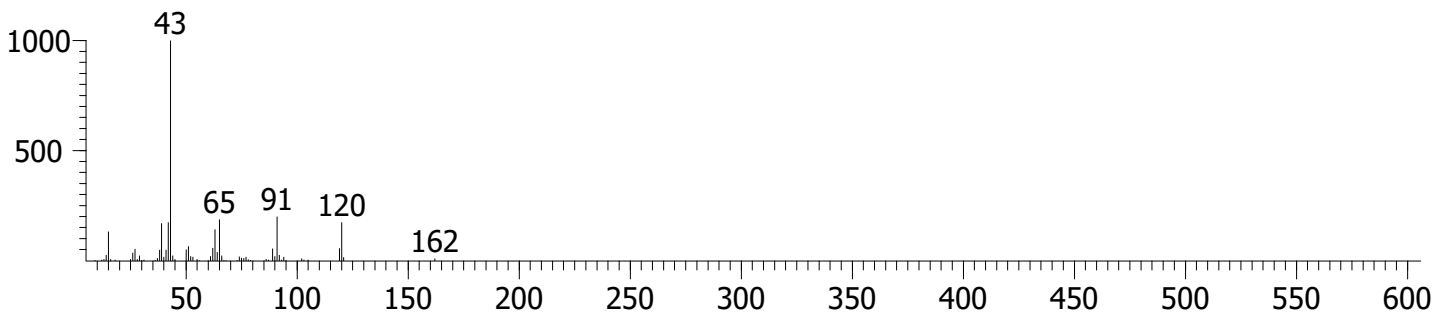
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 869, at 903.258 , 1.795 sec , sec (Spec # 64402)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 869, at 903.258 , 1.795 sec , sec (Spec # 64402)



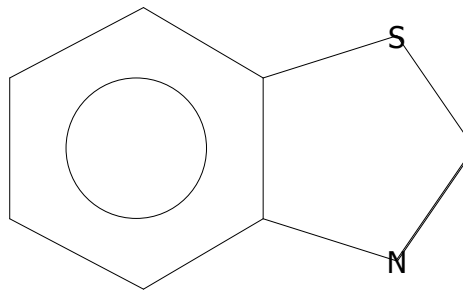
Library Hit - similarity 770, "Phenol, 4-ethenyl-, acetate"



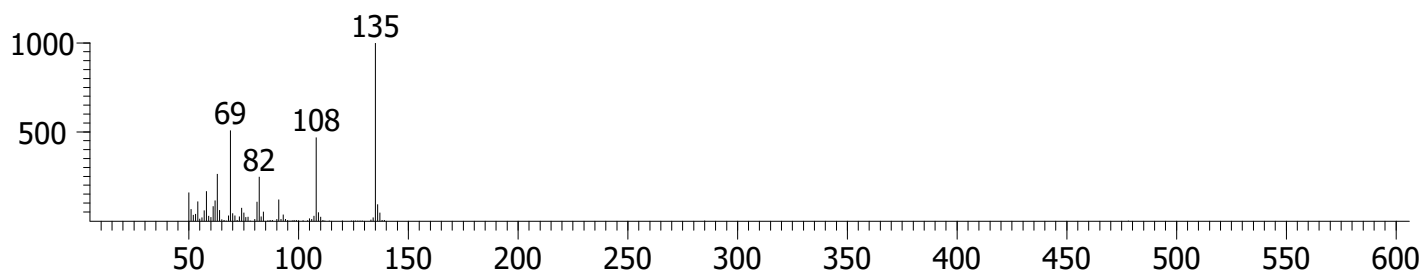
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 4-ethenyl-, acetate	770	3673	2628-16-2	mainlib	C10H10O2	162
2	Benzene, (ethenyloxy)-	760	2593	766-94-9	mainlib	C8H8O	120
3	Benzofuran, 2,3-dihydro-	737	947	496-16-2	mainlib	C8H8O	120
4	6-Methylenebicyclo[3.2.0]hept-3-en-2-one	717	431	0-00-0	mainlib	C8H8O	120
5	2,3,5-Trioxabicyclo[2.1.0]pentane, 1,4-bis(phenylmethyl)-	697	196	56247-48-4	mainlib	C16H14O3	254

Benzothiazole

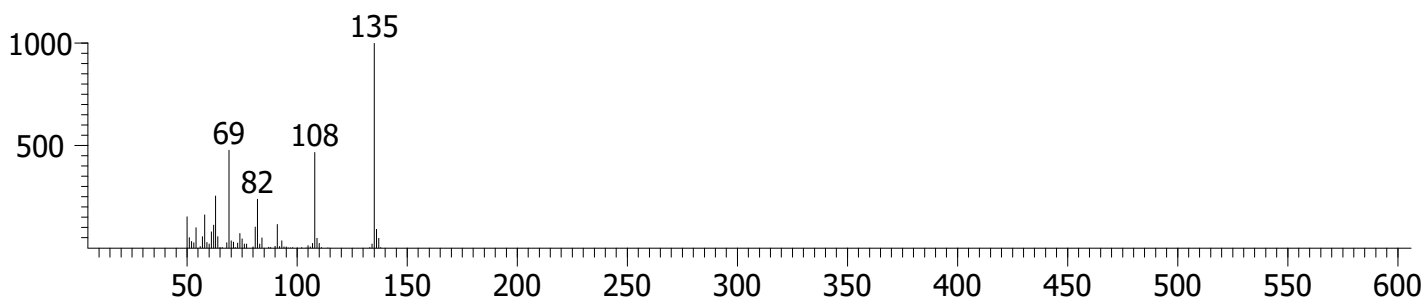
1st Dimension R.T. = 917.25
2nd Dimension R.T. = 2.119
Quant Mass(es) = 135
S/N = 1978.5
Area = 565426
Height = 61299
Similarity = 923



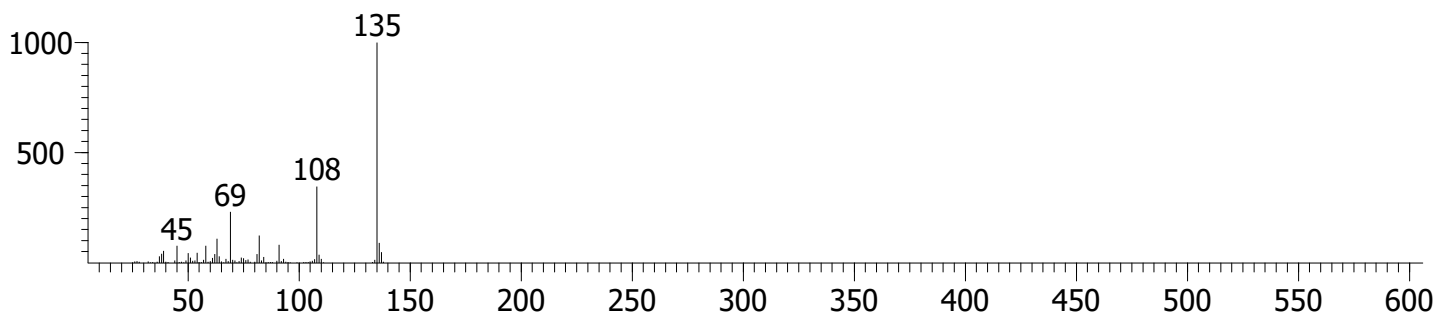
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 895, at 917.25 , 2.119 sec , sec (Spec # 66571)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 895, at 917.25 , 2.119 sec , sec (Spec # 66571)



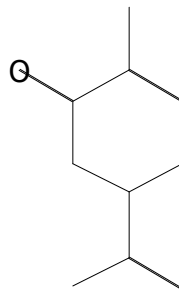
Library Hit - similarity 923, "Benzothiazole"



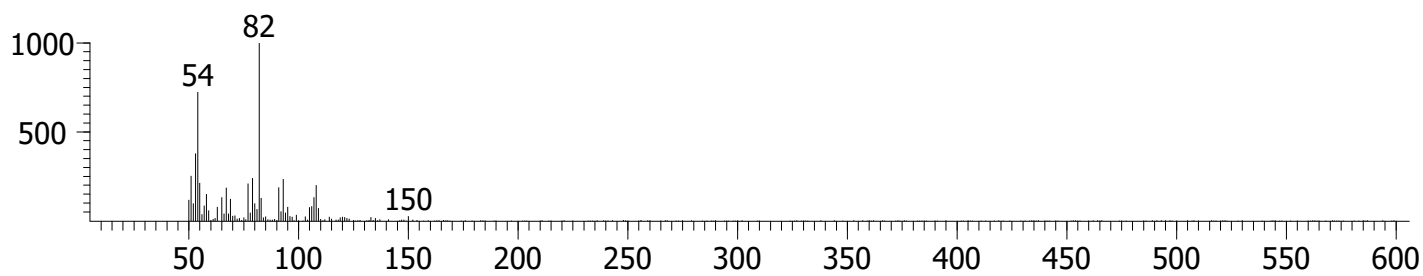
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzothiazole	923	7611	95-16-9	mainlib	C7H5NS	135
2	1,2-Benzisothiazole	886	1852	272-16-2	mainlib	C7H5NS	135
3	Thieno[3,2-c]pyridine	809	226	272-14-0	mainlib	C7H5NS	135
4	Benzothiazole-2-carboxylic acid	798	155	3622-04-6	mainlib	C8H5NO2S	179
5	3-Allylbenzothiazolium bromide	786	103	16407-55-9	mainlib	C10H10BrNS	255

(-)-Carvone

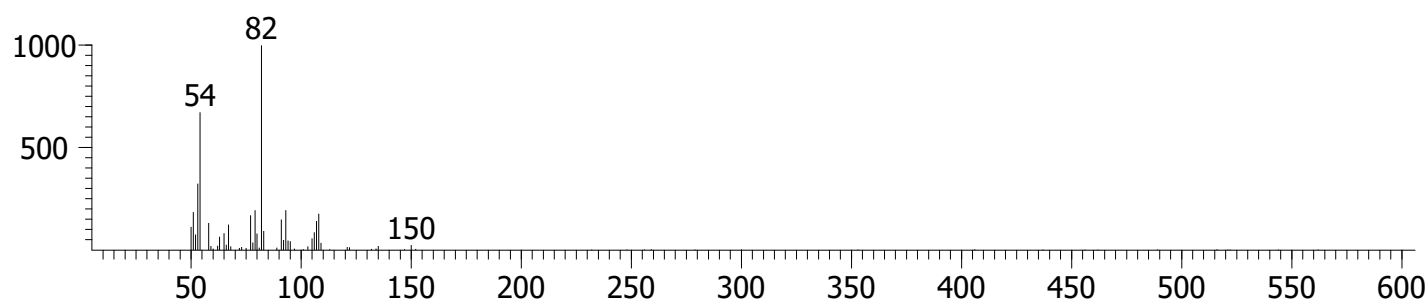
1st Dimension R.T. = 934.74
2nd Dimension R.T. = 1.676
Quant Mass(es) = 82
S/N = 370.17
Area = 85312
Height = 10944
Similarity = 882



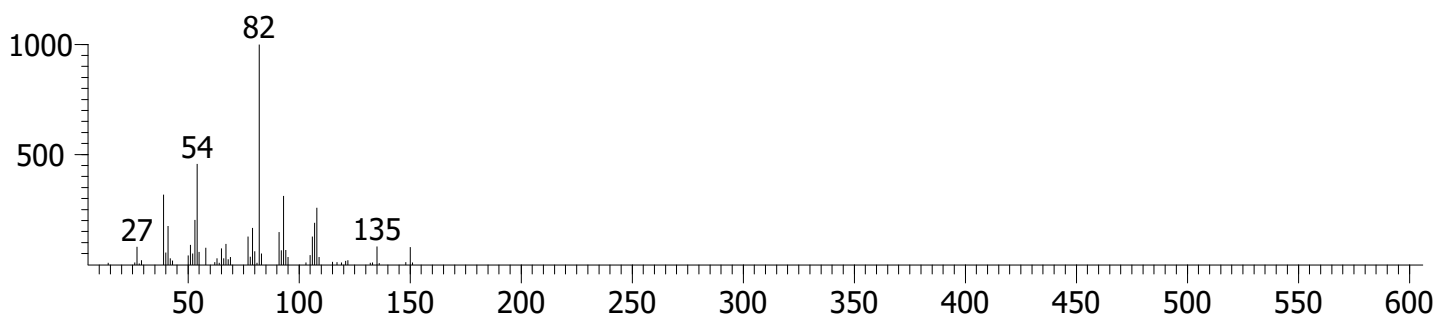
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 924, at 934.74 , 1.676 sec , sec (Spec # 69154)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 924, at 934.74 , 1.676 sec , sec (Spec # 69154)



Library Hit - similarity 882, "(-)-Carvone"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	(-)-Carvone	882	6393	6485-40-1	mainlib	C10H14O	150
2	Carvone	859	2334	99-49-0	mainlib	C10H14O	150
3	D-Carvone	839	1063	2244-16-8	mainlib	C10H14O	150
4	2(3H)-Furanone, 4,5-dihydro-4-(2-methyl-3-methylene-1-buten-4-yl)-	667	22	0-00-0	mainlib	C10H14O2	166
5	Spiro[cyclopropane-1,6'-[3]oxatricyclo[3.2.1.0(2,4)]octane]	658	16	107079-37-8	mainlib	C9H12O	136

Ethosuximide

1st Dimension R.T. = 941.736

2nd Dimension R.T. = 1.927

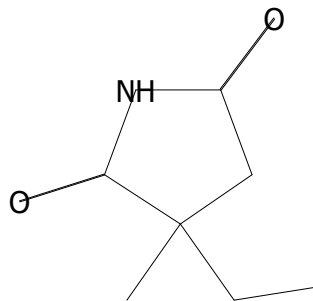
Quant Mass(es) = 113

S/N = 596.19

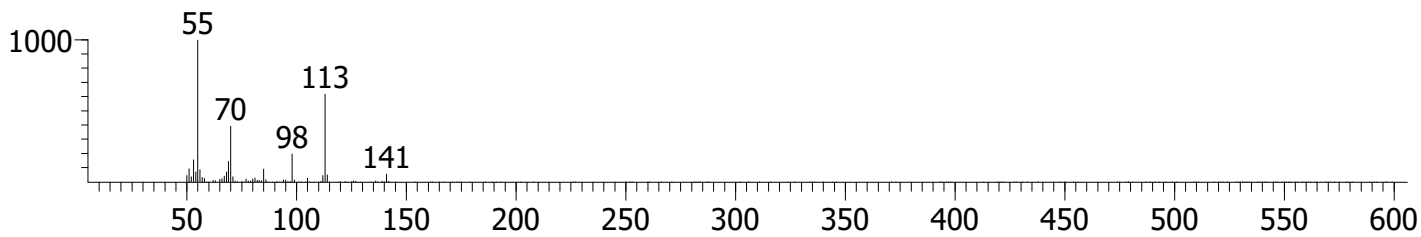
Area = 117972

Height = 14375

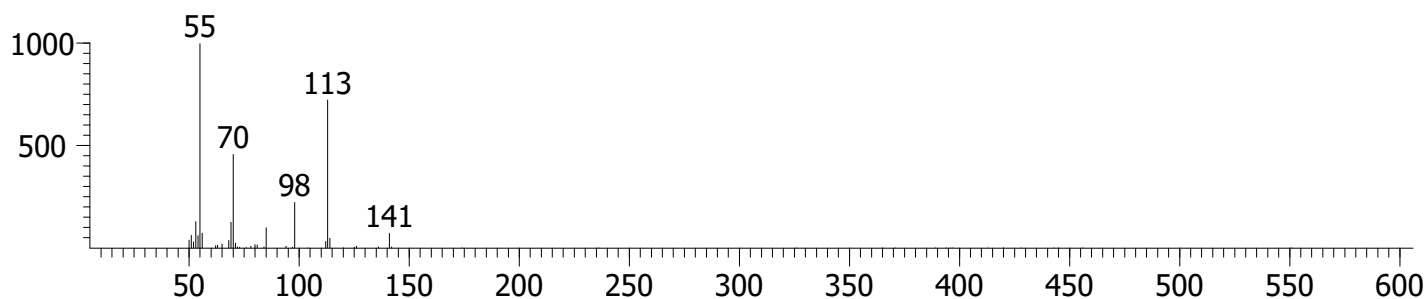
Similarity = 826



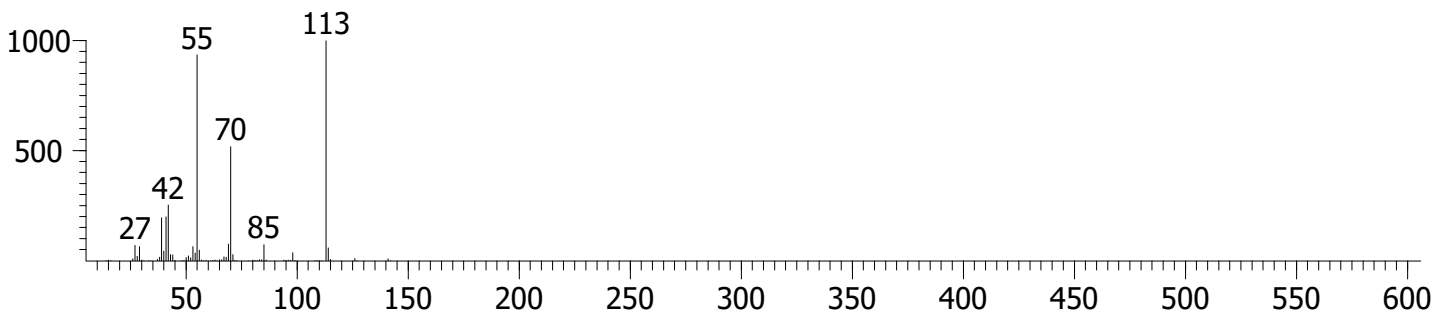
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 941, at 941.736 , 1.927 sec , sec (Spec # 70252)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 941, at 941.736 , 1.927 sec , sec (Spec # 70252)



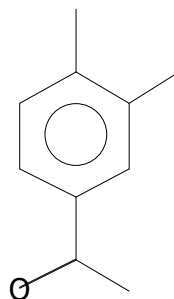
Library Hit - similarity 826, "Ethosuximide"



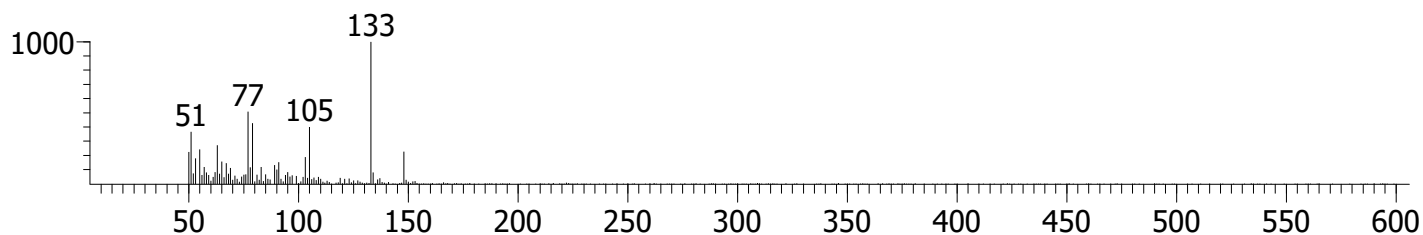
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethosuximide	826	7248	77-67-8	mainlib	C7H11NO2	141
2	2,5-Pyrrolidinedione, 3-methyl-4-propyl-, cis-	740	645	16493-22-4	mainlib	C8H13NO2	155
3	Pyrrolidine, 1-(3-methyl-1-oxohexadecyl)-	697	142	56630-57-0	mainlib	C21H41NO	323
4	Pyrrolidine, 1-(3-methyl-1-oxoheptadecyl)-	694	125	0-00-0	mainlib	C22H43NO	337
5	Octanoic acid, pyrrolidide	688	98	0-00-0	mainlib	C12H23NO	197

Ethanone, 1-(3,4-dimethylphenyl)-

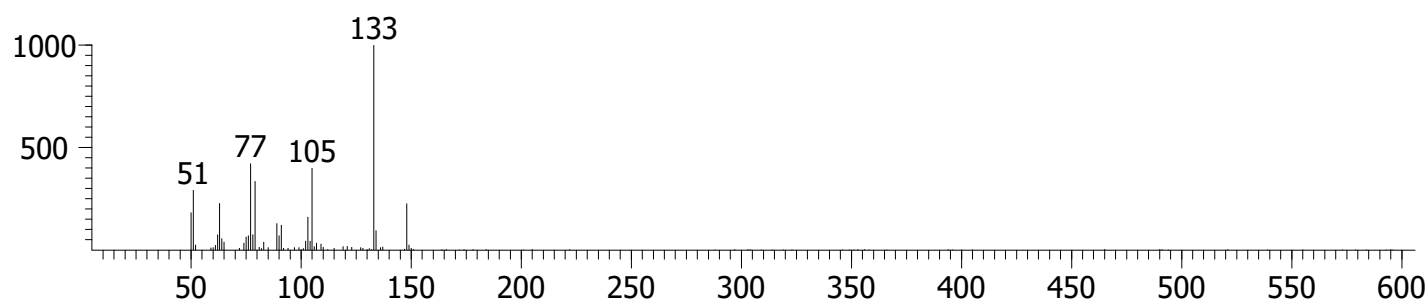
1st Dimension R.T. = 962.724
2nd Dimension R.T. = 1.762
Quant Mass(es) = 133
S/N = 347.53
Area = 59255
Height = 7253.2
Similarity = 873



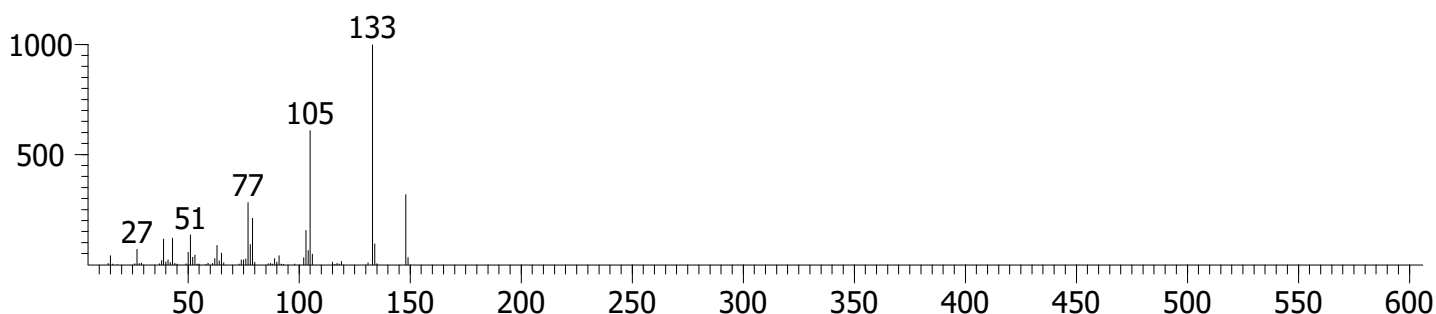
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 980, at 962.724 , 1.762 sec , sec (Spec # 73407)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 980, at 962.724 , 1.762 sec , sec (Spec # 73407)



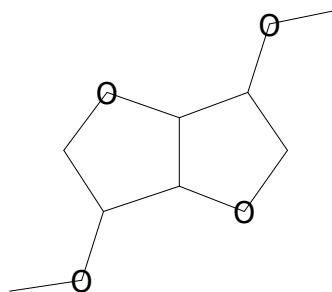
Library Hit - similarity 873, "Ethanone, 1-(3,4-dimethylphenyl)-"



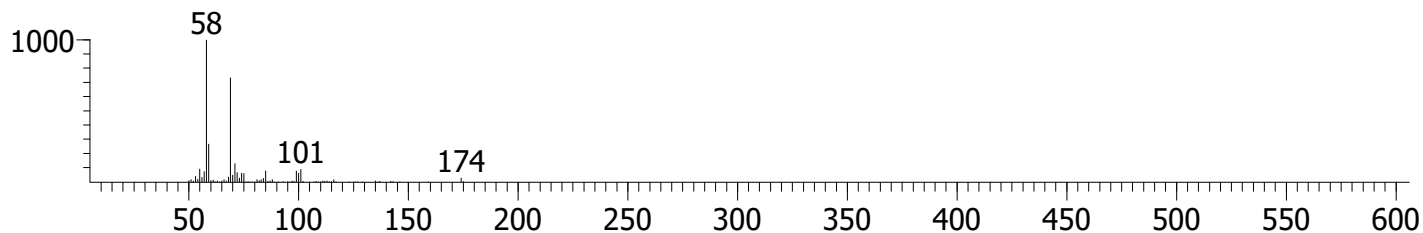
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanone, 1-(3,4-dimethylphenyl)-	873	2343	3637-01-2	mainlib	C10H12O	148
2	m-Ethylacetophenone	861	1560	22699-70-3	mainlib	C10H12O	148
3	Ethanone, 1-(4-ethylphenyl)-	858	1379	937-30-4	mainlib	C10H12O	148
4	4-Ethylbenzoyl chloride	849	1001	16331-45-6	mainlib	C9H9ClO	168
5	Ethanone, 1-(2,5-dimethylphenyl)-	834	606	2142-73-6	mainlib	C10H12O	148

D-Glucitol,
1,4:3,6-dianhydro-2,5-di-O-methyl-

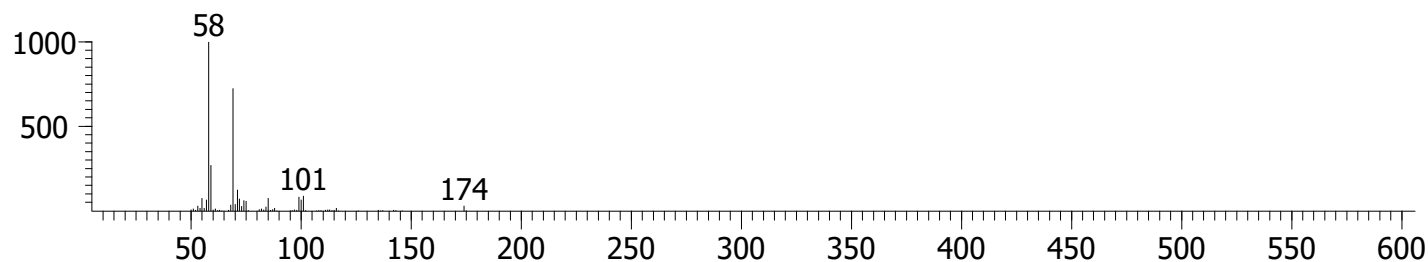
1st Dimension R.T. = 973.218
2nd Dimension R.T. = 1.907
Quant Mass(es) = 58
S/N = 2676.5
Area = 1167593
Height = 132014
Similarity = 868



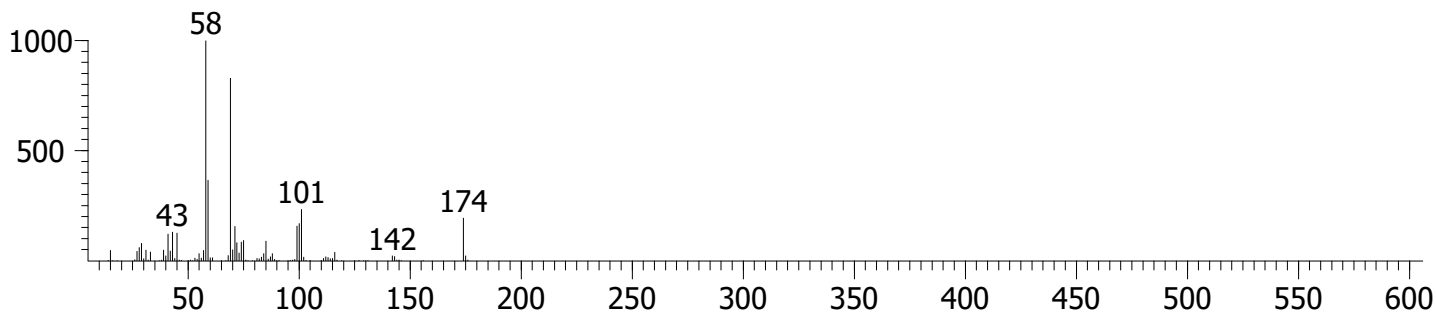
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1005, at 973.218 , 1.907 sec , sec (Spec # 75019)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1005, at 973.218 , 1.907 sec , sec (Spec # 75019)



Library Hit - similarity 868, "D-Glucitol, 1,4:3,6-dianhydro-2,5-di-O-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	D-Glucitol, 1,4:3,6-dianhydro-2,5-di-O-methyl-	868	9360	5306-85-4	mainlib	C8H14O4	174
2	1,3:2,5-Dimethylene-4-methyl-d-rhamnitol	700	213	7464-25-7	mainlib	C9H16O5	204
3	2-Propenoic acid, 2-methyl-, 2-hydroxypropyl ester	683	116	923-26-2	mainlib	C7H12O3	144
4	Cyclopropanecarboxylic acid, 4-methoxy-2-methylbutyl ester	676	89	0-00-0	mainlib	C10H18O3	186
5	2-Pentanone, 5-methoxy-	649	26	17429-04-8	mainlib	C6H12O2	116

Heptadecane, 2,6,10,14-tetramethyl-

1st Dimension R.T. = 983.712

2nd Dimension R.T. = 1.122

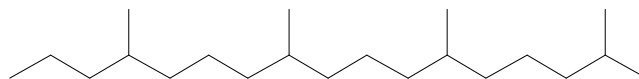
Quant Mass(es) = 71

S/N = 657.71

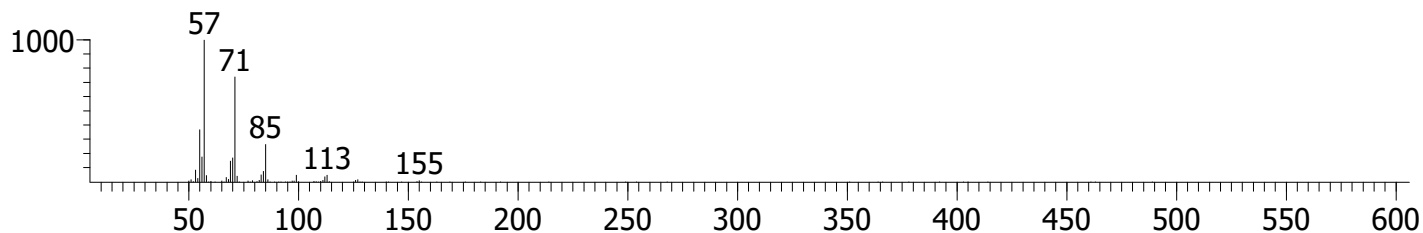
Area = 177535

Height = 25048

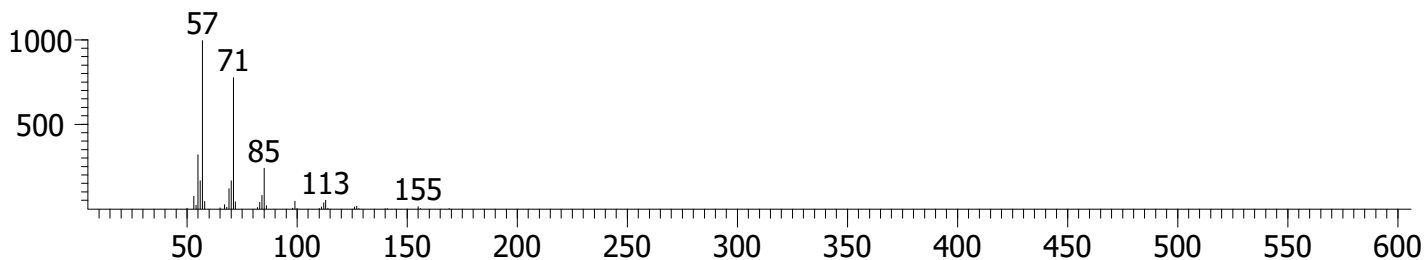
Similarity = 927



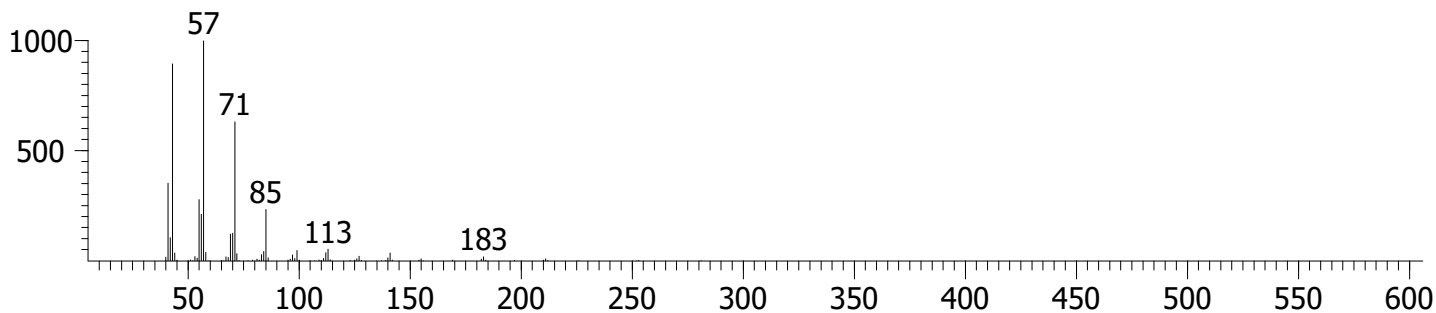
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1021, at 983.712 , 1.122 sec , sec (Spec # 7649 0)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1021, at 983.712 , 1.122 sec , sec (Spec # 7649 0)



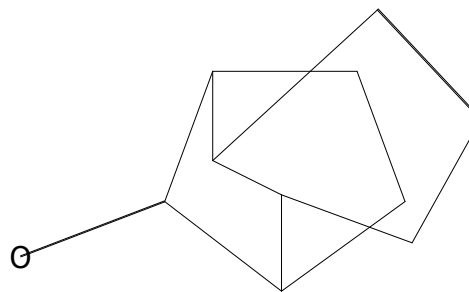
Library Hit - similarity 927, "Heptadecane, 2,6,10,14-tetramethyl-"



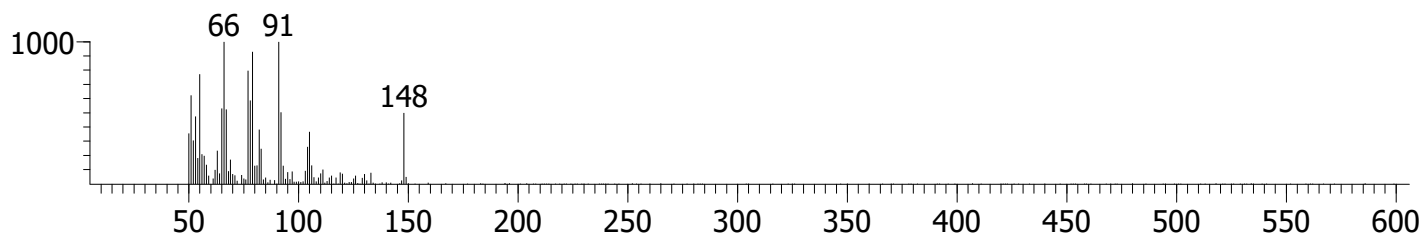
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Heptadecane, 2,6,10,14-tetramethyl-	927	1523	18344-37-1	mainlib	C ₂₁ H ₄₄	296
2	Heptadecane, 2,6-dimethyl-	921	1197	54105-67-8	mainlib	C ₁₉ H ₄₀	268
3	Dodecane, 4,6-dimethyl-	910	821	61141-72-8	mainlib	C ₁₄ H ₃₀	198
4	Decane, 2,3,5,8-tetramethyl-	905	662	192823-15-7	mainlib	C ₁₄ H ₃₀	198
5	2,6,10-Trimethyltridecane	900	533	3891-99-4	mainlib	C ₁₆ H ₃₄	226

Tricyclo[5.2.1.0(2,6)]dec-3-en-10-one

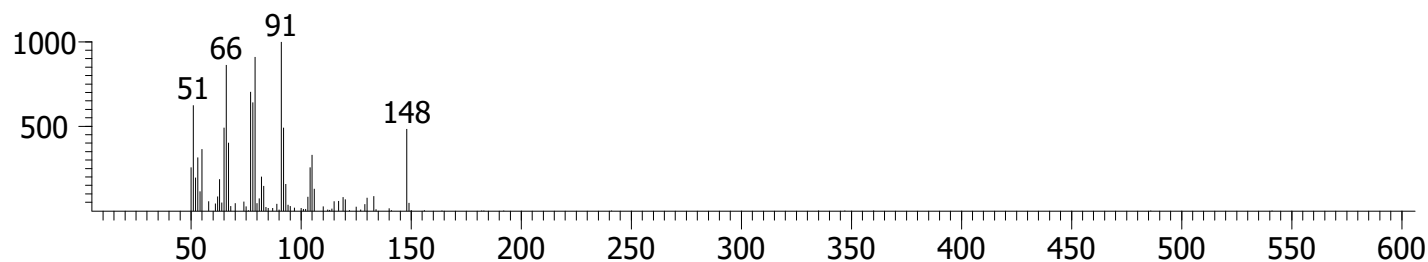
1st Dimension R.T. = 990.708
2nd Dimension R.T. = 1.934
Quant Mass(es) = 148
S/N = 234.19
Area = 45422
Height = 4464.7
Similarity = 899



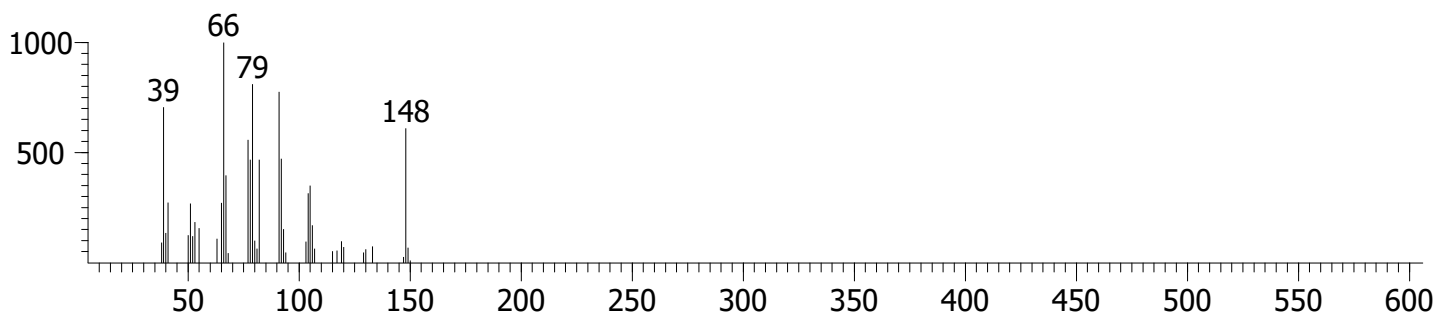
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1037, at 990.708 , 1.934 sec , sec (Spec # 7767 3)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1037, at 990.708 , 1.934 sec , sec (Spec # 7767 3)



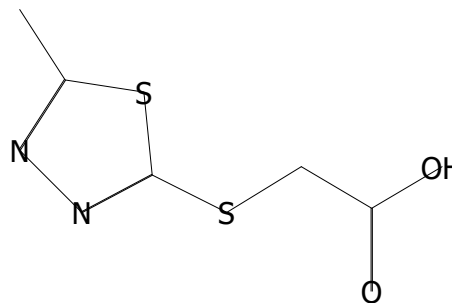
Library Hit - similarity 899, "Tricyclo[5.2.1.0(2,6)]dec-3-en-10-one"



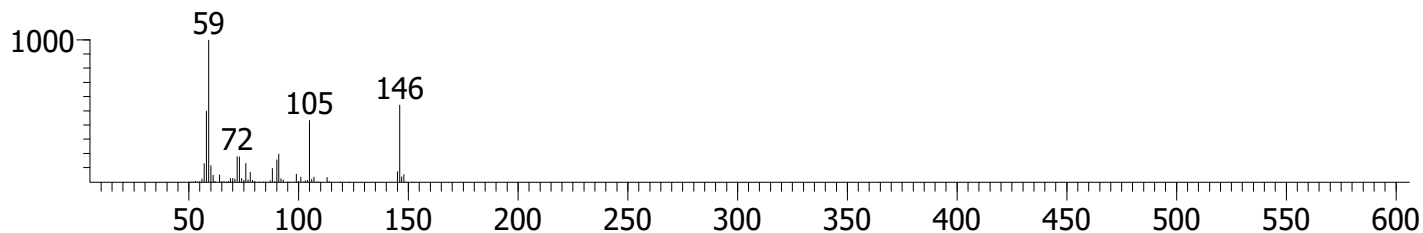
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Tricyclo[5.2.1.0(2,6)]dec-3-en-10-one	899	7653	0-00-0	mainlib	C10H12O	148
2	4,7-Methano-5H-inden-5-one, 3,3a,4,6,7,7a-hexahydro-	840	1383	14888-58-5	mainlib	C10H12O	148
3	Tricyclo[4.2.1.1(2,5)]dec-3-en-9-one	799	315	67009-89-6	mainlib	C10H12O	148
4	Tricyclo[5.2.1.0(2,6)]dec-4-en-8-one	782	172	0-00-0	mainlib	C10H12O	148
5	Tetracyclo[3.3.1.1(3,7).0(4,6)]decan-2-one	758	57	52750-53-5	mainlib	C10H12O	148

Acetic acid,
2-(5-methyl-1,3,4-thiadiazol-2-ylthio)-

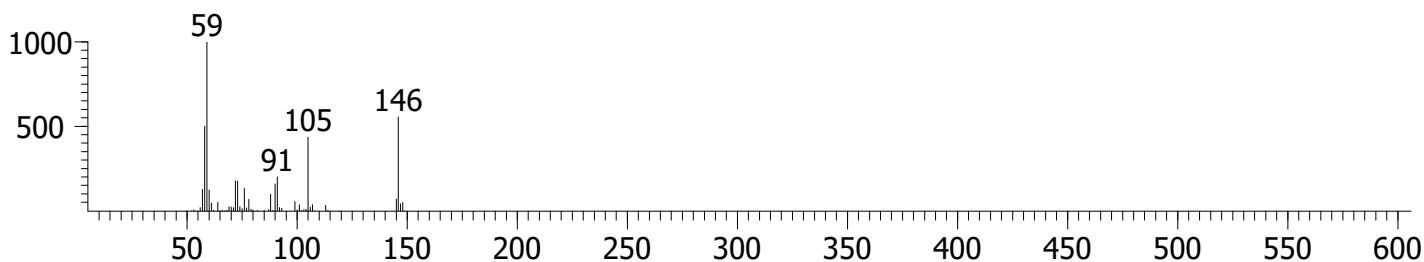
1st Dimension R.T. = 994.206
2nd Dimension R.T. = 2.290
Quant Mass(es) = 146
S/N = 3557.3
Area = 549248
Height = 56680
Similarity = 705



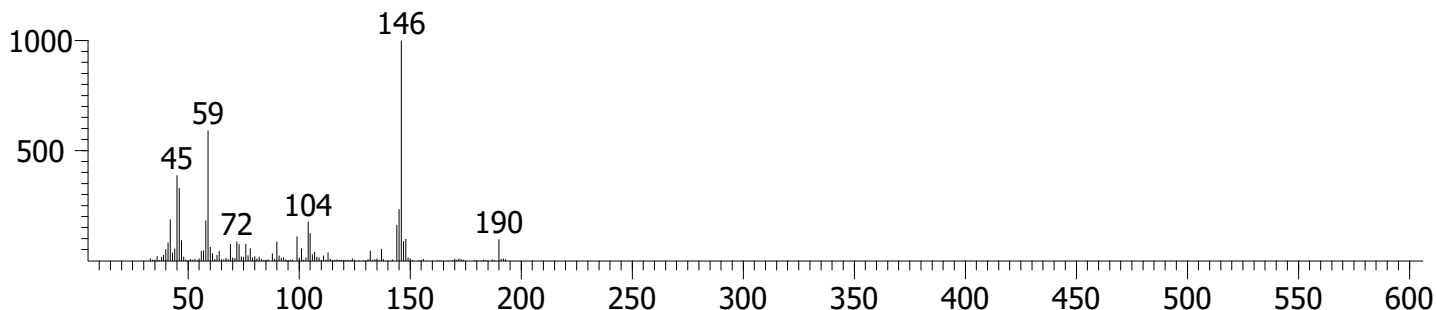
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1049, at 994.206 , 2.290 sec , sec (Spec # 78257)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1049, at 994.206 , 2.290 sec , sec (Spec # 78257)



Library Hit - similarity 705, "Acetic acid, 2-(5-methyl-1,3,4-thiadiazol-2-ylthio)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Acetic acid, 2-(5-methyl-1,3,4-thiadiazol-2-ylthio)-	705	4933	50918-26-8	mainlib	C5H6N2O2S2	190
2	1,3,4-Thiadiazole-2(3H)-thione, 3,5-dimethyl-	694	3384	7111-96-8	mainlib	C4H6N2S2	146
3	5,6-Dimethyl-1,3,4-dithiapyridazine	622	471	21423-60-9	mainlib	C4H6N2S2	146
4	L-Alanine, N-(2-methoxyethoxycarbonyl)-, hexyl ester	580	105	0-00-0	mainlib	C13H25NO5	275
5	L-Alanine, N-(2-methoxyethoxycarbonyl)-, 2-methoxyethyl ester	579	101	0-00-0	mainlib	C10H19NO6	249

2-Pentanamine, N-ethyl-4-methyl-

1st Dimension R.T. = 1008.2

2nd Dimension R.T. = 1.597

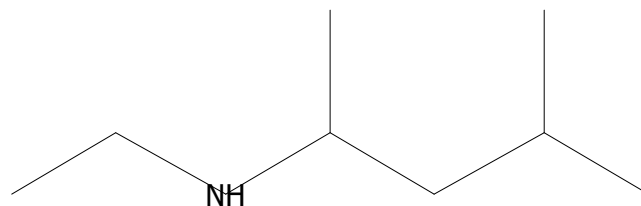
Quant Mass(es) = 72

S/N = 3518.5

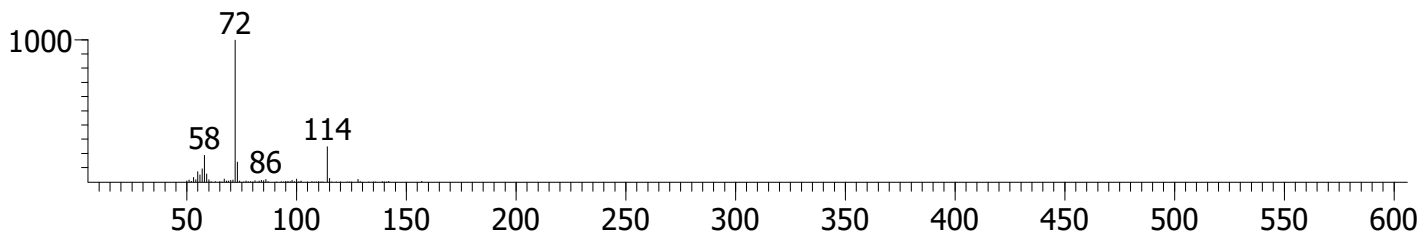
Area = 770193

Height = 92548

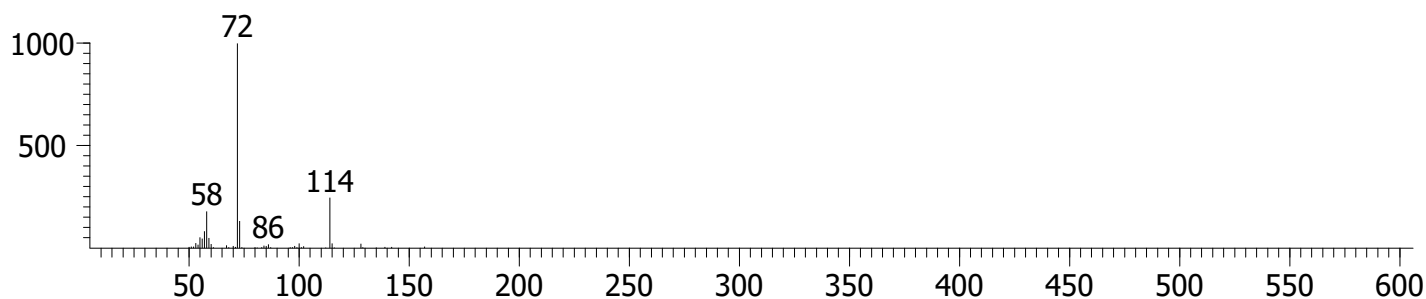
Similarity = 831



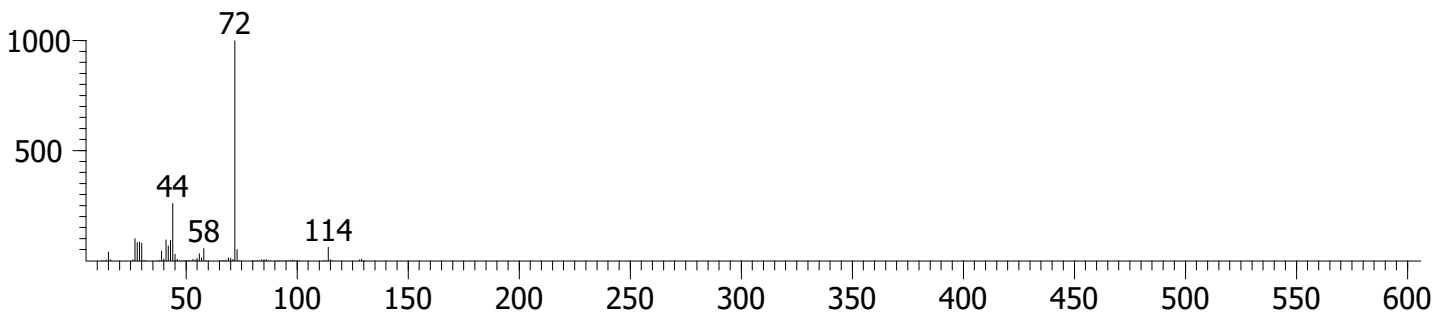
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1073, at 1008.2 , 1.597 sec , sec (Spec # 80272)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1073, at 1008.2 , 1.597 sec , sec (Spec # 80272)



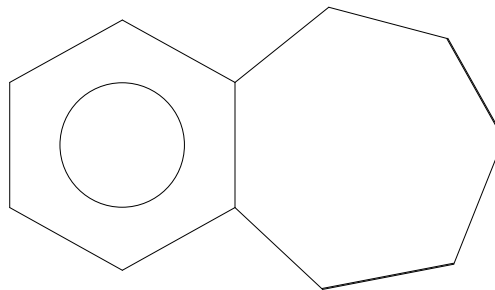
Library Hit - similarity 831, "2-Pentanamine, N-ethyl-4-methyl-"



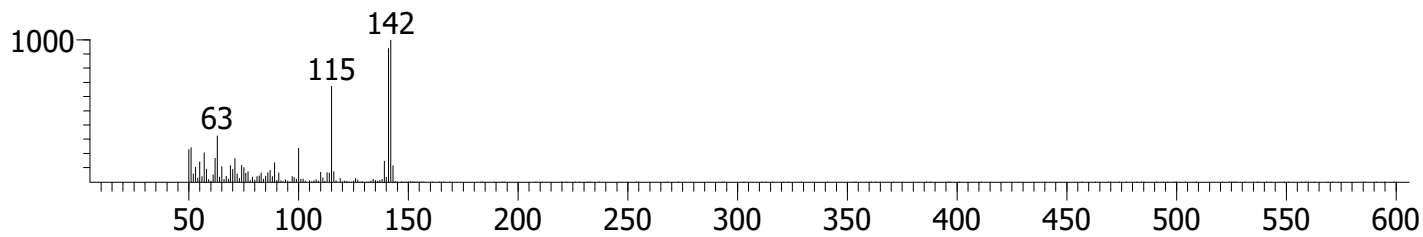
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Pentanamine, N-ethyl-4-methyl-	831	4100	42966-64-3	mainlib	C8H19N	129
2	Formamide, N,N-dibutyl-	830	3941	761-65-9	mainlib	C9H19NO	157
3	Propylneopentylamine	788	884	131229-65-7	mainlib	C8H19N	129
4	1-Hexanamine, N-propyl-	776	589	20193-23-1	mainlib	C9H21N	143
5	Ethylamine, N-methyl-N-hexadecyl-	750	176	66997-40-8	mainlib	C19H41N	283

Benzocycloheptatriene

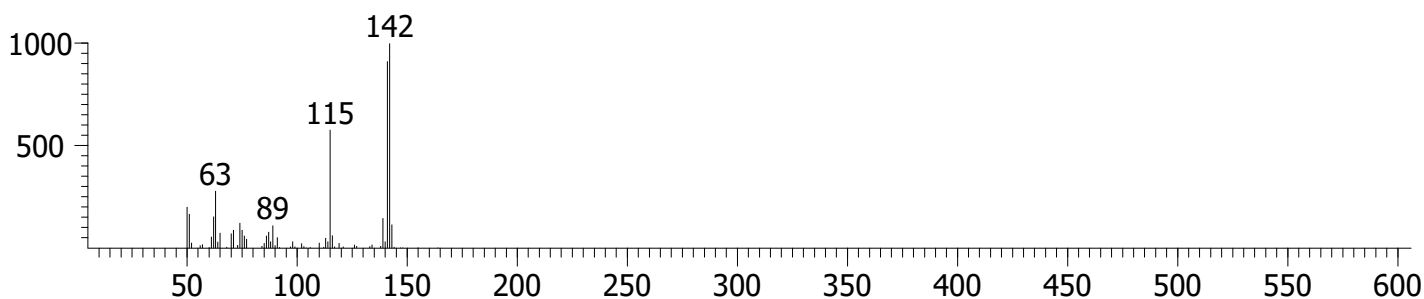
1st Dimension R.T. = 1011.7
2nd Dimension R.T. = 1.815
Quant Mass(es) = 142
S/N = 1627.9
Area = 119932
Height = 16181
Similarity = 922



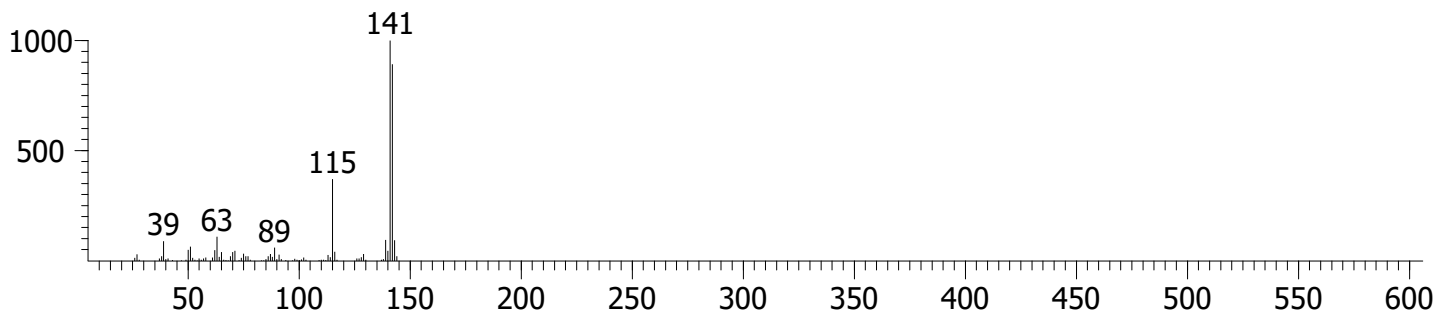
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1088, at 1011.7 , 1.815 sec , sec (Spec # 80835)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1088, at 1011.7 , 1.815 sec , sec (Spec # 80835)



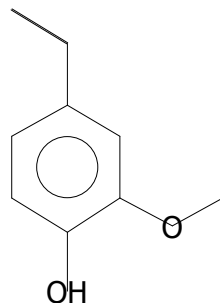
Library Hit - similarity 922, "Benzocycloheptatriene"



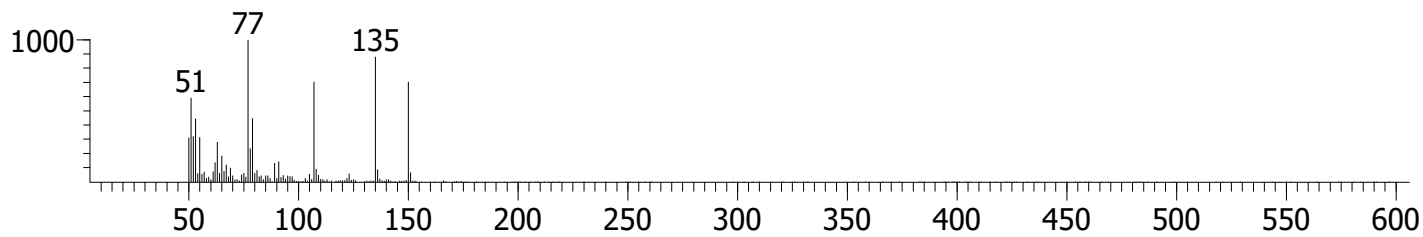
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzocycloheptatriene	922	3541	264-09-5	mainlib	C11H10	142
2	Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene	920	3266	2443-46-1	mainlib	C11H10	142
3	Naphthalene, 1-methyl-	895	996	90-12-0	mainlib	C11H10	142
4	Naphthalene, 2-methyl-	893	919	91-57-6	mainlib	C11H10	142
5	1H-Indene, 1-ethylidene-	892	883	2471-83-2	mainlib	C11H10	142

2-Methoxy-4-vinylphenol

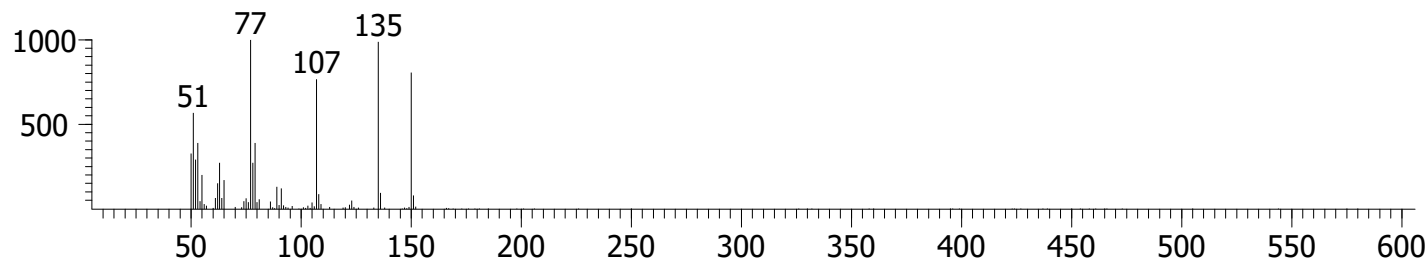
1st Dimension R.T. = 1029.19
2nd Dimension R.T. = 1.835
Quant Mass(es) = 150
S/N = 802.48
Area = 117540
Height = 14559
Similarity = 947



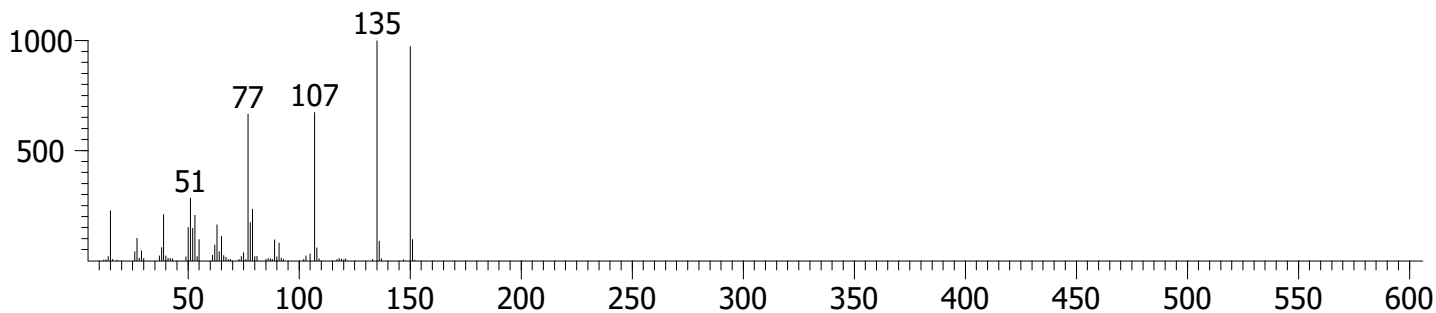
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1138, at 1029.19 , 1.835 sec , sec (Spec # 8348 8)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1138, at 1029.19 , 1.835 sec , sec (Spec # 8348 8)



Library Hit - similarity 947, "2-Methoxy-4-vinylphenol"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Methoxy-4-vinylphenol	947	8586	7786-61-0	mainlib	C ₉ H ₁₀ O ₂	150
2	Phenol, 5-ethenyl-2-methoxy-	859	749	621-58-9	mainlib	C ₉ H ₁₀ O ₂	150
3	4-Hydroxy-2-methylacetophenone	826	196	875-59-2	mainlib	C ₉ H ₁₀ O ₂	150
4	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	823	173	1450-72-2	mainlib	C ₉ H ₁₀ O ₂	150
5	4-Hydroxy-3-methylacetophenone	815	129	876-02-8	mainlib	C ₉ H ₁₀ O ₂	150

Triacetin

1st Dimension R.T. = 1057.17

2nd Dimension R.T. = 1.775

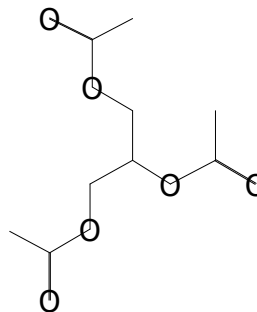
Quant Mass(es) = 103

S/N = 3649.7

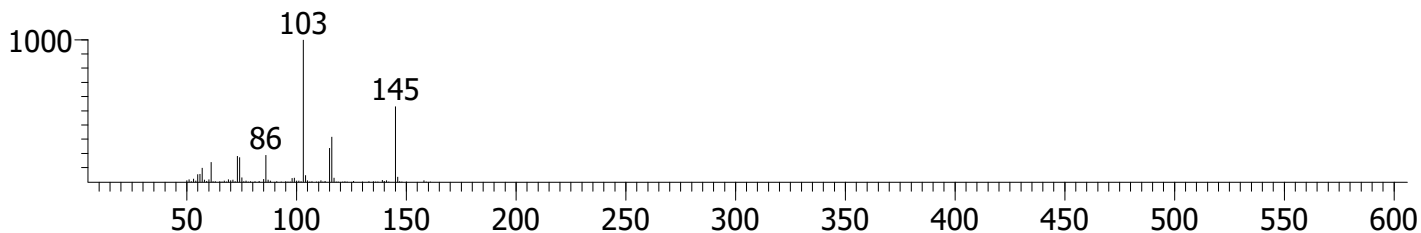
Area = 677014

Height = 76930

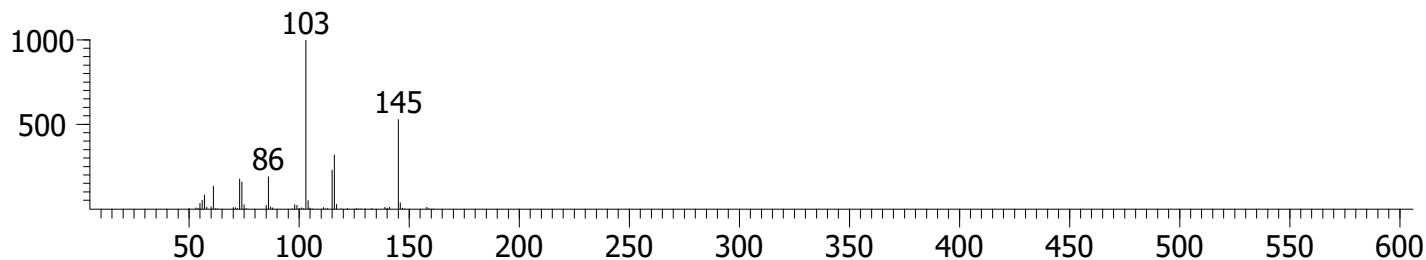
Similarity = 958



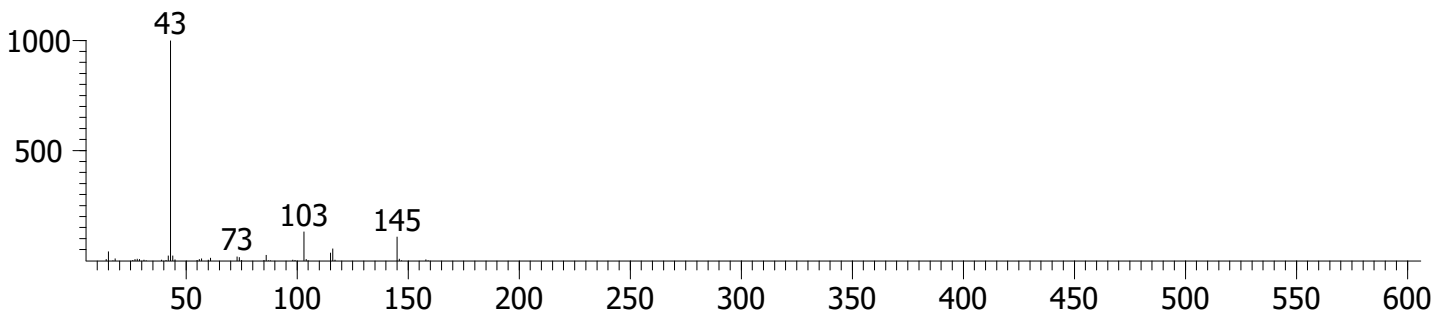
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1198, at 1057.17 , 1.775 sec , sec (Spec # 87719)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1198, at 1057.17 , 1.775 sec , sec (Spec # 87719)



Library Hit - similarity 958, "Triacetin"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Triacetin	958	4950	102-76-1	mainlib	C9H14O6	218
2	Glycerol 1,2-diacetate	953	3989	102-62-5	mainlib	C7H12O5	176
3	1,3-Diacetin	918	1001	0-00-0	mainlib	C7H12O5	176
4	̑-D-Glucopyranose, 2-deoxy-2-fluoro-, tetraacetate	747	21	31077-89-1	mainlib	C14H19FO9	350
5	1,2,3,4-butanetetrol, tetraacetate	741	17	73977-54-5	mainlib	C12H18O8	290

n-Decanoic acid

1st Dimension R.T. = 1081.66

2nd Dimension R.T. = 1.419

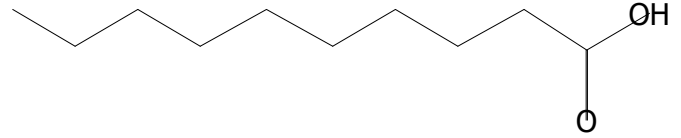
Quant Mass(es) = 60

S/N = 1378.9

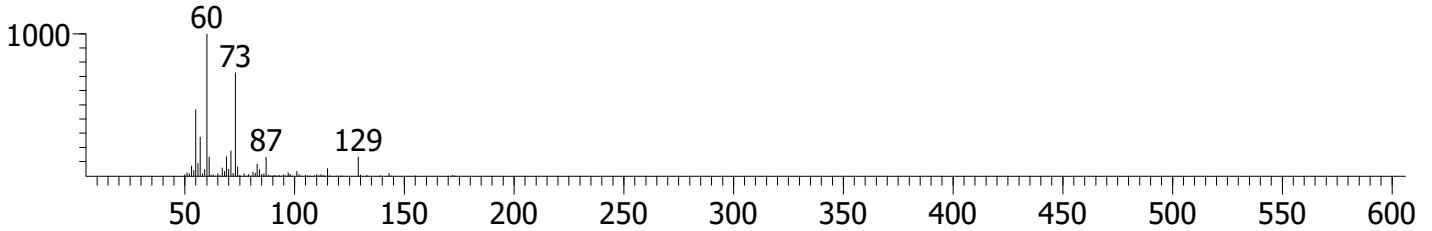
Area = 360398

Height = 53518

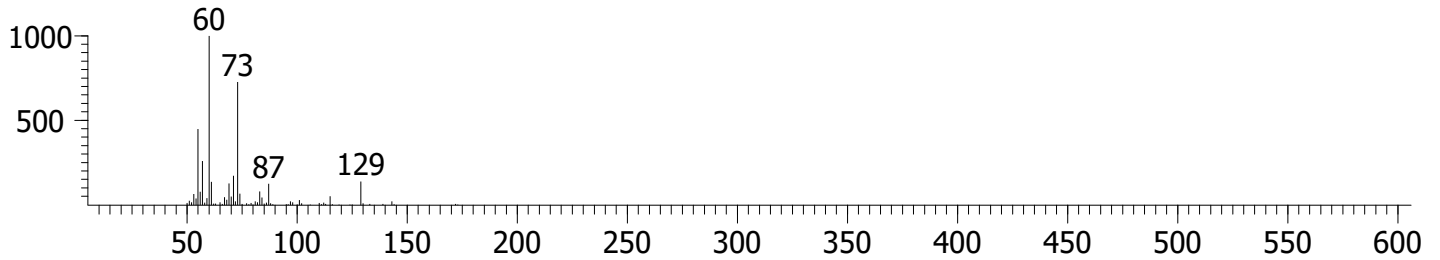
Similarity = 866



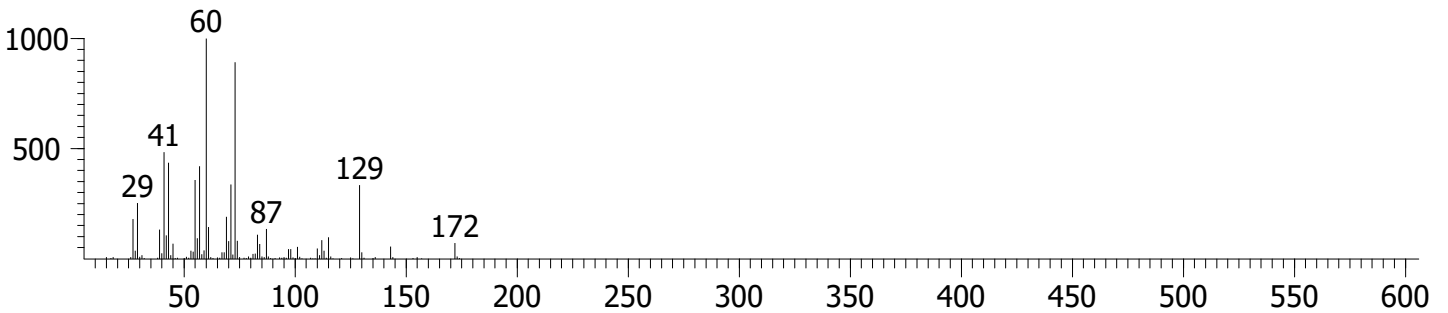
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1242, at 1081.66 , 1.419 sec , sec (Spec # 9137 5)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1242, at 1081.66 , 1.419 sec , sec (Spec # 9137 5)



Library Hit - similarity 866, "n-Decanoic acid"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	n-Decanoic acid	866	6563	334-48-5	mainlib	C10H20O2	172
2	Nonanoic acid	813	1298	112-05-0	mainlib	C9H18O2	158
3	Heptanoic acid	780	339	111-14-8	mainlib	C7H14O2	130
4	n-Hexadecanoic acid	780	339	57-10-3	mainlib	C16H32O2	256
5	8-Methylnonanoic acid	776	287	5963-14-4	mainlib	C10H20O2	172

1(3H)-Isobenzofuranone

1st Dimension R.T. = 1088.65

2nd Dimension R.T. = 2.376

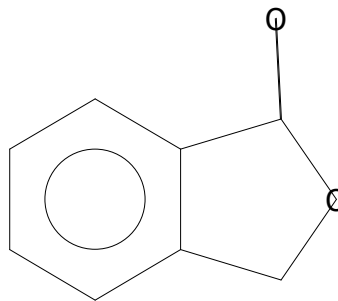
Quant Mass(es) = 105

S/N = 244.19

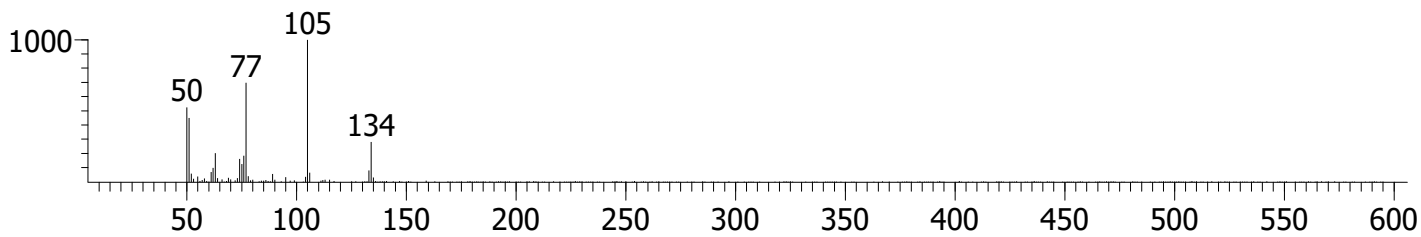
Area = 72519

Height = 7545.4

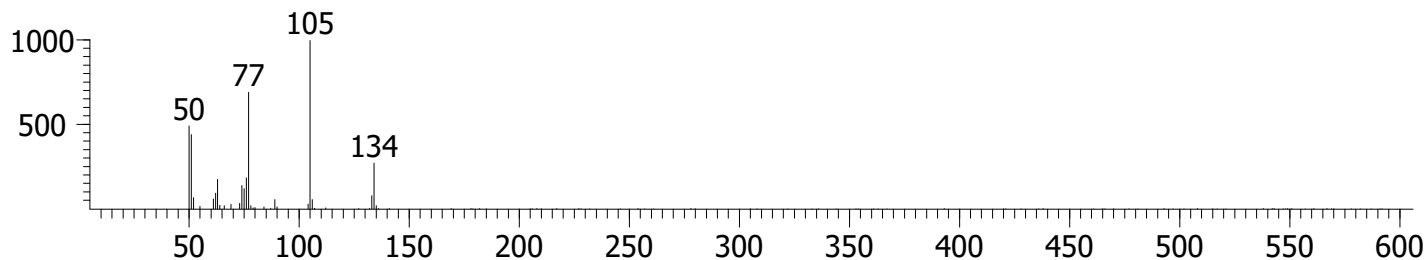
Similarity = 871



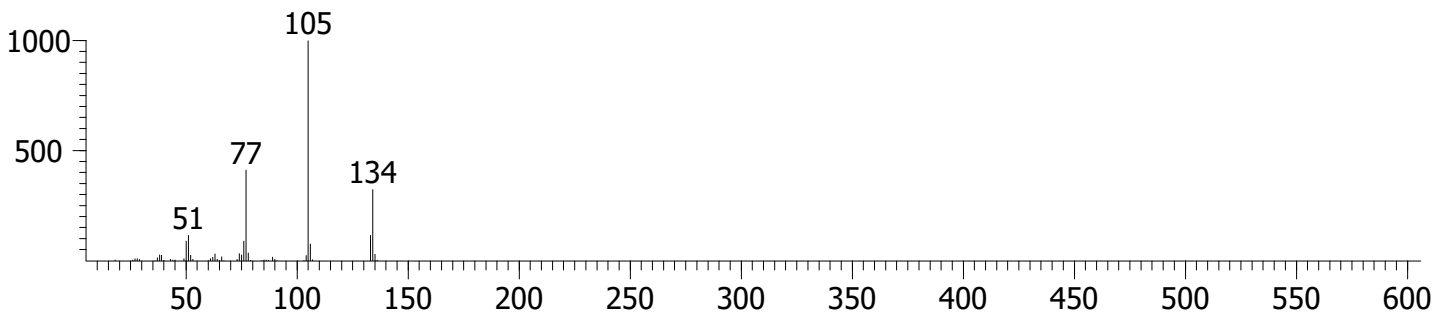
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1270, at 1088.65 , 2.376 sec , sec (Spec # 92580)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1270, at 1088.65 , 2.376 sec , sec (Spec # 92580)



Library Hit - similarity 871, "1(3H)-Isobenzofuranone"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1(3H)-Isobenzofuranone	871	3931	87-41-2	mainlib	C8H6O2	134
2	Benzoic acid, 2-(hydroxymethyl)-	868	3473	612-20-4	mainlib	C8H8O3	152
3	N-[5-(p-Tolyl)-1,3,4-thiadiazol-2-yl]benzamide	789	395	19948-85-7	mainlib	C16H13N3OS	295
4	1,2,3-Benzotriazole-1-benzoate	782	303	54769-36-7	mainlib	C13H9N3O2	239
5	Benzofurazan-5-carbohydrazide, N2-benzoyl-	759	110	0-00-0	mainlib	C14H10N4O3	282

Benzaldehyde, 4-hydroxy-

1st Dimension R.T. = 1109.64

2nd Dimension R.T. = 2.046

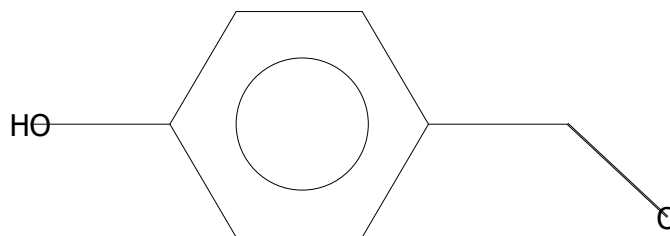
Quant Mass(es) = 122

S/N = 217.85

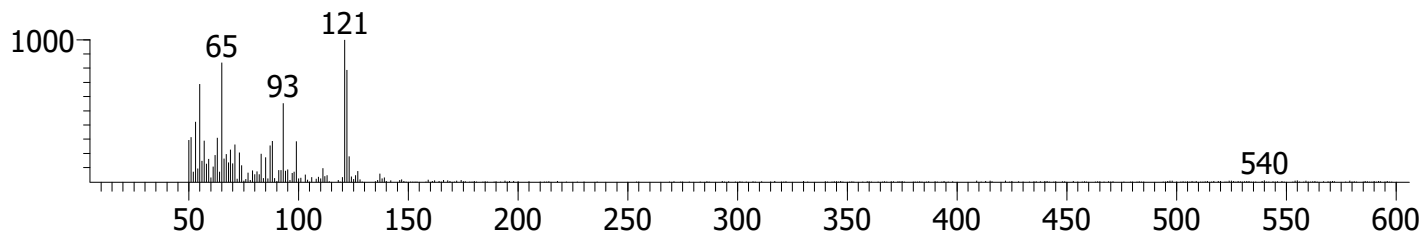
Area = 86409

Height = 9665.6

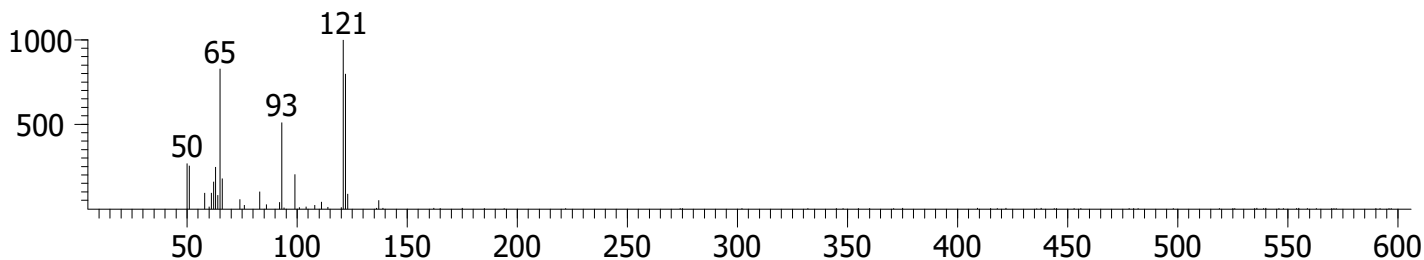
Similarity = 860



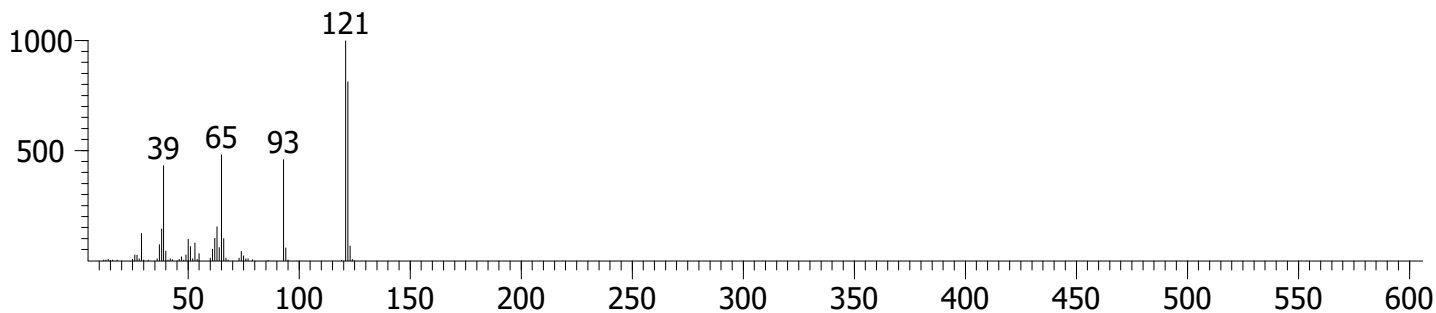
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1309, at 1109.64 , 2.046 sec , sec (Spec # 95710)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1309, at 1109.64 , 2.046 sec , sec (Spec # 95710)



Library Hit - similarity 860, "Benzaldehyde, 4-hydroxy-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzaldehyde, 4-hydroxy-	860	6081	123-08-0	mainlib	C7H6O2	122
2	Propanoic acid, 3-chloro-, 4-formylphenyl ester	832	1756	0-00-0	mainlib	C10H9ClO3	212
3	Benzaldehyde, 3-hydroxy-	825	1345	100-83-4	mainlib	C7H6O2	122
4	4-Acetoxybenzaldehyde	791	344	878-00-2	mainlib	C9H8O3	164
5	3-Acetoxybenzaldehyde	772	167	34231-78-2	mainlib	C9H8O3	164

3-Tetradecene, (E)-

1st Dimension R.T. = 1116.64

2nd Dimension R.T. = 1.188

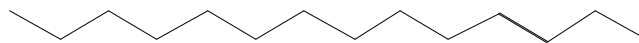
Quant Mass(es) = 70

S/N = 124.02

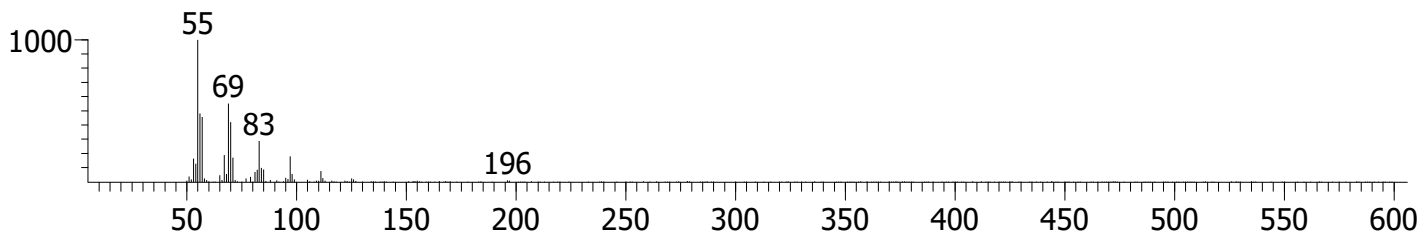
Area = 18148

Height = 2577.3

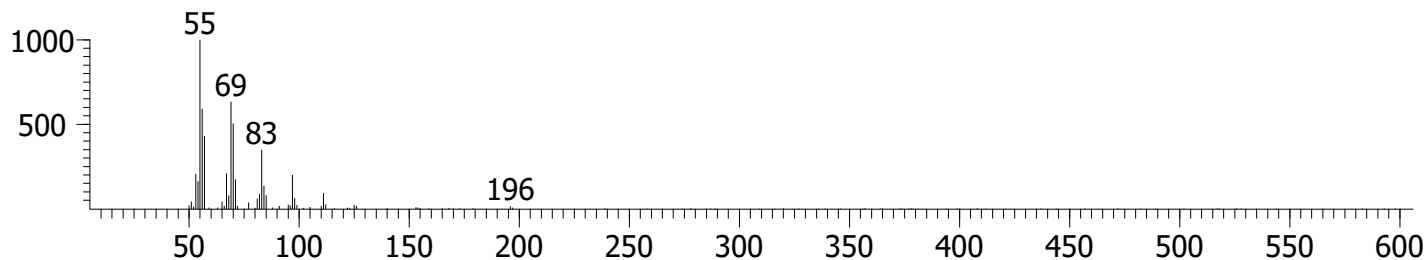
Similarity = 918



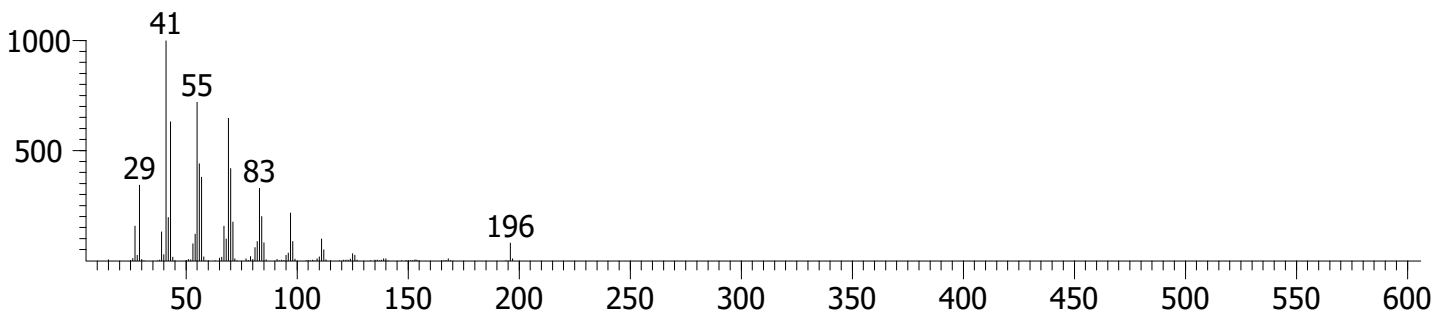
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1318, at 1116.64 , 1.188 sec , sec (Spec # 9664 0)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1318, at 1116.64 , 1.188 sec , sec (Spec # 9664 0)



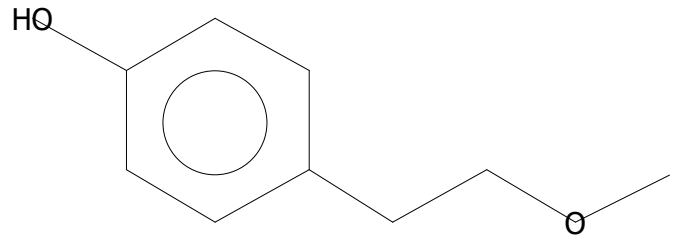
Library Hit - similarity 918, "3-Tetradecene, (E)-"



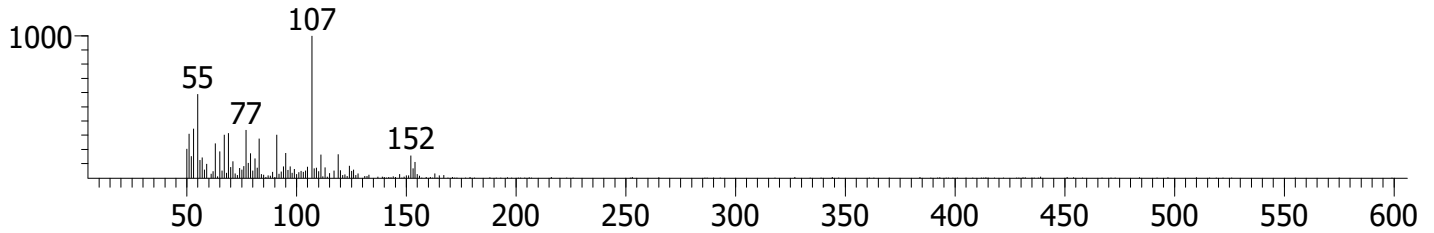
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Tetradecene, (E)-	918	481	41446-68-8	mainlib	C14H28	196
2	7-Hexadecene, (Z)-	912	378	35507-09-6	mainlib	C16H32	224
3	5-Tetradecene, (E)-	910	348	41446-66-6	mainlib	C14H28	196
4	3-Tridecene, (E)-	909	335	41446-57-5	mainlib	C13H26	182
5	3-Tetradecene, (Z)-	909	335	41446-67-7	mainlib	C14H28	196

4-(2-Methoxyethyl)phenol

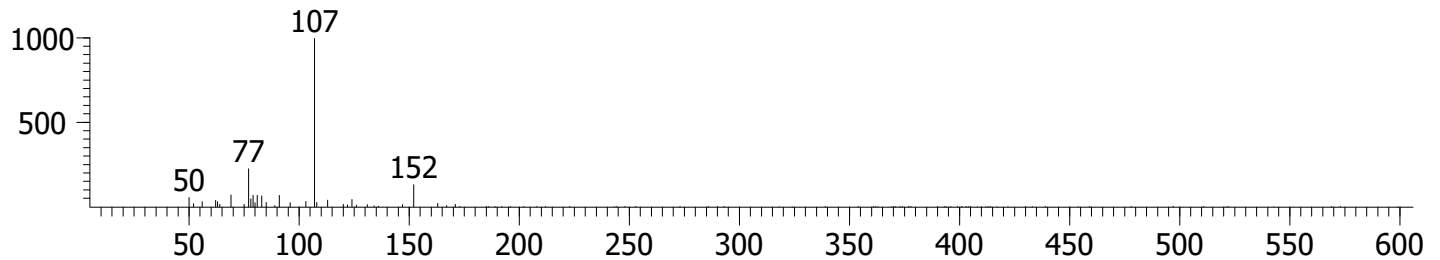
1st Dimension R.T. = 1123.63
2nd Dimension R.T. = 1.914
Quant Mass(es) = 107
S/N = 189.25
Area = 36157
Height = 4201.8
Similarity = 797



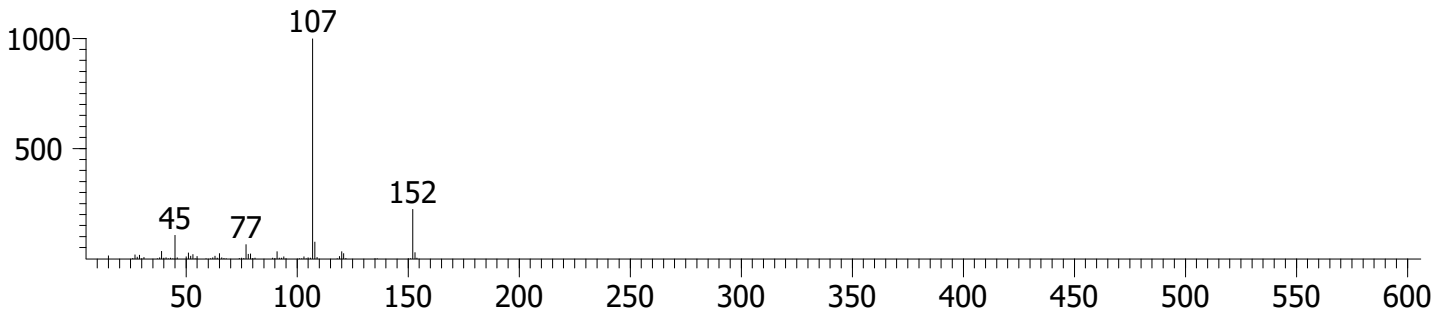
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1345, at 1123.63 , 1.914 sec , sec (Spec # 97810)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1345, at 1123.63 , 1.914 sec , sec (Spec # 97810)



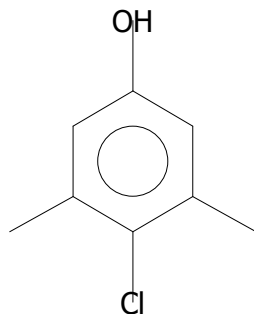
Library Hit - similarity 797, "4-(2-Methoxyethyl)phenol"



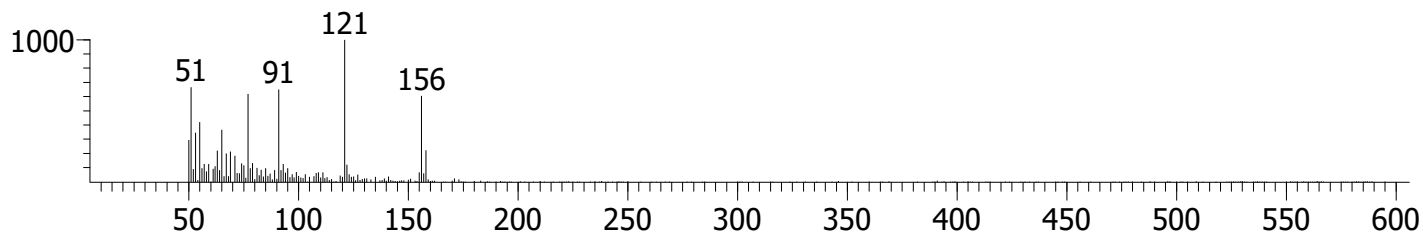
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-(2-Methoxyethyl)phenol	797	5646	56718-71-9	mainlib	C9H12O2	152
2	2-Amino-3-(4-hydroxyphenyl)-propanoic acid	758	1331	556-03-6	mainlib	C9H11NO3	181
3	Benzeneacetic acid, 4-hydroxy-	751	1019	156-38-7	mainlib	C8H8O3	152
4	Pentanoic acid, 5-(4-methylphenylamino)-5-oxo-, 2-propynyl ester	720	278	300726-47-0	mainlib	C15H17NO3	259
5	d-Tyrosine	716	234	556-02-5	mainlib	C9H11NO3	181

Chloroxylenol

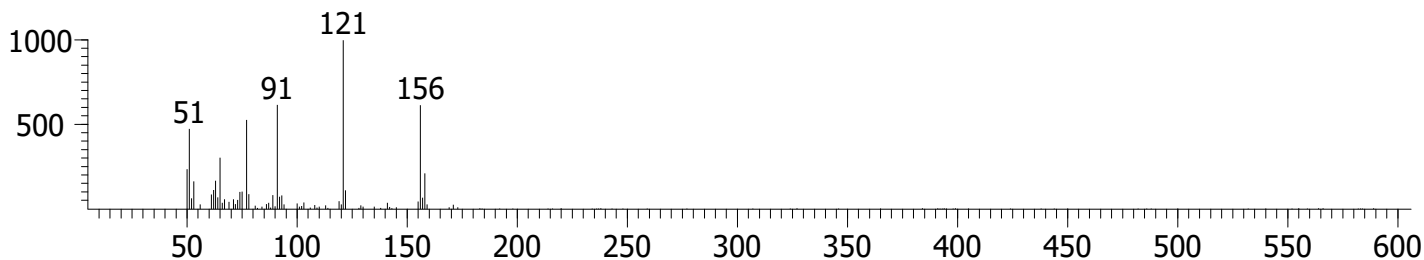
1st Dimension R.T. = 1127.13
2nd Dimension R.T. = 1.828
Quant Mass(es) = 156
S/N = 315.47
Area = 42301
Height = 5367.4
Similarity = 949



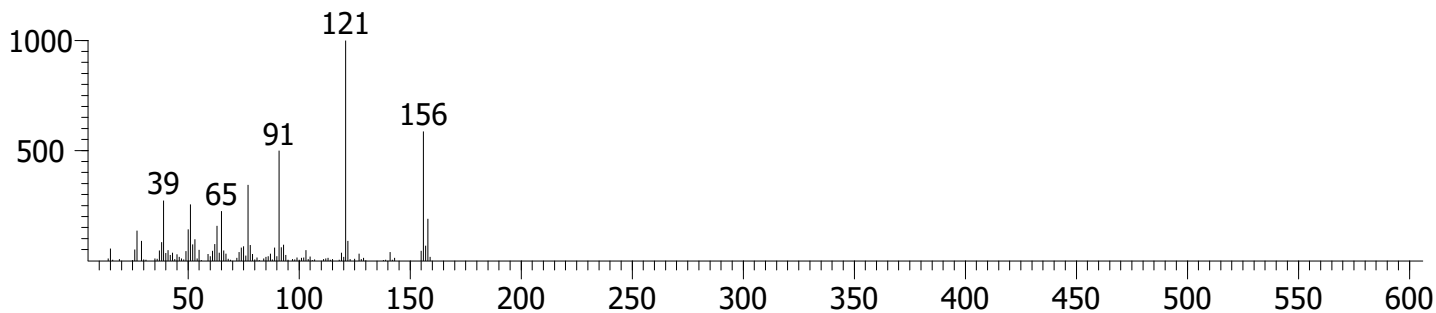
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1350, at 1127.13 , 1.828 sec , sec (Spec # 98327)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1350, at 1127.13 , 1.828 sec , sec (Spec # 98327)



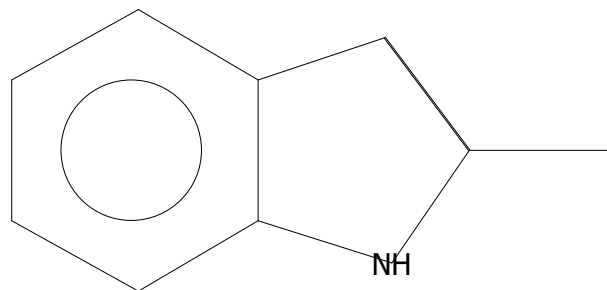
Library Hit - similarity 949, "Chloroxylenol"



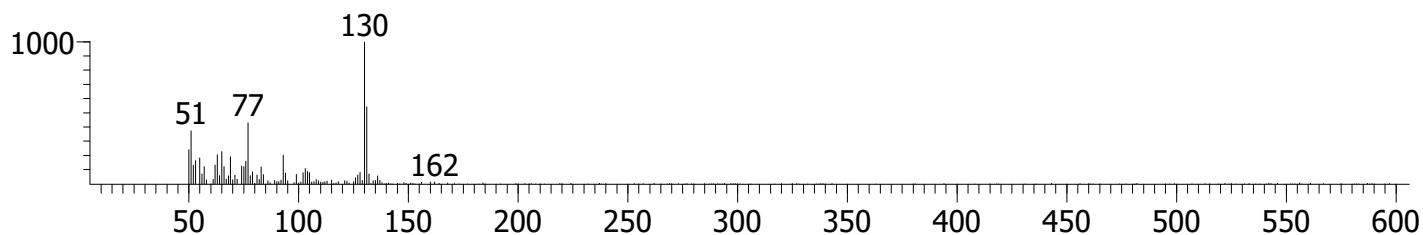
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Chloroxylenol	949	8017	88-04-0	mainlib	C8H9ClO	156
2	4-Chloro-2,6-dimethylphenol	888	1396	1123-63-3	mainlib	C8H9ClO	156
3	Benzene, 1-(chloromethyl)-2-methoxy-	857	380	7035-02-1	mainlib	C8H9ClO	156
4	2-Chloro-4,5-dimethylphenol	819	91	1124-04-5	mainlib	C8H9ClO	156
5	Benzene, 1-(chloromethyl)-3-methoxy-	807	60	824-98-6	mainlib	C8H9ClO	156

1H-Indole, 2-methyl-

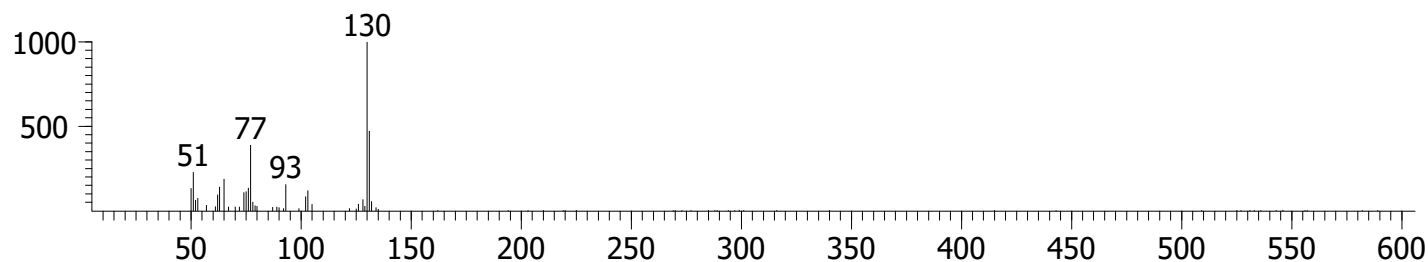
1st Dimension R.T. = 1134.13
2nd Dimension R.T. = 2.152
Quant Mass(es) = 130
S/N = 277.07
Area = 35253
Height = 4133.9
Similarity = 862



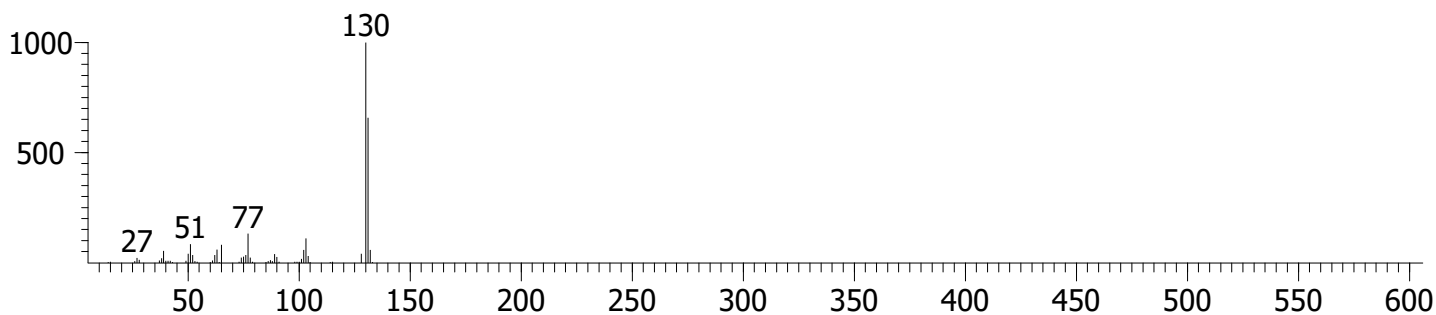
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1369, at 1134.13 , 2.152 sec , sec (Spec # 9943 6)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1369, at 1134.13 , 2.152 sec , sec (Spec # 9943 6)



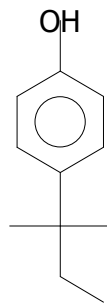
Library Hit - similarity 862, "1H-Indole, 2-methyl-"



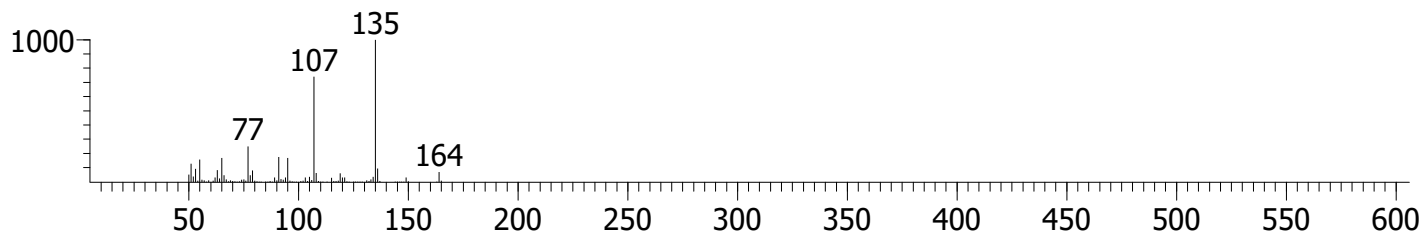
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Indole, 2-methyl-	862	3008	95-20-5	mainlib	C9H9N	131
2	Indole, 3-methyl-	839	1098	83-34-1	mainlib	C9H9N	131
3	Indole, 3-(2-aminopropyl)-, monohydrochloride	838	1056	879-36-7	mainlib	C11H14N2	174
4	1H-Indole-3-ethanamine, à-methyl-	824	661	299-26-3	mainlib	C11H14N2	174
5	1H-Indole, 7-methyl-	810	413	933-67-5	mainlib	C9H9N	131

Phenol, 4-(1,1-dimethylpropyl)-

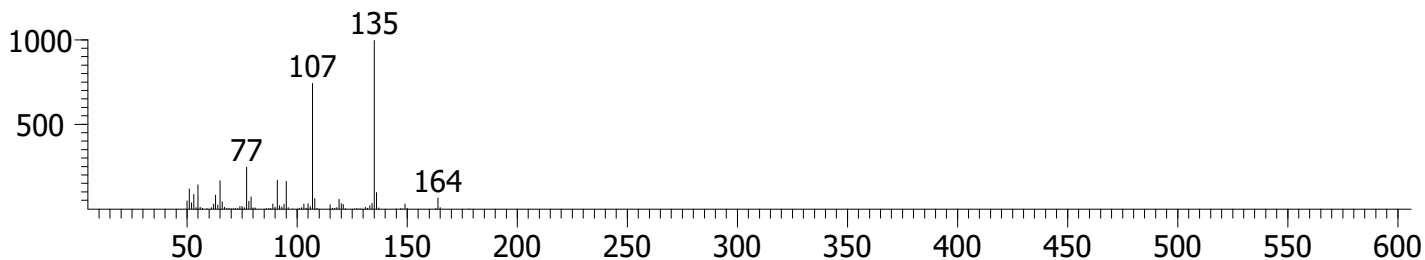
1st Dimension R.T. = 1137.62
2nd Dimension R.T. = 1.723
Quant Mass(es) = 135
S/N = 5818.9
Area = 1115458
Height = 141369
Similarity = 881



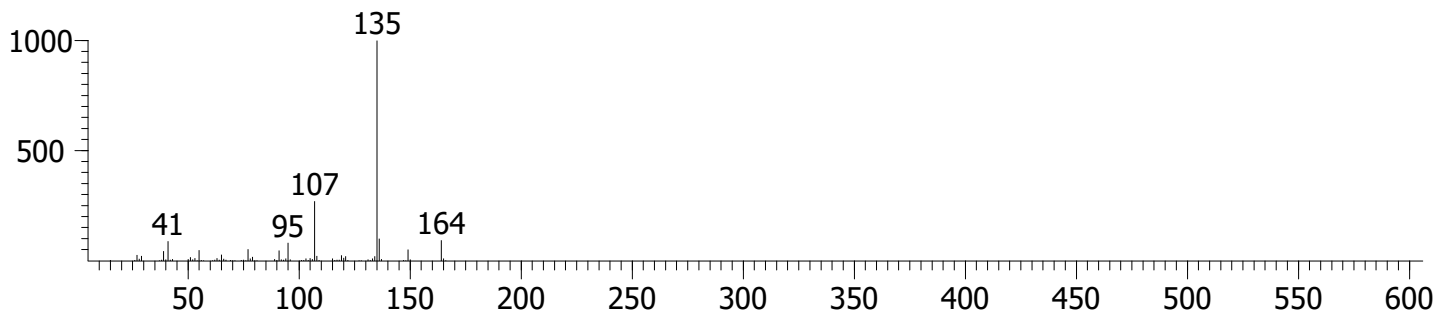
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1372, at 1137.62 , 1.723 sec , sec (Spec # 9990 1)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1372, at 1137.62 , 1.723 sec , sec (Spec # 9990 1)



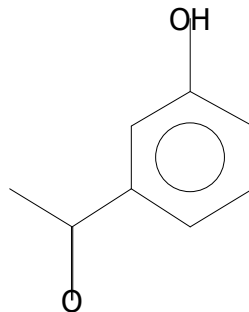
Library Hit - similarity 881, "Phenol, 4-(1,1-dimethylpropyl)-"



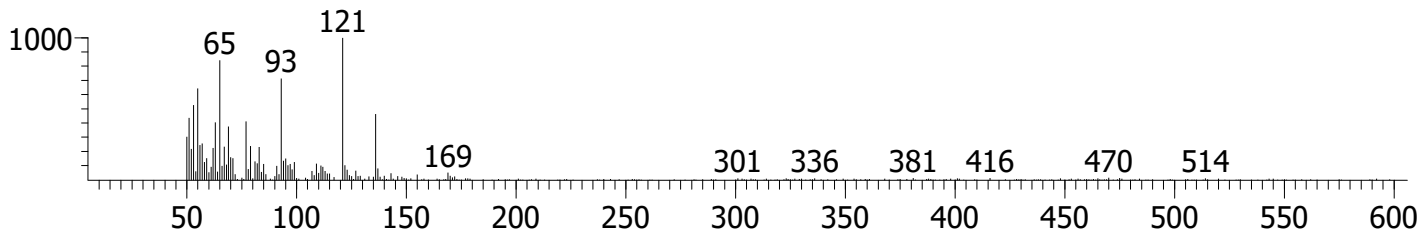
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 4-(1,1-dimethylpropyl)-	881	5921	80-46-6	mainlib	C ₁₁ H ₁₆ O	164
2	Phenol, p-tert-butyl-	810	843	98-54-4	mainlib	C ₁₀ H ₁₄ O	150
3	Hexestrol, O-trifluoroacetyl-	809	810	0-00-0	mainlib	C ₂₀ H ₂₁ F ₃ O ₃	366
4	4-(1,1-Dimethylpropyl)phenyl acetate	806	716	0-00-0	mainlib	C ₁₃ H ₁₈ O ₂	206
5	Hexestrol, O-acetyl-	767	168	0-00-0	mainlib	C ₂₀ H ₂₄ O ₃	312

Ethanone, 1-(3-hydroxyphenyl)-

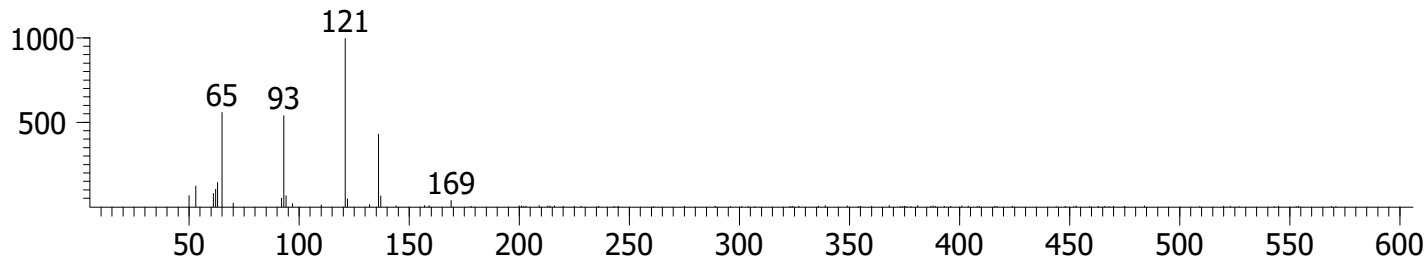
1st Dimension R.T. = 1148.12
2nd Dimension R.T. = 2.046
Quant Mass(es) = 121
S/N = 138.45
Area = 42410
Height = 4877.8
Similarity = 910



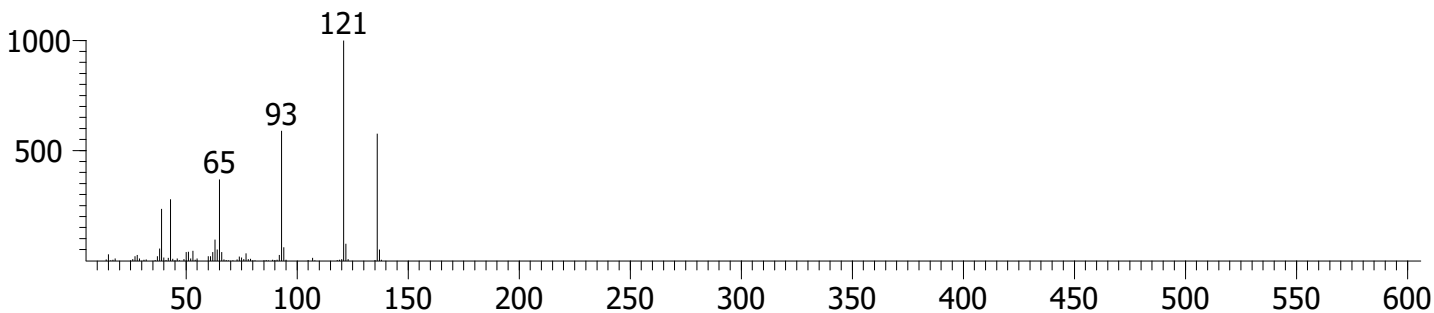
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1393, at 1148.12 , 2.046 sec , sec (Spec # 1015 40)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1393, at 1148.12 , 2.046 sec , sec (Spec # 1015 40)



Library Hit - similarity 910, "Ethanone, 1-(3-hydroxyphenyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanone, 1-(3-hydroxyphenyl)-	910	6614	121-71-1	mainlib	C ₈ H ₈ O ₂	136
2	Ethanone, 1-(2-hydroxyphenyl)-	870	1534	118-93-4	mainlib	C ₈ H ₈ O ₂	136
3	Acetophenone, 4'-hydroxy-	845	468	99-93-4	mainlib	C ₈ H ₈ O ₂	136
4	1-Butanone, 4-chloro-1-(4-hydroxyphenyl)-	838	358	7150-55-2	mainlib	C ₁₀ H ₁₁ ClO ₂	198
5	Methanol, (4-carboxymethoxy)benzoyl-	824	224	80099-44-1	mainlib	C ₁₀ H ₁₀ O ₅	210

1,1'-Biphenyl, 4-methyl-

1st Dimension R.T. = 1186.6

2nd Dimension R.T. = 1.921

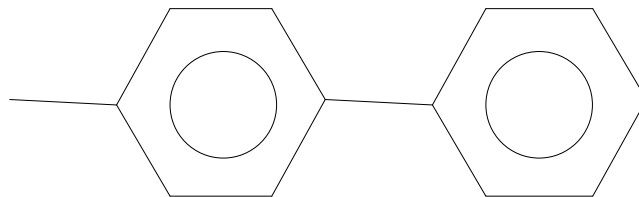
Quant Mass(es) = 167

S/N = 643.69

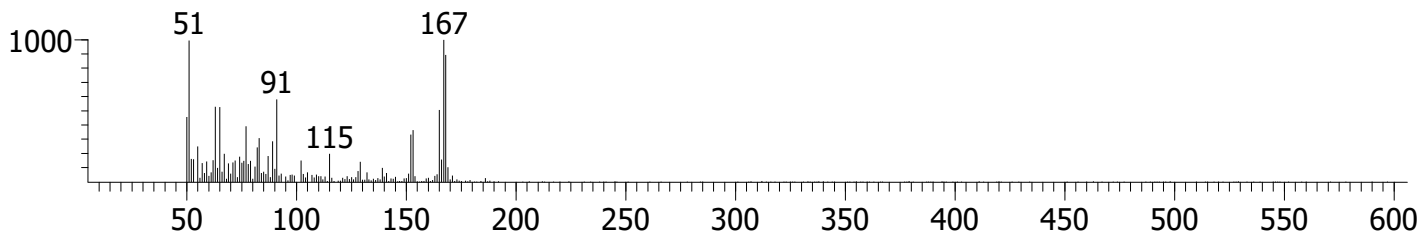
Area = 50383

Height = 6363.9

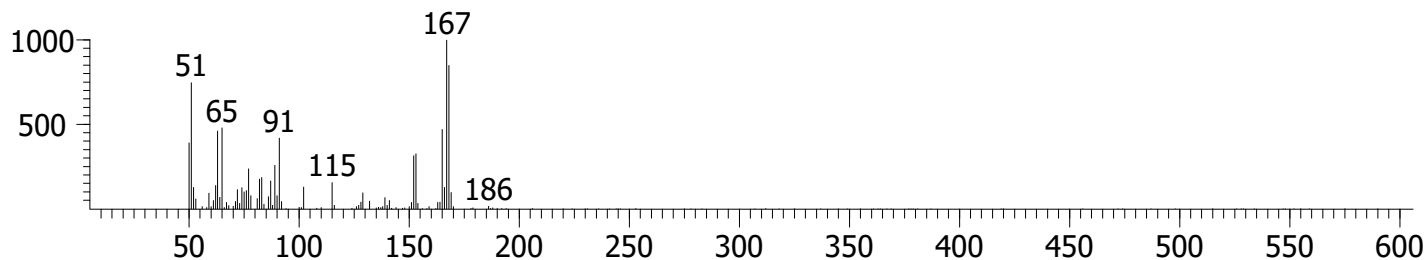
Similarity = 828



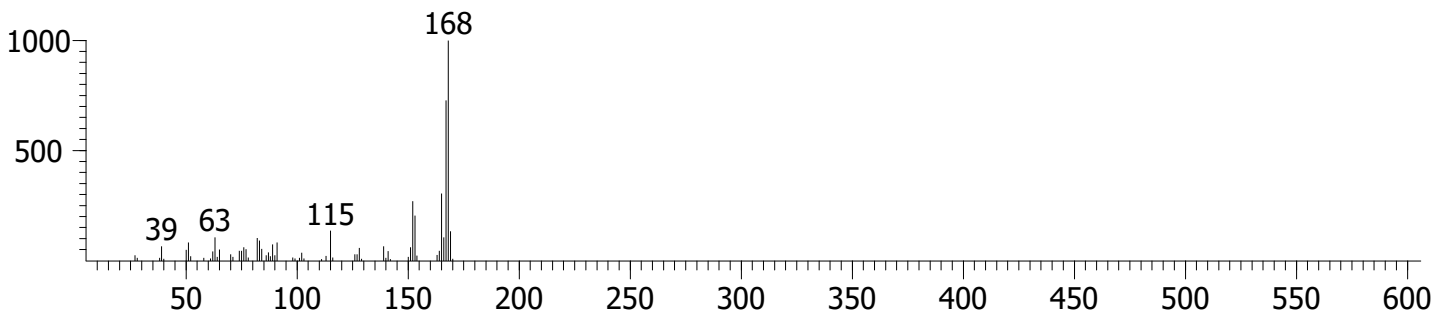
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1471, at 1186.6 , 1.921 sec , sec (Spec # 10735 1)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1471, at 1186.6 , 1.921 sec , sec (Spec # 10735 1)



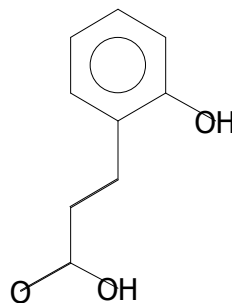
Library Hit - similarity 828, "1,1'-Biphenyl, 4-methyl-"



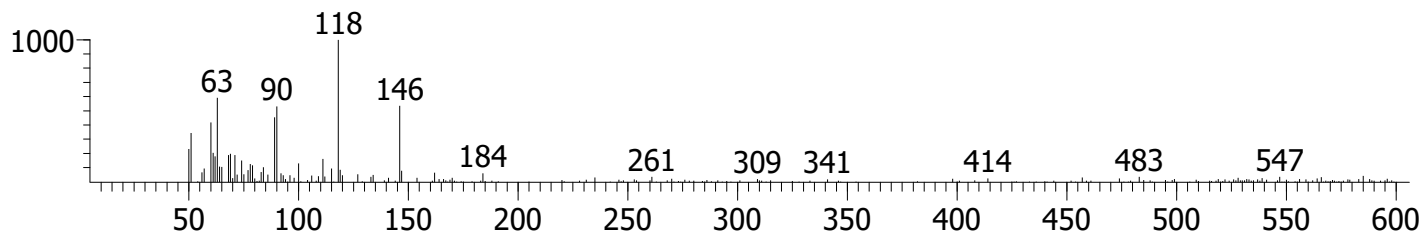
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,1'-Biphenyl, 4-methyl-	828	3000	644-08-6	mainlib	C13H12	168
2	1,1'-Biphenyl, 2-methyl-	821	2298	643-58-3	mainlib	C13H12	168
3	Diphenylmethane	812	1668	101-81-5	mainlib	C13H12	168
4	2-Allylnaphthalene	781	454	2489-87-4	mainlib	C13H12	168
5	Naphthalene, 1-(2-propenyl)-	780	437	2489-86-3	mainlib	C13H12	168

2-Propenoic acid, 3-(2-hydroxyphenyl)-,
(E)-

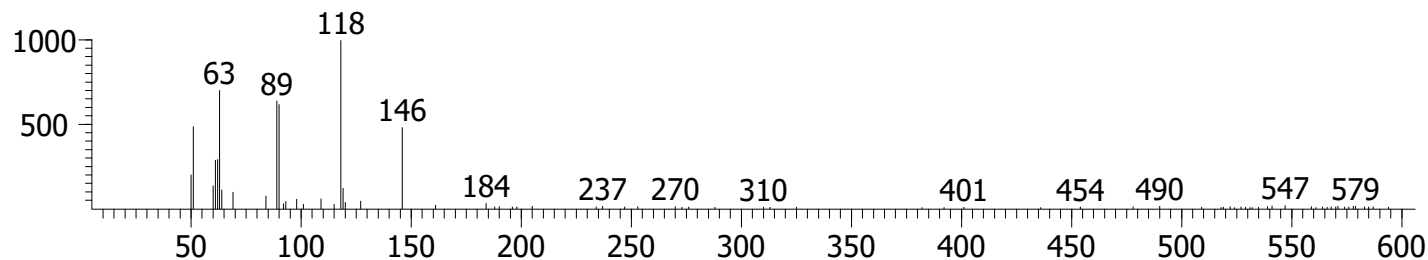
1st Dimension R.T. = 1204.09
 2nd Dimension R.T. = 2.363
 Quant Mass(es) = 118
 S/N = 62.148
 Area = 12600
 Height = 1203.2
 Similarity = 761



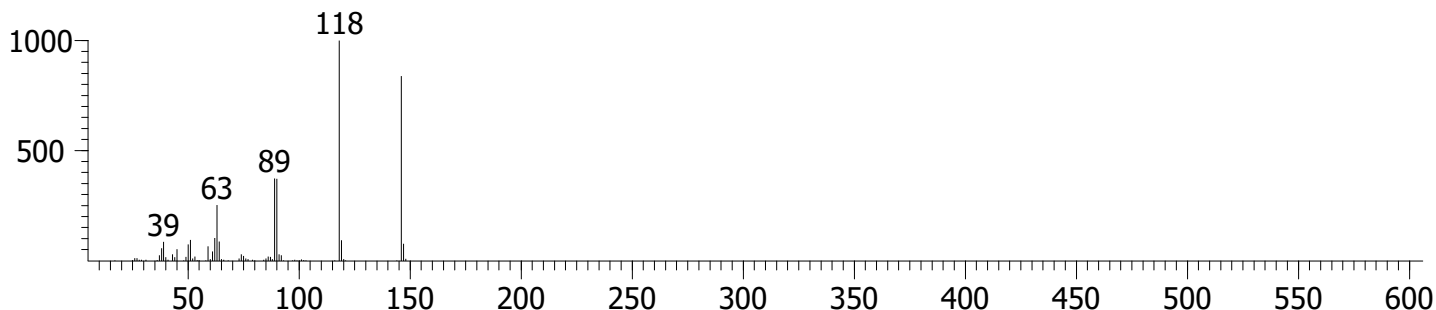
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1506, at 1204.09 , 2.363 sec , sec (Spec # 1100 68)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1506, at 1204.09 , 2.363 sec , sec (Spec # 1100 68)



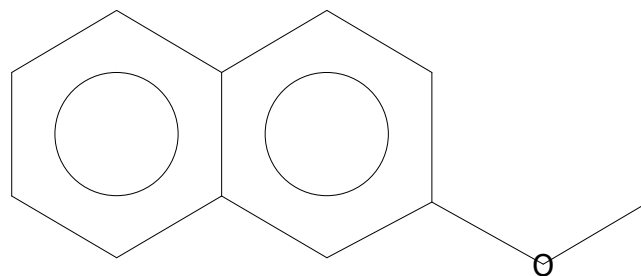
Library Hit - similarity 761, "2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-"



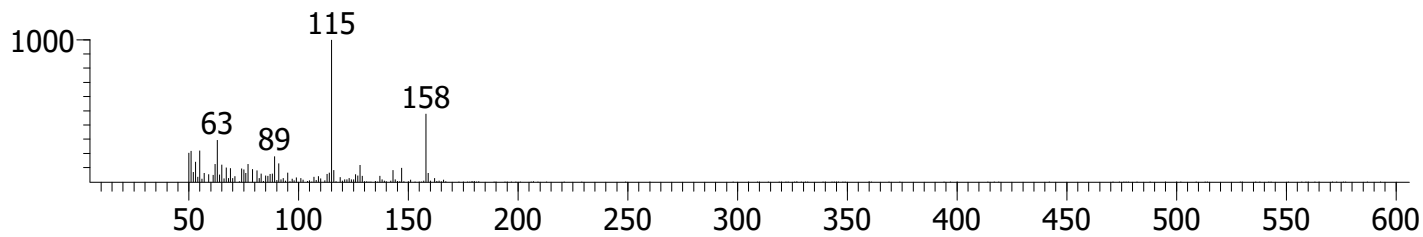
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-	761	2829	614-60-8	mainlib	C9H8O3	164
2	2H-1-Benzopyran-3-carboxaldehyde, 2-oxo-	752	2053	95306-75-5	mainlib	C10H6O3	174
3	2-Aminoethyl 2-oxo-2H-chromene-3-carboxylate	749	1814	0-00-0	mainlib	C12H11NO4	233
4	2-Propenoic acid, 3-(2-hydroxyphenyl)-	743	1426	583-17-5	mainlib	C9H8O3	164
5	1(2H)-Naphthalenone, 3,4-dihydro-	704	336	529-34-0	mainlib	C10H10O	146

Naphthalene, 2-methoxy-

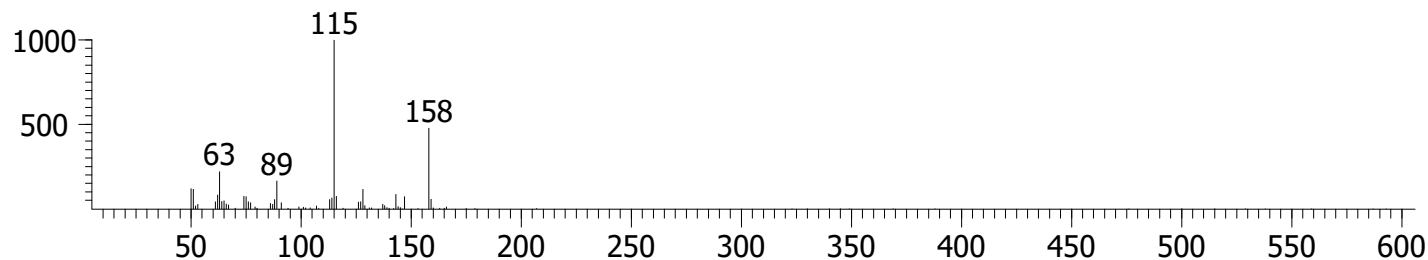
1st Dimension R.T. = 1214.58
2nd Dimension R.T. = 2.006
Quant Mass(es) = 158
S/N = 419.74
Area = 35917
Height = 4111.0
Similarity = 891



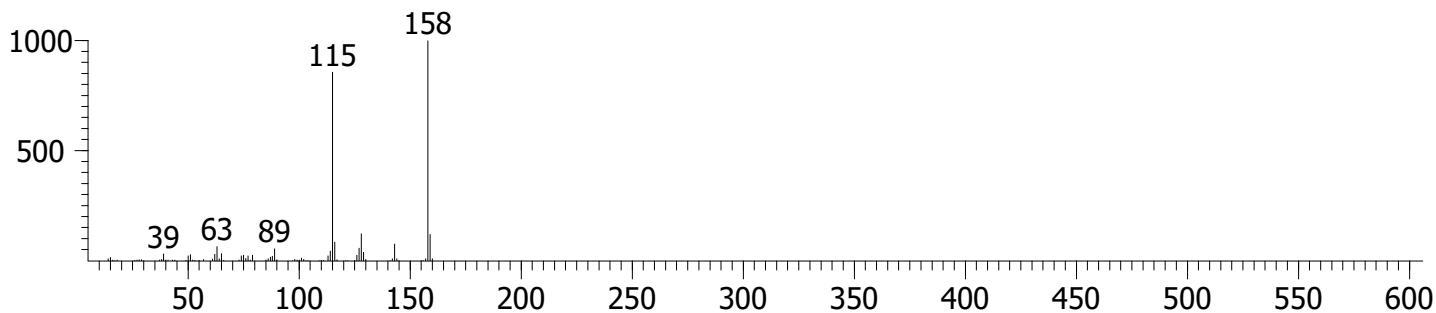
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1533, at 1214.58 , 2.006 sec , sec (Spec # 1116 04)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1533, at 1214.58 , 2.006 sec , sec (Spec # 1116 04)



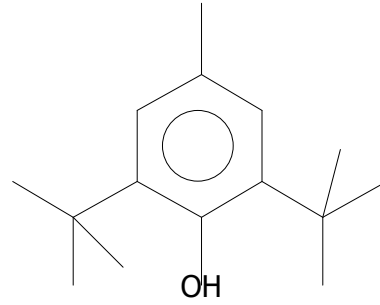
Library Hit - similarity 891, "Naphthalene, 2-methoxy-"



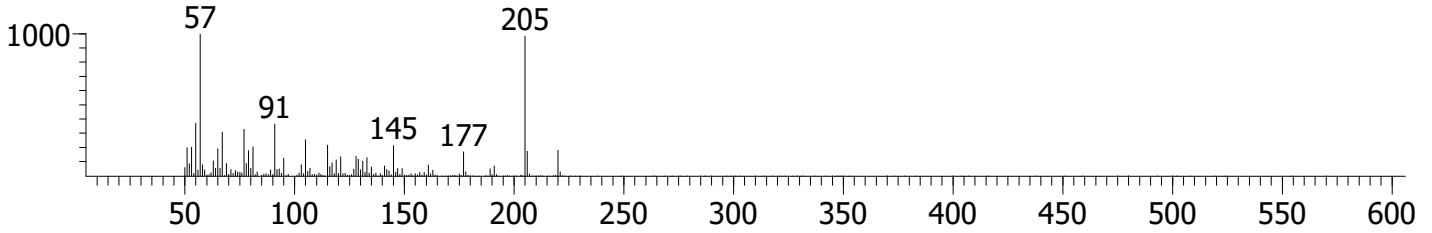
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Naphthalene, 2-methoxy-	891	7944	93-04-9	mainlib	C11H10O	158
2	Naphthalene, 1-methoxy-	840	1601	2216-69-5	mainlib	C11H10O	158
3	(1-Benzyl-3-phenyl-prop-2-ynyl)-dimethyl-amine	727	98	0-00-0	mainlib	C18H19N	249
4	Cinnoline, 3,4-dimethyl-	724	87	3929-83-7	mainlib	C10H10N2	158
5	Hydrazine, 2-naphthalenyl-	723	83	2243-57-4	mainlib	C10H10N2	158

Butylated Hydroxytoluene

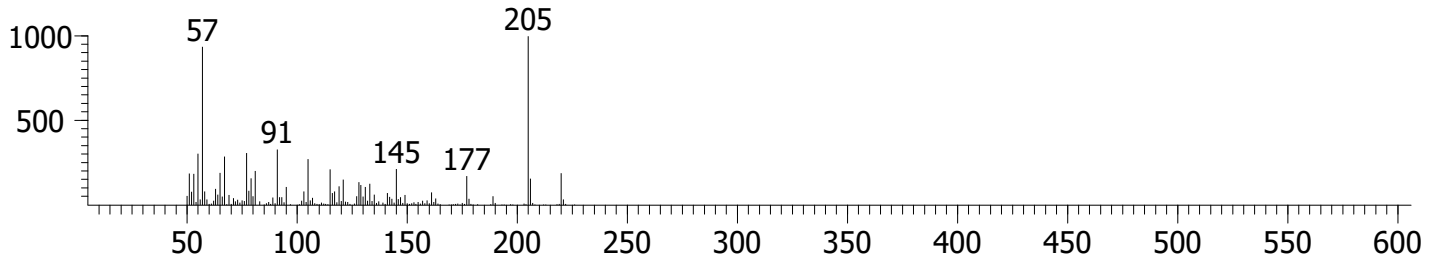
1st Dimension R.T. = 1277.54
 2nd Dimension R.T. = 1.564
 Quant Mass(es) = 205
 S/N = 2933.7
 Area = 229761
 Height = 31611
 Similarity = 883



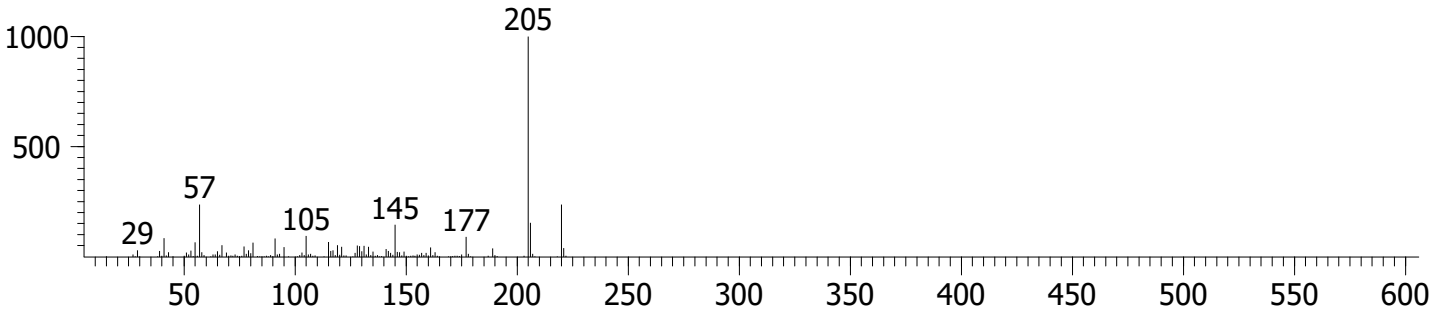
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1688, at 1277.54 , 1.564 sec , sec (Spec # 1210 77)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1688, at 1277.54 , 1.564 sec , sec (Spec # 1210 77)



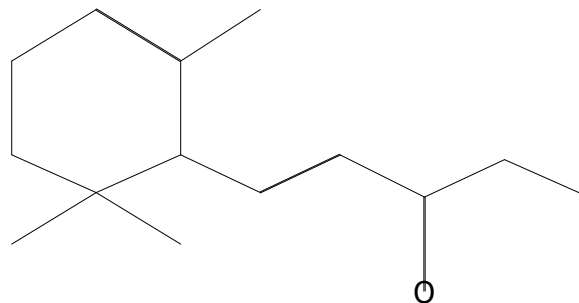
Library Hit - similarity 883, "Butylated Hydroxytoluene"



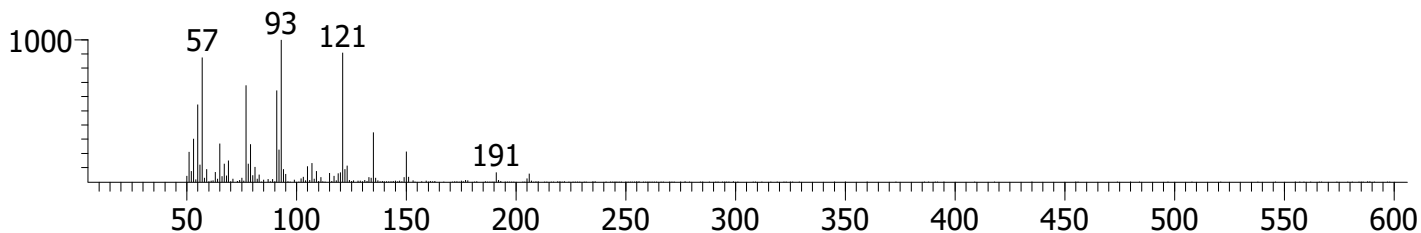
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Butylated Hydroxytoluene	883	8390	128-37-0	mainlib	C15H24O	220
2	Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-	795	732	616-55-7	mainlib	C15H24O	220
3	4,6-di-tert-Butyl-m-cresol	780	443	497-39-2	mainlib	C15H24O	220
4	Ethanone, 1-(5,6,7,8-tetrahydro-2,8,8-trimethyl-4H-cyclohepta[b]furan-5-yl)-	750	123	71596-88-8	mainlib	C14H20O2	220
5	Cyclopropanecarboxylic acid, 1-hydroxy-, (2,6-di-t-butyl-4-methylphenyl) ester	749	118	108546-75-4	mainlib	C19H28O3	304

1-Penten-3-one,
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-

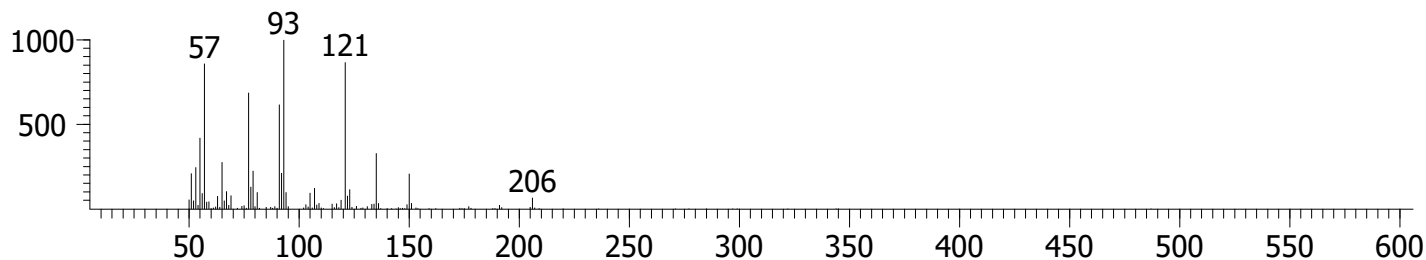
1st Dimension R.T. = 1288.04
 2nd Dimension R.T. = 1.551
 Quant Mass(es) = 121
 S/N = 549.56
 Area = 87067
 Height = 11107
 Similarity = 894



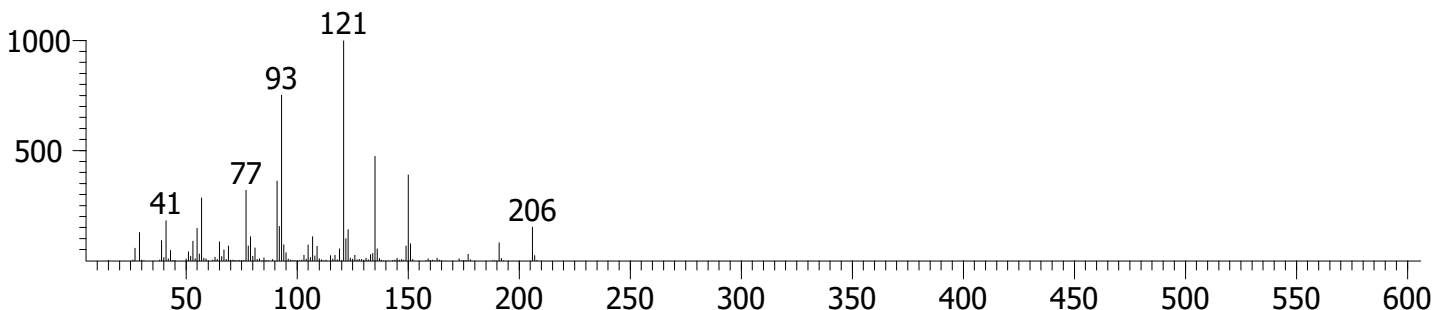
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1703, at 1288.04 , 1.551 sec , sec (Spec # 1226 65)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1703, at 1288.04 , 1.551 sec , sec (Spec # 1226 65)



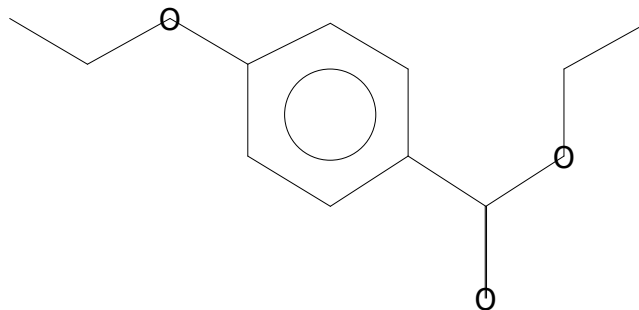
Library Hit - similarity 894, "1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-"



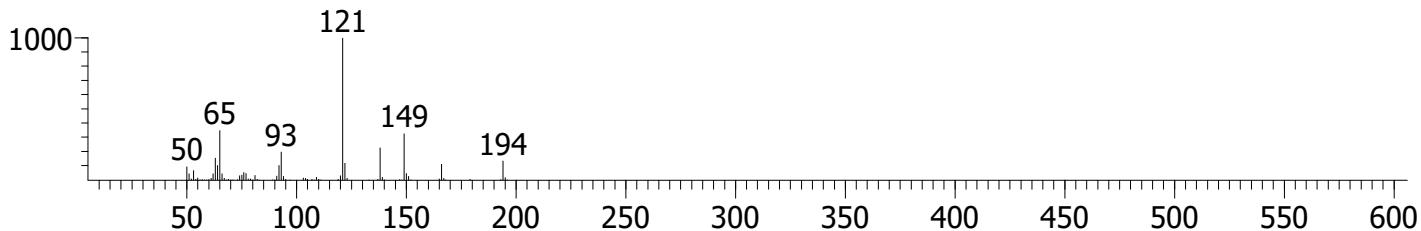
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	894	7714	7779-30-8	mainlib	C14H22O	206
2	1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-	830	1267	93302-56-8	mainlib	C14H22O	206
3	2-Isopropylidene-3-methylhexa-3,5-dienal	734	101	0-00-0	mainlib	C10H14O	150
4	3-Nonen-5-yne, 4-ethyl-, (E)-	729	81	74744-60-8	mainlib	C11H18	150
5	3-Nonen-5-yne, 4-ethyl-, (Z)-	721	60	74744-26-6	mainlib	C11H18	150

Benzoic acid, 4-ethoxy-, ethyl ester

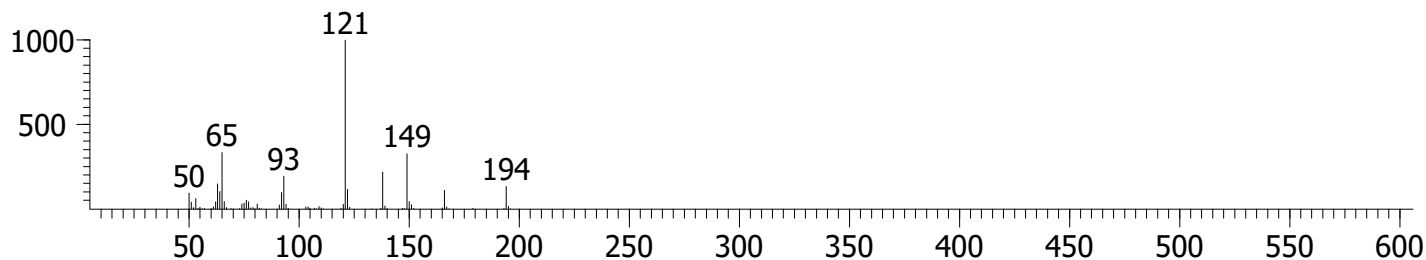
1st Dimension R.T. = 1291.54
2nd Dimension R.T. = 1.795
Quant Mass(es) = 121
S/N = 18939
Area = 3152268
Height = 373733
Similarity = 921



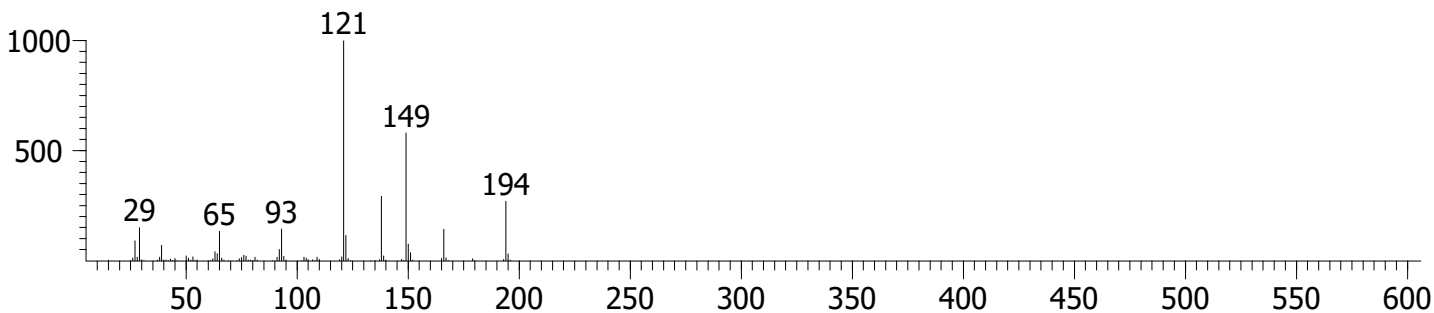
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1713, at 1291.54 , 1.795 sec , sec (Spec # 1232 32)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1713, at 1291.54 , 1.795 sec , sec (Spec # 1232 32)

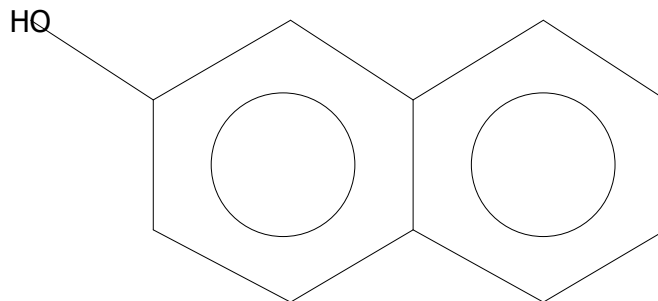


Library Hit - similarity 921, "Benzoic acid, 4-ethoxy-, ethyl ester"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzoic acid, 4-ethoxy-, ethyl ester	921	8866	23676-09-7	mainlib	C11H14O3	194
2	Benzoic acid, 3-ethoxy-, ethyl ester	791	367	0-00-0	mainlib	C11H14O3	194
3	2-Ethoxybenzhydrazide	773	189	21018-13-3	mainlib	C9H12N2O2	180
4	4-Ethoxybenzoyl chloride	754	92	16331-46-7	mainlib	C9H9ClO2	184
5	3-(4-Ethoxyphenyl)-3-oxopropanenitrile	754	92	54605-62-8	mainlib	C11H11NO2	189

2-Naphthalenol



1st Dimension R.T. = 1291.54

2nd Dimension R.T. = 2.191

Quant Mass(es) = 144

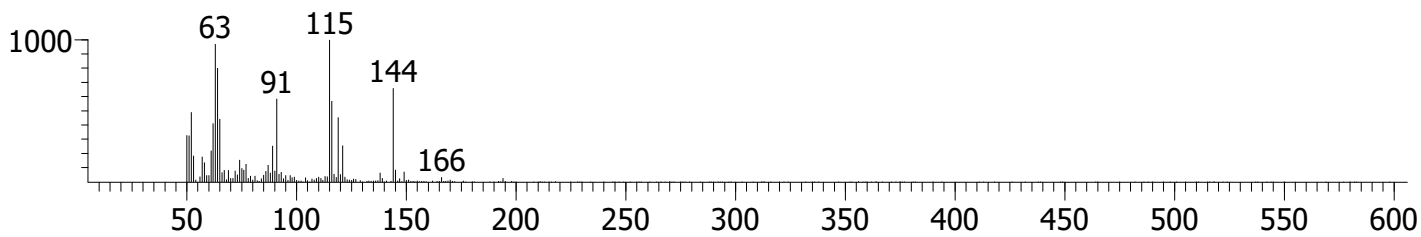
S/N = 590.07

Area = 87577

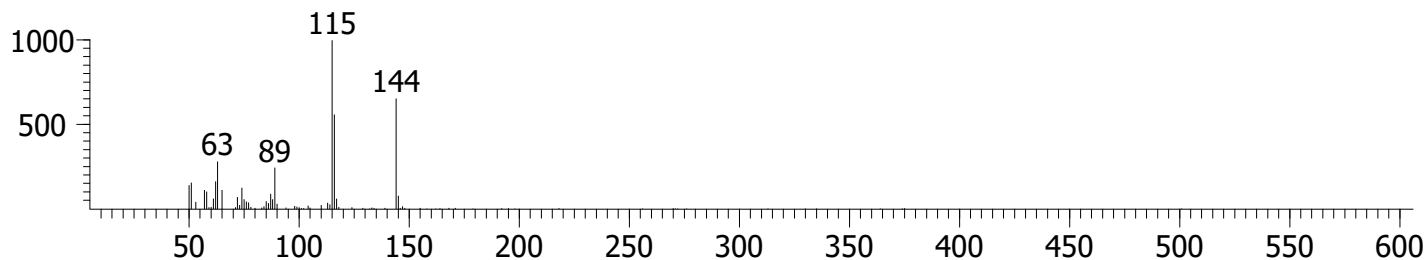
Height = 9980.4

Similarity = 874

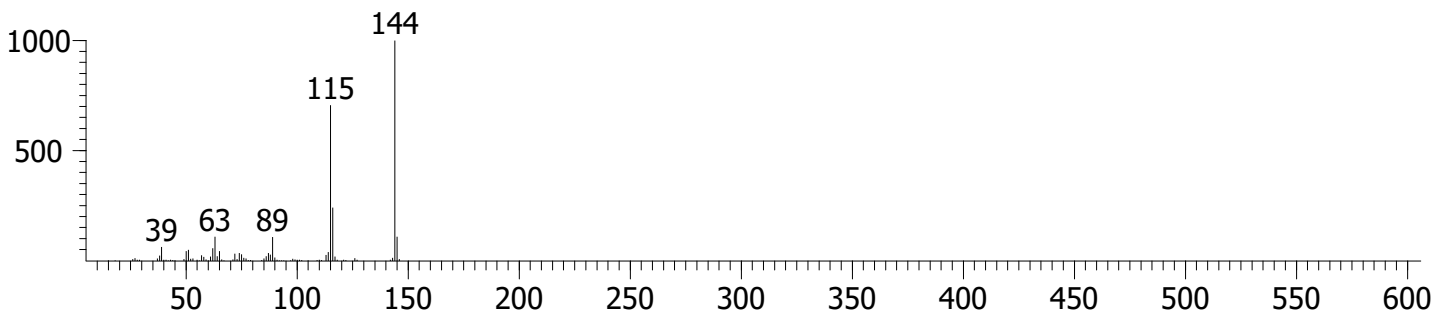
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1715, at 1291.54 , 2.191 sec , sec (Spec # 1232 92)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1715, at 1291.54 , 2.191 sec , sec (Spec # 1232 92)



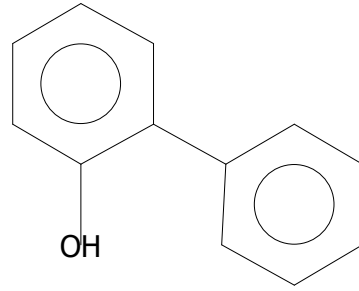
Library Hit - similarity 874, "2-Naphthalenol"



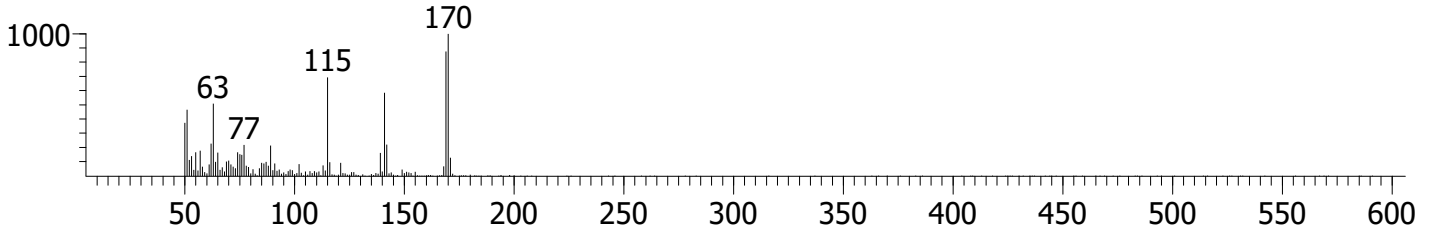
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Naphthalenol	874	4457	135-19-3	mainlib	C10H8O	144
2	1-Naphthyl n-propylcarbamate	856	2298	25216-27-7	mainlib	C14H15NO2	229
3	1-Naphthalenol	842	1439	90-15-3	mainlib	C10H8O	144
4	Cinnoline, 3-methyl-	790	287	17372-78-0	mainlib	C9H8N2	144
5	Furan, 3-phenyl-	780	202	13679-41-9	mainlib	C10H8O	144

o-Hydroxybiphenyl

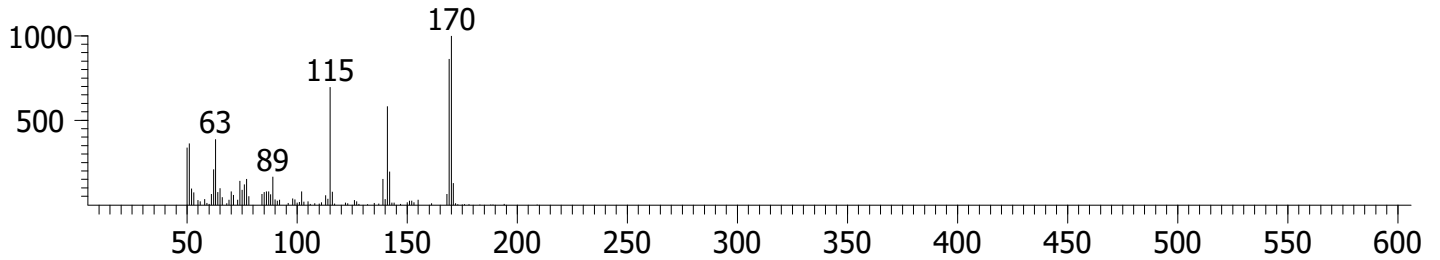
1st Dimension R.T. = 1295.03
2nd Dimension R.T. = 2.072
Quant Mass(es) = 170
S/N = 2296.9
Area = 258373
Height = 28663
Similarity = 892



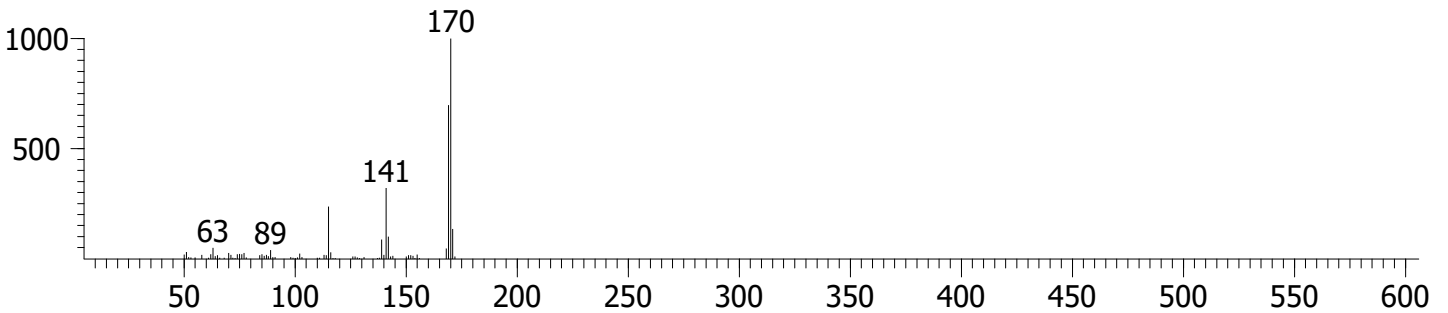
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1723, at 1295.03 , 2.072 sec , sec (Spec # 1238 04)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1723, at 1295.03 , 2.072 sec , sec (Spec # 1238 04)



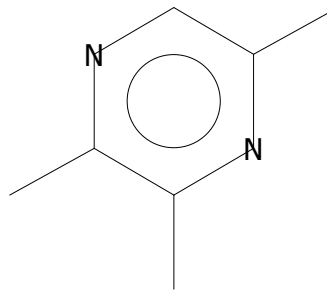
Library Hit - similarity 892, "o-Hydroxybiphenyl"



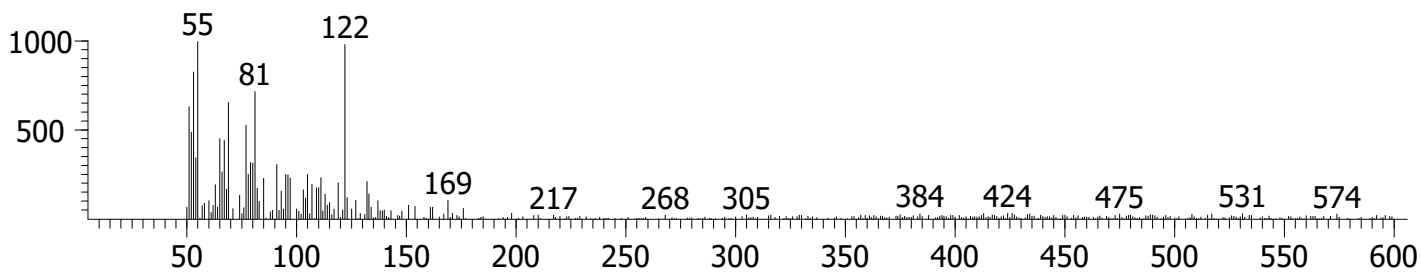
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	o-Hydroxybiphenyl	892	6881	90-43-7	mainlib	C12H10O	170
2	1-Naphthalenecarboxaldehyde, 4-methyl-	863	1950	33738-48-6	mainlib	C12H10O	170
3	Spiro[cyclopropane-1,1'(4'H)-naphthalen]-4'-one	825	467	33498-24-7	mainlib	C12H10O	170
4	1,1'-Biphenyl, 2-butoxy-	789	115	55059-22-8	mainlib	C16H18O	226
5	1H,3H-Naphtho[1,8-cd]pyran	787	106	203-84-9	mainlib	C12H10O	170

Pyrazine, trimethyl-

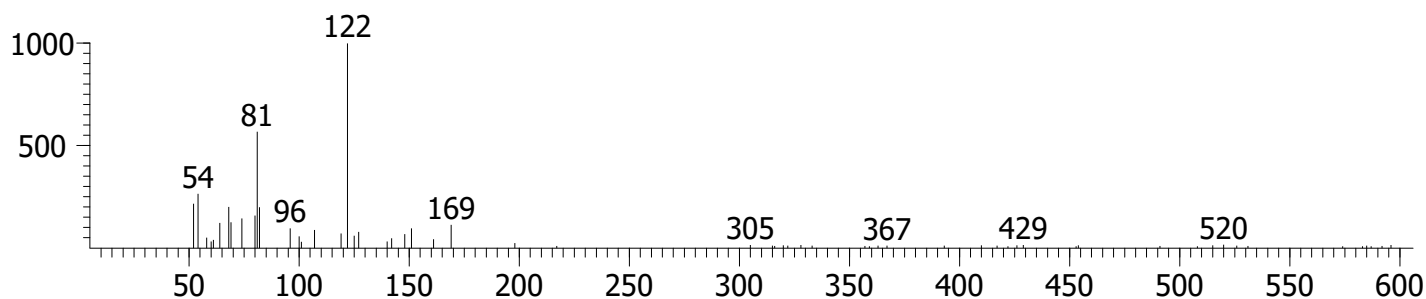
1st Dimension R.T. = 1358
2nd Dimension R.T. = 2.330
Quant Mass(es) = 122
S/N = 75.602
Area = 14006
Height = 1387.9
Similarity = 518



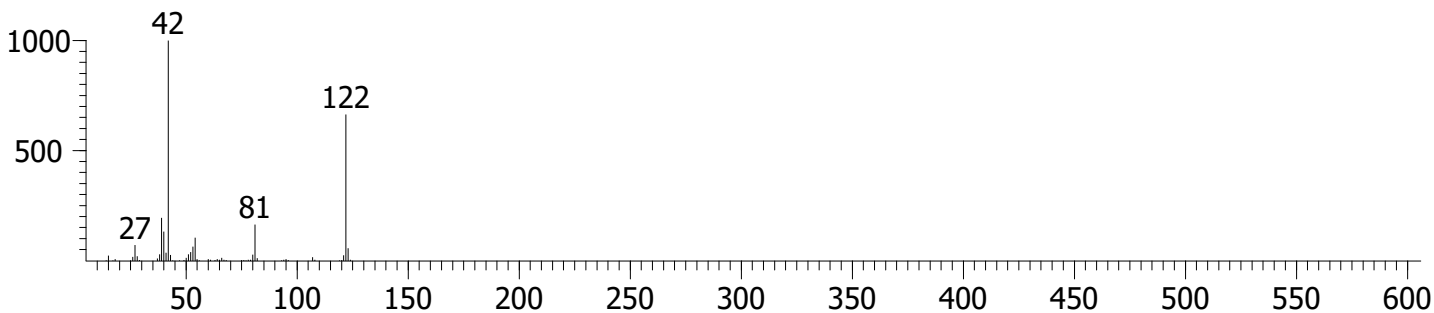
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1856, at 1358 , 2.330 sec , sec (Spec # 133383)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1856, at 1358 , 2.330 sec , sec (Spec # 133383)



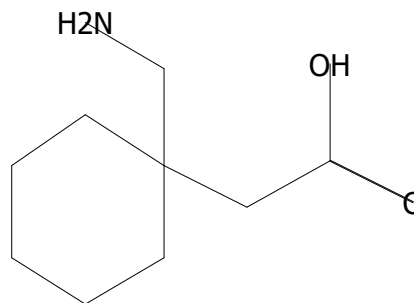
Library Hit - similarity 518, "Pyrazine, trimethyl-"



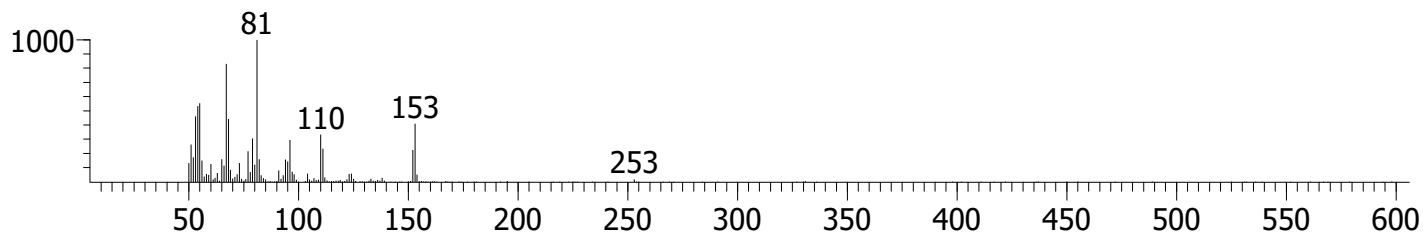
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pyrazine, trimethyl-	518	1494	14667-55-1	mainlib	C7H10N2	122
2	Bicyclo[3.3.1]nonan-3-ol, exo-	516	1378	10036-08-5	mainlib	C9H16O	140
3	(5-Methyl-2H-[1,2,4]triazolo-3-yl)acetonitrile	511	1111	0-00-0	mainlib	C5H6N4	122
4	Cyclohexanecarboxylic acid, 2-(2-propenyl)-, methyl ester	507	938	84694-72-4	mainlib	C11H18O2	182
5	Bicyclo[3.3.1]nonan-9-ol	502	756	15598-80-8	mainlib	C9H16O	140

Gabapentin

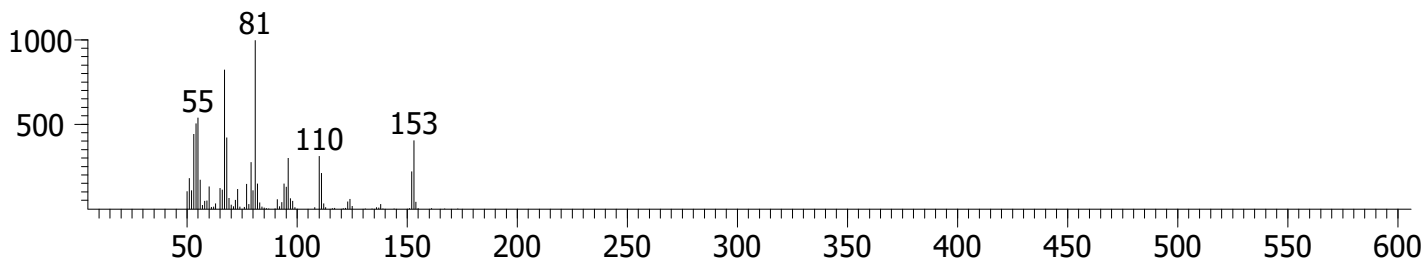
1st Dimension R.T. = 1368.49
2nd Dimension R.T. = 2.330
Quant Mass(es) = 153
S/N = 693.63
Area = 149504
Height = 13545
Similarity = 914



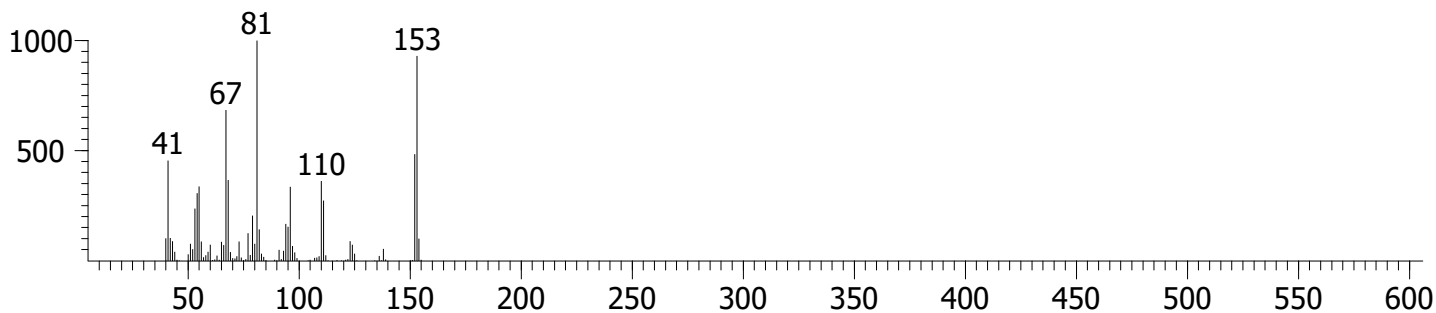
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1879, at 1368.49 , 2.330 sec , sec (Spec # 1349 73)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1879, at 1368.49 , 2.330 sec , sec (Spec # 1349 73)



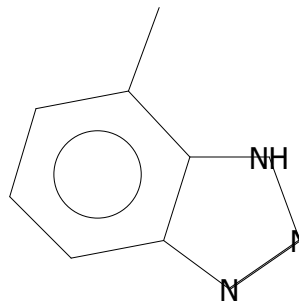
Library Hit - similarity 914, "Gabapentin"



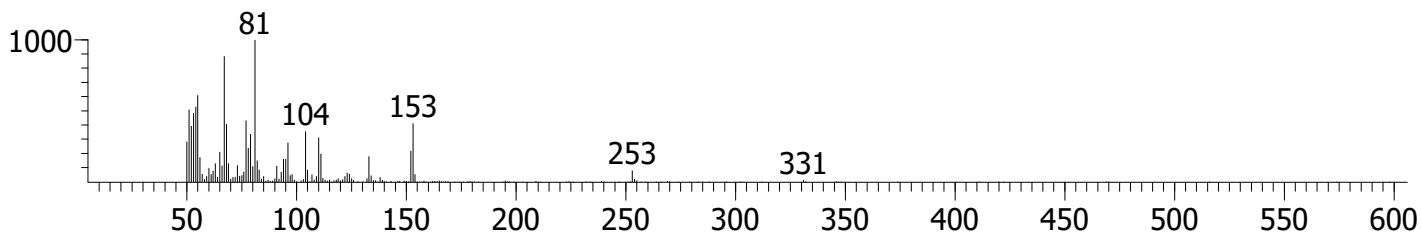
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Gabapentin	914	5335	60142-96-3	mainlib	C9H17NO2	171
2	Gabapentin lactam	906	3980	64744-50-9	mainlib	C9H15NO	153
3	5-Decen-1-ol, acetate, (E)-	725	70	38421-90-8	mainlib	C12H22O2	198
4	Spiro[3.5]nonan-1-one	705	31	29800-45-1	mainlib	C9H14O	138
5	1,3-Octadiene	699	25	1002-33-1	mainlib	C8H14	110

1H-Benzotriazole, 4-methyl-

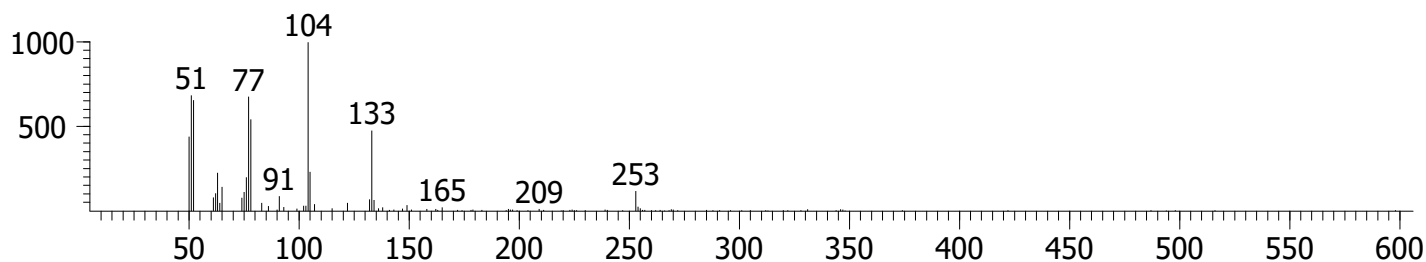
1st Dimension R.T. = 1368.49
2nd Dimension R.T. = 2.356
Quant Mass(es) = 104
S/N = 257.20
Area = 91829
Height = 9482.0
Similarity = 853



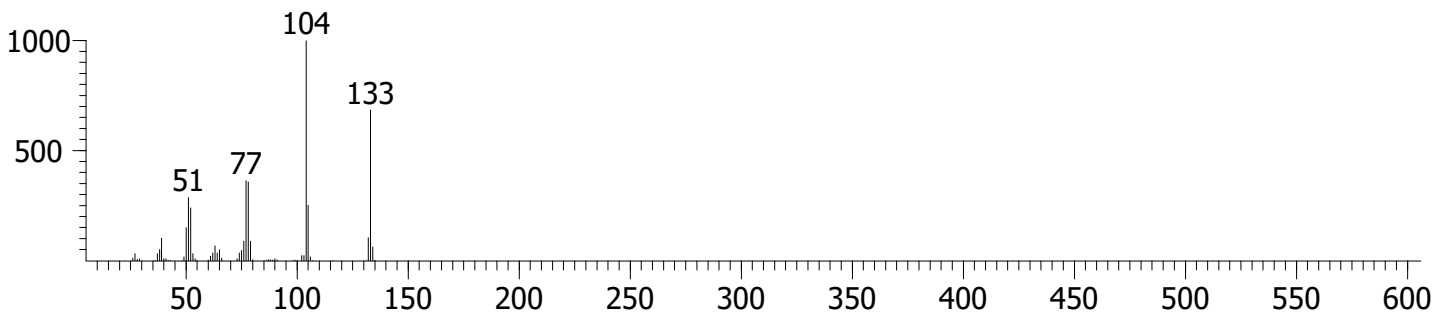
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1880, at 1368.49 , 2.356 sec , sec (Spec # 1349 77)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1880, at 1368.49 , 2.356 sec , sec (Spec # 1349 77)



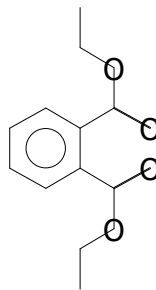
Library Hit - similarity 853, "1H-Benzotriazole, 4-methyl-"



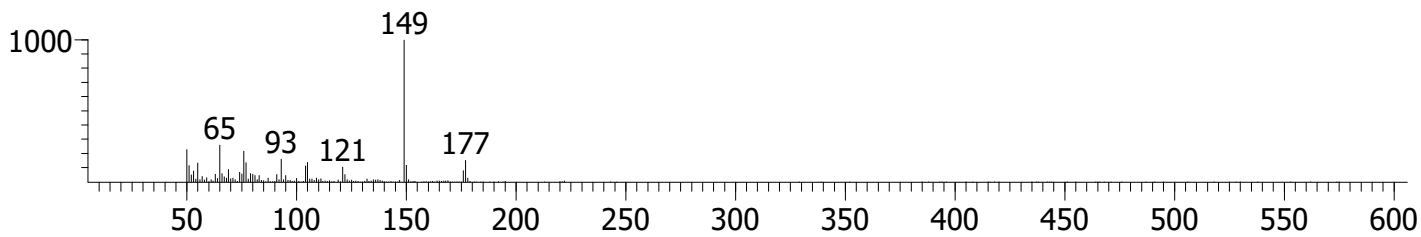
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Benzotriazole, 4-methyl-	853	5417	29878-31-7	mainlib	C7H7N3	133
2	1H-Benzotriazole, 5-methyl-	799	1061	136-85-6	mainlib	C7H7N3	133
3	1-Benzofuran-7-amine	790	770	67830-55-1	mainlib	C8H7NO	133
4	2H-Indol-2-one, 1,3-dihydro-	785	621	59-48-3	mainlib	C8H7NO	133
5	Benzene, (azidomethyl)-	767	320	622-79-7	mainlib	C7H7N3	133

Diethyl Phthalate

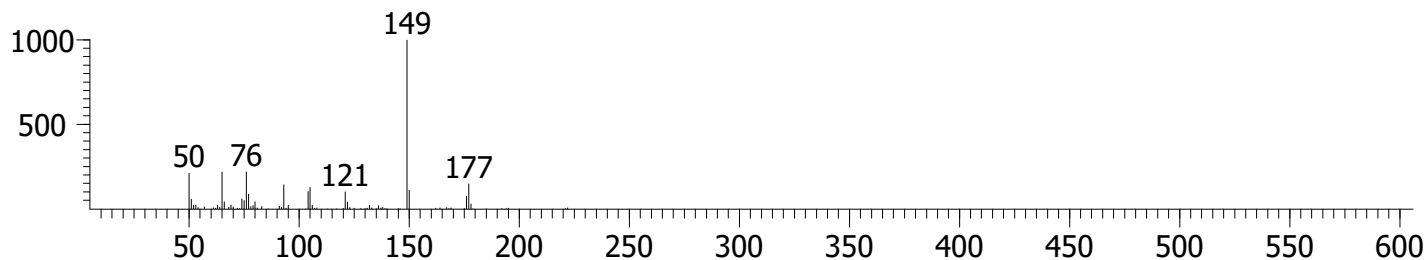
1st Dimension R.T. = 1375.49
2nd Dimension R.T. = 2.020
Quant Mass(es) = 149
S/N = 1568.4
Area = 344554
Height = 34991
Similarity = 927



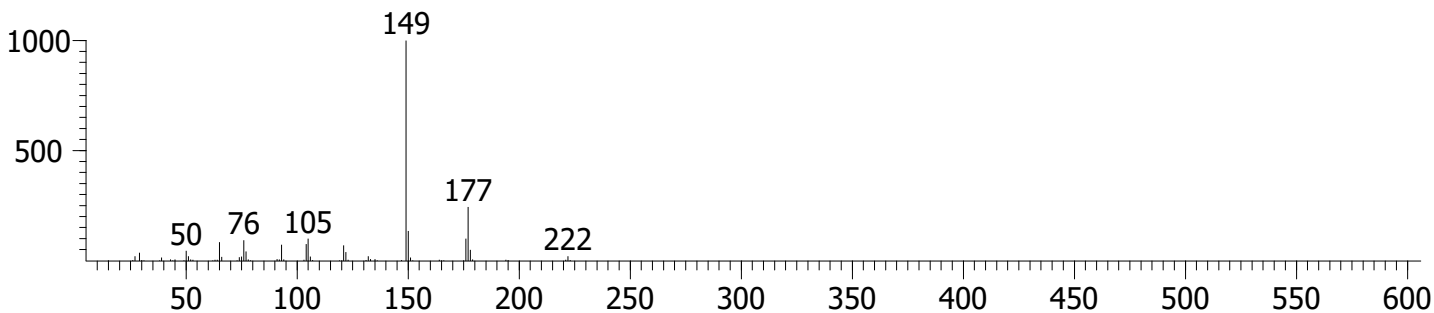
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1898, at 1375.49 , 2.020 sec , sec (Spec # 1359 86)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1898, at 1375.49 , 2.020 sec , sec (Spec # 1359 86)



Library Hit - similarity 927, "Diethyl Phthalate"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Diethyl Phthalate	927	6960	84-66-2	mainlib	C12H14O4	222
2	Benzoic acid, 2-(1-oxopropyl)-	847	765	2360-45-4	mainlib	C10H10O3	178
3	2-Acetylbenzoic acid	830	417	577-56-0	mainlib	C9H8O3	164
4	Phthalic acid, di-(1-hexen-5-yl) ester	819	286	0-00-0	mainlib	C20H26O4	330
5	Phthalic acid, monoethyl ester	804	173	2306-33-4	mainlib	C10H10O4	194

Benzophenone

1st Dimension R.T. = 1424.46

2nd Dimension R.T. = 2.185

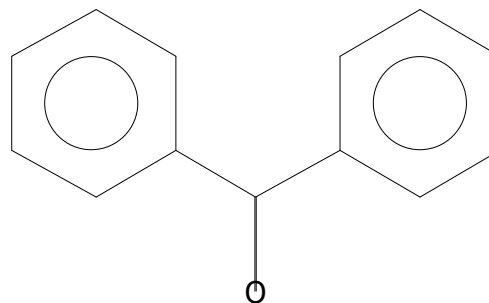
Quant Mass(es) = 105

S/N = 5030.3

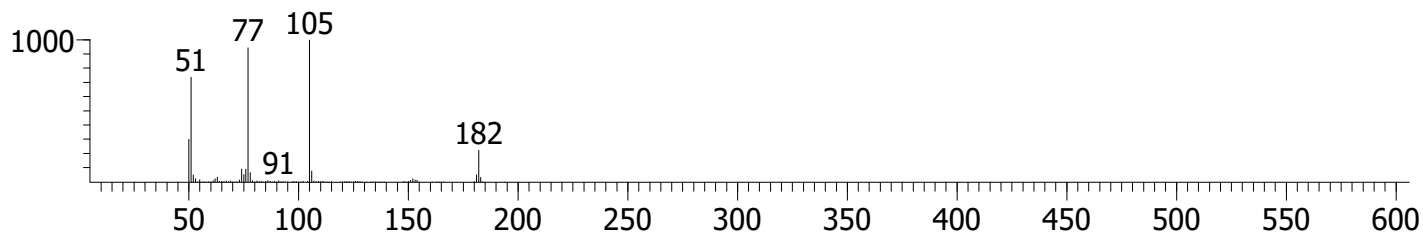
Area = 1969521

Height = 196516

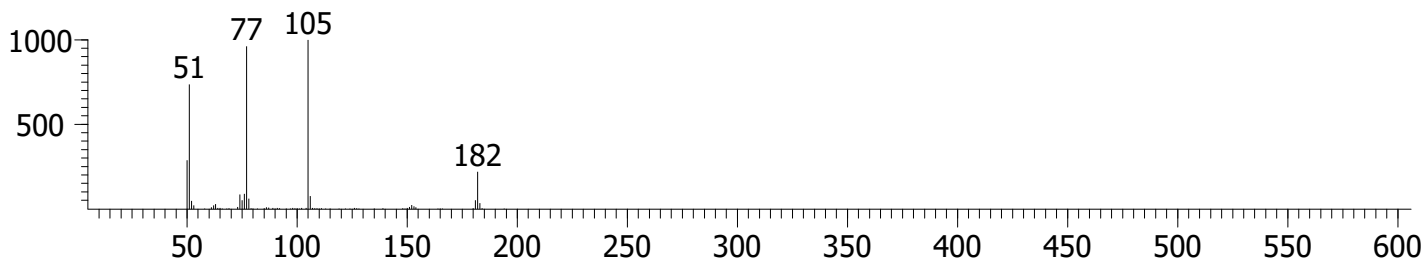
Similarity = 888



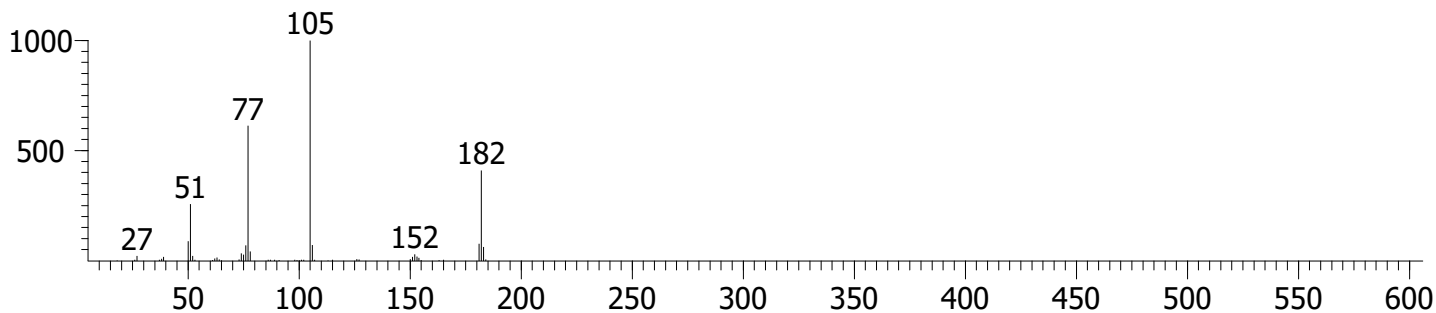
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1996, at 1424.46 , 2.185 sec , sec (Spec # 1434 31)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1996, at 1424.46 , 2.185 sec , sec (Spec # 1434 31)



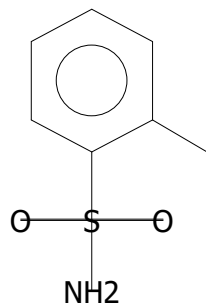
Library Hit - similarity 888, "Benzophenone"



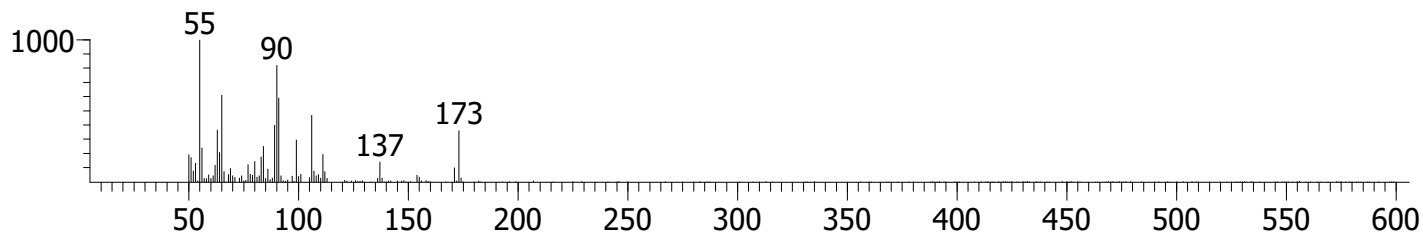
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzophenone	888	981	119-61-9	mainlib	C13H10O	182
2	2(5H)-Thiazolone, 4-(benzoyloxy)-	884	829	0-00-0	mainlib	C10H7NO3S	221
3	Benzeneacetic acid, à-oxo-, methyl ester	877	635	15206-55-0	mainlib	C9H8O3	164
4	N-(1H-Tetrazol-5-yl)benzamide	872	512	4847-62-5	mainlib	C8H7N5O	189
5	Benzoylformic acid	870	472	611-73-4	mainlib	C8H6O3	150

Benzenesulfonamide, 2-methyl-

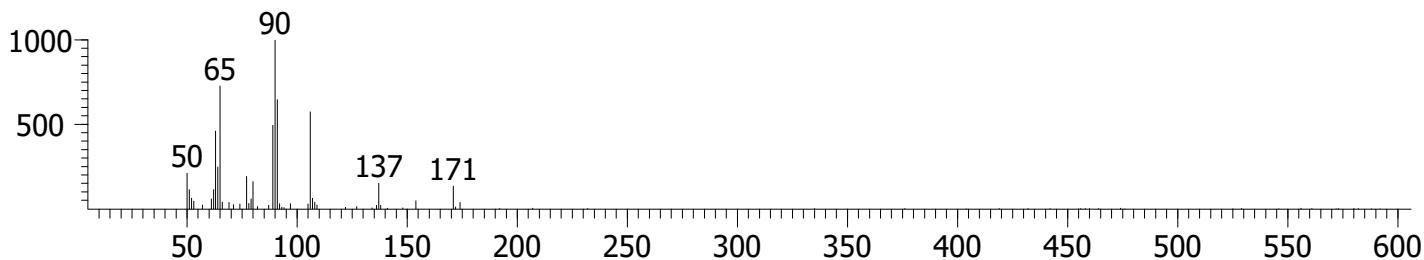
1st Dimension R.T. = 1431.46
2nd Dimension R.T. = 2.666
Quant Mass(es) = 90
S/N = 296.37
Area = 62089
Height = 5949.8
Similarity = 800



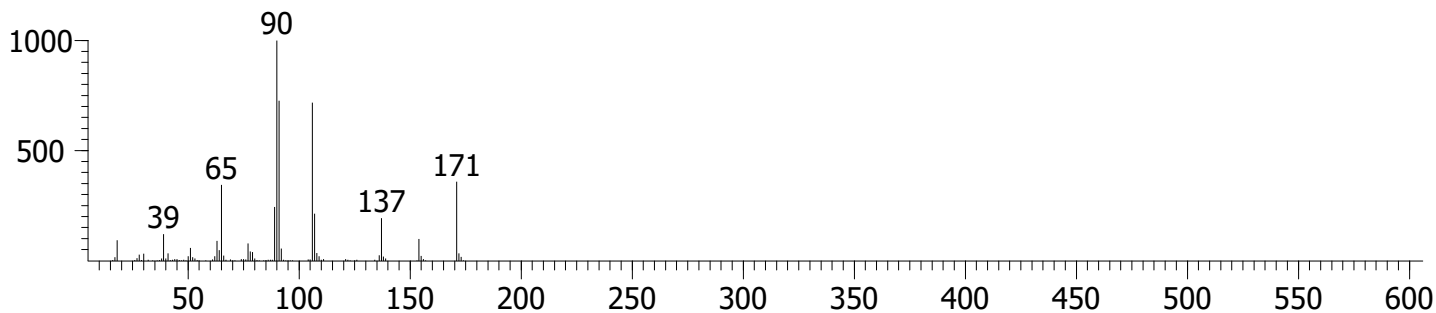
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2013, at 1431.46 , 2.666 sec , sec (Spec # 1445 64)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2013, at 1431.46 , 2.666 sec , sec (Spec # 1445 64)



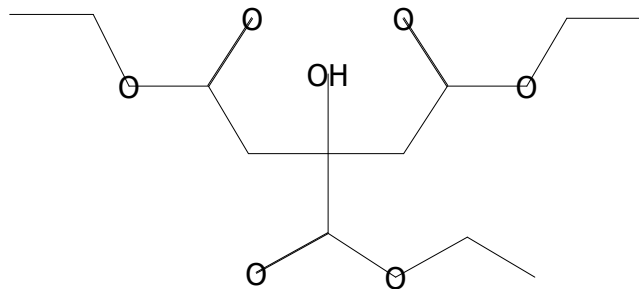
Library Hit - similarity 800, "Benzenesulfonamide, 2-methyl-"



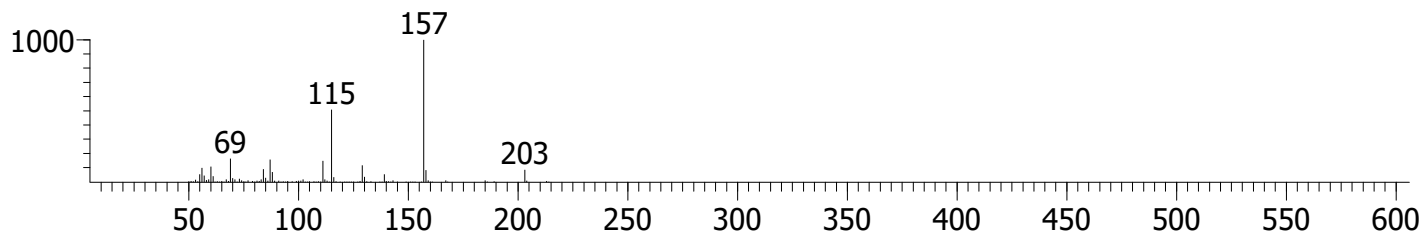
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenesulfonamide, 2-methyl-	800	7005	88-19-7	mainlib	C ₇ H ₉ NO ₂ S	171
2	4-(2-Aminoethyl)benzenesulfonamide	721	798	35303-76-5	mainlib	C ₈ H ₁₂ N ₂ O ₂ S	200
3	2-Iodoamphetamine	716	643	22080-10-0	mainlib	C ₉ H ₁₂ I ₂ N	261
4	Phenethylamine, 4-iodo-à-methyl-, hydrochloride	709	493	21894-58-6	mainlib	C ₉ H ₁₂ I ₂ N	261
5	Phenethylamine, 3-iodo-à-methyl-, hydrochloride	707	454	20110-28-5	mainlib	C ₉ H ₁₂ I ₂ N	261

Triethyl citrate

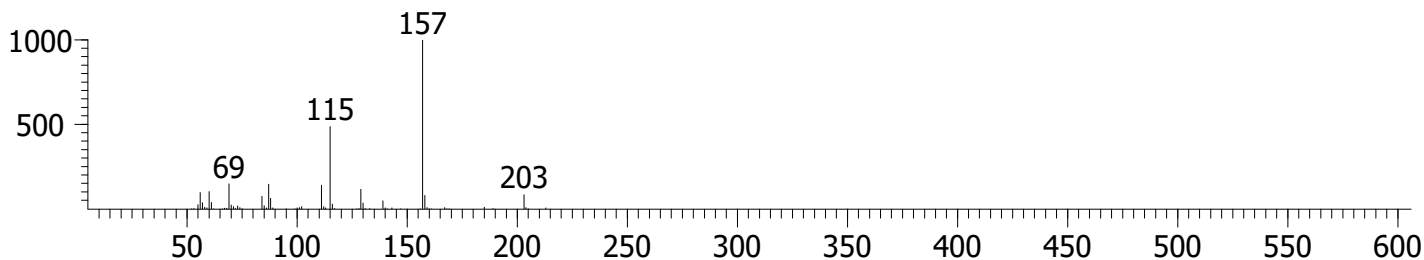
1st Dimension R.T. = 1438.45
2nd Dimension R.T. = 1.835
Quant Mass(es) = 157
S/N = 11171
Area = 1108966
Height = 124590
Similarity = 907



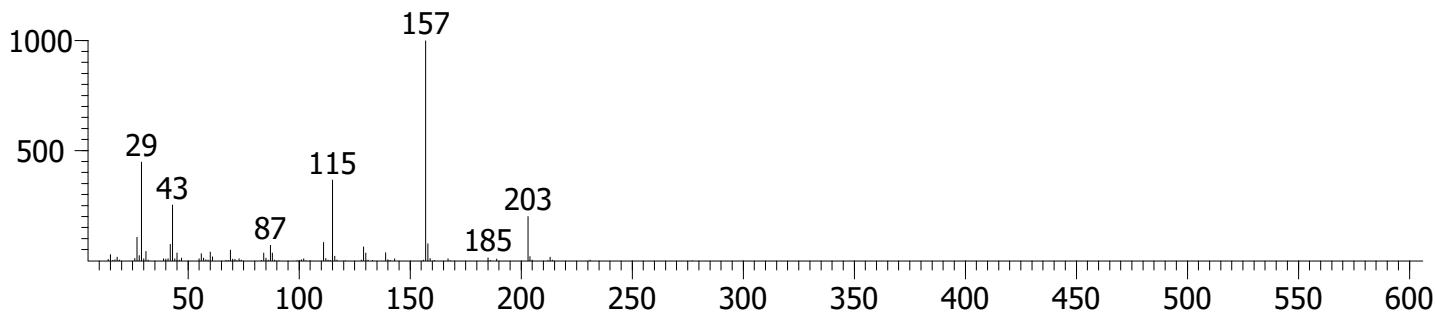
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2029, at 1438.45 , 1.835 sec , sec (Spec # 1454 98)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2029, at 1438.45 , 1.835 sec , sec (Spec # 1454 98)



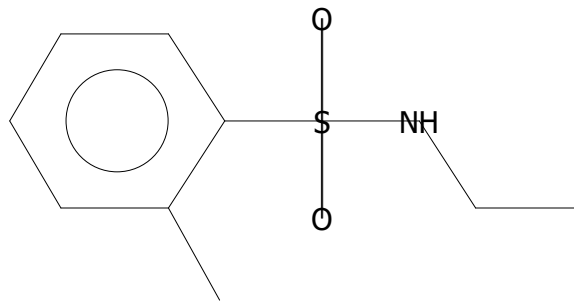
Library Hit - similarity 907, "Triethyl citrate"



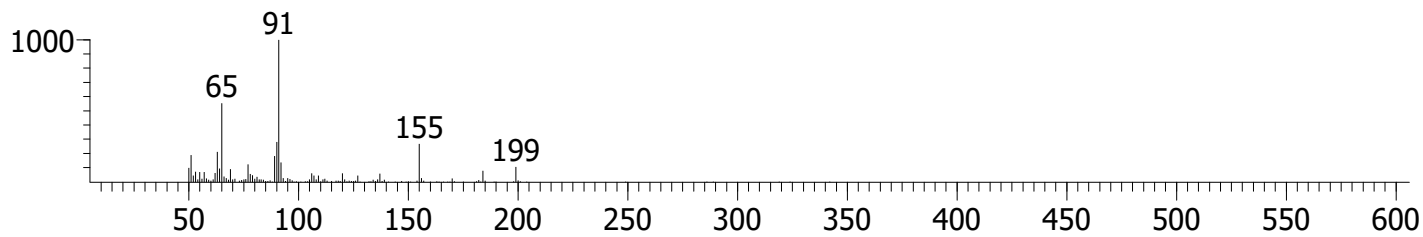
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Triethyl citrate	907	9558	77-93-0	mainlib	C12H20O7	276
2	à-l-Mannopyranose, 6-deoxy-, tetraacetate	743	231	27821-11-0	mainlib	C14H20O9	332
3	Glutaric acid, 2-methylpent-3-yl propyl ester	713	64	0-00-0	mainlib	C14H26O4	258
4	Glutaric acid, 4-heptyl propyl ester	708	51	0-00-0	mainlib	C15H28O4	272
5	Glutaric acid, 2-octyl propyl ester	673	13	0-00-0	mainlib	C16H30O4	286

Benzenesulfonamide, N-ethyl-2-methyl-

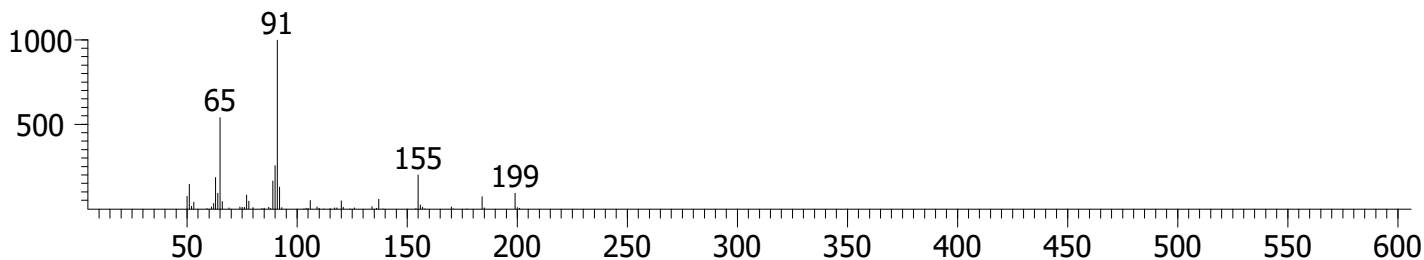
1st Dimension R.T. = 1455.94
2nd Dimension R.T. = 2.376
Quant Mass(es) = 91
S/N = 816.60
Area = 340473
Height = 31371
Similarity = 800



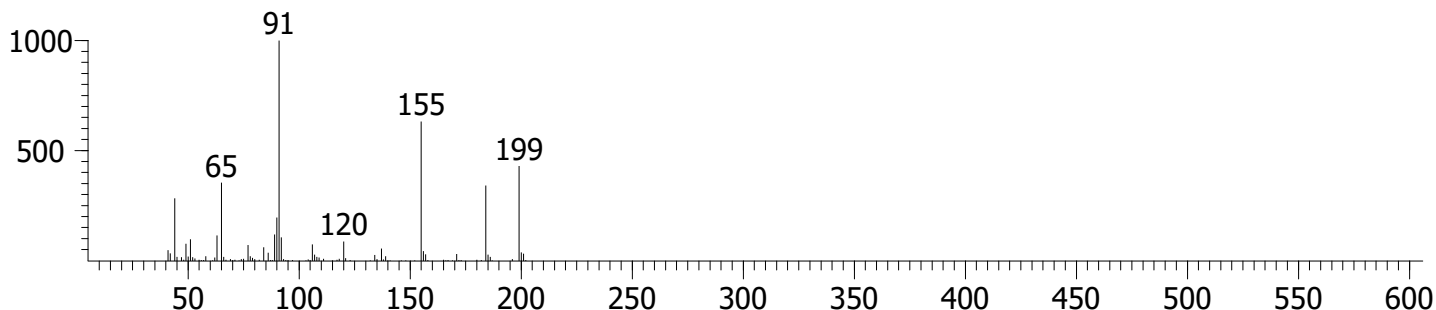
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2065, at 1455.94 , 2.376 sec , sec (Spec # 1482 30)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2065, at 1455.94 , 2.376 sec , sec (Spec # 1482 30)



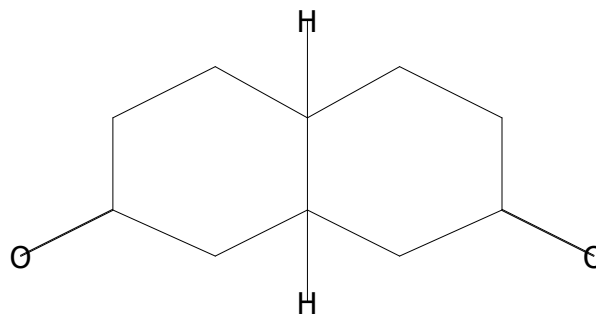
Library Hit - similarity 800, "Benzenesulfonamide, N-ethyl-2-methyl-"



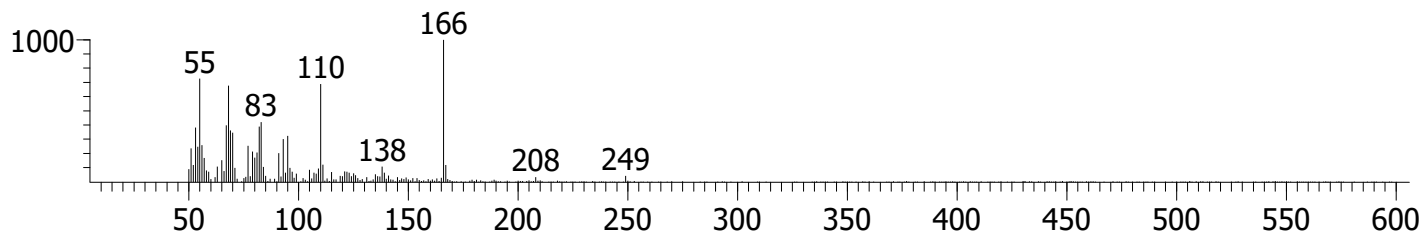
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenesulfonamide, N-ethyl-2-methyl-	800	2512	1077-56-1	mainlib	C9H13NO2S	199
2	p-Toluenesulfonylacetonitrile	787	1622	5697-44-9	mainlib	C9H9NO2S	195
3	2-(Toluene-4-sulfonyloxy)propionic acid	773	1015	0-00-0	mainlib	C10H12O5S	244
4	Benzenesulfonyl chloride, 2-methyl-	756	554	133-59-5	mainlib	C7H7ClO2S	190
5	4-Methyl-N-[2-(3-nitro-[1,2,4]triazol-1-yl)-ethyl]-benzenesulfonamide	745	380	0-00-0	mainlib	C11H13N5O4S	311

2,7(1H,3H)-Naphthalenedione, hexahydro-

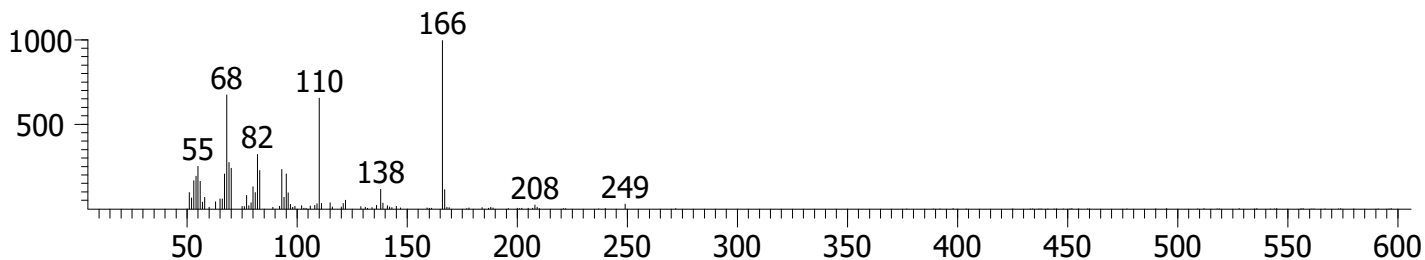
1st Dimension R.T. = 1462.94
2nd Dimension R.T. = 1.874
Quant Mass(es) = 166
S/N = 617.91
Area = 83103
Height = 9824.8
Similarity = 762



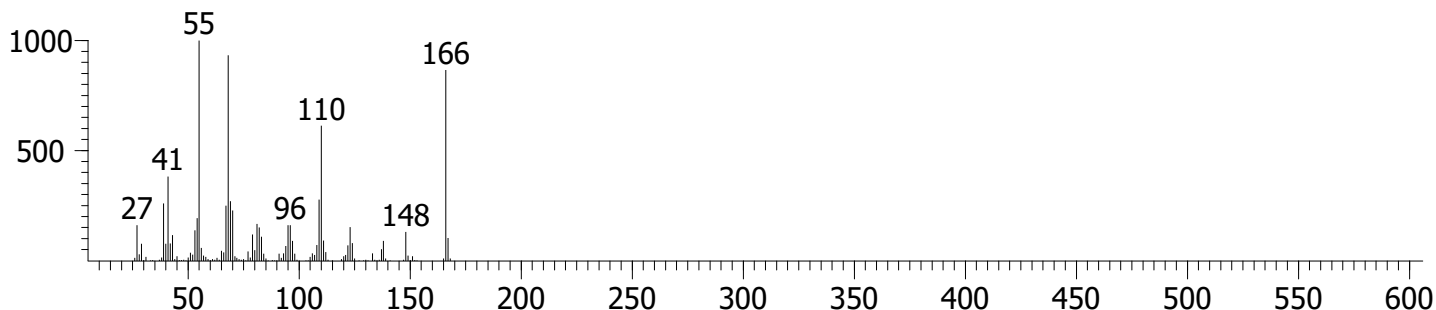
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2078, at 1462.94 , 1.874 sec , sec (Spec # 1492 14)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2078, at 1462.94 , 1.874 sec , sec (Spec # 1492 14)



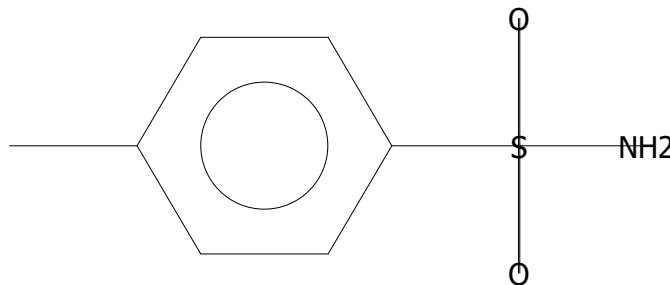
Library Hit - similarity 762, "2,7(1H,3H)-Naphthalenedione, hexahydro-"



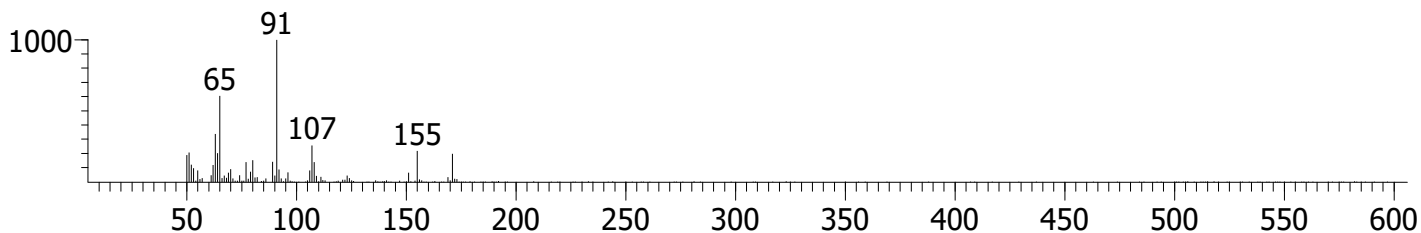
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,7(1H,3H)-Naphthalenedione, hexahydro-	762	3941	46048-64-0	mainlib	C10H14O2	166
2	3,6-Diazahomoadamantan-9-one	715	824	126126-45-2	mainlib	C9H14N2O	166
3	11-Oxadispiro[4.0.4.1]undecan-1-one	698	450	36803-49-3	mainlib	C10H14O2	166
4	3,5-Dibutylhexahydro-1H-pyrrolizine	695	397	150044-83-0	mainlib	C15H29N	223
5	(1R,4R,9aS)-1-Ethyl-4-(pent-4-en-1-yl)octahydro-1H-quinolizine	684	272	957792-07-3	mainlib	C16H29N	235

Benzenesulfonamide, 4-methyl-

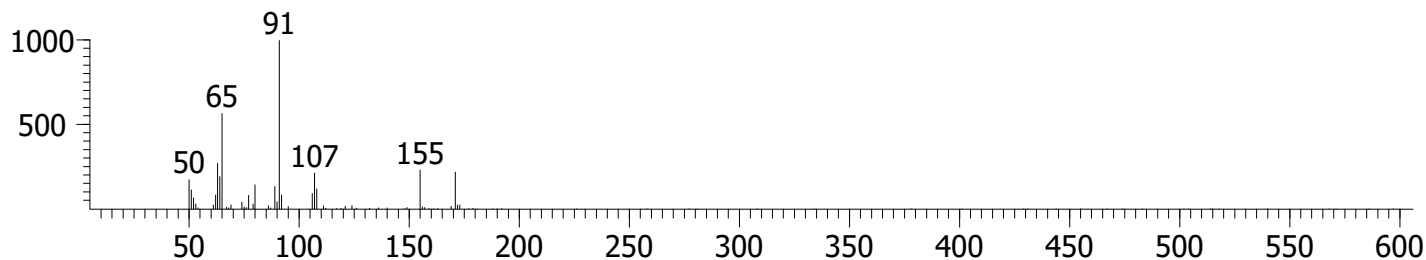
1st Dimension R.T. = 1476.93
2nd Dimension R.T. = 2.633
Quant Mass(es) = 171
S/N = 213.15
Area = 43637
Height = 3786.4
Similarity = 848



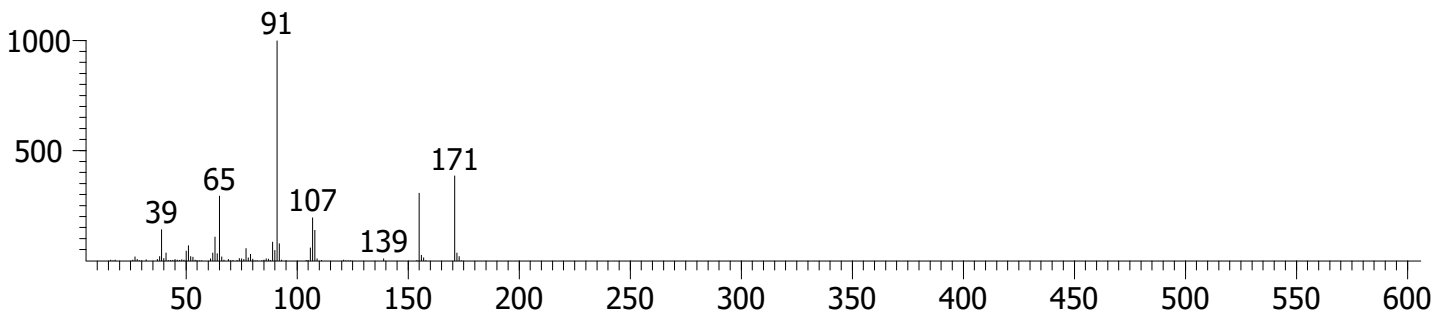
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2120, at 1476.93 , 2.633 sec , sec (Spec # 1514 49)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2120, at 1476.93 , 2.633 sec , sec (Spec # 1514 49)



Library Hit - similarity 848, "Benzenesulfonamide, 4-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	O-p-toluenesulfonyl-N-acetylserine, methyl ester	888	5431	0-00-0	mainlib	C13H17NO6S	315
2	N-p-toluenesulfonyl-L-threonine, benzyl ester	866	2147	0-00-0	mainlib	C18H21NO5S	363
3	Benzenesulfonamide, 4-methyl-	848	1107	70-55-3	mainlib	C7H9NO2S	171
4	Thiosulfuric acid, S-[2-[3-(4-methylbenzenesulfonamido)propionamidino]ethyl] ester	844	935	0-00-0	mainlib	C12H19N3O5S3	381
5	N3, Nà-bis*(ptoluenesulfonyl)histidineamide	799	199	0-00-0	mainlib	C20H22N4O5S2	462

Tri(2-chloroethyl) phosphate

1st Dimension R.T. = 1560.88

2nd Dimension R.T. = 2.237

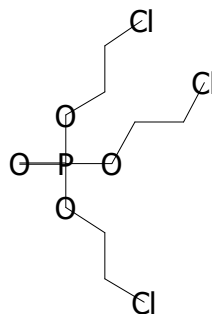
Quant Mass(es) = 63

S/N = 2556.4

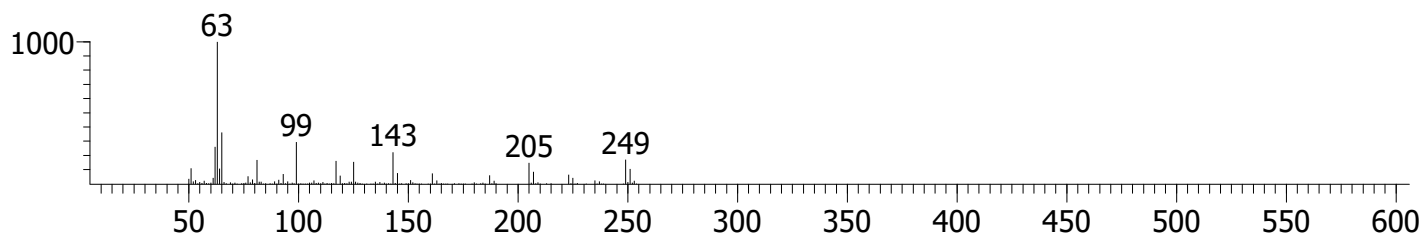
Area = 863582

Height = 71990

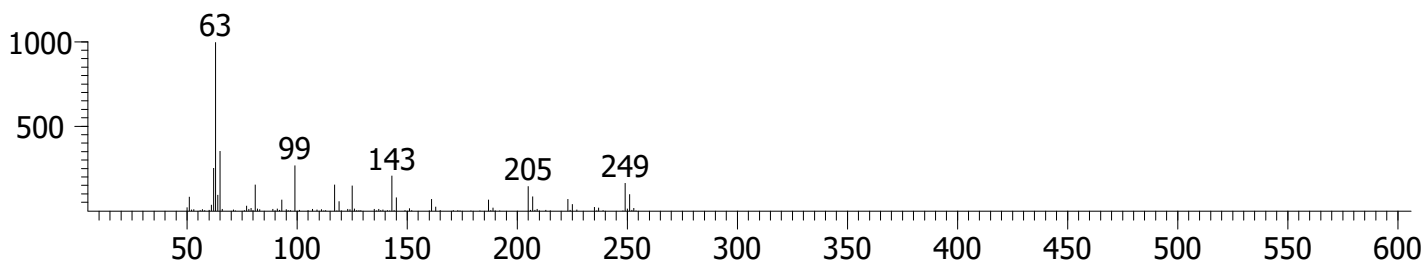
Similarity = 907



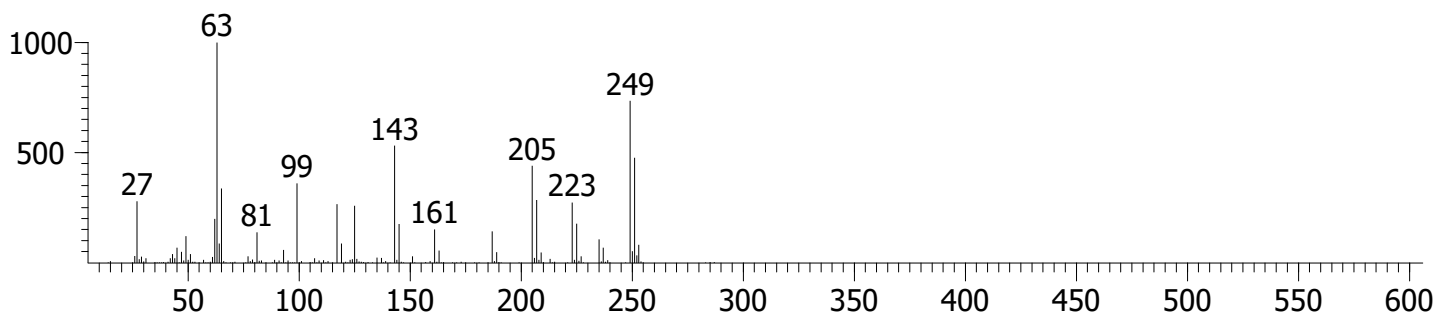
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2310, at 1560.88 , 2.237 sec , sec (Spec # 1641 09)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2310, at 1560.88 , 2.237 sec , sec (Spec # 1641 09)



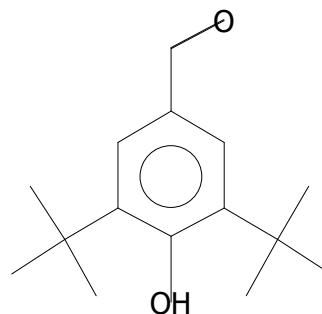
Library Hit - similarity 907, "Tri(2-chloroethyl) phosphate"



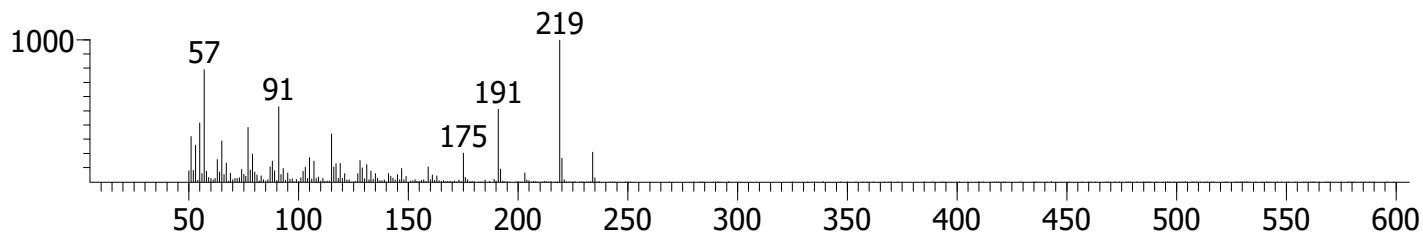
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Tri(2-chloroethyl) phosphate	907	9880	115-96-8	mainlib	C6H12Cl3O4P	284
2	Phosphoric acid, 1,2-ethanediyl tetrakis(2-chloroethyl) ester	666	98	33125-86-9	mainlib	C10H20Cl4O8P2	470
3	2-(2-Chloroethoxy)ethyl bis(2-chloroethyl) phosphate	602	16	137888-36-9	mainlib	C8H16Cl3O5P	328
4	1-Chloroethyl sulfone	525	1	10038-07-0	mainlib	C4H8Cl2O2S	190
5	4-Bromo-3-chloroacetanilide	463	0	22459-81-0	mainlib	C8H7BrClNO	247

3,5-di-tert-Butyl-4-hydroxybenzaldehyde

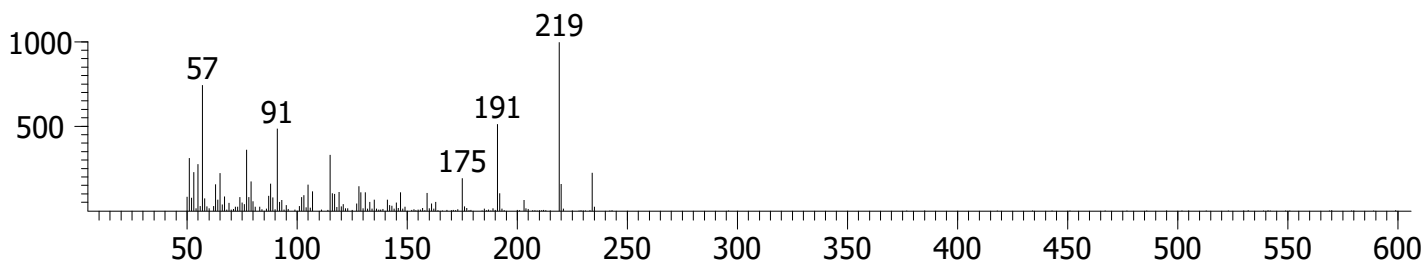
1st Dimension R.T. = 1567.88
2nd Dimension R.T. = 1.789
Quant Mass(es) = 219
S/N = 1732.2
Area = 116008
Height = 13254
Similarity = 876



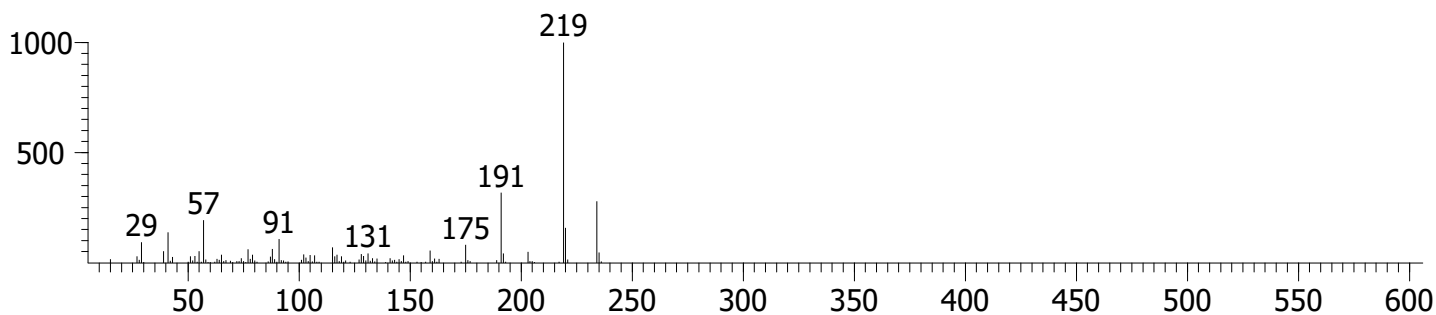
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2321, at 1567.88 , 1.789 sec , sec (Spec # 1651 01)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2321, at 1567.88 , 1.789 sec , sec (Spec # 1651 01)



Library Hit - similarity 876, "3,5-di-tert-Butyl-4-hydroxybenzaldehyde"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	876	7274	1620-98-0	mainlib	C15H22O2	234
2	2,3,5,6-Detetrahydrocyclohexanone, 2,6-di-t-butyl-4-hydroxymethylene-	850	2179	101100-38-3	mainlib	C15H22O2	234
3	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-	789	379	4130-42-1	mainlib	C16H26O	234
4	3,5-Di-tert-butylbenzoic acid	764	115	16225-26-6	mainlib	C15H22O2	234
5	3,5-Di-tert-butyl-2-hydroxybenzaldehyde	707	21	37942-07-7	mainlib	C15H22O2	234

Benzyl Benzoate

1st Dimension R.T. = 1571.38

2nd Dimension R.T. = 2.119

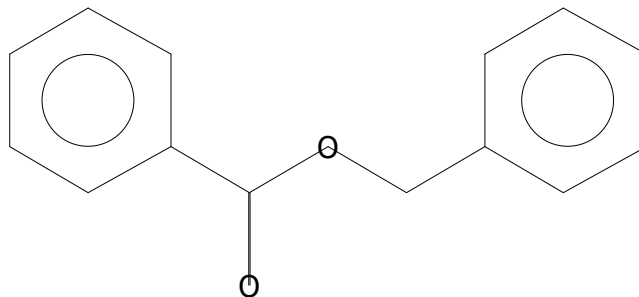
Quant Mass(es) = 105

S/N = 252.15

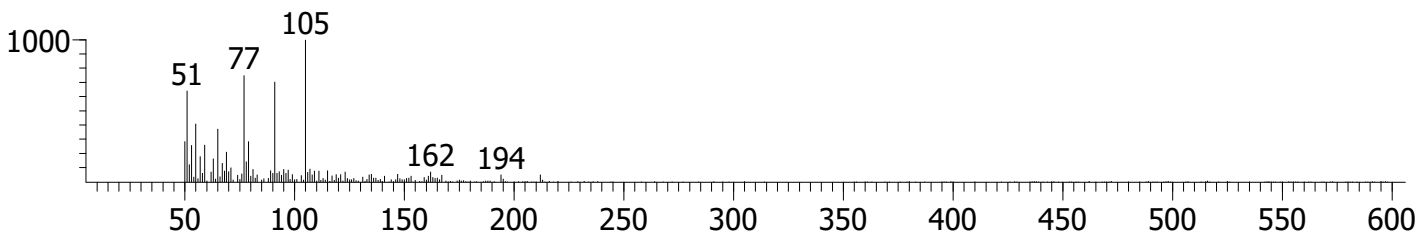
Area = 87748

Height = 7129.9

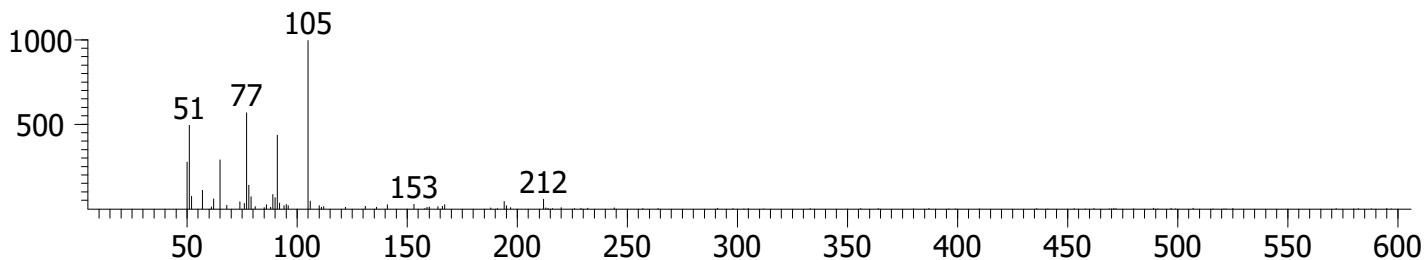
Similarity = 849



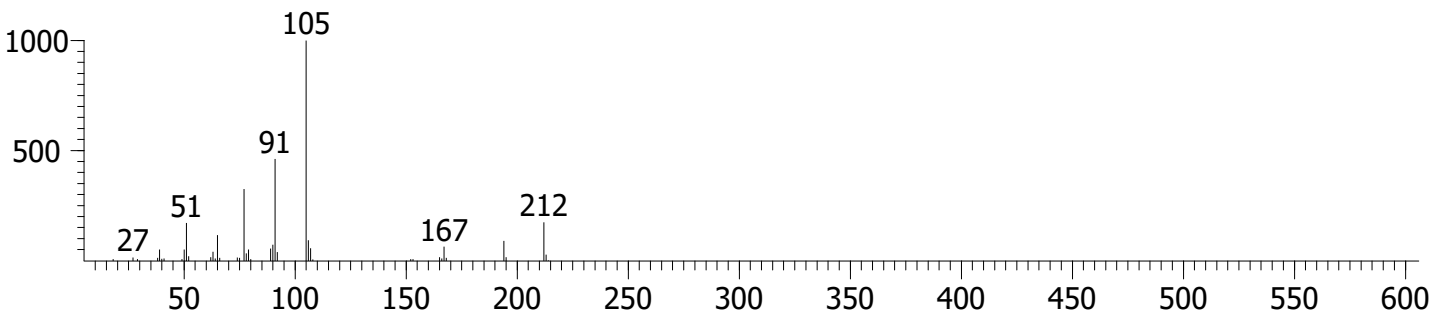
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2331, at 1571.38 , 2.119 sec , sec (Spec # 1656 81)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2331, at 1571.38 , 2.119 sec , sec (Spec # 1656 81)



Library Hit - similarity 849, "Benzyl Benzoate"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzyl Benzoate	849	4021	120-51-4	mainlib	C14H12O2	212
2	Ethanone, 1-phenyl-2-(4H-1,2,4-triazol-3-ylthio)-	777	560	32189-00-7	mainlib	C10H9N3OS	219
3	Acetic acid, 2-benzoylthio-, 2-oxo-2-phenylethyl ester	773	473	0-00-0	mainlib	C17H14O4S	314
4	Ethanone, 2-bromo-1-phenyl-	772	454	70-11-1	mainlib	C8H7BrO	198
5	7-Benzoyloxybicyclo[2.2.1]hepta-2,5-diene	765	348	4796-68-3	mainlib	C14H12O2	212

2-Propanol, 1-chloro-, phosphate (3:1)

1st Dimension R.T. = 1599.36

2nd Dimension R.T. = 1.947

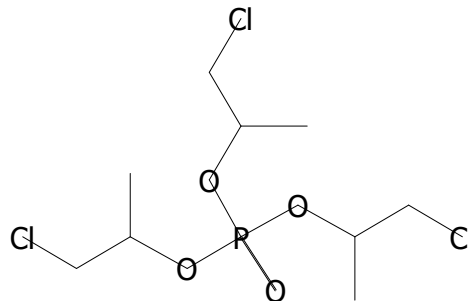
Quant Mass(es) = 99

S/N = 5564.6

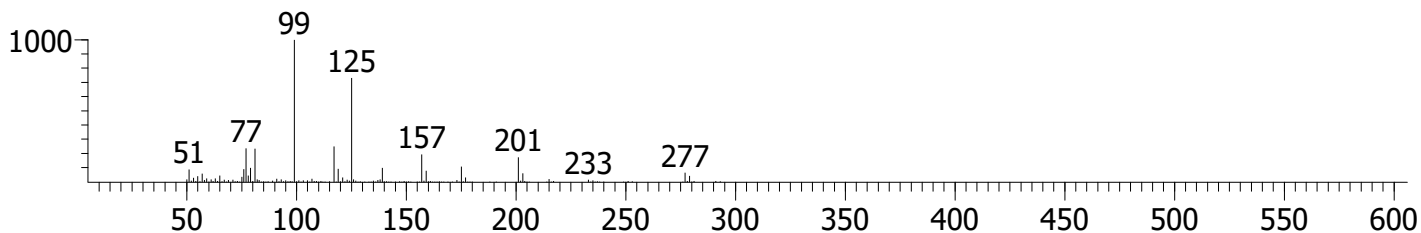
Area = 1289369

Height = 120801

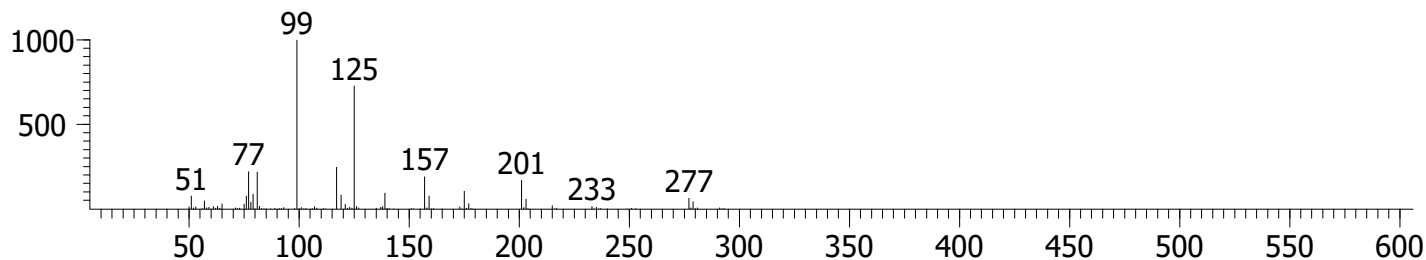
Similarity = 779



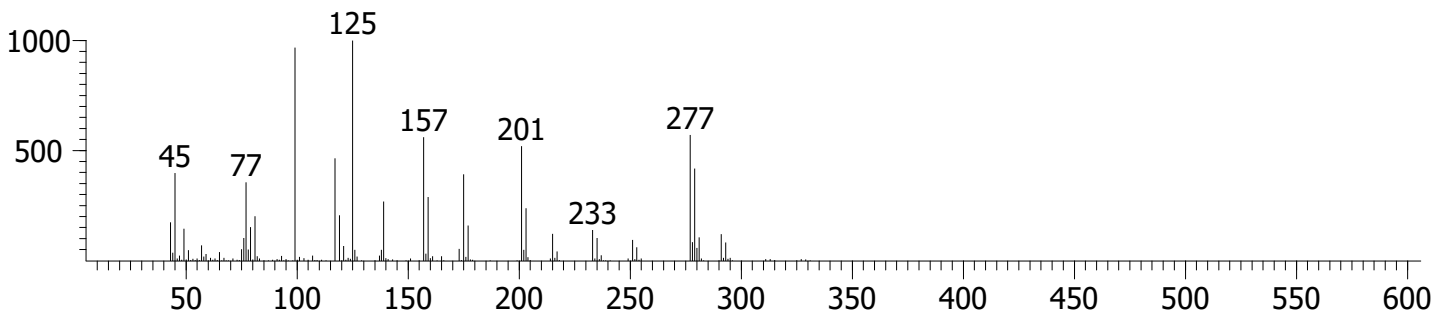
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2390, at 1599.36 , 1.947 sec , sec (Spec # 1698 95)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2390, at 1599.36 , 1.947 sec , sec (Spec # 1698 95)

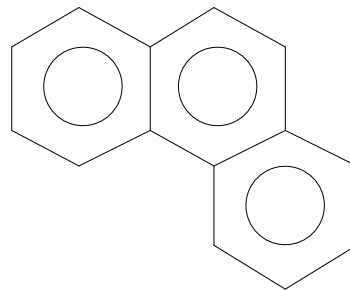


Library Hit - similarity 779, "2-Propanol, 1-chloro-, phosphate (3:1)"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Propanol, 1-chloro-, phosphate (3:1)	779	4654	13674-84-5	mainlib	C9H18Cl3O4P	326
2	Bis(1-chloro-2-propyl)(3-chloro-1-propyl)phosphate	776	4112	137909-40-1	mainlib	C9H18Cl3O4P	326
3	Bis(3-chloro-1-propyl)(1-chloro-2-propyl)phosphate	718	757	137888-35-8	mainlib	C9H18Cl3O4P	326
4	Tris(3-chloropropyl) phosphate	702	436	1067-98-7	mainlib	C9H18Cl3O4P	326
5	2-Butyl methylphosphonofluoridate	589	26	352-52-3	mainlib	C5H12FO2P	154

Phenanthrene



1st Dimension R.T. = 1599.36

2nd Dimension R.T. = 2.284

Quant Mass(es) = 178

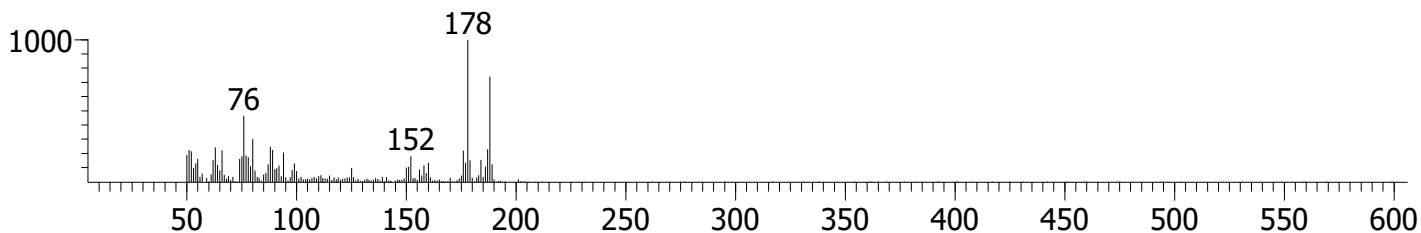
S/N = 1514.5

Area = 231887

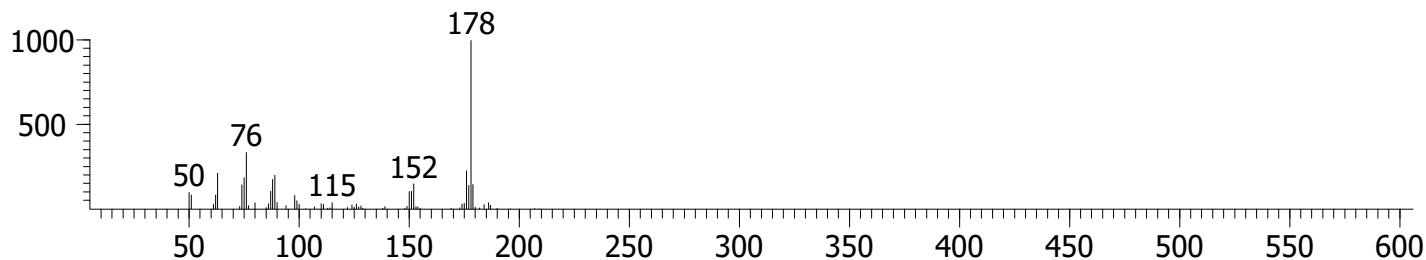
Height = 21763

Similarity = 952

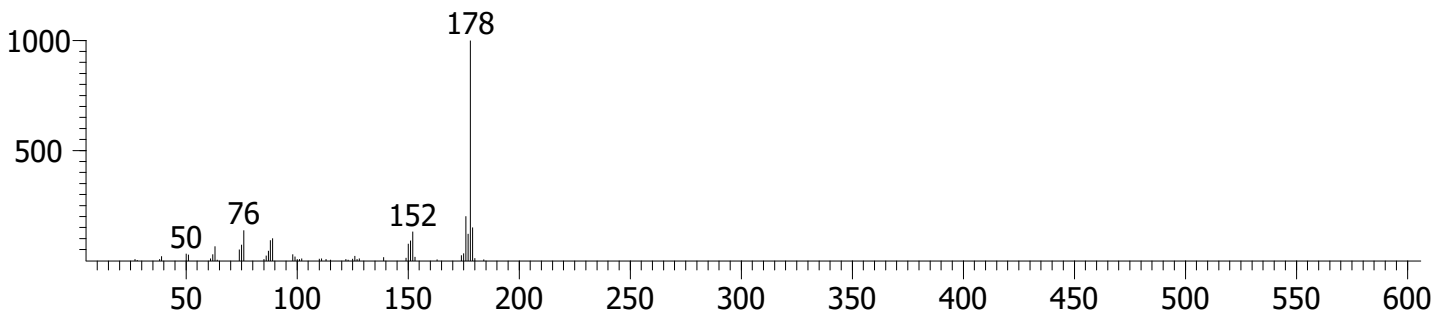
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2394, at 1599.36 , 2.284 sec , sec (Spec # 1699 46)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2394, at 1599.36 , 2.284 sec , sec (Spec # 1699 46)



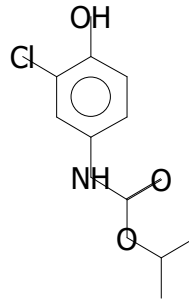
Library Hit - similarity 952, "Phenanthrene"



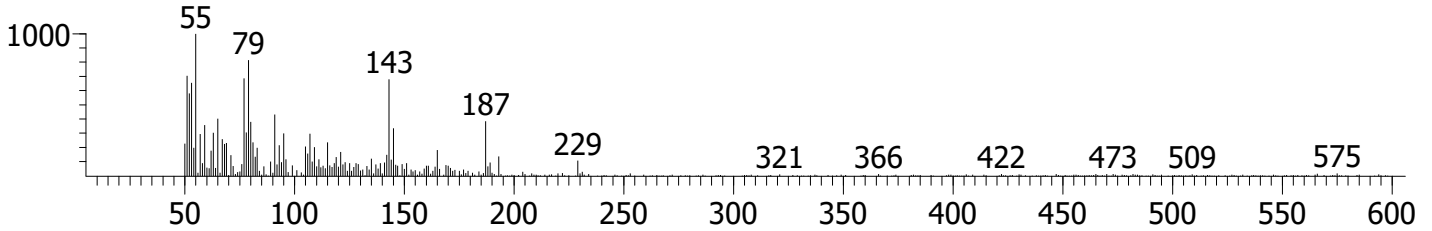
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenanthrene	952	5659	85-01-8	mainlib	C14H10	178
2	9H-Fluorene, 9-methylene-	915	1377	4425-82-5	mainlib	C14H10	178
3	2-Biphenylacetylene	904	944	52889-62-0	mainlib	C14H10	178
4	Anthracene	880	316	120-12-7	mainlib	C14H10	178
5	7,8-Diphenylbicyclo[4.2.1]nona-2,4,7-triene	877	279	54049-09-1	mainlib	C21H18	270

Carbamic acid,
(3-chloro-4-hydroxyphenyl)-, 1-methylethyl

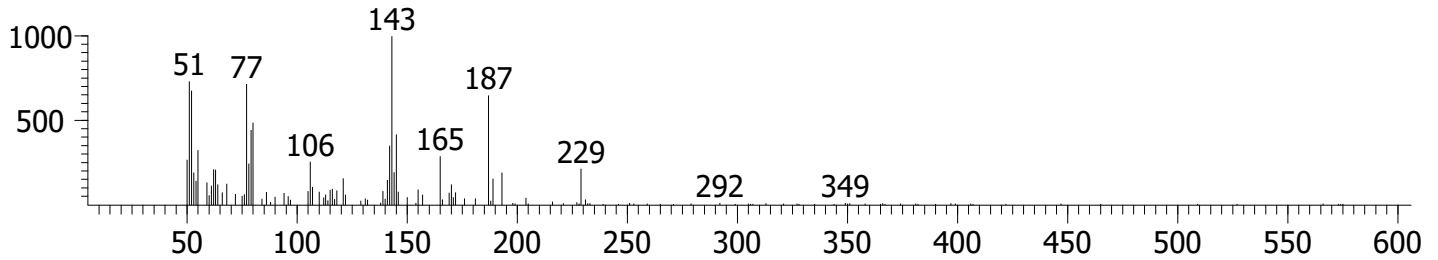
1st Dimension R.T. = 1606.36
2nd Dimension R.T. = 2.033
Quant Mass(es) = 143
S/N = 111.77
Area = 21691
Height = 2016.0
Similarity = 613



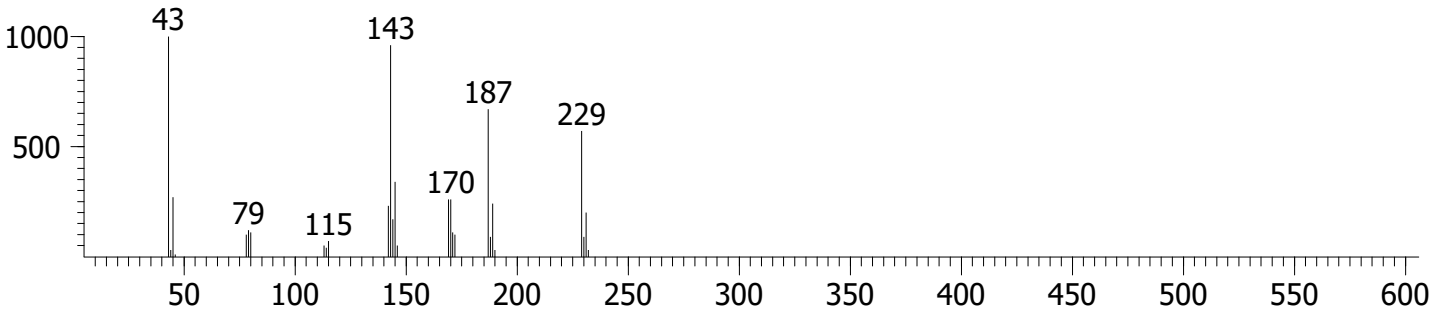
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2407, at 1606.36 , 2.033 sec , sec (Spec # 1709 68)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2407, at 1606.36 , 2.033 sec , sec (Spec # 1709 68)



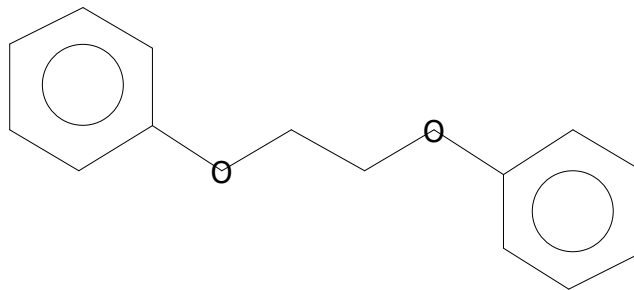
Library Hit - similarity 613, "Carbamic acid, (3-chloro-4-hydroxyphenyl)-, 1-methylethyl ester"



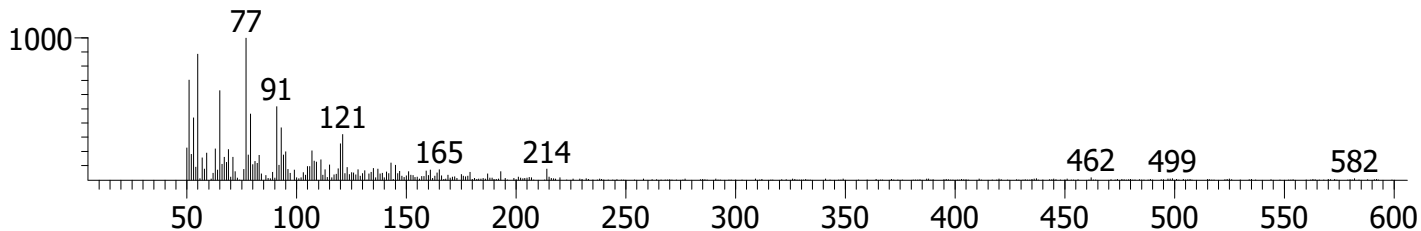
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Carbamic acid, (3-chloro-4-hydroxyphenyl)-, 1-methylethyl ester	613	3761	28705-96-6	mainlib	C10H12ClNO3	229
2	Cyclohex-3-en-2-one-1-carboxylic acid, 3-chloro-1-methyl-, methyl ester	601	2505	0-00-0	mainlib	C9H11ClO3	202
3	Carbamic acid, (5-chloro-2-hydroxyphenyl)-, 1-methylethyl ester	548	495	27898-06-2	mainlib	C10H12ClNO3	229
4	Carbamic acid, (3-chloro-5-hydroxyphenyl)-, 1-methylethyl ester	537	339	34061-87-5	mainlib	C10H12ClNO3	229
5	acetamide, N-(3-chloro-4-hydroxyphenyl)-	534	300	0-00-0	mainlib	C8H8ClNO2	185

Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-

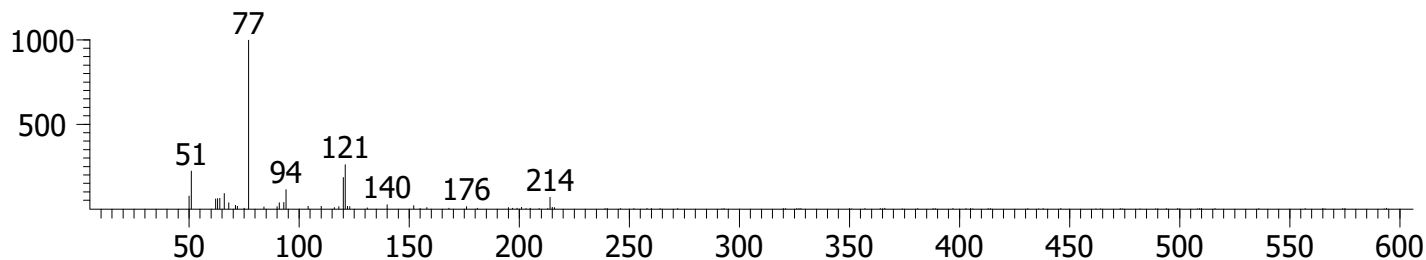
1st Dimension R.T. = 1606.36
2nd Dimension R.T. = 2.079
Quant Mass(es) = 214
S/N = 63.990
Area = 2233.7
Height = 259.51
Similarity = 718



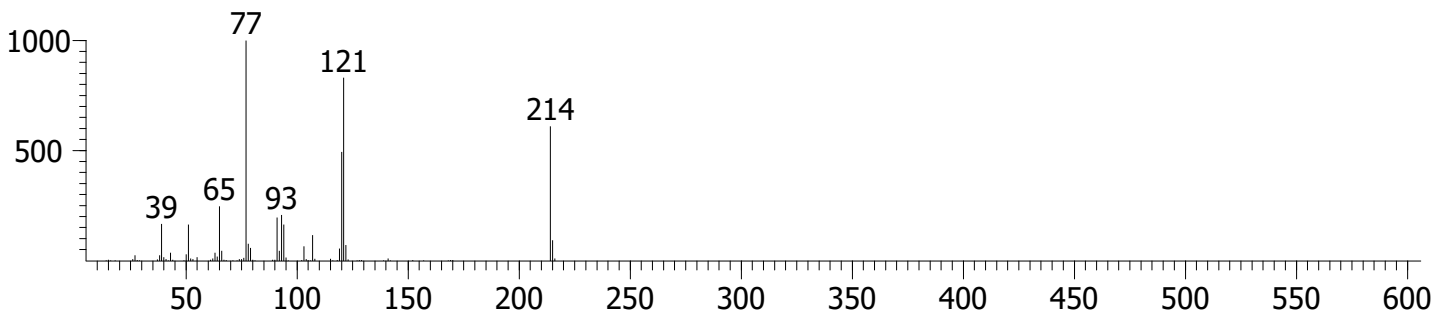
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2408, at 1606.36 , 2.079 sec , sec (Spec # 1709 75)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2408, at 1606.36 , 2.079 sec , sec (Spec # 1709 75)



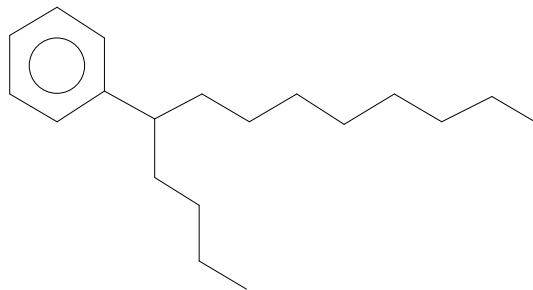
Library Hit - similarity 718, "Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-"



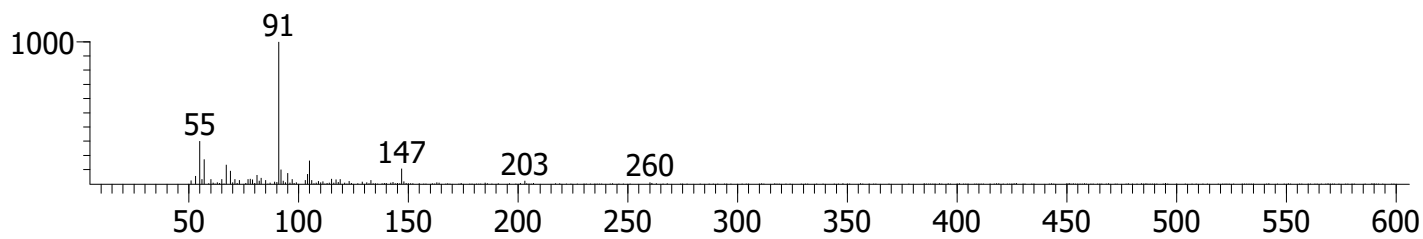
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-	718	6204	104-66-5	mainlib	C ₁₄ H ₁₄ O ₂	214
2	Propanoyl chloride, 2-phenoxy-	679	1462	122-35-0	mainlib	C ₉ H ₉ ClO ₂	184
3	6-(Dimethylamino)fulvene	659	666	696-68-4	mainlib	C ₈ H ₁₁ N	121
4	Chloroacetic acid, 4-methoxybenzyl ester	645	417	164011-15-8	mainlib	C ₁₀ H ₁₁ ClO ₃	214
5	Benzene, 1,1'-[oxybis(2,1-ethanediyloxy-2,1-ethanediyloxy)]bis-	637	311	20768-77-8	mainlib	C ₂₀ H ₂₆ O ₅	346

Benzene, (1-butylonyl)-

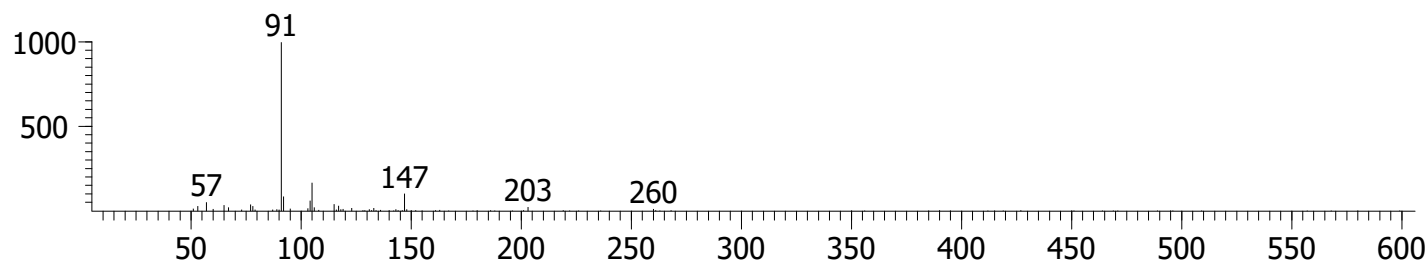
1st Dimension R.T. = 1623.85
2nd Dimension R.T. = 1.386
Quant Mass(es) = 91
S/N = 210.50
Area = 66469
Height = 8641.0
Similarity = 895



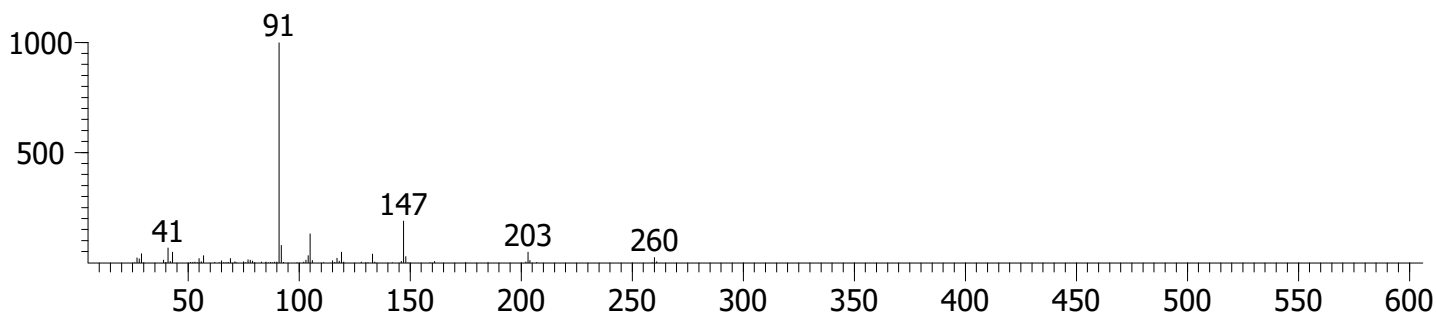
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2439, at 1623.85 , 1.386 sec , sec (Spec # 1735 20)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2439, at 1623.85 , 1.386 sec , sec (Spec # 1735 20)



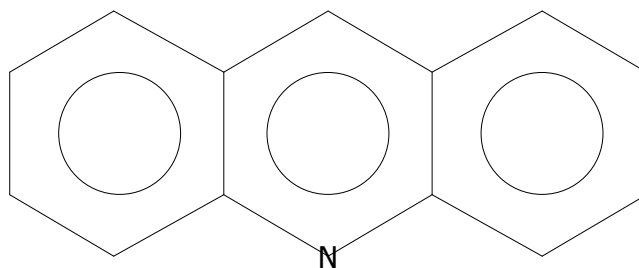
Library Hit - similarity 895, "Benzene, (1-butylonyl)-"



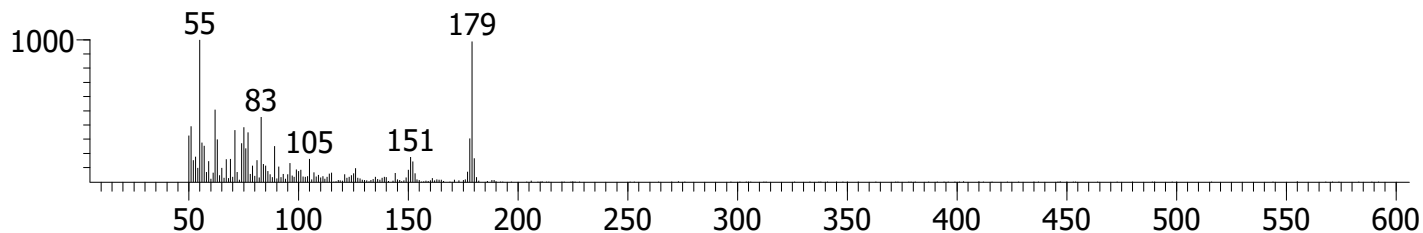
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, (1-butylonyl)-	895	4619	4534-50-3	mainlib	C19H32	260
2	Benzene, (1-butylheptyl)-	884	3168	4537-15-9	mainlib	C17H28	232
3	3-Benzoyl-8-oxo-6-azabicyclo[3.2.1]octan-6,7-dicarboxylic acid, dibenzyl ester	847	771	0-00-0	mainlib	C30H27NO6	497
4	Benzene, (3-iodo-2,2-dimethylpropyl)-	812	193	40548-64-9	mainlib	C11H15I	274
5	Hexanal benzyl hexyl acetal	810	178	0-00-0	mainlib	C19H32O2	292

Acridine

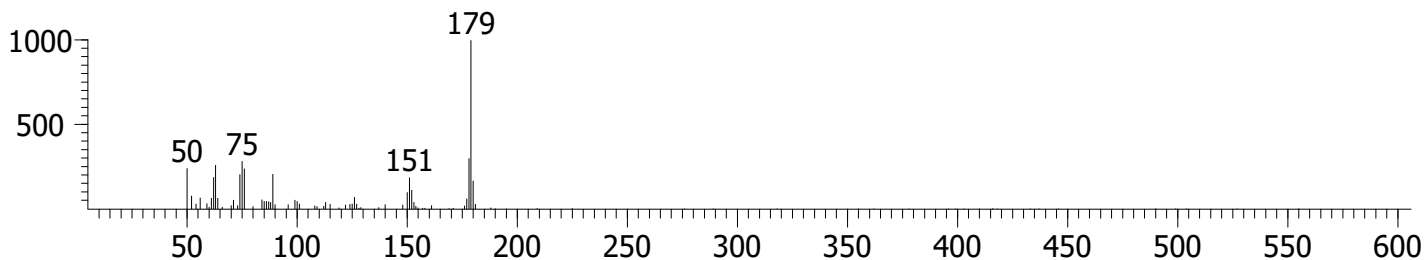
1st Dimension R.T. = 1623.85
2nd Dimension R.T. = 2.376
Quant Mass(es) = 179
S/N = 664.38
Area = 96327
Height = 8713.4
Similarity = 918



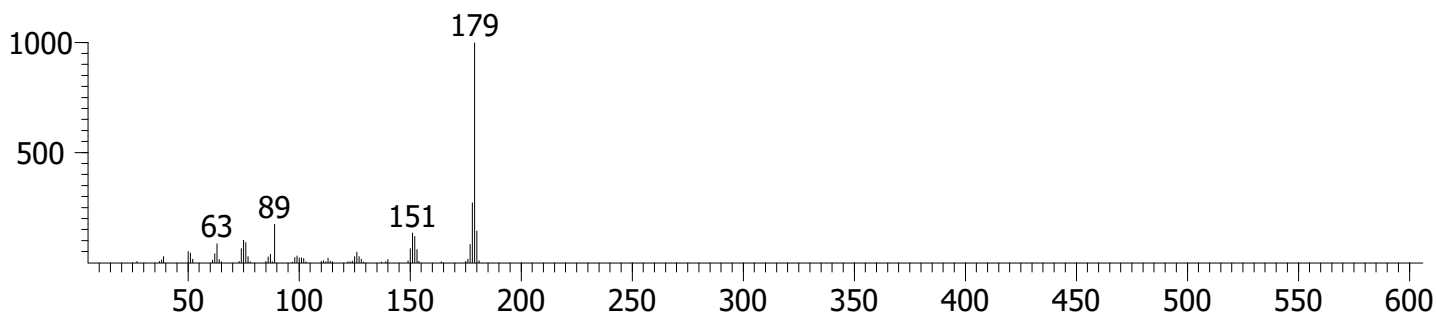
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2443, at 1623.85 , 2.376 sec , sec (Spec # 1736 70)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2443, at 1623.85 , 2.376 sec , sec (Spec # 1736 70)



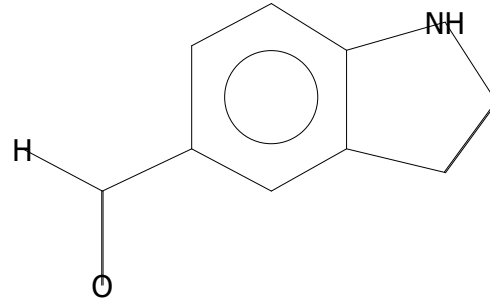
Library Hit - similarity 918, "Acridine"



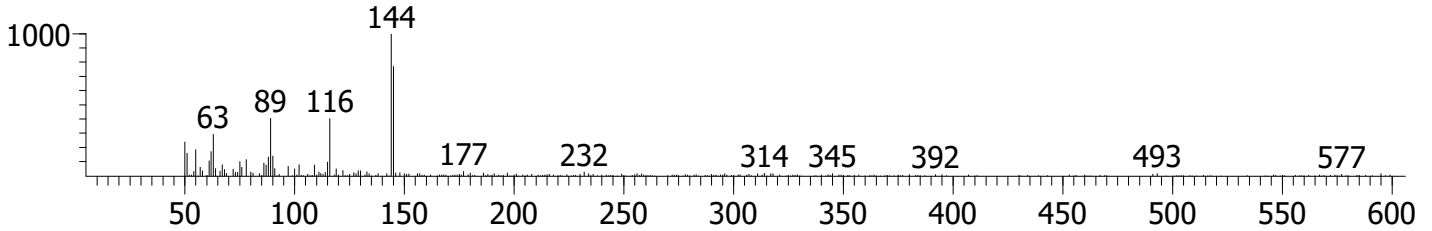
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Acridine	918	6103	260-94-6	mainlib	C13H9N	179
2	Benzo[f]quinoline	891	1795	85-02-9	mainlib	C13H9N	179
3	Phenanthridine	868	655	229-87-8	mainlib	C13H9N	179
4	p-Phenylbenzotrile	849	318	2920-38-9	mainlib	C13H9N	179
5	Benzo[h]quinoline	844	256	230-27-3	mainlib	C13H9N	179

Indole-5-aldehyde

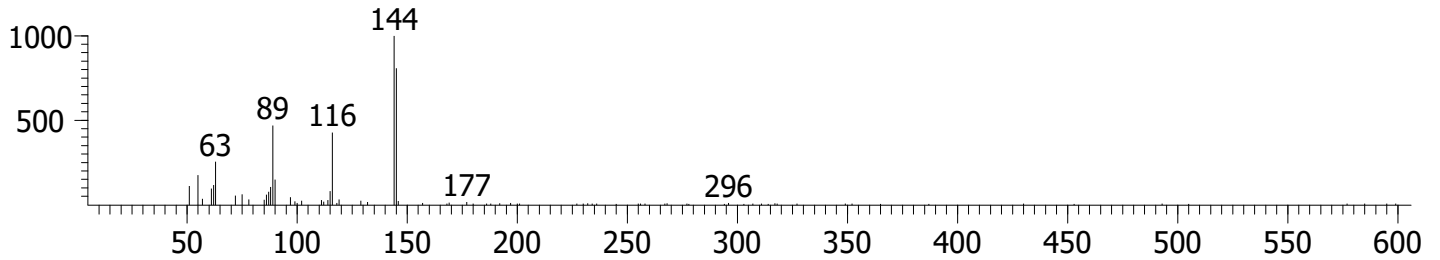
1st Dimension R.T. = 1634.34
2nd Dimension R.T. = 2.891
Quant Mass(es) = 144
S/N = 144.63
Area = 13349
Height = 1202.0
Similarity = 866



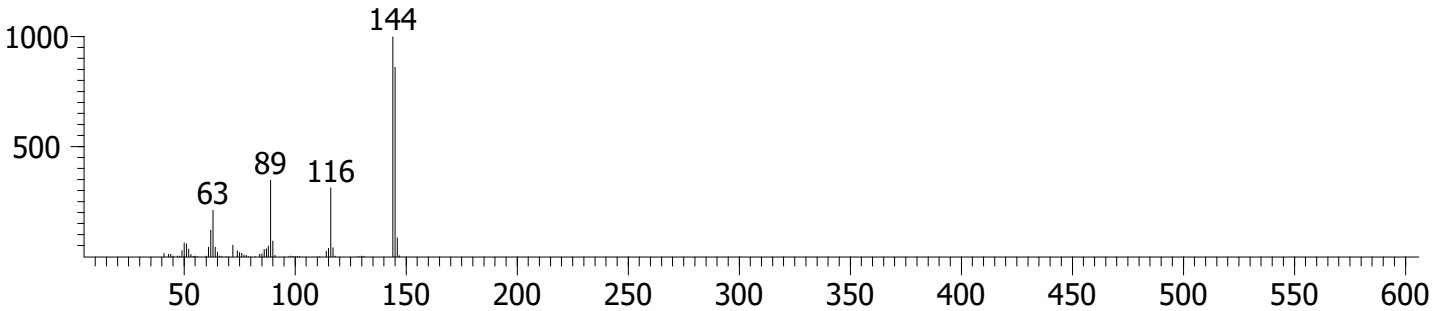
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2463, at 1634.34 , 2.891 sec , sec (Spec # 1753 38)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2463, at 1634.34 , 2.891 sec , sec (Spec # 1753 38)



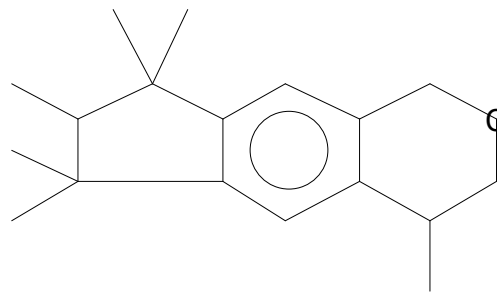
Library Hit - similarity 866, "Indole-5-aldehyde"



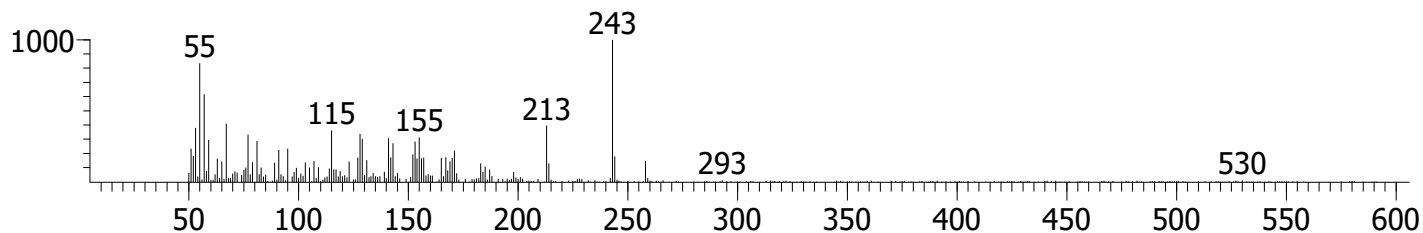
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Indole-5-aldehyde	866	3757	1196-69-6	mainlib	C9H7NO	145
2	Indole-6-carboxaldehyde	854	2502	1196-70-9	mainlib	C9H7NO	145
3	1H-Indole-3-carboxaldehyde	851	2211	487-89-8	mainlib	C9H7NO	145
4	Indole-7-carboxaldehyde	823	638	1074-88-0	mainlib	C9H7NO	145
5	1H-Indole-4-carboxaldehyde	807	367	1074-86-8	mainlib	C9H7NO	145

Cyclopenta[g]-2-benzopyran,
3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl

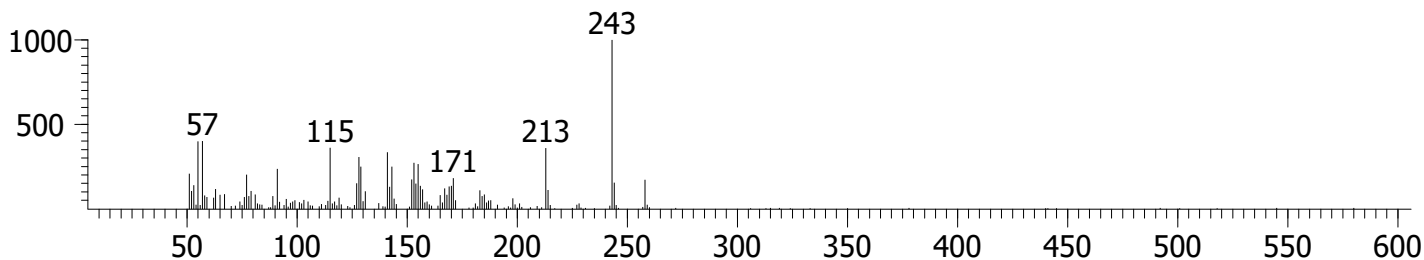
1st Dimension R.T. = 1658.83
2nd Dimension R.T. = 1.789
Quant Mass(es) = 243
S/N = 297.47
Area = 26691
Height = 3199.3
Similarity = 813



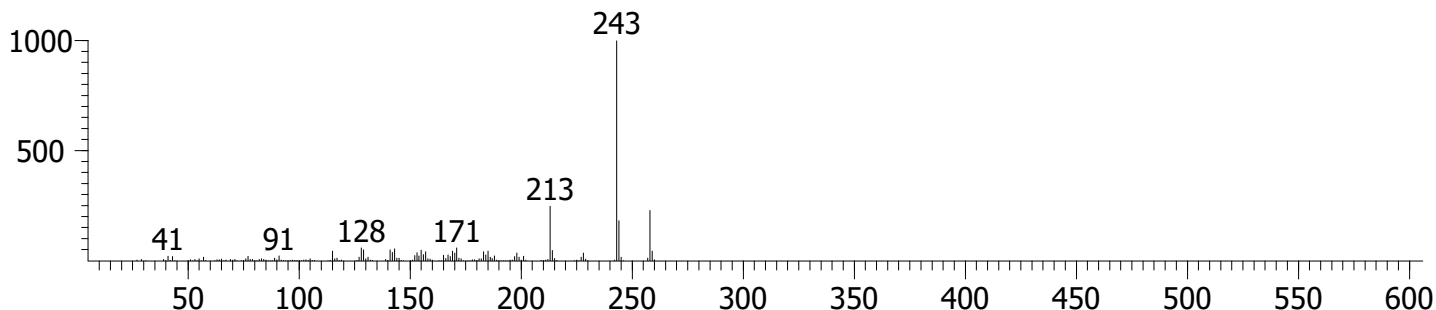
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2500, at 1658.83 , 1.789 sec , sec (Spec # 1788 81)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2500, at 1658.83 , 1.789 sec , sec (Spec # 1788 81)



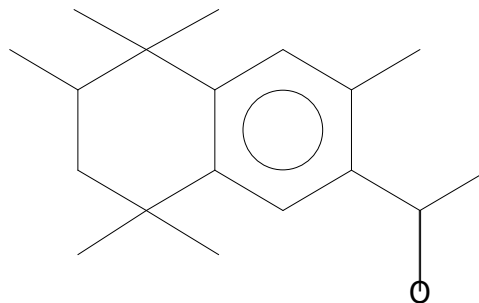
Library Hit - similarity 813, "Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-"



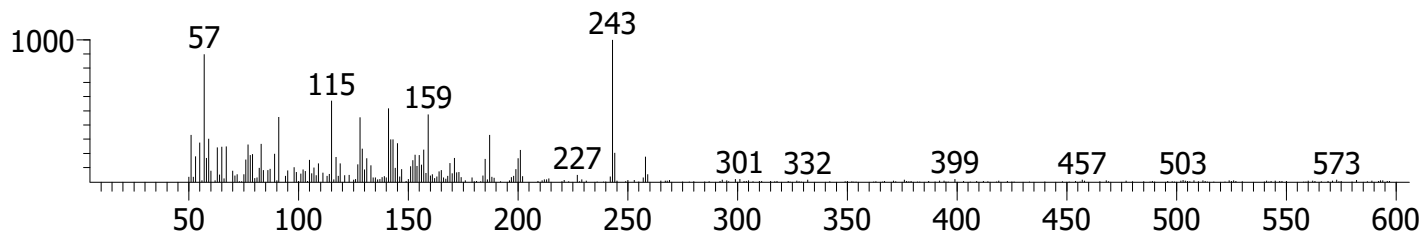
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	813	8535	1222-05-5	mainlib	C18H26O	258
2	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-, [1S-(1à,4aà,10aà)]-	694	460	57345-30-9	mainlib	C17H22O2	258
3	Pyrazole, 1,3-dimethyl-4-[2-(4-nitrophenyl)ethenyl]-	675	223	84547-52-4	mainlib	C13H13N3O2	243
4	7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	661	140	88-29-9	mainlib	C18H26O	258
5	5,8,11-Heptadecatriynoic acid, methyl ester	660	134	56554-57-5	mainlib	C18H24O2	272

Tonalid

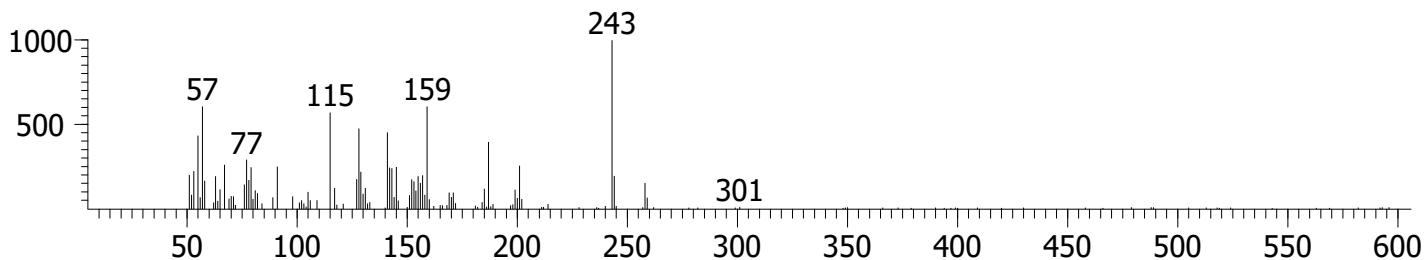
1st Dimension R.T. = 1669.32
 2nd Dimension R.T. = 1.742
 Quant Mass(es) = 243
 S/N = 195.33
 Area = 15685
 Height = 1833.3
 Similarity = 756



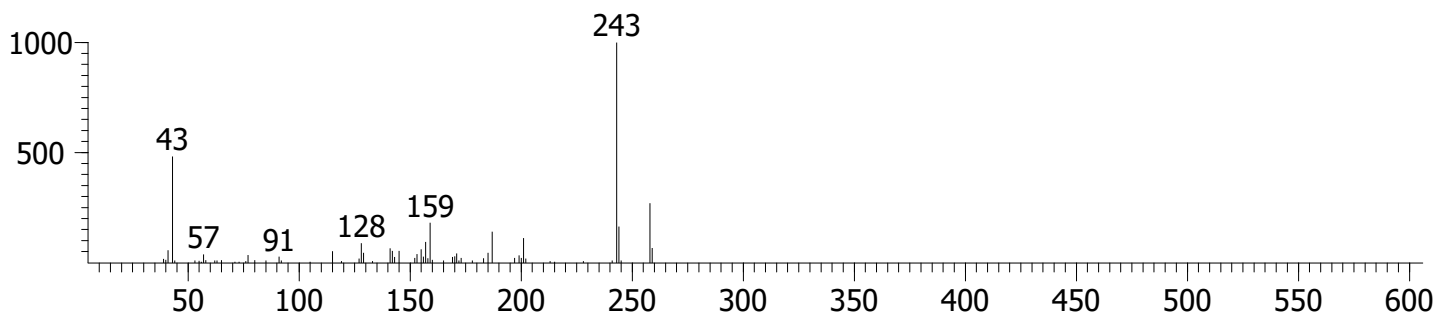
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2521, at 1669.32 , 1.742 sec , sec (Spec # 1804 64)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2521, at 1669.32 , 1.742 sec , sec (Spec # 1804 64)



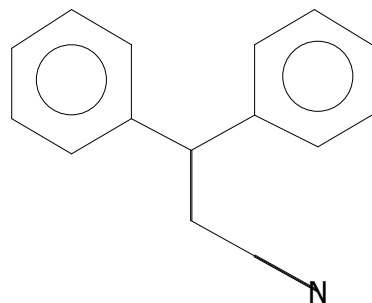
Library Hit - similarity 756, "Tonalid"



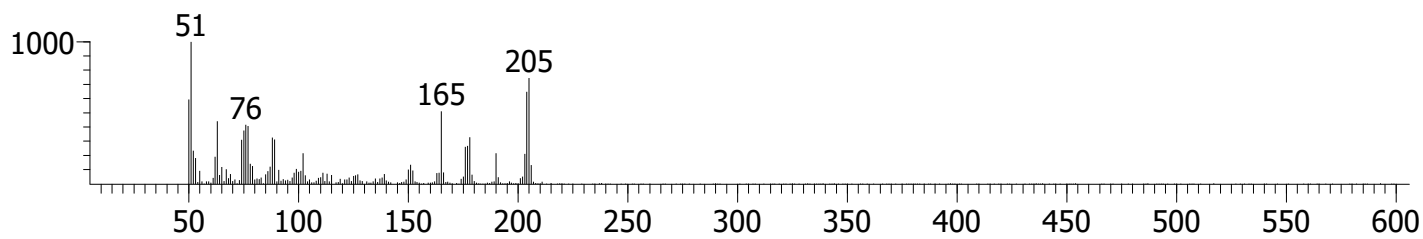
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Tonalid	756	7086	21145-77-7	mainlib	C18H26O	258
2	7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	720	1751	88-29-9	mainlib	C18H26O	258
3	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	667	346	1222-05-5	mainlib	C18H26O	258
4	5,8,11-Eicosatriynoic acid, methyl ester	641	103	0-00-0	mainlib	C21H30O2	314
5	Furo[2,3-H]coumarine, 2-(1-hydroxyethyl)-1,6-dimethyl-	635	81	350682-01-8	mainlib	C15H14O4	258

2-Propenenitrile, 3,3-diphenyl-

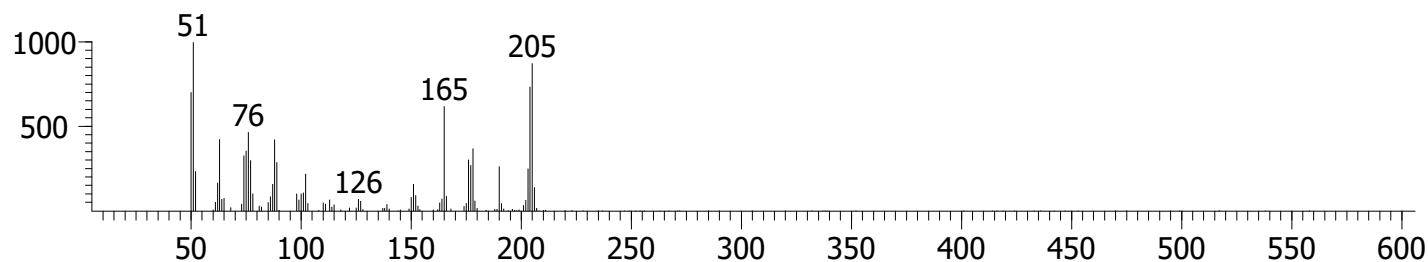
1st Dimension R.T. = 1683.31
2nd Dimension R.T. = 2.356
Quant Mass(es) = 204
S/N = 696.06
Area = 69511
Height = 6224.9
Similarity = 892



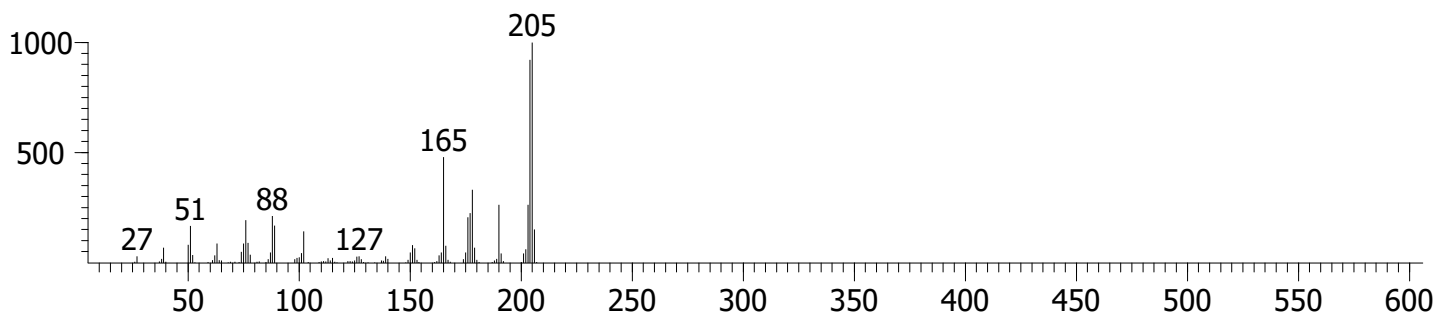
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2547, at 1683.31 , 2.356 sec , sec (Spec # 1826 77)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2547, at 1683.31 , 2.356 sec , sec (Spec # 1826 77)



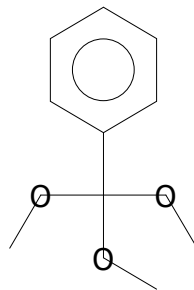
Library Hit - similarity 892, "2-Propenenitrile, 3,3-diphenyl-"



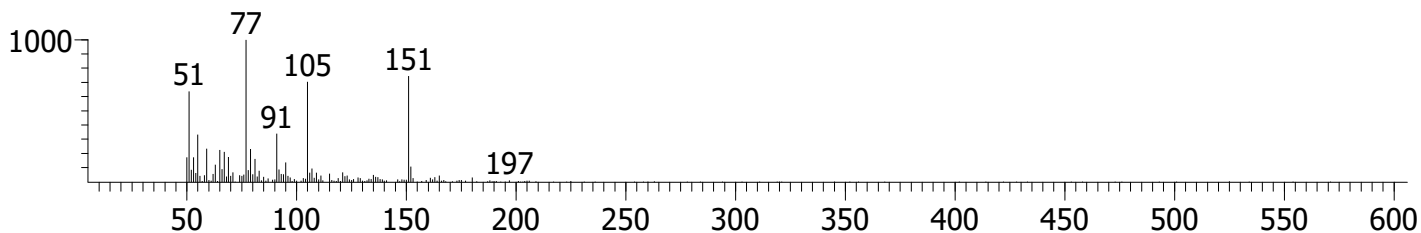
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Propenenitrile, 3,3-diphenyl-	892	7254	3531-24-6	mainlib	C15H11N	205
2	Benzeneacetonitrile, à-(phenylmethylene)-	839	1435	2510-95-4	mainlib	C15H11N	205
3	Benzonitrile, 4-(2-phenylethenyl)-	809	398	1552-58-5	mainlib	C15H11N	205
4	Benzene, 1,1'-(1-isocyano-1,2-ethenediyl)bis-, (Z)-	802	305	56701-14-5	mainlib	C15H11N	205
5	Benzonitrile, 3-(2-phenylethenyl)-, (E)-	791	209	14064-35-8	mainlib	C15H11N	205

Benzene, (trimethoxymethyl)-

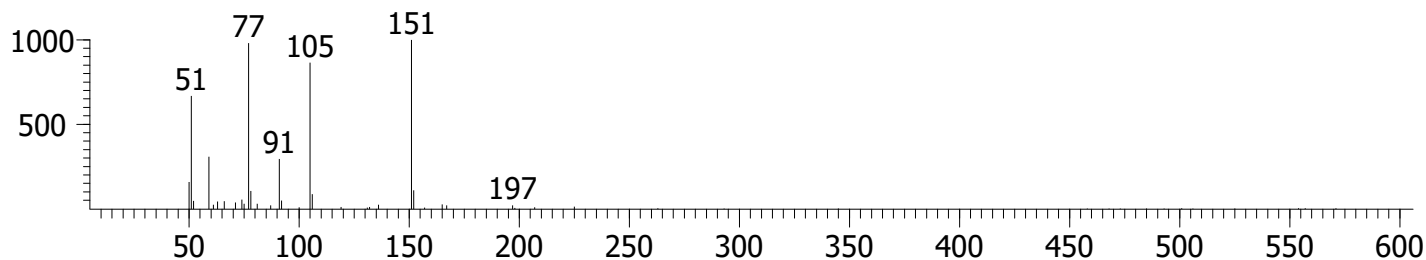
1st Dimension R.T. = 1690.31
2nd Dimension R.T. = 2.251
Quant Mass(es) = 151
S/N = 414.03
Area = 63480
Height = 5464.1
Similarity = 858



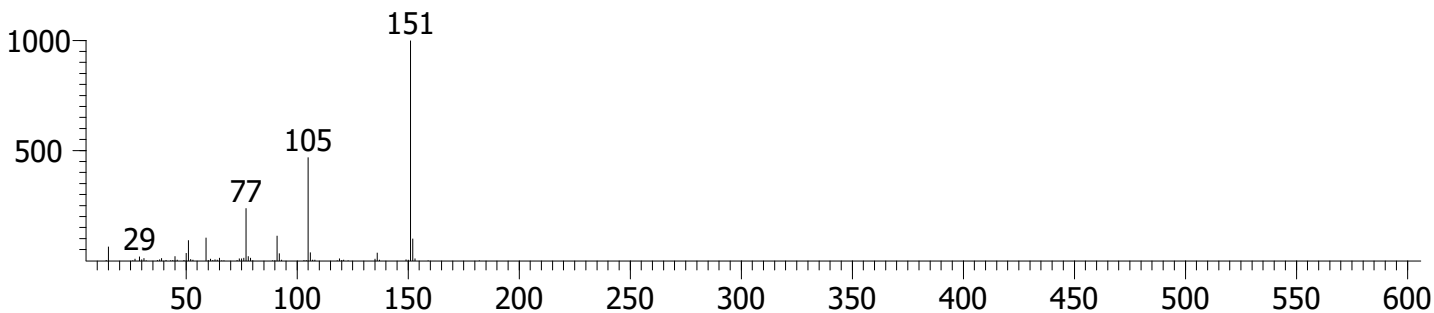
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2565, at 1690.31 , 2.251 sec , sec (Spec # 1837 21)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2565, at 1690.31 , 2.251 sec , sec (Spec # 1837 21)



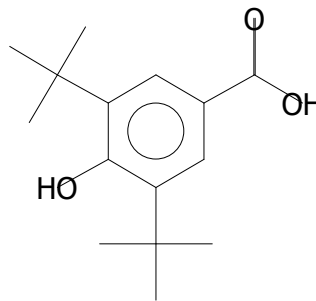
Library Hit - similarity 858, "Benzene, (trimethoxymethyl)-"



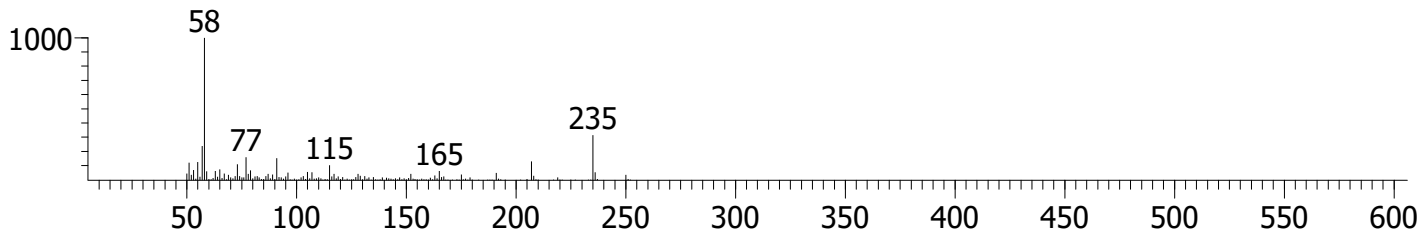
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, (trimethoxymethyl)-	858	5568	707-07-3	mainlib	C10H14O3	182
2	Ethanone, 2,2-dimethoxy-1,2-diphenyl-	844	3485	24650-42-8	mainlib	C16H16O3	256
3	5-Nitro-m-xylene	744	259	99-12-7	mainlib	C8H9NO2	151
4	2-Amino-1-(o-hydroxyphenyl)propane	734	183	73470-00-5	mainlib	C9H13NO	151
5	Benzoic acid, 1-cyanoquinuclidin-1-yl ester	724	129	0-00-0	mainlib	C15H16N2O2	256

Benzoic acid,
3,5-bis(1,1-dimethylethyl)-4-hydroxy-

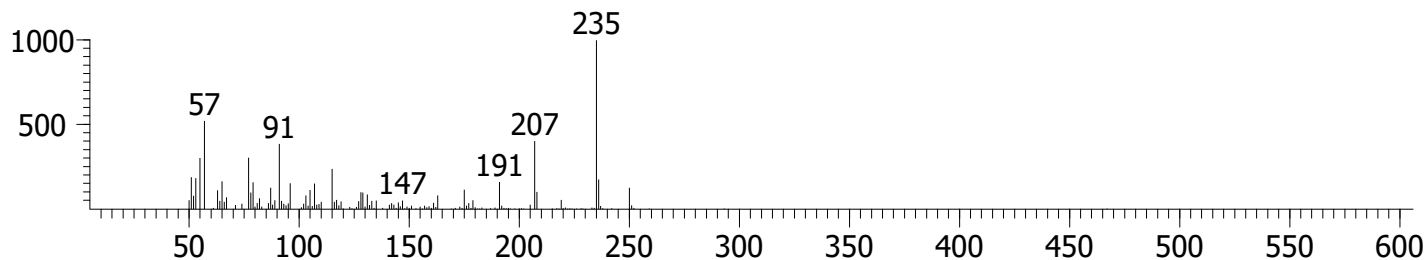
1st Dimension R.T. = 1697.3
 2nd Dimension R.T. = 1.934
 Quant Mass(es) = 235
 S/N = 1703.0
 Area = 260734
 Height = 27941
 Similarity = 888



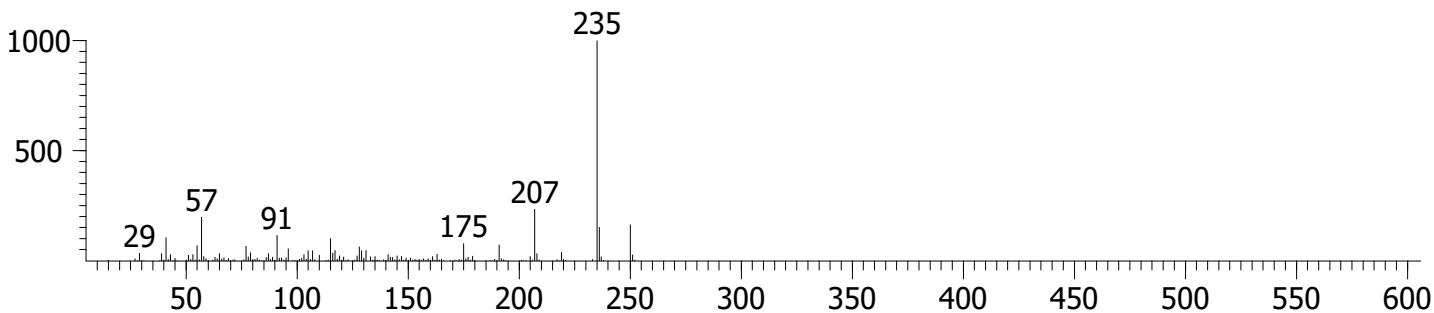
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2577, at 1697.3 , 1.934 sec , sec (Spec # 18473 3)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2577, at 1697.3 , 1.934 sec , sec (Spec # 18473 3)



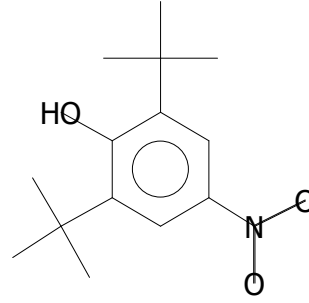
Library Hit - similarity 888, "Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-"



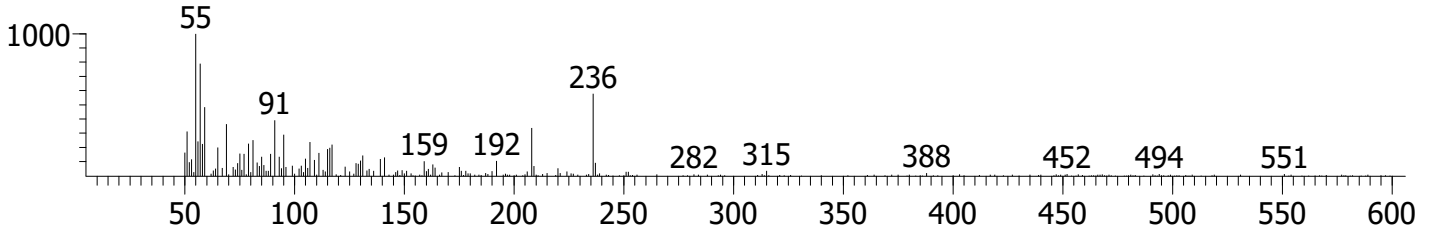
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-	888	9664	1421-49-4	mainlib	C15H22O3	250
2	1,3-Benzenedicarboxylic acid, 5-(1,1-dimethylethyl)-, dimethyl ester	678	96	16308-65-9	mainlib	C14H18O4	250
3	Phenol, 2,6-bis(1,1-dimethylethyl)-4-(methoxymethyl)-	660	49	87-97-8	mainlib	C16H26O2	250
4	2-tert-Butyl-4-ethylphenol, trimethylsilyl ether	659	47	0-00-0	mainlib	C15H26OSi	250
5	3-Cyclohexen-1-one, 2,2,4-trimethyl-3-[2-(2-methyl-1,3-dioxolan-2-yl)-1-ethenyl]	644	29	0-00-0	mainlib	C15H22O3	250

Bayer 28,589

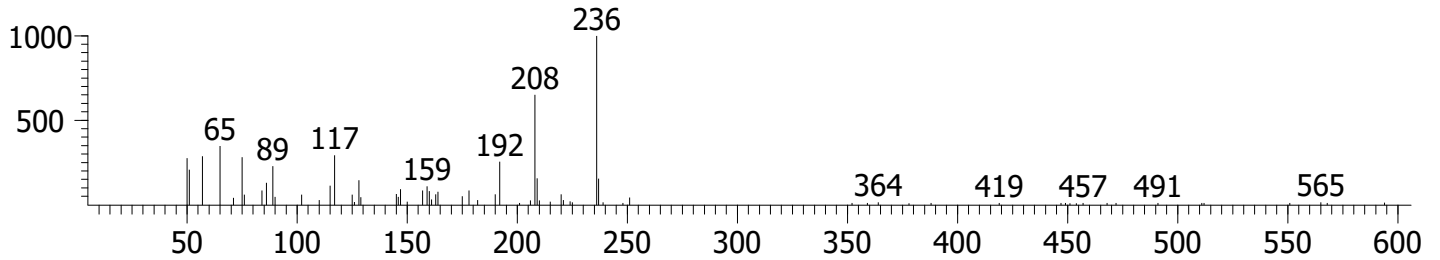
1st Dimension R.T. = 1711.3
2nd Dimension R.T. = 1.802
Quant Mass(es) = 236
S/N = 112.42
Area = 9032.0
Height = 1101.2
Similarity = 678



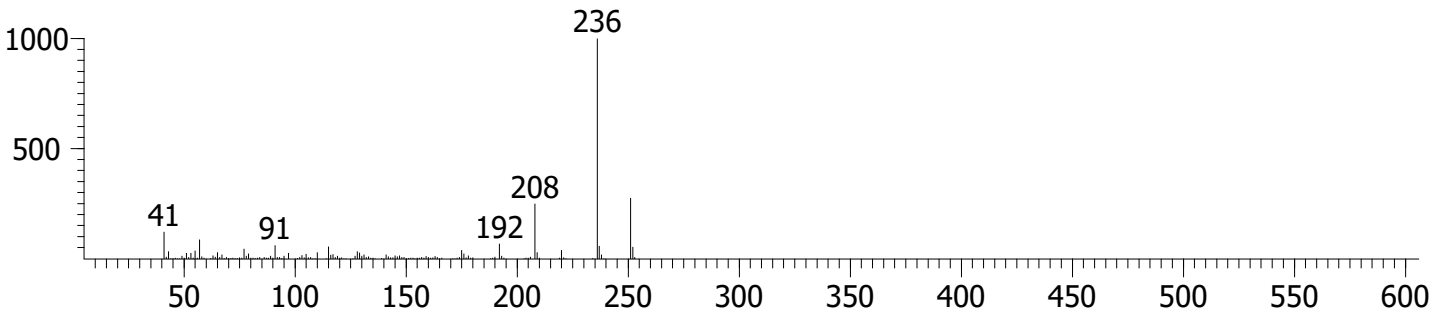
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2596, at 1711.3 , 1.802 sec , sec (Spec # 18683 3)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2596, at 1711.3 , 1.802 sec , sec (Spec # 18683 3)



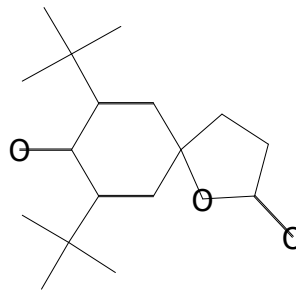
Library Hit - similarity 678, "Bayer 28,589"



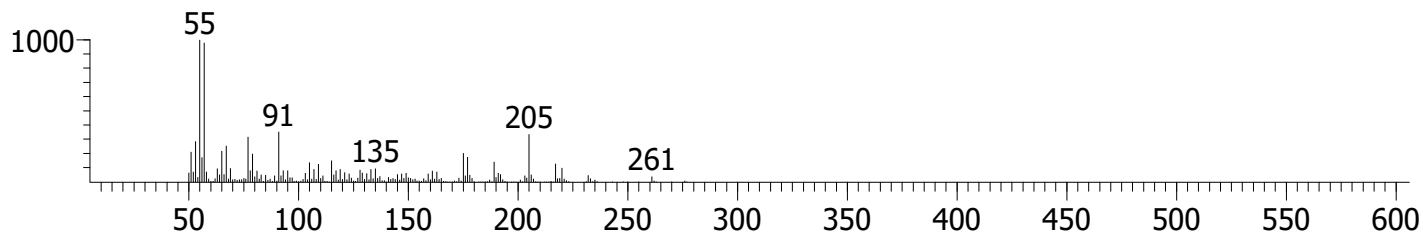
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Bayer 28,589	678	5824	728-40-5	mainlib	C14H21NO3	251
2	6H,12H-Indazolo[2,1-a]indazole-6,12-dione	597	617	18428-89-2	mainlib	C14H8N2O2	236
3	2-Tetrazaboroline, 5-methyl-1,4-diphenyl-	597	617	20534-05-8	mainlib	C13H13BN4	236
4	4-(3-Pyridyl)-4-oxo-butyrac acid tbdms	581	355	0-00-0	mainlib	C15H23NO3Si	293
5	Dendroban-12-one, 10-hydroxy-	576	286	29414-86-6	mainlib	C16H25NO3	279

-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8

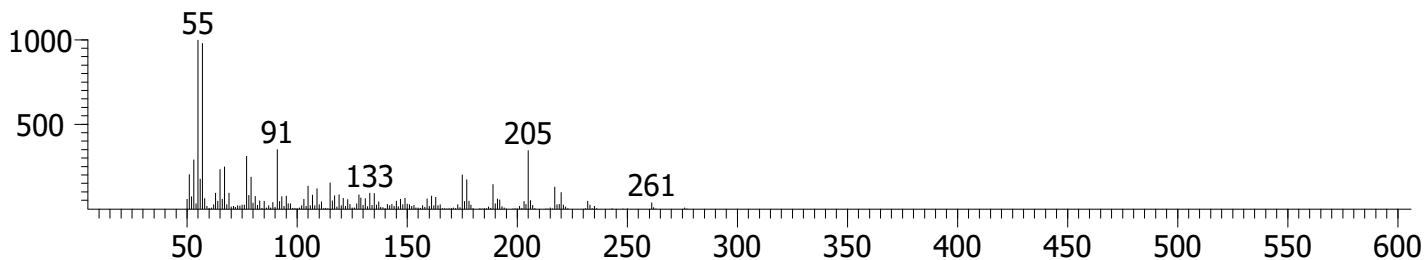
1st Dimension R.T. = 1718.29
2nd Dimension R.T. = 1.855
Quant Mass(es) = 205
S/N = 2606.4
Area = 234238
Height = 27302
Similarity = 871



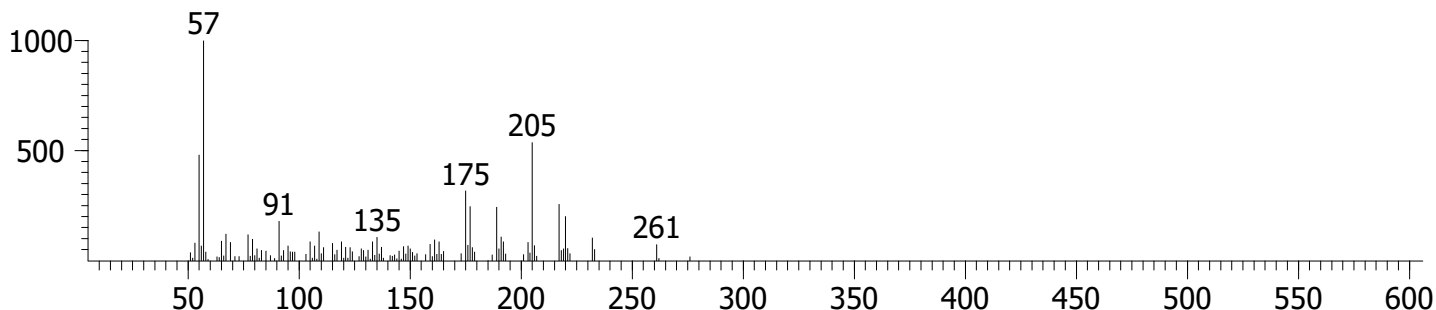
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2608, at 1718.29 , 1.855 sec , sec (Spec # 1879 01)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2608, at 1718.29 , 1.855 sec , sec (Spec # 1879 01)



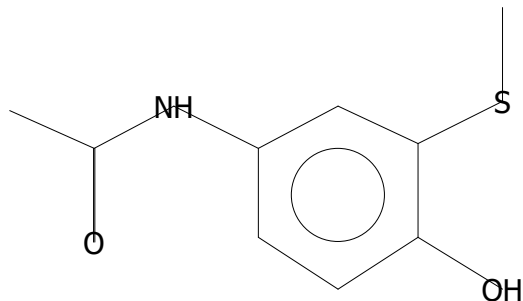
Library Hit - similarity 871, "7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione"



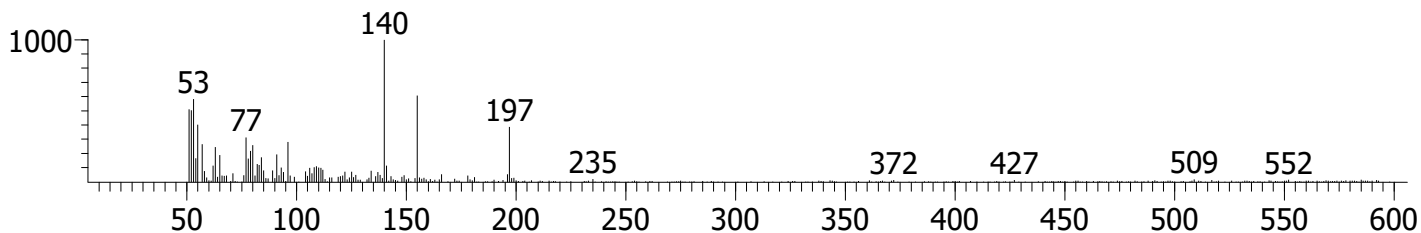
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	871	8696	82304-66-3	mainlib	C17H24O3	276
2	Trichothec-9-en-8-one, 12,13-epoxy-3,4,7,15-tetrahydroxy-, (3à,4á,7à)-	718	233	23282-20-4	mainlib	C15H20O7	312
3	9-Isopropyl-1-methyl-2-methylene-5-oxatricyclo[5.4.0.0(3,8)]undecane	704	145	0-00-0	mainlib	C15H24O	220
4	11,14-Octadecadiynoic acid, methyl ester	699	117	56554-58-6	mainlib	C19H30O2	290
5	1H-2,8a-Methanocyclopenta[a]cyclopropa[e]cyclodecen-11-one, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,4-bis(hydroxymethyl)-1,7,9-trimethyl-, [1S-(1à,1aà,2à,5á,5aá,6á,8aà,9à,10aà)]-	694	94	52557-29-6	mainlib	C20H28O6	364

Acetamide,
N-[4-hydroxy-3-(methylthio)phenyl]-

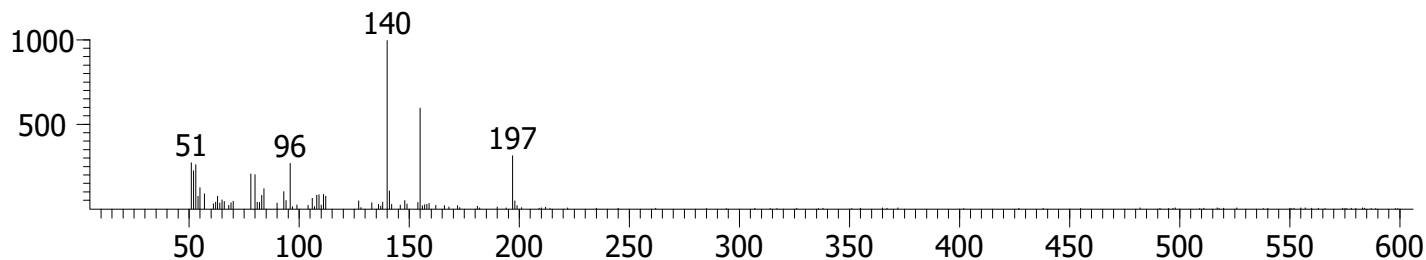
1st Dimension R.T. = 1721.79
2nd Dimension R.T. = 2.620
Quant Mass(es) = 140
S/N = 218.97
Area = 46926
Height = 4017.7
Similarity = 773



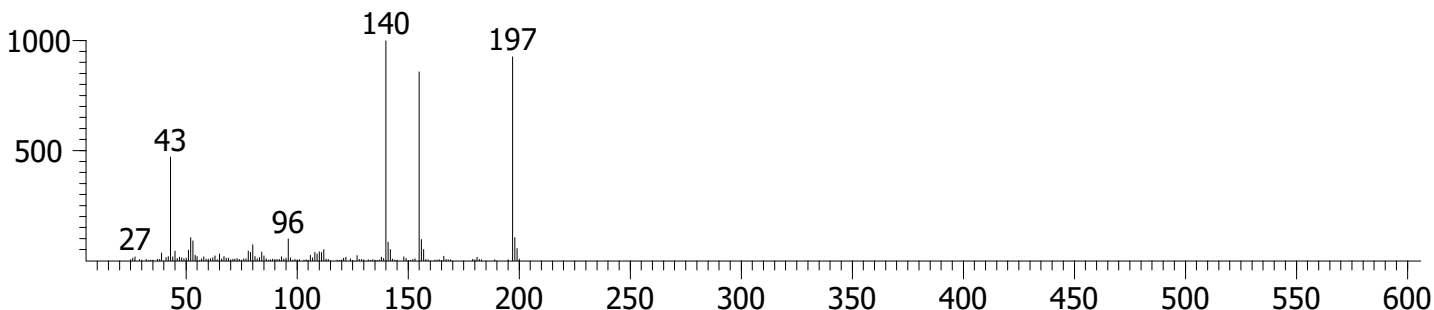
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2622, at 1721.79 , 2.620 sec , sec (Spec # 1885 47)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2622, at 1721.79 , 2.620 sec , sec (Spec # 1885 47)

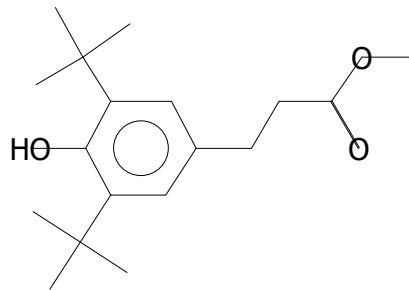


Library Hit - similarity 773, "Acetamide, N-[4-hydroxy-3-(methylthio)phenyl]-"



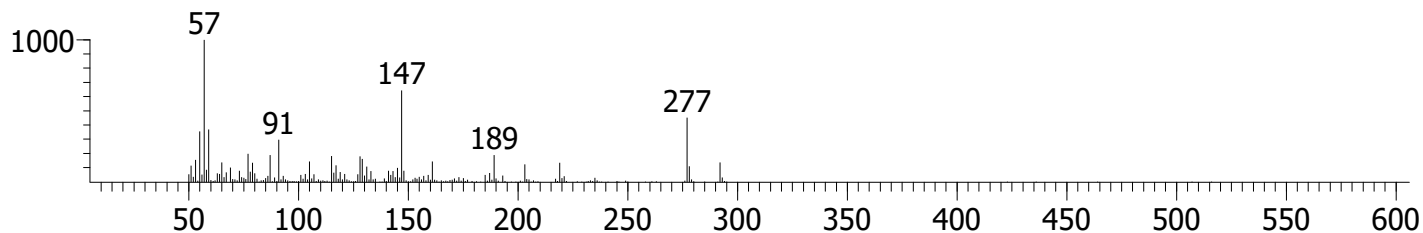
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Acetamide, N-[4-hydroxy-3-(methylthio)phenyl]-	773	9171	37398-23-5	mainlib	C9H11NO2S	197
2	Pent-1-en-3-one, 4,4-dimethyl-1-(4-morpholino)-	615	232	0-00-0	mainlib	C11H19NO2	197
3	5-Ethyl-6-imino-5-(1-methyl-butyl)-dihydro-pyrimidine-2,4-dione	582	60	0-00-0	mainlib	C11H19N3O2	225
4	3-Butanone, 2-(2,6-dioxo-3-piperidyl)-2-methyl-	569	39	198283-36-2	mainlib	C10H15NO3	197
5	5a-Methoxy-9a-methyl-3,4,5a,6,7,8,9a,10-octahydropyrano [4,3-b]chromene-1,9-dione	567	36	0-00-0	mainlib	C14H18O5	266

Benzenepropanoic acid,
3,5-bis(1,1-dimethylethyl)-4-hydroxy-,

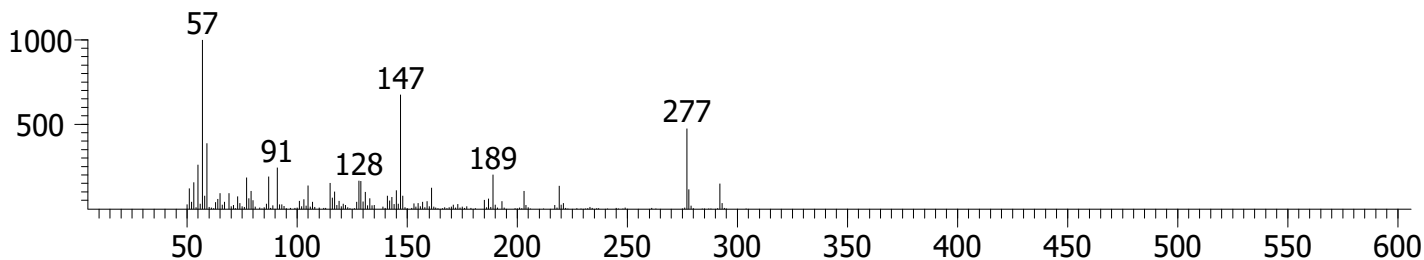


1st Dimension R.T. = 1735.78
 2nd Dimension R.T. = 1.775
 Quant Mass(es) = 277
 S/N = 1306.9
 Area = 70121
 Height = 7786.1
 Similarity = 816

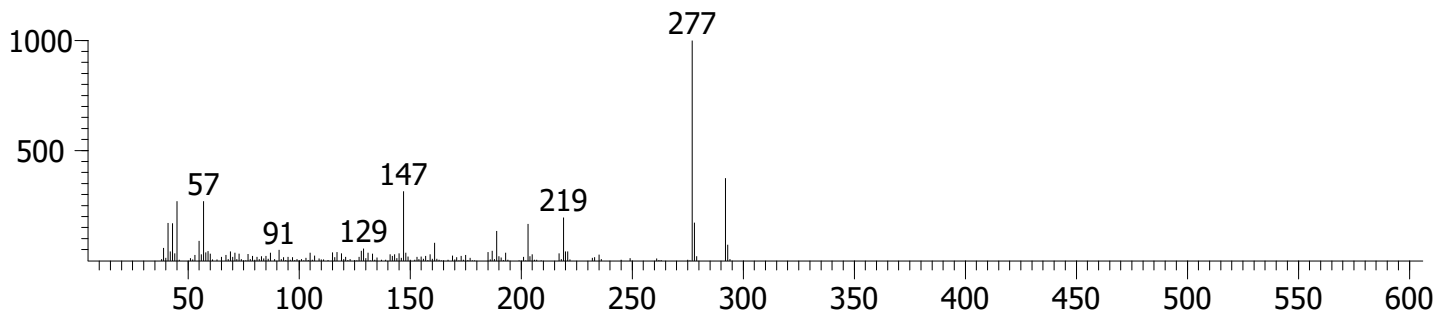
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2647, at 1735.78 , 1.775 sec , sec (Spec # 1905 39)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2647, at 1735.78 , 1.775 sec , sec (Spec # 1905 39)



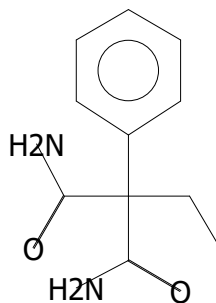
Library Hit - similarity 816, "Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester"



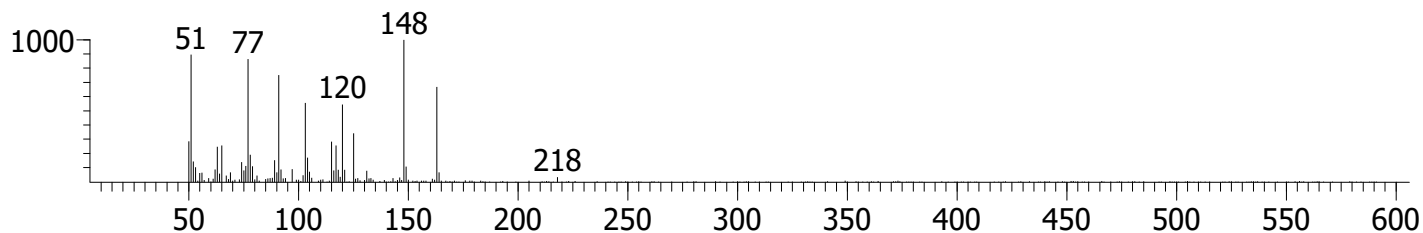
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	816	9562	6386-38-5	mainlib	C18H28O3	292
2	Butylated Hydroxytoluene, TMS derivative	629	149	18510-49-1	mainlib	C18H32OSi	292
3	Propanamide, 3-[3,5-di(tert-butyl)-4-hydroxyphenyl]-N-(2-hydroxyethyl)-	591	35	0-00-0	mainlib	C19H31NO3	321
4	9-Heptadecene-4,6-diyne-8-ol, (Z)-	583	26	32768-90-4	mainlib	C17H26O	246
5	2,6-Dimethyl-N-[3-(trimethylsilyl)-1,3-thiazinan-2-ylidene]aniline	573	18	0-00-0	mainlib	C15H24N2SSi	292

Propanediamide, 2-ethyl-2-phenyl-

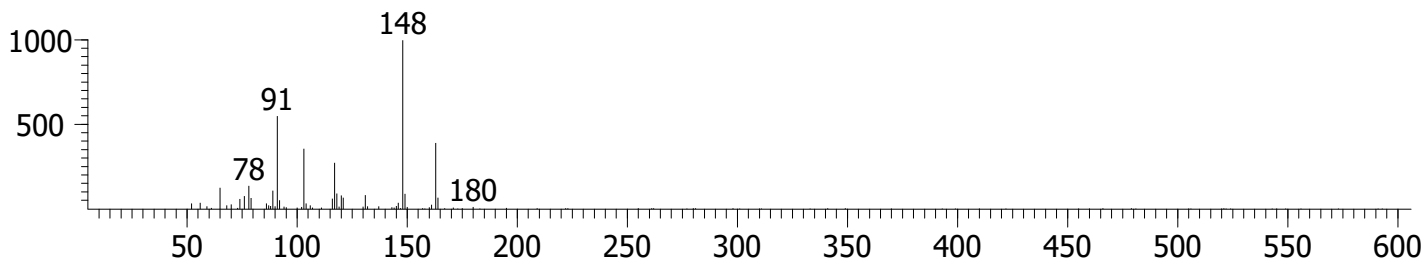
1st Dimension R.T. = 1739.28
2nd Dimension R.T. = 2.818
Quant Mass(es) = 148
S/N = 370.85
Area = 67046
Height = 5535.6
Similarity = 823



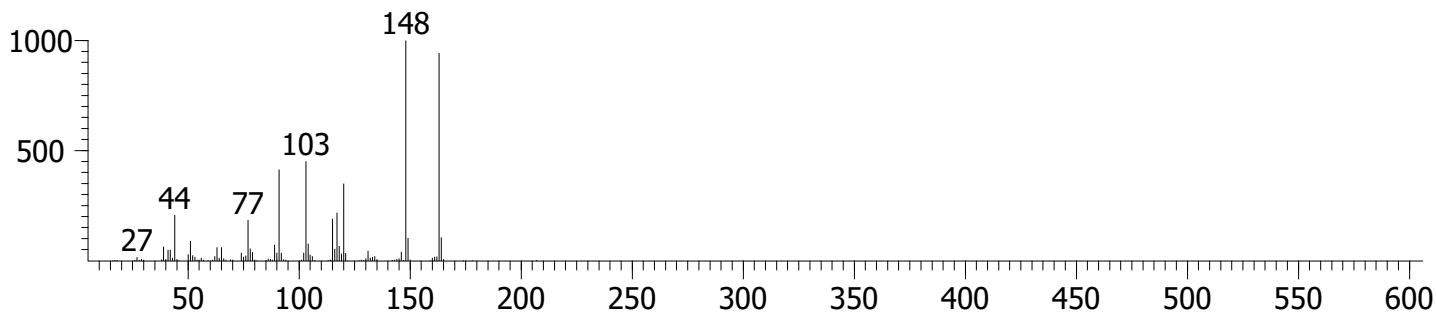
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2660, at 1739.28 , 2.818 sec , sec (Spec # 1912 27)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2660, at 1739.28 , 2.818 sec , sec (Spec # 1912 27)



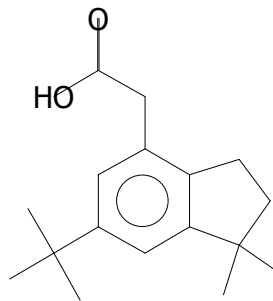
Library Hit - similarity 823, "Propanediamide, 2-ethyl-2-phenyl-"



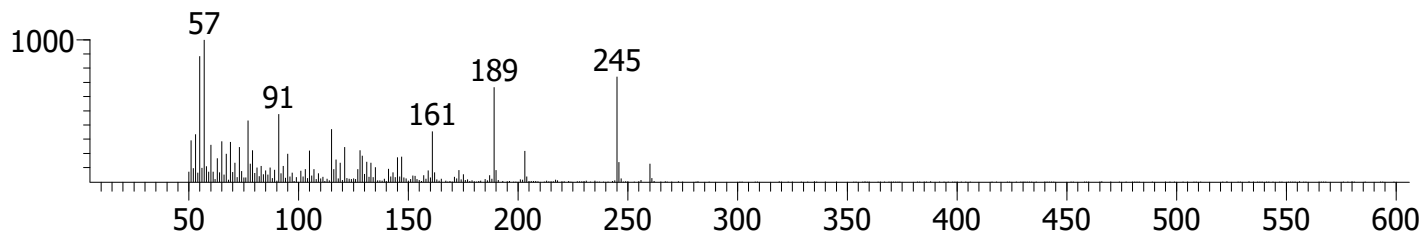
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Propanediamide, 2-ethyl-2-phenyl-	823	7690	7206-76-0	mainlib	C11H14N2O2	206
2	Benzene, 1-acetyl-2-amino-3-ethyl-	717	516	108562-67-0	mainlib	C10H13NO	163
3	Benzenamine, N,N-diethyl-2-methyl-	705	344	606-46-2	mainlib	C11H17N	163
4	2-tert-Butyl-6-methylaniline	705	344	13117-94-7	mainlib	C11H17N	163
5	Benzenamine, N,N-diethyl-4-methyl-	695	242	613-48-9	mainlib	C11H17N	163

1H-Indene-4-acetic acid,
-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl

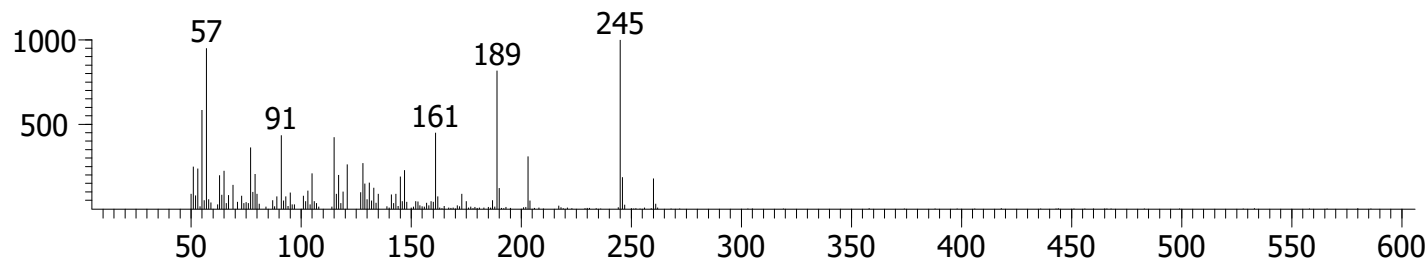
1st Dimension R.T. = 1742.78
 2nd Dimension R.T. = 1.940
 Quant Mass(es) = 245
 S/N = 900.27
 Area = 52502
 Height = 5213.6
 Similarity = 679



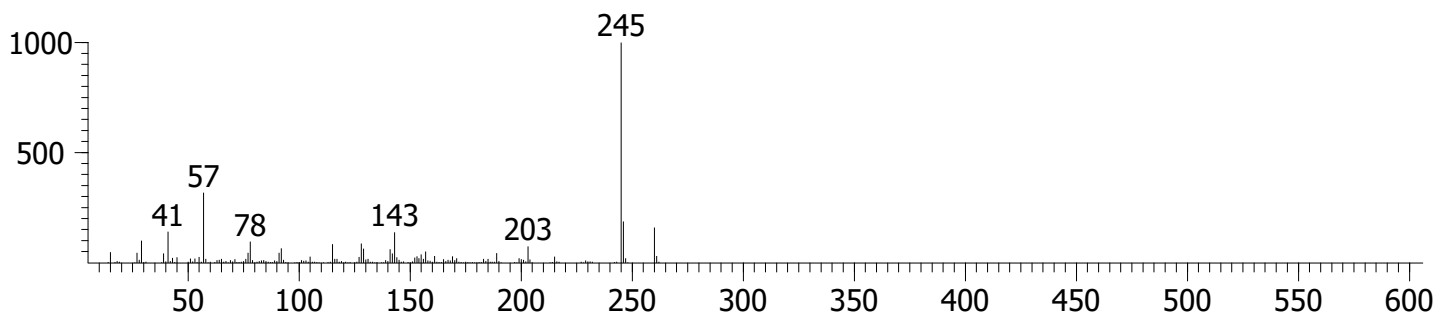
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2664, at 1742.78 , 1.940 sec , sec (Spec # 1916 24)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2664, at 1742.78 , 1.940 sec , sec (Spec # 1916 24)



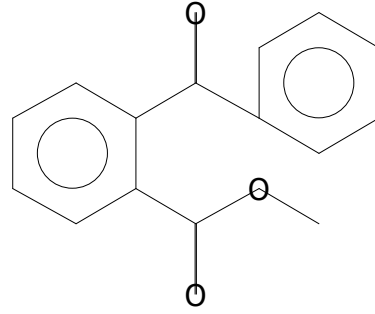
Library Hit - similarity 679, "1H-Indene-4-acetic acid, 6-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-"



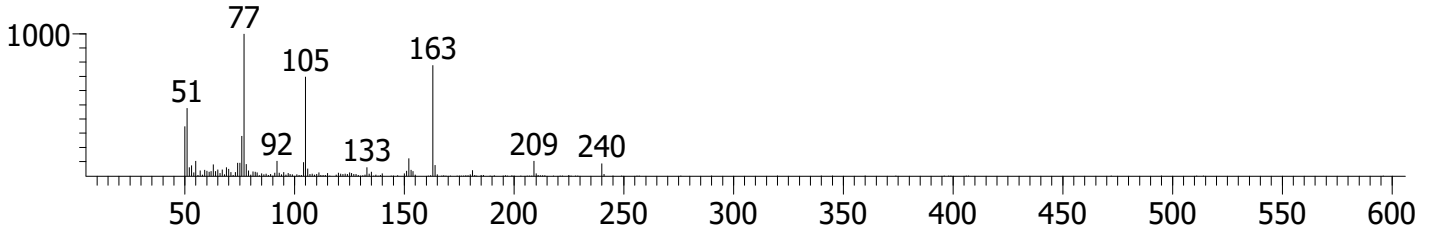
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Indene-4-acetic acid, 6-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-	679	3492	55591-05-4	mainlib	C17H24O2	260
2	Acetate, (2-cyclohexenyl-3-[1-methyl-3-oxo-1-butenyl]-2,4,4-trimethyl) ester	637	783	0-00-0	mainlib	C16H24O3	264
3	Bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propyl] maleate	621	451	0-00-0	mainlib	C38H56O6	608
4	9-Heptadecene-4,6-diy-8-ol, (Z)-	606	273	32768-90-4	mainlib	C17H26O	246
5	Naphthalene, 2,3,4,4a,5,6-hexahydro-1,4a-dimethyl-7-(1-methylethyl)-	604	252	473-14-3	mainlib	C15H24	204

Benzoic acid, 2-benzoyl-, methyl ester

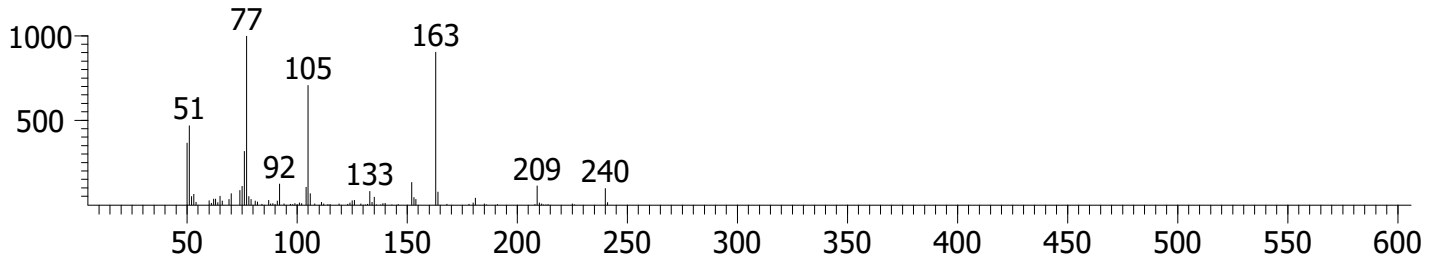
1st Dimension R.T. = 1746.28
2nd Dimension R.T. = 2.521
Quant Mass(es) = 163
S/N = 1119.8
Area = 173443
Height = 14318
Similarity = 825



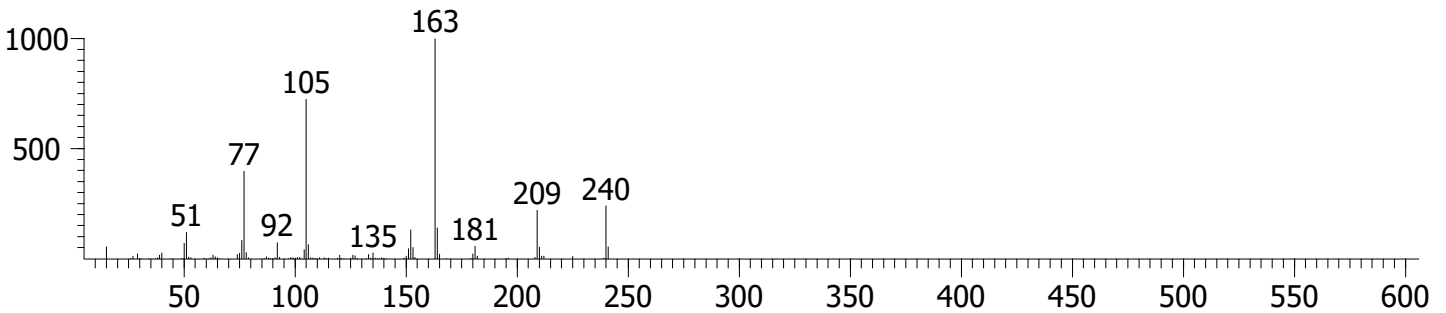
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2673, at 1746.28 , 2.521 sec , sec (Spec # 1922 42)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2673, at 1746.28 , 2.521 sec , sec (Spec # 1922 42)



Library Hit - similarity 825, "Benzoic acid, 2-benzoyl-, methyl ester"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzoic acid, 2-benzoyl-, methyl ester	825	8290	606-28-0	mainlib	C15H12O3	240
2	Benzoic acid, 2-(1-oxopropyl)-, methyl ester	730	671	32025-37-9	mainlib	C11H12O3	192
3	Benzoic acid, 4-benzoyl-, methyl ester	723	514	6158-54-9	mainlib	C15H12O3	240
4	1,3-Dioxolane, 2,4-dimethyl-2-phenyl-	689	131	4359-30-2	mainlib	C11H14O2	178
5	Ethanone, 2-(2-methylpropoxy)-1,2-diphenyl-	676	85	22499-12-3	mainlib	C18H20O2	268

2,4(1H,3H)-Pteridinedione, 1,3-dimethyl-

1st Dimension R.T. = 1760.27

2nd Dimension R.T. = 2.792

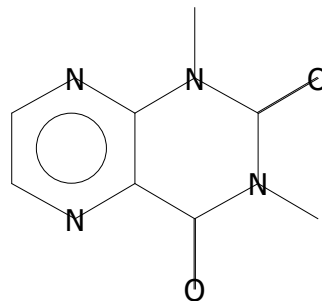
Quant Mass(es) = 85

S/N = 589.46

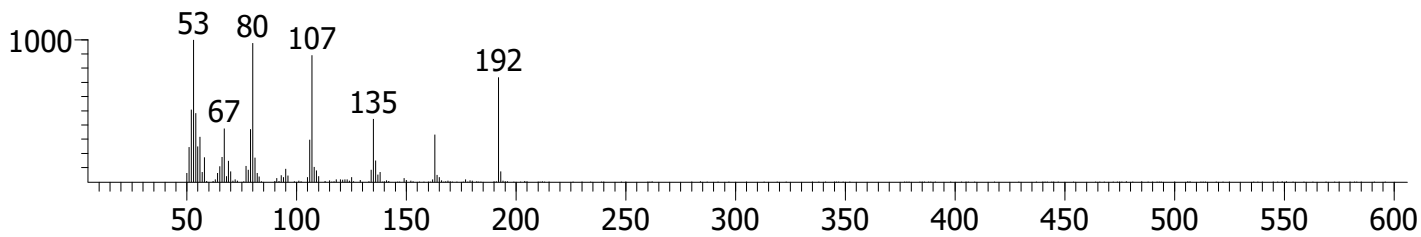
Area = 2395.9

Height = 502.47

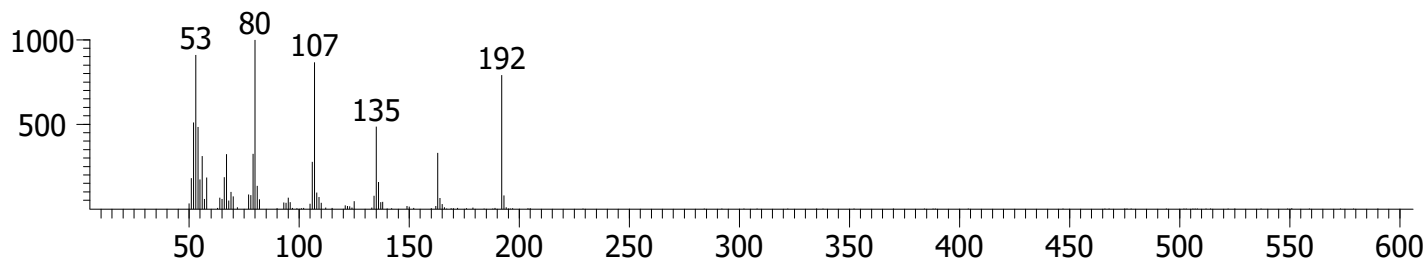
Similarity = 743



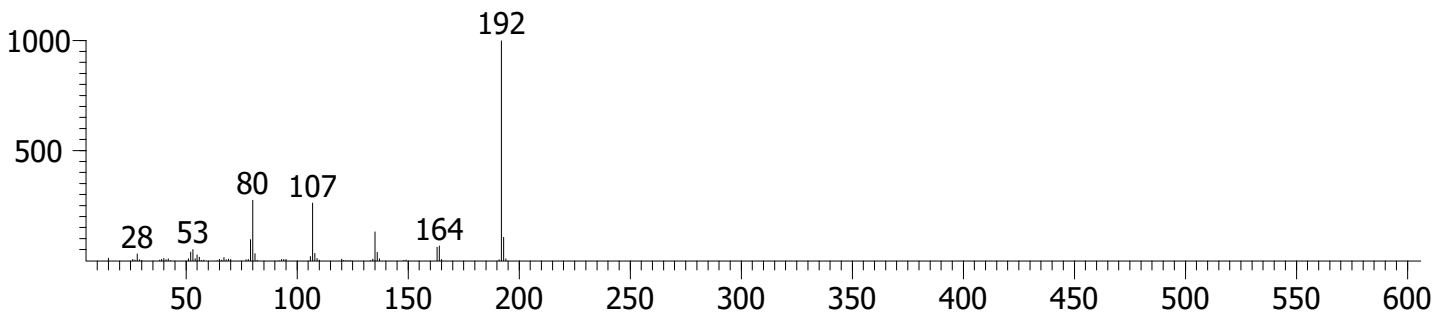
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2702, at 1760.27 , 2.792 sec , sec (Spec # 1944 03)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2702, at 1760.27 , 2.792 sec , sec (Spec # 1944 03)

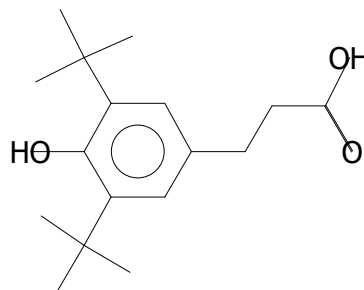


Library Hit - similarity 743, "2,4(1H,3H)-Pteridinedione, 1,3-dimethyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,4(1H,3H)-Pteridinedione, 1,3-dimethyl-	743	6964	13401-18-8	mainlib	C8H8N4O2	192
2	4(3H)-Pteridinone, 3-methoxy-6-methyl-	681	1190	24898-65-5	mainlib	C8H8N4O2	192
3	4(3H)-Pteridinone, 3-hydroxy-6,7-dimethyl-	638	262	18106-61-1	mainlib	C8H8N4O2	192
4	6-Methoxy-2,4-dihydroxy-1,5-naphthyridine	633	211	0-00-0	mainlib	C9H8N2O3	192
5	5-Amino-1-(4-amino-furazan-3-yl)-1H-[1,2,3]triazole-4-carbonitrile	618	128	0-00-0	mainlib	C5H4N8O	192

3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid



1st Dimension R.T. = 1784.75

2nd Dimension R.T. = 1.881

Quant Mass(es) = 263

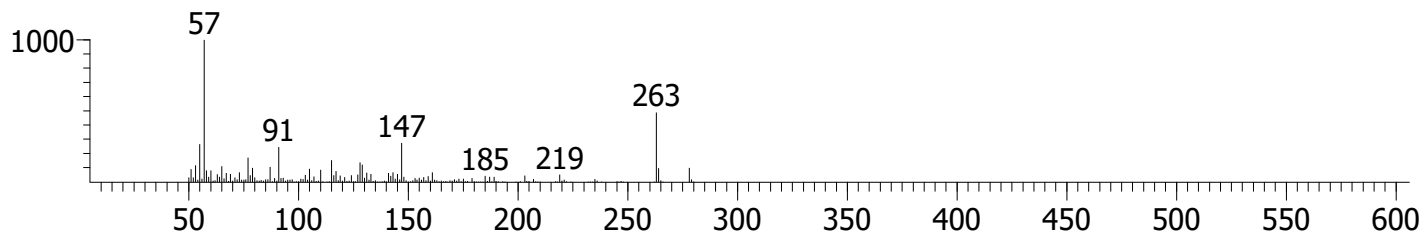
S/N = 2991.9

Area = 397001

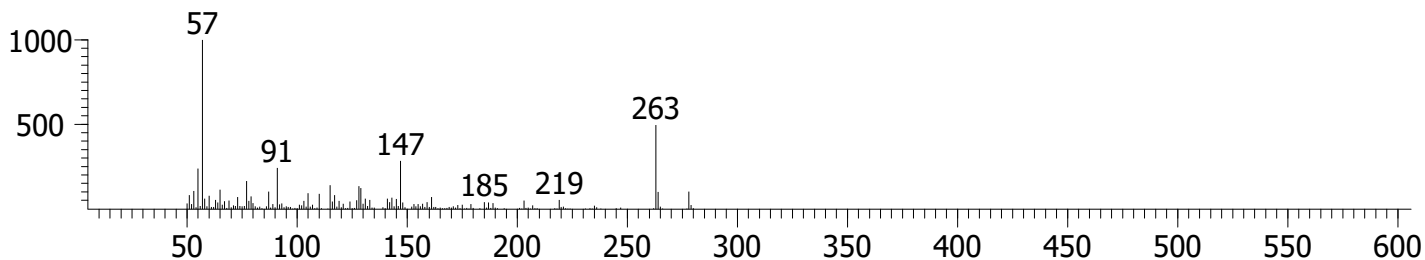
Height = 41175

Similarity = 798

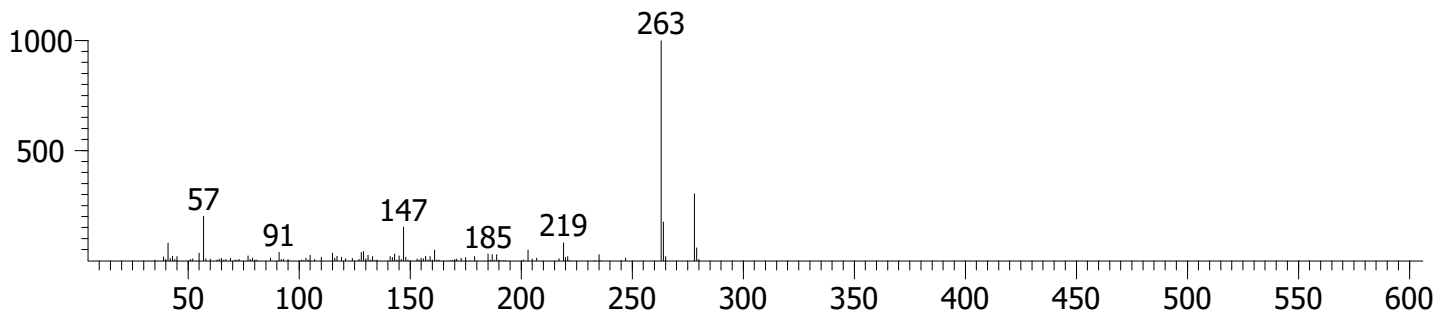
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2741, at 1784.75 , 1.881 sec , sec (Spec # 1979 75)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2741, at 1784.75 , 1.881 sec , sec (Spec # 1979 75)



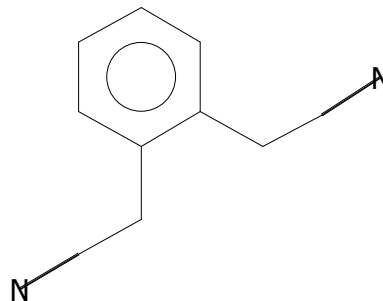
Library Hit - similarity 798, "3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid"



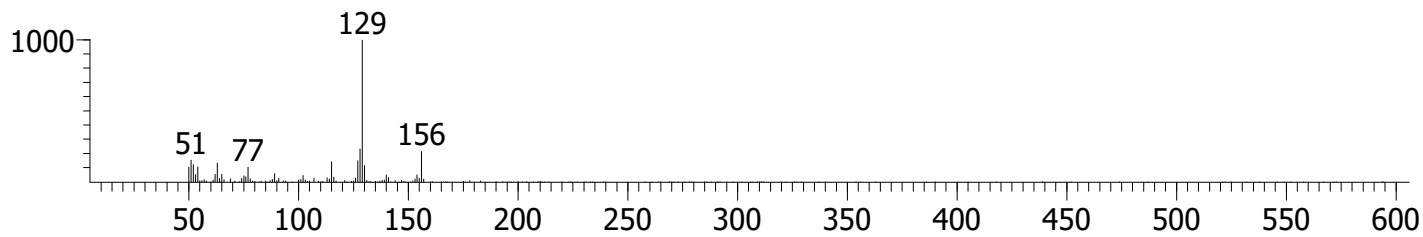
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid	798	9043	20170-32-5	mainlib	C17H26O3	278
2	Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, ethyl ester	692	607	1620-64-0	mainlib	C17H26O3	278
3	1,4-Dihydrophenacetic acid, 3,5-di-t-butyl-, ethyl ester	665	178	0-00-0	mainlib	C18H30O2	278
4	2,4,6-Tri-t-butylbenzenethiol	629	44	961-39-7	mainlib	C18H30S	278
5	Panaxydol	610	21	72800-72-7	mainlib	C17H24O2	260

1,2-Benzenediacetonitrile

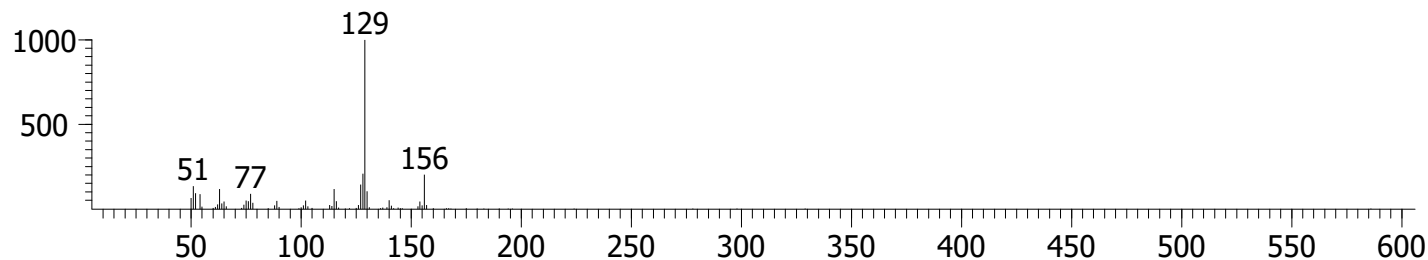
1st Dimension R.T. = 1788.25
2nd Dimension R.T. = 2.732
Quant Mass(es) = 129
S/N = 738.88
Area = 144650
Height = 10559
Similarity = 801



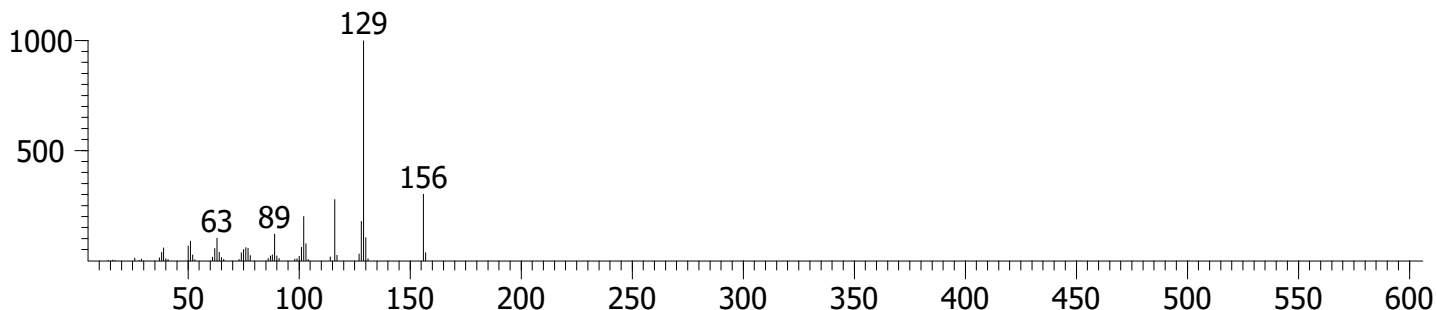
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2753, at 1788.25 , 2.732 sec , sec (Spec # 1986 34)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2753, at 1788.25 , 2.732 sec , sec (Spec # 1986 34)



Library Hit - similarity 801, "1,2-Benzenediacetonitrile"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,2-Benzenediacetonitrile	801	1770	613-73-0	mainlib	C10H8N2	156
2	2-Phenyl-2-(prop-2-en-1-yl)pent-4-enenitrile	799	1632	28049-67-4	mainlib	C14H15N	197
3	Cyclopropene, 2,3-dimethyl-3-phenyl-	782	891	0-00-0	mainlib	C11H12	144
4	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	779	787	57964-39-3	mainlib	C14H14N2	210
5	3-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	771	587	57964-40-6	mainlib	C14H14N2	210

6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline

1st Dimension R.T. = 1837.22

2nd Dimension R.T. = 1.881

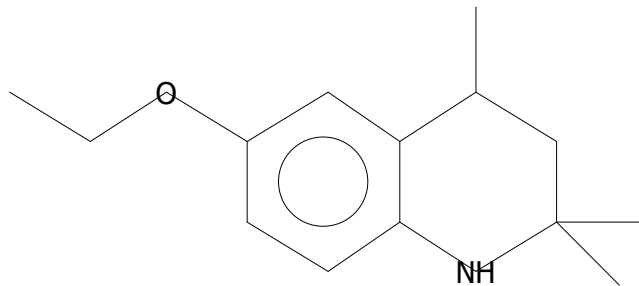
Quant Mass(es) = 204

S/N = 452.33

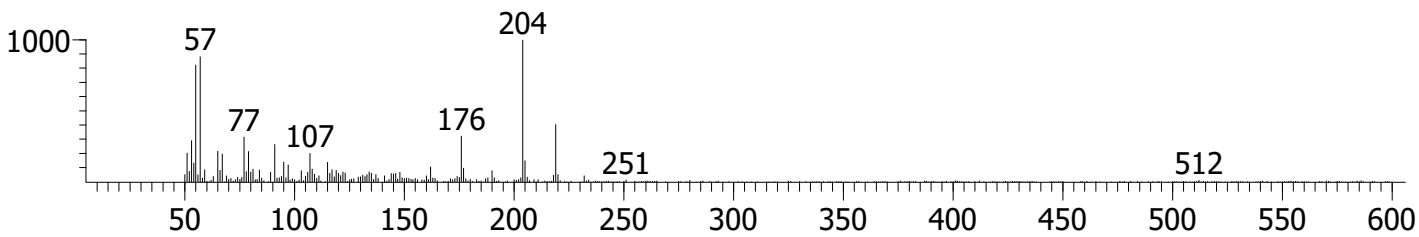
Area = 35340

Height = 3755.8

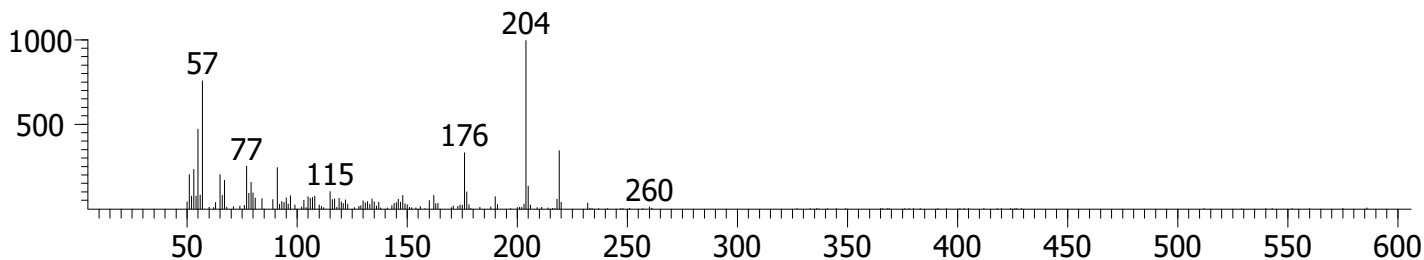
Similarity = 704



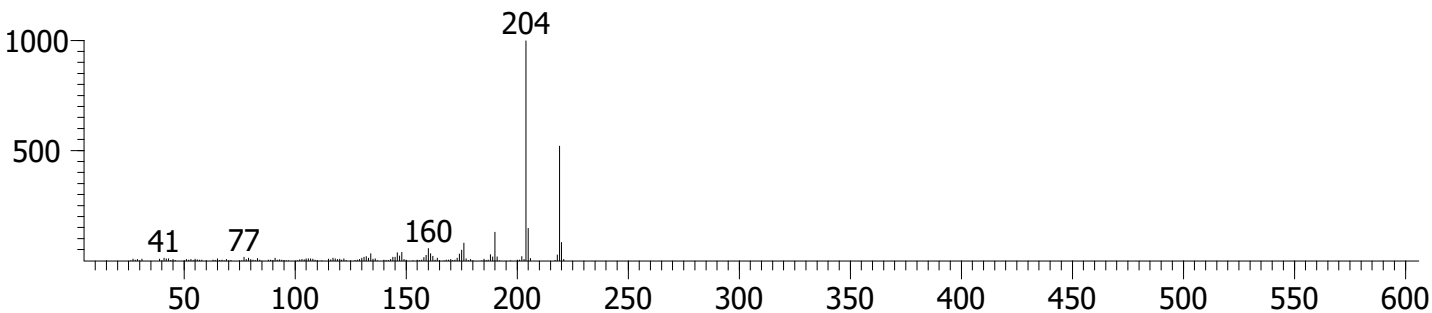
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2818, at 1837.22 , 1.881 sec , sec (Spec # 2059 25)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2818, at 1837.22 , 1.881 sec , sec (Spec # 2059 25)



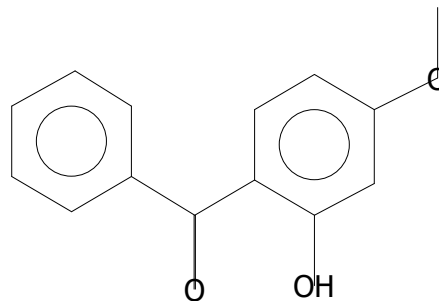
Library Hit - similarity 704, "6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline"



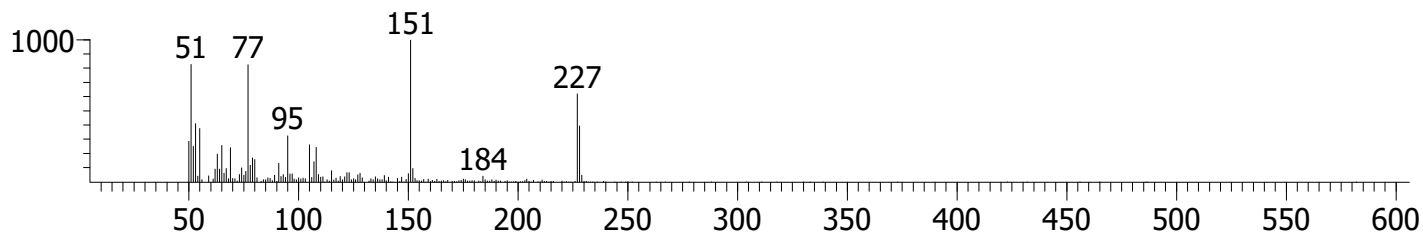
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline	704	3467	16489-90-0	mainlib	C14H21NO	219
2	6,7-Dimethoxy-3,3-dimethyl-4H-isoquinoline	680	1161	148319-42-0	mainlib	C13H17NO2	219
3	Pyrrole-3-carbonitrile, 2-amino-1-butyl-(1,1-dimethylethyl)-	676	981	340180-56-5	mainlib	C13H21N3	219
4	1-Ethyl-1,2,3,4-tetrahydro-6,7-methylenedioxy-4-oxoquinoline	664	653	132767-88-5	mainlib	C12H13NO3	219
5	2(1H)-Quinolinone, 5,8-dimethoxy-4-methyl-	649	396	0-00-0	mainlib	C12H13NO3	219

Oxybenzone

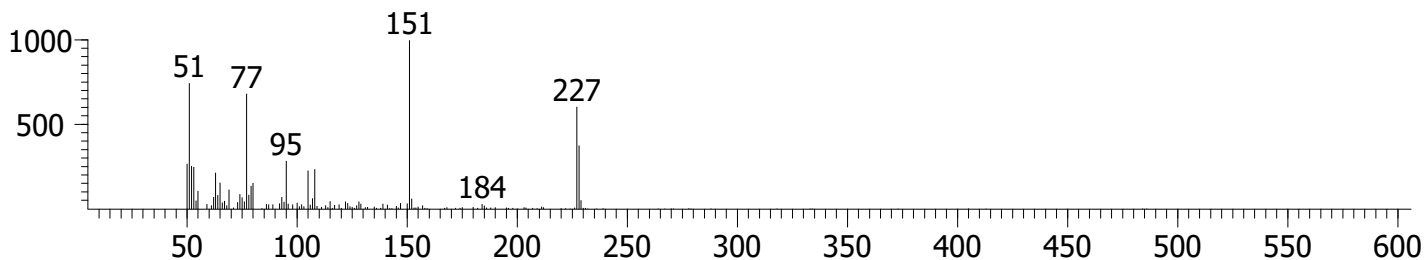
1st Dimension R.T. = 1837.22
 2nd Dimension R.T. = 2.303
 Quant Mass(es) = 227
 S/N = 621.42
 Area = 45986
 Height = 4486.6
 Similarity = 879



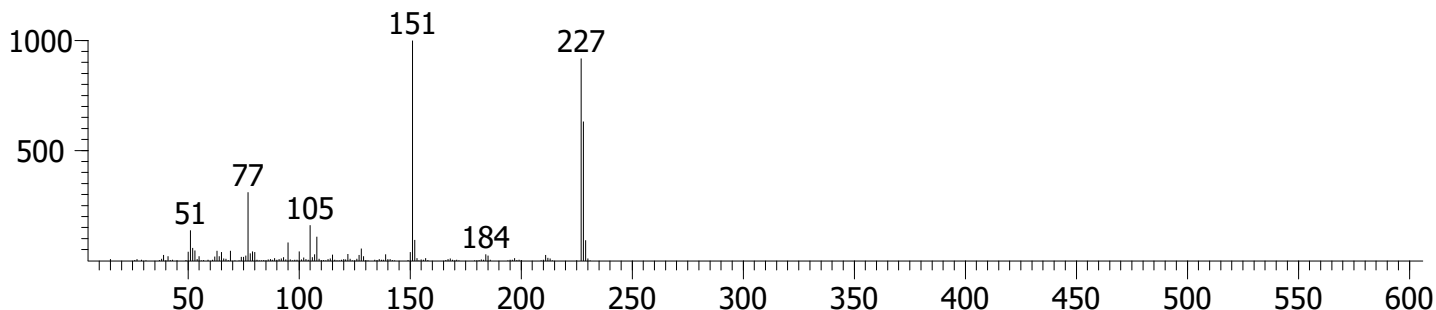
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2819, at 1837.22 , 2.303 sec , sec (Spec # 2059 89)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2819, at 1837.22 , 2.303 sec , sec (Spec # 2059 89)



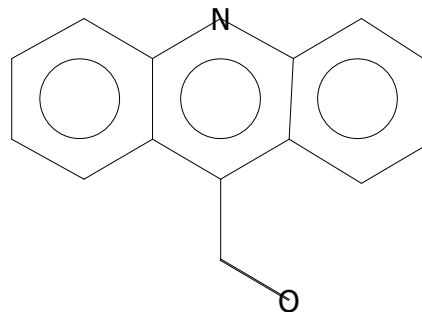
Library Hit - similarity 879, "Oxybenzone"



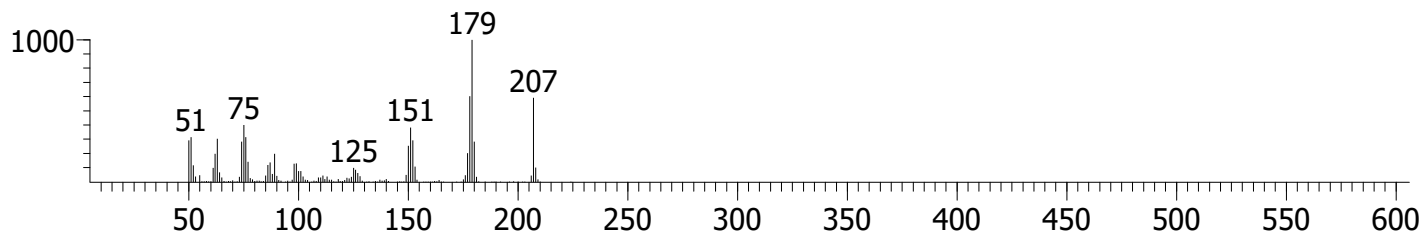
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Oxybenzone	879	9745	131-57-7	mainlib	C14H12O3	228
2	Benzophenone, 2'-hydroxy-5'-methoxy-	697	167	14770-96-8	mainlib	C14H12O3	228
3	Sulisobenzone	653	36	4065-45-6	mainlib	C14H12O6S	308
4	Benzoic acid, 1-cyanoquinuclidin-1-yl ester	600	7	0-00-0	mainlib	C15H16N2O2	256
5	Thiourea, 1-(3-hydroxyphenyl)-3-(4-phenoxyphenyl)-	590	5	0-00-0	mainlib	C19H16N2O2S	336

Acridine-9-carbaldehyde

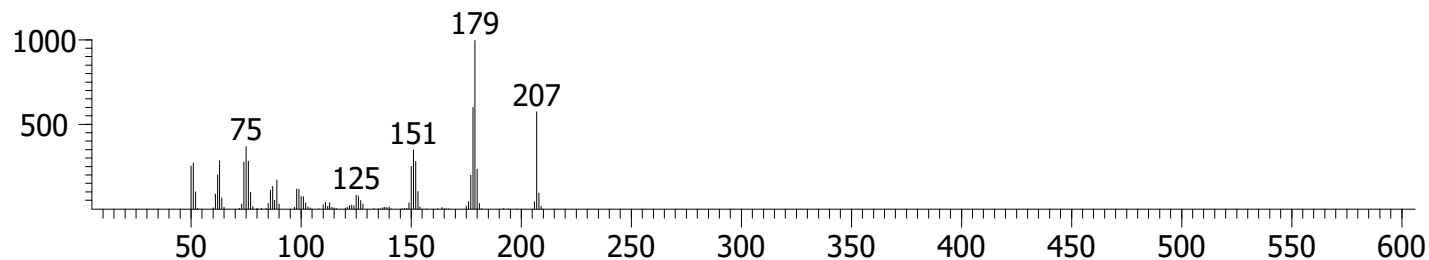
1st Dimension R.T. = 1879.2
2nd Dimension R.T. = 2.607
Quant Mass(es) = 179
S/N = 3366.6
Area = 878318
Height = 74132
Similarity = 763



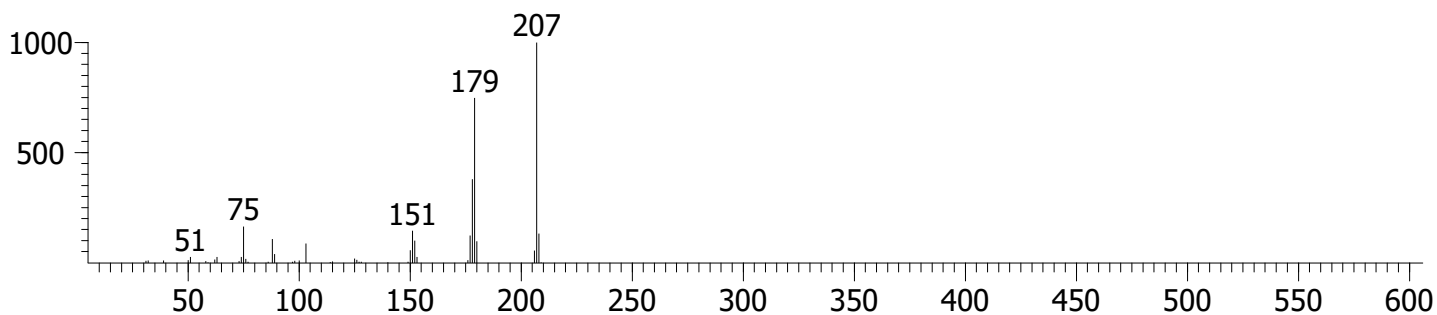
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2876, at 1879.2 , 2.607 sec , sec (Spec # 21239 5)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2876, at 1879.2 , 2.607 sec , sec (Spec # 21239 5)



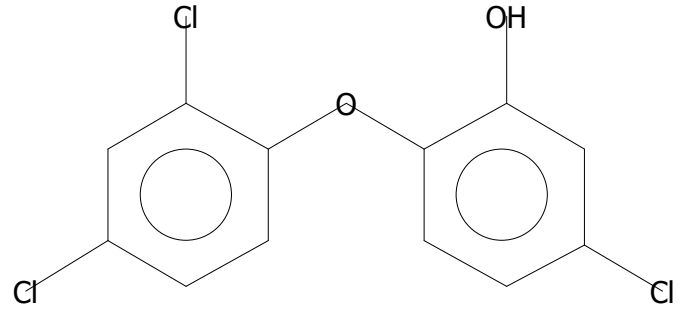
Library Hit - similarity 763, "Acridine-9-carbaldehyde"



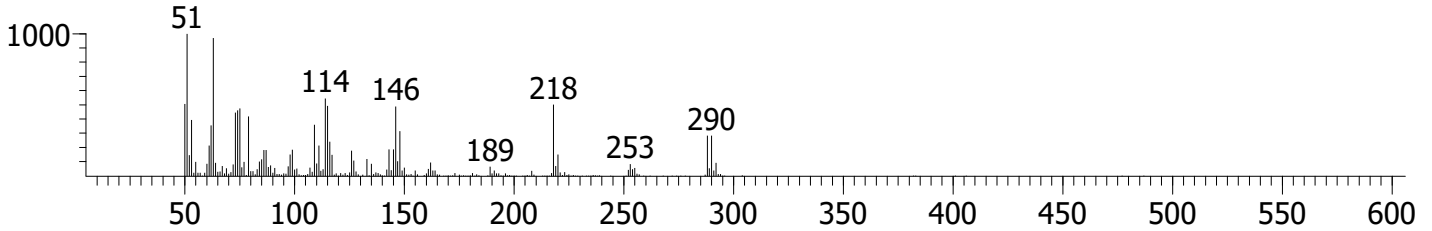
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Acridine	807	3584	260-94-6	mainlib	C13H9N	179
2	Phenanthridine	801	2817	229-87-8	mainlib	C13H9N	179
3	Benzo[f]quinoline	775	844	85-02-9	mainlib	C13H9N	179
4	Acridine-9-carbaldehyde	763	562	0-00-0	mainlib	C14H9NO	207
5	p-Phenylbenzotrile	752	385	2920-38-9	mainlib	C13H9N	179

Triclosan

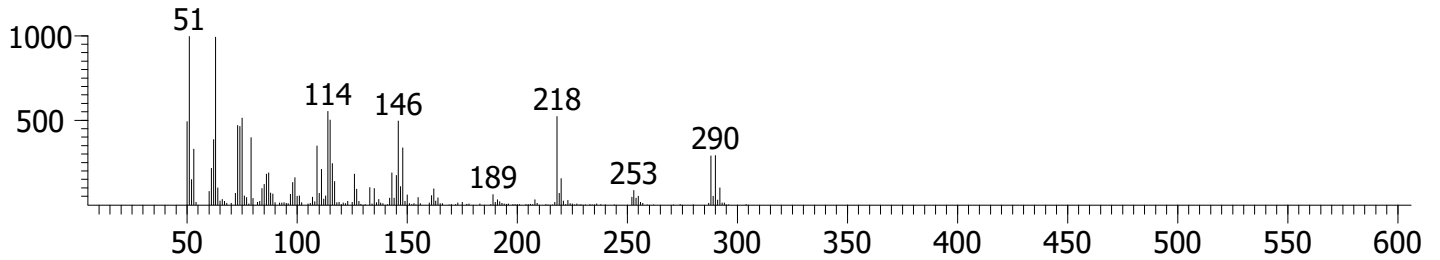
1st Dimension R.T. = 1910.68
 2nd Dimension R.T. = 2.125
 Quant Mass(es) = 218
 S/N = 928.03
 Area = 104651
 Height = 10772
 Similarity = 847



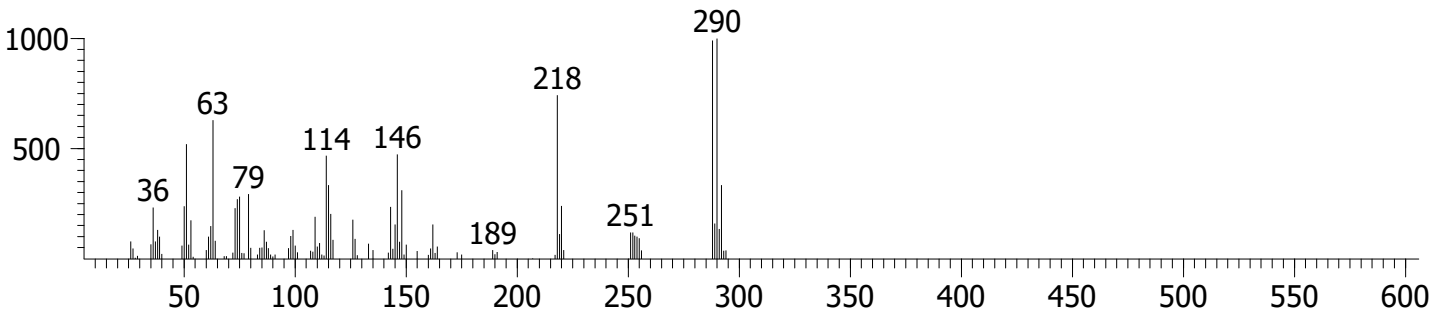
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2911, at 1910.68 , 2.125 sec , sec (Spec # 2170 92)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2911, at 1910.68 , 2.125 sec , sec (Spec # 2170 92)



Library Hit - similarity 847, "Triclosan"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Triclosan	847	9845	3380-34-5	mainlib	C ₁₂ H ₇ Cl ₃ O ₂	288
2	Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-, acetate	643	98	4623-99-8	mainlib	C ₁₄ H ₉ Cl ₃ O ₃	330
3	6-Chloro-N-(2-chlorophenyl)quinolin-4-amine	620	35	0-00-0	mainlib	C ₁₅ H ₁₀ Cl ₂ N ₂	288
4	6-Chloro-N-(3-chlorophenyl)quinolin-4-amine	588	9	0-00-0	mainlib	C ₁₅ H ₁₀ Cl ₂ N ₂	288
5	1,1'-Biphenyl, 2,3,3',4,4',5-hexachloro-	498	0	38380-08-4	mainlib	C ₁₂ H ₄ Cl ₆	358

Benzene.

4-chloro-1-(2,4-dichlorophenoxy)-2-methoxy-

1st Dimension R.T. = 1921.18

2nd Dimension R.T. = 2.178

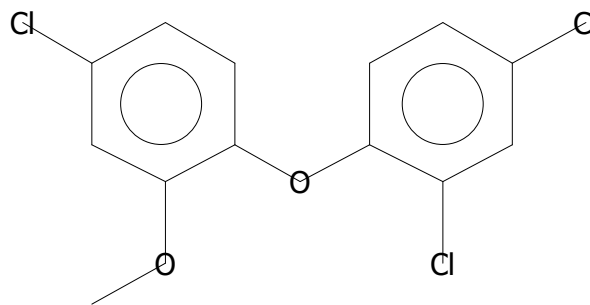
Quant Mass(es) = 252

S/N = 1389.9

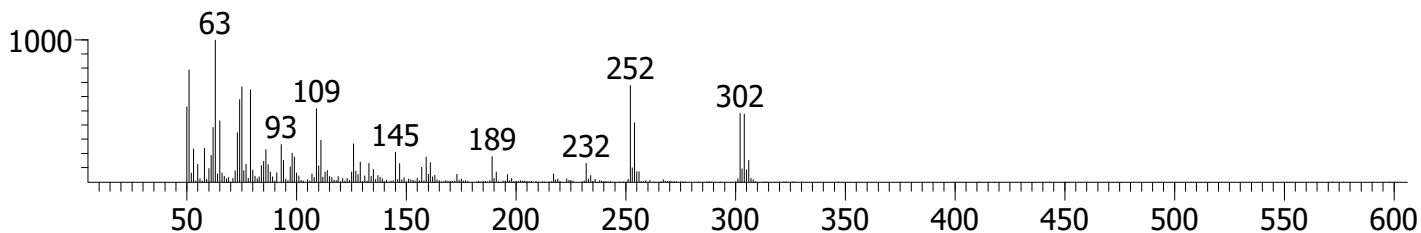
Area = 93740

Height = 9329.4

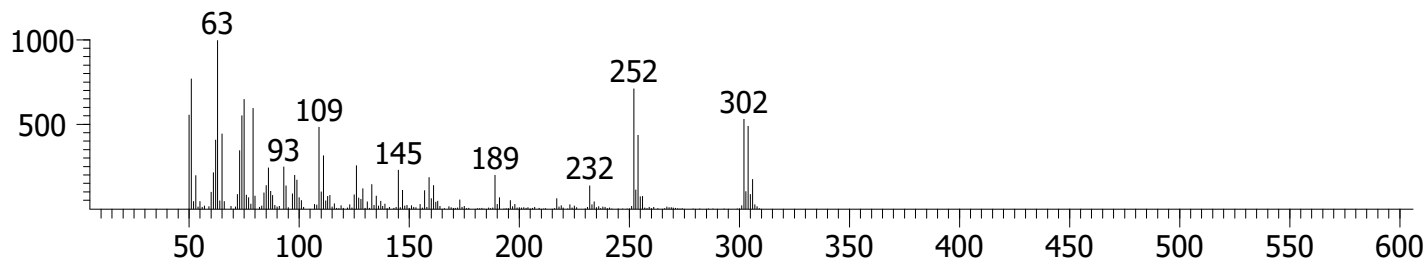
Similarity = 855



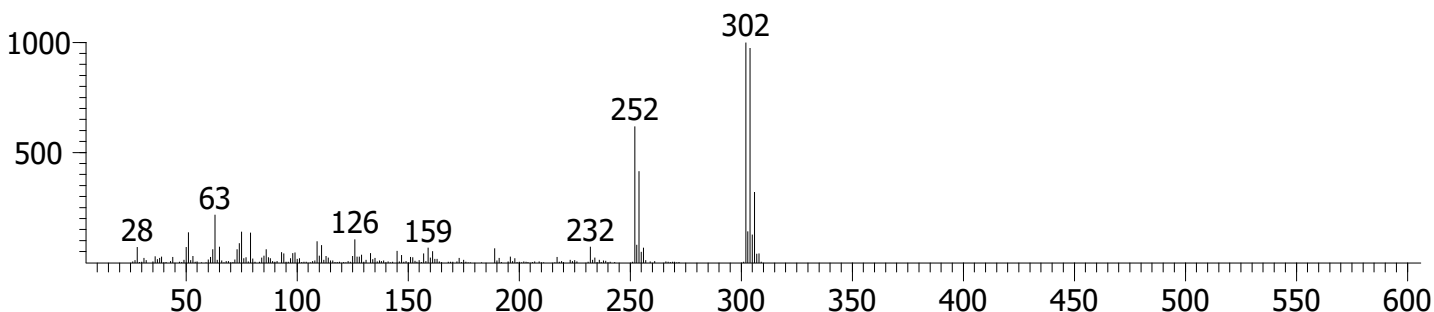
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2926, at 1921.18 , 2.178 sec , sec (Spec # 2186 90)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2926, at 1921.18 , 2.178 sec , sec (Spec # 2186 90)



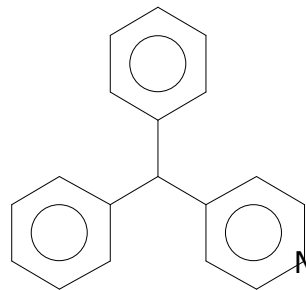
Library Hit - similarity 855, "Benzene, 4-chloro-1-(2,4-dichlorophenoxy)-2-methoxy-"



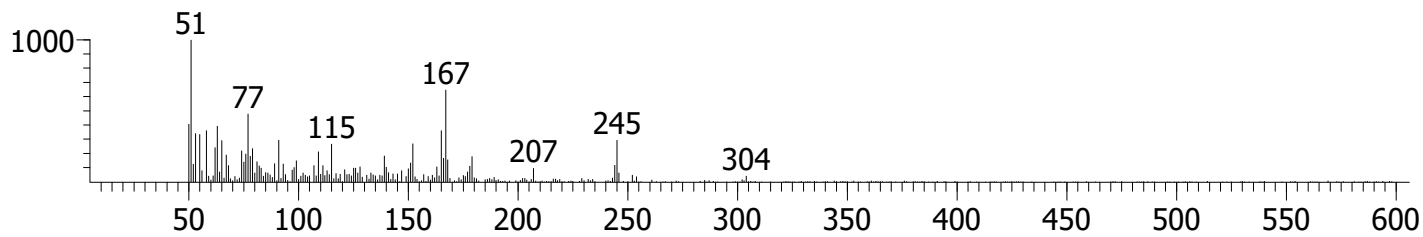
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 4-chloro-1-(2,4-dichlorophenoxy)-2-methoxy-	855	9773	4640-01-1	mainlib	C13H9Cl3O2	302
2	Dibenzo[b,e][1,4]dioxin, 2,3-dichloro-	559	97	29446-15-9	mainlib	C12H6Cl2O2	252
3	1,6-Methano-1H-indene, 2,3,4,5,7-pentachloro-3a,6,7,7a-tetrahydro-	517	21	69743-79-9	mainlib	C10H7Cl5	302
4	5-Bromo-2,2,3,3-tetrafluoro-2,3-dihydrobenzo[b]thiophen-1-oxide	506	15	146431-26-7	mainlib	C8H3BrF4OS	302
5	4-Chloro-2-methoxyphenol, pentafluoropropionate	500	11	0-00-0	mainlib	C10H6ClF5O3	304

Pyridine, 4-(diphenylmethyl)-

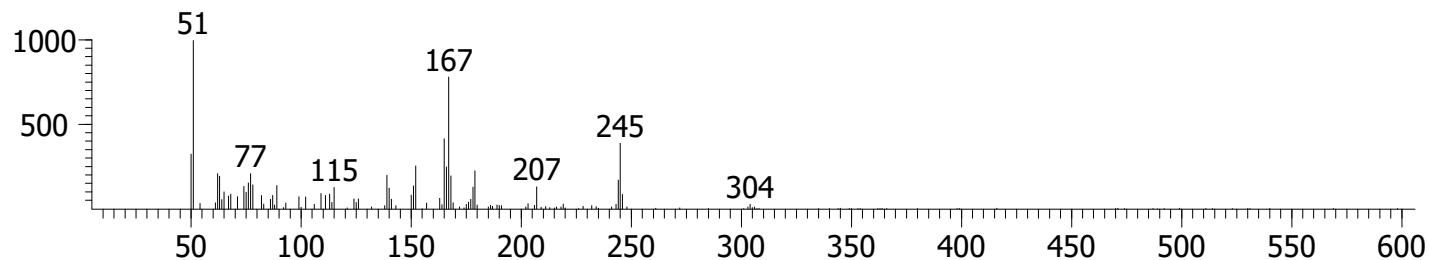
1st Dimension R.T. = 1921.18
2nd Dimension R.T. = 2.402
Quant Mass(es) = 167
S/N = 229.97
Area = 36379
Height = 2862.6
Similarity = 716



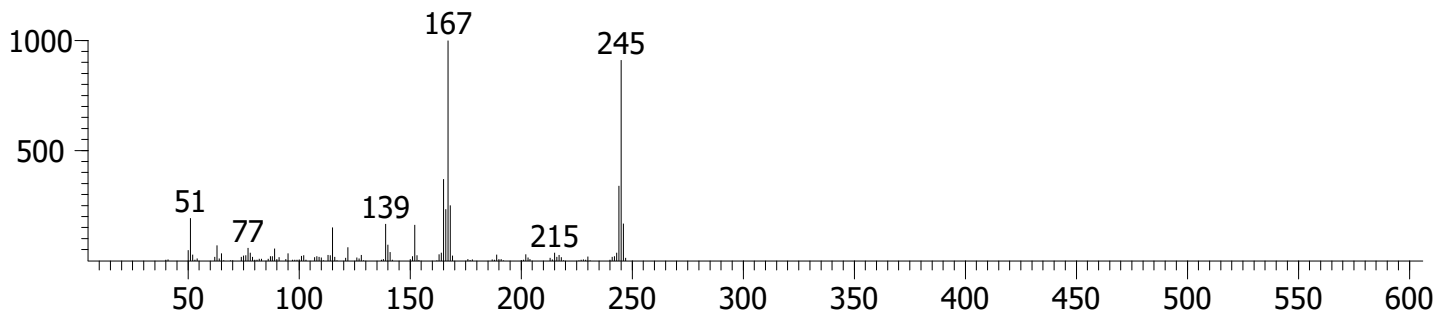
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2929, at 1921.18 , 2.402 sec , sec (Spec # 2187 24)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2929, at 1921.18 , 2.402 sec , sec (Spec # 2187 24)



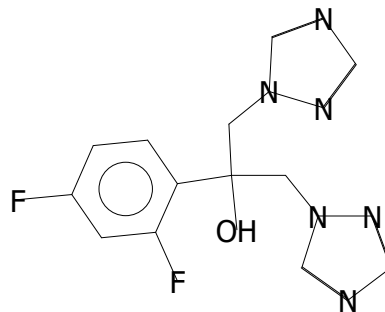
Library Hit - similarity 716, "Pyridine, 4-(diphenylmethyl)-"



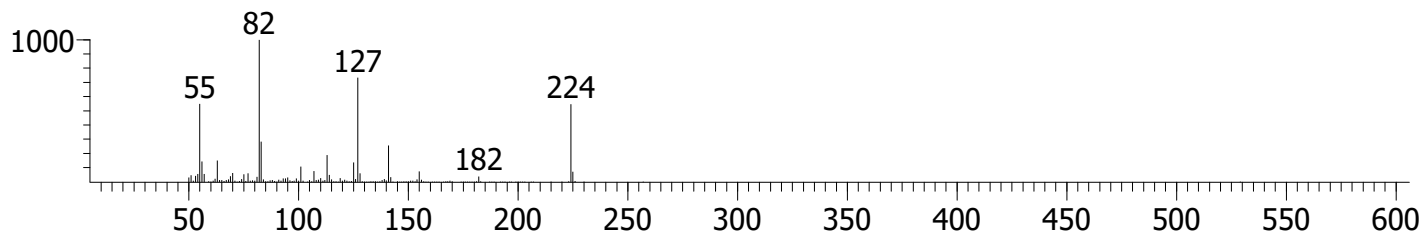
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pyridine, 4-(diphenylmethyl)-	716	3605	3678-72-6	mainlib	C18H15N	245
2	Pyridine, 3-(diphenylmethyl)-	700	2076	3678-71-5	mainlib	C18H15N	245
3	Pyridine, 2-(diphenylmethyl)-	698	1915	3678-70-4	mainlib	C18H15N	245
4	Benzene, 1,1'-(2,2-dichloroethylidene)bis-	680	987	2387-16-8	mainlib	C14H12Cl2	250
5	4-Benzylphenylacetonitrile	655	301	101096-72-4	mainlib	C15H13N	207

Fluconazole

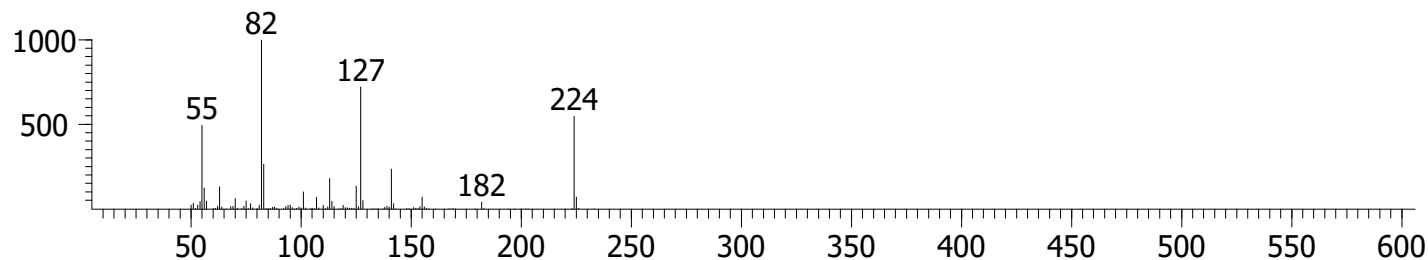
1st Dimension R.T. = 1938.67
 2nd Dimension R.T. = 2.442
 Quant Mass(es) = 224
 S/N = 3820.1
 Area = 378309
 Height = 32993
 Similarity = 908



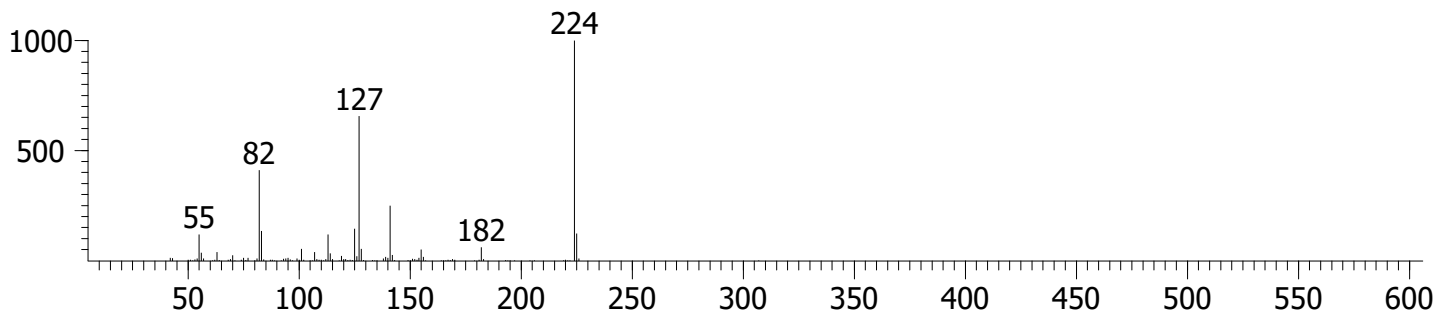
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 2959, at 1938.67 , 2.442 sec , sec (Spec # 2213 80)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 2959, at 1938.67 , 2.442 sec , sec (Spec # 2213 80)



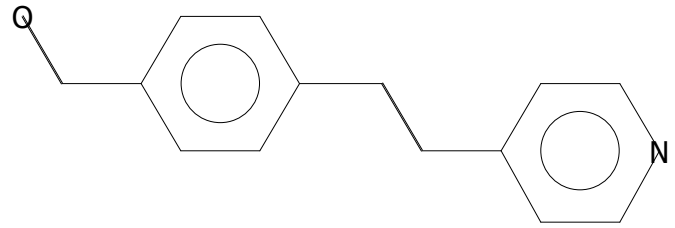
Library Hit - similarity 908, "Fluconazole"



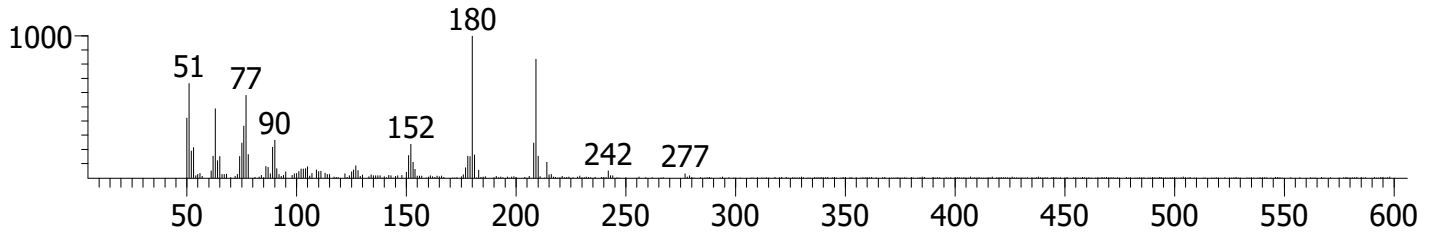
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Fluconazole	908	9347	86386-73-4	mainlib	C ₁₃ H ₁₂ F ₂ N ₆ O	306
2	3-Naphthalen-2-yl-3-piperidin-1-yl-propan-1-ol	524	93	0-00-0	mainlib	C ₁₈ H ₂₃ NO	269
3	Voriconazole	509	56	137234-62-9	mainlib	C ₁₆ H ₁₄ F ₃ N ₅ O	349
4	1,3,2-Dioxaborolane, 2-(cyclohexyloxy)-	505	47	55089-04-8	mainlib	C ₈ H ₁₅ BO ₃	170
5	1-[2-(2,4-Difluoro-phenyl)-oxiranylmethyl]-1H-[1,2,4]triazole	503	44	0-00-0	mainlib	C ₁₁ H ₉ F ₂ N ₃ O	237

4-(2-(4-Formylphenyl)ethenyl)pyridine

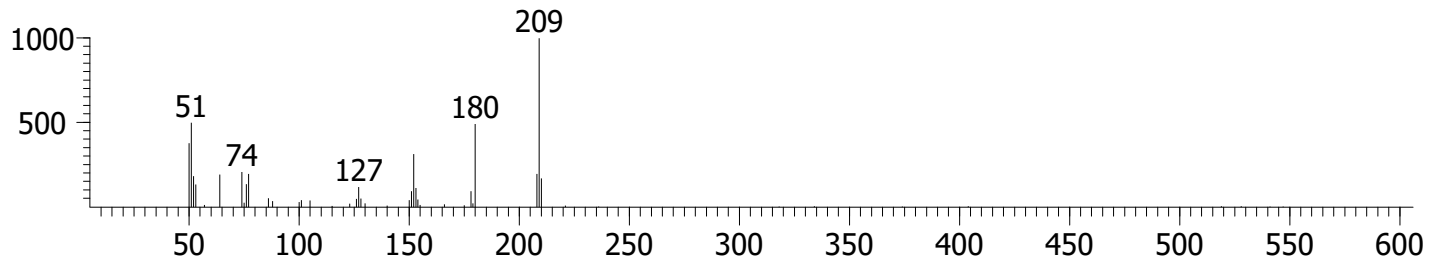
1st Dimension R.T. = 1970.15
2nd Dimension R.T. = 2.805
Quant Mass(es) = 209
S/N = 305.85
Area = 44343
Height = 3399.4
Similarity = 816



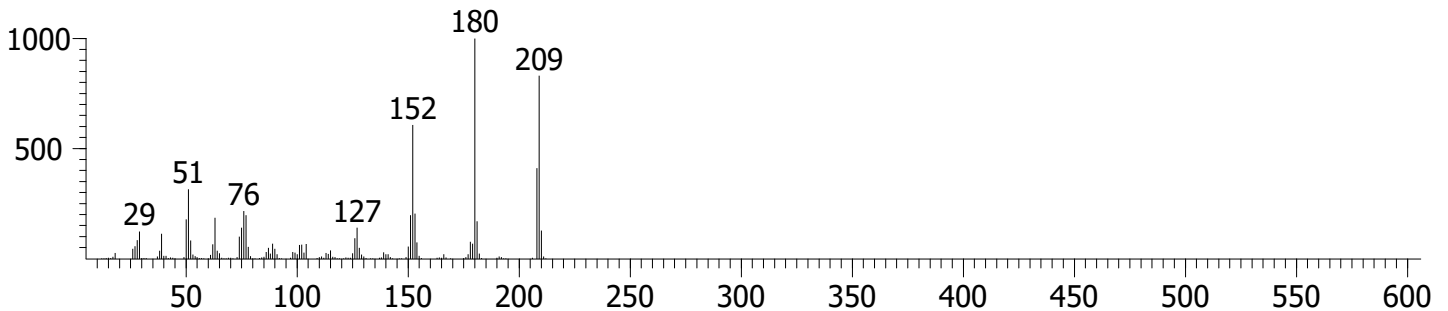
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3005, at 1970.15 , 2.805 sec , sec (Spec # 2262 05)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3005, at 1970.15 , 2.805 sec , sec (Spec # 2262 05)



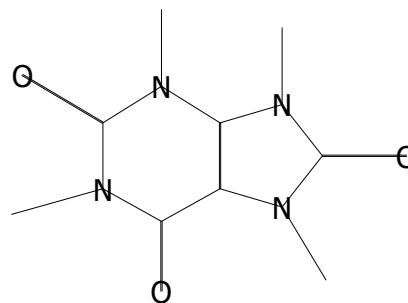
Library Hit - similarity 816, "4-(2-(4-Formylphenyl)ethenyl)pyridine"



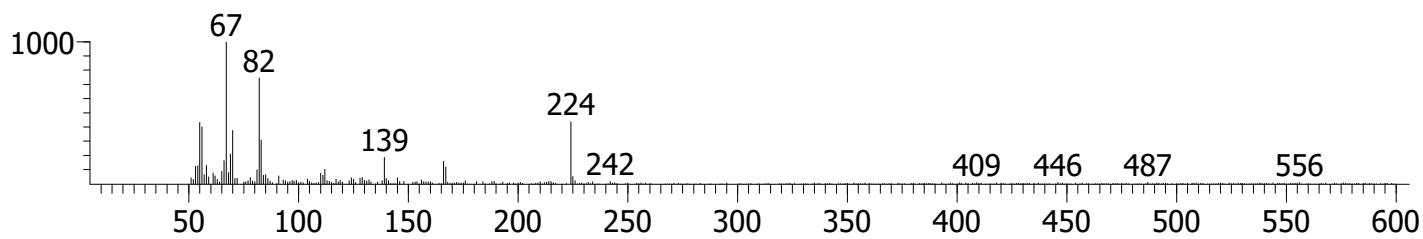
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-(2-(4-Formylphenyl)ethenyl)pyridine	816	2704	74401-03-9	mainlib	C14H11NO	209
2	5-Benzofuranamine, 2-phenyl-	805	1855	0-00-0	mainlib	C14H11NO	209
3	4-Methyl-acridone	804	1783	68506-36-5	mainlib	C14H11NO	209
4	5,11-Dihydro-10H-dibenzo[b,f]azepin-10-one	795	1294	21737-58-6	mainlib	C14H11NO	209
5	Benzo[f]quinolin-1-ol, 3-methyl-	772	472	1210-03-3	mainlib	C14H11NO	209

1,3,7,9-Tetramethyluric acid

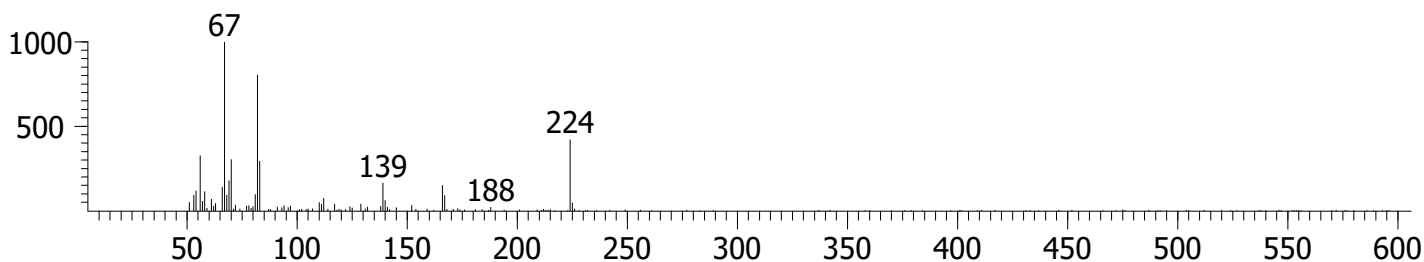
1st Dimension R.T. = 2036.61
2nd Dimension R.T. = 3.010
Quant Mass(es) = 224
S/N = 163.87
Area = 21481
Height = 1768.8
Similarity = 807



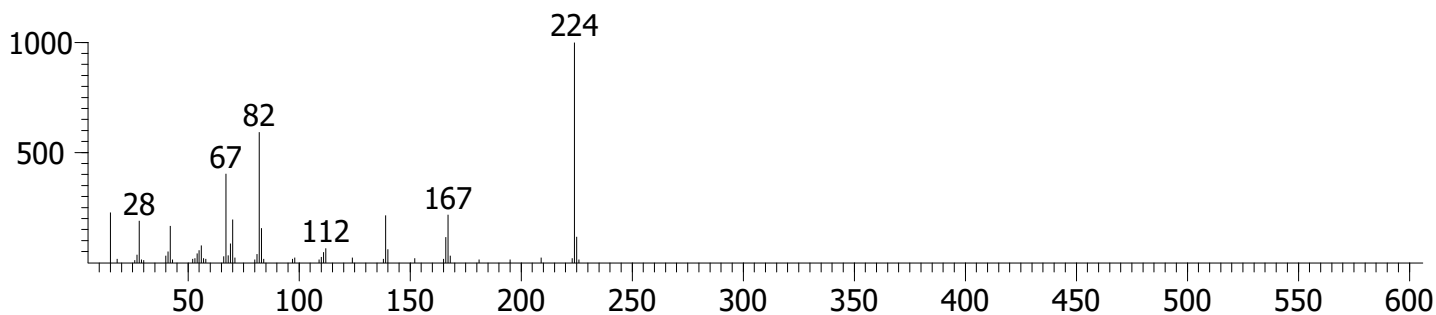
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3079, at 2036.61 , 3.010 sec , sec (Spec # 2363 06)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3079, at 2036.61 , 3.010 sec , sec (Spec # 2363 06)



Library Hit - similarity 807, "1,3,7,9-Tetramethyluric acid"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,3,7,9-Tetramethyluric acid	807	9390	2309-49-1	mainlib	C9H12N4O3	224
2	1H-Purine-2,6-dione, 3,7-dihydro-8-(hydroxymethyl)-1,3,7-trimethyl-	633	191	4921-51-1	mainlib	C9H12N4O3	224
3	Acetic acid, trifluoro-, cyclohexyl ester	559	25	1549-45-7	mainlib	C8H11F3O2	196
4	1H-1,2,3-Triazole-5-carboxylic acid, 1-(4-amino-1,2,5-oxadiazol-3-yl)-4-methyl-, methyl ester	559	25	0-00-0	mainlib	C7H8N6O3	224
5	Cyclohexanol, 2-(aminomethyl)-, trans-	544	15	5691-09-8	mainlib	C7H15NO	129

1,2-Benzenedicarboxylic acid,
2-butoxyethyl butyl ester

1st Dimension R.T. = 2064.59

2nd Dimension R.T. = 2.066

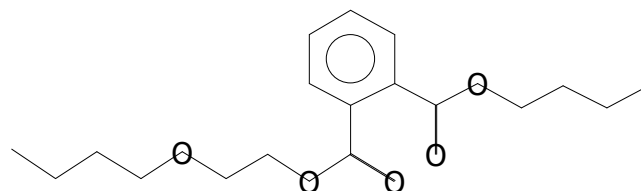
Quant Mass(es) = 149

S/N = 502.35

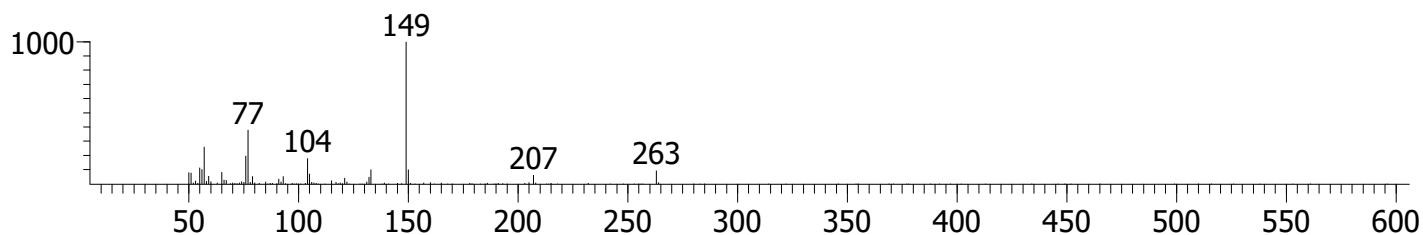
Area = 68186

Height = 6414.7

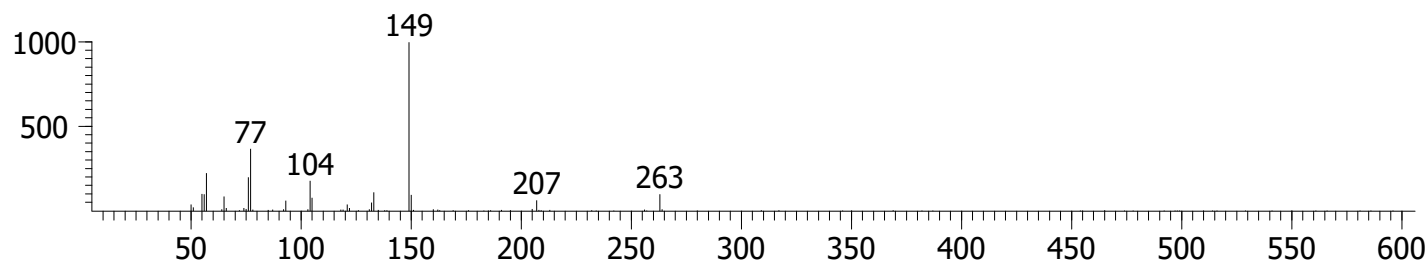
Similarity = 893



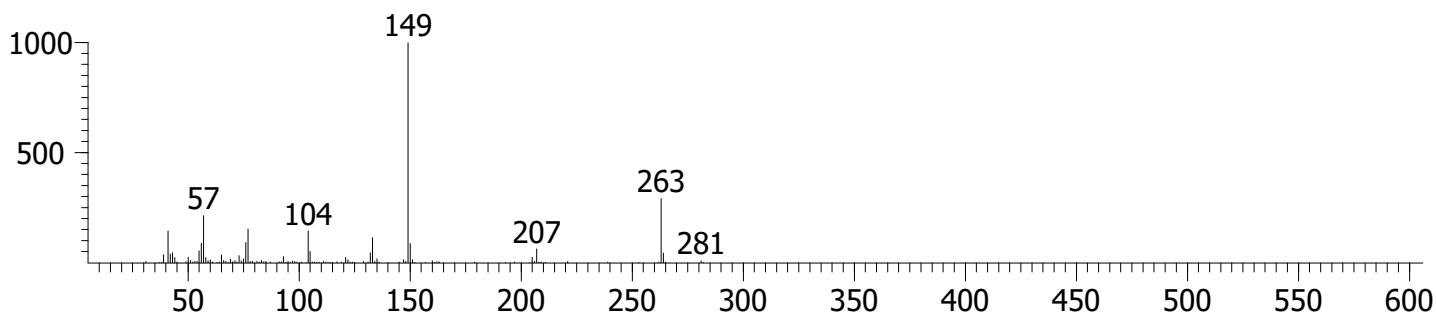
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3109, at 2064.59 , 2.066 sec , sec (Spec # 2404 03)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3109, at 2064.59 , 2.066 sec , sec (Spec # 2404 03)

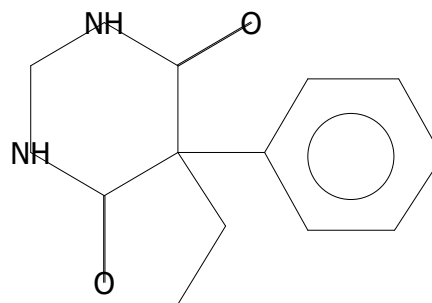


Library Hit - similarity 893, "1,2-Benzenedicarboxylic acid, 2-butoxyethyl butyl ester"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,2-Benzenedicarboxylic acid, 2-butoxyethyl butyl ester	893	8095	33374-28-6	mainlib	C18H26O5	322
2	Phthalic acid, butyl ester, ester with butyl glycolate	808	728	85-70-1	mainlib	C18H24O6	336
3	Phthalic acid, heptyl pentyl ester	740	110	0-00-0	mainlib	C20H30O4	334
4	Phthalic acid, 2-chloropropyl isobutyl ester	739	106	0-00-0	mainlib	C15H19ClO4	298
5	Phthalic acid, isobutyl octyl ester	731	79	0-00-0	mainlib	C20H30O4	334

Primidone



1st Dimension R.T. = 2064.59

2nd Dimension R.T. = 3.485

Quant Mass(es) = 146

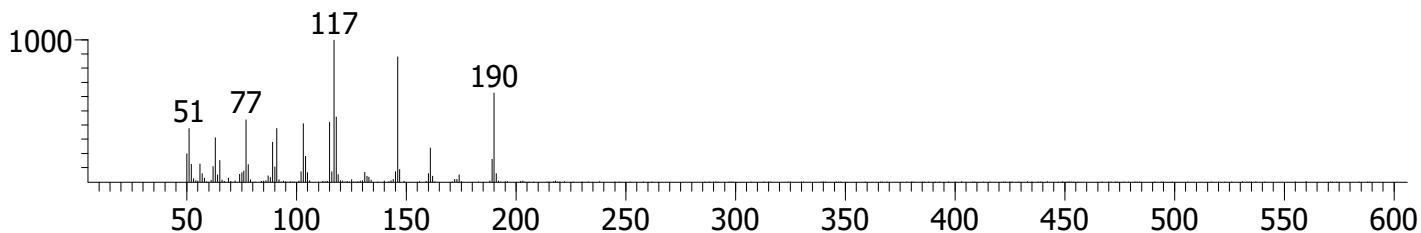
S/N = 625.69

Area = 132903

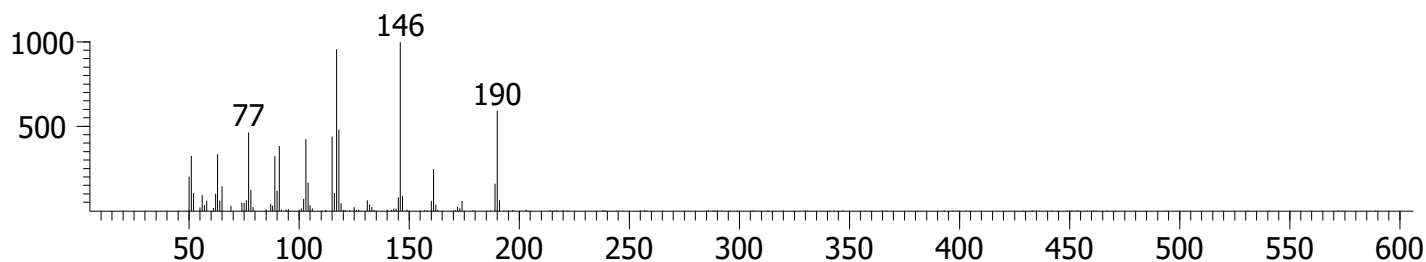
Height = 9054.8

Similarity = 833

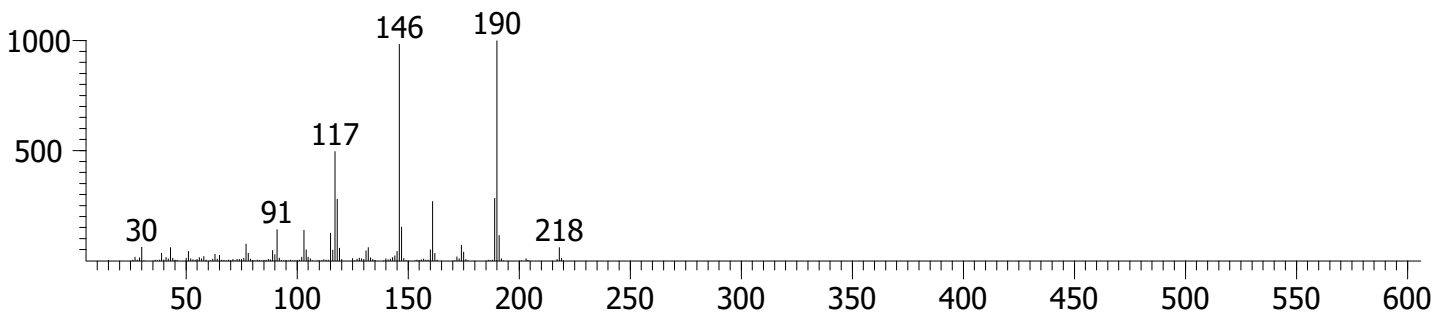
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3110, at 2064.59 , 3.485 sec , sec (Spec # 2406 18)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3110, at 2064.59 , 3.485 sec , sec (Spec # 2406 18)



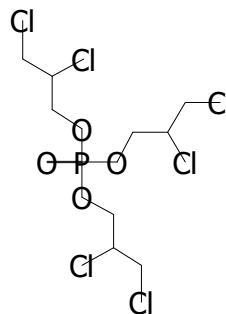
Library Hit - similarity 833, "Primidone"



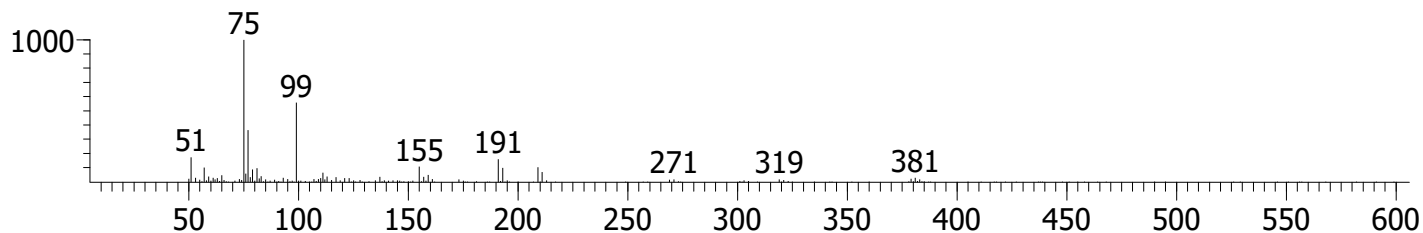
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Primidone	833	7730	125-33-7	mainlib	C12H14N2O2	218
2	2,4-Azetidinedione, 3-ethyl-3-phenyl-	726	513	42282-82-6	mainlib	C11H11NO2	189
3	Primidone, N,N'-diacetyl-	715	352	0-00-0	mainlib	C16H18N2O4	302
4	7-Methylindan-1-one	710	283	39627-61-7	mainlib	C10H10O	146
5	3-Ethyl-3-phenyl-1-methylazetidin-2,4-dione	690	129	0-00-0	mainlib	C12H13NO2	203

1-Propanol, 2,3-dichloro-, phosphate (3:1)

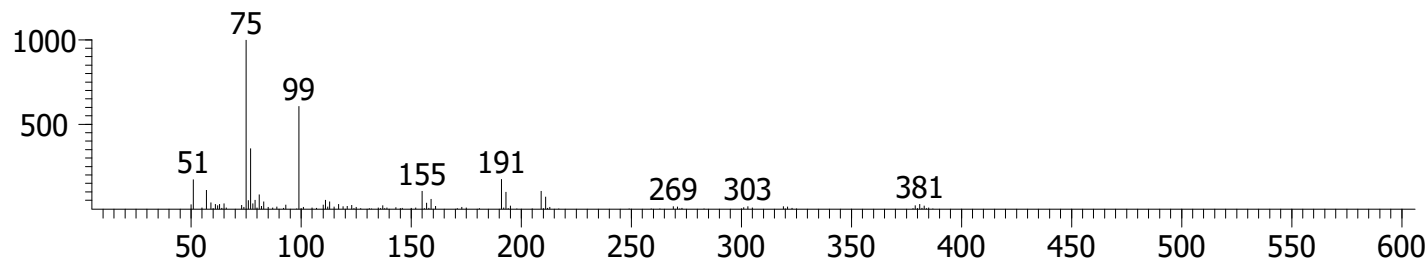
1st Dimension R.T. = 2092.58
2nd Dimension R.T. = 2.178
Quant Mass(es) = 75
S/N = 618.56
Area = 190283
Height = 16470
Similarity = 884



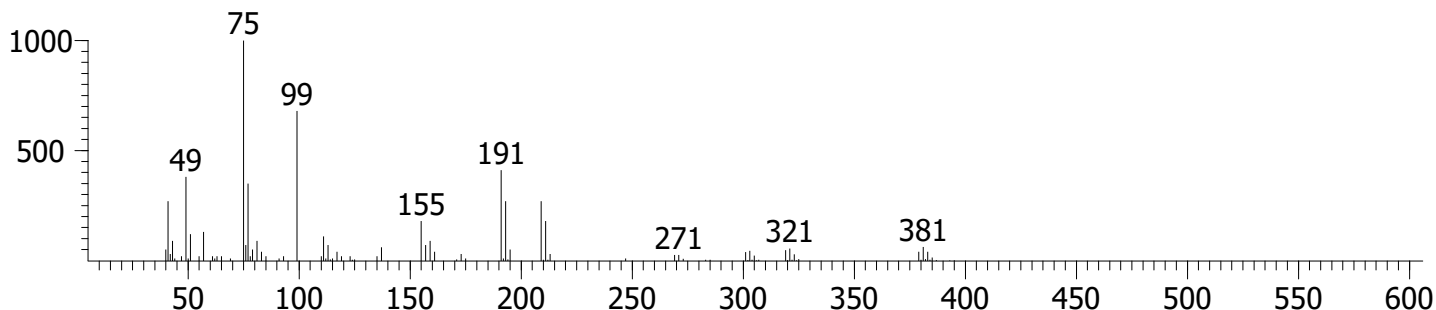
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3141, at 2092.58 , 2.178 sec , sec (Spec # 2446 60)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3141, at 2092.58 , 2.178 sec , sec (Spec # 2446 60)



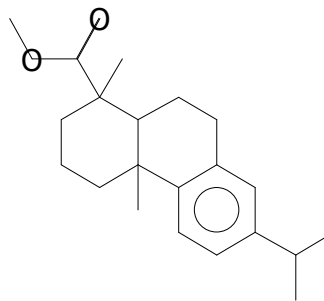
Library Hit - similarity 884, "1-Propanol, 2,3-dichloro-, phosphate (3:1)"



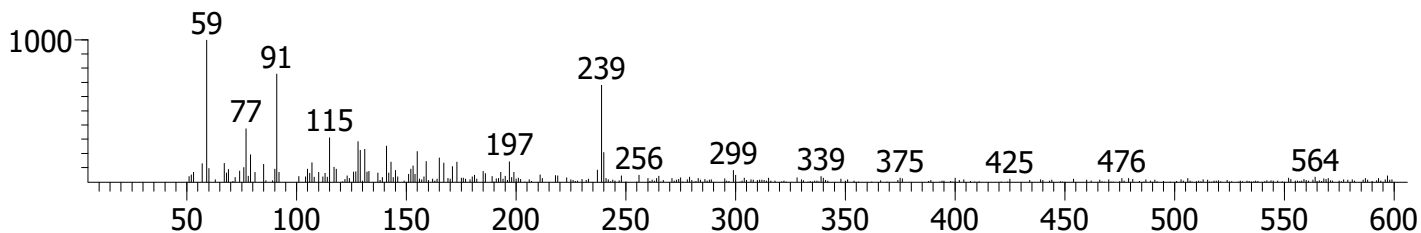
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1-Propanol, 2,3-dichloro-, phosphate (3:1)	884	9573	78-43-3	mainlib	C9H15Cl6O4P	428
2	Tris(1,3-dichloroisopropyl)phosphate	756	410	13674-87-8	mainlib	C9H15Cl6O4P	428
3	Phosphoric acid, bis[2-chloro-1-(chloromethyl)ethyl] 2,3-dichloropropyl ester	614	13	68460-03-7	mainlib	C9H15Cl6O4P	428
4	Propane, 2,2'-oxybis[1,3-dichloro-	527	1	59440-89-0	mainlib	C6H10Cl4O	238
5	Propane, 1,2-dichloro-3-[2-chloro-1-(chloromethyl)ethoxy]-	521	0	59440-90-3	mainlib	C6H10Cl4O	238

Methyl dehydroabietate

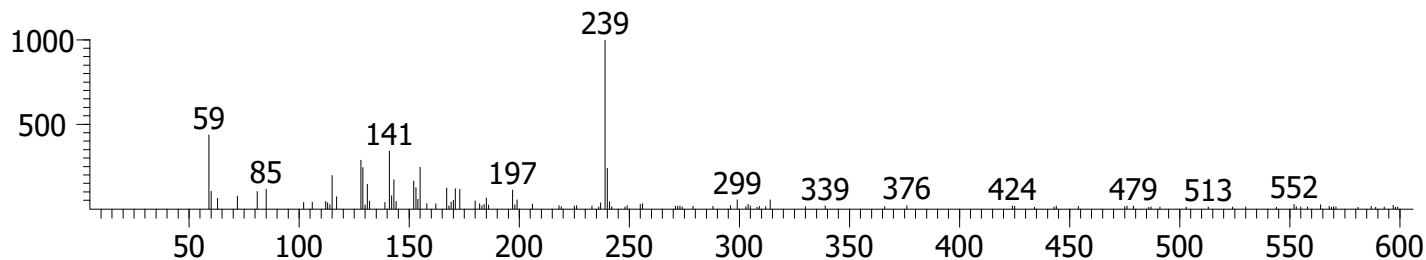
1st Dimension R.T. = 2103.07
 2nd Dimension R.T. = 2.059
 Quant Mass(es) = 239
 S/N = 78.094
 Area = 5732.3
 Height = 514.60
 Similarity = 805



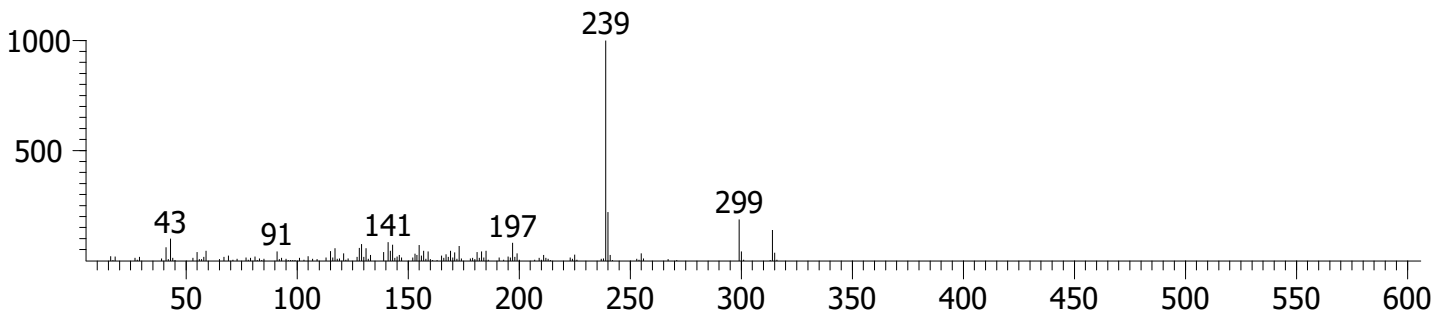
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3153, at 2103.07 , 2.059 sec , sec (Spec # 2462 32)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3153, at 2103.07 , 2.059 sec , sec (Spec # 2462 32)



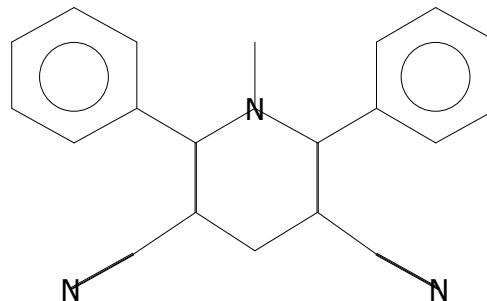
Library Hit - similarity 805, "Methyl dehydroabietate"



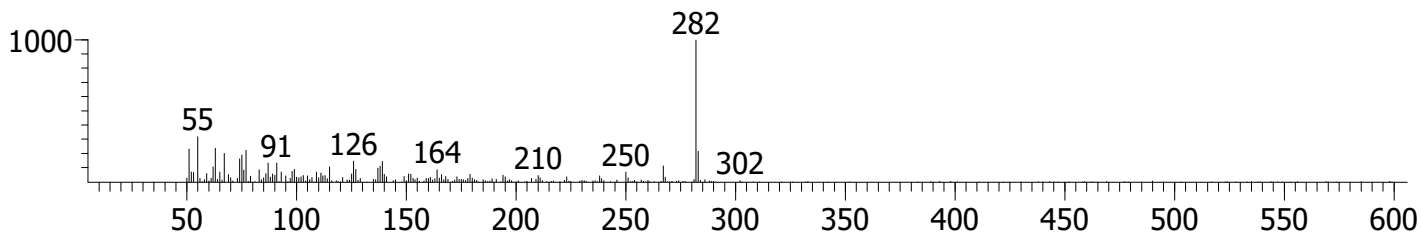
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Methyl dehydroabietate	805	9407	1235-74-1	mainlib	C21H30O2	314
2	Isobutyl dehydroabietate	672	370	0-00-0	mainlib	C24H36O2	356
3	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1S-(1à,4aà,10aà)]-	620	74	24035-60-7	mainlib	C21H30O2	314
4	Noroxycodone, N,O-bis(heptafluorobutyl)-	593	21	0-00-0	mainlib	C25H17F14NO6	693
5	1H,9H-Pyrrolo[3,2-H]quinolin-6-one, 1,2,3,8-tetramethyl-	583	15	0-00-0	mainlib	C15H16N2O	240

2,6-diphenyl-4-methyl-1,4-dihydropyridine-3,5-dicarbonitrile

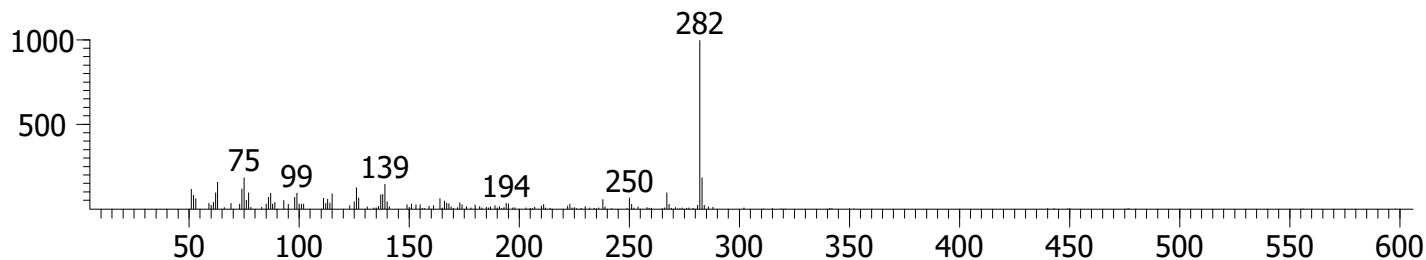
1st Dimension R.T. = 2106.57
2nd Dimension R.T. = 2.772
Quant Mass(es) = 282
S/N = 443.62
Area = 48243
Height = 3732.7
Similarity = 717



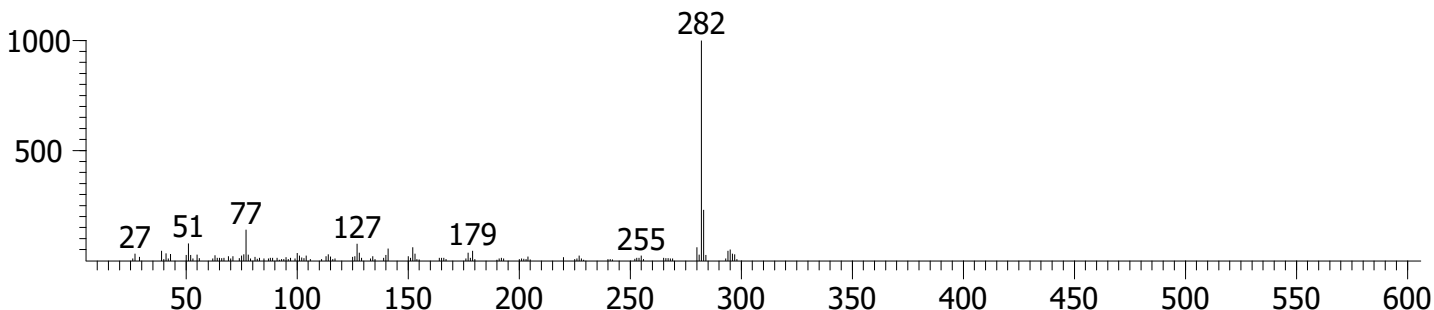
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3157, at 2106.57 , 2.772 sec , sec (Spec # 2468 70)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3157, at 2106.57 , 2.772 sec , sec (Spec # 2468 70)



Library Hit - similarity 717, "2,6-Diphenyl-4-methyl-1,4-dihydropyridine-3,5-dicarbonitrile"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,6-Diphenyl-4-methyl-1,4-dihydropyridine-3,5-dicarbonitrile	717	3626	15521-04-7	mainlib	C20H15N3	297
2	1,3,6-Trimethyl-5-[3-(2-acetylamino-2-methoxycarbonylethyl)-1H-indol-2-yl]-1,3-dihydropyrimidin-2,4-dione	689	1047	123760-39-4	mainlib	C21H24N4O5	412
3	Carbamic acid, N-[10,11-dihydro-5-(2-methylamino-1-oxoethyl)-3-5H-dibenzo[b,f]azepinyl]-, ethyl ester	682	802	102821-92-1	mainlib	C20H23N3O3	353
4	4-Methoxy-6-[2-(4-methoxyphenyl)ethynyl]-2H-1,3-benzodioxole	677	646	0-00-0	mainlib	C17H14O4	282
5	2-Methoxyethylamine, N,N-dinonyl-	670	495	0-00-0	mainlib	C21H45NO	327

Hexanedioic acid, bis(2-ethylhexyl) ester

1st Dimension R.T. = 2120.56

2nd Dimension R.T. = 1.518

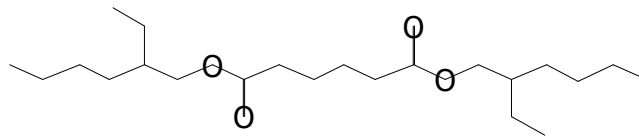
Quant Mass(es) = 129

S/N = 487.27

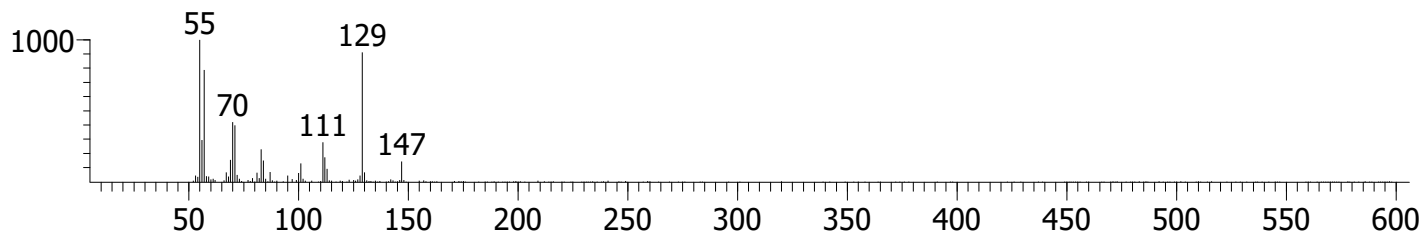
Area = 63962

Height = 8176.0

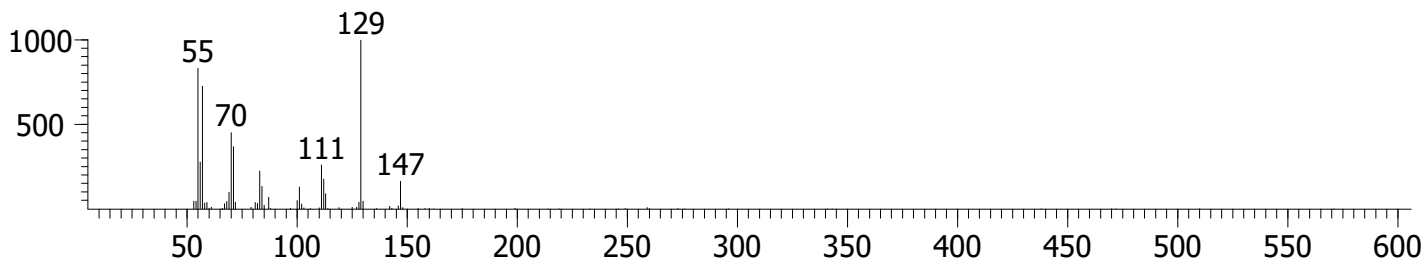
Similarity = 904



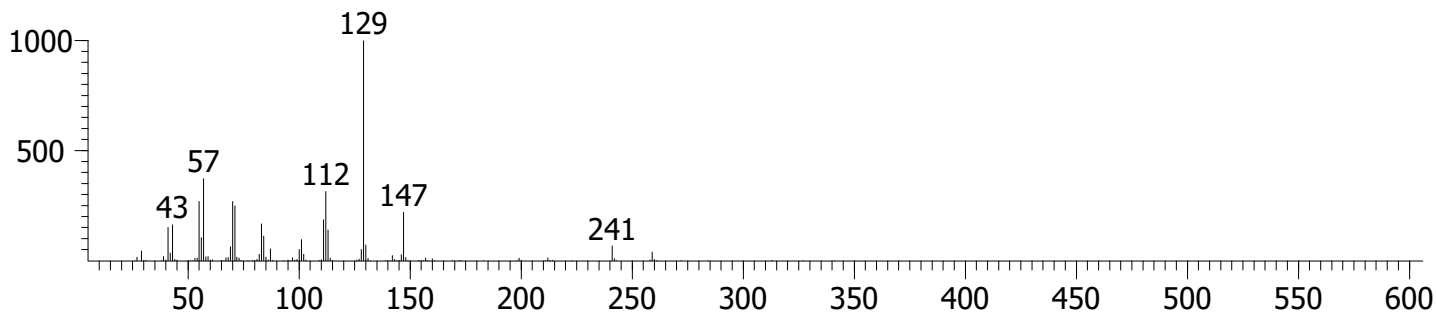
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3175, at 2120.56 , 1.518 sec , sec (Spec # 2488 00)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3175, at 2120.56 , 1.518 sec , sec (Spec # 2488 00)



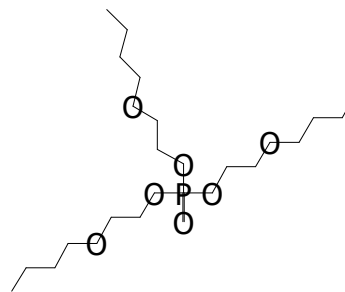
Library Hit - similarity 904, "Hexanedioic acid, bis(2-ethylhexyl) ester"



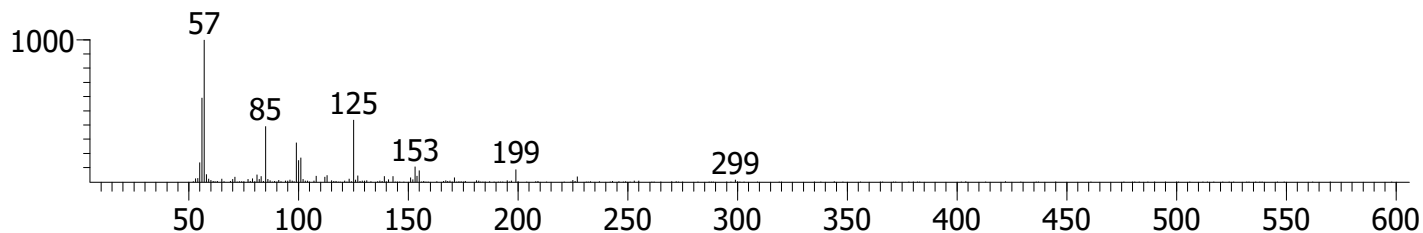
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Hexanedioic acid, bis(2-ethylhexyl) ester	904	4597	103-23-1	mainlib	C22H42O4	370
2	Diisooctyl adipate	888	2647	1330-86-5	mainlib	C22H42O4	370
3	Hexanedioic acid, mono(2-ethylhexyl)ester	832	504	4337-65-9	mainlib	C14H26O4	258
4	Hexanedioic acid, dioctyl ester	825	386	123-79-5	mainlib	C22H42O4	370
5	Adipic acid, 2-ethylhexyl pentadecyl ester	820	311	0-00-0	mainlib	C29H56O4	468

Ethanol, 2-butoxy-, phosphate (3:1)

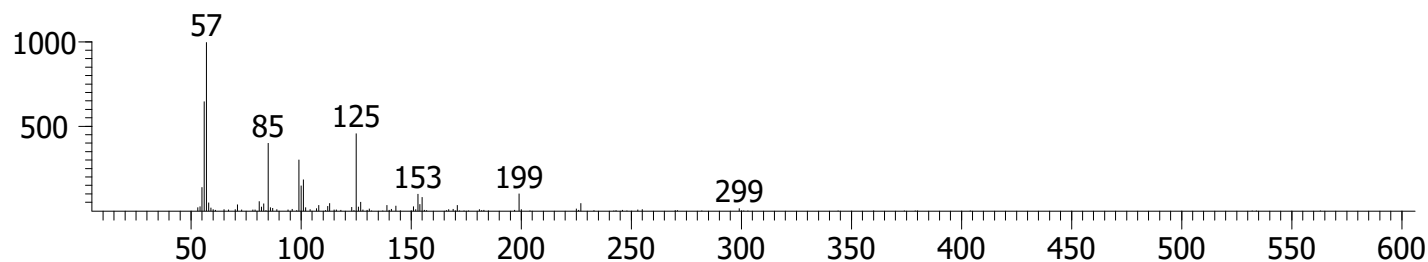
1st Dimension R.T. = 2134.55
2nd Dimension R.T. = 1.795
Quant Mass(es) = 125
S/N = 359.71
Area = 33313
Height = 3782.3
Similarity = 850



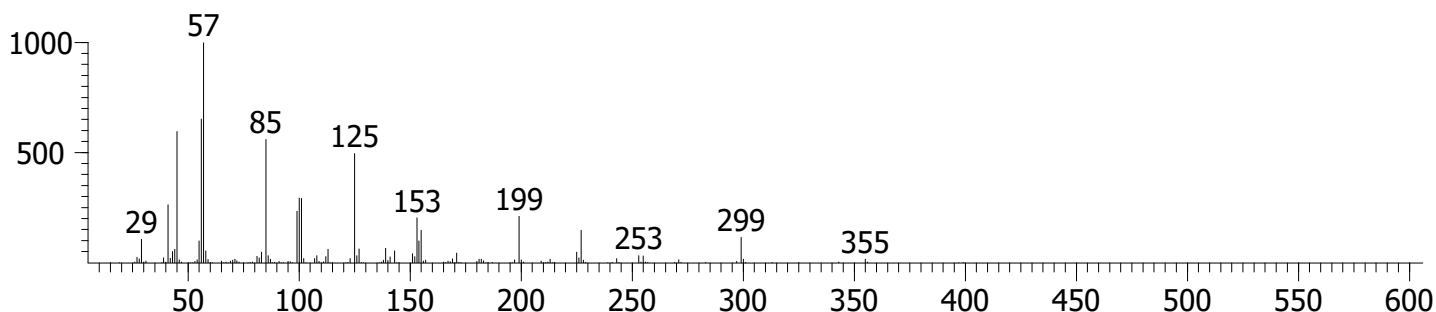
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3191, at 2134.55 , 1.795 sec , sec (Spec # 2509 62)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3191, at 2134.55 , 1.795 sec , sec (Spec # 2509 62)



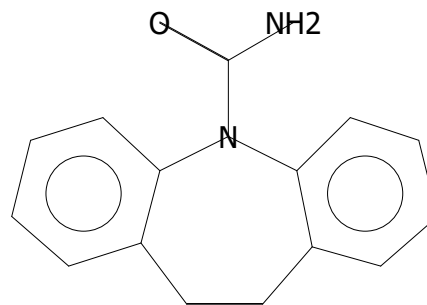
Library Hit - similarity 850, "Ethanol, 2-butoxy-, phosphate (3:1)"



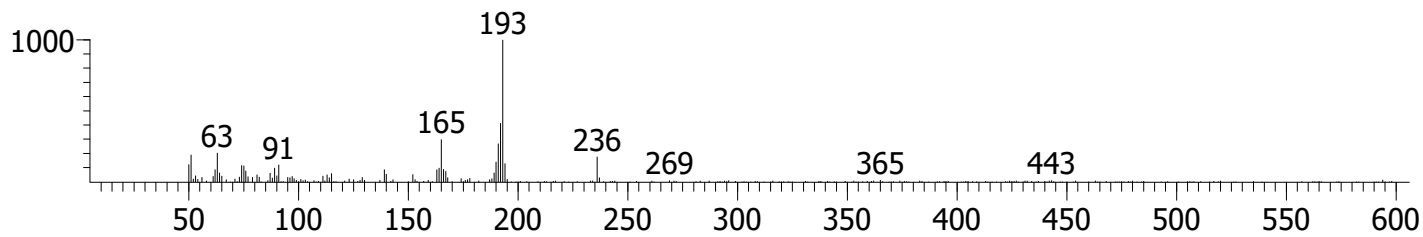
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanol, 2-butoxy-, phosphate (3:1)	850	9332	78-51-3	mainlib	C18H39O7P	398
2	2,2,7,7-Tetramethyloctane	592	93	1071-31-4	mainlib	C12H26	170
3	Butyl lactate	591	89	138-22-7	mainlib	C7H14O3	146
4	Heptane, 2,2,4,6,6-pentamethyl-	590	86	13475-82-6	mainlib	C12H26	170
5	Hexane, 2-methyl-	583	66	591-76-4	mainlib	C7H16	100

Carbamazepine

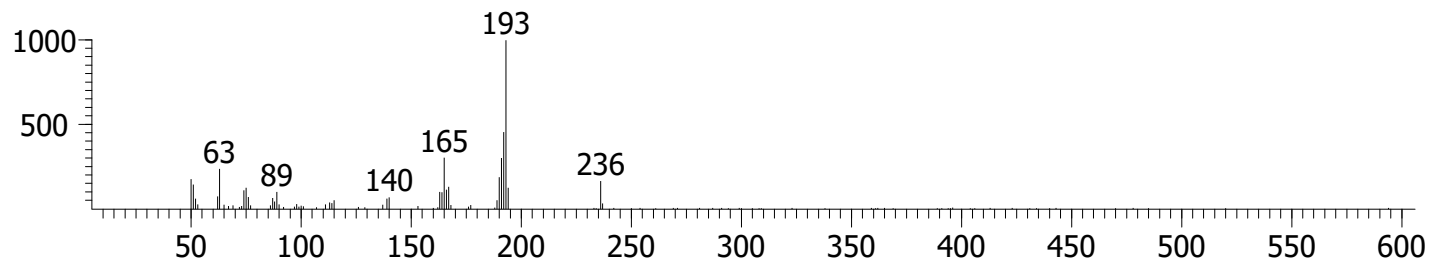
1st Dimension R.T. = 2134.55
2nd Dimension R.T. = 3.247
Quant Mass(es) = 193
S/N = 210.33
Area = 53165
Height = 3873.5
Similarity = 881



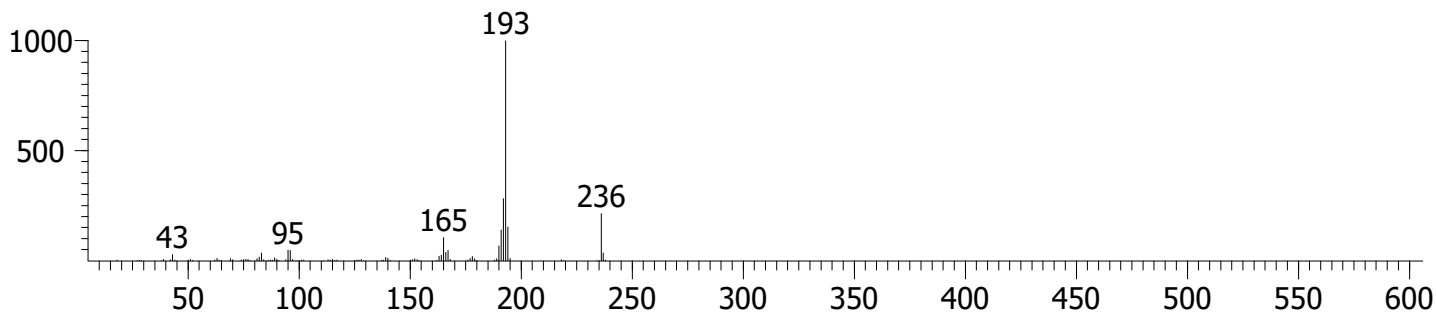
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3193, at 2134.55 , 3.247 sec , sec (Spec # 251182)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3193, at 2134.55 , 3.247 sec , sec (Spec # 251182)



Library Hit - similarity 881, "Carbamazepine"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Carbamazepine	881	4728	298-46-4	mainlib	C15H12N2O	236
2	5-Acetyl-5H-dibenz[b,f]azepine	853	1365	19209-60-0	mainlib	C16H13NO	235
3	3-Methyl-acridine	844	991	4740-12-9	mainlib	C14H11N	193
4	2-Phenylindolizine	837	759	25379-20-8	mainlib	C14H11N	193
5	Iminostilbene	827	536	256-96-2	mainlib	C14H11N	193

Triphenyl phosphate

1st Dimension R.T. = 2148.55

2nd Dimension R.T. = 2.627

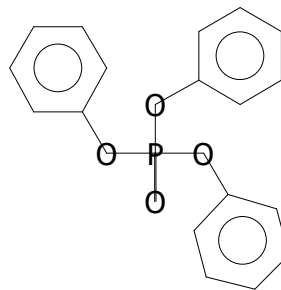
Quant Mass(es) = 326

S/N = 65.888

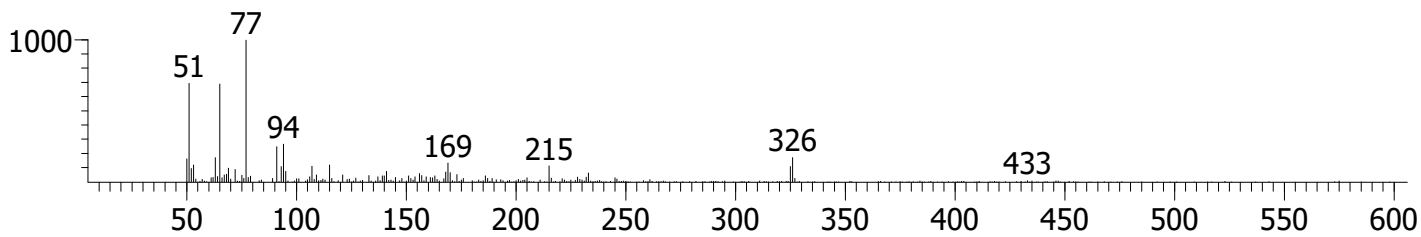
Area = 4181.2

Height = 373.64

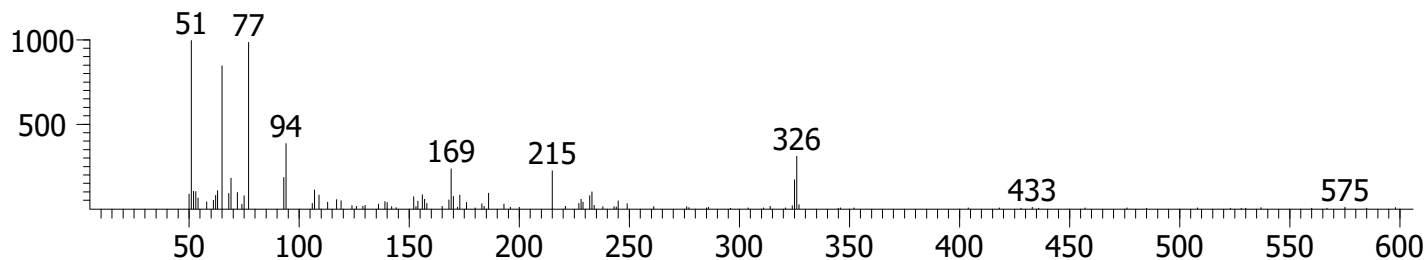
Similarity = 662



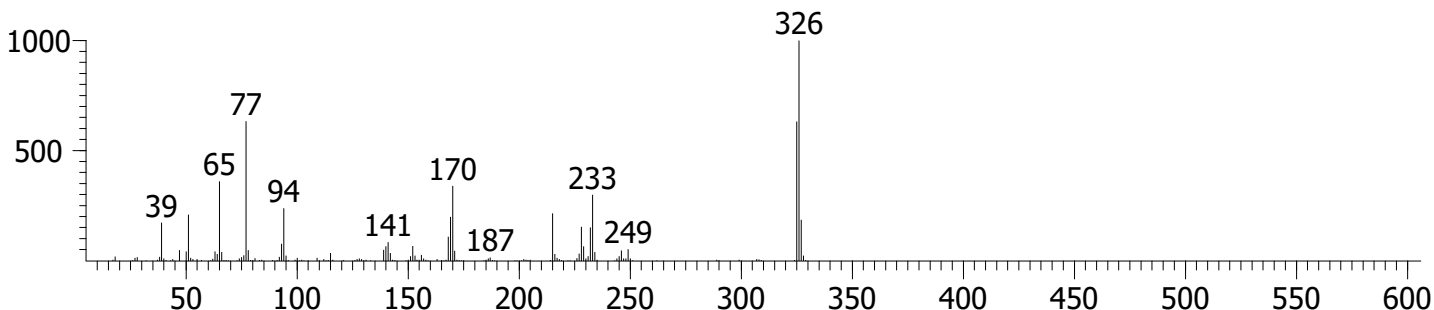
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3209, at 2148.55 , 2.627 sec , sec (Spec # 2532 08)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3209, at 2148.55 , 2.627 sec , sec (Spec # 2532 08)



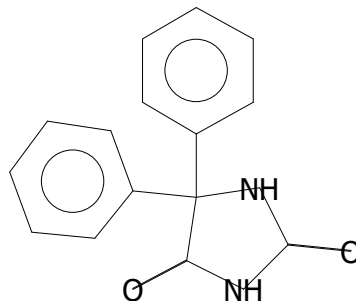
Library Hit - similarity 662, "Triphenyl phosphate"



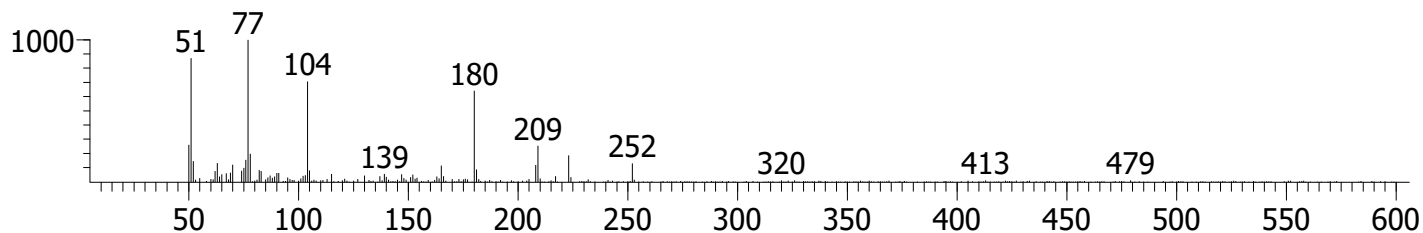
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Triphenyl phosphate	662	8754	115-86-6	mainlib	C18H15O4P	326
2	2-[(4-Fluorophenyl)carbonyl]-5H,6H,7H,8H-thieno[2,3-b]quinolin-3-amine	485	168	0-00-0	mainlib	C18H15FN2OS	326
3	Metaraminol	484	161	54-49-9	mainlib	C9H13NO2	167
4	Pyridazine-3,4,5(2H)-trione, 6-(4-chlorophenyl)-, 5-phenylhydrazone	480	136	299921-97-4	mainlib	C16H11ClN4O2	326
5	Phosphinic acid, di(phenoxymethyl)-	472	101	21993-10-2	mainlib	C14H15O4P	278

Phenytoin

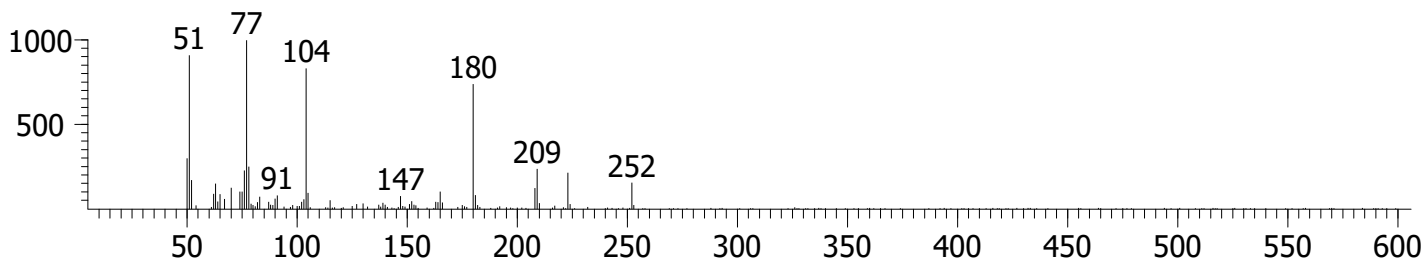
1st Dimension R.T. = 2148.55
 2nd Dimension R.T. = 3.003
 Quant Mass(es) = 180
 S/N = 254.08
 Area = 40958
 Height = 2952.5
 Similarity = 859



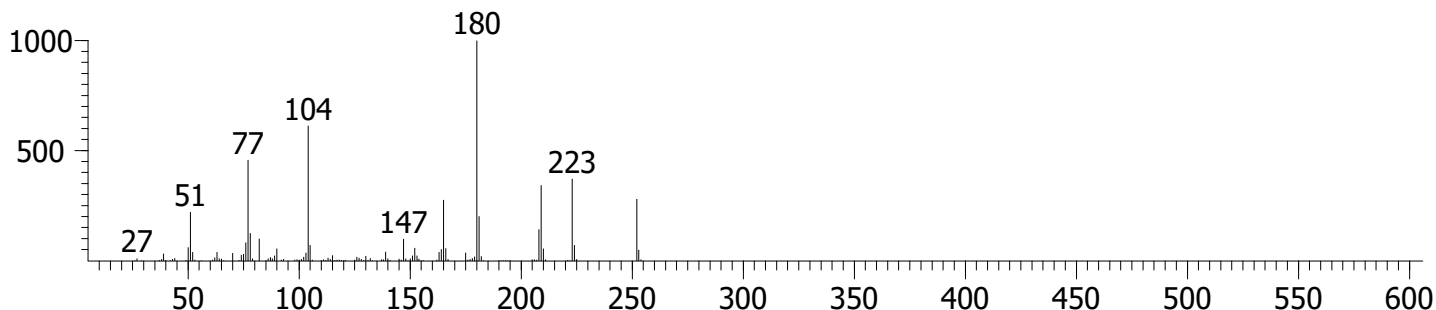
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3210, at 2148.55 , 3.003 sec , sec (Spec # 2532 65)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3210, at 2148.55 , 3.003 sec , sec (Spec # 2532 65)



Library Hit - similarity 859, "Phenytoin"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenytoin	859	9319	57-41-0	mainlib	C15H12N2O2	252
2	Methyl 8-((2-(N-(4-amino-2-methyl-5,6-dihydro-5-pyrimidinylmethyl)-N-formylamino)-1-(2-hydroxyethyl)-1-propenyl)dithio)-6-(acetylthio)octanoate	734	419	0-00-0	mainlib	C23H38N4O5S3	546
3	Diphenylmethyleimine, N-acetyl-	699	105	22800-71-1	mainlib	C15H13NO	223
4	3-Benzyl-benzotriazin-4-one	651	21	15561-72-5	mainlib	C14H11N3O	237
5	5,5-Diphenylhydantoin, 3-trifluoroacetyl-	650	20	0-00-0	mainlib	C17H11F3N2O3	348

Triethylene glycol di(2-ethylhexoate)

1st Dimension R.T. = 2183.53

2nd Dimension R.T. = 1.657

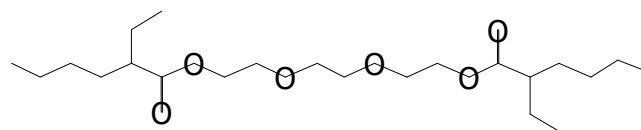
Quant Mass(es) = 171

S/N = 79.629

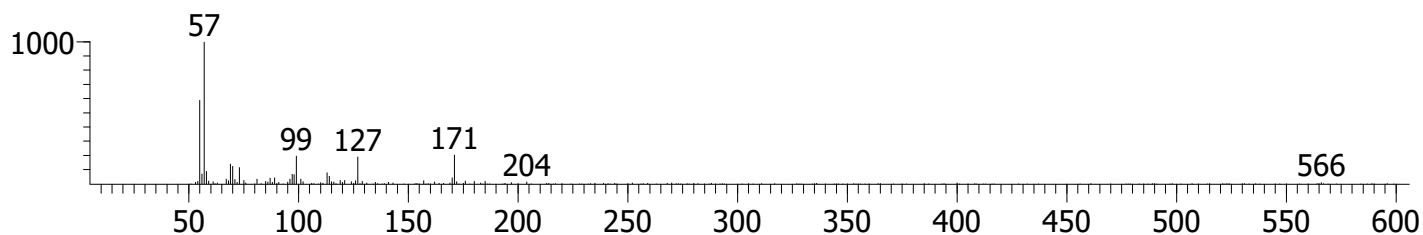
Area = 5019.2

Height = 615.89

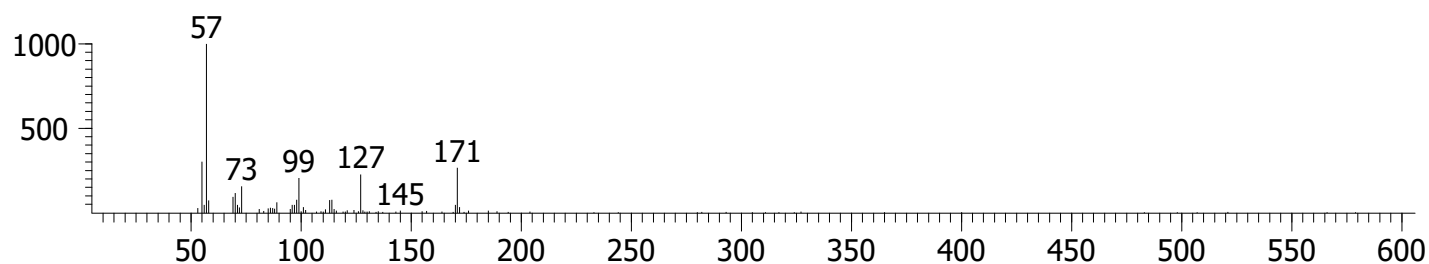
Similarity = 819



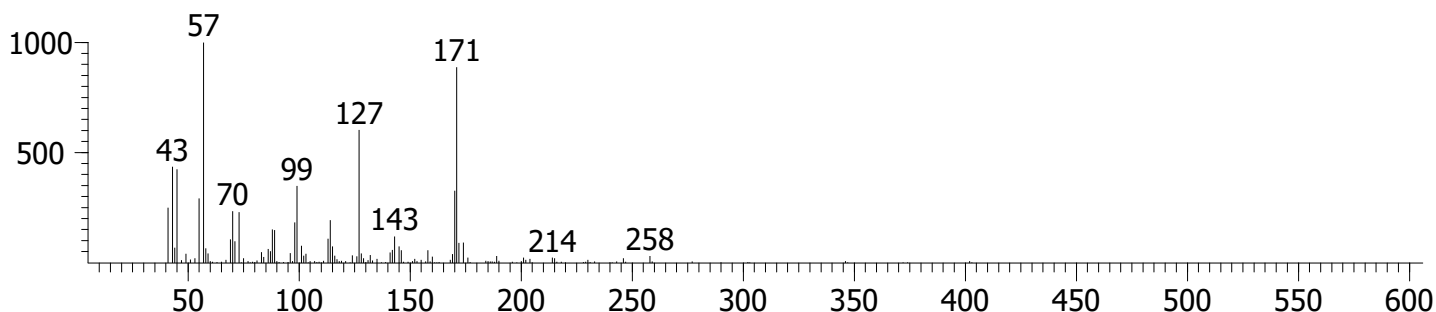
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 3255, at 2183.53 , 1.657 sec , sec (Spec # 2583 61)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 3255, at 2183.53 , 1.657 sec , sec (Spec # 2583 61)



Library Hit - similarity 819, "Triethylene glycol di(2-ethylhexoate)"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Triethylene glycol di(2-ethylhexoate)	819	8294	94-28-0	mainlib	C22H42O6	402
2	Hexanoic acid, 2-ethyl-, oxybis(2,1-ethanedioxy-2,1-ethanedioyl) ester	746	1129	18268-70-7	mainlib	C24H46O7	446
3	1-Hexanol, 2,2-dimethyl-	682	185	2370-13-0	mainlib	C8H18O	130
4	à-D-Glucopyranoside, methyl-2,3,4-tri-O-acetyl-6-O-heptyl-	653	52	0-00-0	mainlib	C20H34O9	418
5	9,9-Dimethyl-1,4-dioxa-7-azaspiro[4.4]nonan-8-one	651	48	0-00-0	mainlib	C8H13NO3	171

Tetrasulfide, dimethyl

1st Dimension R.T. = 906.756

2nd Dimension R.T. = 2.000

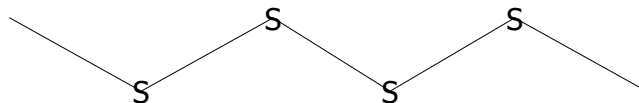
Quant Mass(es) = 158

S/N = 112.25

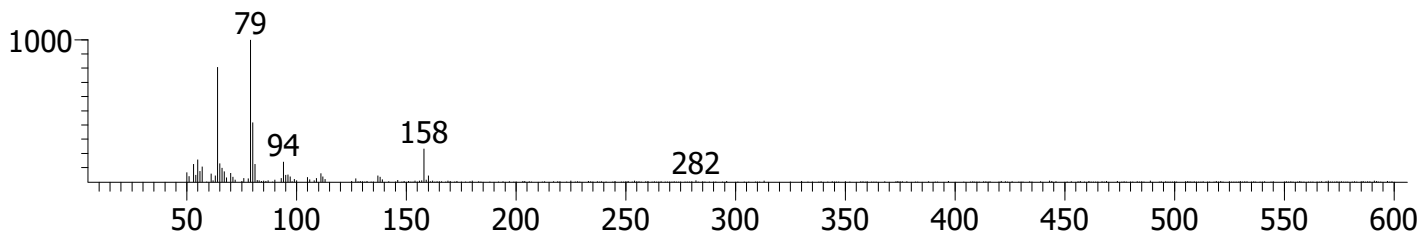
Area = 9846.2

Height = 1388.9

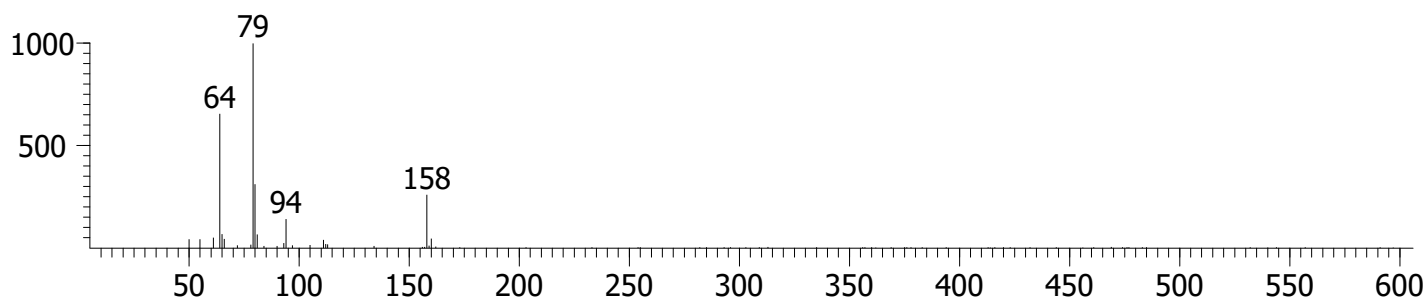
Similarity = 782



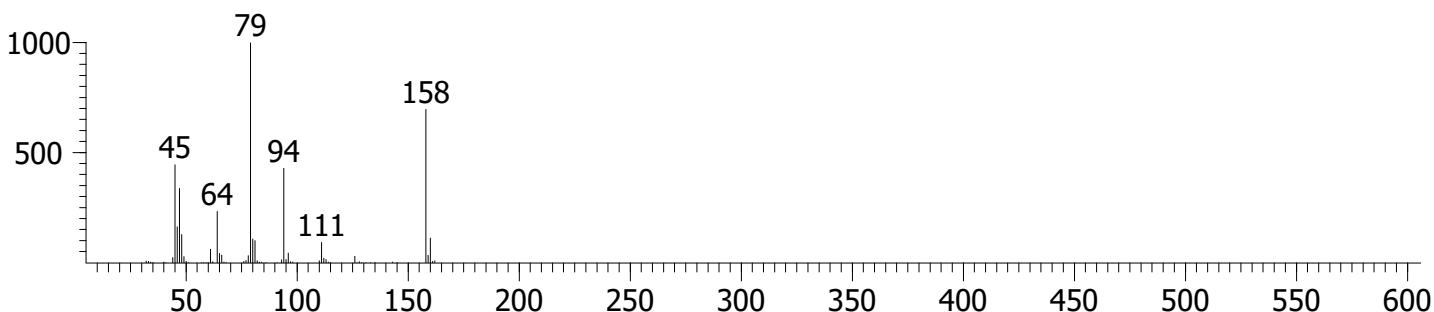
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 874, at 906.756 , 2.000 sec , sec (Spec # 64963)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 874, at 906.756 , 2.000 sec , sec (Spec # 64963)

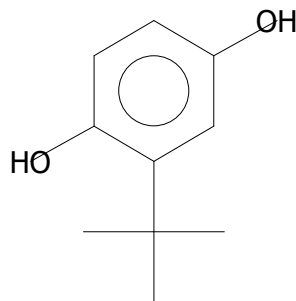


Library Hit - similarity 782, "Tetrasulfide, dimethyl"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Tetrasulfide, dimethyl	782	8203	5756-24-1	mainlib	C ₂ H ₆ S ₄	158
2	Pentasulfide, dimethyl	731	1653	7330-31-6	mainlib	C ₂ H ₆ S ₅	190
3	1,2-Ethanediol dimethanesulphonate	583	47	4672-49-5	mainlib	C ₄ H ₁₀ O ₆ S ₂	218
4	N-Chloro-N,O-bis(methylsulfonyl)hydroxylamine	545	11	96733-44-7	mainlib	C ₂ H ₆ ClNO ₅ S ₂	223
5	N,O-Bis(methylsulfonyl)hydroxylamine	543	10	96088-56-1	mainlib	C ₂ H ₇ NO ₅ S ₂	189

t-Butylhydroquinone



1st Dimension R.T. = 1333.51

2nd Dimension R.T. = 1.987

Quant Mass(es) = 151

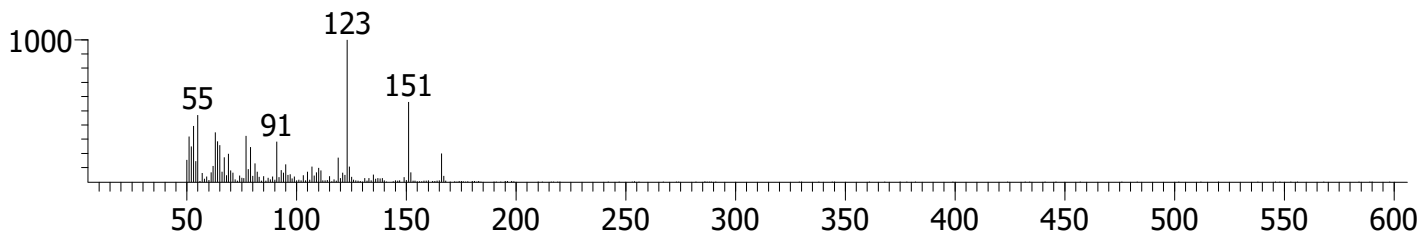
S/N = 915.27

Area = 151016

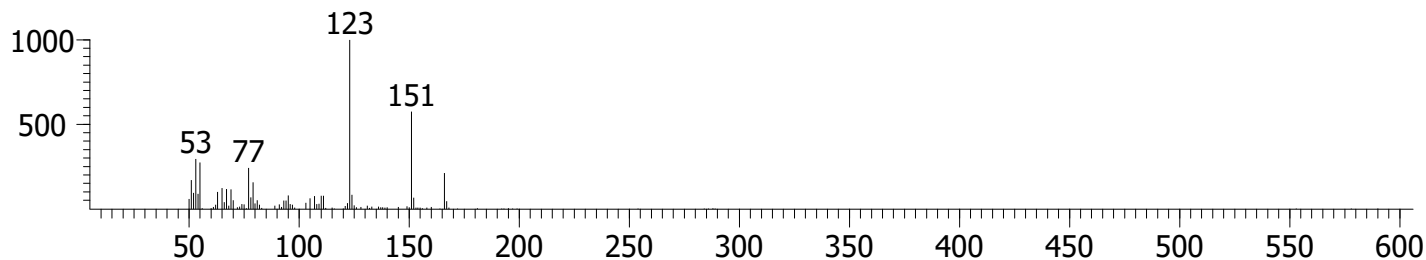
Height = 15806

Similarity = 867

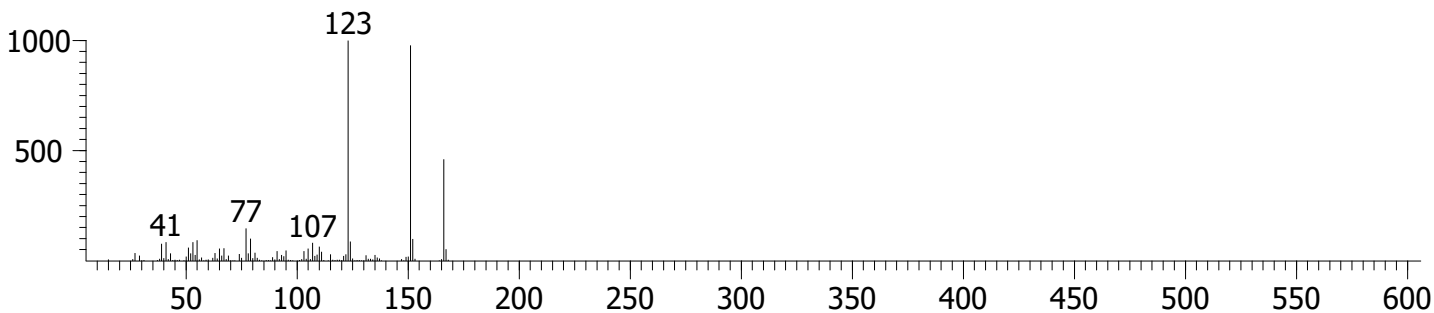
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 2024, at 1333.51 , 1.987 sec , sec (Spec # 1296 21)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 2024, at 1333.51 , 1.987 sec , sec (Spec # 1296 21)



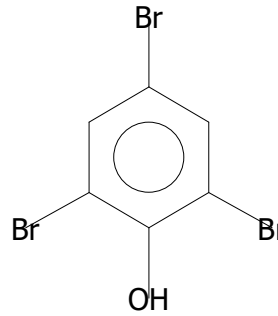
Library Hit - similarity 867, "t-Butylhydroquinone"



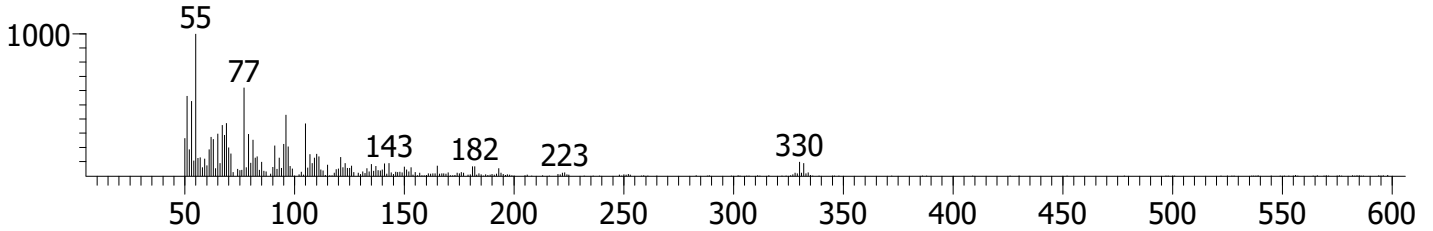
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	t-Butylhydroquinone	867	8115	1948-33-0	mainlib	C10H14O2	166
2	Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	759	532	1197-92-8	mainlib	C11H18O	166
3	5-Hepten-3-yn-2-ol, 6-methyl-5-(1-methylethyl)-	739	242	63922-41-8	mainlib	C11H18O	166
4	7a-Methyl-3-methylenehexahydrobenzofuran-2-one	729	171	67498-53-7	mainlib	C10H14O2	166
5	p-tert.-Butylcatechol	723	134	98-29-3	mainlib	C10H14O2	166

Phenol, 2,4,6-tribromo-

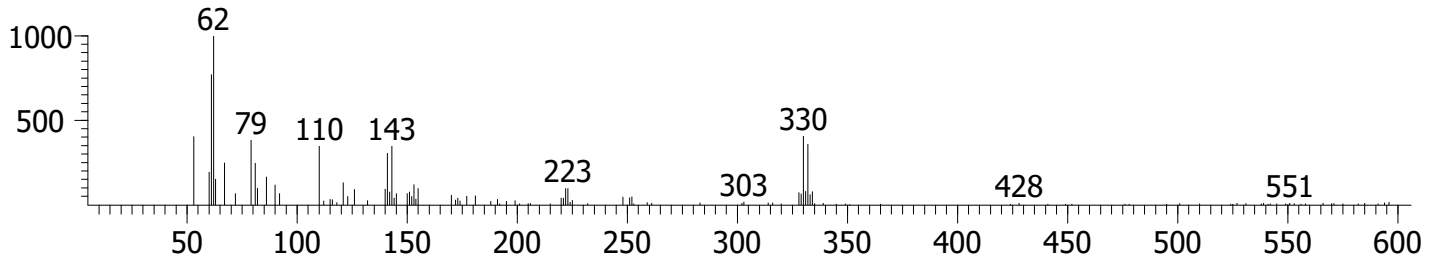
1st Dimension R.T. = 1445.45
2nd Dimension R.T. = 2.125
Quant Mass(es) = 332
S/N = 66.712
Area = 5788.8
Height = 694.87
Similarity = 668



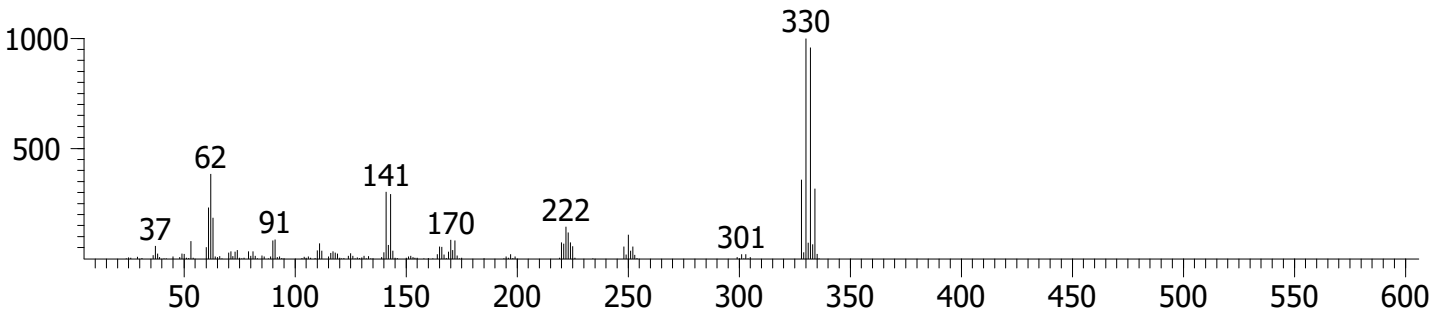
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 2347, at 1445.45 , 2.125 sec , sec (Spec # 1466 02)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 2347, at 1445.45 , 2.125 sec , sec (Spec # 1466 02)



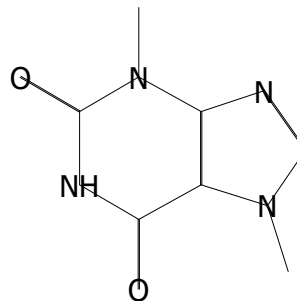
Library Hit - similarity 668, "Phenol, 2,4,6-tribromo-"



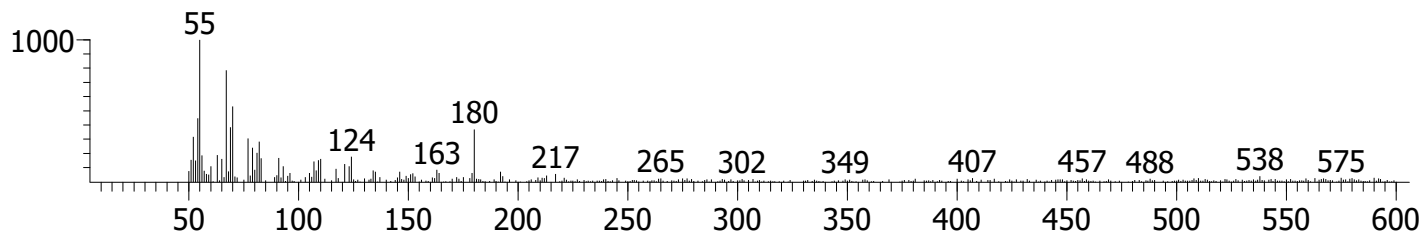
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 2,4,6-tribromo-	668	3601	118-79-6	mainlib	C6H3Br3O	328
2	2,4,5-Tribromophenol, acetate	645	1315	0-00-0	mainlib	C8H5Br3O2	370
3	2,3,4-Tribromophenol, acetate	641	1111	0-00-0	mainlib	C8H5Br3O2	370
4	2,4,5-Tribromophenol	635	873	14401-61-7	mainlib	C6H3Br3O	328
5	2,3,4-Tribromophenol	625	616	138507-65-0	mainlib	C6H3Br3O	328

Theobromine

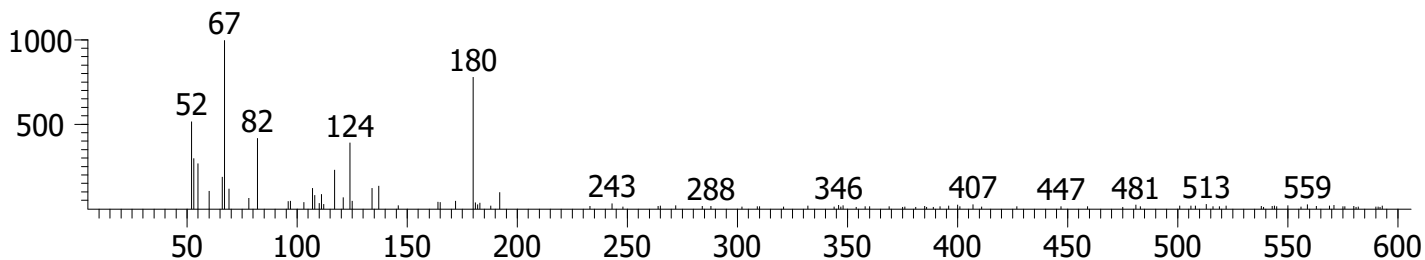
1st Dimension R.T. = 1690.31
 2nd Dimension R.T. = 2.812
 Quant Mass(es) = 180
 S/N = 51.210
 Area = 5017.4
 Height = 402.48
 Similarity = 596



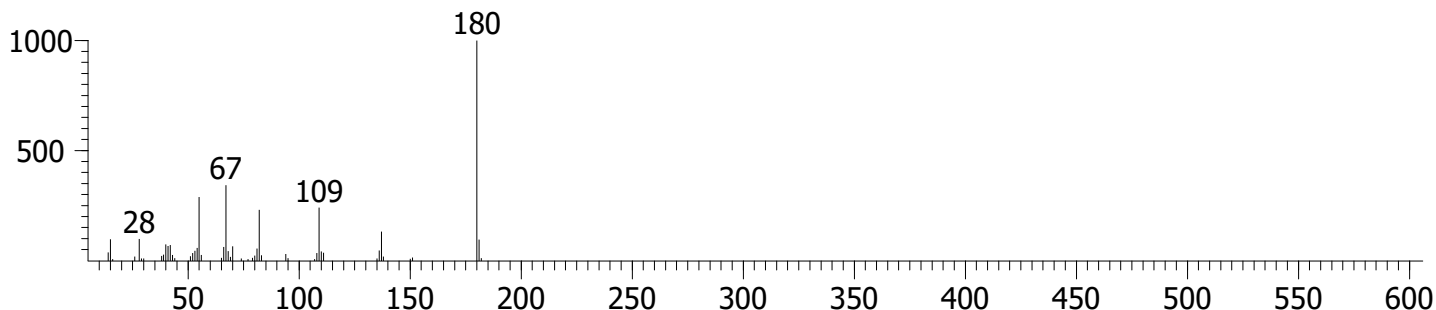
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3096, at 1690.31 , 2.812 sec , sec (Spec # 1838 06)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3096, at 1690.31 , 2.812 sec , sec (Spec # 1838 06)



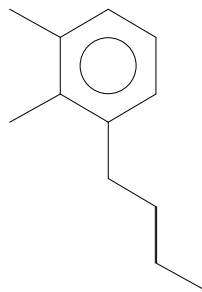
Library Hit - similarity 596, "Theobromine"



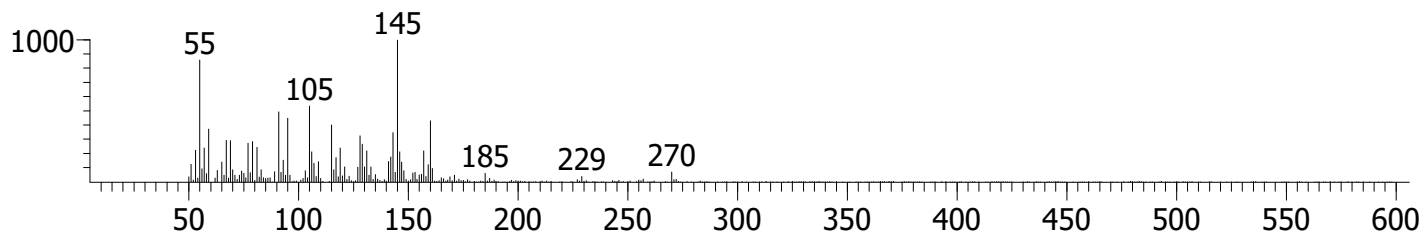
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Theobromine	596	3827	83-67-0	mainlib	C7H8N4O2	180
2	Purine-2,6(1H,3H)-dione, 1-(2-ethenylxyethyl)-3,7-dimethyl-	533	641	0-00-0	mainlib	C11H14N4O3	250
3	2-Piperidinecarboxylic acid, 1-(trifluoroacetyl)-, butyl ester	528	517	54965-28-5	mainlib	C12H18F3NO3	281
4	Diethylboryl-ε-capryllactam	526	476	0-00-0	mainlib	C12H24BNO	209
5	(2S,4aS,5R,8aR)-2,5-Dipropyldecahydroquinoline	521	384	68365-90-2	mainlib	C15H29N	223

Benzene, 1-(2-butenyl)-2,3-dimethyl-

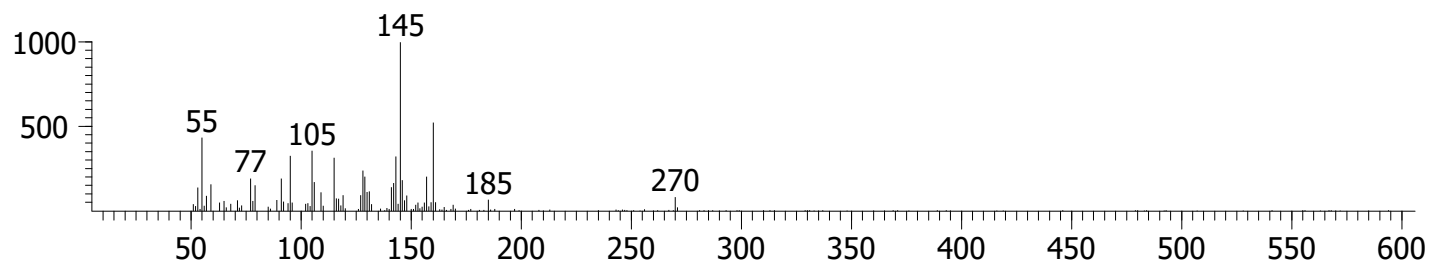
1st Dimension R.T. = 1704.3
2nd Dimension R.T. = 1.597
Quant Mass(es) = 145
S/N = 297.62
Area = 76849
Height = 7063.5
Similarity = 726



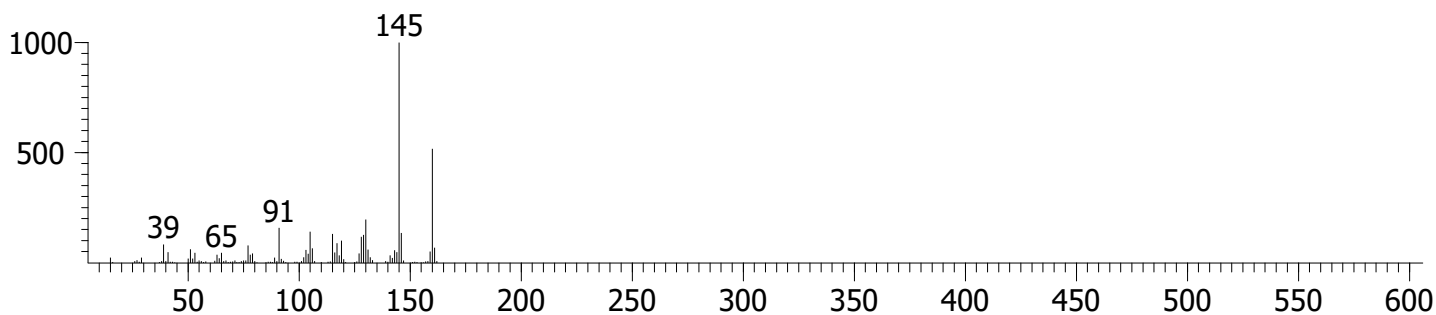
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3133, at 1704.3 , 1.597 sec , sec (Spec # 18574 2)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3133, at 1704.3 , 1.597 sec , sec (Spec # 18574 2)



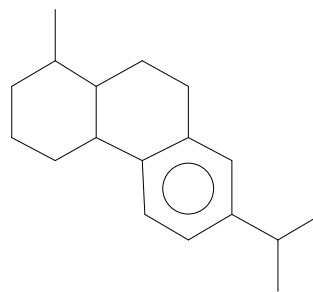
Library Hit - similarity 726, "Benzene, 1-(2-butenyl)-2,3-dimethyl-"



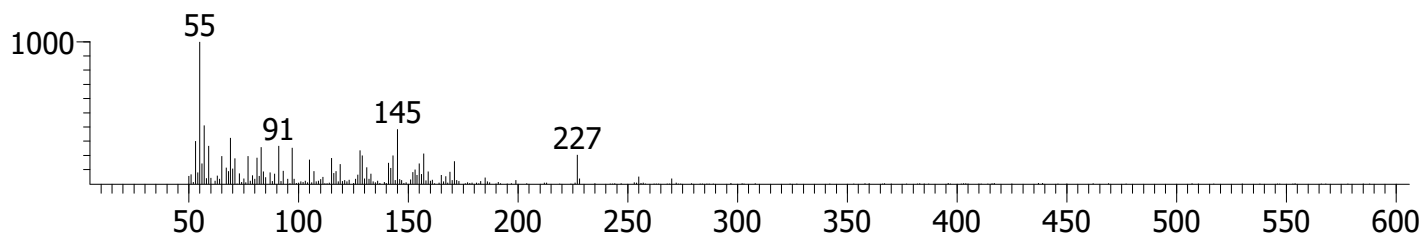
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-(2-butenyl)-2,3-dimethyl-	726	1925	54340-85-1	mainlib	C12H16	160
2	Benzene, 4-(2-butenyl)-1,2-dimethyl-, (E)-	717	1397	54340-86-2	mainlib	C12H16	160
3	Naphthalene, 1,2,3,4-tetrahydro-6,7-dimethyl-	708	1014	1076-61-5	mainlib	C12H16	160
4	Benzene, 1,2,4-trimethyl-5-(1-methylethenyl)-	696	675	54340-84-0	mainlib	C12H16	160
5	Benzene, 1,3,5-trimethyl-2-(1-methylethenyl)-	694	623	14679-13-1	mainlib	C12H16	160

10,18-Bisnorabieta-8,11,13-triene

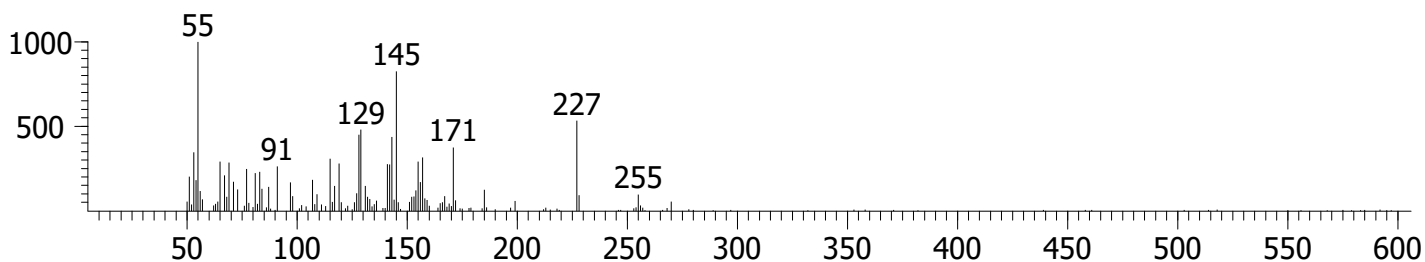
1st Dimension R.T. = 1753.27
2nd Dimension R.T. = 1.676
Quant Mass(es) = 227
S/N = 126.60
Area = 7234.0
Height = 817.73
Similarity = 684



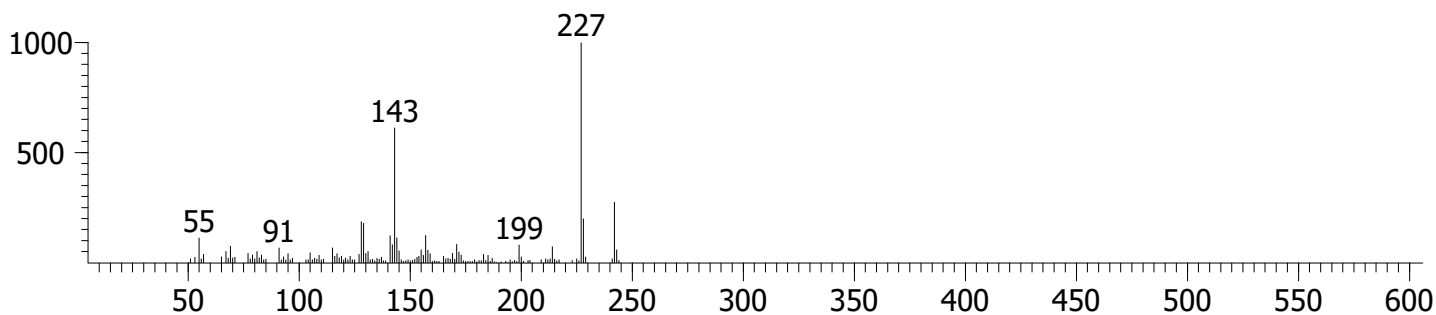
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3308, at 1753.27 , 1.676 sec , sec (Spec # 193174)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3308, at 1753.27 , 1.676 sec , sec (Spec # 193174)



Library Hit - similarity 684, "10,18-Bisnorabieta-8,11,13-triene"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	10,18-Bisnorabieta-8,11,13-triene	684	4450	32624-67-2	mainlib	C18H26	242
2	Benzene, 1,3,5-tris(3-methyl-3-butenyl)-	657	1309	55124-94-2	mainlib	C21H30	282
3	5,8,11-Eicosatriynoic acid, methyl ester	645	872	0-00-0	mainlib	C21H30O2	314
4	5-Pentyl-2-phenylcyclohex-1-ene-1-carbaldehyde	634	598	0-00-0	mainlib	C18H24O	256
5	5,8,11-Heptadecatriynoic acid, methyl ester	617	326	56554-57-5	mainlib	C18H24O2	272

Benzyl chloride

1st Dimension R.T. = 612.924

2nd Dimension R.T. = 1.637

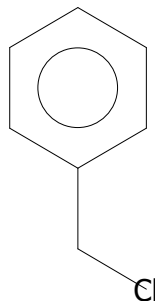
Quant Mass(es) = 91

S/N = 1939.3

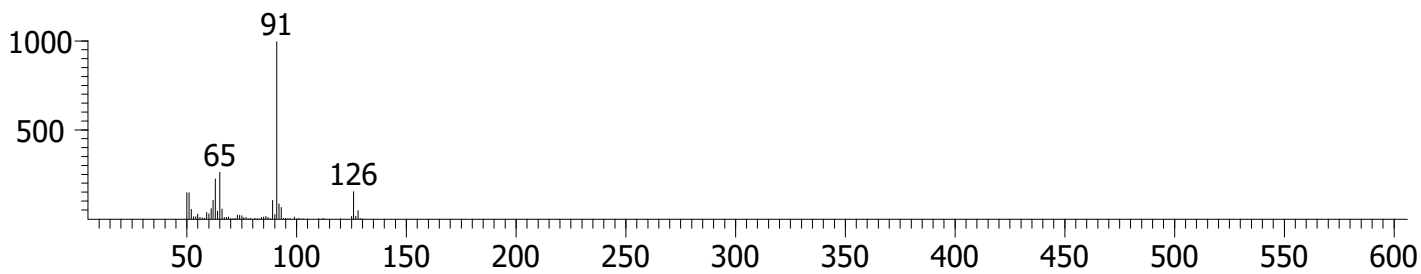
Area = 644388

Height = 94739

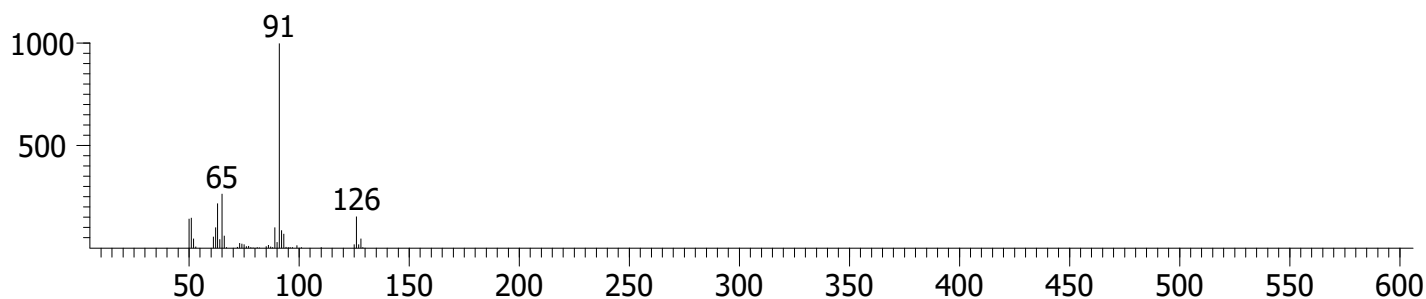
Similarity = 839



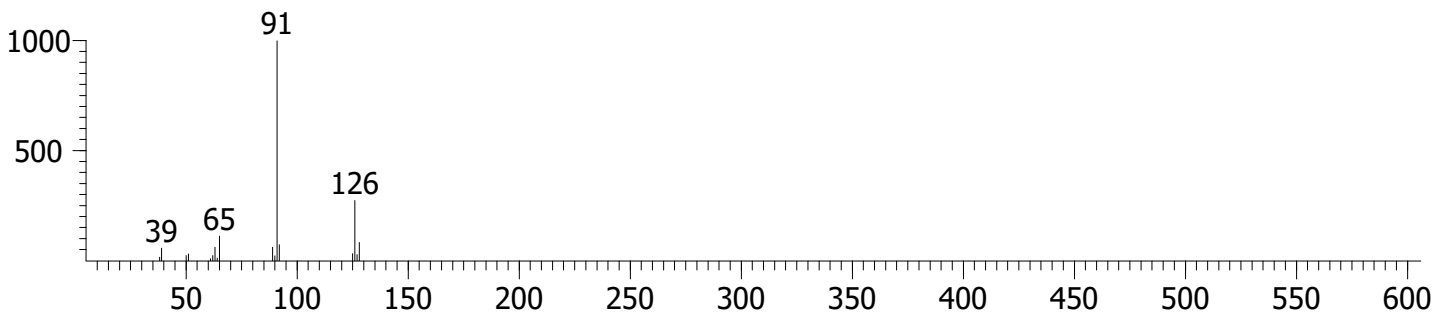
Peak Apex - sample "AnBxr B (20191121):1", peak 360, at 612.924 , 1.637 sec , sec (Spec # 20388)



Peak True - sample "AnBxr B (20191121):1", peak 360, at 612.924 , 1.637 sec , sec (Spec # 20388)



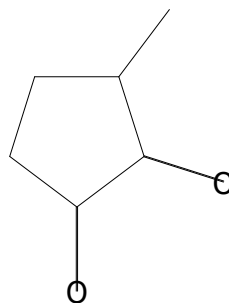
Library Hit - similarity 839, "Benzyl chloride"



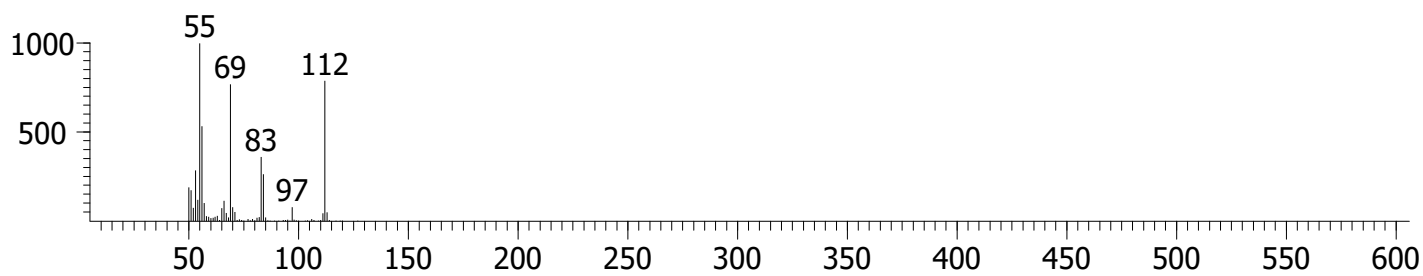
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzyl chloride	839	4023	100-44-7	replib	C7H7Cl	126
2	Benzene, 1-chloro-3-methyl-	798	918	108-41-8	replib	C7H7Cl	126
3	1,6-Heptadien-3-yne	794	809	5150-80-1	mainlib	C7H8	92
4	1,6-Heptadien-3-yne	792	721	5150-80-1	replib	C7H8	92
5	Benzyl chloride	789	4023	100-44-7	replib	C7H7Cl	126

1,2-Cyclopentanedione, 3-methyl-

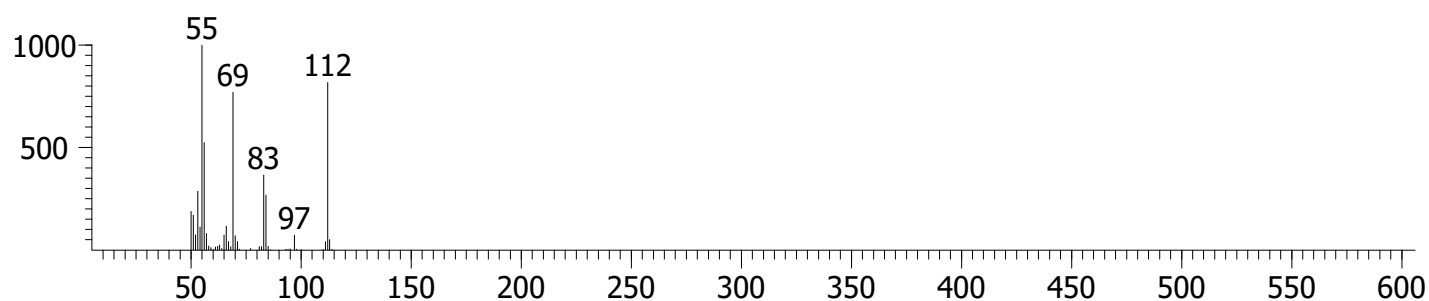
1st Dimension R.T. = 630.414
2nd Dimension R.T. = 1.729
Quant Mass(es) = 112
S/N = 2976.8
Area = 417177
Height = 55107
Similarity = 963



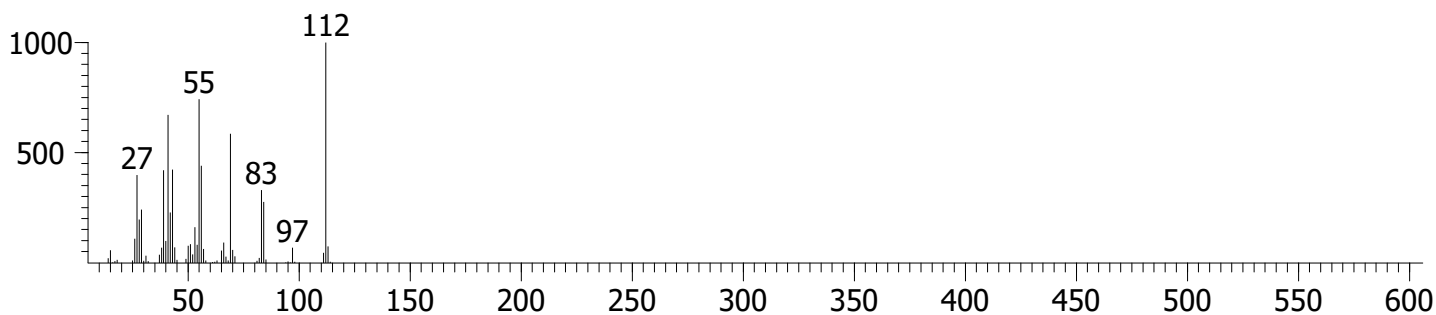
Peak Apex - sample "AnBxr B (20191121):1", peak 423, at 630.414 , 1.729 sec , sec (Spec # 23052)



Peak True - sample "AnBxr B (20191121):1", peak 423, at 630.414 , 1.729 sec , sec (Spec # 23052)

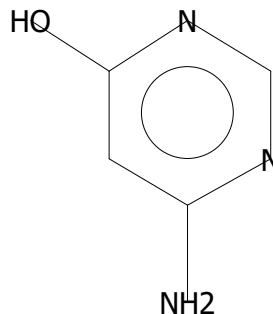


Library Hit - similarity 963, "1,2-Cyclopentanedione, 3-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,2-Cyclopentanedione, 3-methyl-	963	8108	765-70-8	mainlib	C6H8O2	112
2	1,2-Cyclopentanedione, 3-methyl-	959	7117	765-70-8	replib	C6H8O2	112
3	1,2-Cyclopentanedione, 3-methyl-	939	7117	765-70-8	replib	C6H8O2	112
4	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	936	2599	80-71-7	replib	C6H8O2	112
5	1,2-Cyclopentanedione, 3-methyl-	911	7117	765-70-8	replib	C6H8O2	112

4-Amino-6-hydroxypyrimidine



1st Dimension R.T. = 693.378

2nd Dimension R.T. = 1.921

Quant Mass(es) = 111

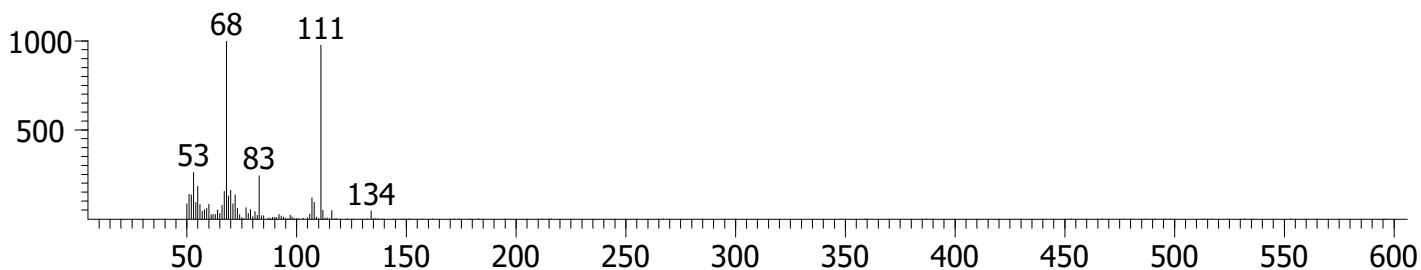
S/N = 854.72

Area = 212790

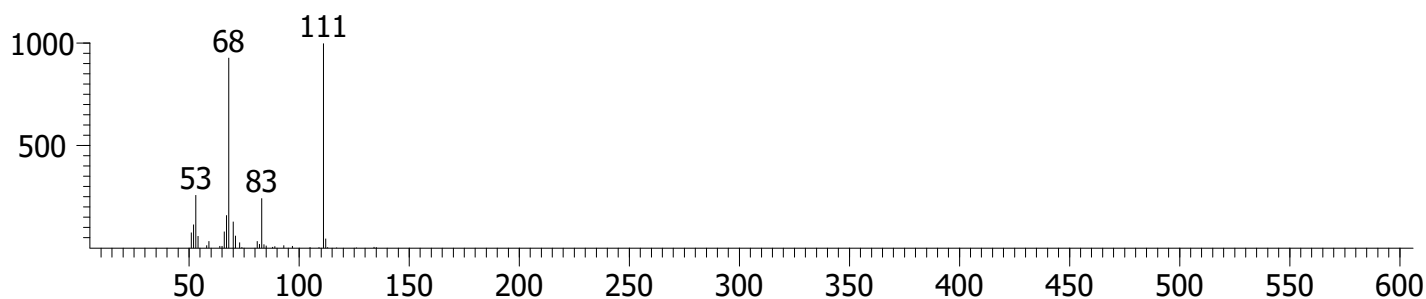
Height = 27570

Similarity = 736

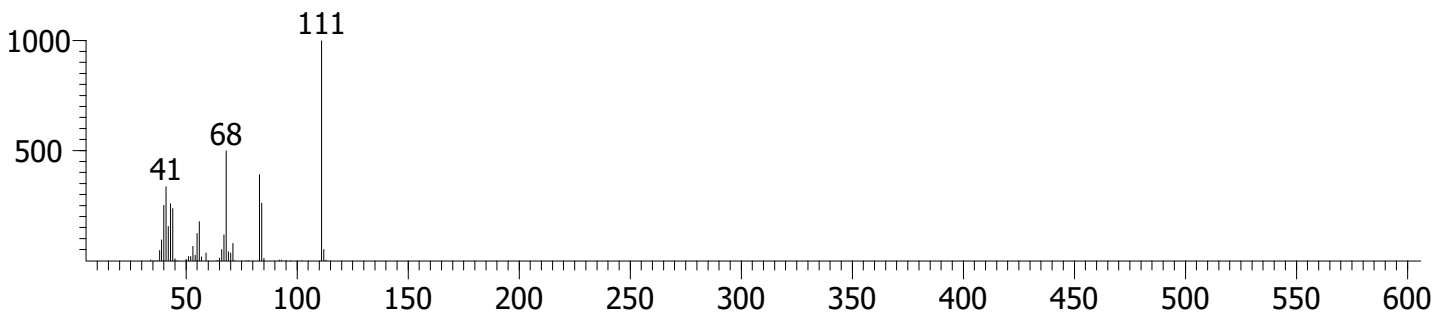
Peak Apex - sample "AnBxr B (20191121):1", peak 599, at 693.378 , 1.921 sec , sec (Spec # 32621)



Peak True - sample "AnBxr B (20191121):1", peak 599, at 693.378 , 1.921 sec , sec (Spec # 32621)



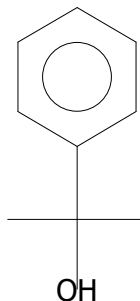
Library Hit - similarity 736, "4-Amino-6-hydroxypyrimidine"



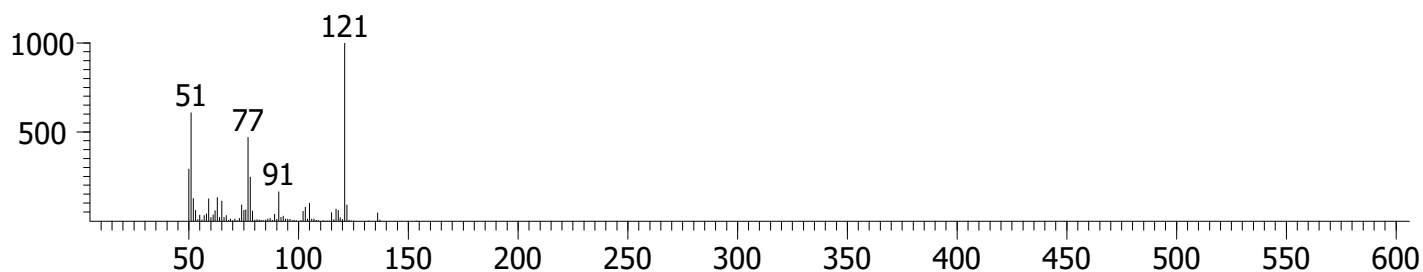
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Amino-6-hydroxypyrimidine	736	4293	1193-22-2	replib	C4H5N3O	111
2	2(1H)-Pyridinone, 6-hydroxy-	730	3375	626-06-2	replib	C5H5NO2	111
3	Isocytosine	723	4297	108-53-2	mainlib	C4H5N3O	111
4	4-Amino-6-hydroxypyrimidine	708	4293	1193-22-2	replib	C4H5N3O	111
5	4-Amino-6-hydroxypyrimidine	700	1569	1193-22-2	mainlib	C4H5N3O	111

Benzenemethanol, à,à-dimethyl-

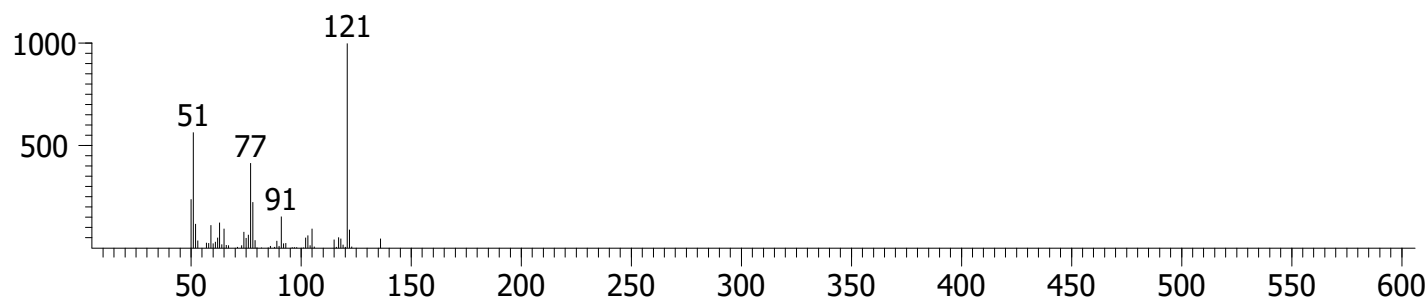
1st Dimension R.T. = 710.868
2nd Dimension R.T. = 1.663
Quant Mass(es) = 121
S/N = 6207.4
Area = 1156130
Height = 156902
Similarity = 867



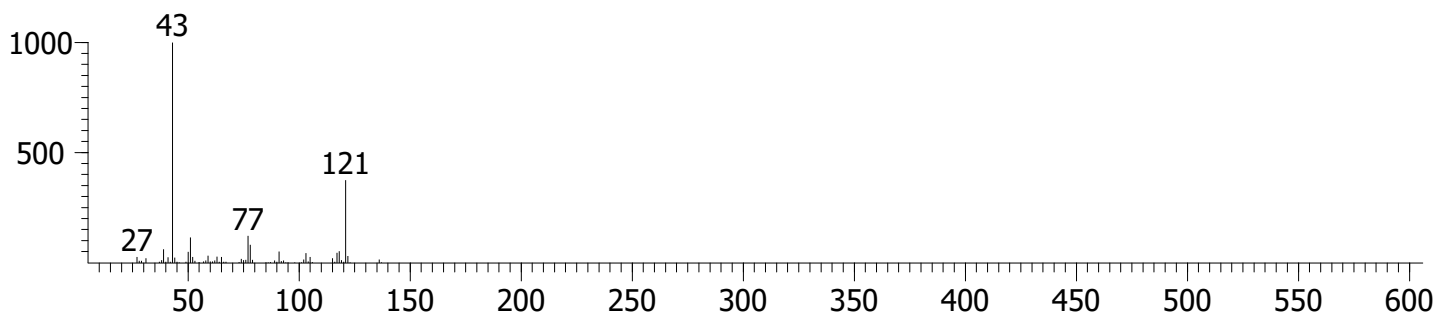
Peak Apex - sample "AnBxr B (20191121):1", peak 666, at 710.868 , 1.663 sec , sec (Spec # 35232)



Peak True - sample "AnBxr B (20191121):1", peak 666, at 710.868 , 1.663 sec , sec (Spec # 35232)



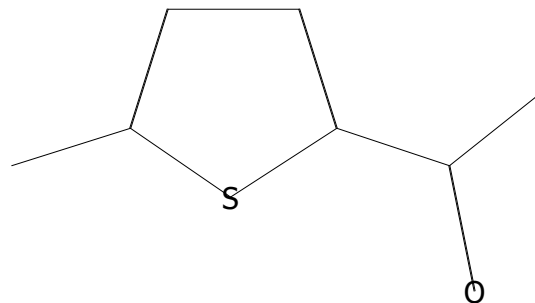
Library Hit - similarity 867, "Benzenemethanol, à,à-dimethyl-"



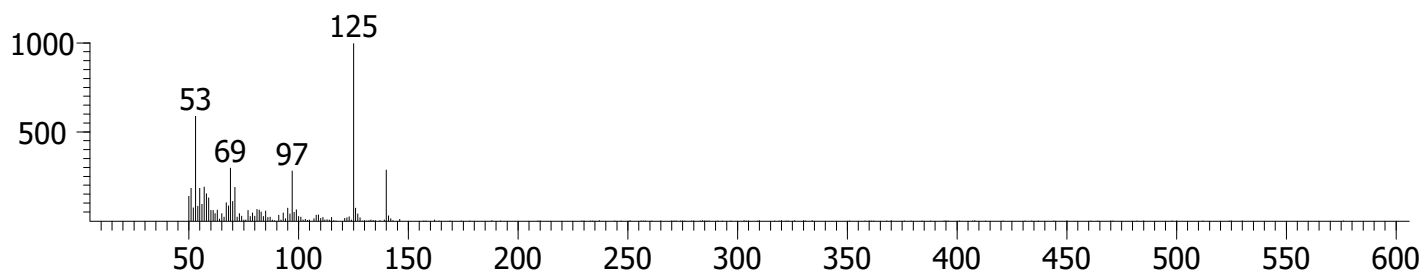
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenemethanol, à,à-dimethyl-	867	5475	617-94-7	replib	C9H12O	136
2	Benzene, (1-methoxyethyl)-	831	2021	4013-34-7	mainlib	C9H12O	136
3	Benzeneacetic acid, à-hydroxy-à-methyl-, methyl ester	824	1548	20731-95-7	mainlib	C10H12O3	180
4	à-Ethyl-à-methylbenzyl alcohol	821	1368	1565-75-9	mainlib	C10H14O	150
5	Atrolactic acid	820	1145	515-30-0	replib	C9H10O3	166

2-Acetyl-5-methylthiophene

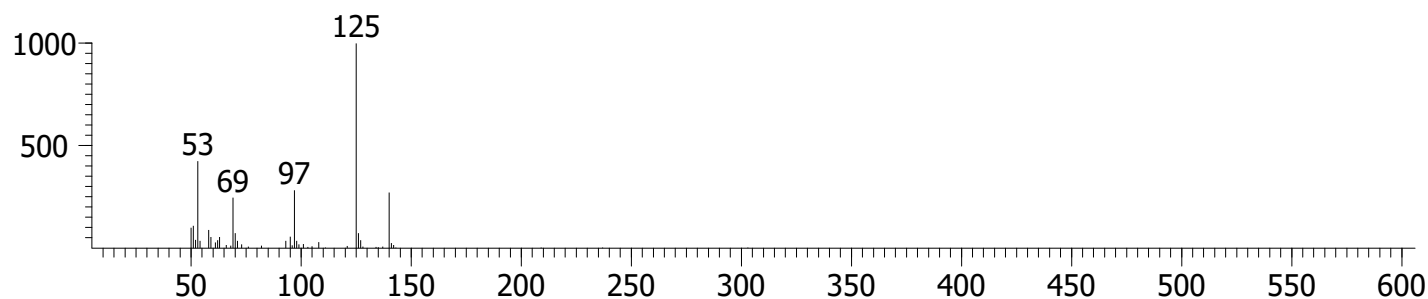
1st Dimension R.T. = 882.27
2nd Dimension R.T. = 1.921
Quant Mass(es) = 125
S/N = 784.78
Area = 124920
Height = 14811
Similarity = 925



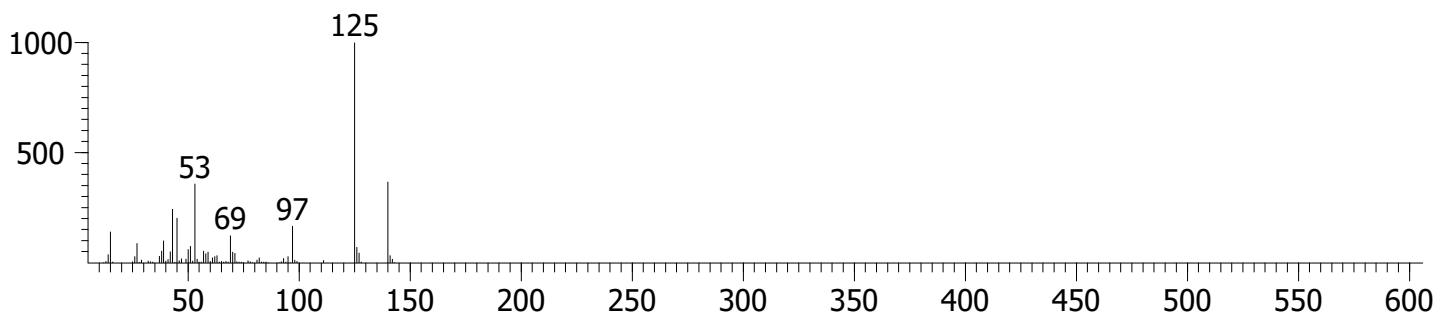
Peak Apex - sample "AnBxr B (20191121):1", peak 1393, at 882.27 , 1.921 sec , sec (Spec # 61241)



Peak True - sample "AnBxr B (20191121):1", peak 1393, at 882.27 , 1.921 sec , sec (Spec # 61241)



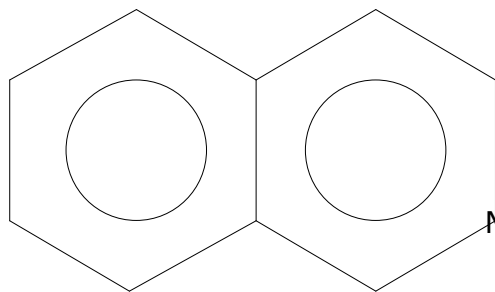
Library Hit - similarity 925, "2-Acetyl-5-methylthiophene"



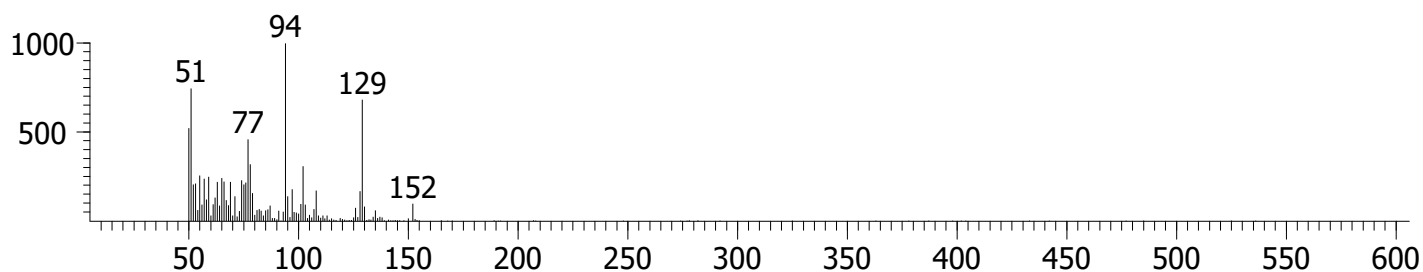
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Acetyl-5-methylthiophene	925	6770	13679-74-8	mainlib	C7H8OS	140
2	Ethanone, 1-(4-methyl-2-thienyl)-	890	1699	13679-73-7	mainlib	C7H8OS	140
3	2-Acetyl-3-methylthiophene	889	6543	13679-72-6	replib	C7H8OS	140
4	2-Acetyl-3-methylthiophene	877	1097	13679-72-6	mainlib	C7H8OS	140
5	2-Acetyl-5-methylthiophene	867	2586	13679-74-8	replib	C7H8OS	140

Isoquinoline

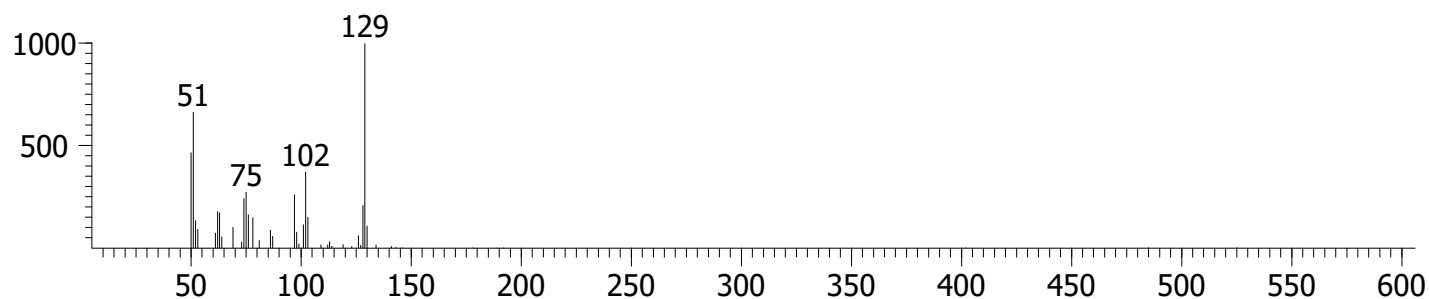
1st Dimension R.T. = 934.74
2nd Dimension R.T. = 2.079
Quant Mass(es) = 129
S/N = 547.95
Area = 150067
Height = 15869
Similarity = 825



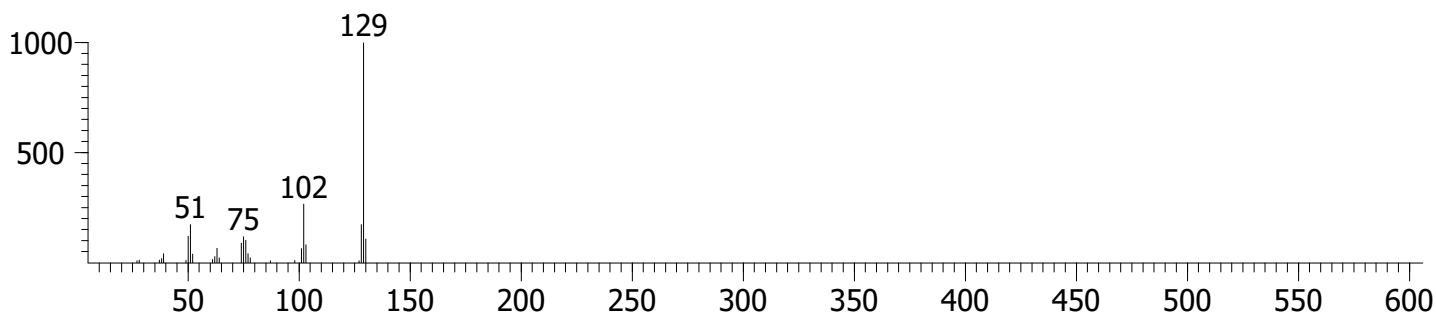
Peak Apex - sample "AnBxr B (20191121):1", peak 1691, at 934.74 , 2.079 sec , sec (Spec # 69215)



Peak True - sample "AnBxr B (20191121):1", peak 1691, at 934.74 , 2.079 sec , sec (Spec # 69215)



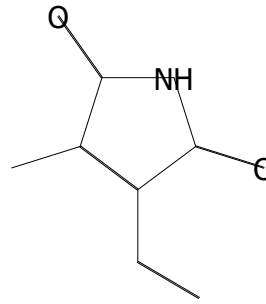
Library Hit - similarity 825, "Isoquinoline"



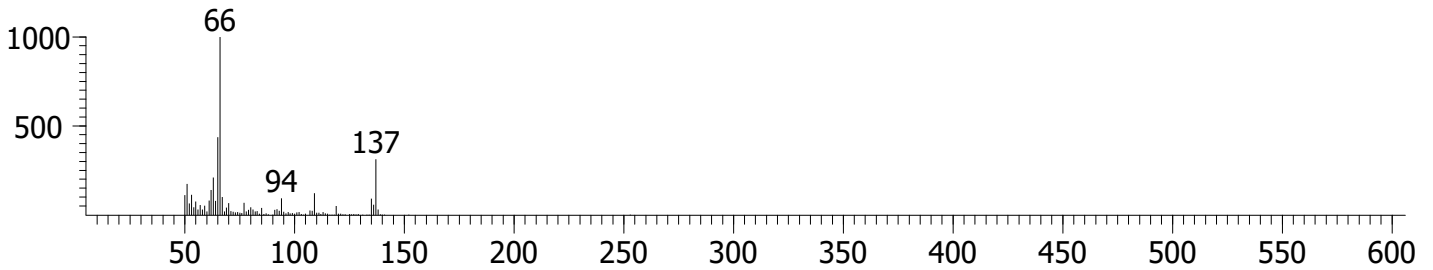
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Isoquinoline	825	4016	119-65-3	replib	C9H7N	129
2	Isoquinoline	821	4016	119-65-3	replib	C9H7N	129
3	Quinoline	817	2996	91-22-5	replib	C9H7N	129
4	2-Propenenitrile, 3-phenyl-, (E)-	812	2415	1885-38-7	replib	C9H7N	129
5	Isoquinoline	776	4016	119-65-3	replib	C9H7N	129

1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-

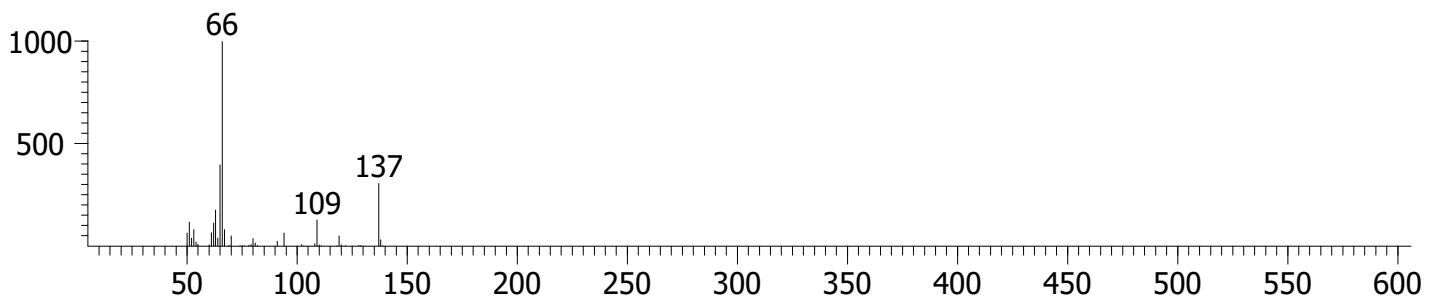
1st Dimension R.T. = 952.23
2nd Dimension R.T. = 1.987
Quant Mass(es) = 66
S/N = 1814.6
Area = 967416
Height = 113150
Similarity = 890



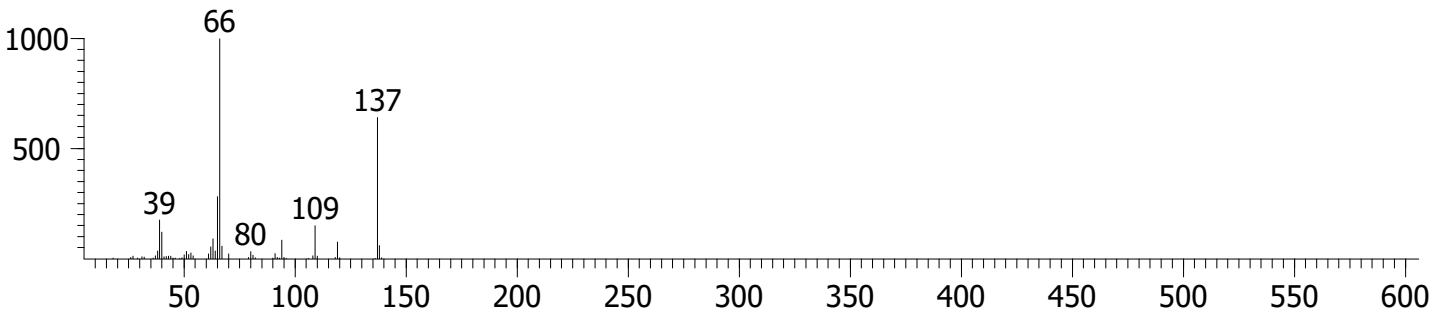
Peak Apex - sample "AnBxr B (20191121):1", peak 1770, at 952.23 , 1.987 sec , sec (Spec # 71851)



Peak True - sample "AnBxr B (20191121):1", peak 1770, at 952.23 , 1.987 sec , sec (Spec # 71851)



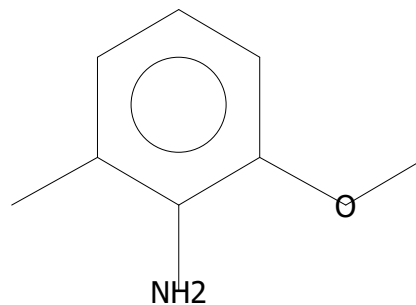
Library Hit - similarity 890, "1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-"



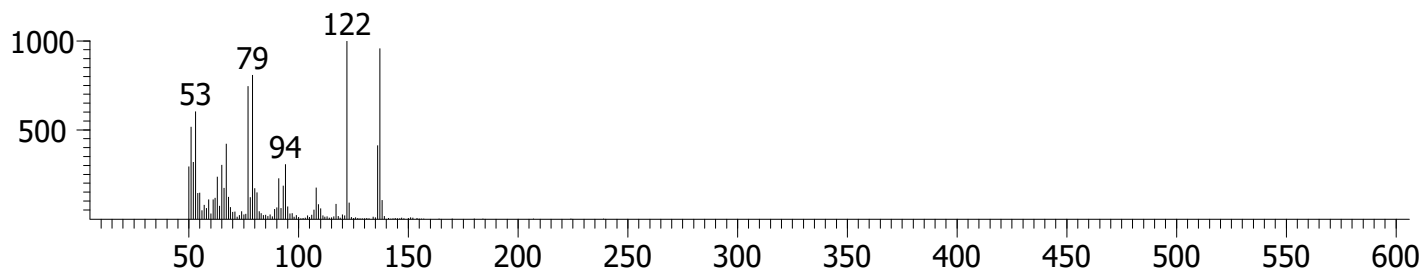
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	890	9277	21494-57-5	replib	C7H7NO2	137
2	1-Penten-3-yne	762	3604	646-05-9	mainlib	C5H6	66
3	1-Buten-3-yne, 2-methyl-	746	285	78-80-8	replib	C5H6	66
4	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	745	1967	21494-57-5	mainlib	C7H7NO2	137
5	3-Penten-1-yne, (E)-	743	252	2004-69-5	replib	C5H6	66

2-Methoxy-6-methylaniline

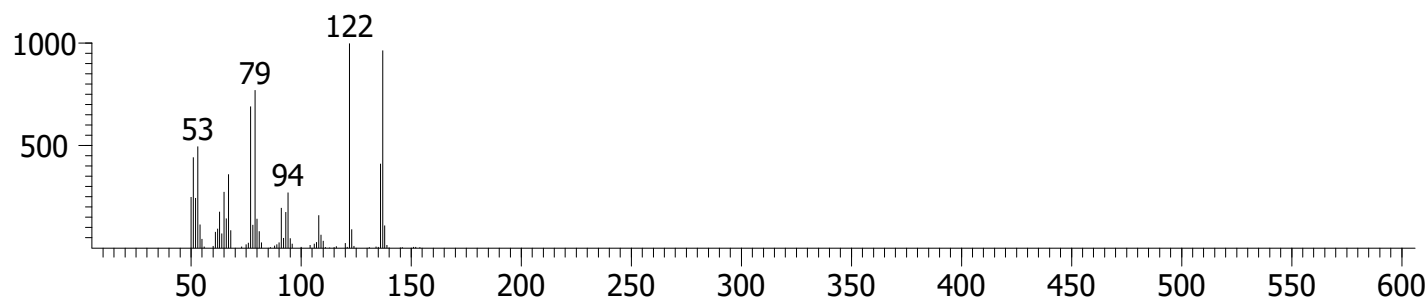
1st Dimension R.T. = 1050.17
2nd Dimension R.T. = 2.020
Quant Mass(es) = 137
S/N = 2045.5
Area = 574155
Height = 64791
Similarity = 755



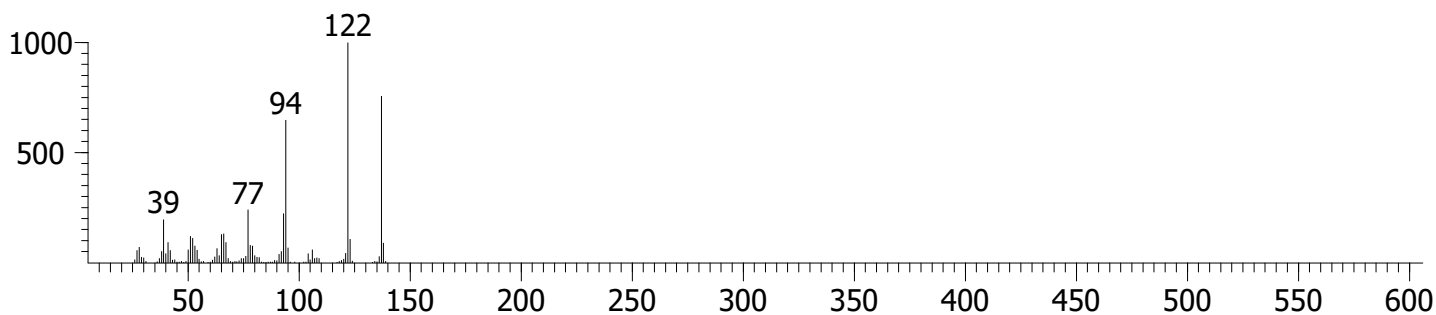
Peak Apex - sample "AnBxr B (20191121):1", peak 2329, at 1050.17 , 2.020 sec , sec (Spec # 86696)



Peak True - sample "AnBxr B (20191121):1", peak 2329, at 1050.17 , 2.020 sec , sec (Spec # 86696)



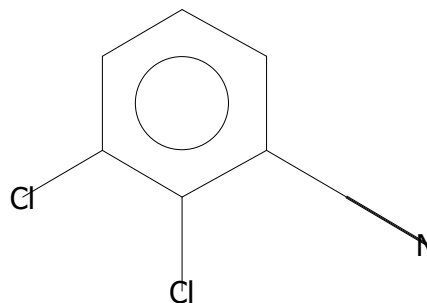
Library Hit - similarity 755, "2-Methoxy-6-methylaniline"



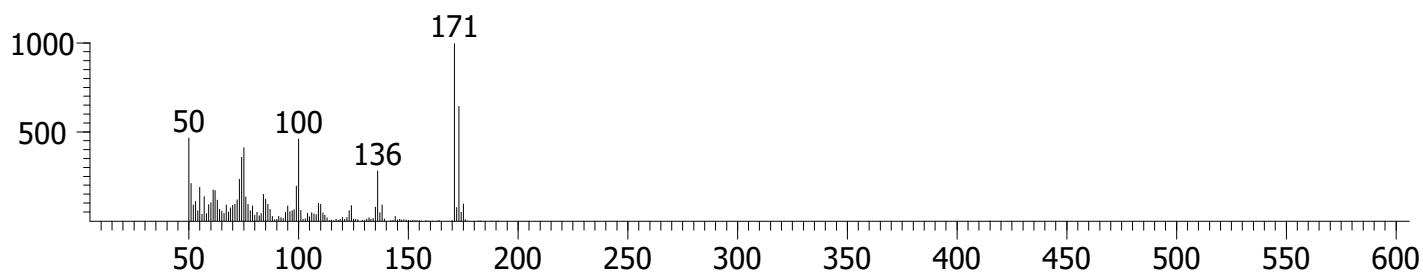
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Methoxy-6-methylaniline	755	5468	50868-73-0	replib	C8H11NO	137
2	Phenol, 4-(ethylamino)-	738	1427	659-34-7	mainlib	C8H11NO	137
3	Phenol, 2-(ethylamino)-	733	1150	614-70-0	mainlib	C8H11NO	137
4	Benzeneamine, 3-ethyl-4-hydroxy-	733	1150	178698-88-9	mainlib	C8H11NO	137
5	m-Ethylaminophenol	728	1608	621-31-8	replib	C8H11NO	137

2,3-Dichlorobenzonitrile

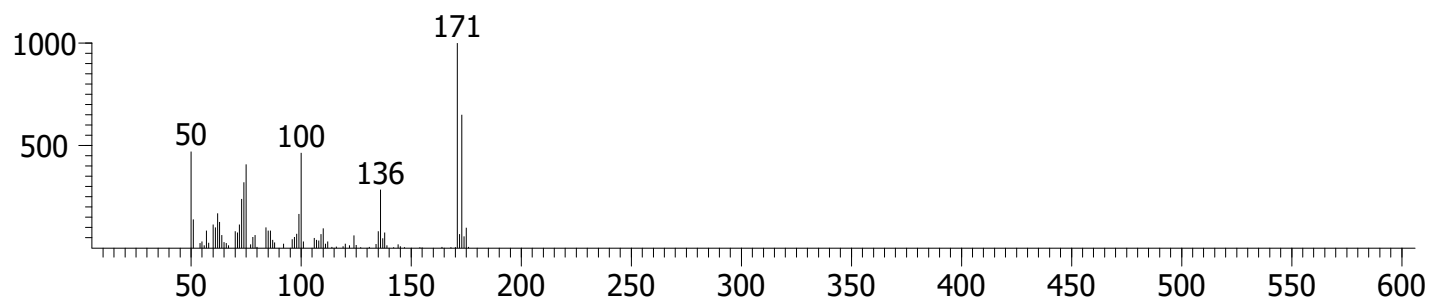
1st Dimension R.T. = 1060.67
2nd Dimension R.T. = 2.066
Quant Mass(es) = 171
S/N = 2306.7
Area = 264302
Height = 30569
Similarity = 867



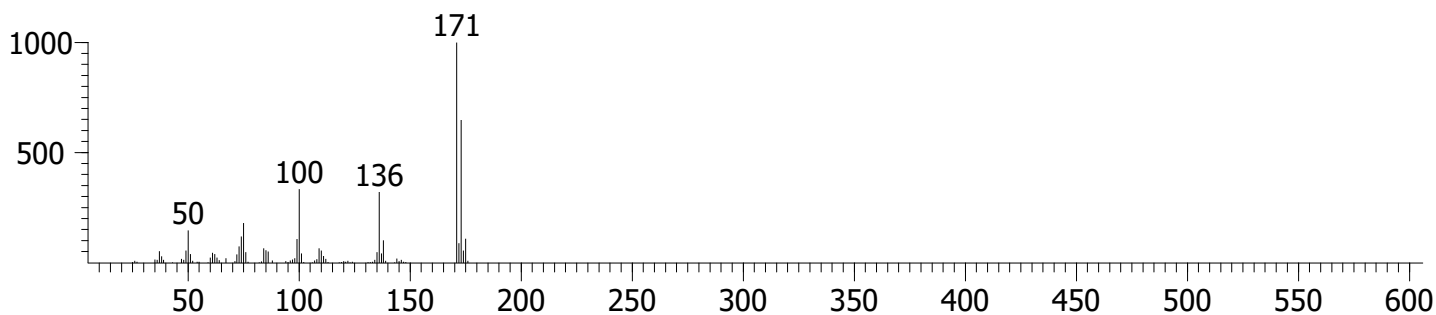
Peak Apex - sample "AnBxr B (20191121):1", peak 2395, at 1060.67 , 2.066 sec , sec (Spec # 88293)



Peak True - sample "AnBxr B (20191121):1", peak 2395, at 1060.67 , 2.066 sec , sec (Spec # 88293)



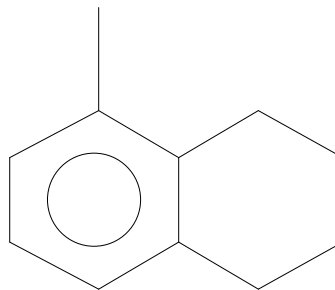
Library Hit - similarity 867, "2,3-Dichlorobenzonitrile"



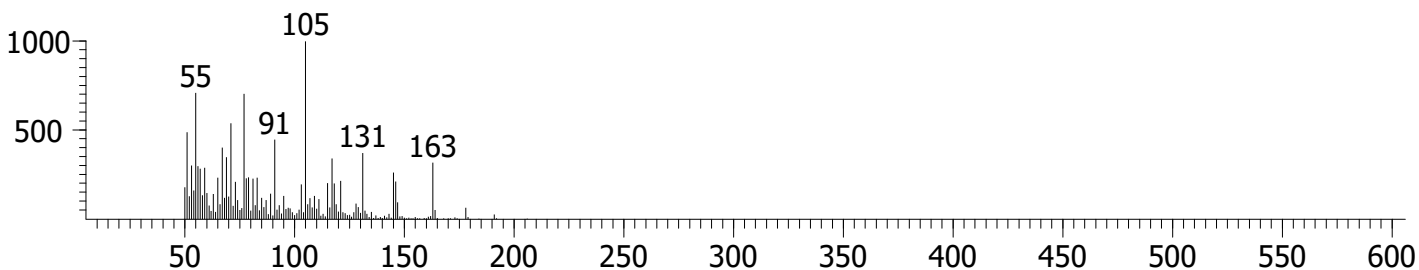
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,3-Dichlorobenzonitrile	867	3214	6574-97-6	mainlib	C7H3Cl2N	171
2	2,5-Dichlorobenzonitrile	864	2840	21663-61-6	mainlib	C7H3Cl2N	171
3	3,5-Dichlorobenzonitrile	855	5128	6575-00-4	replib	C7H3Cl2N	171
4	Benzonitrile, 2,6-dichloro-	853	4730	1194-65-6	replib	C7H3Cl2N	171
5	Benzonitrile, 2,6-dichloro-	850	4730	1194-65-6	replib	C7H3Cl2N	171

Naphthalene, 1,2,3,4-tetrahydro-5-methyl-

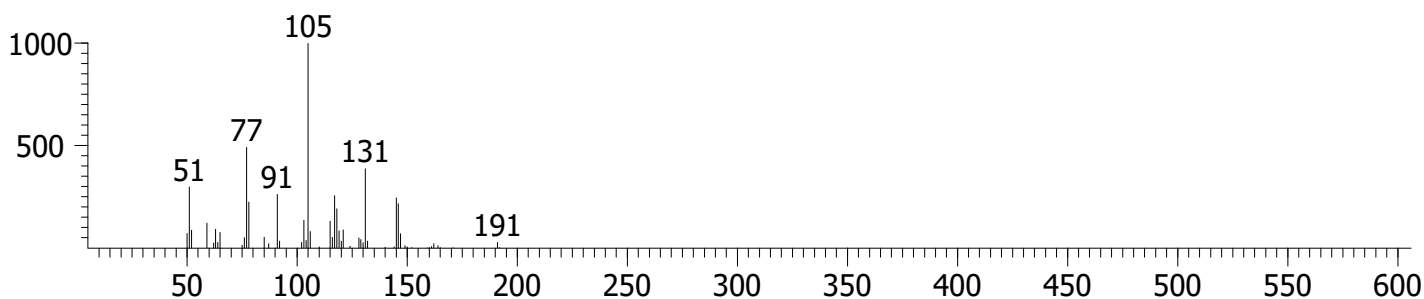
1st Dimension R.T. = 1081.66
2nd Dimension R.T. = 1.630
Quant Mass(es) = 105
S/N = 701.39
Area = 440534
Height = 45378
Similarity = 742



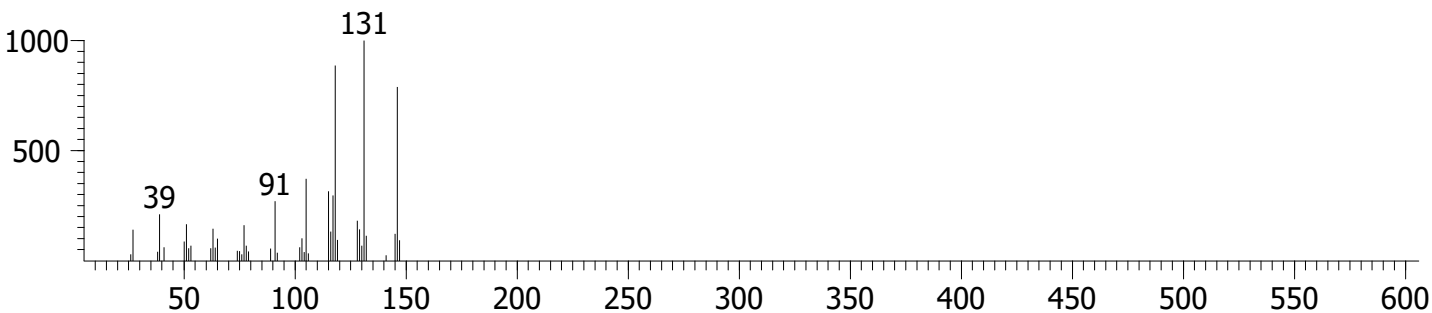
Peak Apex - sample "AnBxr B (20191121):1", peak 2488, at 1081.66 , 1.630 sec , sec (Spec # 91407)



Peak True - sample "AnBxr B (20191121):1", peak 2488, at 1081.66 , 1.630 sec , sec (Spec # 91407)



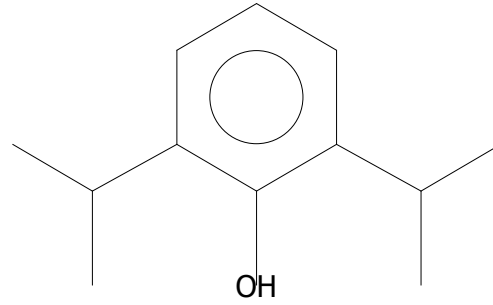
Library Hit - similarity 742, "Naphthalene, 1,2,3,4-tetrahydro-5-methyl-"



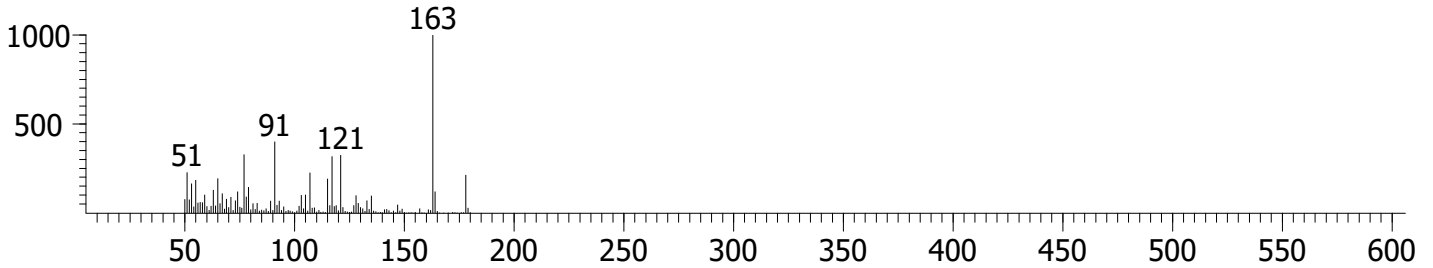
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	742	3342	2809-64-5	replib	C11H14	146
2	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	733	2426	1680-51-9	replib	C11H14	146
3	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	733	1578	1680-51-9	mainlib	C11H14	146
4	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	732	2426	1680-51-9	replib	C11H14	146
5	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	731	1456	2809-64-5	mainlib	C11H14	146

Propofol

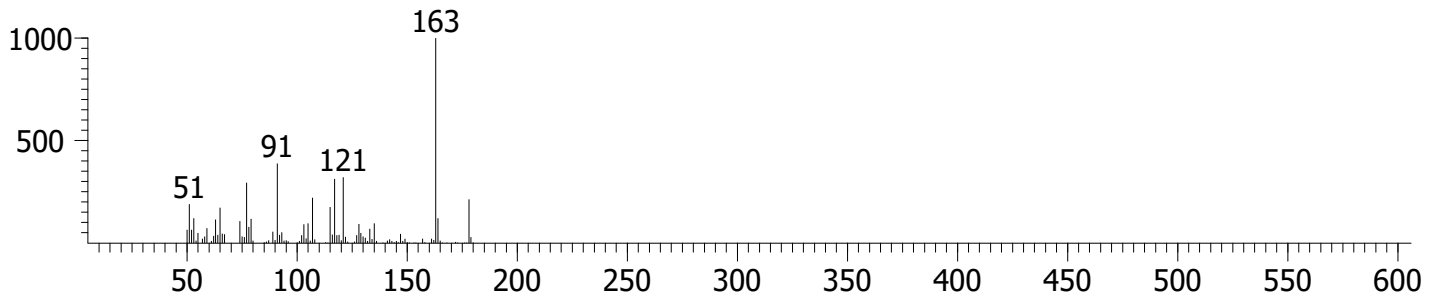
1st Dimension R.T. = 1085.15
2nd Dimension R.T. = 1.657
Quant Mass(es) = 163
S/N = 11918
Area = 1967761
Height = 272241
Similarity = 908



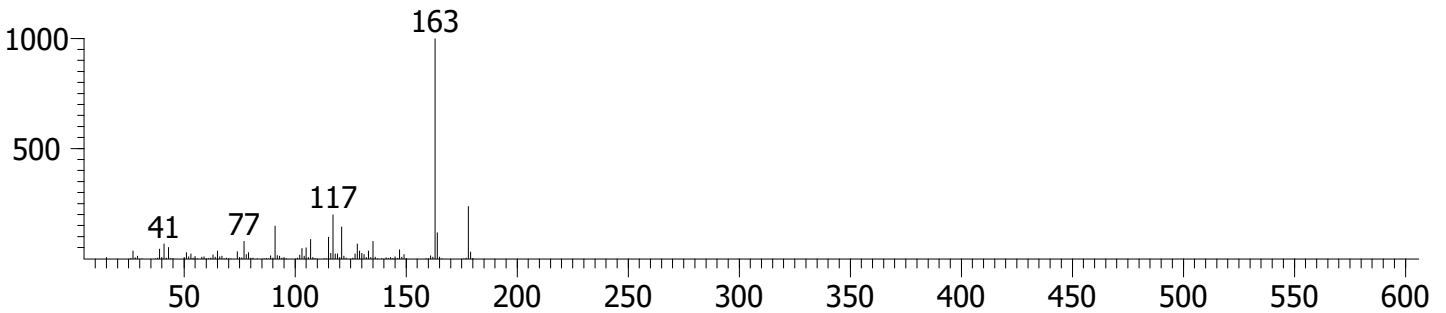
Peak Apex - sample "AnBxr B (20191121):1", peak 2510, at 1085.15 , 1.657 sec , sec (Spec # 91941)



Peak True - sample "AnBxr B (20191121):1", peak 2510, at 1085.15 , 1.657 sec , sec (Spec # 91941)



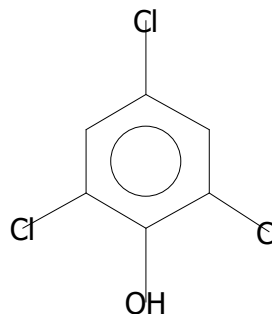
Library Hit - similarity 908, "Propofol"



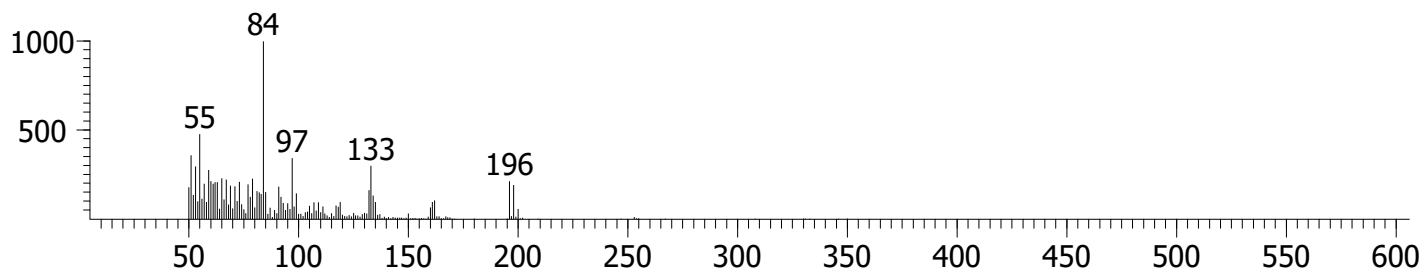
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Propofol	908	8989	2078-54-8	replib	C12H18O	178
2	Propofol	889	8989	2078-54-8	replib	C12H18O	178
3	Propofol	885	8989	2078-54-8	replib	C12H18O	178
4	Phenol, 2,5-bis(1-methylethyl)-	874	4227	35946-91-9	mainlib	C12H18O	178
5	Propofol	873	4063	2078-54-8	mainlib	C12H18O	178

Phenol, 2,4,6-trichloro-

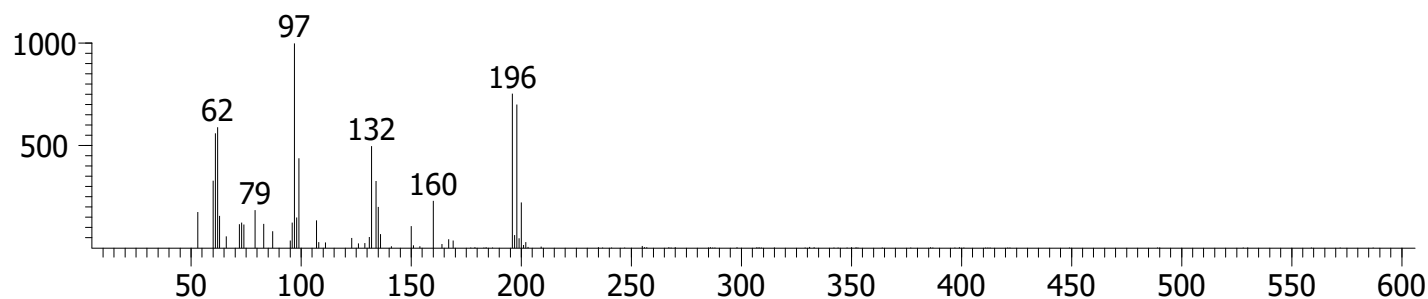
1st Dimension R.T. = 1088.65
2nd Dimension R.T. = 1.795
Quant Mass(es) = 196
S/N = 631.83
Area = 57536
Height = 7495.2
Similarity = 861



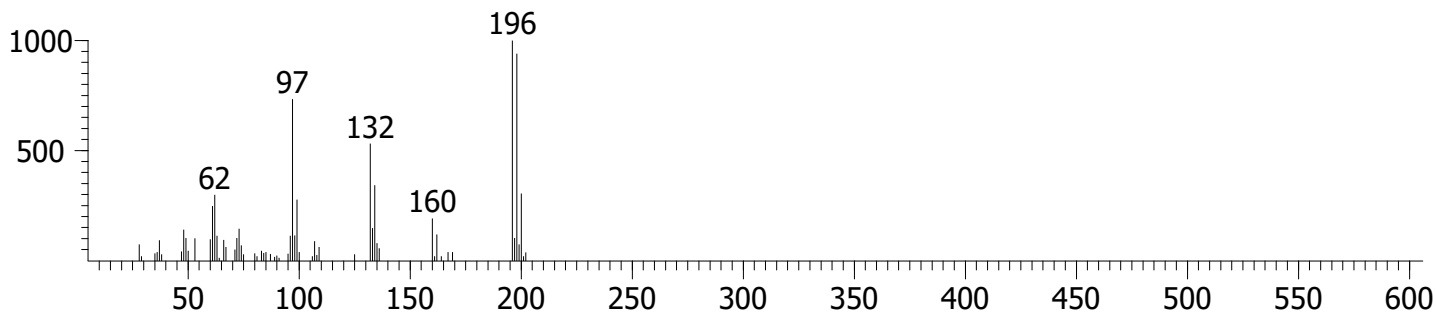
Peak Apex - sample "AnBxr B (20191121):1", peak 2533, at 1088.65 , 1.795 sec , sec (Spec # 92492)



Peak True - sample "AnBxr B (20191121):1", peak 2533, at 1088.65 , 1.795 sec , sec (Spec # 92492)



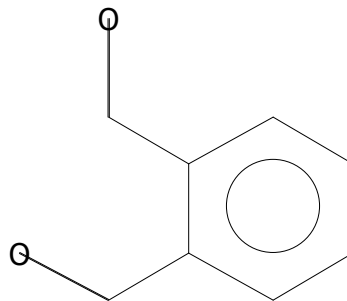
Library Hit - similarity 861, "Phenol, 2,4,6-trichloro-"



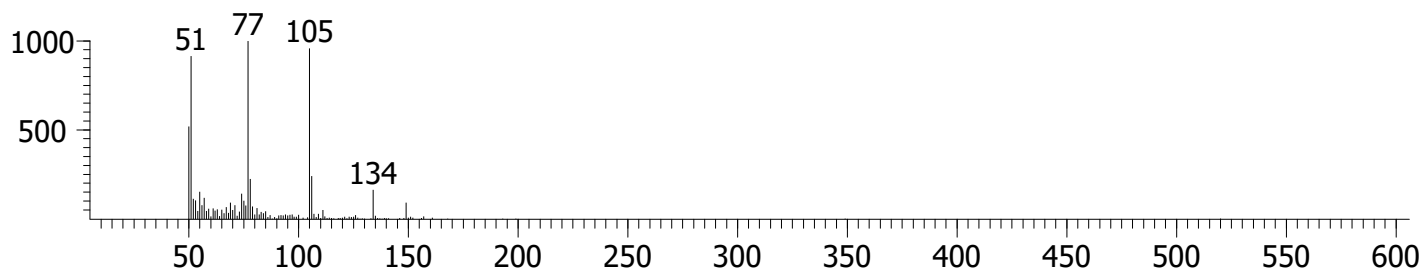
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 2,4,6-trichloro-	861	2778	88-06-2	replib	C6H3Cl3O	196
2	Phenol, 2,3,6-trichloro-	861	2778	933-75-5	replib	C6H3Cl3O	196
3	Phenol, 2,4,6-trichloro-	856	2778	88-06-2	replib	C6H3Cl3O	196
4	Phenol, 2,3,5-trichloro-	852	2017	933-78-8	replib	C6H3Cl3O	196
5	Phenol, 2,4,5-trichloro-	847	1625	95-95-4	replib	C6H3Cl3O	196

1,2-Benzenedicarboxaldehyde

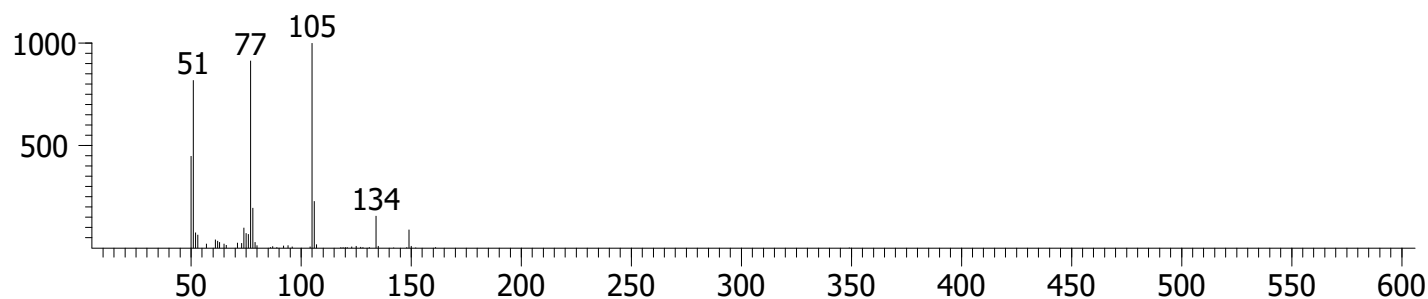
1st Dimension R.T. = 1148.12
2nd Dimension R.T. = 2.336
Quant Mass(es) = 105
S/N = 585.72
Area = 284621
Height = 30147
Similarity = 883



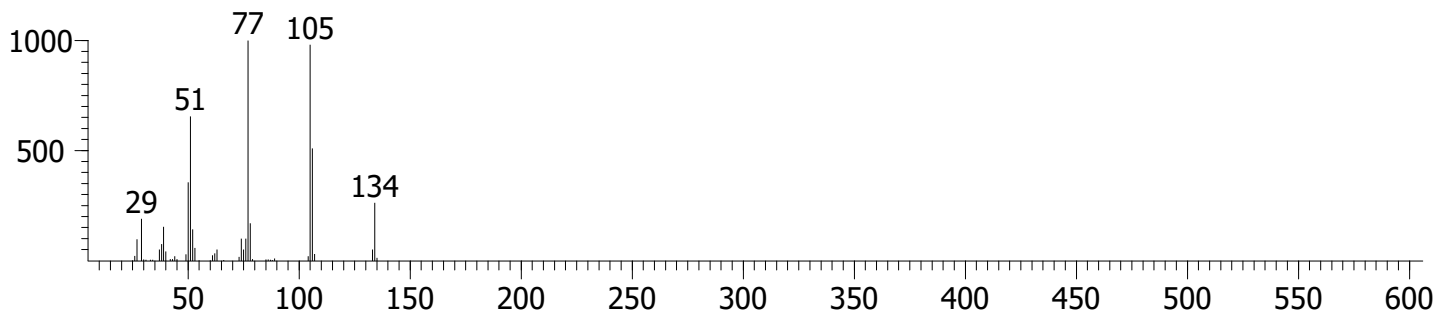
Peak Apex - sample "AnBxr B (20191121):1", peak 2894, at 1148.12 , 2.336 sec , sec (Spec # 101584)



Peak True - sample "AnBxr B (20191121):1", peak 2894, at 1148.12 , 2.336 sec , sec (Spec # 101584)



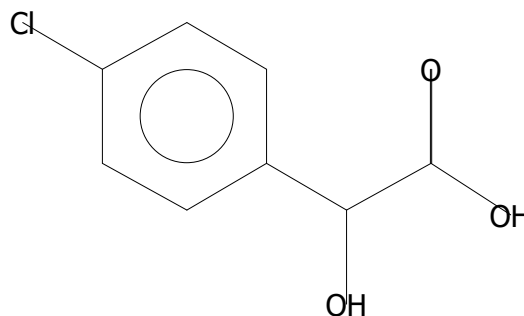
Library Hit - similarity 883, "1,2-Benzenedicarboxaldehyde"



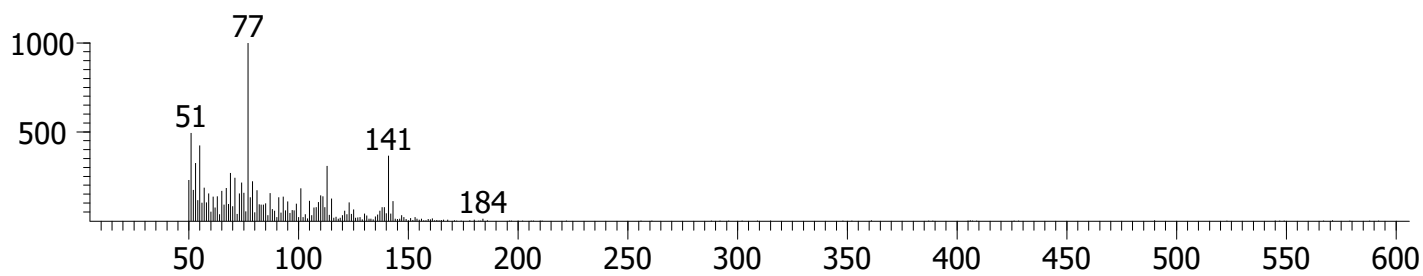
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,2-Benzenedicarboxaldehyde	883	5589	643-79-8	replib	C8H6O2	134
2	ethanone, 2-chloro-2,2-difluoro-1-phenyl-	871	3247	0-00-0	mainlib	C8H5ClF2O	190
3	1,2-Benzenedicarboxaldehyde	865	5589	643-79-8	replib	C8H6O2	134
4	1,2-Benzenedicarboxaldehyde	852	1577	643-79-8	mainlib	C8H6O2	134
5	1,2-Benzenedicarboxaldehyde	841	5589	643-79-8	replib	C8H6O2	134

p-Chloromandelic acid

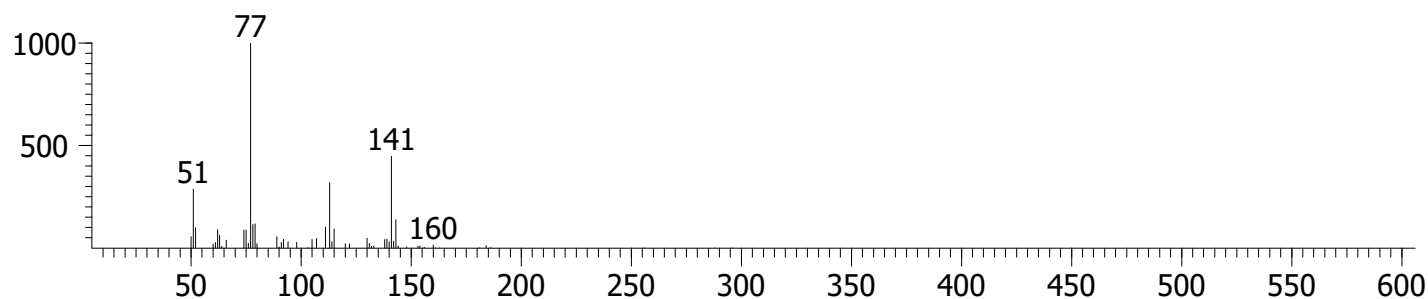
1st Dimension R.T. = 1165.61
2nd Dimension R.T. = 2.039
Quant Mass(es) = 141
S/N = 360.30
Area = 76169
Height = 7800.6
Similarity = 807



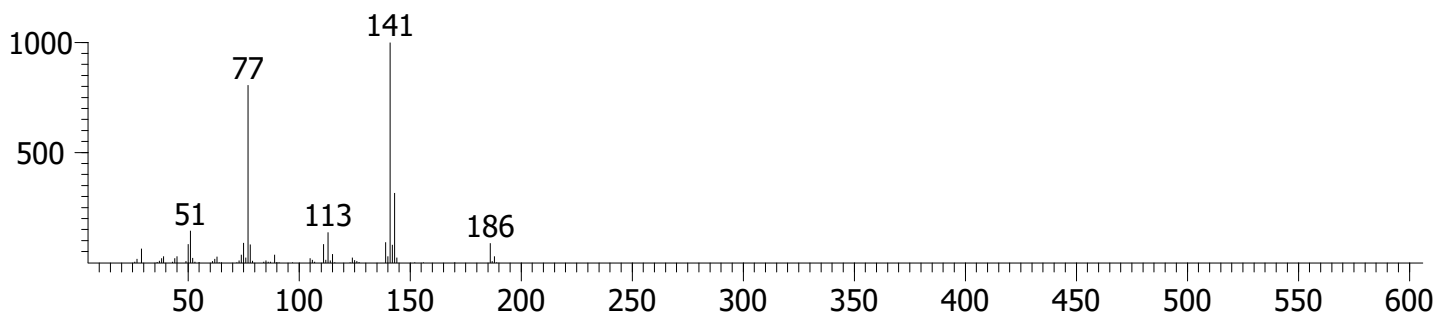
Peak Apex - sample "AnBxr B (20191121):1", peak 2991, at 1165.61 , 2.039 sec , sec (Spec # 104189)



Peak True - sample "AnBxr B (20191121):1", peak 2991, at 1165.61 , 2.039 sec , sec (Spec # 104189)



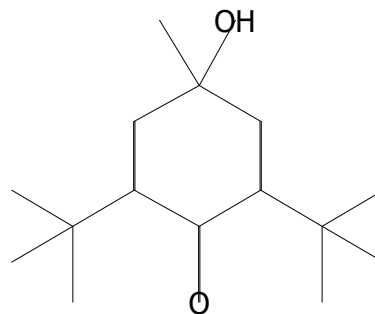
Library Hit - similarity 807, "p-Chloromandelic acid"



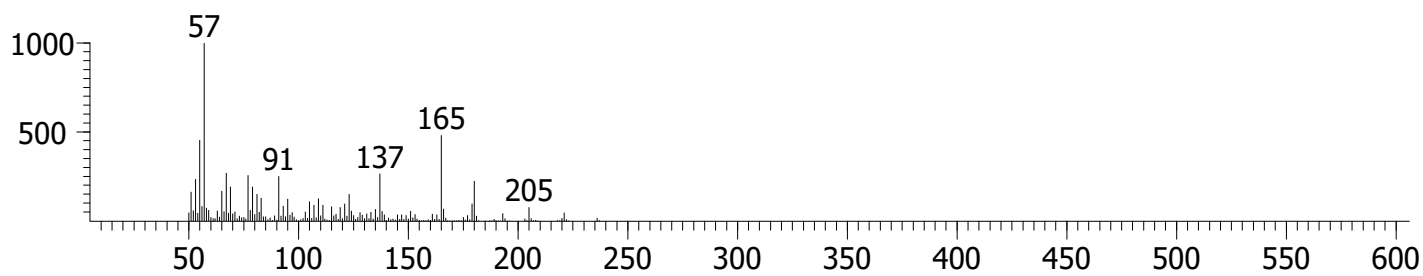
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	p-Chloromandelic acid	807	4824	492-86-4	mainlib	C8H7ClO3	186
2	p-Chloromandelic acid	794	6999	492-86-4	replib	C8H7ClO3	186
3	1,2-Bis(4-chlorophenyl)ethane-1,2-diol	793	3019	38152-44-2	mainlib	C14H12Cl2O2	282
4	p-Chloromandelic acid	787	6999	492-86-4	replib	C8H7ClO3	186
5	Benzenemethanol, 4-chloro-à-(2-nitrocyclopentyl)-, [1à(R*),2à]-	737	575	103130-03-6	mainlib	C12H14ClNO3	255

rt-butyl-4-hydroxy-4-methylcyclohexa-2,5-die

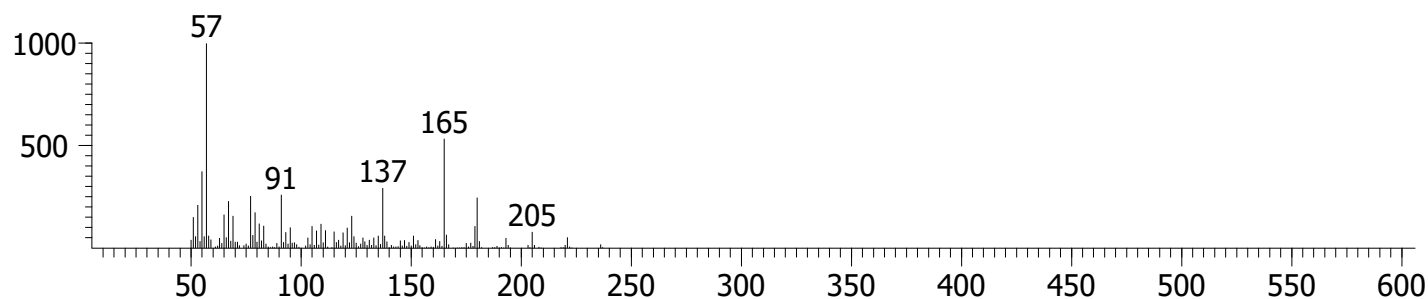
1st Dimension R.T. = 1221.58
2nd Dimension R.T. = 1.498
Quant Mass(es) = 165
S/N = 4079.9
Area = 694679
Height = 89267
Similarity = 869



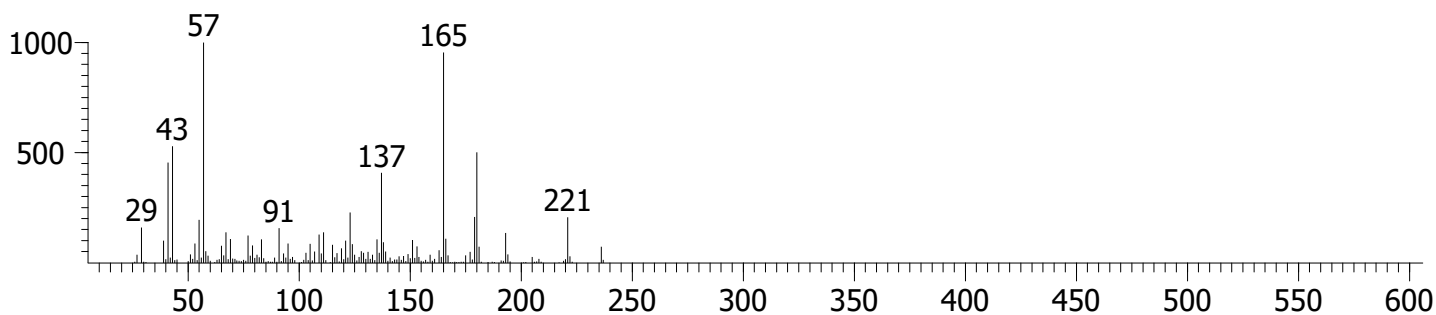
Peak Apex - sample "AnBxr B (20191121):1", peak 3300, at 1221.58 , 1.498 sec , sec (Spec # 112587)



Peak True - sample "AnBxr B (20191121):1", peak 3300, at 1221.58 , 1.498 sec , sec (Spec # 112587)



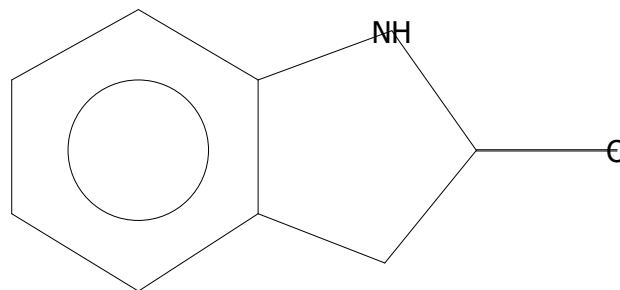
Library Hit - similarity 869, "2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one"



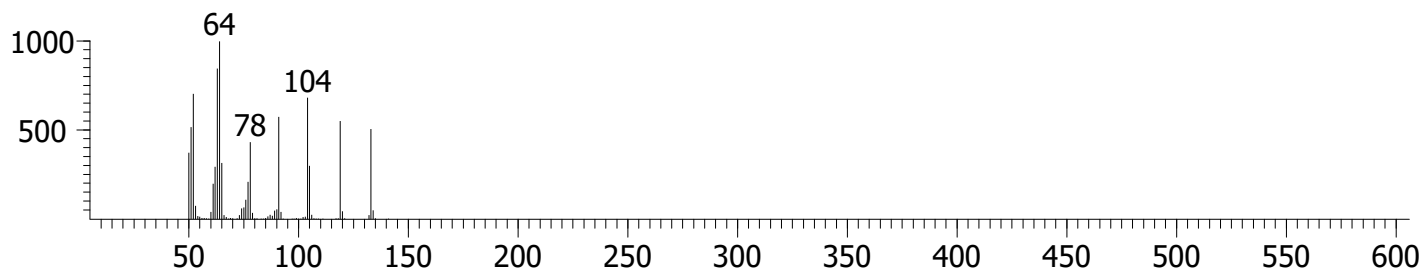
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one	869	8150	10396-80-2	mainlib	C15H24O2	236
2	Menthol, 1'-(butyn-3-one-1-yl)-, (1S,2S,5R)-	713	210	0-00-0	mainlib	C14H22O2	222
3	1H-Inden-1-ol, 2,4,5,6,7,7a-hexahydro-4,4,7a-trimethyl-	711	193	43125-89-9	mainlib	C12H20O	180
4	Menthol, 1'-(butyn-3-one-1-yl)-, (1R,2S,5R)-	707	163	0-00-0	mainlib	C14H22O2	222
5	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1-methoxy-	703	138	70703-08-1	mainlib	C11H16O2	180

2H-Indol-2-one, 1,3-dihydro-

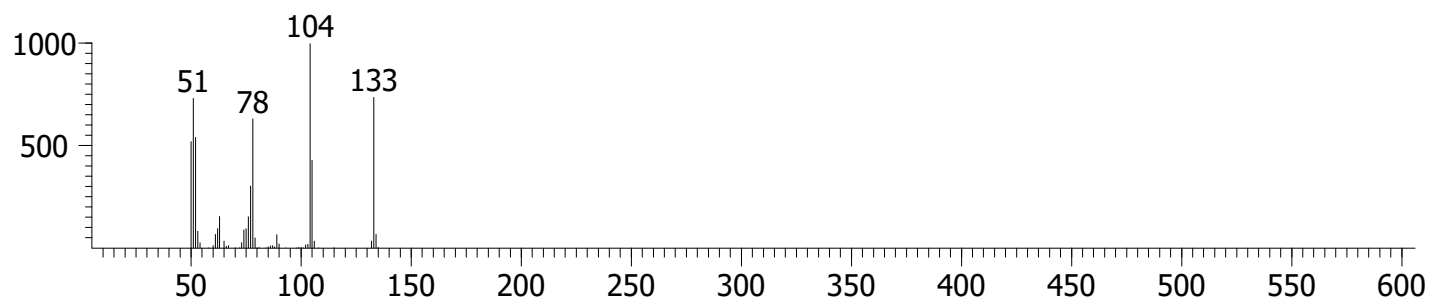
1st Dimension R.T. = 1246.06
2nd Dimension R.T. = 2.488
Quant Mass(es) = 104
S/N = 1324.1
Area = 3694117
Height = 260299
Similarity = 917



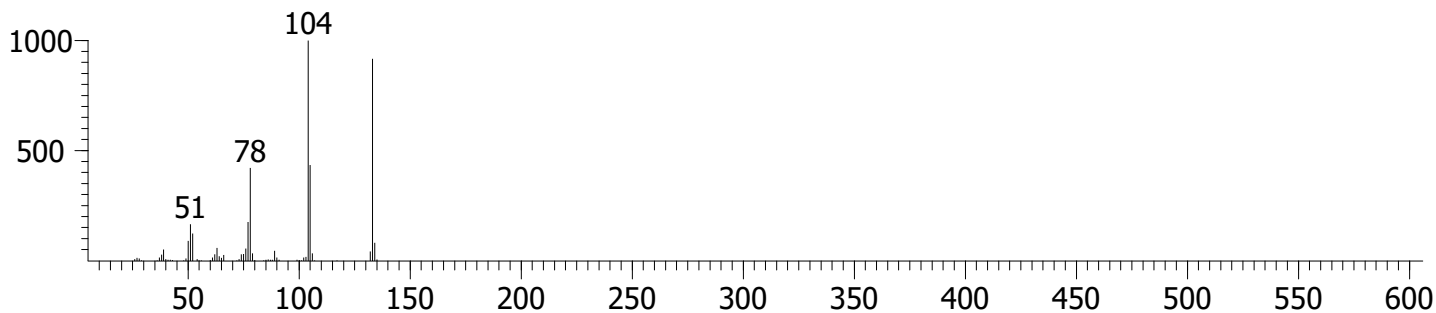
Peak Apex - sample "AnBxr B (20191121):1", peak 3476, at 1246.06 , 2.488 sec , sec (Spec # 116447)



Peak True - sample "AnBxr B (20191121):1", peak 3476, at 1246.06 , 2.488 sec , sec (Spec # 116447)



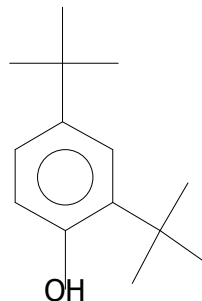
Library Hit - similarity 917, "2H-Indol-2-one, 1,3-dihydro-"



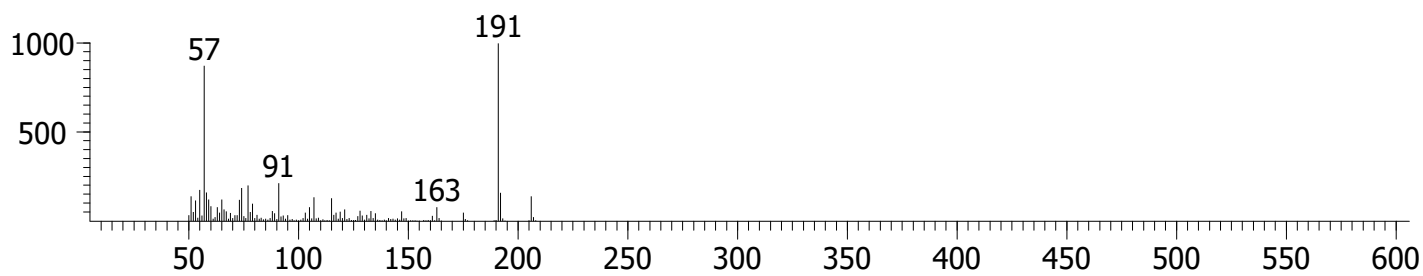
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2H-Indol-2-one, 1,3-dihydro-	917	7586	59-48-3	replib	C8H7NO	133
2	2H-Indol-2-one, 1,3-dihydro-	914	7586	59-48-3	replib	C8H7NO	133
3	2H-Indol-2-one, 1,3-dihydro-	910	7434	59-48-3	mainlib	C8H7NO	133
4	2H-Indol-2-one, 1,3-dihydro-	894	7586	59-48-3	replib	C8H7NO	133
5	2H-Indol-2-one, 1,3-dihydro-	885	7586	59-48-3	replib	C8H7NO	133

2,4-Di-tert-butylphenol

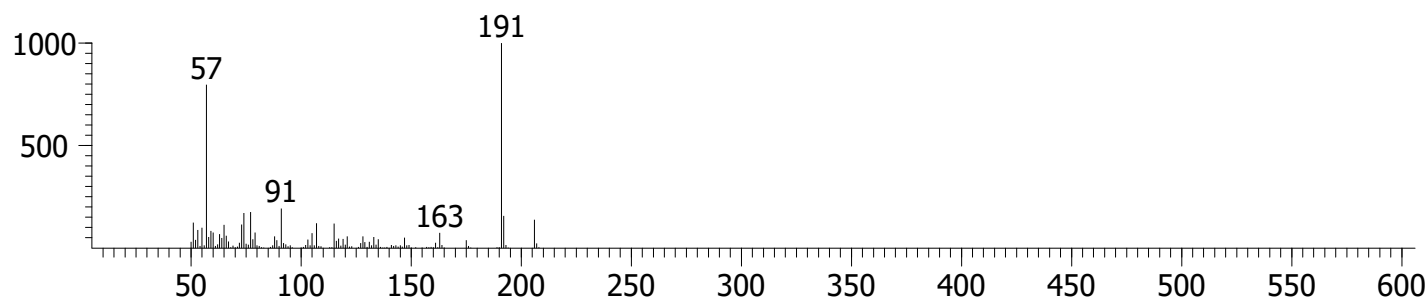
1st Dimension R.T. = 1270.55
2nd Dimension R.T. = 1.617
Quant Mass(es) = 191
S/N = 18072
Area = 1964943
Height = 257702
Similarity = 899



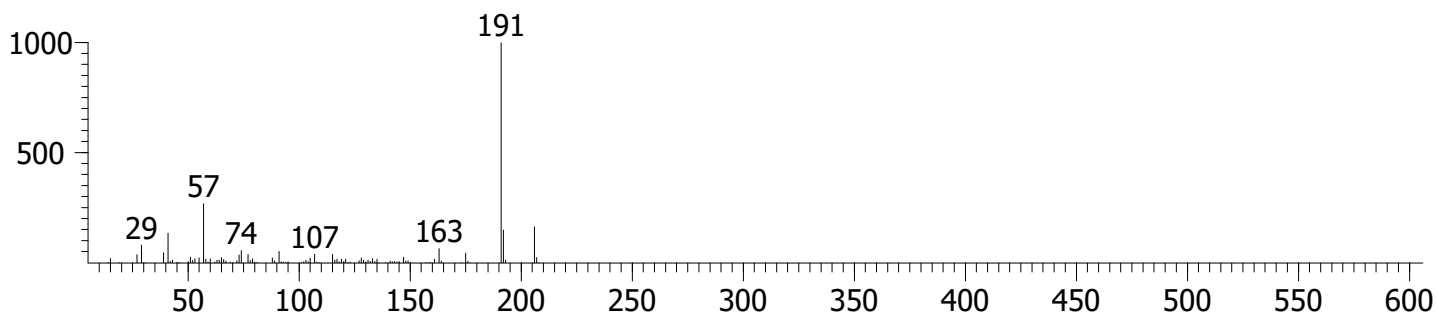
Peak Apex - sample "AnBxr B (20191121):1", peak 3617, at 1270.55 , 1.617 sec , sec (Spec # 120025)



Peak True - sample "AnBxr B (20191121):1", peak 3617, at 1270.55 , 1.617 sec , sec (Spec # 120025)



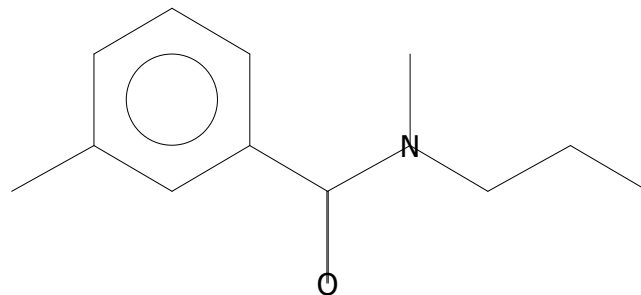
Library Hit - similarity 899, "2,4-Di-tert-butylphenol"



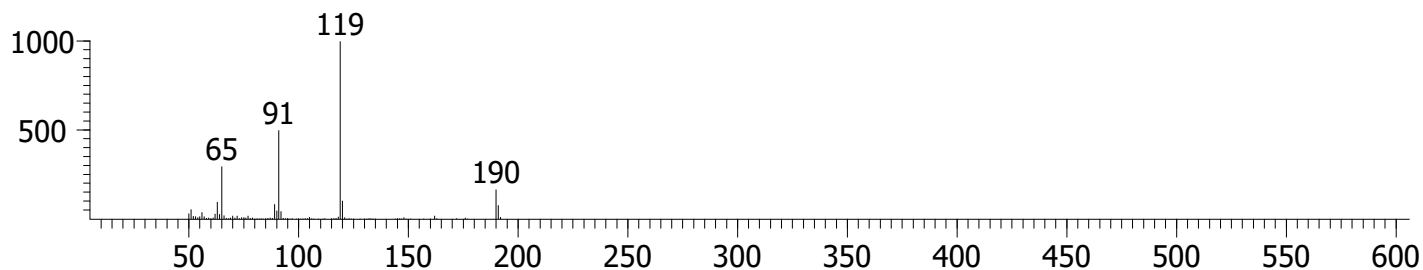
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,4-Di-tert-butylphenol	899	4829	96-76-4	replib	C ₁₄ H ₂₂ O	206
2	Phenol, 2,5-bis(1,1-dimethylethyl)-	892	3699	5875-45-6	replib	C ₁₄ H ₂₂ O	206
3	2,4-Di-tert-butylphenol	890	7557	96-76-4	mainlib	C ₁₄ H ₂₂ O	206
4	2,4-Di-tert-butylphenol	880	4829	96-76-4	replib	C ₁₄ H ₂₂ O	206
5	2,4-Di-tert-butylphenol	877	4829	96-76-4	replib	C ₁₄ H ₂₂ O	206

Benzamide, 3-methyl-N-methyl-N-propyl-

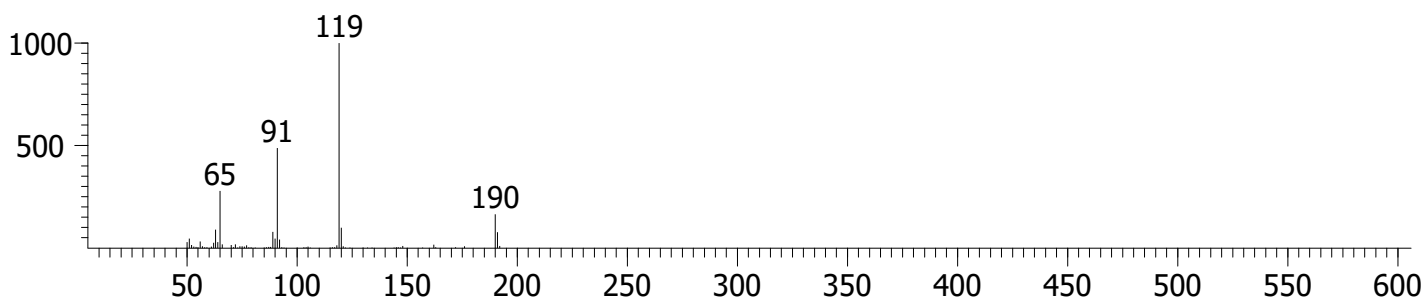
1st Dimension R.T. = 1361.5
2nd Dimension R.T. = 1.993
Quant Mass(es) = 119
S/N = 36621
Area = 12419449
Height = 946726
Similarity = 930



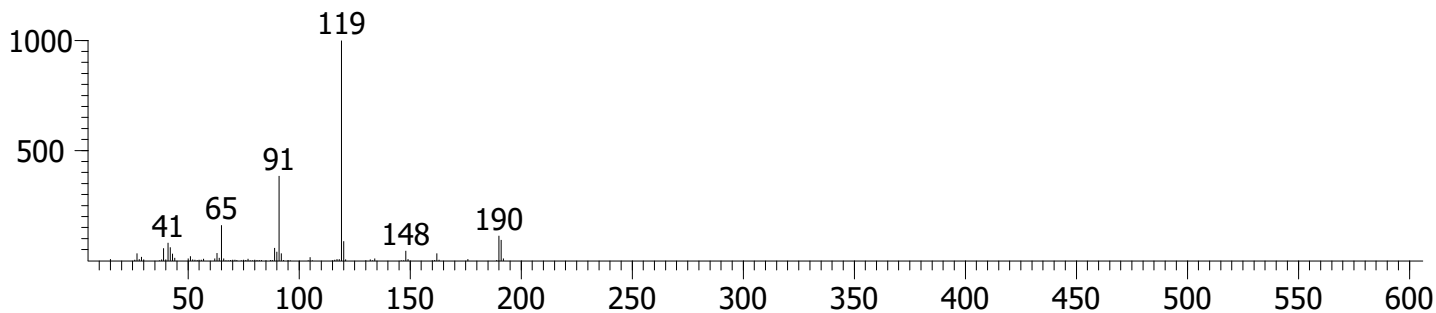
Peak Apex - sample "AnBxr B (20191121):1", peak 4204, at 1361.5 , 1.993 sec , sec (Spec # 133862)



Peak True - sample "AnBxr B (20191121):1", peak 4204, at 1361.5 , 1.993 sec , sec (Spec # 133862)



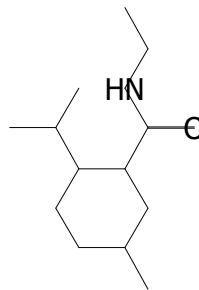
Library Hit - similarity 930, "Benzamide, 3-methyl-N-methyl-N-propyl-"



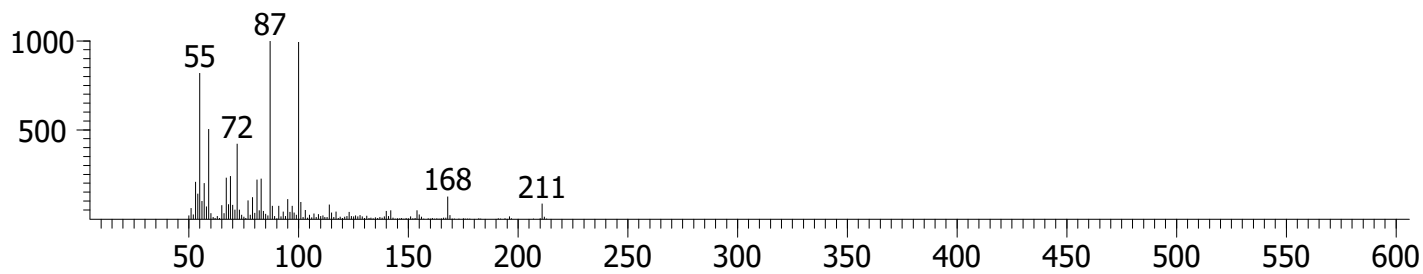
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzamide, 3-methyl-N-methyl-N-propyl-	930	2900	0-00-0	mainlib	C ₁₂ H ₁₇ NO	191
2	Diethyltoluamide	930	6970	134-62-3	replib	C ₁₂ H ₁₇ NO	191
3	Diethyltoluamide	916	6970	134-62-3	replib	C ₁₂ H ₁₇ NO	191
4	Diethyltoluamide	910	6970	134-62-3	replib	C ₁₂ H ₁₇ NO	191
5	Diethyltoluamide	892	6970	134-62-3	replib	C ₁₂ H ₁₇ NO	191

Cyclohexanecarboxamide,
N-ethyl-5-methyl-2-(1-methylethyl)-

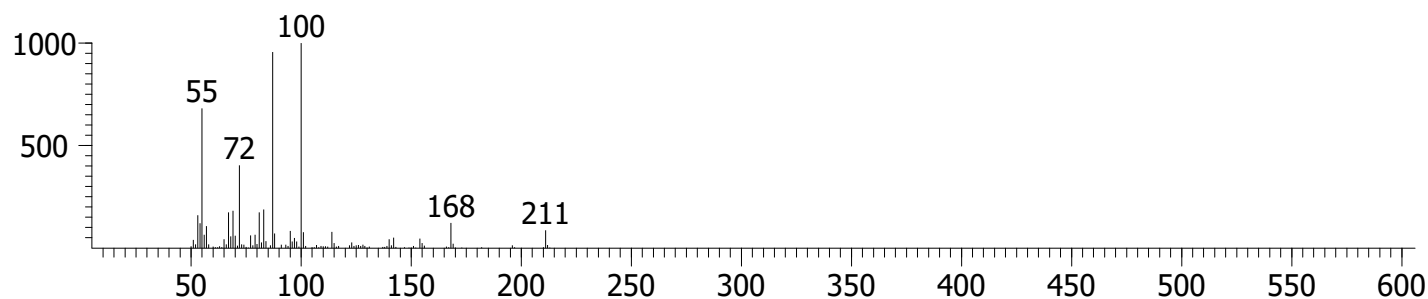
1st Dimension R.T. = 1378.99
 2nd Dimension R.T. = 1.696
 Quant Mass(es) = 100
 S/N = 7867.3
 Area = 1399039
 Height = 134357
 Similarity = 884



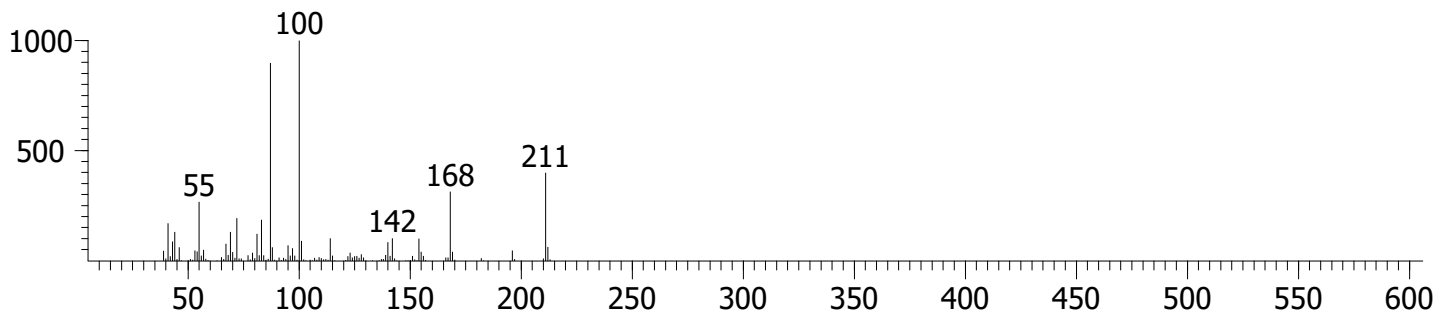
Peak Apex - sample "AnBxr B (20191121):1", peak 4328, at 1378.99 , 1.696 sec , sec (Spec # 136467)



Peak True - sample "AnBxr B (20191121):1", peak 4328, at 1378.99 , 1.696 sec , sec (Spec # 136467)



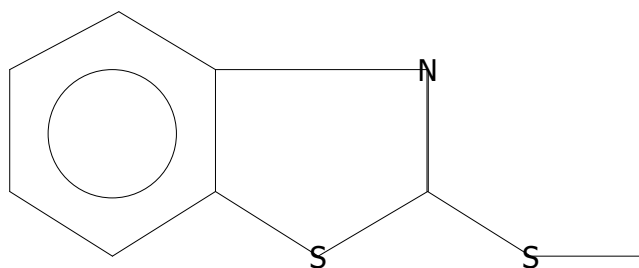
Library Hit - similarity 884, "Cyclohexanecarboxamide, N-ethyl-5-methyl-2-(1-methylethyl)-"



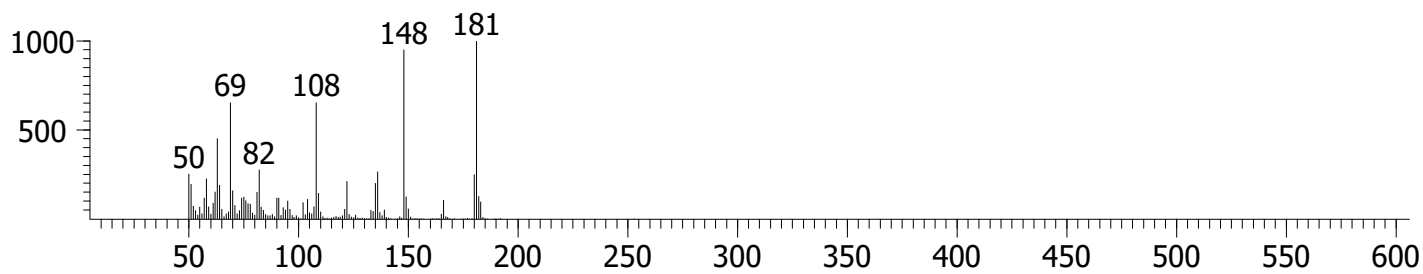
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cyclohexanecarboxamide, N-ethyl-5-methyl-2-(1-methylethyl)-	884	9193	39711-79-0	mainlib	C13H25NO	211
2	2-Decanone, O-methyloxime	699	147	36382-61-3	mainlib	C11H23NO	185
3	Propanamide, 3-cyclopentyl-N-ethyl-	689	103	0-00-0	mainlib	C10H19NO	169
4	Non-7-enoic acid, dimethylamide	682	79	0-00-0	mainlib	C11H21NO	183
5	2-Nonanone, O-methyloxime	680	73	56292-72-9	mainlib	C10H21NO	171

2-(Methylmercapto)benzothiazole

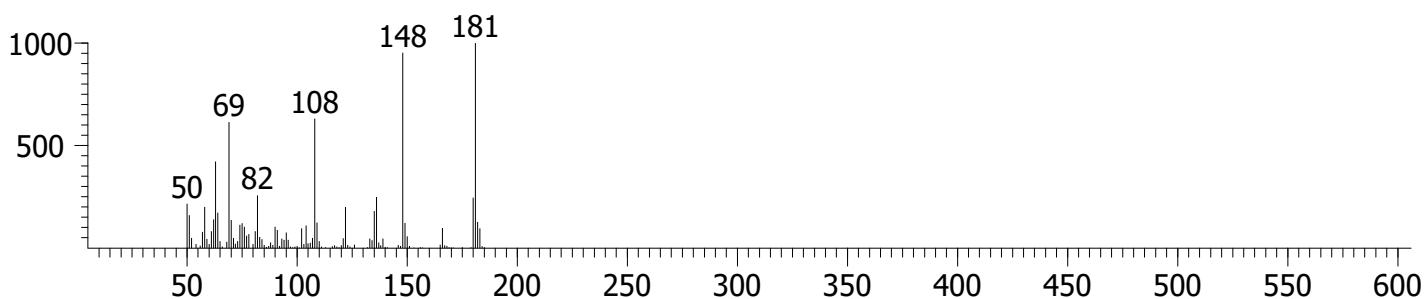
1st Dimension R.T. = 1399.97
2nd Dimension R.T. = 2.277
Quant Mass(es) = 181
S/N = 6676.1
Area = 1218083
Height = 122667
Similarity = 961



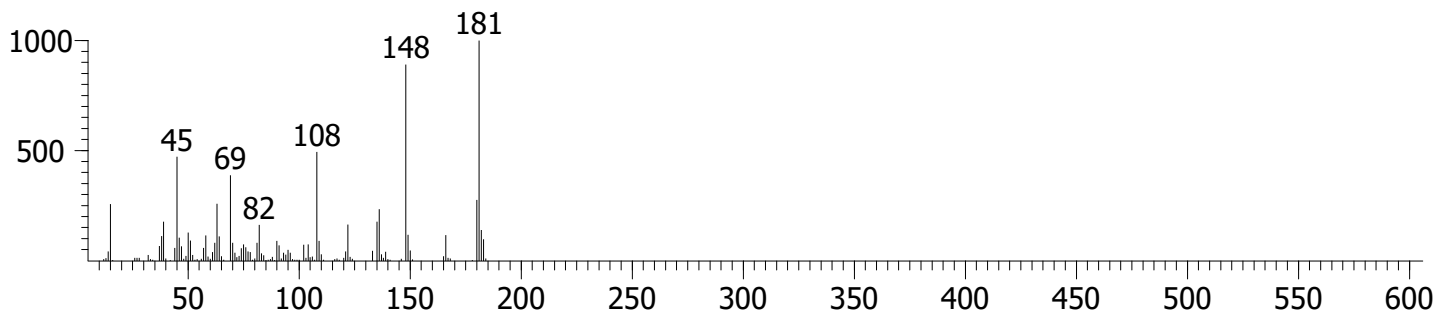
Peak Apex - sample "AnBxr B (20191121):1", peak 4485, at 1399.97 , 2.277 sec , sec (Spec # 139735)



Peak True - sample "AnBxr B (20191121):1", peak 4485, at 1399.97 , 2.277 sec , sec (Spec # 139735)



Library Hit - similarity 961, "2-(Methylmercapto)benzothiazole"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-(Methylmercapto)benzothiazole	961	9614	615-22-5	replib	C ₈ H ₇ NS ₂	181
2	2-(Methylmercapto)benzothiazole	926	9614	615-22-5	replib	C ₈ H ₇ NS ₂	181
3	2-(Methylmercapto)benzothiazole	905	7110	615-22-5	mainlib	C ₈ H ₇ NS ₂	181
4	2-(Methylmercapto)benzothiazole	900	9614	615-22-5	replib	C ₈ H ₇ NS ₂	181
5	2-(Methylthio)phenyl isothiocyanate	870	1784	51333-75-6	mainlib	C ₈ H ₇ NS ₂	181

Cinnamaldehyde, à-pentyl-

1st Dimension R.T. = 1434.95

2nd Dimension R.T. = 1.762

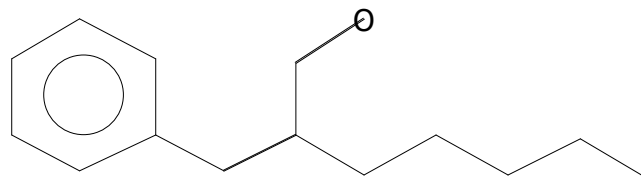
Quant Mass(es) = 129

S/N = 809.57

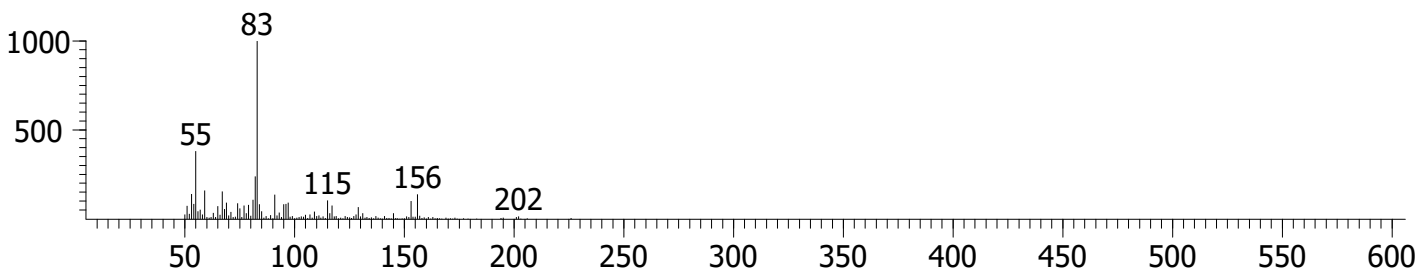
Area = 172502

Height = 15004

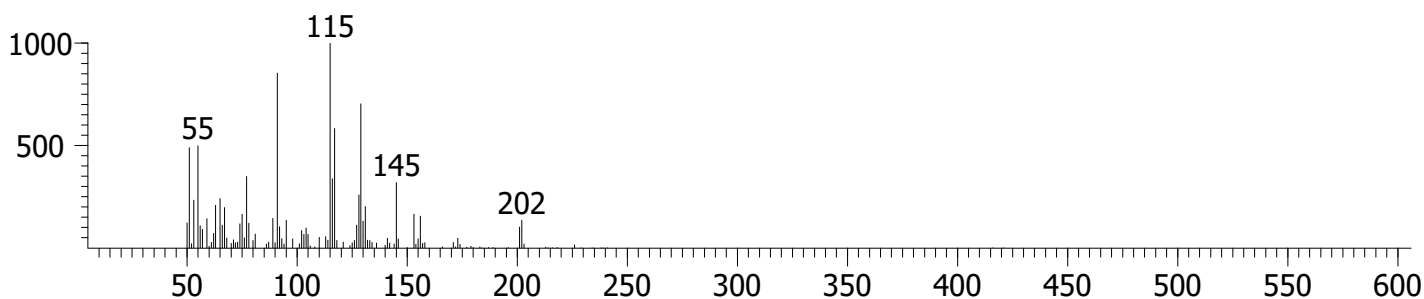
Similarity = 788



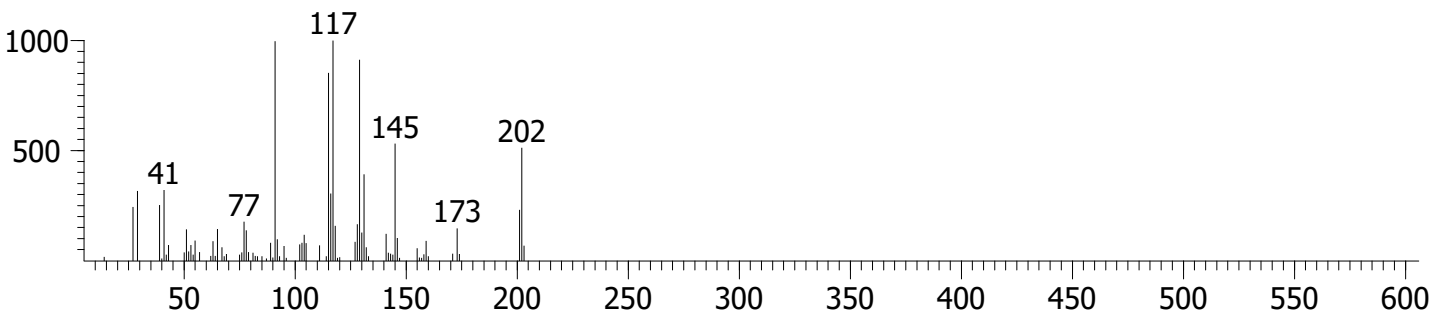
Peak Apex - sample "AnBxr B (20191121):1", peak 4727, at 1434.95 , 1.762 sec , sec (Spec # 144957)



Peak True - sample "AnBxr B (20191121):1", peak 4727, at 1434.95 , 1.762 sec , sec (Spec # 144957)



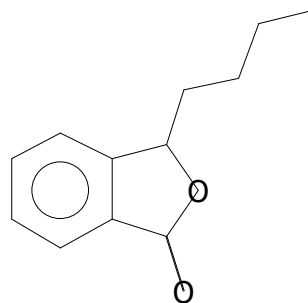
Library Hit - similarity 788, "Cinnamaldehyde, à-pentyl-"



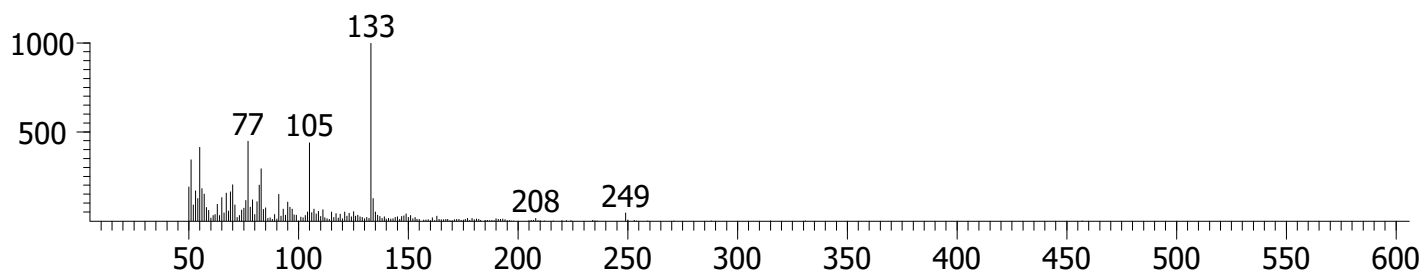
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cinnamaldehyde, à-pentyl-	788	6899	122-40-7	replib	C14H18O	202
2	Cinnamaldehyde, à-pentyl-	775	6899	122-40-7	replib	C14H18O	202
3	Cinnamaldehyde, à-pentyl-	771	6899	122-40-7	replib	C14H18O	202
4	Octanal, 2-(phenylmethylene)-	735	1364	101-86-0	replib	C15H20O	216
5	5-APDI	729	1072	13396-94-6	replib	C12H17N	175

3-Butylisobenzofuran-1(3H)-one

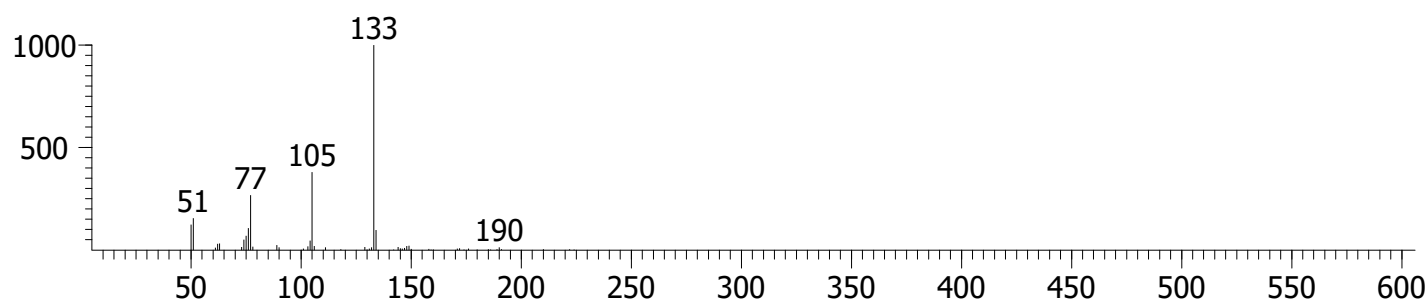
1st Dimension R.T. = 1452.44
2nd Dimension R.T. = 2.039
Quant Mass(es) = 133
S/N = 1292.5
Area = 559233
Height = 51885
Similarity = 887



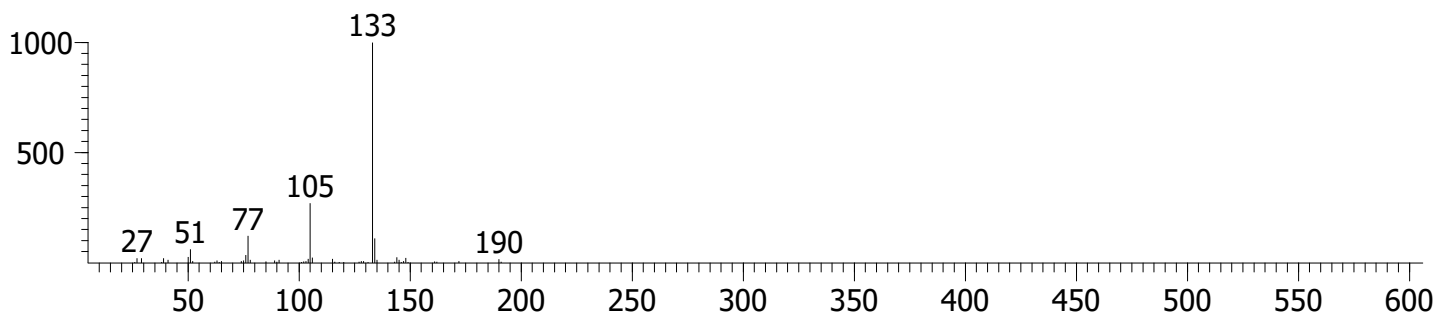
Peak Apex - sample "AnBxr B (20191121):1", peak 4839, at 1452.44 , 2.039 sec , sec (Spec # 147649)



Peak True - sample "AnBxr B (20191121):1", peak 4839, at 1452.44 , 2.039 sec , sec (Spec # 147649)



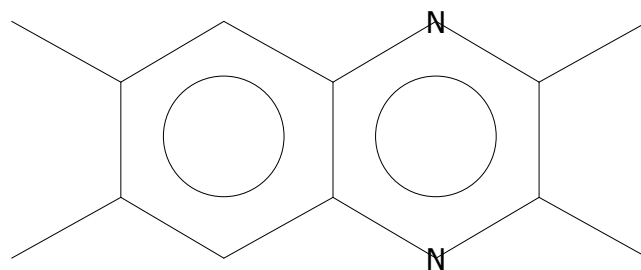
Library Hit - similarity 887, "3-Butylisobenzofuran-1(3H)-one"



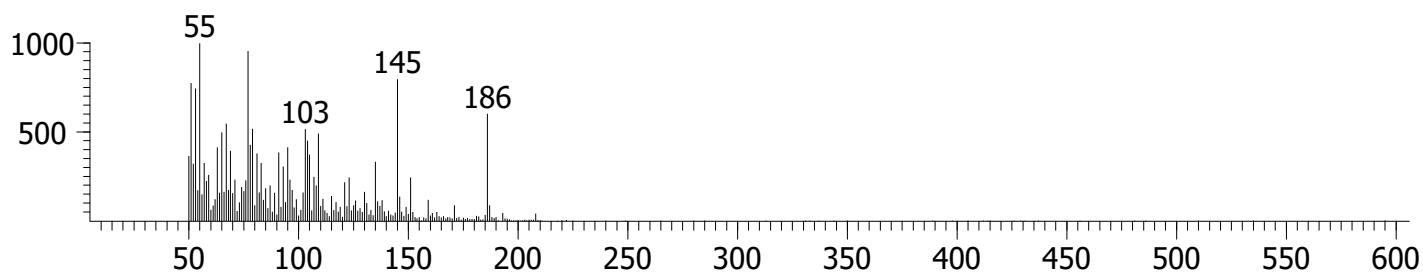
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Butylisobenzofuran-1(3H)-one	887	3660	6066-49-5	mainlib	C ₁₂ H ₁₄ O ₂	190
2	3-Butylisobenzofuran-1(3H)-one	884	7482	6066-49-5	replib	C ₁₂ H ₁₄ O ₂	190
3	Benzoic acid, 4-formyl-, 4-nitrophenyl(ester)	853	938	131266-90-5	mainlib	C ₁₄ H ₉ NO ₅	271
4	Scopoletin	838	6425	92-61-5	nist_msms	C ₁₀ H ₈ O ₄	192
5	Furazan-3-carboxylic acid, 4-amino-, 2-(2,5-dimethylphenyl)-2-oxoethyl ester	836	512	296244-74-1	mainlib	C ₁₃ H ₁₃ N ₃ O ₄	275

2,3,6,7-Tetramethylquinoxaline

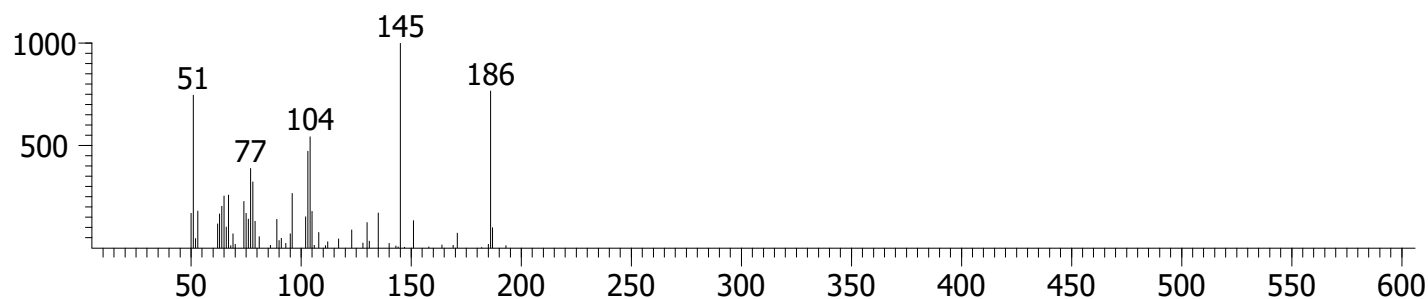
1st Dimension R.T. = 1473.43
2nd Dimension R.T. = 1.993
Quant Mass(es) = 186
S/N = 983.37
Area = 130189
Height = 13241
Similarity = 665



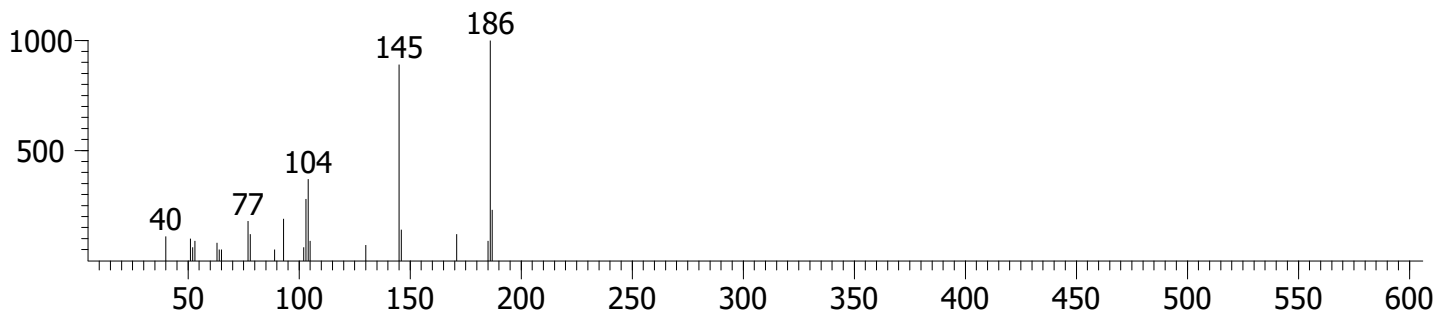
Peak Apex - sample "AnBxr B (20191121):1", peak 4967, at 1473.43 , 1.993 sec , sec (Spec # 150822)



Peak True - sample "AnBxr B (20191121):1", peak 4967, at 1473.43 , 1.993 sec , sec (Spec # 150822)



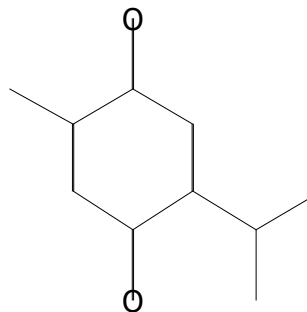
Library Hit - similarity 665, "2,3,6,7-Tetramethylquinoxaline"



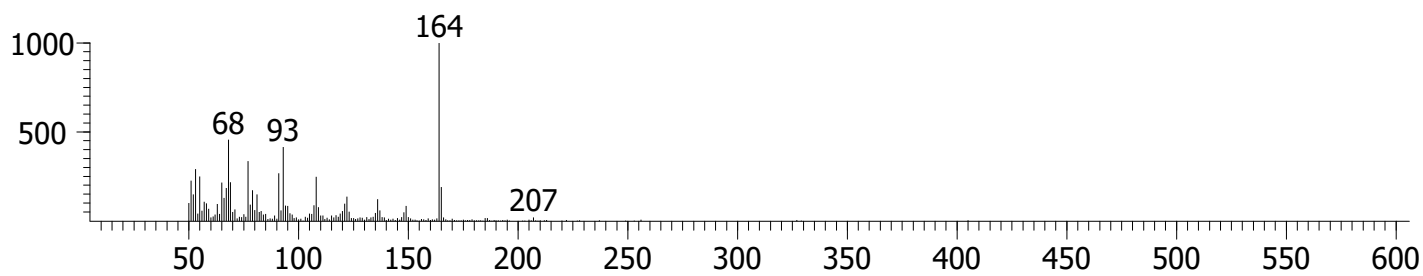
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,3,6,7-Tetramethylquinoxaline	665	5197	6957-19-3	mainlib	C12H14N2	186
2	Benzenesulfonic acid, 2,5-dimethyl-	593	4179	609-54-1	replib	C8H10O3S	186
3	Benzenesulfonic acid, 2,5-dimethyl-	570	421	609-54-1	mainlib	C8H10O3S	186
4	Benzeneacetic acid, 4-(5-methyl-1H-1,2,3,4-tetrazol-1-yl)-	560	297	0-00-0	mainlib	C10H10N4O2	218
5	1-Methyl-4-oxo-N-(1,3,4-thiadiazol-2-yl)quinoline-3-carboxamide	560	297	0-00-0	mainlib	C13H10N4O2S	286

Thymoquinone

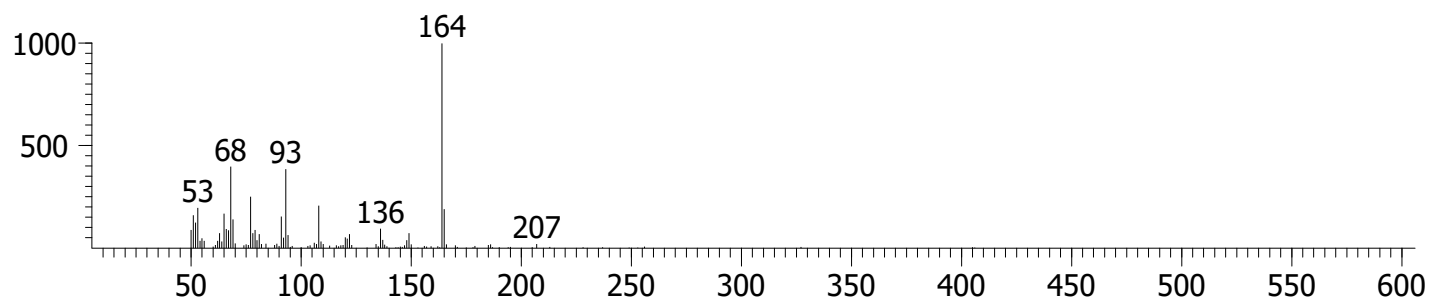
1st Dimension R.T. = 1508.41
2nd Dimension R.T. = 1.921
Quant Mass(es) = 164
S/N = 5184.8
Area = 704966
Height = 71115
Similarity = 746



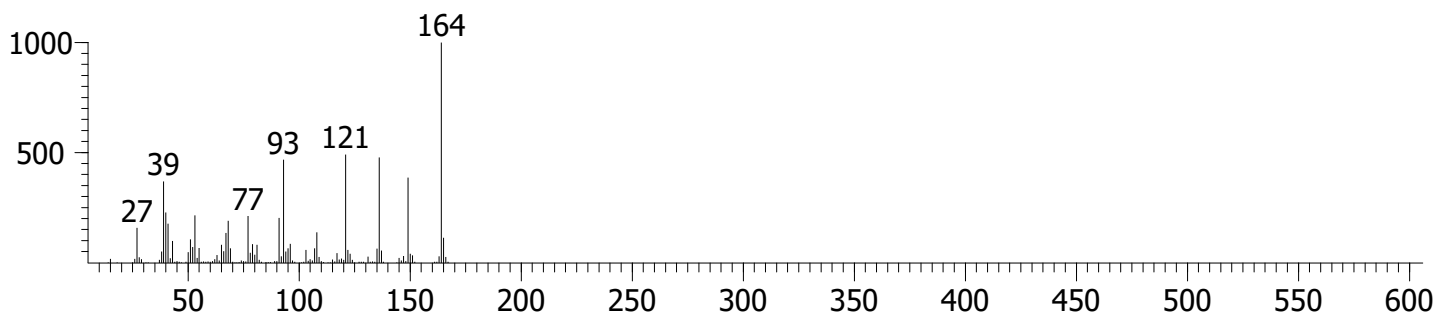
Peak Apex - sample "AnBxr B (20191121):1", peak 5208, at 1508.41 , 1.921 sec , sec (Spec # 156111)



Peak True - sample "AnBxr B (20191121):1", peak 5208, at 1508.41 , 1.921 sec , sec (Spec # 156111)



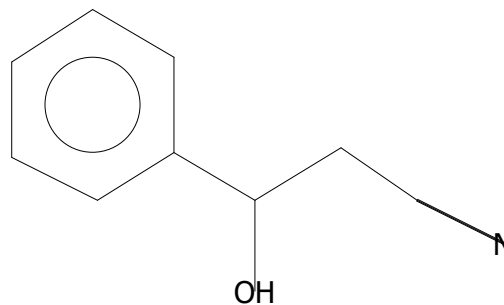
Library Hit - similarity 746, "Thymoquinone"



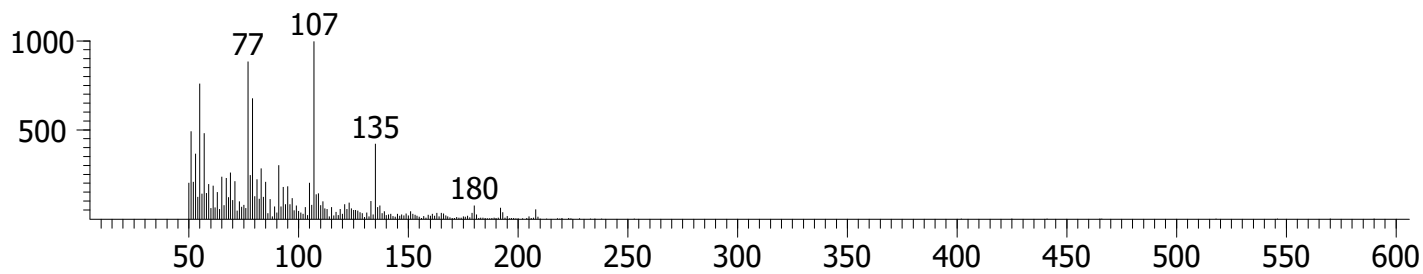
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Thymoquinone	746	3396	490-91-5	mainlib	C10H12O2	164
2	Thymoquinone	743	6465	490-91-5	replib	C10H12O2	164
3	Thymoquinone	708	6465	490-91-5	replib	C10H12O2	164
4	Inden-5(4H)-one, 2,6,7,7a-tetrahydro-4,4-dimethyl-	697	697	18366-35-3	mainlib	C11H16O	164
5	Tricyclo[3.3.3.0]undecan-3-one	687	492	83043-47-4	mainlib	C11H16O	164

Benzenepropanenitrile, á-hydroxy-

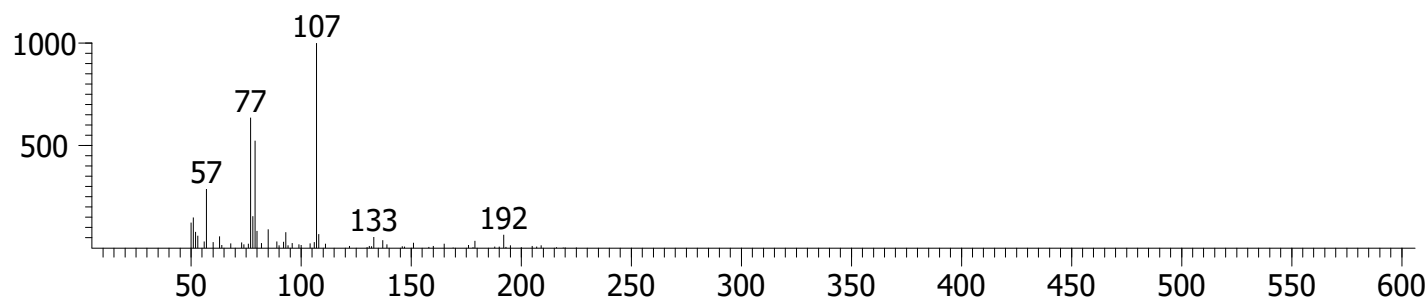
1st Dimension R.T. = 1529.4
2nd Dimension R.T. = 2.079
Quant Mass(es) = 107
S/N = 123.80
Area = 334846
Height = 30950
Similarity = 783



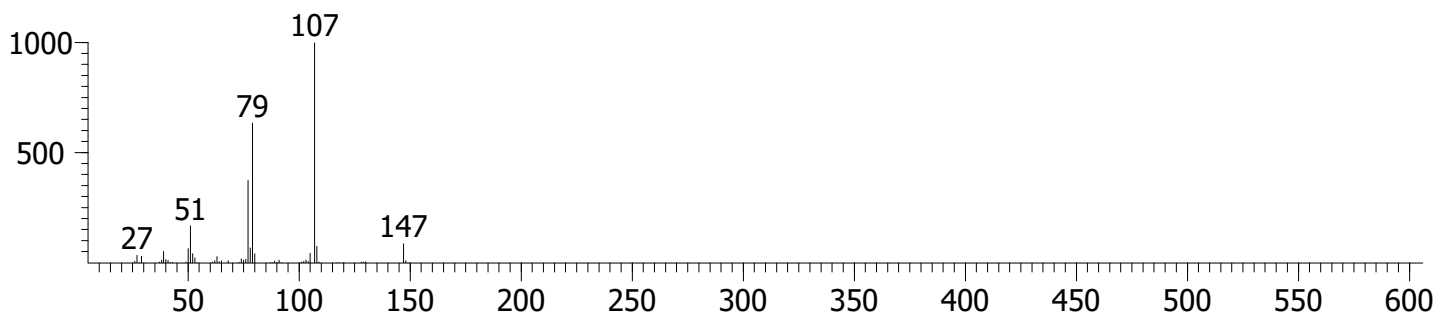
Peak Apex - sample "AnBxr B (20191121):1", peak 5364, at 1529.4 , 2.079 sec , sec (Spec # 159315)



Peak True - sample "AnBxr B (20191121):1", peak 5364, at 1529.4 , 2.079 sec , sec (Spec # 159315)



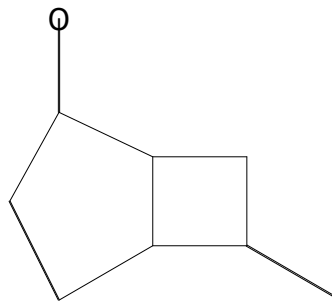
Library Hit - similarity 783, "Benzenepropanenitrile, á-hydroxy-"



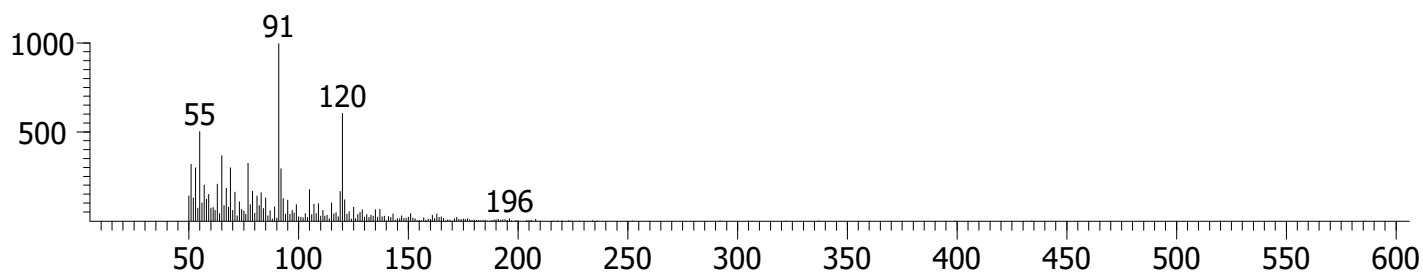
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenepropanenitrile, á-hydroxy-	783	1506	17190-29-3	mainlib	C9H9NO	147
2	Benzenemethanol, à-(2,2-dimethylpropyl)-	780	1331	62338-03-8	mainlib	C12H18O	178
3	Benzenemethanol, à-2-propenyl-	778	1643	936-58-3	replib	C10H12O	148
4	Mandelic acid	767	1127	90-64-2	replib	C8H8O3	152
5	Tricyclo[2.2.1.0(1,4)]heptan-2-one, 6-nitro-	765	806	56666-50-3	mainlib	C7H7NO3	153

6-Methylenebicyclo[3.2.0]hept-3-en-2-one

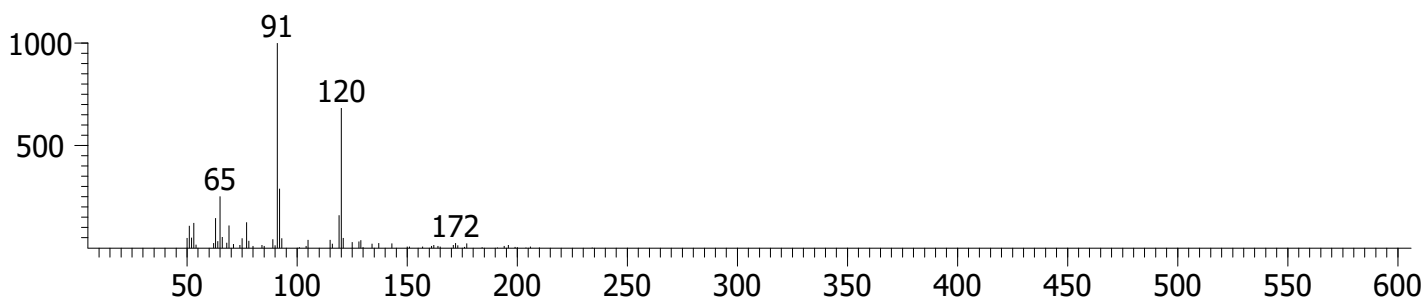
1st Dimension R.T. = 1543.39
2nd Dimension R.T. = 2.198
Quant Mass(es) = 120
S/N = 779.85
Area = 162959
Height = 14685
Similarity = 837



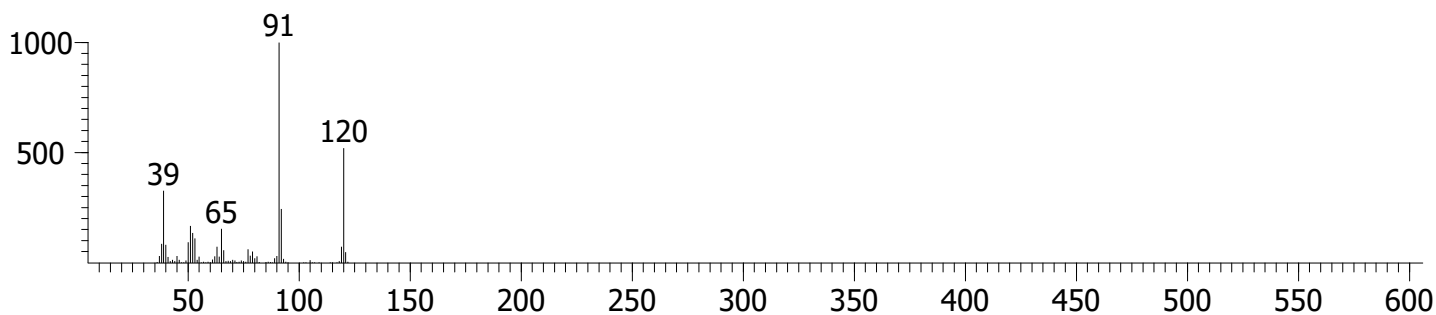
Peak Apex - sample "AnBxr B (20191121):1", peak 5457, at 1543.39 , 2.198 sec , sec (Spec # 161453)



Peak True - sample "AnBxr B (20191121):1", peak 5457, at 1543.39 , 2.198 sec , sec (Spec # 161453)



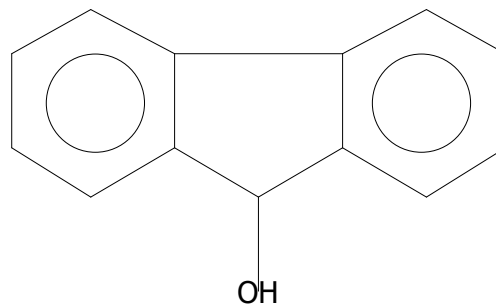
Library Hit - similarity 837, "6-Methylenebicyclo[3.2.0]hept-3-en-2-one"



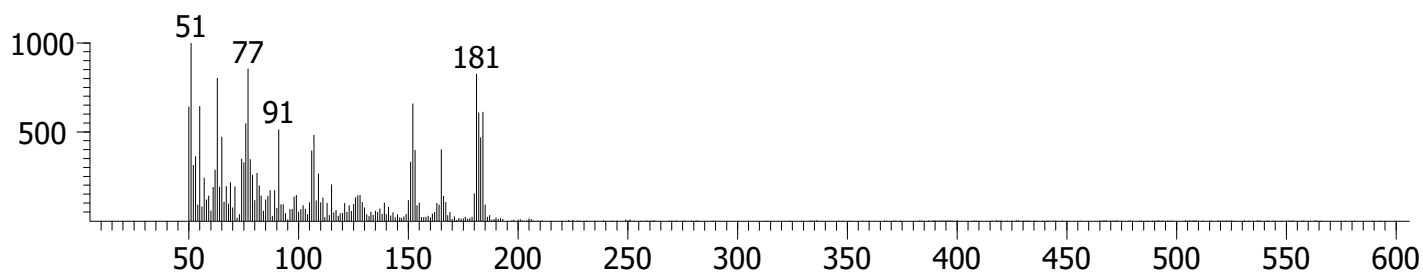
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	6-Methylenebicyclo[3.2.0]hept-3-en-2-one	837	5201	0-00-0	mainlib	C8H8O	120
2	4,5-Dihydro-2(1H)-pentalenone	815	2056	0-00-0	mainlib	C8H8O	120
3	Benzeneacetaldehyde	806	4696	122-78-1	replib	C8H8O	120
4	Phthalan	768	1125	496-14-0	replib	C8H8O	120
5	Benzeneacetaldehyde	768	4696	122-78-1	replib	C8H8O	120

9H-Fluoren-9-ol

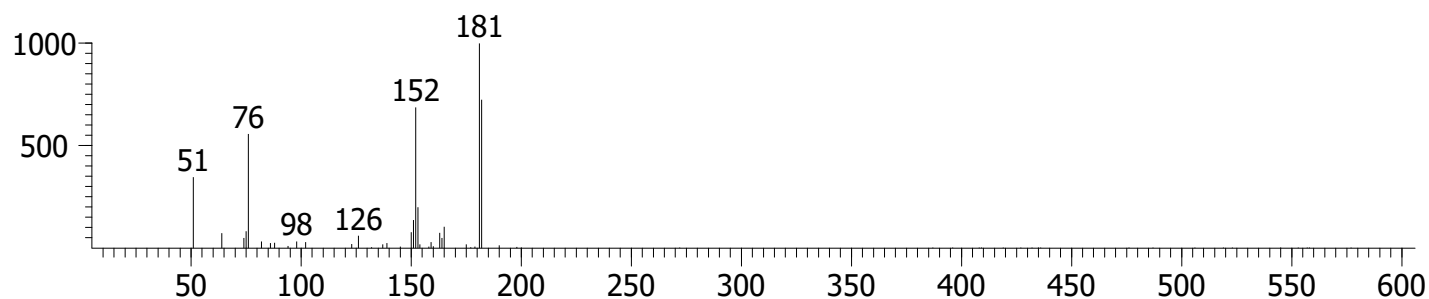
1st Dimension R.T. = 1557.38
2nd Dimension R.T. = 2.317
Quant Mass(es) = 181
S/N = 779.98
Area = 185039
Height = 14618
Similarity = 878



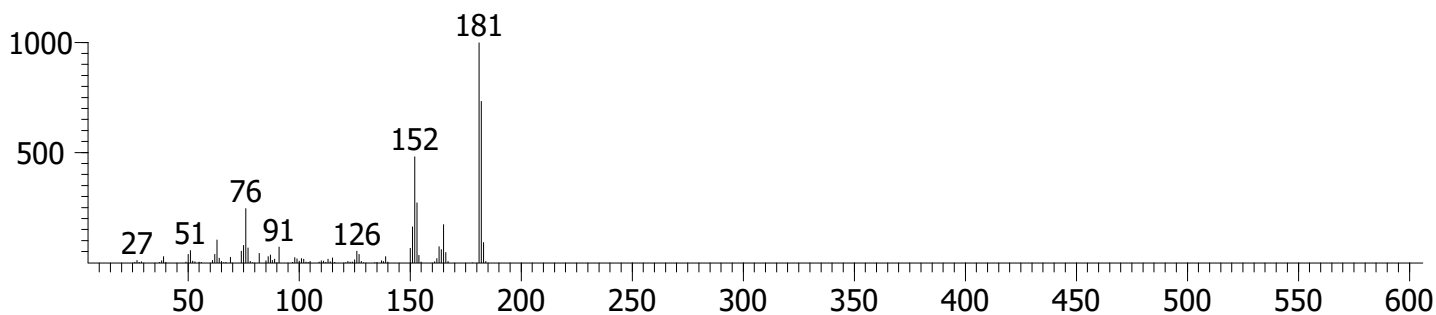
Peak Apex - sample "AnBxr B (20191121):1", peak 5565, at 1557.38 , 2.317 sec , sec (Spec # 163591)



Peak True - sample "AnBxr B (20191121):1", peak 5565, at 1557.38 , 2.317 sec , sec (Spec # 163591)



Library Hit - similarity 878, "9H-Fluoren-9-ol"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	9H-Fluoren-9-ol	878	7633	1689-64-1	replib	C13H10O	182
2	9H-Fluoren-9-ol	839	7633	1689-64-1	replib	C13H10O	182
3	6H-Dibenzo[b,d]pyran	819	3355	229-95-8	mainlib	C13H10O	182
4	9H-Fluoren-9-ol	808	7633	1689-64-1	replib	C13H10O	182
5	9H-Xanthene	804	1016	92-83-1	replib	C13H10O	182

4S,9aS)-4-Allyl-1-ethyloctahydro-1H-quinoli:

1st Dimension R.T. = 1578.37

2nd Dimension R.T. = 1.967

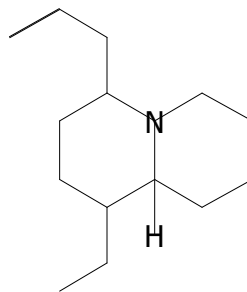
Quant Mass(es) = 166

S/N = 2407.2

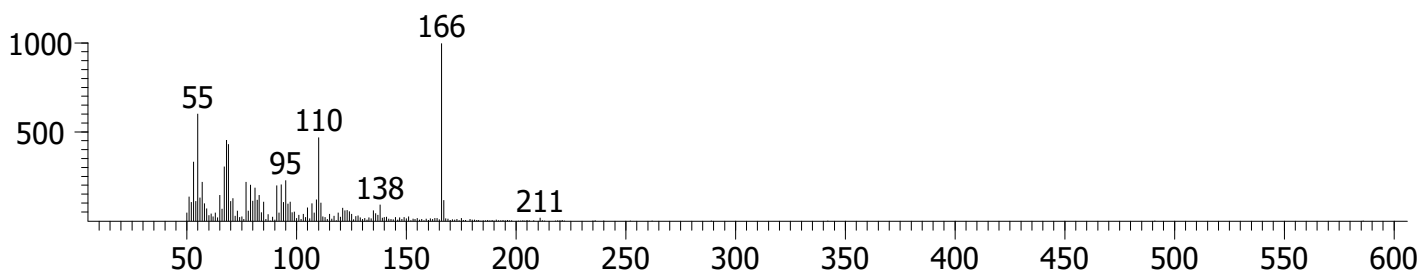
Area = 416015

Height = 38020

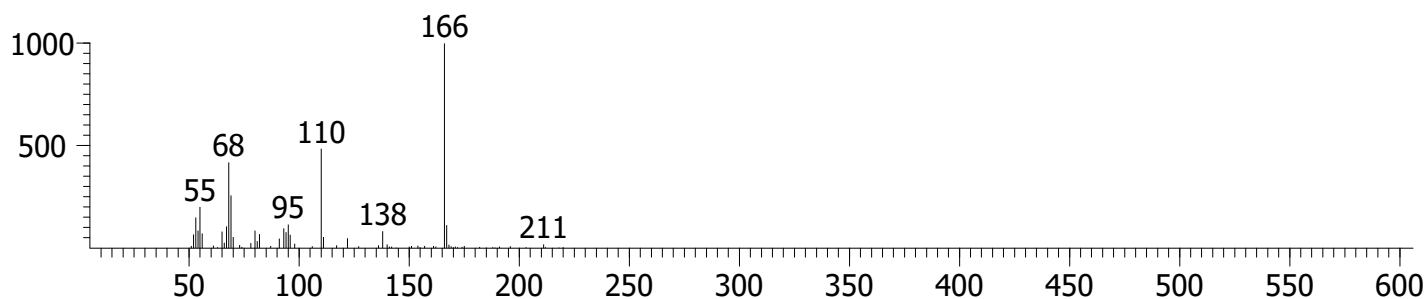
Similarity = 759



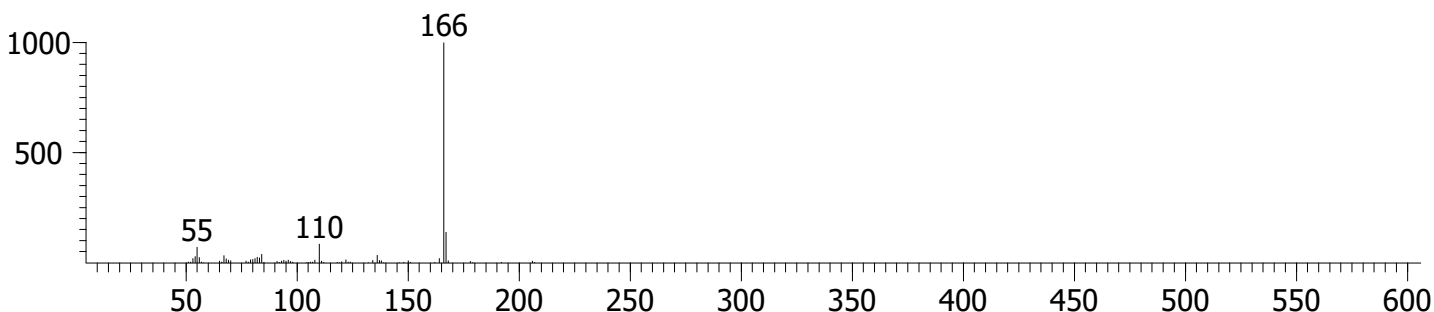
Peak Apex - sample "AnBxr B (20191121):1", peak 5695, at 1578.37 , 1.967 sec , sec (Spec # 166718)



Peak True - sample "AnBxr B (20191121):1", peak 5695, at 1578.37 , 1.967 sec , sec (Spec # 166718)



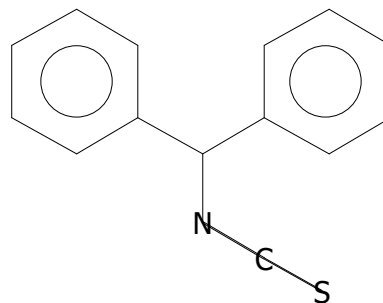
Library Hit - similarity 759, "(1S,4S,9aS)-4-Allyl-1-ethyloctahydro-1H-quinoline"



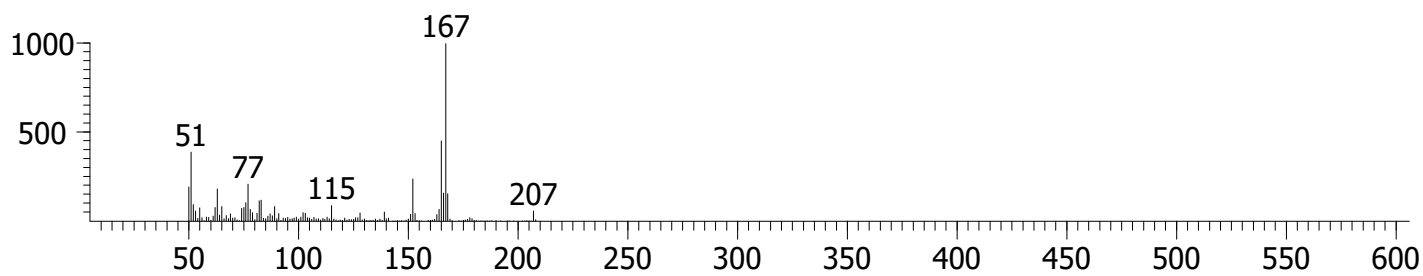
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	(1S,4S,9aS)-4-Allyl-1-ethyloctahydro-1H-quinoline	759	1565	151805-12-8	mainlib	C14H25N	207
2	(1R,4R,9aS)-1-Ethyl-4-(pent-4-en-1-yl)octahydro-1H-quinoline	758	1504	957792-07-3	mainlib	C16H29N	235
3	2,7(1H,3H)-Naphthalenedione, hexahydro-	740	775	46048-64-0	mainlib	C10H14O2	166
4	Imidazo[4,5-e][1,4]diazepine-5,8-dione, 1,4,6,7-tetrahydro-	738	715	119584-65-5	mainlib	C6H6N4O2	166
5	1-Aminocyclopentanecarboxylic acid, n-propargyloxycarbonyl-, pentadecyl ester	729	519	0-00-0	mainlib	C25H43NO4	421

Benzhydryl isothiocyanate

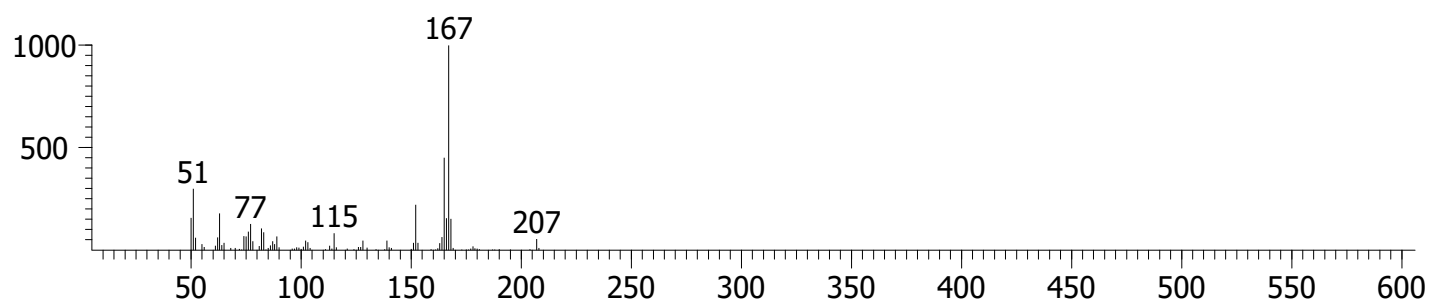
1st Dimension R.T. = 1655.33
2nd Dimension R.T. = 2.435
Quant Mass(es) = 167
S/N = 5006.8
Area = 1232115
Height = 103275
Similarity = 915



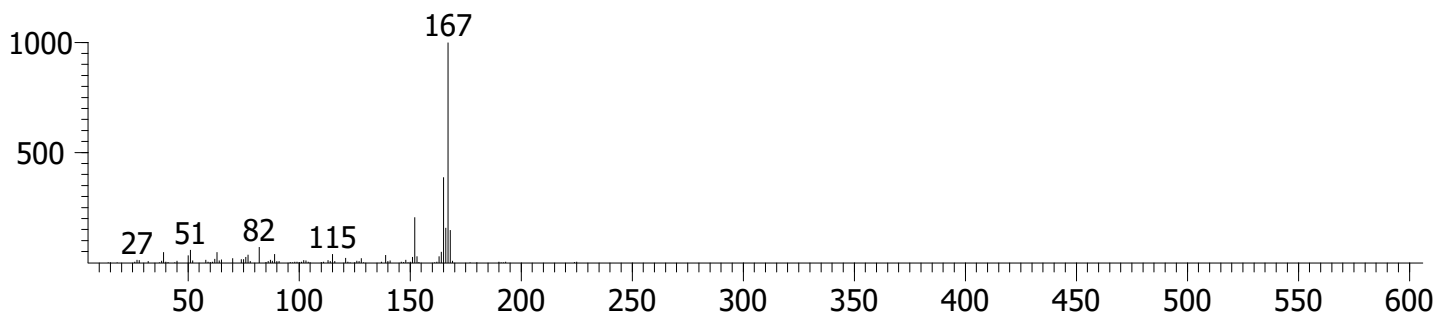
Peak Apex - sample "AnBxr B (20191121):1", peak 6182, at 1655.33 , 2.435 sec , sec (Spec # 178449)



Peak True - sample "AnBxr B (20191121):1", peak 6182, at 1655.33 , 2.435 sec , sec (Spec # 178449)

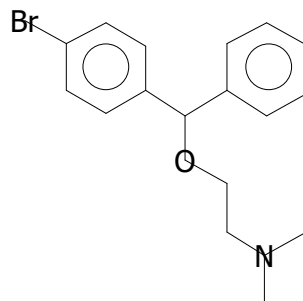


Library Hit - similarity 915, "Benzhydryl isothiocyanate"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzhydryl isothiocyanate	915	1787	3550-21-8	mainlib	C14H11NS	225
2	Benzene, 1,1'-[(methylthio)methylene]bis-	911	1510	15733-08-1	mainlib	C14H14S	214
3	2-Propanone, 1,1-diphenyl-	907	1276	781-35-1	mainlib	C15H14O	210
4	Benzenepropanenitrile, α -phenyl-	903	1077	2286-54-6	mainlib	C15H13N	207
5	Benzenemethanethiol, α -phenyl-	902	1652	4237-48-3	replib	C13H12S	200

Amodryl



1st Dimension R.T. = 1700.8

2nd Dimension R.T. = 1.960

Quant Mass(es) = 58

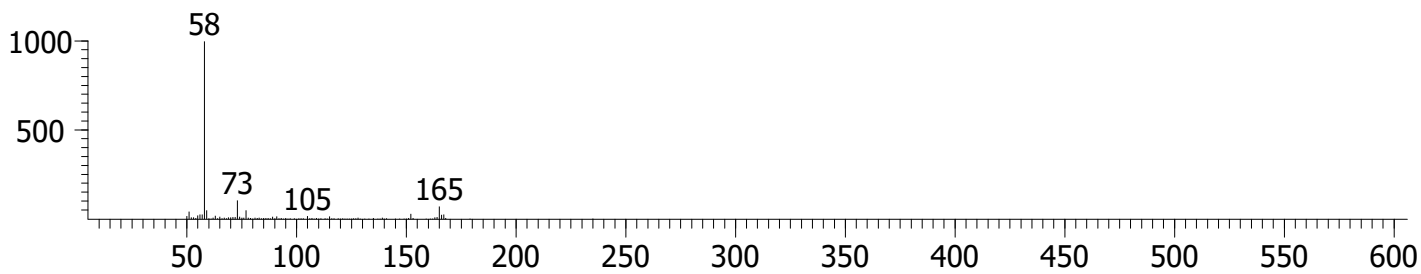
S/N = 12379

Area = 14115498

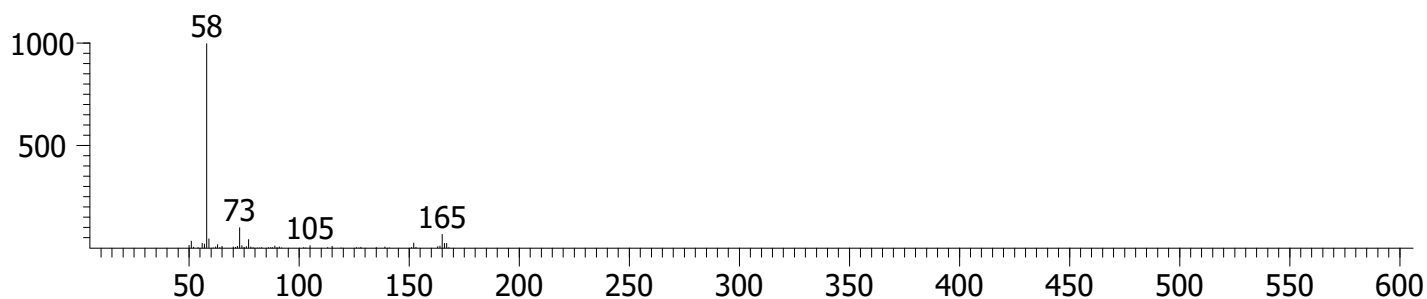
Height = 1127996

Similarity = 938

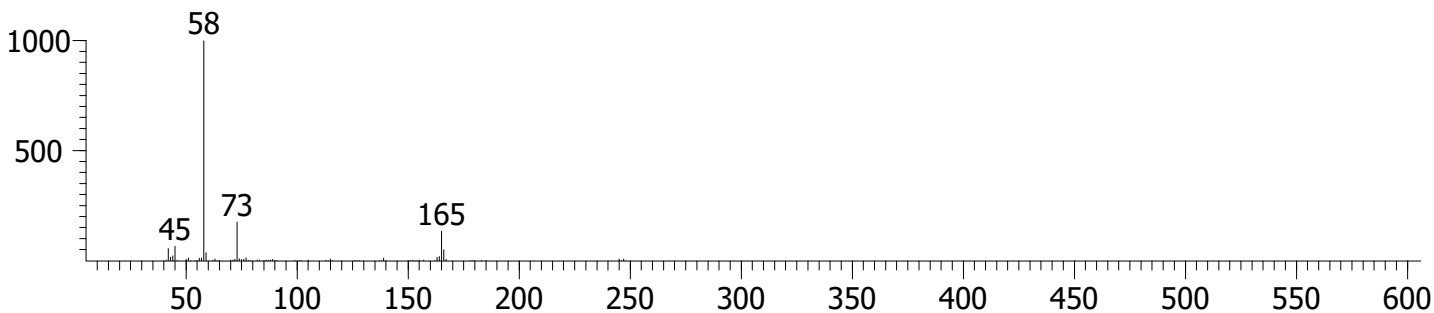
Peak Apex - sample "AnBxr B (20191121):1", peak 6461, at 1700.8 , 1.960 sec , sec (Spec # 185267)



Peak True - sample "AnBxr B (20191121):1", peak 6461, at 1700.8 , 1.960 sec , sec (Spec # 185267)



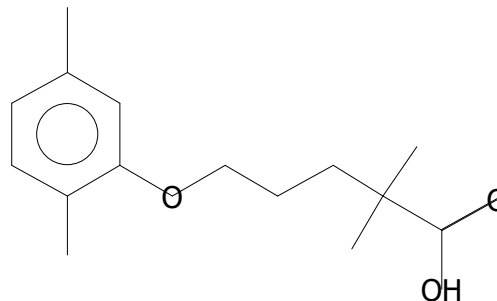
Library Hit - similarity 938, "Amodryl"



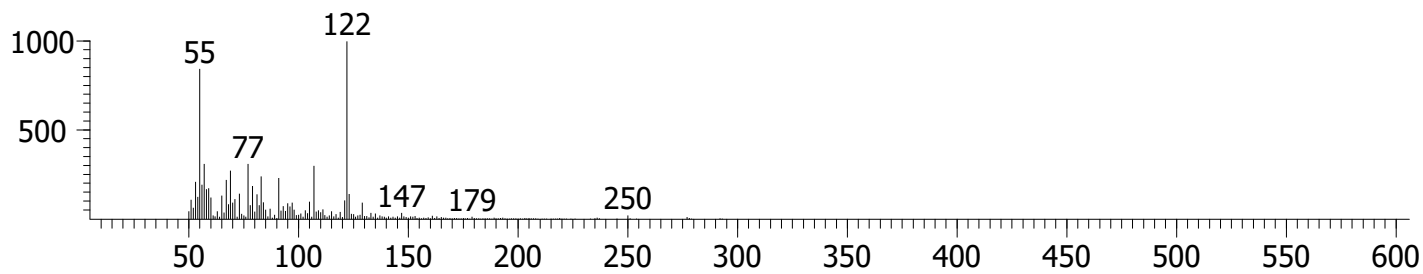
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Amodryl	938	3918	118-23-0	mainlib	C17H20BrNO	333
2	Orphenadrine	914	3665	83-98-7	replib	C18H23NO	269
3	Benadryl	905	2661	58-73-1	replib	C17H21NO	255
4	N,N-Dimethyl-2-phenoxyethylamine	902	968	13468-02-5	mainlib	C10H15NO	165
5	Tramadol, O-trimethylsilyl-	901	931	0-00-0	mainlib	C19H33NO2Si	335

Gemfibrozil

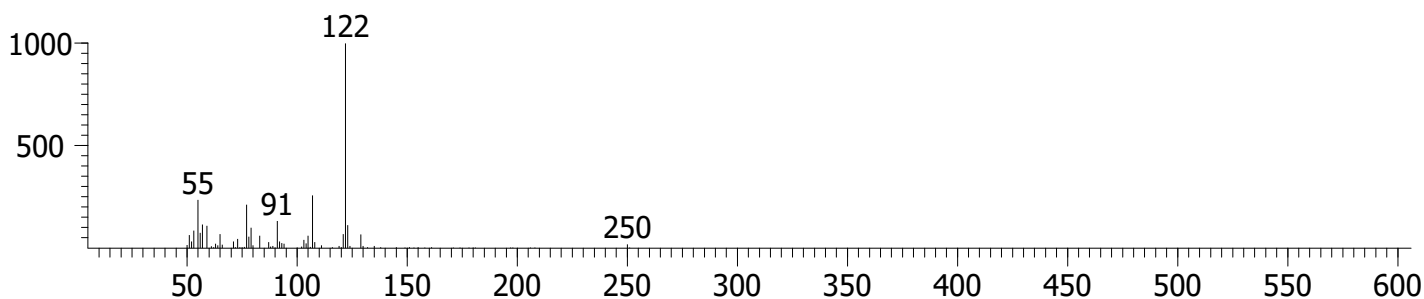
1st Dimension R.T. = 1732.28
2nd Dimension R.T. = 1.874
Quant Mass(es) = 122
S/N = 4396.7
Area = 1126899
Height = 123546
Similarity = 852



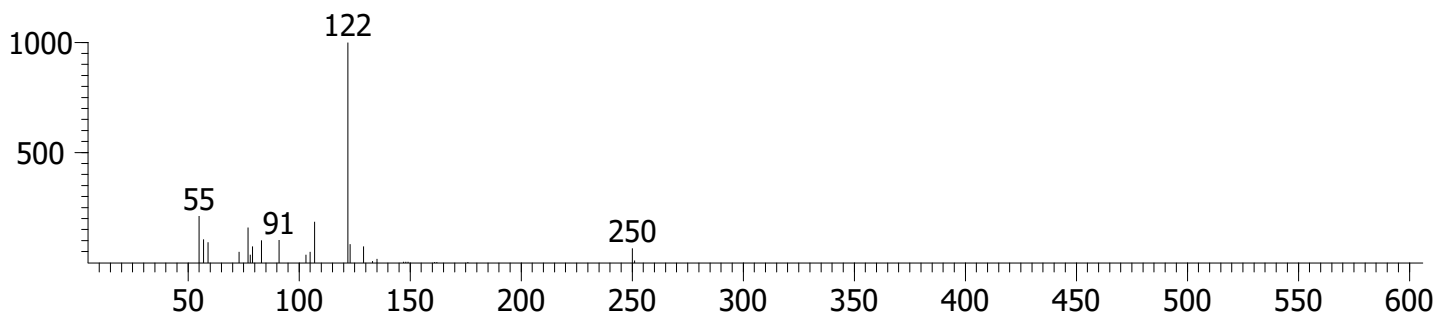
Peak Apex - sample "AnBxr B (20191121):1", peak 6657, at 1732.28 , 1.874 sec , sec (Spec # 190024)



Peak True - sample "AnBxr B (20191121):1", peak 6657, at 1732.28 , 1.874 sec , sec (Spec # 190024)



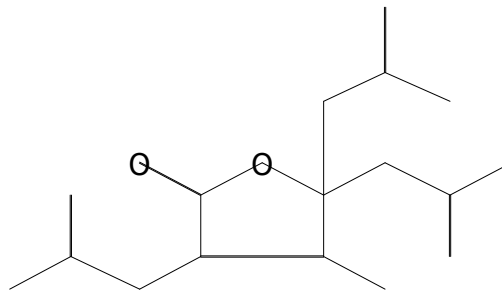
Library Hit - similarity 852, "Gemfibrozil"



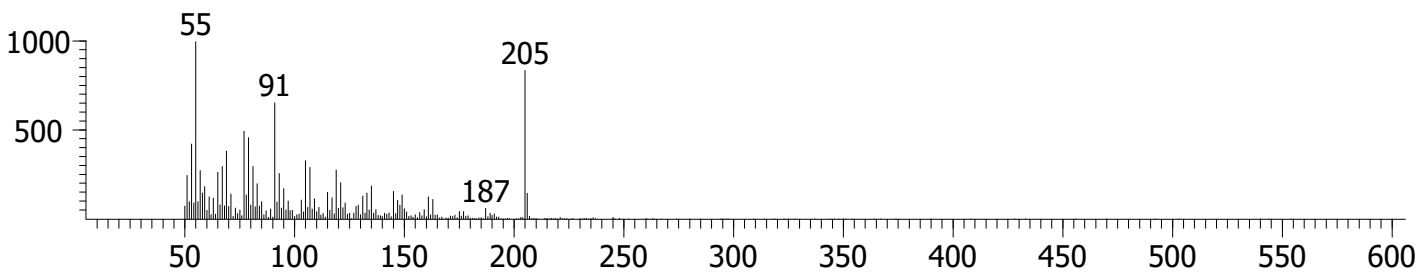
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Gemfibrozil	852	5453	25812-30-0	replib	C ₁₅ H ₂₂ O ₃	250
2	Gemfibrozil	829	1183	25812-30-0	mainlib	C ₁₅ H ₂₂ O ₃	250
3	Carbonic acid, butyl 3,5-dimethylphenyl ester	824	953	0-00-0	mainlib	C ₁₃ H ₁₈ O ₃	222
4	butanedioic acid, mono(3,4-dimethylphenyl) ester	804	434	0-00-0	mainlib	C ₁₂ H ₁₄ O ₄	222
5	Carbonic acid, isobutyl 3,5-dimethylphenyl ester	801	383	0-00-0	mainlib	C ₁₃ H ₁₈ O ₃	222

2(5H)-Furanone,
4-methyl-3,5,5-tris(2-methyl-2-propenyl)-

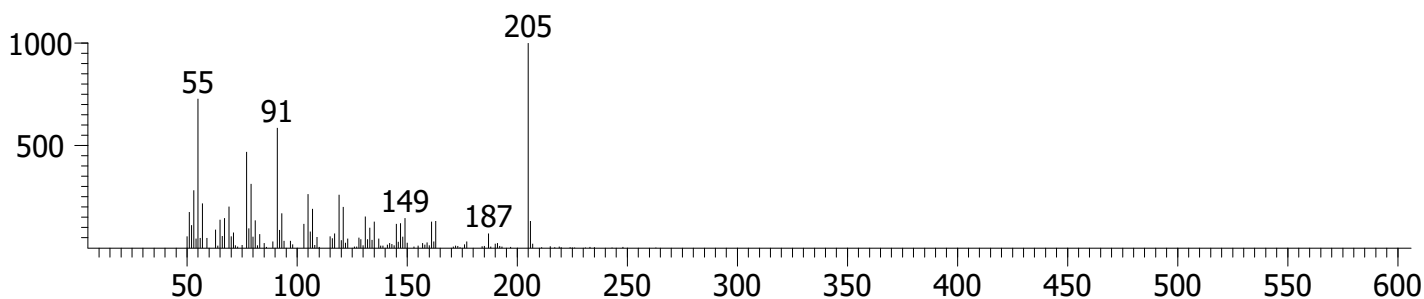
1st Dimension R.T. = 1739.28
 2nd Dimension R.T. = 2.059
 Quant Mass(es) = 205
 S/N = 2282.2
 Area = 438028
 Height = 36577
 Similarity = 767



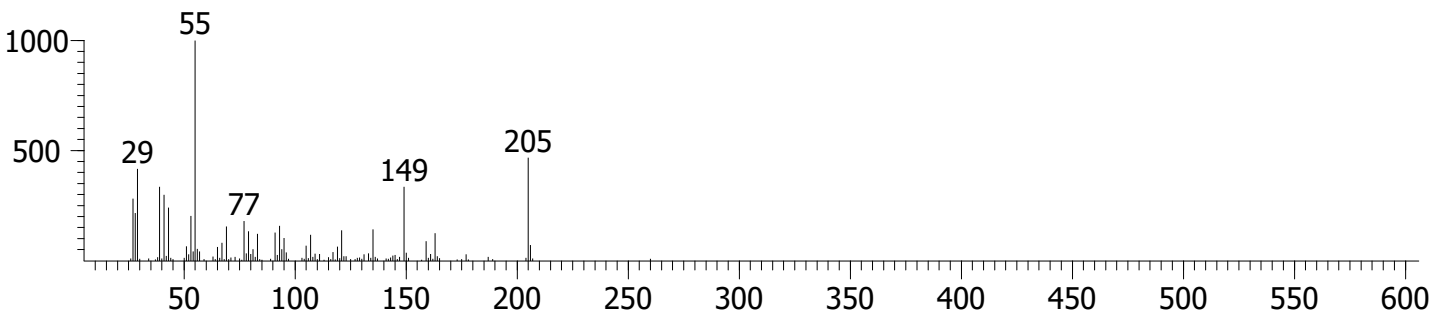
Peak Apex - sample "AnBxr B (20191121):1", peak 6700, at 1739.28 , 2.059 sec , sec (Spec # 191112)



Peak True - sample "AnBxr B (20191121):1", peak 6700, at 1739.28 , 2.059 sec , sec (Spec # 191112)



Library Hit - similarity 767, "2(5H)-Furanone, 4-methyl-3,5,5-tris(2-methyl-2-propenyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2(5H)-Furanone, 4-methyl-3,5,5-tris(2-methyl-2-propenyl)-	767	4005	89902-28-3	mainlib	C17H24O2	260
2	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1aà,4aà,7á,7aá,7bà)]-	734	5437	6750-60-3	replib	C15H24O	220
3	(1aR,3aR,4R,7R,8aS)-1a,4,9,9-Tetramethyloctahydro-3a,7-methanoazuleno[1,8a-b]oxirene	733	1027	25570-94-9	mainlib	C15H24O	220
4	Ethanone, 1-(5,6,7,8-tetrahydro-2,8,8-trimethyl-4H-cyclohepta[b]furan-5-yl)-	728	827	71596-88-8	mainlib	C14H20O2	220
5	11,14-Octadecadiynoic acid, methyl ester	723	667	56554-58-6	mainlib	C19H30O2	290

Diphenyl sulfone

1st Dimension R.T. = 1742.78

2nd Dimension R.T. = 2.765

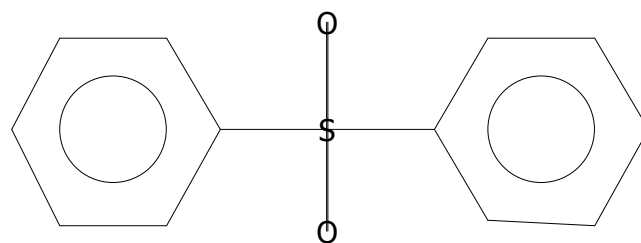
Quant Mass(es) = 125

S/N = 4199.4

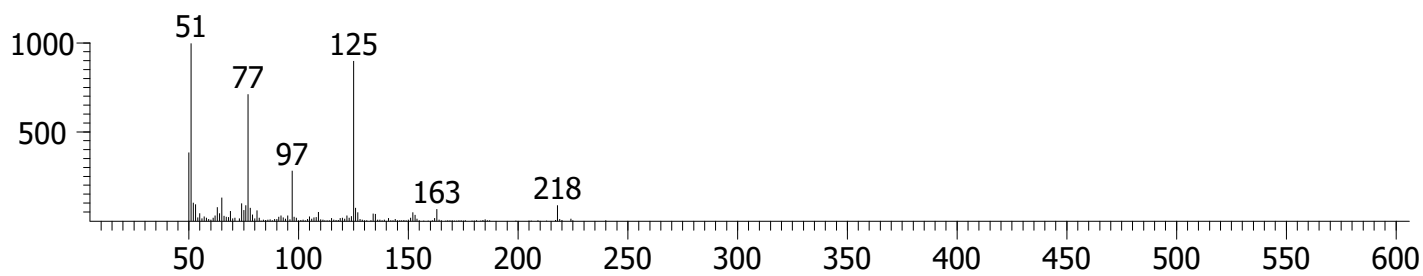
Area = 1557283

Height = 118567

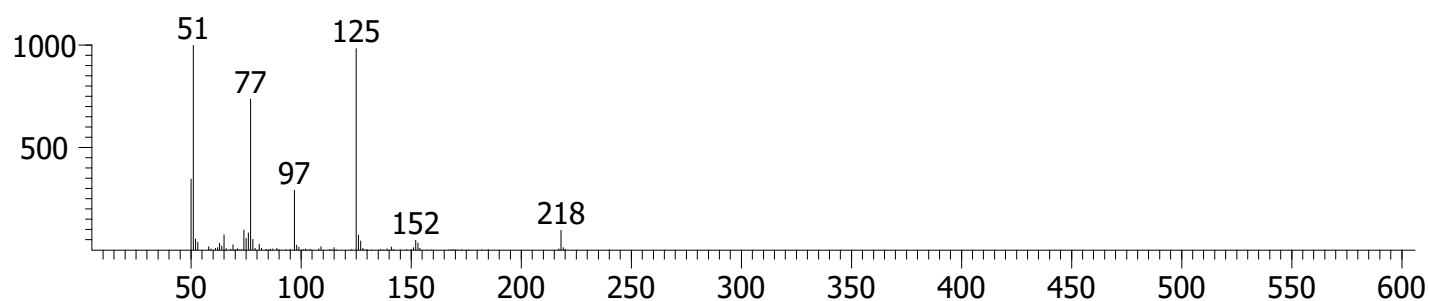
Similarity = 874



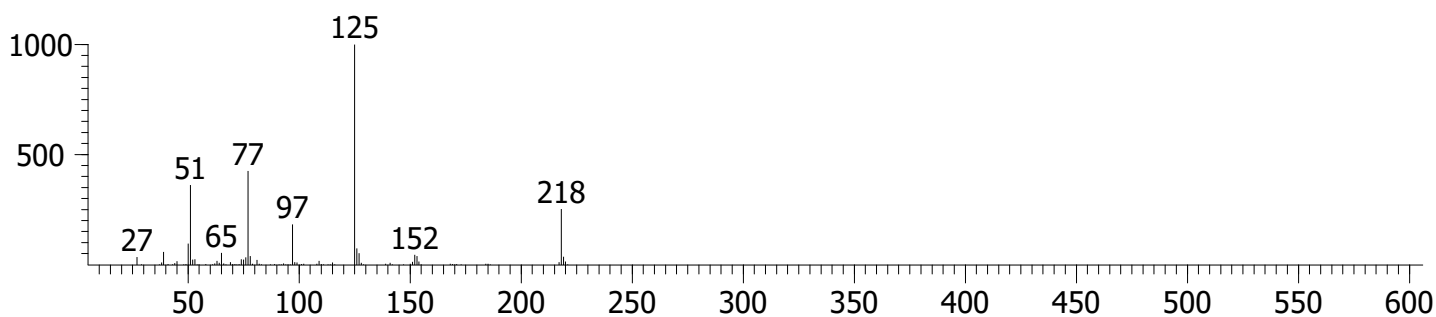
Peak Apex - sample "AnBxr B (20191121):1", peak 6729, at 1742.78 , 2.765 sec , sec (Spec # 191749)



Peak True - sample "AnBxr B (20191121):1", peak 6729, at 1742.78 , 2.765 sec , sec (Spec # 191749)



Library Hit - similarity 874, "Diphenyl sulfone"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Diphenyl sulfone	874	9078	127-63-9	replib	C12H10O2S	218
2	Diphenyl sulfone	834	9078	127-63-9	replib	C12H10O2S	218
3	Bis[phenylsulfonyl]-4-trichloromethylphenyl chloromethane	824	5763	81269-12-7	mainlib	C20H14Cl4O4S2	522
4	2-Propenenitrile, 3-(phenylsulfonyl)-	803	2451	1424-51-7	mainlib	C9H7NO2S	193
5	2-Propenenitrile, 3-(phenylsulfonyl)-	787	800	1424-51-7	replib	C9H7NO2S	193

Carbinoxamine

1st Dimension R.T. = 1756.77

2nd Dimension R.T. = 2.039

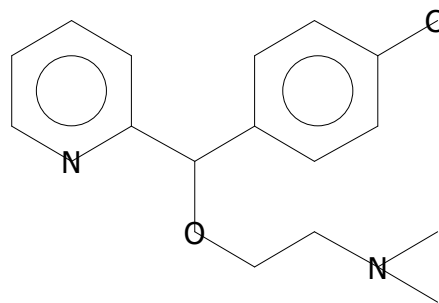
Quant Mass(es) = 58

S/N = 3419.9

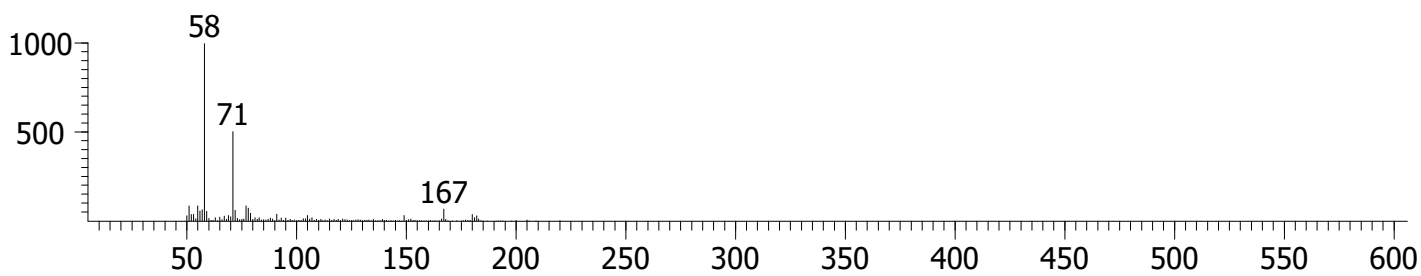
Area = 2057163

Height = 196568

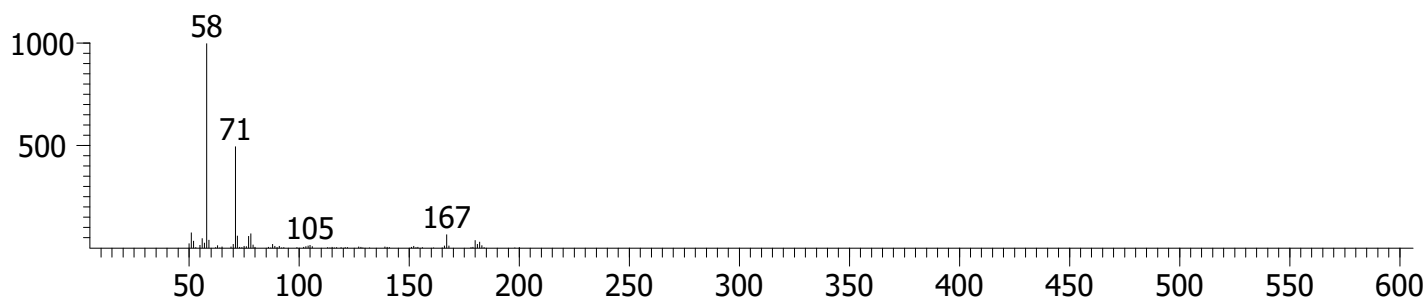
Similarity = 900



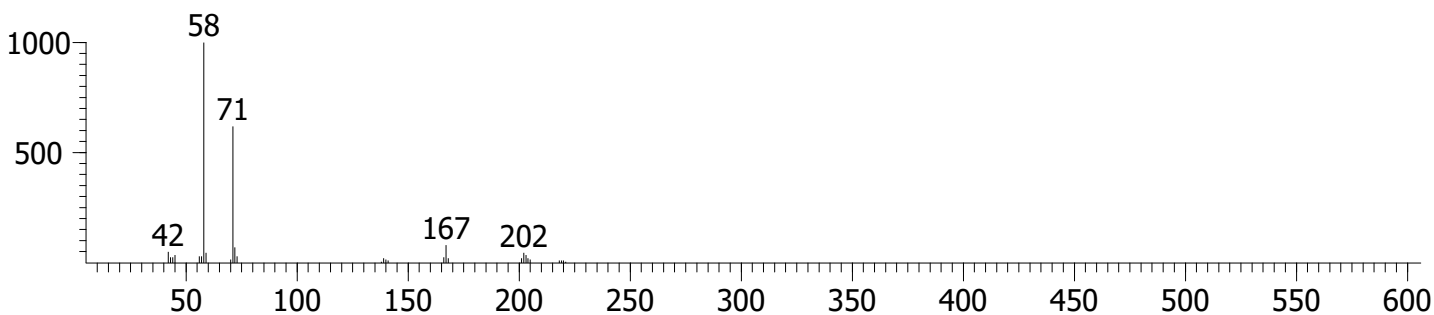
Peak Apex - sample "AnBxr B (20191121):1", peak 6807, at 1756.77 , 2.039 sec , sec (Spec # 193759)



Peak True - sample "AnBxr B (20191121):1", peak 6807, at 1756.77 , 2.039 sec , sec (Spec # 193759)



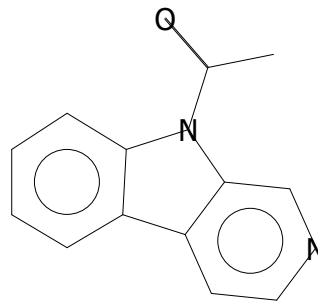
Library Hit - similarity 900, "Carbinoxamine"



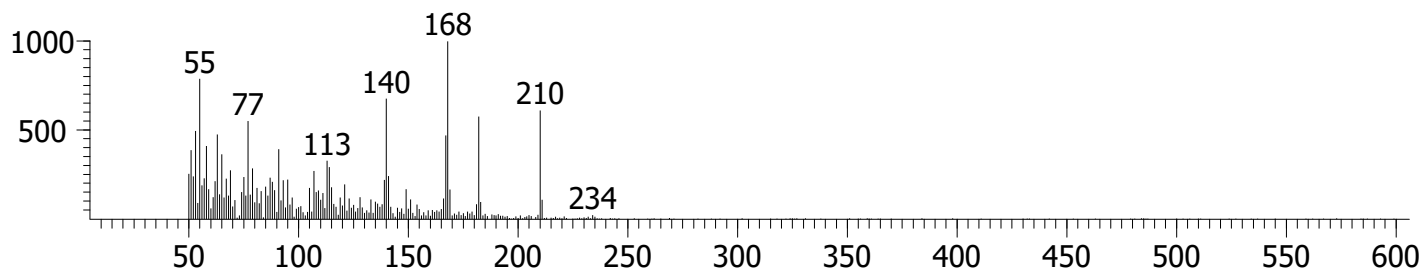
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Carbinoxamine	900	7896	486-16-8	replib	C16H19ClN2O	290
2	O-Ethyl S-2-dimethylaminoethyl ethylphosphonothiolate	856	3333	98543-25-0	mainlib	C8H20NO2PS	225
3	O-Ethyl S-2-dimethylaminoethyl methylphosphonothiolate	840	1919	20820-80-8	mainlib	C7H18NO2PS	211
4	Suberohydroxamic acid	835	8620	38937-66-5	nist_msms	C8H16N2O4	204
5	Acetic acid, (dodecahydro-7-hydroxy-1,4b,8,8-tetramethyl-10-oxo-2(1H)-phenanthrenylidene)-,2-(dimethylamino)ethyl ester	830	1355	0-00-0	mainlib	C24H39NO4	405

Norharmane, N-acetyl-

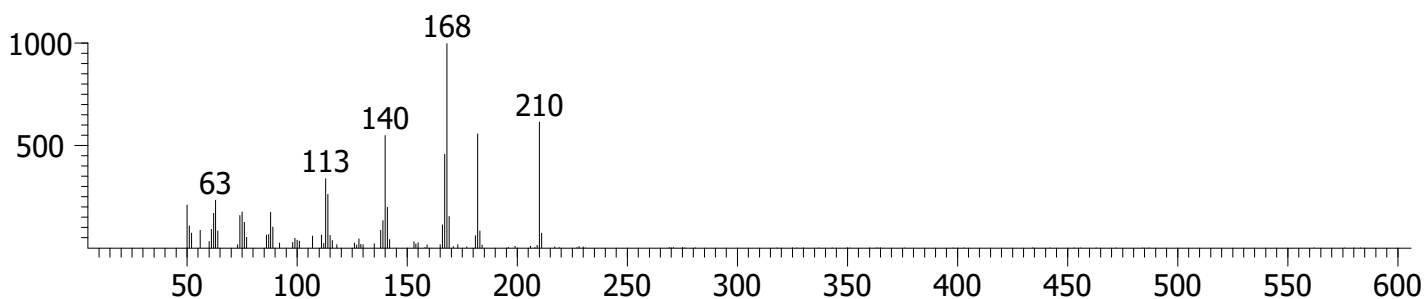
1st Dimension R.T. = 1823.23
2nd Dimension R.T. = 2.330
Quant Mass(es) = 168
S/N = 827.11
Area = 114224
Height = 10206
Similarity = 706



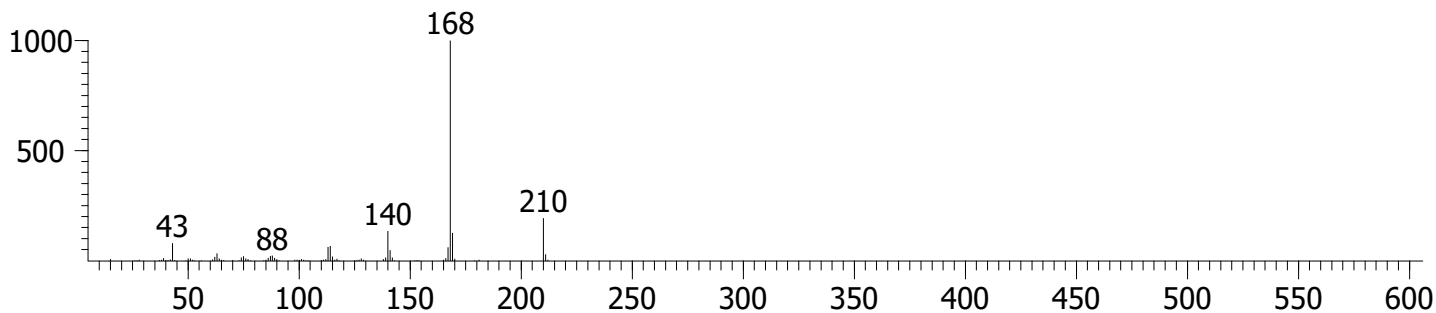
Peak Apex - sample "AnBxr B (20191121):1", peak 7153, at 1823.23 , 2.330 sec , sec (Spec # 203873)



Peak True - sample "AnBxr B (20191121):1", peak 7153, at 1823.23 , 2.330 sec , sec (Spec # 203873)



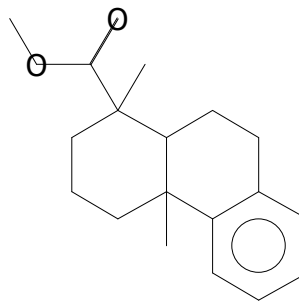
Library Hit - similarity 706, "Norharmane, N-acetyl-"



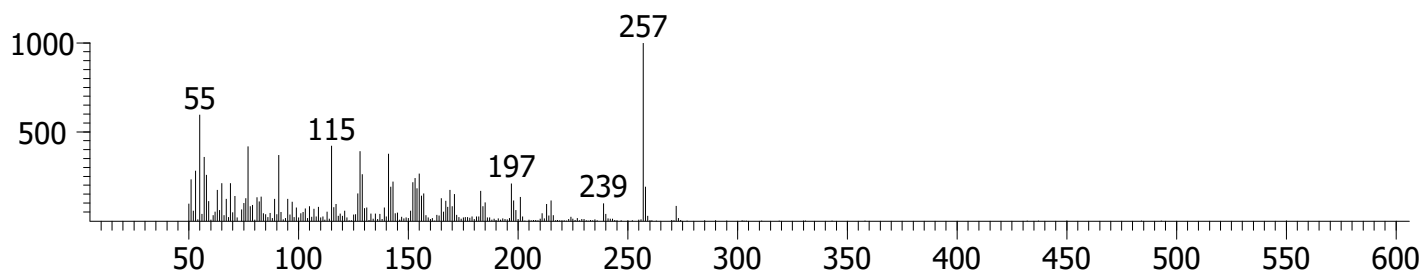
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Norharmane, N-acetyl-	706	3372	0-00-0	mainlib	C ₁₃ H ₁₀ N ₂ O	210
2	6-Methylquinoline-2-carbonitrile	687	1637	0-00-0	mainlib	C ₁₁ H ₈ N ₂	168
3	á-Carboline-3-carboxylic acid propyl ester	666	696	76808-18-9	mainlib	C ₁₅ H ₁₄ N ₂ O ₂	254
4	9H-Pyrido[3,4-b]indole	663	4471	244-63-3	replib	C ₁₁ H ₈ N ₂	168
5	9H-Pyrido[3,4-b]indole	662	4471	244-63-3	replib	C ₁₁ H ₈ N ₂	168

1-Phenanthrenecarboxylic acid,
2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-

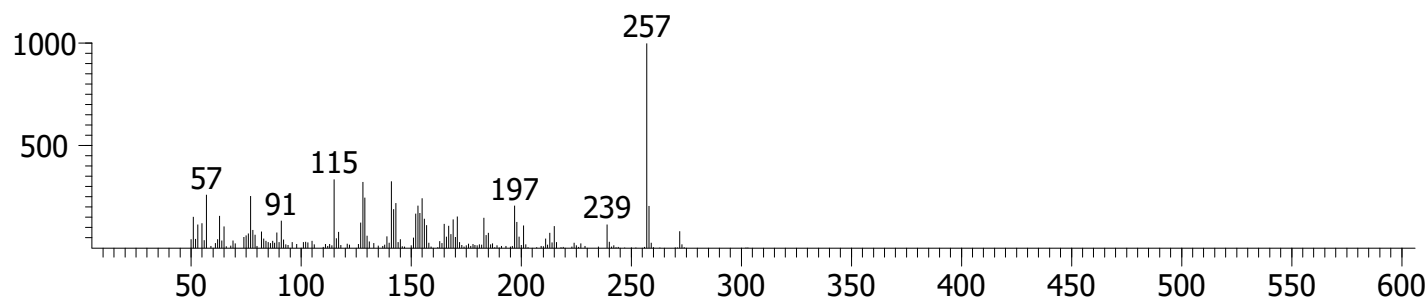
1st Dimension R.T. = 1973.65
2nd Dimension R.T. = 2.211
Quant Mass(es) = 257
S/N = 1891.9
Area = 256365
Height = 19571
Similarity = 697



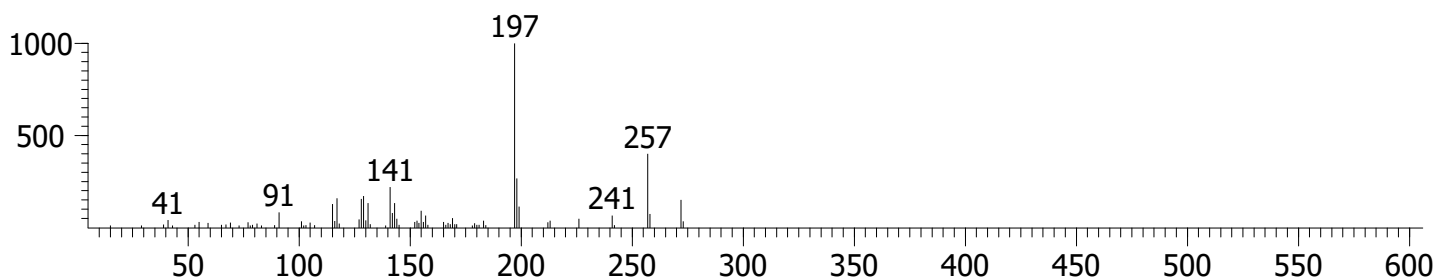
Peak Apex - sample "AnBxr B (20191121):1", peak 7716, at 1973.65 , 2.211 sec , sec (Spec # 226645)



Peak True - sample "AnBxr B (20191121):1", peak 7716, at 1973.65 , 2.211 sec , sec (Spec # 226645)



Library Hit - similarity 697, "1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-, methyl ester, [1S-(1à,4aà,10aá)]-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-, methyl ester, [1S-(1à,4aà,10aá)]-	697	3606	2651-34-5	mainlib	C18H24O2	272
2	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-, methyl ester	667	1002	108395-86-4	mainlib	C18H24O2	272
3	5,8,11-Heptadecatriynoic acid, methyl ester	662	808	56554-57-5	mainlib	C18H24O2	272
4	5,8,11-Eicosatriynoic acid, methyl ester	658	682	0-00-0	mainlib	C21H30O2	314
5	5à-Podocarpa-8,11,13-trien-16-oic acid, methyl ester	657	656	3745-36-6	mainlib	C18H24O2	272

Phenol, 4,4'-(1-methylethylidene)bis-

1st Dimension R.T. = 1973.65

2nd Dimension R.T. = 2.633

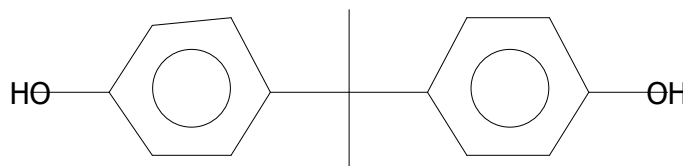
Quant Mass(es) = 213

S/N = 7815.3

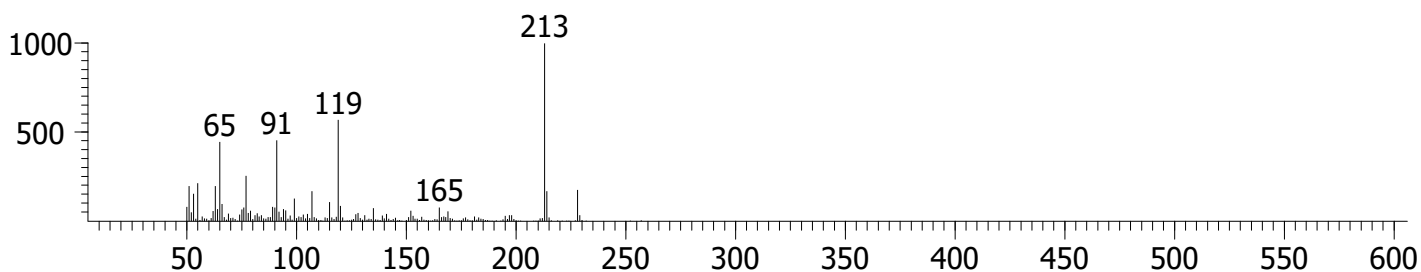
Area = 1788254

Height = 133294

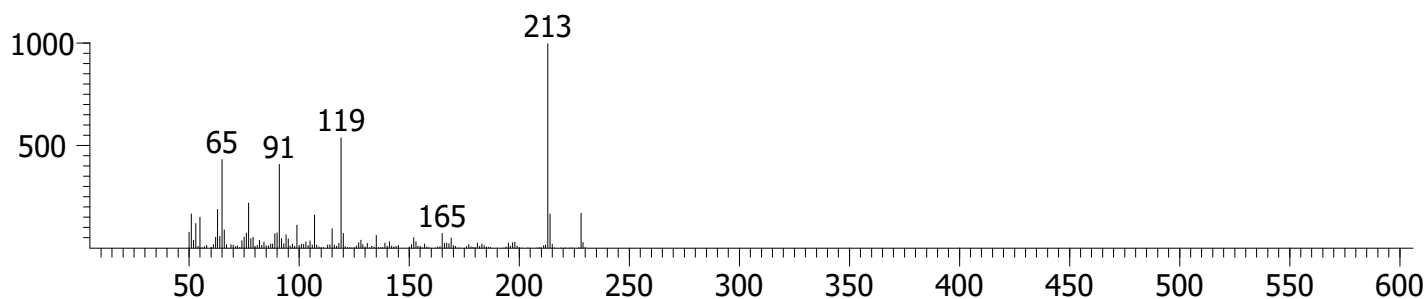
Similarity = 881



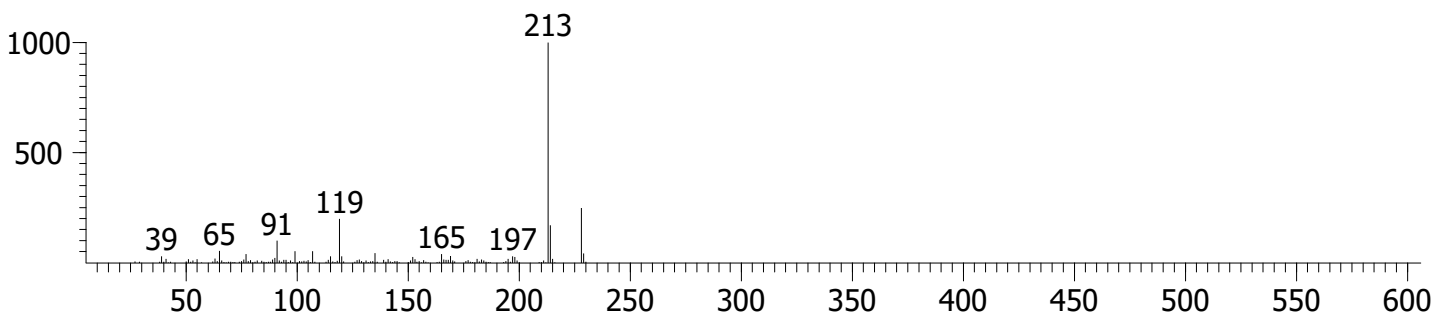
Peak Apex - sample "AnBxr B (20191121):1", peak 7719, at 1973.65 , 2.633 sec , sec (Spec # 226709)



Peak True - sample "AnBxr B (20191121):1", peak 7719, at 1973.65 , 2.633 sec , sec (Spec # 226709)



Library Hit - similarity 881, "Phenol, 4,4'-(1-methylethylidene)bis-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 4,4'-(1-methylethylidene)bis-	881	8664	80-05-7	replib	C15H16O2	228
2	3,4'-Isopropylidenediphenol	871	7502	46765-25-7	mainlib	C15H16O2	228
3	Phenol, 4,4'-(1-methylethylidene)bis-	821	1526	80-05-7	mainlib	C15H16O2	228
4	Phenol, 4,4'-(1-methylethylidene)bis-	818	8664	80-05-7	replib	C15H16O2	228
5	Phenol, 2,4'-isopropylidenedi-	794	449	837-08-1	mainlib	C15H16O2	228

Adipic acid, 2-decyl isobutyl ester

1st Dimension R.T. = 2194.02

2nd Dimension R.T. = 1.663

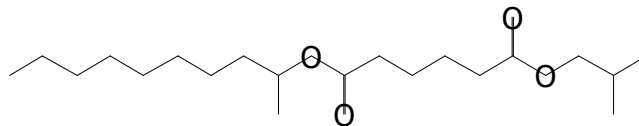
Quant Mass(es) = 185

S/N = 1180.1

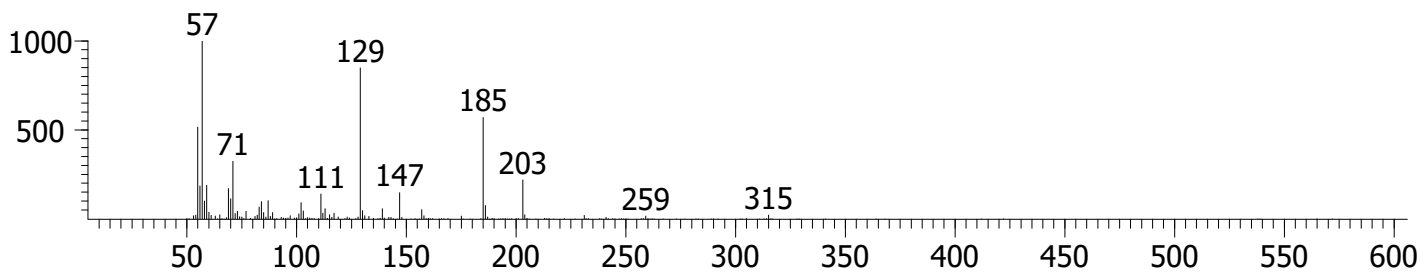
Area = 110927

Height = 11658

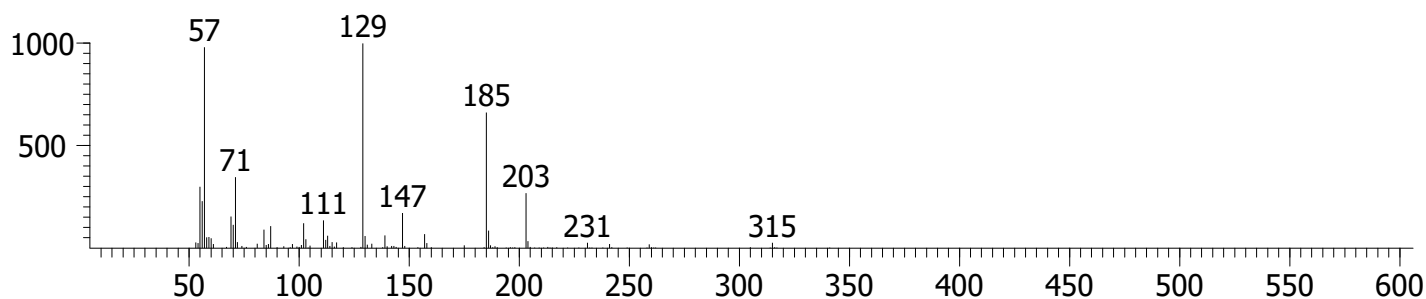
Similarity = 694



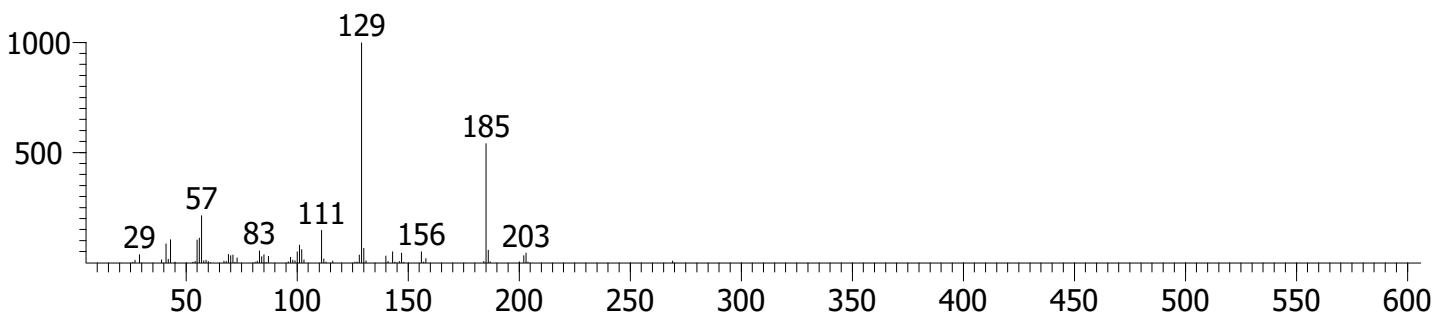
Peak Apex - sample "AnBxr B (20191121):1", peak 8358, at 2194.02 , 1.663 sec , sec (Spec # 259952)



Peak True - sample "AnBxr B (20191121):1", peak 8358, at 2194.02 , 1.663 sec , sec (Spec # 259952)



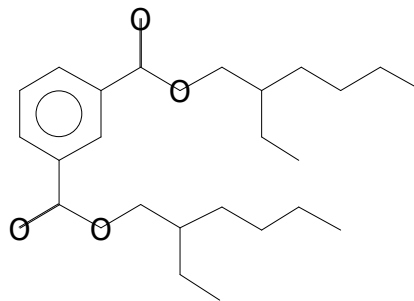
Library Hit - similarity 694, "Adipic acid, 2-decyl isobutyl ester"



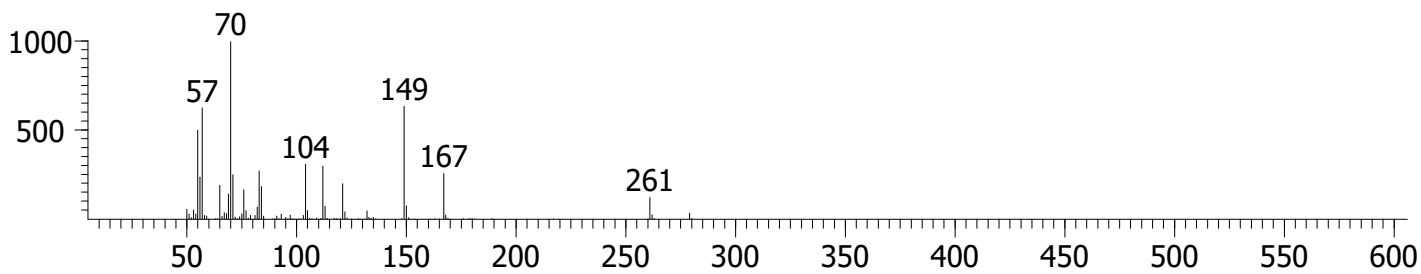
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Adipic acid, 2-decyl isobutyl ester	694	1072	0-00-0	mainlib	C20H38O4	342
2	Adipic acid, 2-ethylhexyl isobutyl ester	693	1031	0-00-0	mainlib	C18H34O4	314
3	Butyl citrate	691	5631	77-94-1	replib	C18H32O7	360
4	Adipic acid, isobutyl octadecyl ester	688	830	0-00-0	mainlib	C28H54O4	454
5	Adipic acid, butyl 2-ethylhexyl ester	687	798	0-00-0	mainlib	C18H34O4	314

1,3-Benzenedicarboxylic acid,
bis(2-ethylhexyl) ester

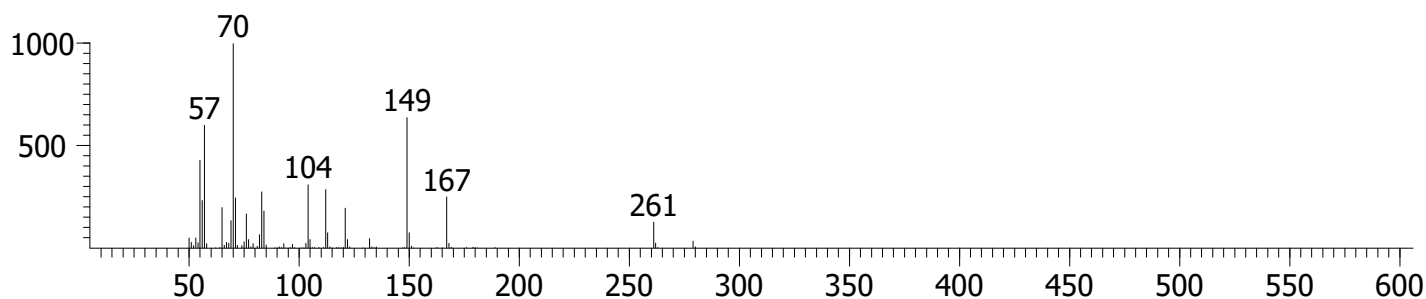
1st Dimension R.T. = 2382.91
2nd Dimension R.T. = 1.604
Quant Mass(es) = 149
S/N = 2433.0
Area = 384542
Height = 41692
Similarity = 802



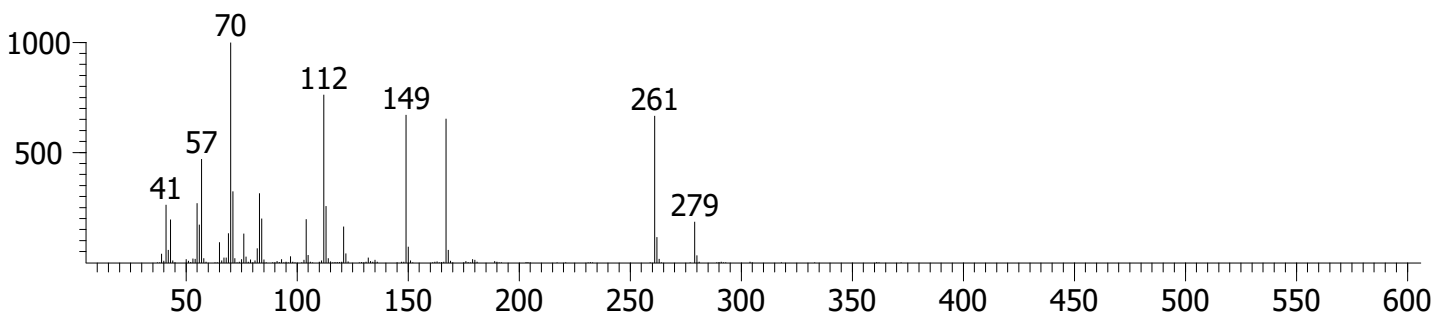
Peak Apex - sample "AnBxr B (20191121):1", peak 8736, at 2382.91 , 1.604 sec , sec (Spec # 288563)



Peak True - sample "AnBxr B (20191121):1", peak 8736, at 2382.91 , 1.604 sec , sec (Spec # 288563)



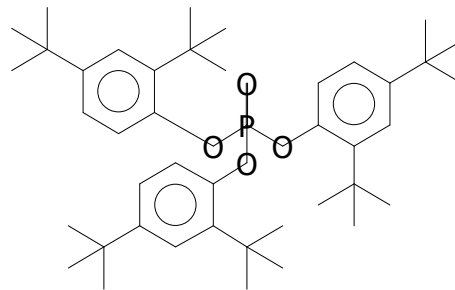
Library Hit - similarity 802, "1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester"



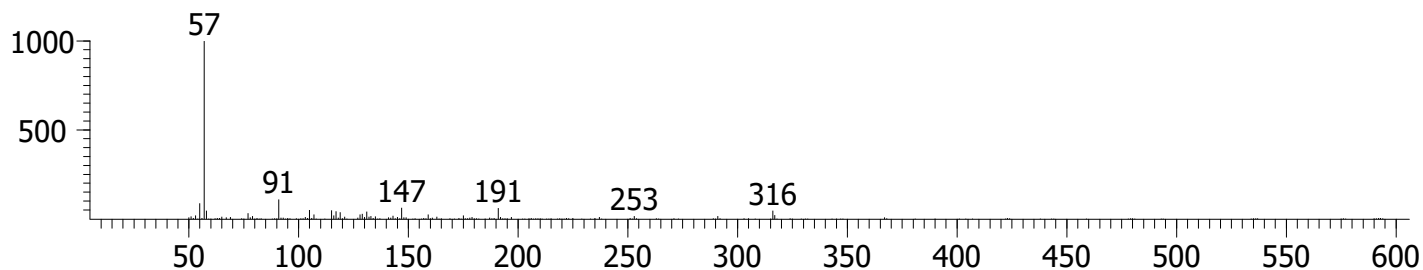
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	802	7442	137-89-3	mainlib	C ₂₄ H ₃₈ O ₄	390
2	1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	798	5082	137-89-3	replib	C ₂₄ H ₃₈ O ₄	390
3	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	788	3588	6422-86-2	replib	C ₂₄ H ₃₈ O ₄	390
4	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	763	3588	6422-86-2	replib	C ₂₄ H ₃₈ O ₄	390
5	Mono(2-ethylhexyl) phthalate	760	1036	4376-20-9	replib	C ₁₆ H ₂₂ O ₄	278

Tris(2,4-di-tert-butylphenyl) phosphate

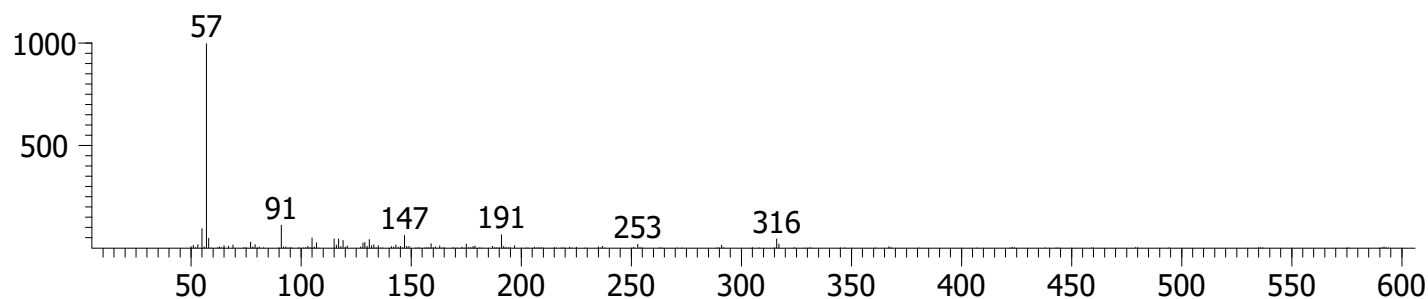
1st Dimension R.T. = 3358.85
2nd Dimension R.T. = 1.914
Quant Mass(es) = 57
S/N = 883.54
Area = 6128276
Height = 181801
Similarity = 649



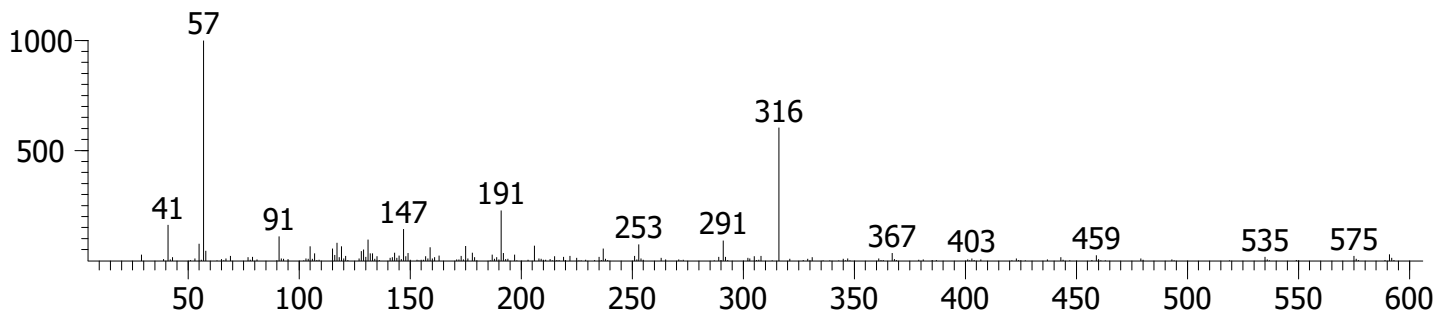
Peak Apex - sample "AnBxr B (20191121):1", peak 9729, at 3358.85 , 1.914 sec , sec (Spec # 436480)



Peak True - sample "AnBxr B (20191121):1", peak 9729, at 3358.85 , 1.914 sec , sec (Spec # 436480)



Library Hit - similarity 649, "Tris(2,4-di-tert-butylphenyl) phosphate"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Tris(2,4-di-tert-butylphenyl) phosphate	649	1948	95906-11-9	mainlib	C42H63O4P	662
2	̑-Hydroxybutyric acid	647	915	20016-85-7	nist_msms	C4H8O3	104
3	2-Decanol	647	915	1120-06-5	nist_msms	C10H22O	158
4	Aziridine, 1-methyl-	645	3017	1072-44-2	replib	C3H7N	57
5	Butoxyacetic acid	643	772	2516-93-0	nist_msms	C6H12O3	132

5-Hepten-2-one, 6-methyl-

1st Dimension R.T. = 563.952

2nd Dimension R.T. = 1.432

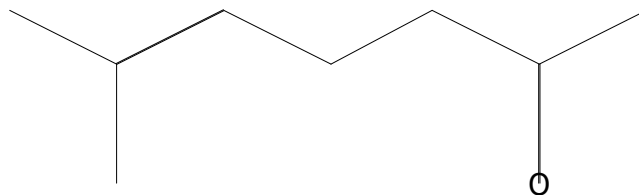
Quant Mass(es) = 108

S/N = 593.58

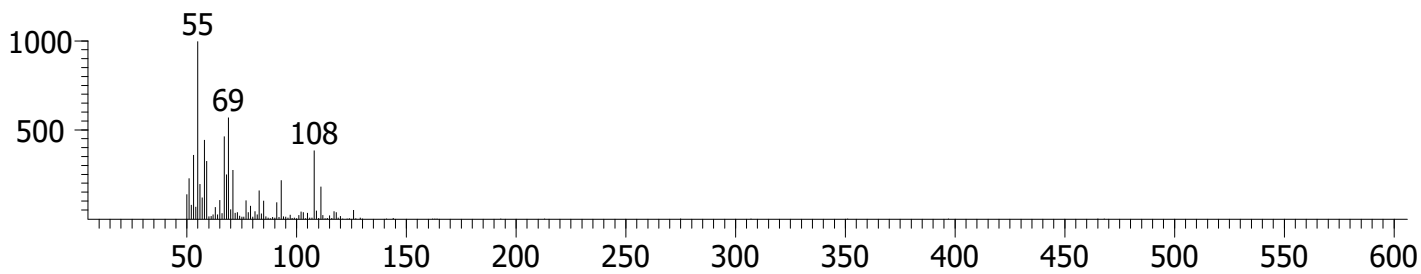
Area = 101105

Height = 10009

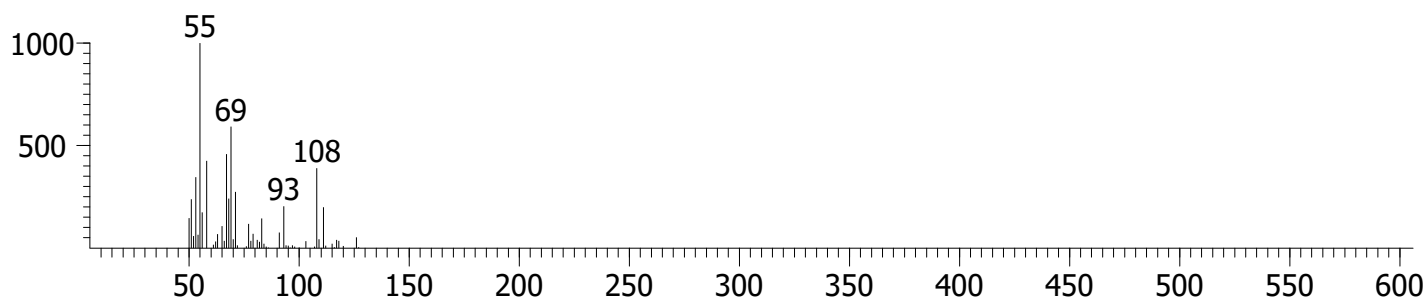
Similarity = 894



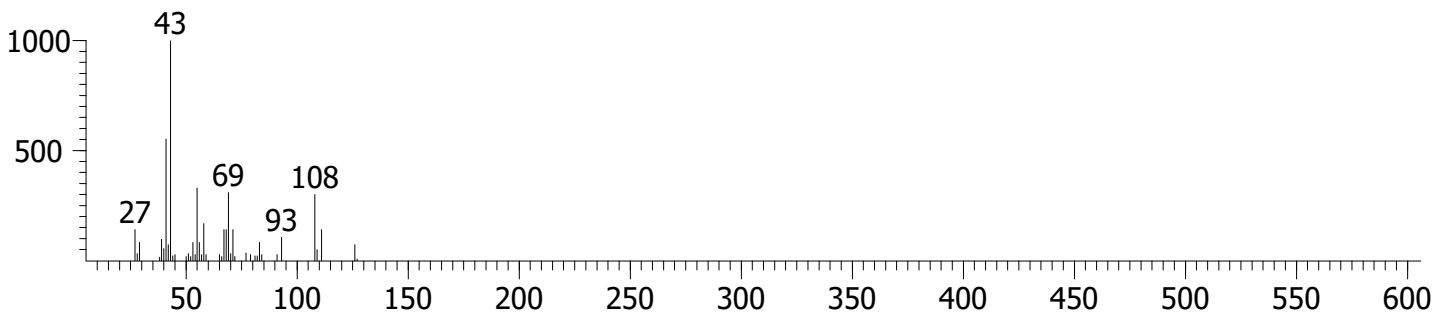
Peak Apex - sample "AnBxr C 091919 (20191122):1", peak 147, at 563.952 , 1.432 sec , sec (Spec # 12937)



Peak True - sample "AnBxr C 091919 (20191122):1", peak 147, at 563.952 , 1.432 sec , sec (Spec # 12937)



Library Hit - similarity 894, "5-Hepten-2-one, 6-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-Hepten-2-one, 6-methyl-	894	9556	110-93-0	replib	C8H14O	126
2	5-Hepten-2-one, 6-methyl-	867	9556	110-93-0	replib	C8H14O	126
3	5-Hepten-2-one, 6-methyl-	849	9556	110-93-0	replib	C8H14O	126
4	5-Hepten-2-one, 6-methyl-	826	7341	110-93-0	mainlib	C8H14O	126
5	5-Hepten-2-one, 6-methyl-	817	9556	110-93-0	replib	C8H14O	126

2-Pentenoic acid, ethyl ester

1st Dimension R.T. = 1221.58

2nd Dimension R.T. = 2.092

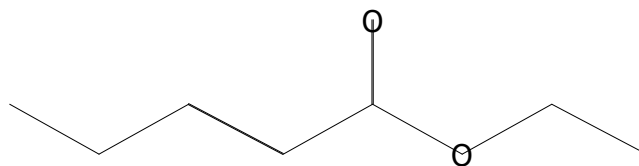
Quant Mass(es) = 83

S/N = 571.11

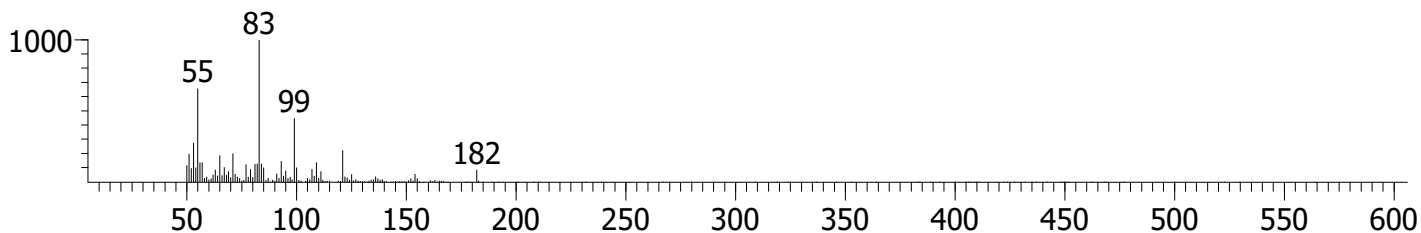
Area = 346135

Height = 35414

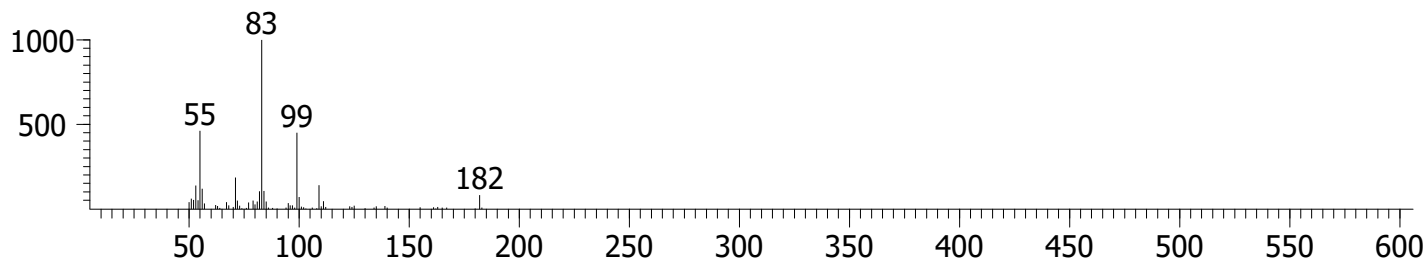
Similarity = 759



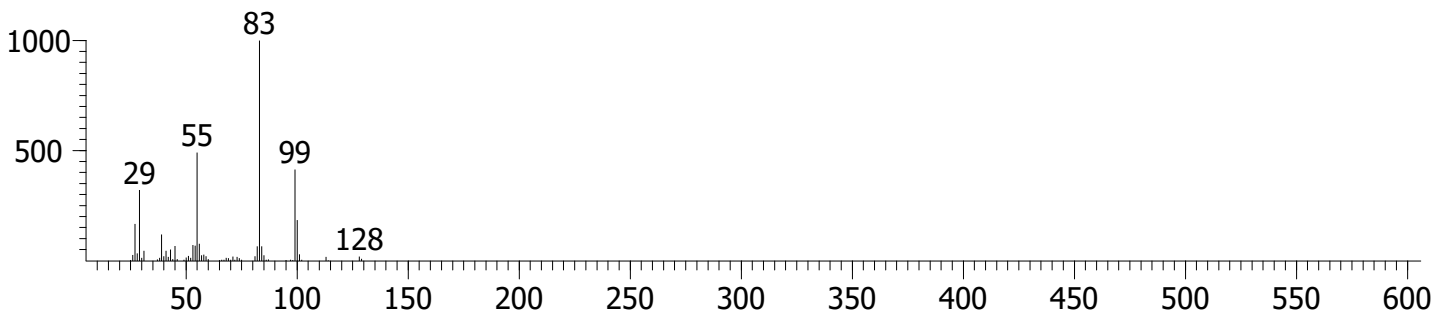
Peak Apex - sample "AnBxr C 091919 (20191122):1", peak 2598, at 1221.58 , 2.092 sec , sec (Spec # 112677)



Peak True - sample "AnBxr C 091919 (20191122):1", peak 2598, at 1221.58 , 2.092 sec , sec (Spec # 112677)



Library Hit - similarity 759, "2-Pentenoic acid, ethyl ester"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Pentenoic acid, ethyl ester	759	4155	2445-93-4	mainlib	C7H12O2	128
2	2,2-Dimethyl-4-octenal	731	1200	30390-60-4	mainlib	C10H18O	154
3	Ethyl trans-2-pentenoate	730	1153	24410-84-2	mainlib	C7H12O2	128
4	2-Butynoic acid, 4-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester	728	1063	69511-49-5	mainlib	C10H14O4	198
5	5-Octen-2-one, 3,6-dimethyl-	721	814	64165-21-5	mainlib	C10H18O	154

Benzene, 1-chloro-3-phenoxy-

1st Dimension R.T. = 1382.48

2nd Dimension R.T. = 1.934

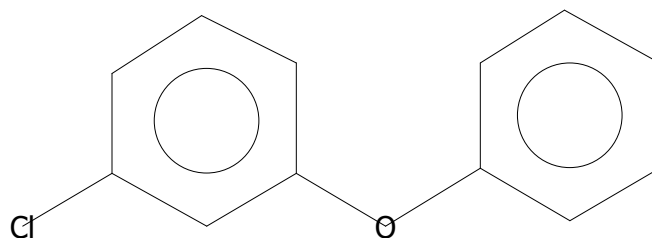
Quant Mass(es) = 204

S/N = 739.11

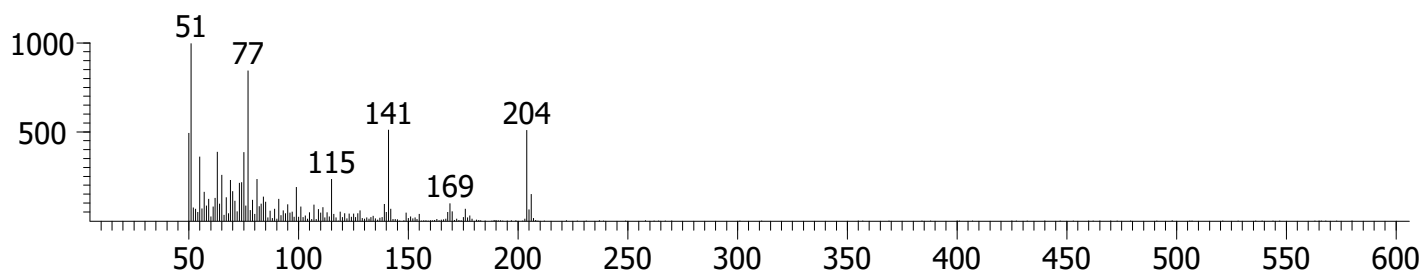
Area = 56993

Height = 7130.3

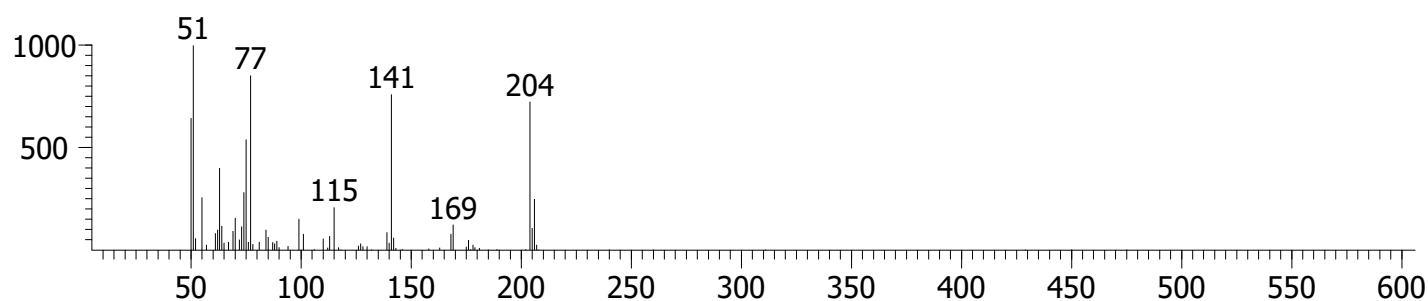
Similarity = 796



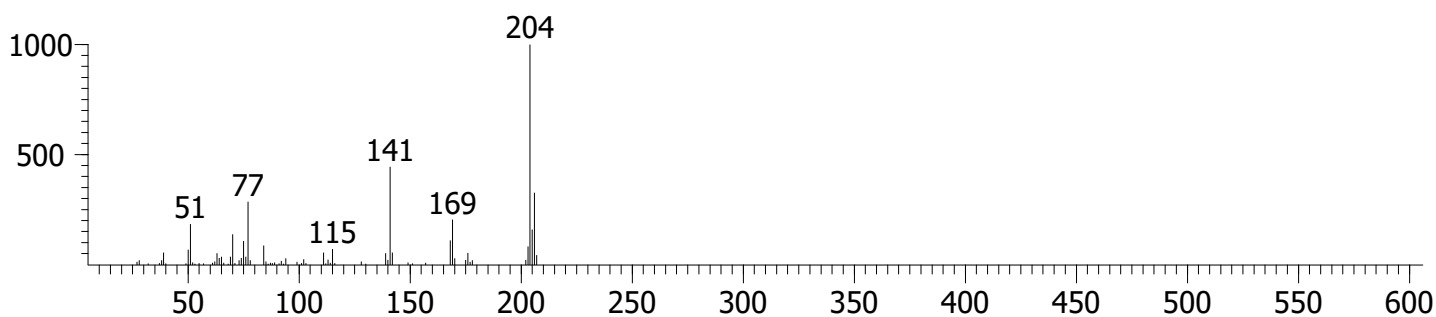
Peak Apex - sample "AnMbr B (20191120):1", peak 3448, at 1382.48 , 1.934 sec , sec (Spec # 137033)



Peak True - sample "AnMbr B (20191120):1", peak 3448, at 1382.48 , 1.934 sec , sec (Spec # 137033)

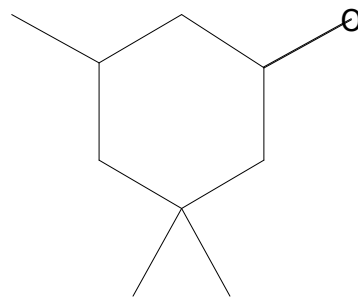


Library Hit - similarity 796, "Benzene, 1-chloro-3-phenoxy-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-chloro-3-phenoxy-	796	5789	6452-49-9	mainlib	C ₁₂ H ₉ ClO	204
2	Benzene, 1-chloro-4-phenoxy-	781	3508	7005-72-3	mainlib	C ₁₂ H ₉ ClO	204
3	[1,1'-Biphenyl-4-ol], 2-chloro-	678	247	23719-22-4	mainlib	C ₁₂ H ₉ ClO	204
4	[1,1'-Biphenyl]-4-ol, 4'-chloro-	646	66	28034-99-3	mainlib	C ₁₂ H ₉ ClO	204
5	4-Hydroxy-2-chlorobiphenyl, acetate	638	49	0-00-0	mainlib	C ₁₄ H ₁₁ ClO ₂	246

Cyclohexanone, 3,3,5-trimethyl-



1st Dimension R.T. = 647.904

2nd Dimension R.T. = 1.465

Quant Mass(es) = 83

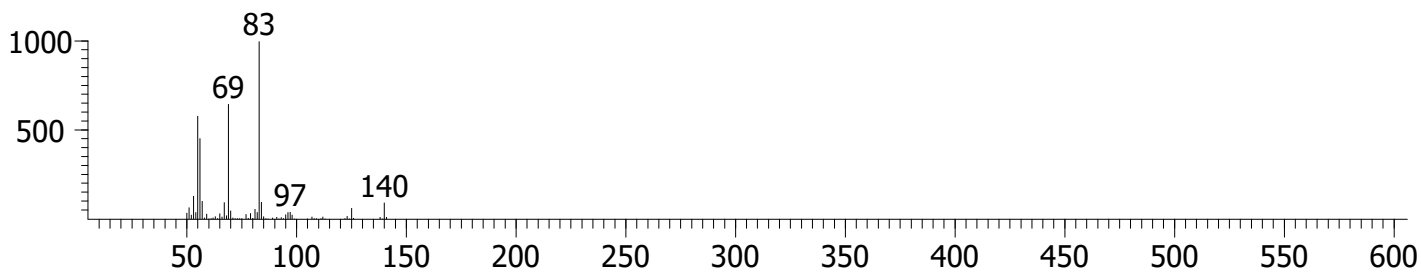
S/N = 5769.4

Area = 2230935

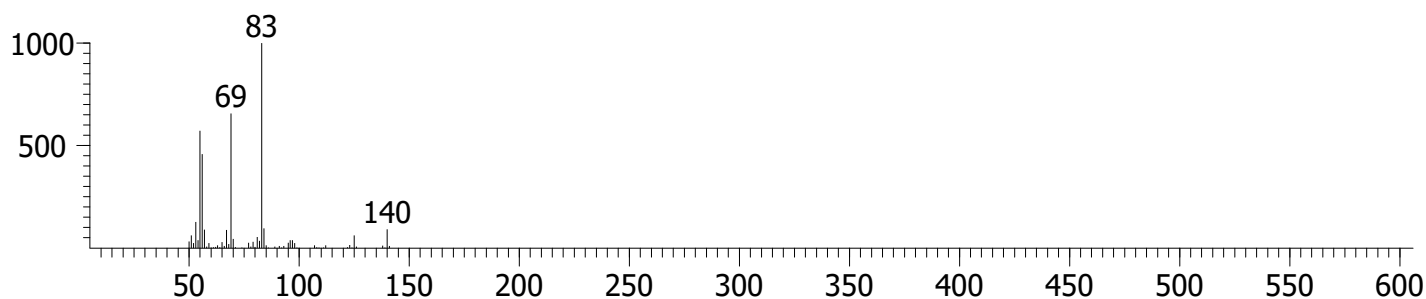
Height = 266284

Similarity = 854

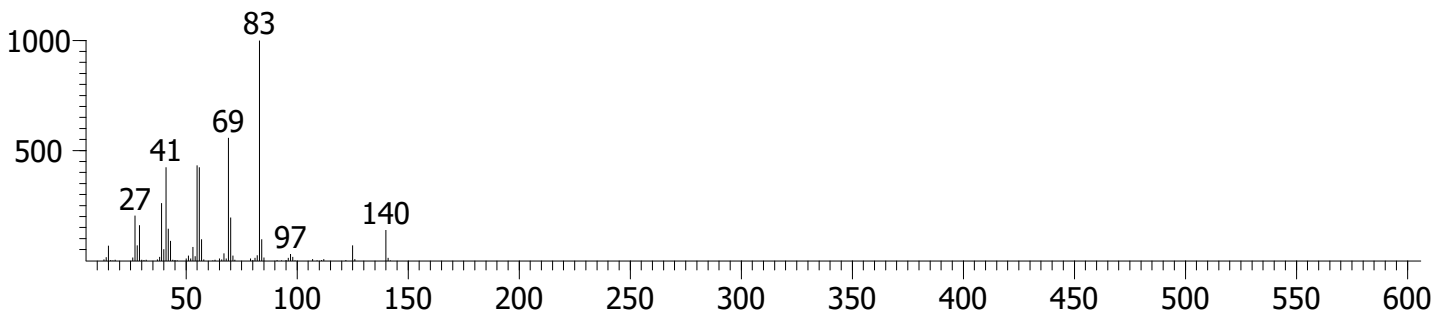
Peak Apex - sample "AnMbr C (20191120):1", peak 413, at 647.904 , 1.465 sec , sec (Spec # 25662)



Peak True - sample "AnMbr C (20191120):1", peak 413, at 647.904 , 1.465 sec , sec (Spec # 25662)



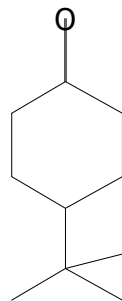
Library Hit - similarity 854, "Cyclohexanone, 3,3,5-trimethyl-"



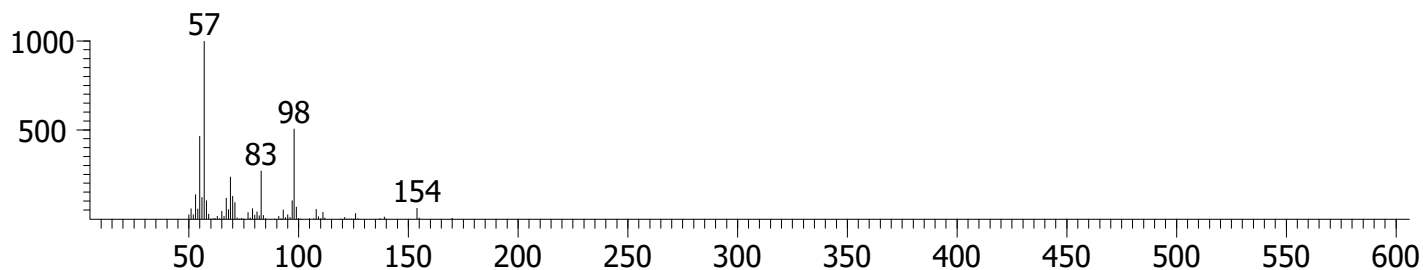
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cyclohexanone, 3,3,5-trimethyl-	854	6277	873-94-9	mainlib	C9H16O	140
2	2,4,6-Trimethyl-3-heptene	807	1313	0-00-0	mainlib	C10H20	140
3	2,4-Dimethylsulfolane	780	386	1003-78-7	mainlib	C6H12O2S	148
4	4-Pentenal	759	164	2100-17-6	mainlib	C5H8O	84
5	3-Octene, 2,2-dimethyl-	758	157	86869-76-3	mainlib	C10H20	140

Cyclohexanone, 4-(1,1-dimethylethyl)-

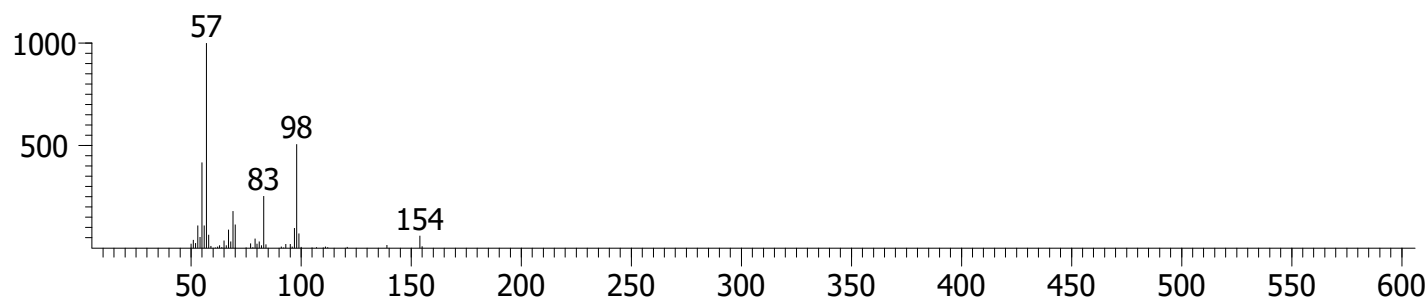
1st Dimension R.T. = 913.752
2nd Dimension R.T. = 1.630
Quant Mass(es) = 98
S/N = 9906.0
Area = 1533717
Height = 184111
Similarity = 935



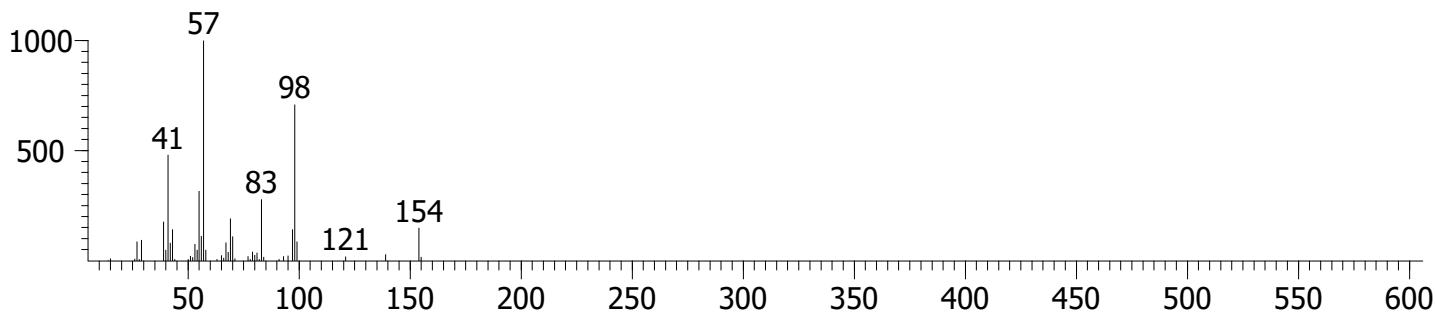
Peak Apex - sample "AnMbr C (20191120):1", peak 1355, at 913.752 , 1.630 sec , sec (Spec # 65967)



Peak True - sample "AnMbr C (20191120):1", peak 1355, at 913.752 , 1.630 sec , sec (Spec # 65967)



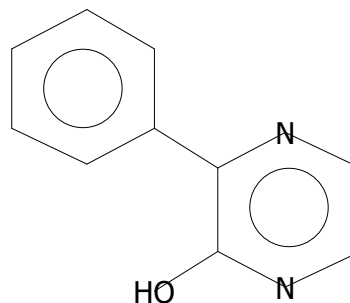
Library Hit - similarity 935, "Cyclohexanone, 4-(1,1-dimethylethyl)-"



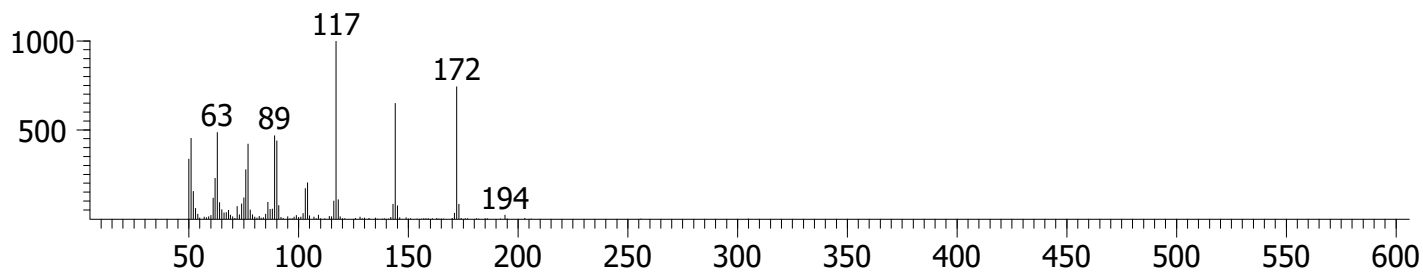
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cyclohexanone, 4-(1,1-dimethylethyl)-	935	8262	98-53-3	mainlib	C10H18O	154
2	4-Octylcyclohexanone	859	1041	0-00-0	mainlib	C14H26O	210
3	1,2-Cyclopentanediol, 3-methyl-	826	272	27583-37-5	mainlib	C6H12O2	116
4	Ether, tert-butyl isopropylidencyclopropyl	795	74	24524-56-9	mainlib	C10H18O	154
5	1-Hexene, 2,4,4-triethyl-	783	49	0-00-0	mainlib	C12H24	168

3-Phenylpyrazin-2-ol

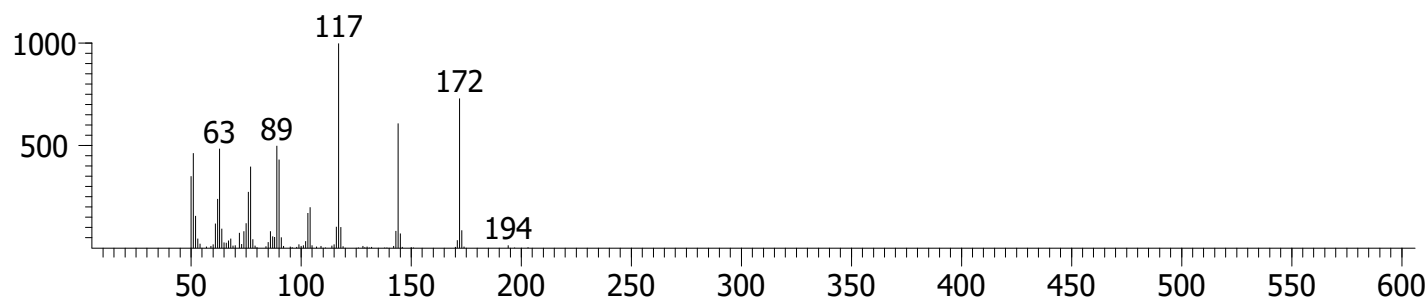
1st Dimension R.T. = 1676.32
2nd Dimension R.T. = 2.812
Quant Mass(es) = 172
S/N = 1744.4
Area = 560231
Height = 46101
Similarity = 880



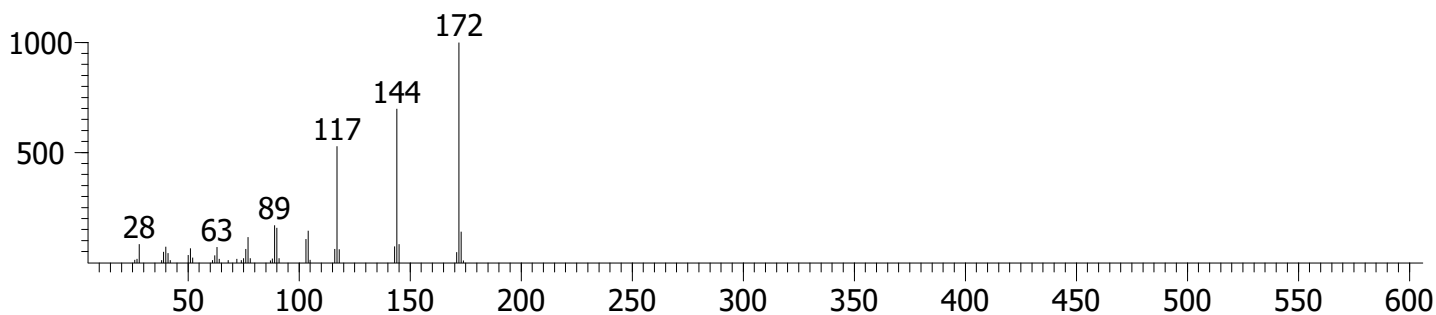
Peak Apex - sample "AnMbr C (20191120):1", peak 5598, at 1676.32 , 2.812 sec , sec (Spec # 181686)



Peak True - sample "AnMbr C (20191120):1", peak 5598, at 1676.32 , 2.812 sec , sec (Spec # 181686)



Library Hit - similarity 880, "3-Phenylpyrazin-2-ol"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Phenylpyrazin-2-ol	880	7872	73200-73-4	mainlib	C10H8N2O	172
2	Pyrazine, 2-hydroxy-5-phenyl-	820	1397	25844-72-8	mainlib	C10H8N2O	172
3	1-Acetyl-2-phenylimidazole	768	279	182481-13-6	mainlib	C11H10N2O	186
4	1H-Imidazole, 1-phenyl-	738	77	7164-98-9	mainlib	C9H8N2	144
5	1H-Imidazole-2-carbaldehyde, 1-phenyl-	731	59	0-00-0	mainlib	C10H8N2O	172

4-Hexen-2-one, 3-methyl-

1st Dimension R.T. = 595.434

2nd Dimension R.T. = 1.802

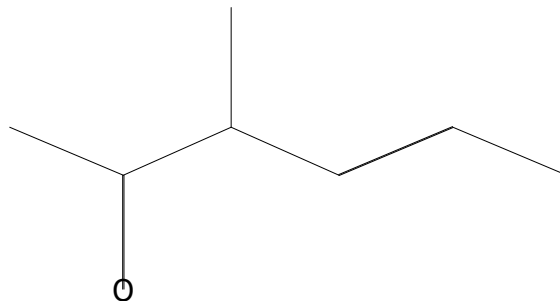
Quant Mass(es) = 114

S/N = 69.694

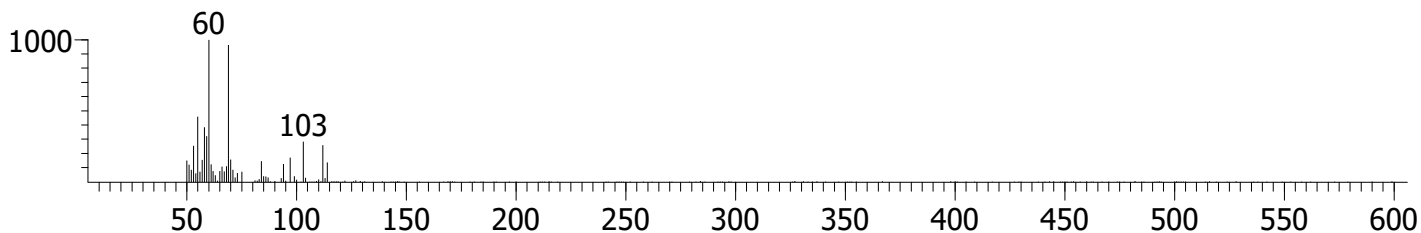
Area = 45939

Height = 5618.6

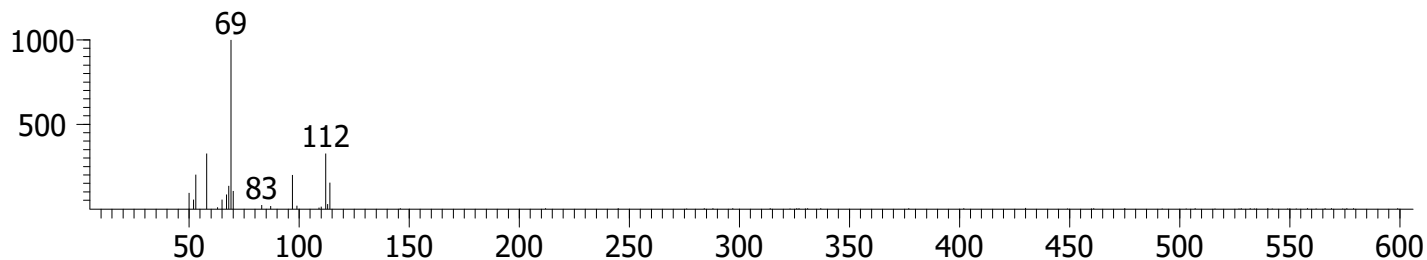
Similarity = 820



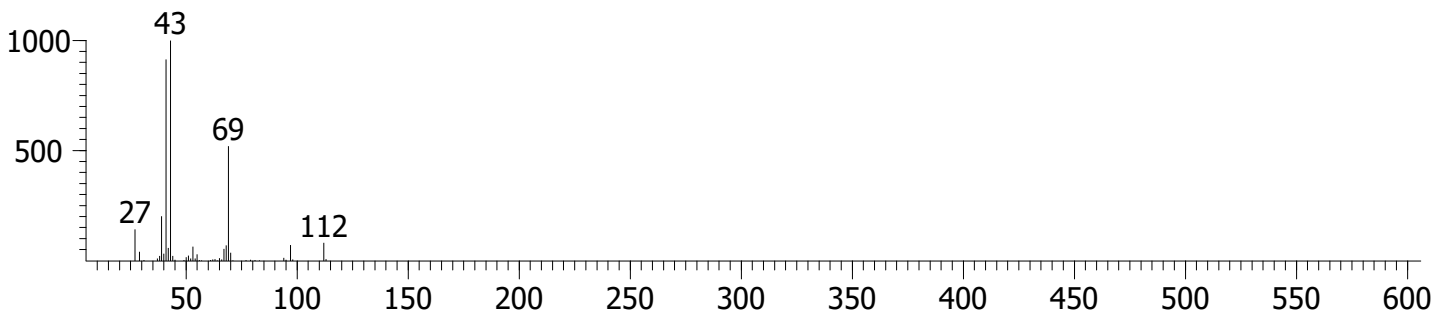
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 277, at 595.434 , 1.802 sec , sec (Spec # 17763)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 277, at 595.434 , 1.802 sec , sec (Spec # 17763)



Library Hit - similarity 820, "4-Hexen-2-one, 3-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Hexen-2-one, 3-methyl-	820	6670	72189-24-3	mainlib	C7H12O	112
2	2-Furanone, 2,5-dihydro-3,5-dimethyl	780	1547	0-00-0	mainlib	C6H8O2	112
3	3-Penten-2-one, 3,4-dimethyl-	765	937	684-94-6	mainlib	C7H12O	112
4	5-Hexen-2-one, 5-methyl-	718	196	3240-09-3	mainlib	C7H12O	112
5	3-Hexen-2-one, 3-methyl-	716	180	1187-80-0	mainlib	C7H12O	112

2-Decanone

1st Dimension R.T. = 707.37

2nd Dimension R.T. = 1.366

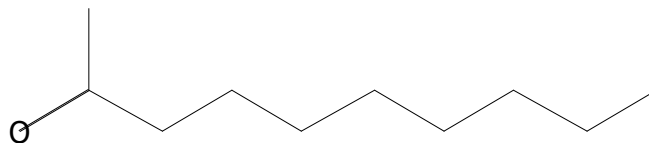
Quant Mass(es) = 58

S/N = 10416

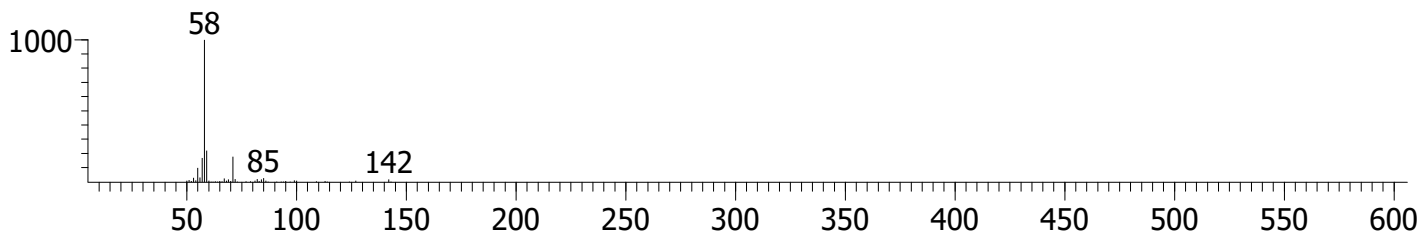
Area = 3539591

Height = 524926

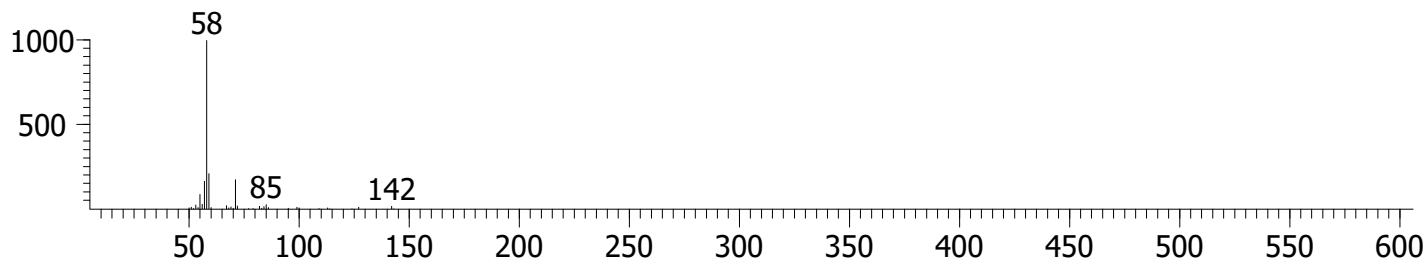
Similarity = 940



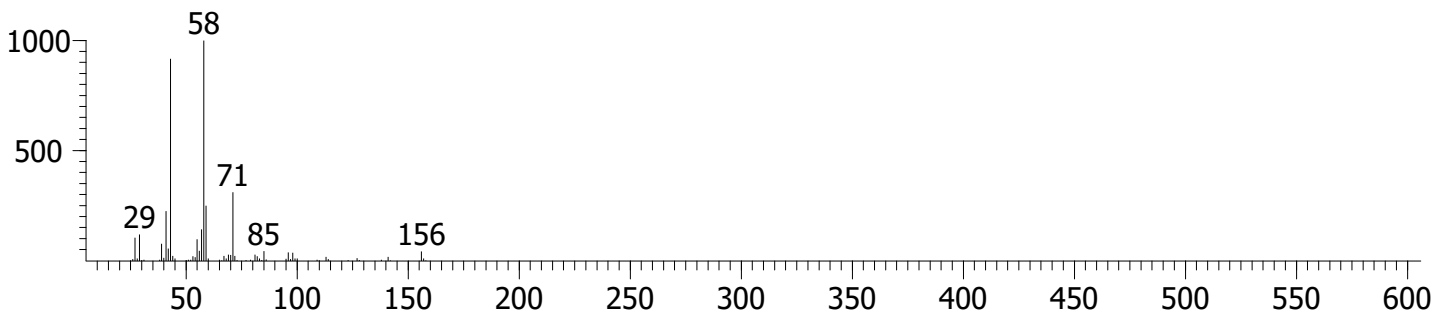
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 601, at 707.37 , 1.366 sec , sec (Spec # 34657)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 601, at 707.37 , 1.366 sec , sec (Spec # 34657)



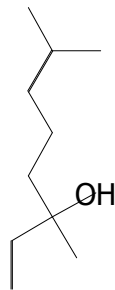
Library Hit - similarity 940, "2-Decanone"



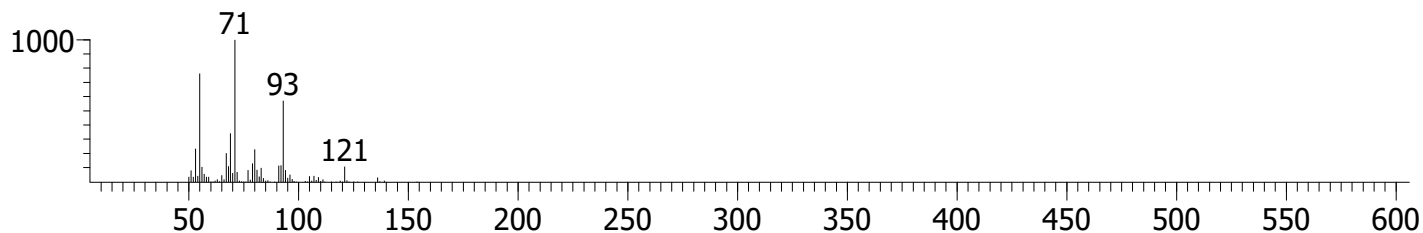
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Decanone	940	3625	693-54-9	mainlib	C10H20O	156
2	2-Hexanone, 5-methyl-	922	1869	110-12-3	mainlib	C7H14O	114
3	2-Dodecanone	911	1282	6175-49-1	mainlib	C12H24O	184
4	2-Octanone	896	777	111-13-7	mainlib	C8H16O	128
5	2-Nonanone	896	777	821-55-6	mainlib	C9H18O	142

Linalool

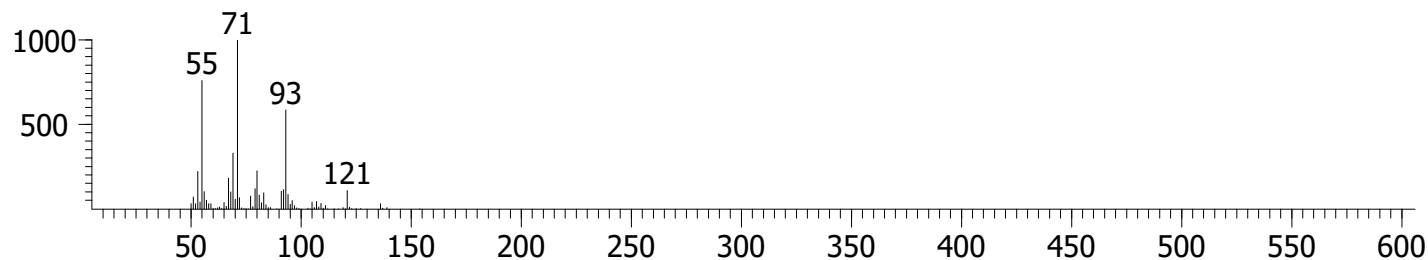
1st Dimension R.T. = 721.362
2nd Dimension R.T. = 1.386
Quant Mass(es) = 71
S/N = 24255
Area = 13212837
Height = 1660846
Similarity = 931



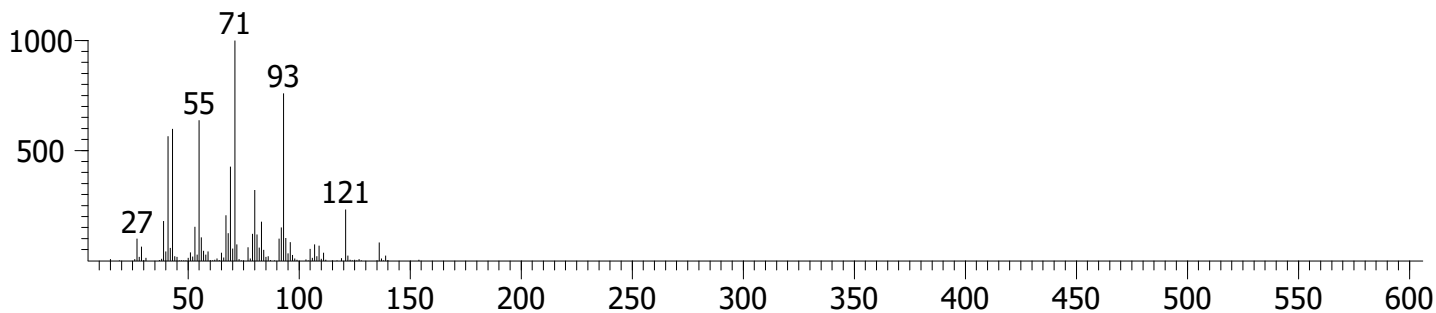
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 647, at 721.362 , 1.386 sec , sec (Spec # 36780)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 647, at 721.362 , 1.386 sec , sec (Spec # 36780)



Library Hit - similarity 931, "Linalool"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Linalool	931	8537	78-70-6	mainlib	C10H18O	154
2	(-)-Isopinocampheol, 2-methylpropionate	800	348	0-00-0	mainlib	C14H24O2	224
3	1,6-Octadien-3-ol, 3,7-dimethyl-, formate	794	273	115-99-1	mainlib	C11H18O2	182
4	Ethylinalool	785	198	0-00-0	mainlib	C11H20O	168
5	Linalyl acetate	775	140	115-95-7	mainlib	C12H20O2	196

2(3H)-Furanone, 5-acetyldihydro-

1st Dimension R.T. = 770.334

2nd Dimension R.T. = 2.343

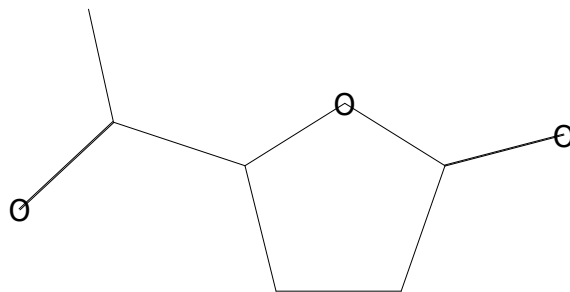
Quant Mass(es) = 85

S/N = 1249.4

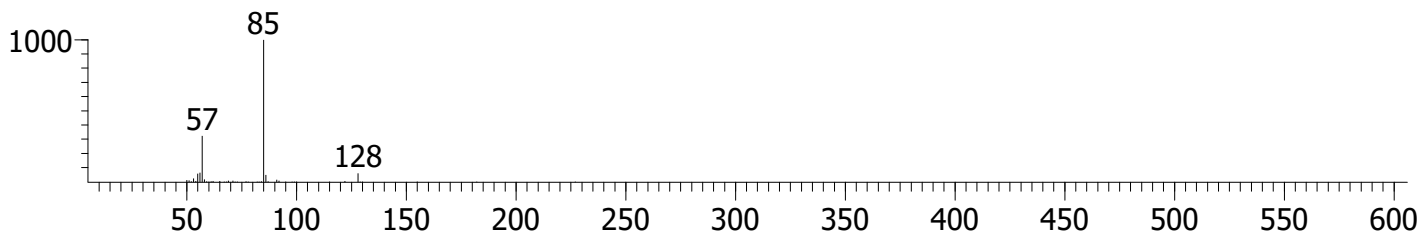
Area = 548976

Height = 54850

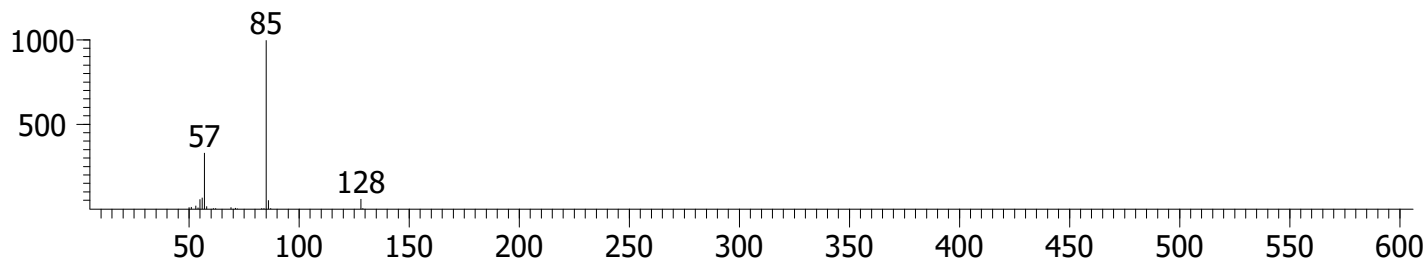
Similarity = 937



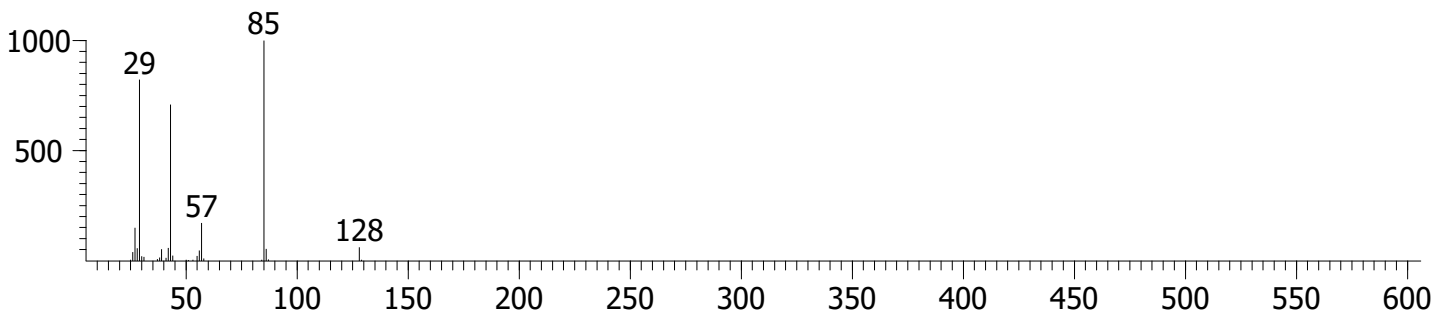
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 808, at 770.334 , 2.343 sec , sec (Spec # 443 45)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 808, at 770.334 , 2.343 sec , sec (Spec # 4434 5)



Library Hit - similarity 937, "2(3H)-Furanone, 5-acetyldihydro-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2(3H)-Furanone, 5-acetyldihydro-	937	5141	29393-32-6	mainlib	C ₆ H ₈ O ₃	128
2	Valeric anhydride	890	1075	2082-59-9	mainlib	C ₁₀ H ₁₈ O ₃	186
3	2-Furanmethanol, tetrahydro-5-methyl-, trans-	886	908	54774-28-6	mainlib	C ₆ H ₁₂ O ₂	116
4	Ethanone, 1-(3-methyloxiranyl)-	866	413	17257-79-3	mainlib	C ₅ H ₈ O ₂	100
5	Furfuryl alcohol, tetrahydro-5-methyl-, cis-	863	365	16015-08-0	mainlib	C ₆ H ₁₂ O ₂	116

Amyl cyclopentenone

1st Dimension R.T. = 1064.17

2nd Dimension R.T. = 1.861

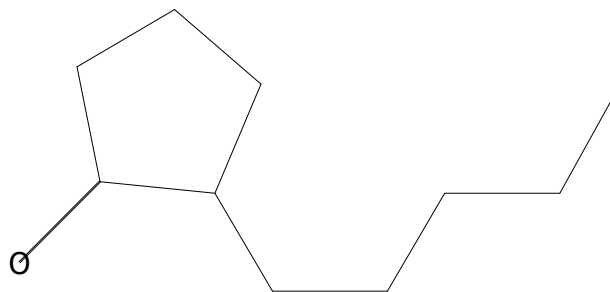
Quant Mass(es) = 84

S/N = 1113.2

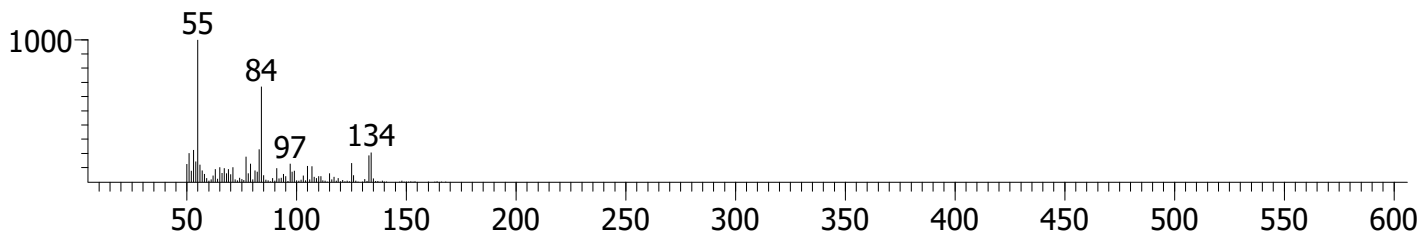
Area = 317416

Height = 36654

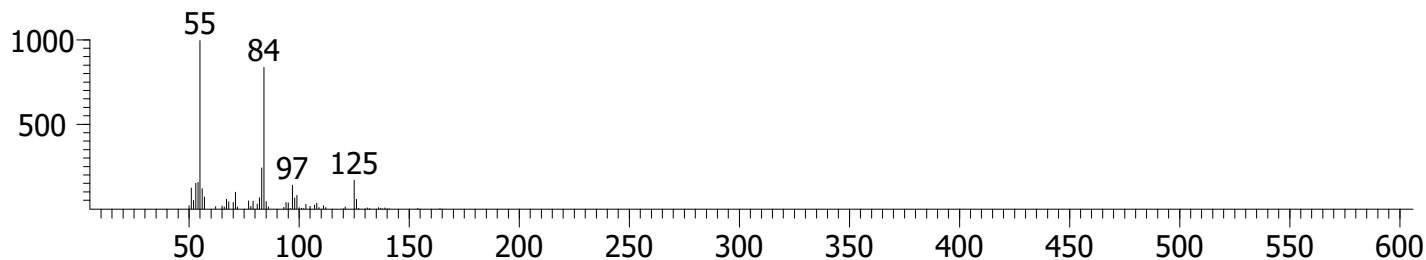
Similarity = 719



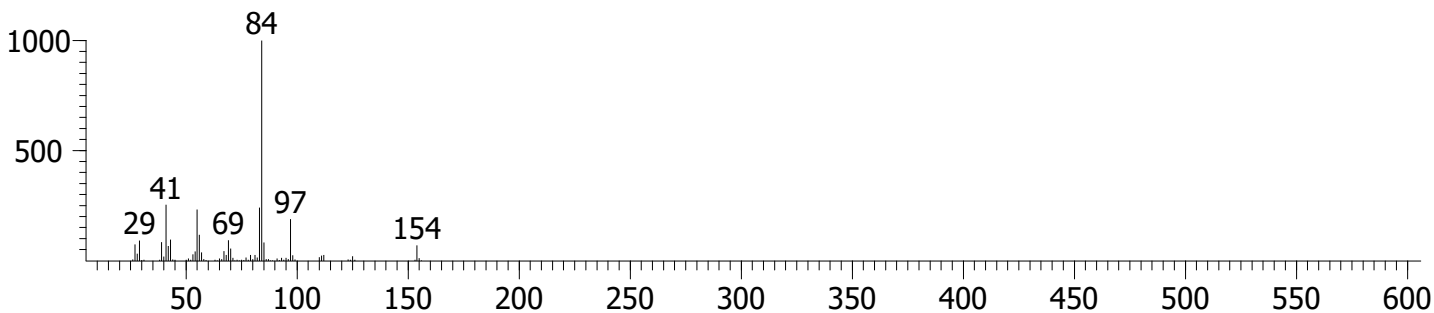
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 2120, at 1064.17 , 1.861 sec , sec (Spec # 88792)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 2120, at 1064.17 , 1.861 sec , sec (Spec # 88792)



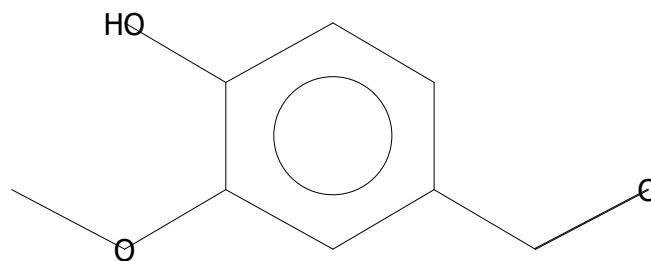
Library Hit - similarity 719, "Amyl cyclopentenone"



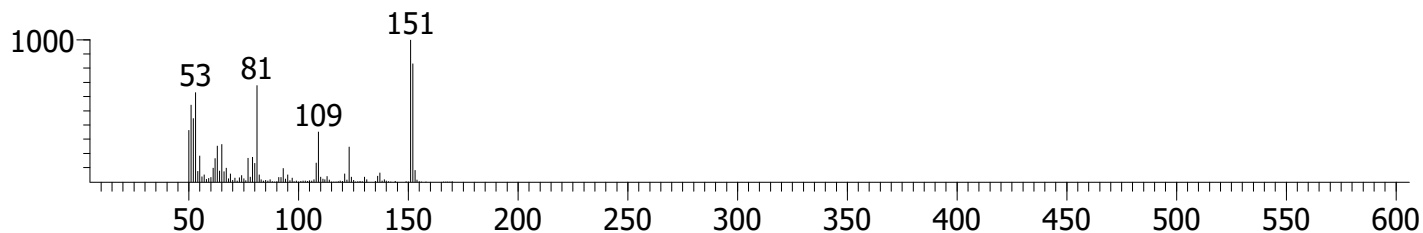
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Amyl cyclopentenone	719	963	4819-67-4	mainlib	C10H18O	154
2	2,5-Heptadien-4-ol, 3,5-dimethyl-4-[2-(pyrrolidin-1-yl)ethyl]-	701	496	178763-04-7	mainlib	C15H27NO	237
3	cyclopentanone, 2-decyl-	700	477	0-00-0	mainlib	C15H28O	224
4	Furan, 2,3-dihydro-4-methyl-	695	384	34314-83-5	mainlib	C5H8O	84
5	2-Butenal, 2-methyl-, (E)-	693	354	497-03-0	mainlib	C5H8O	84

Vanillin

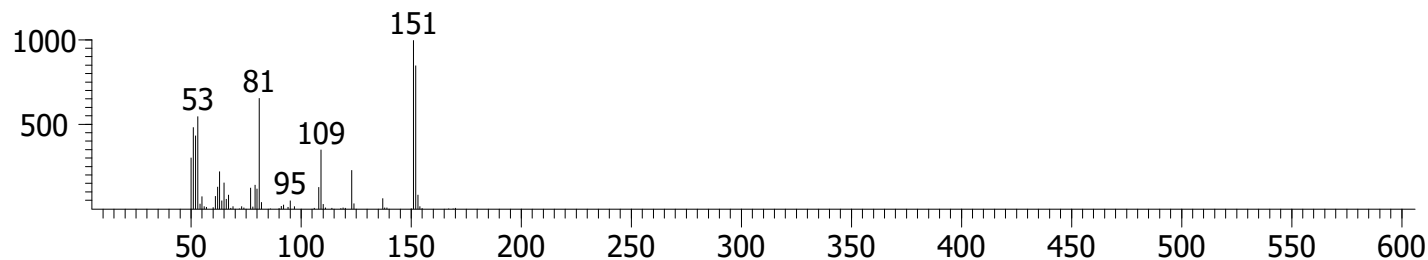
1st Dimension R.T. = 1144.62
2nd Dimension R.T. = 2.165
Quant Mass(es) = 151
S/N = 2875.5
Area = 690292
Height = 74211
Similarity = 931



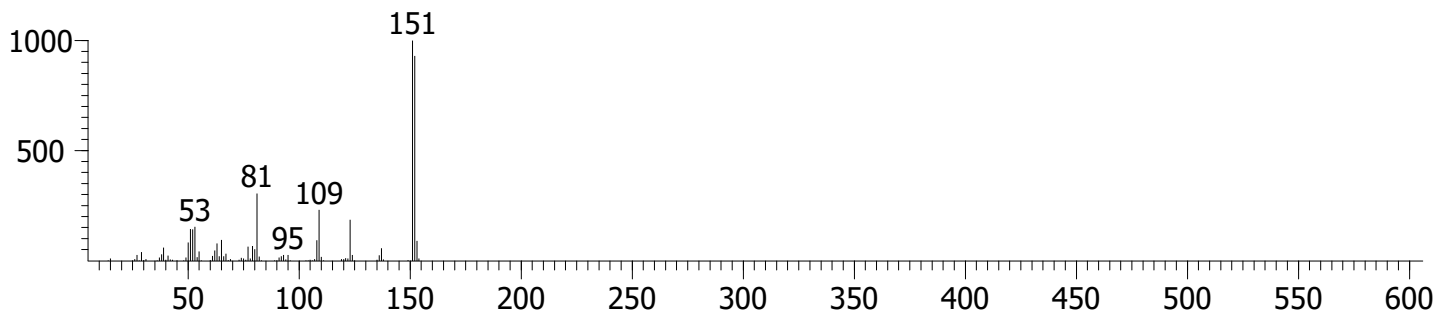
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 2536, at 1144.62 , 2.165 sec , sec (Spec # 101028)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 2536, at 1144.62 , 2.165 sec , sec (Spec # 101028)



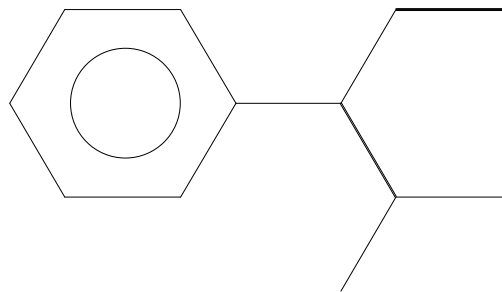
Library Hit - similarity 931, "Vanillin"



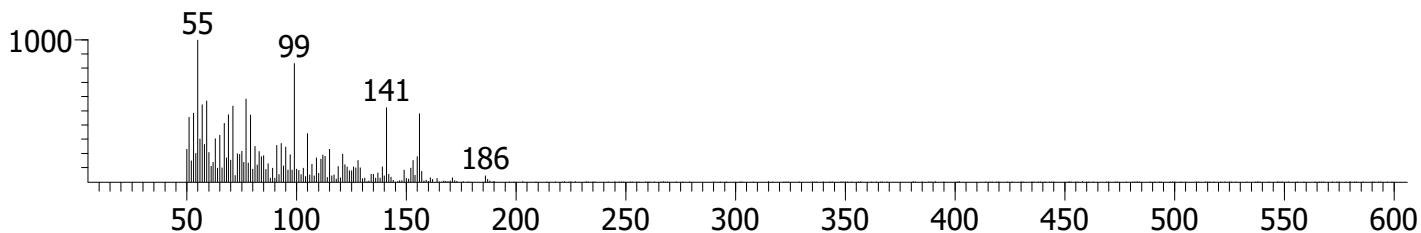
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Vanillin	931	4492	121-33-5	mainlib	C8H8O3	152
2	Benzaldehyde, 3-hydroxy-4-methoxy-	922	3261	621-59-0	mainlib	C8H8O3	152
3	3-Methoxy-4-hydroxy mandelonitrile	877	694	0-00-0	mainlib	C9H9NO3	179
4	4-Hydroxy-2-methoxybenzaldehyde	877	694	18278-34-7	mainlib	C8H8O3	152
5	Benzaldehyde, 3-(chloroacetoxy)-4-methoxy-	871	546	66267-38-7	mainlib	C10H9ClO4	228

Pent-1-yn-3-ene, 4-methyl-3-phenyl-

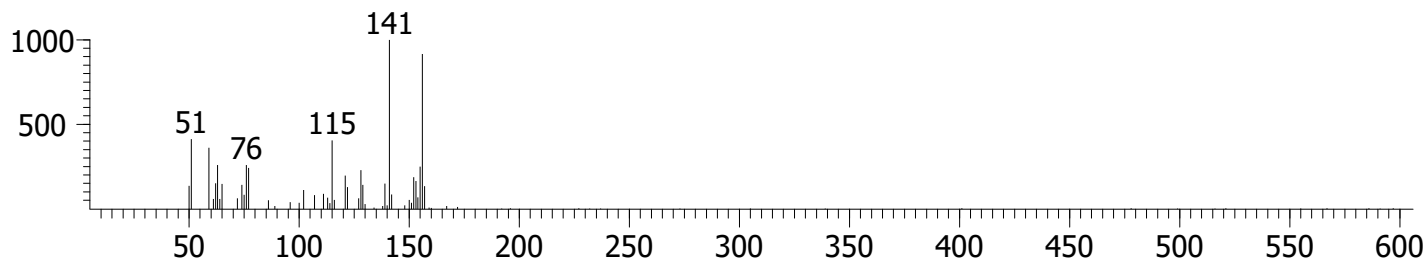
1st Dimension R.T. = 1176.1
2nd Dimension R.T. = 1.848
Quant Mass(es) = 156
S/N = 304.66
Area = 38522
Height = 4787.5
Similarity = 843



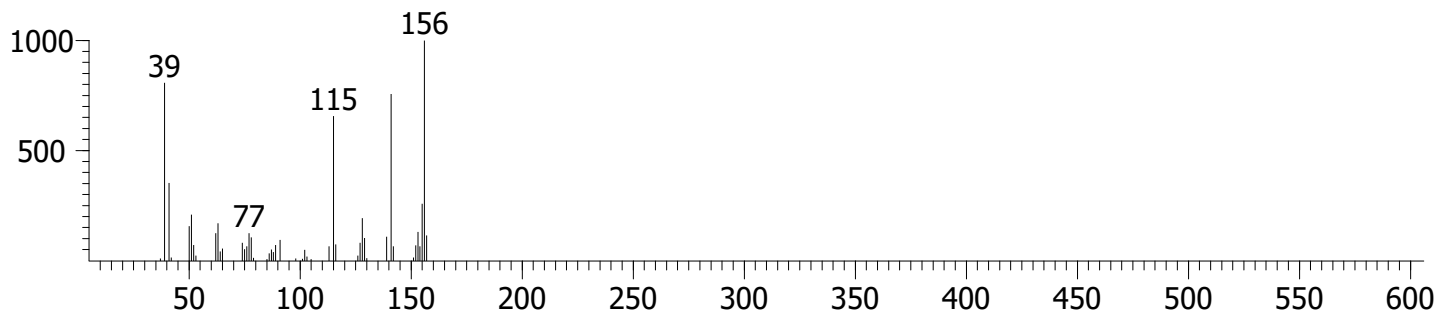
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 2709, at 1176.1 , 1.848 sec , sec (Spec # 105750)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 2709, at 1176.1 , 1.848 sec , sec (Spec # 105750)



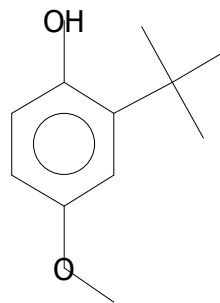
Library Hit - similarity 843, "Pent-1-yn-3-ene, 4-methyl-3-phenyl-"



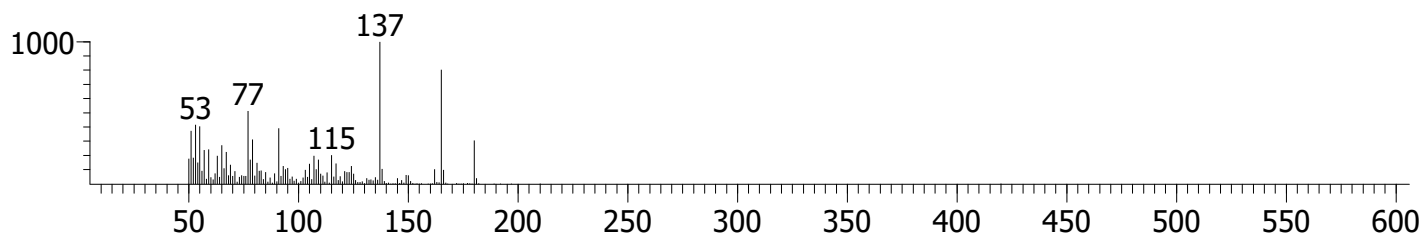
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pent-1-yn-3-ene, 4-methyl-3-phenyl-	843	4159	65050-80-8	mainlib	C12H12	156
2	Naphthalene, 2,3-dimethyl-	804	980	581-40-8	mainlib	C12H12	156
3	Naphthalene, 1,7-dimethyl-	797	751	575-37-1	mainlib	C12H12	156
4	Naphthalene, 2,6-dimethyl-	791	590	581-42-0	mainlib	C12H12	156
5	1,4-Dimethylazulene	786	475	1127-69-1	mainlib	C12H12	156

3-tert-Butyl-4-hydroxyanisole

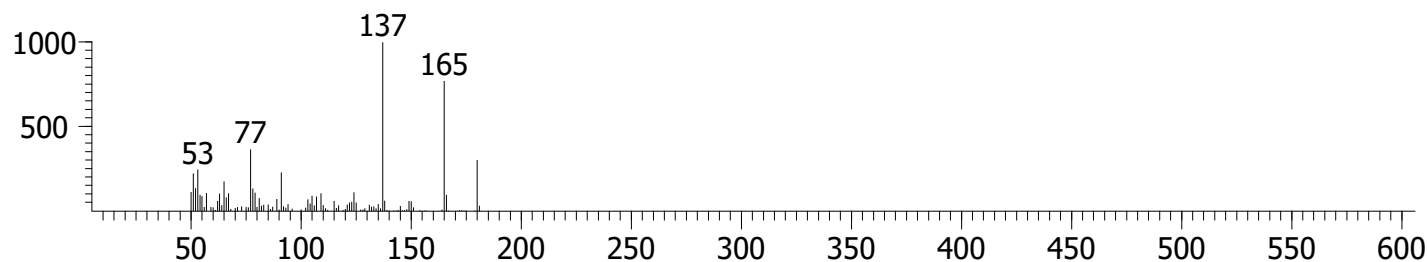
1st Dimension R.T. = 1246.06
2nd Dimension R.T. = 1.841
Quant Mass(es) = 137
S/N = 1570.9
Area = 240324
Height = 29692
Similarity = 884



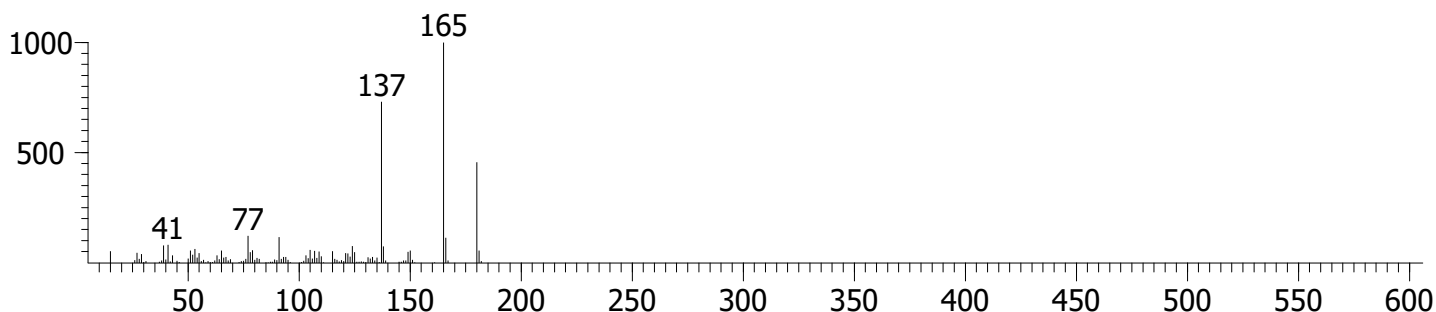
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 3121, at 1246.06 , 1.841 sec , sec (Spec # 116349)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 3121, at 1246.06 , 1.841 sec , sec (Spec # 116349)



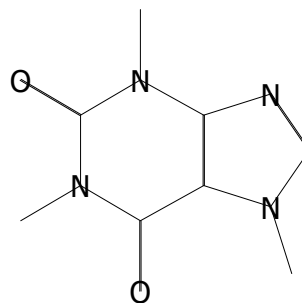
Library Hit - similarity 884, "3-tert-Butyl-4-hydroxyanisole"



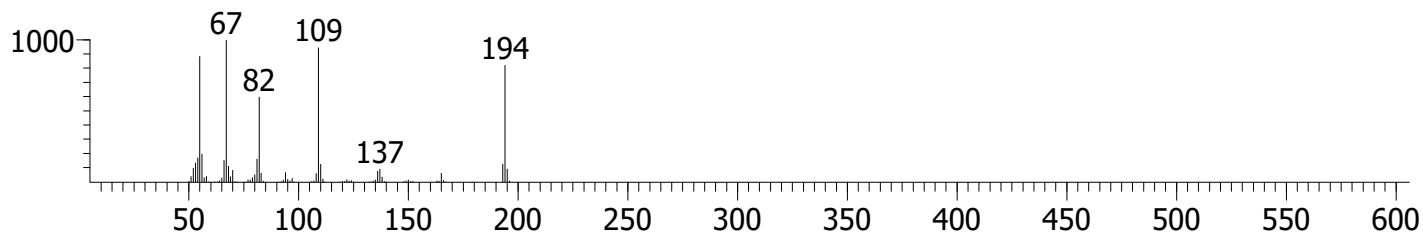
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-tert-Butyl-4-hydroxyanisole	884	8688	121-00-6	mainlib	C ₁₁ H ₁₆ O ₂	180
2	Phenol, 3-(1,1-dimethylethyl)-4-methoxy-	771	535	88-32-4	mainlib	C ₁₁ H ₁₆ O ₂	180
3	3-tert-Butyl-4-hydroxyanisole, acetate	766	431	91401-26-2	mainlib	C ₁₃ H ₁₈ O ₃	222
4	3-(tert-Butyl)-4-methoxyphenyl acetate	711	83	0-00-0	mainlib	C ₁₃ H ₁₈ O ₃	222
5	1-(2,4-Diethoxy-phenyl)-ethanone	706	67	22924-18-1	mainlib	C ₁₂ H ₁₆ O ₃	208

Caffeine

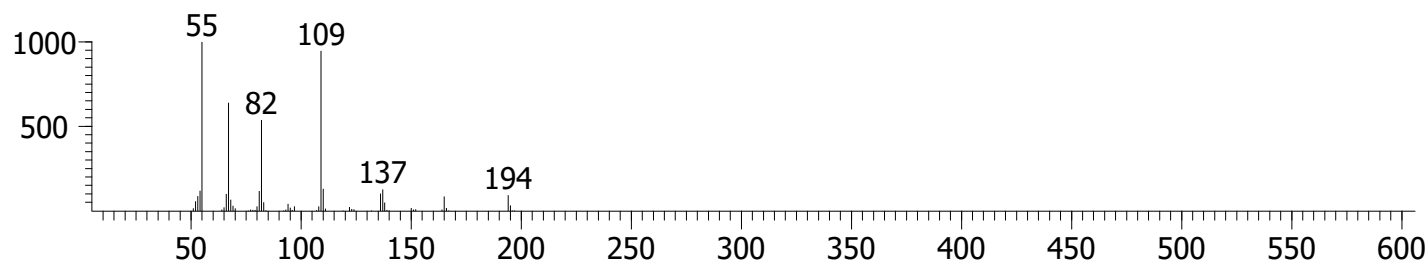
1st Dimension R.T. = 1665.82
 2nd Dimension R.T. = 3.016
 Quant Mass(es) = 109
 S/N = 10146
 Area = 174685496
 Height = 4821059
 Similarity = 766



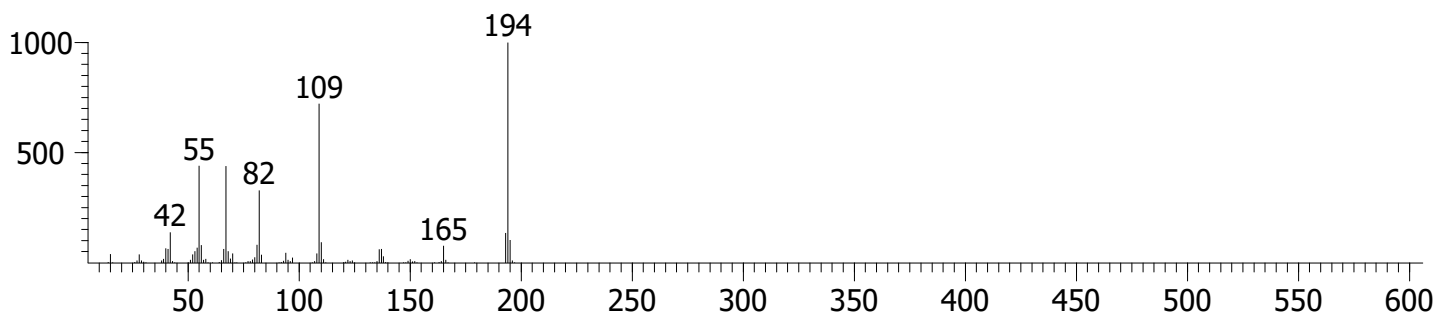
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 5799, at 1665.82 , 3.016 sec , sec (Spec # 18 0127)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 5799, at 1665.82 , 3.016 sec , sec (Spec # 180 127)



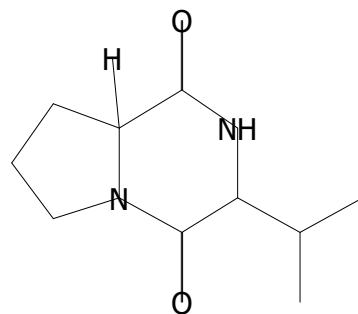
Library Hit - similarity 766, "Caffeine"



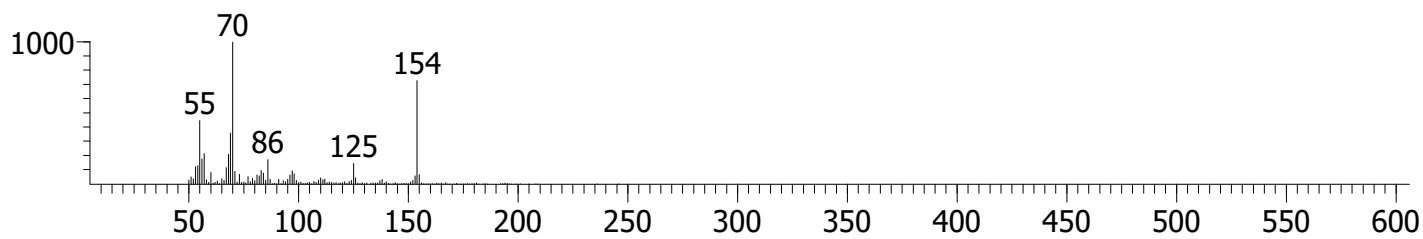
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Caffeine	766	7403	58-08-2	mainlib	C ₈ H ₁₀ N ₄ O ₂	194
2	Cyclooctene,1-(diethylboryl)oxy-	683	725	57387-71-0	mainlib	C ₁₂ H ₂₃ BO	194
3	1-Pyrrolidinylacetonitrile	666	396	29134-29-0	mainlib	C ₆ H ₁₀ N ₂	110
4	Cyclohexane, decylidene-	644	156	62338-40-3	mainlib	C ₁₆ H ₃₀	222
5	2-Amino-4-methylpyrimidine	637	119	108-52-1	mainlib	C ₅ H ₇ N ₃	109

Cyclo(L-prolyl-L-valine)

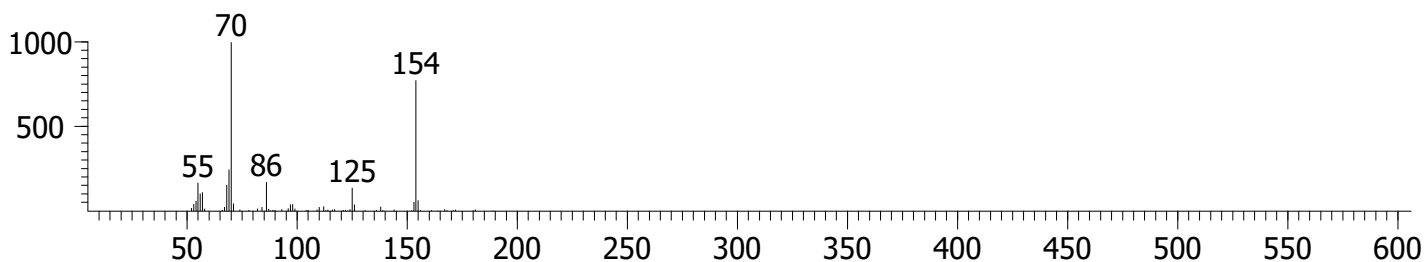
1st Dimension R.T. = 1732.28
2nd Dimension R.T. = 2.567
Quant Mass(es) = 154
S/N = 3069.9
Area = 641611
Height = 54280
Similarity = 836



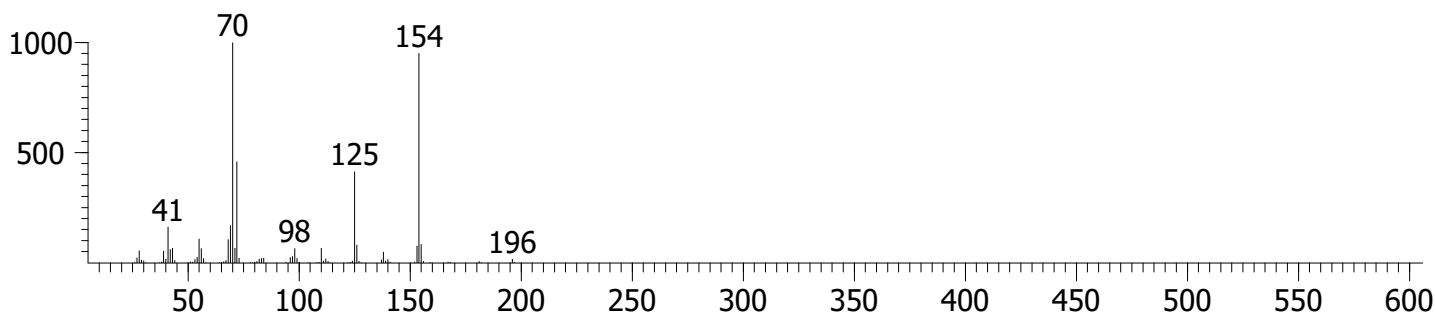
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 6224, at 1732.28 , 2.567 sec , sec (Spec # 19 0129)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 6224, at 1732.28 , 2.567 sec , sec (Spec # 190 129)



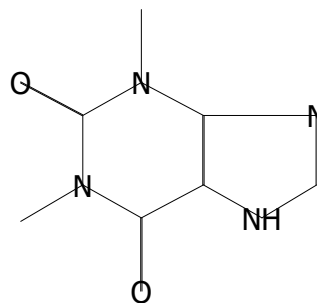
Library Hit - similarity 836, "Cyclo(L-prolyl-L-valine)"



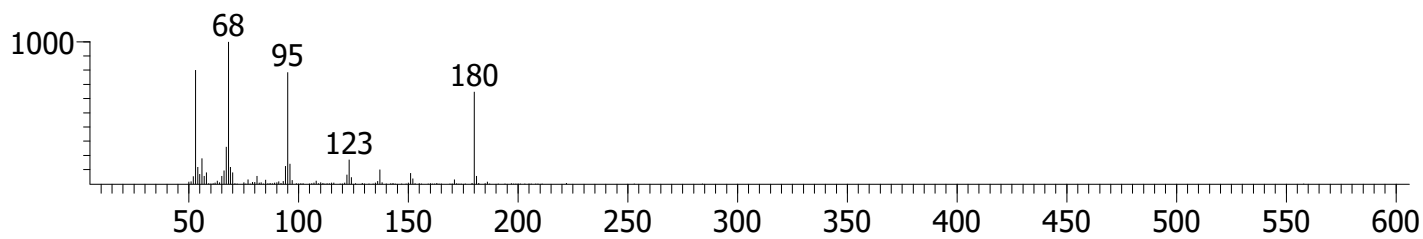
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cyclo(L-prolyl-L-valine)	836	7232	2854-40-2	mainlib	C10H16N2O2	196
2	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	791	1540	5654-86-4	mainlib	C11H18N2O2	210
3	L-Proline, N-valeryl-, pentadecyl ester	723	233	0-00-0	mainlib	C25H47NO3	409
4	L-Proline, N-valeryl-, nonyl ester	712	160	0-00-0	mainlib	C19H35NO3	325
5	L-Proline, N-valeryl-, dodecyl ester	711	154	0-00-0	mainlib	C22H41NO3	367

Theophylline

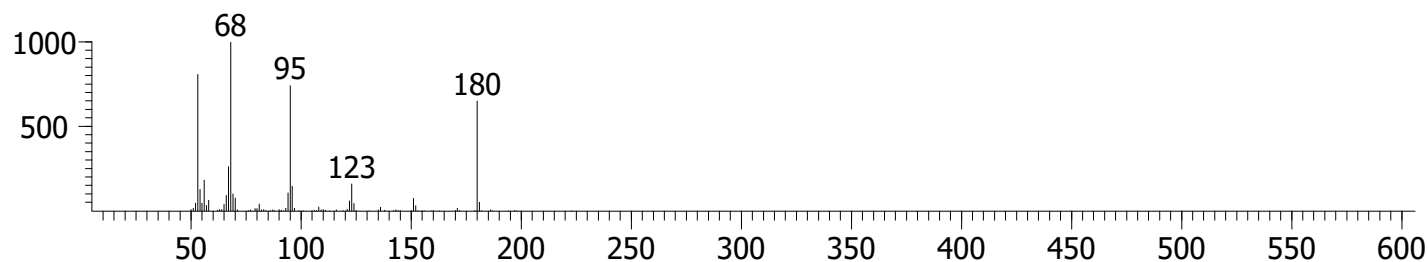
1st Dimension R.T. = 1823.23
 2nd Dimension R.T. = 2.911
 Quant Mass(es) = 180
 S/N = 1874.0
 Area = 669297
 Height = 50091
 Similarity = 895



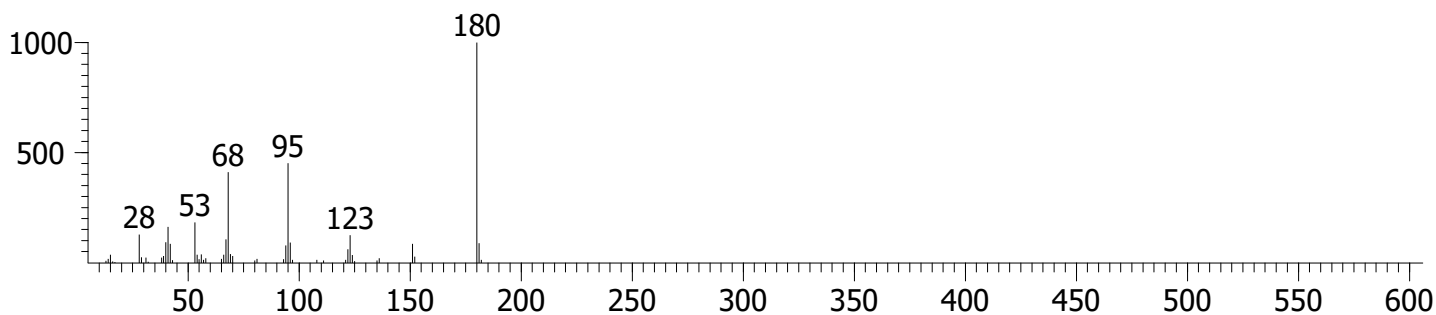
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 6720, at 1823.23 , 2.911 sec , sec (Spec # 203961)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 6720, at 1823.23 , 2.911 sec , sec (Spec # 203961)



Library Hit - similarity 895, "Theophylline"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Theophylline	895	7047	58-55-9	mainlib	C7H8N4O2	180
2	7-Acetyl-1,3-dimethyl-1H-purine-2,6(3H,7H)-dione	857	1688	0-00-0	mainlib	C9H10N4O3	222
3	Theophylline, N-acetyl-	845	1124	0-00-0	mainlib	C9H10N4O3	222
4	7H-Purine-2,6(1H,3H)-dione, 1,3-dimethyl-7-(4-methyl-1,2,5-oxadiazol-3-ylaminomethyl)-	762	110	0-00-0	mainlib	C11H13N7O3	291
5	1,7-Dimethylxanthine	694	16	611-59-6	mainlib	C7H8N4O2	180

Adipic acid, 3-heptyl isobutyl ester

1st Dimension R.T. = 1952.66

2nd Dimension R.T. = 1.736

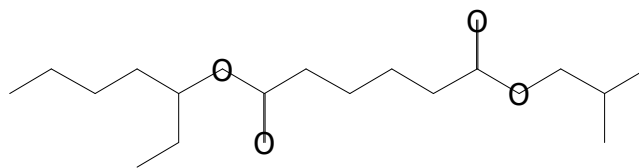
Quant Mass(es) = 185

S/N = 7898.3

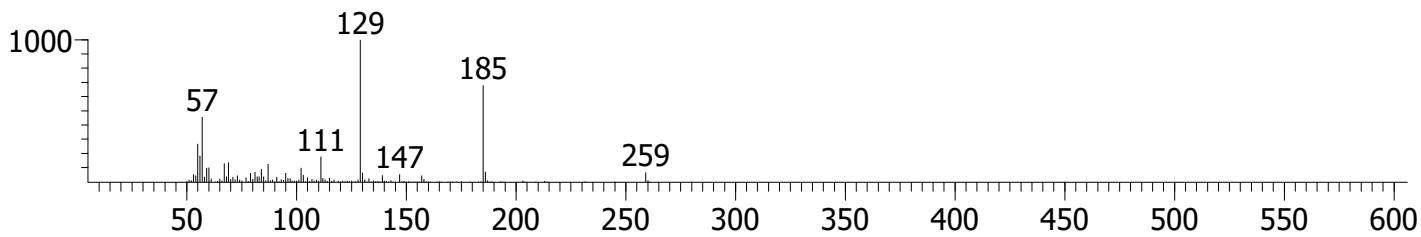
Area = 823894

Height = 79615

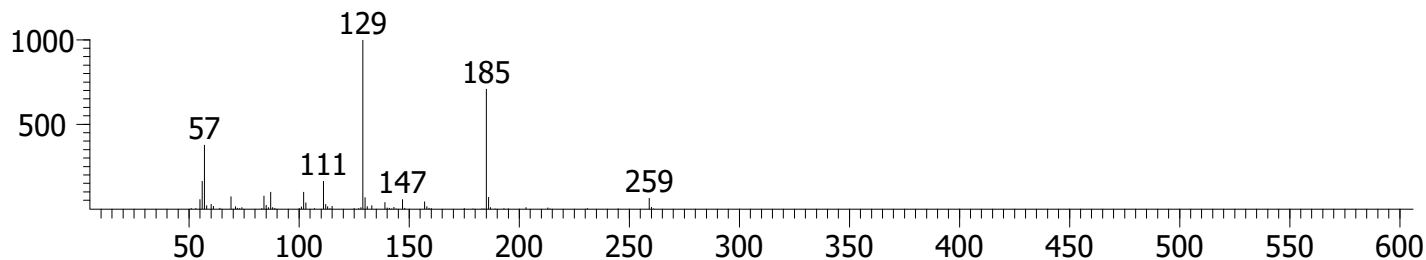
Similarity = 842



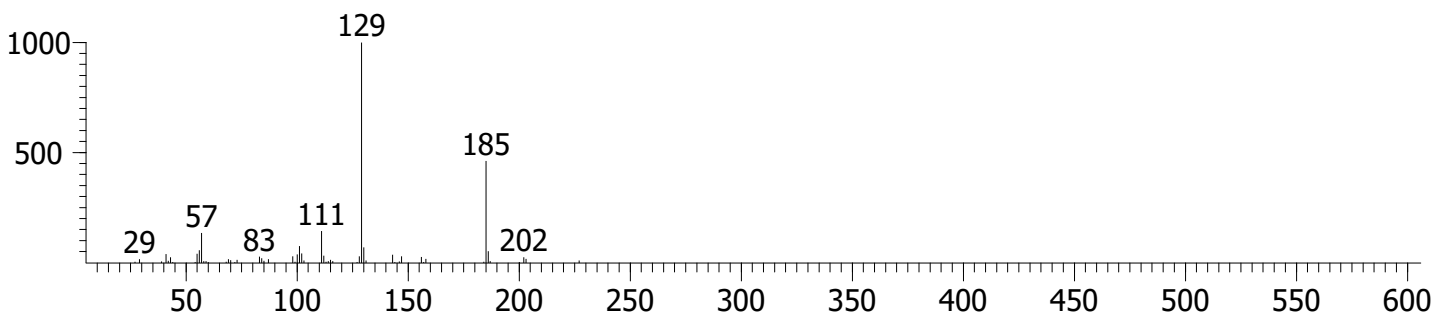
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 7215, at 1952.66 , 1.736 sec , sec (Spec # 223393)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 7215, at 1952.66 , 1.736 sec , sec (Spec # 223393)



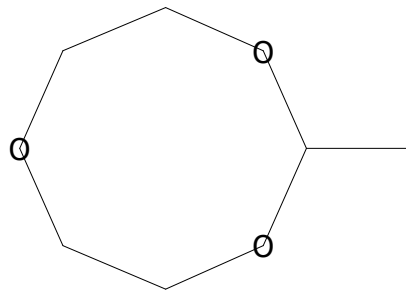
Library Hit - similarity 842, "Adipic acid, 3-heptyl isobutyl ester"



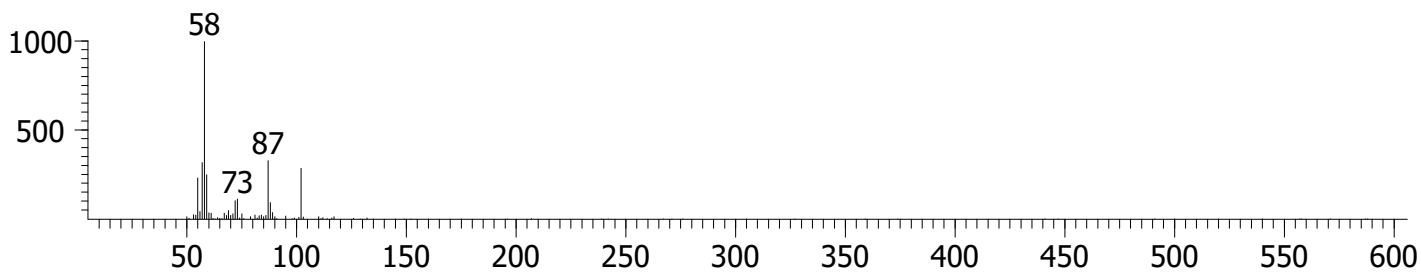
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Adipic acid, 3-heptyl isobutyl ester	842	3356	0-00-0	mainlib	C17H32O4	300
2	Adipic acid, 2-decyl isobutyl ester	838	2835	0-00-0	mainlib	C20H38O4	342
3	Adipic acid, 2-heptyl isobutyl ester	813	864	0-00-0	mainlib	C17H32O4	300
4	Adipic acid, 4-heptyl isobutyl ester	806	662	0-00-0	mainlib	C17H32O4	300
5	Adipic acid, 2-hexyl isobutyl ester	790	381	0-00-0	mainlib	C16H30O4	286

1,3,6-Trioxocane, 2-methyl-

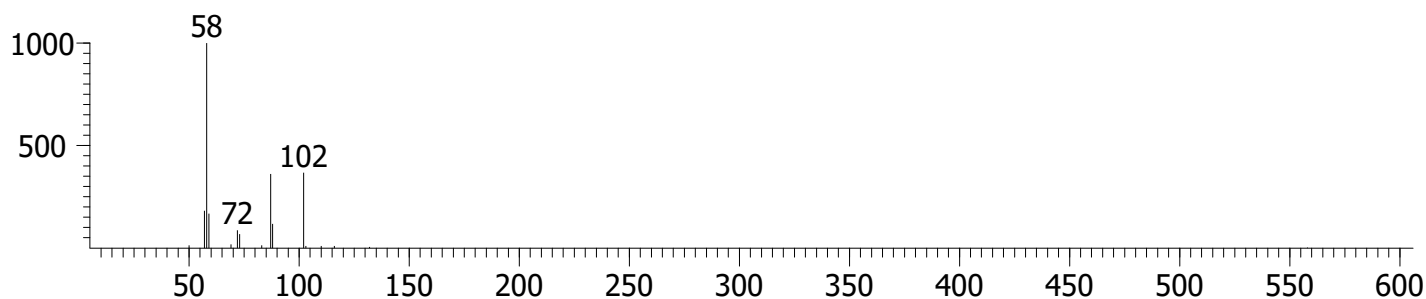
1st Dimension R.T. = 507.984
2nd Dimension R.T. = 1.505
Quant Mass(es) = 58
S/N = 151.07
Area = 104469
Height = 10621
Similarity = 896



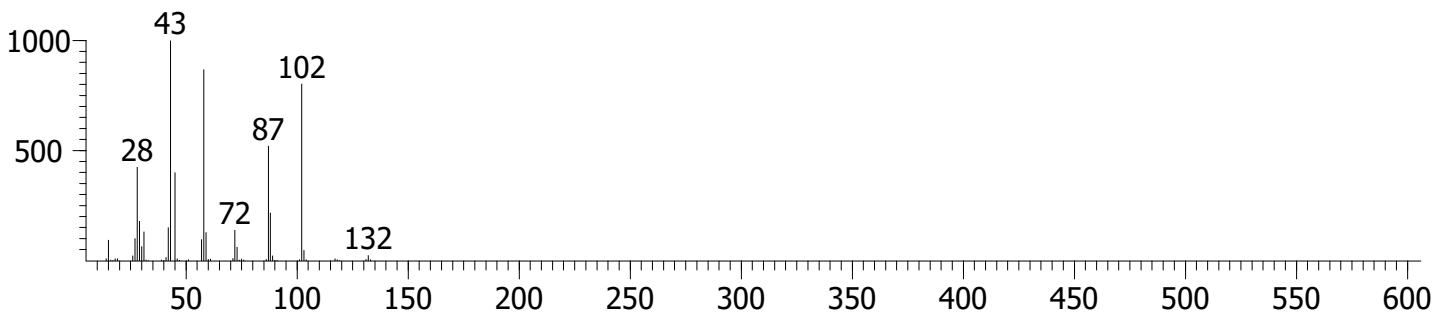
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 41, at 507.984 , 1.505 sec , sec (Spec # 4468)



Peak True - sample "INF-C comp 091919 (111419):1", peak 41, at 507.984 , 1.505 sec , sec (Spec # 4468)

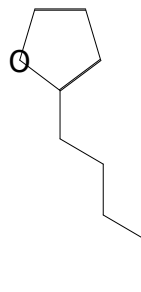


Library Hit - similarity 896, "1,3,6-Trioxocane, 2-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,3,6-Trioxocane, 2-methyl-	896	9402	2781-01-3	mainlib	C6H12O3	132
2	3-[Carbamoyl(methyl)amino]propanoic acid	764	377	72054-55-8	mainlib	C5H10N2O3	146
3	2H-Pyran-3-ol, tetrahydro-6-methoxy-2-methyl-, [2R-(2à,3á,6á)]-	708	71	21317-50-0	mainlib	C7H14O3	146
4	N,N-Dimethyl-3-isopropoxypropylamine	694	45	71126-66-4	mainlib	C8H19NO	145
5	3-Cyclohexyloxypropylamine, N,N-dimethyl-	692	41	71126-67-5	mainlib	C11H23NO	185

Furan, 2-pentyl-



1st Dimension R.T. = 563.952

2nd Dimension R.T. = 1.300

Quant Mass(es) = 81

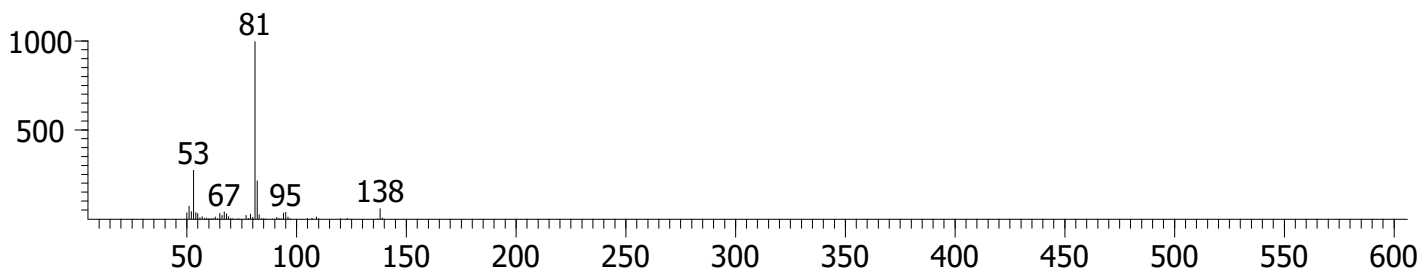
S/N = 8848.6

Area = 4580066

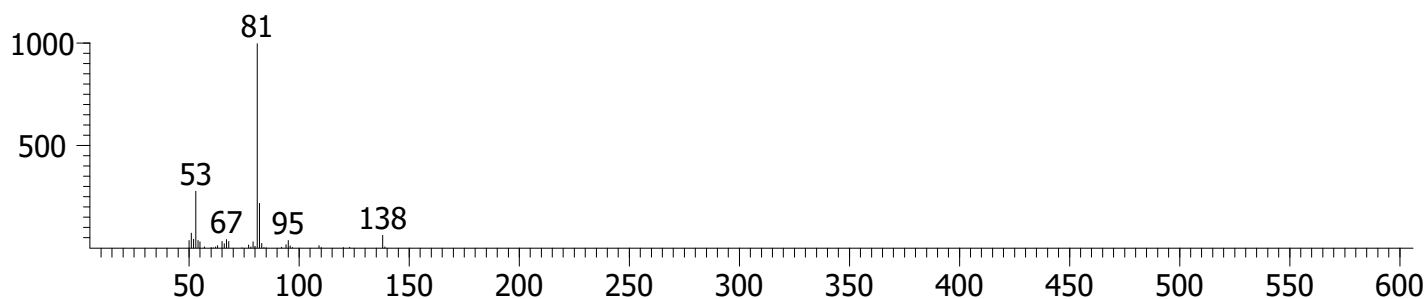
Height = 756031

Similarity = 875

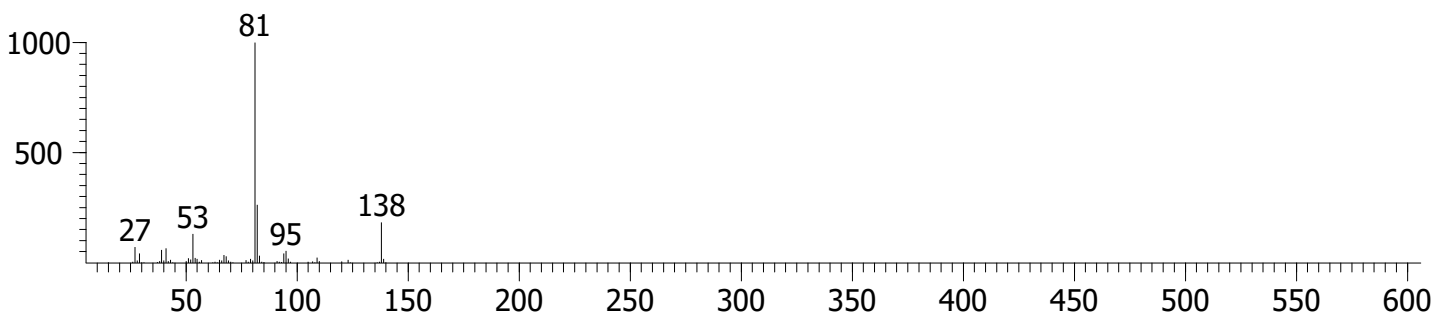
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 194, at 563.952 , 1.300 sec , sec (Spec # 12917)



Peak True - sample "INF-C comp 091919 (111419):1", peak 194, at 563.952 , 1.300 sec , sec (Spec # 12917)



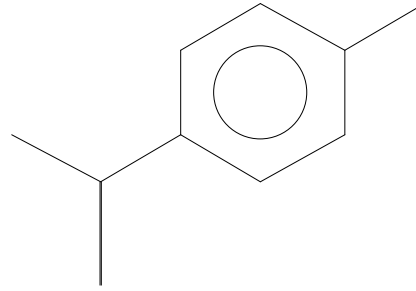
Library Hit - similarity 875, "Furan, 2-pentyl-"



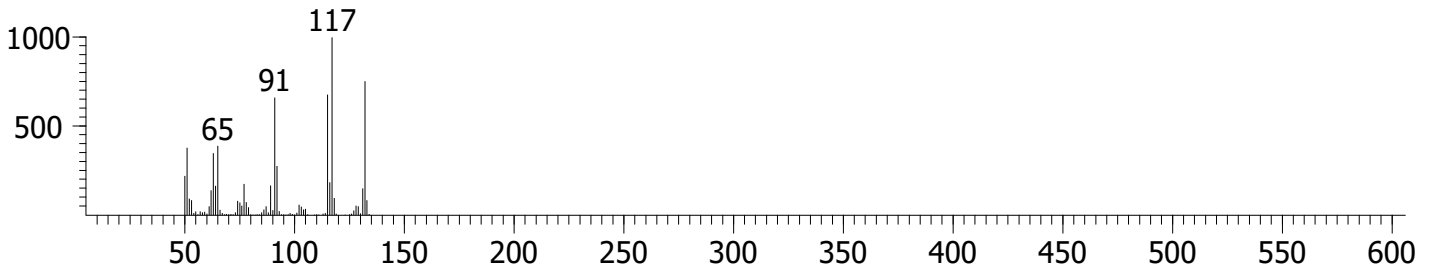
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Furan, 2-pentyl-	875	2640	3777-69-3	mainlib	C9H14O	138
2	E-2-Methyl-5-(fur-3-yl)-pent-2-enal	872	2333	0-00-0	mainlib	C10H12O2	164
3	2-n-Butyl furan	870	2152	4466-24-4	mainlib	C8H12O	124
4	2,4-Nonadienal, (E,E)-	836	551	5910-87-2	mainlib	C9H14O	138
5	2-furfuryl 2-oxo-3-pentyl disulfide	831	444	0-00-0	mainlib	C10H14O2S2	230

Benzene, 1-methyl-4-(1-methylethenyl)-

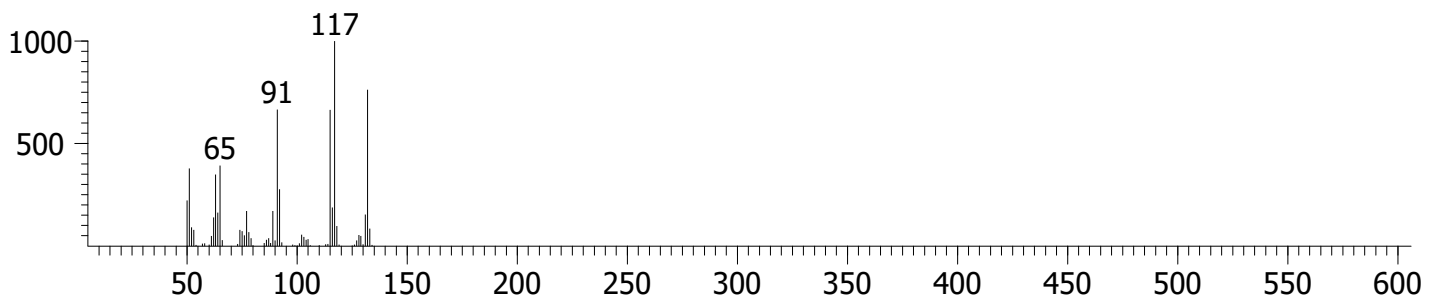
1st Dimension R.T. = 707.37
2nd Dimension R.T. = 1.505
Quant Mass(es) = 132
S/N = 10968
Area = 1267463
Height = 201699
Similarity = 966



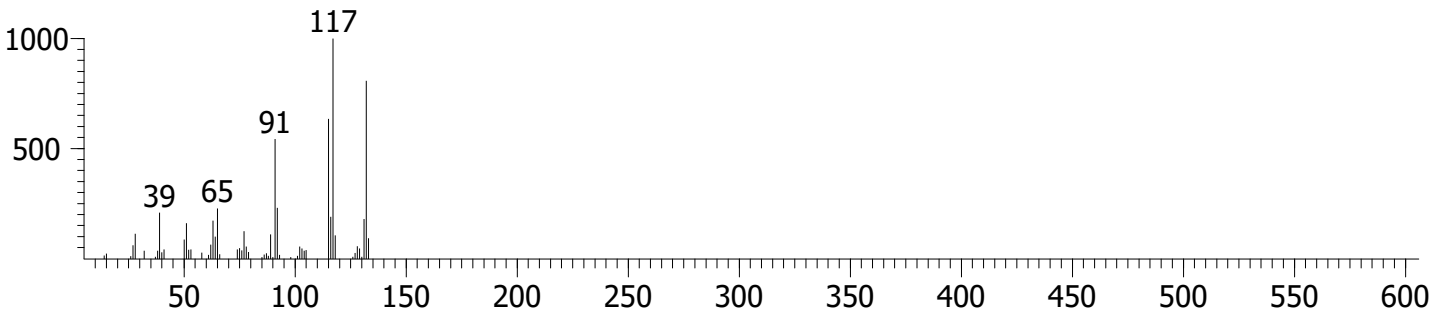
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 569, at 707.37 , 1.505 sec , sec (Spec # 34678)



Peak True - sample "INF-C comp 091919 (111419):1", peak 569, at 707.37 , 1.505 sec , sec (Spec # 34678)



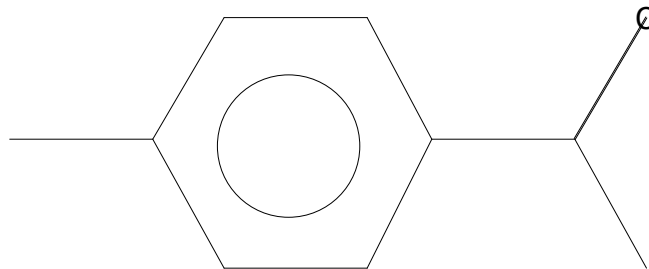
Library Hit - similarity 966, "Benzene, 1-methyl-4-(1-methylethenyl)-"



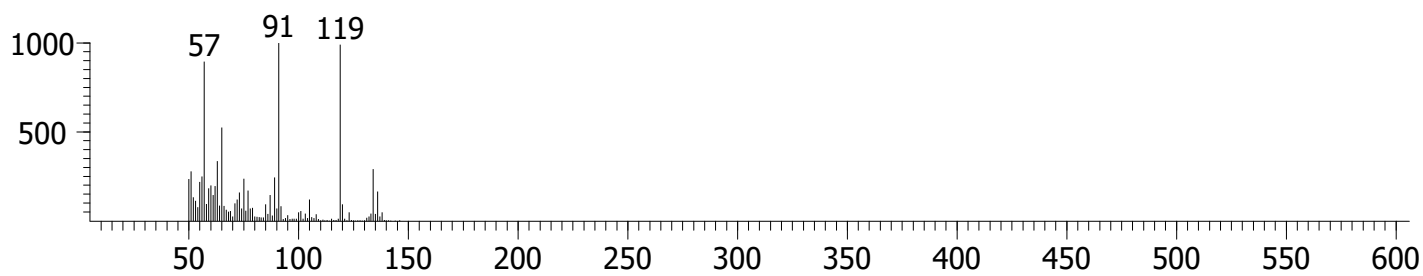
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-methyl-4-(1-methylethenyl)-	966	4285	1195-32-0	mainlib	C10H12	132
2	o-Isopropenyltoluene	956	3025	7399-49-7	mainlib	C10H12	132
3	p-(1-Propenyl)-toluene	924	808	0-00-0	mainlib	C10H12	132
4	Benzene, 1-methyl-3-(1-methylethenyl)-	919	651	1124-20-5	mainlib	C10H12	132
5	Benzene, (2-methyl-1-propenyl)-	886	170	768-49-0	mainlib	C10H12	132

Ethanone, 1-(4-methylphenyl)-

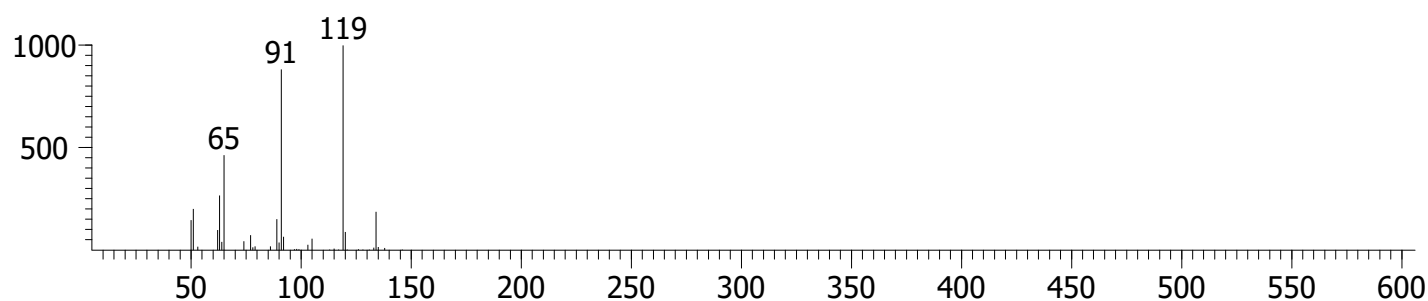
1st Dimension R.T. = 847.29
2nd Dimension R.T. = 1.835
Quant Mass(es) = 119
S/N = 2224.5
Area = 802770
Height = 97042
Similarity = 881



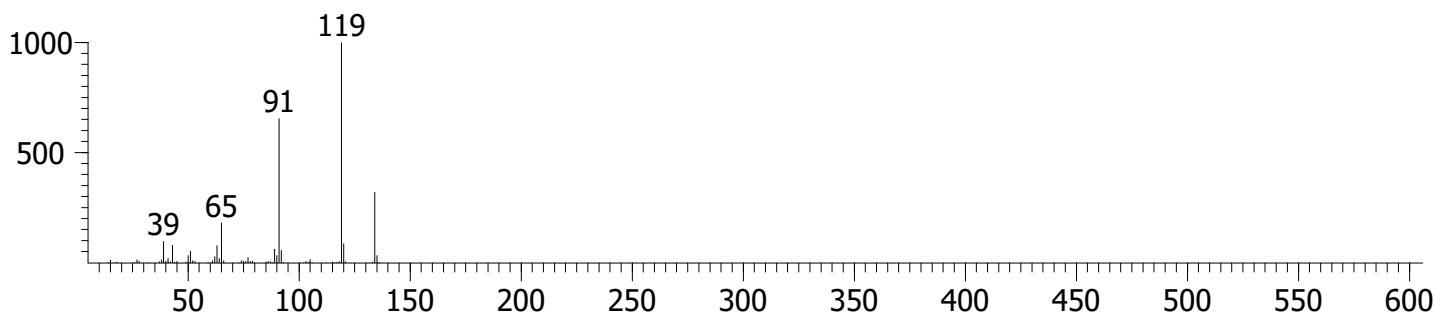
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 1021, at 847.29 , 1.835 sec , sec (Spec # 55928)



Peak True - sample "INF-C comp 091919 (111419):1", peak 1021, at 847.29 , 1.835 sec , sec (Spec # 55928)



Library Hit - similarity 881, "Ethanone, 1-(4-methylphenyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanone, 1-(4-methylphenyl)-	881	1674	122-00-9	mainlib	C ₉ H ₁₀ O	134
2	Ethanone, 1-(3-methylphenyl)-	878	1479	585-74-0	mainlib	C ₉ H ₁₀ O	134
3	Ethanone, 1-(2-methylphenyl)-	861	807	577-16-2	mainlib	C ₉ H ₁₀ O	134
4	2-fluoro-1-(p-tolyl)ethanone	857	682	0-00-0	mainlib	C ₉ H ₉ FO	152
5	2-Methylbenzoyl isothiocyanate	841	392	28115-85-7	mainlib	C ₉ H ₇ NOS	177

Diphenyl ether

1st Dimension R.T. = 1137.62

2nd Dimension R.T. = 1.967

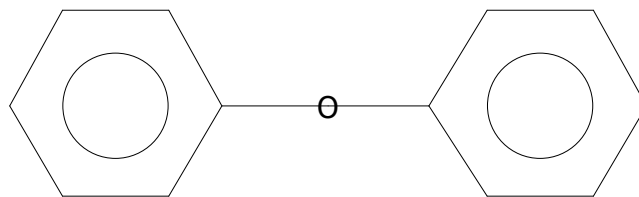
Quant Mass(es) = 170

S/N = 1185.4

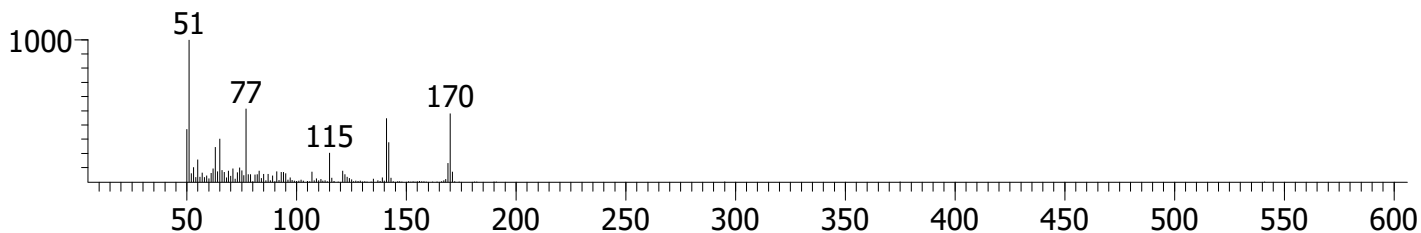
Area = 125146

Height = 14903

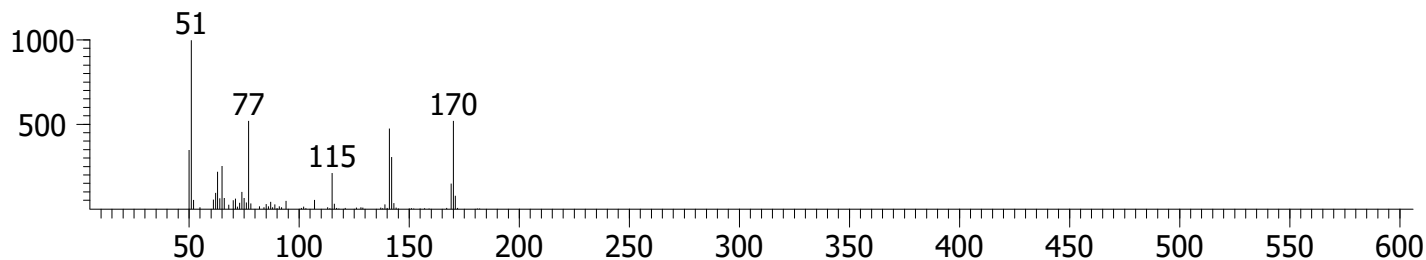
Similarity = 826



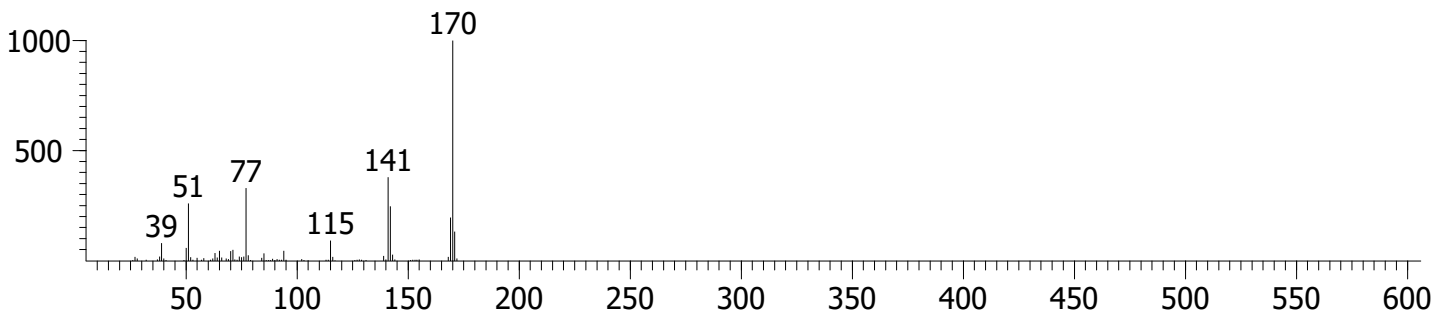
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 2170, at 1137.62 , 1.967 sec , sec (Spec # 99938)



Peak True - sample "INF-C comp 091919 (111419):1", peak 2170, at 1137.62 , 1.967 sec , sec (Spec # 99938)



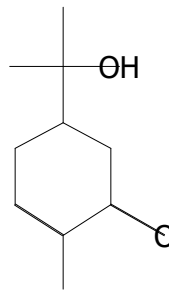
Library Hit - similarity 826, "Diphenyl ether"



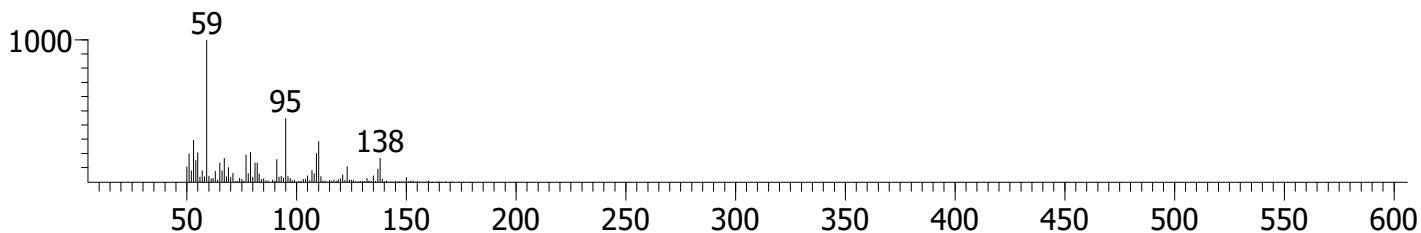
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Diphenyl ether	826	8352	101-84-8	mainlib	C12H10O	170
2	Spiro[cyclopropane-1,1'(4'H)-naphthalen]-4'-one	732	684	33498-24-7	mainlib	C12H10O	170
3	1H,3H-Naphtho[1,8-cd]pyran	702	190	203-84-9	mainlib	C12H10O	170
4	methanone, 1,3-cyclopentadien-1-ylphenyl-	698	160	0-00-0	mainlib	C12H10O	170
5	Diphenyl oxalate	688	113	3155-16-6	mainlib	C14H10O4	242

-Hydroxy-1-methylethyl)-2-methyl-2-cyclohe:

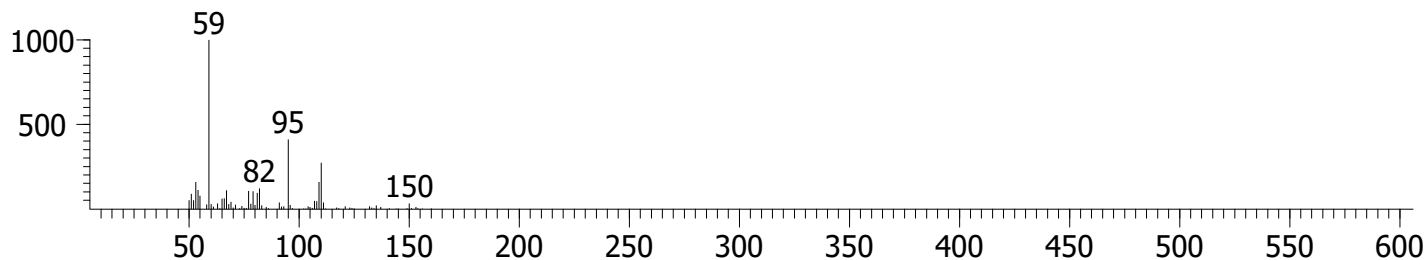
1st Dimension R.T. = 1172.6
2nd Dimension R.T. = 1.987
Quant Mass(es) = 59
S/N = 751.83
Area = 611723
Height = 68847
Similarity = 889



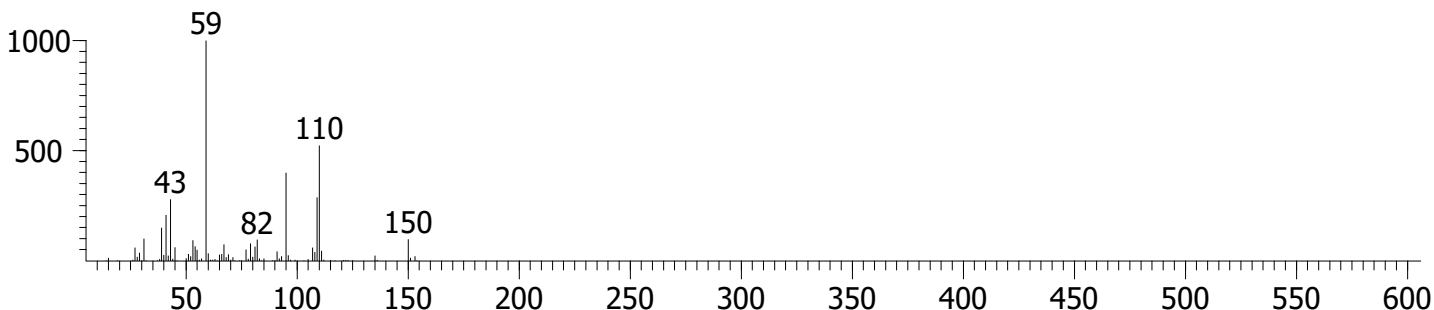
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 2329, at 1172.6 , 1.987 sec , sec (Spec # 105241)



Peak True - sample "INF-C comp 091919 (111419):1", peak 2329, at 1172.6 , 1.987 sec , sec (Spec # 105241)



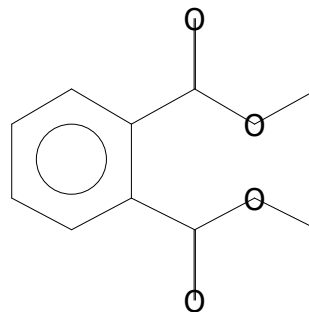
Library Hit - similarity 889, "S-(+)-5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one"



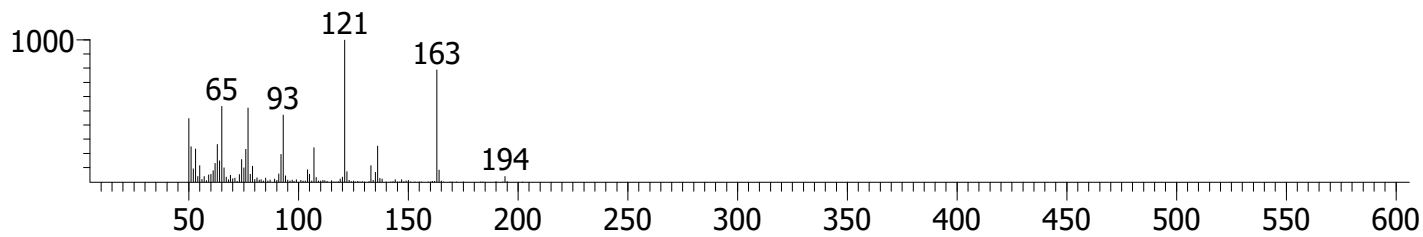
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	S-(+)-5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one	889	7913	60593-11-5	mainlib	C10H16O2	168
2	8-Hydroxycarvotanacetone	846	1745	7712-46-1	mainlib	C10H16O2	168
3	1,2-cis-1,5-trans-2,5-dihydroxy-4-methyl-1-(1-hydroxy-1-isopropyl)cyclohex-3-ene	752	142	87096-70-6	mainlib	C10H18O3	186
4	3-(2-Hydroxy-2-methyl-propyl)-cyclohex-2-enone	732	65	0-00-0	mainlib	C10H16O2	168
5	7-Oxabicyclo[4.1.0]heptane, 2-methylene-	714	33	98126-49-9	mainlib	C7H10O	110

Dimethyl phthalate

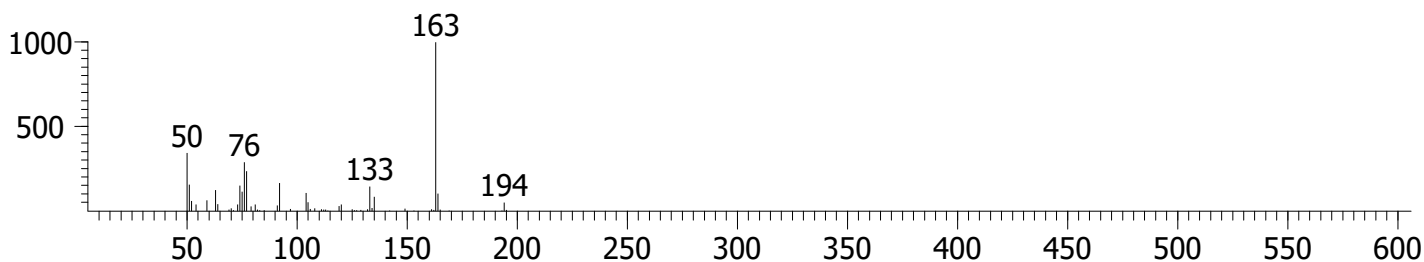
1st Dimension R.T. = 1200.59
2nd Dimension R.T. = 2.198
Quant Mass(es) = 163
S/N = 1672.0
Area = 318048
Height = 29040
Similarity = 884



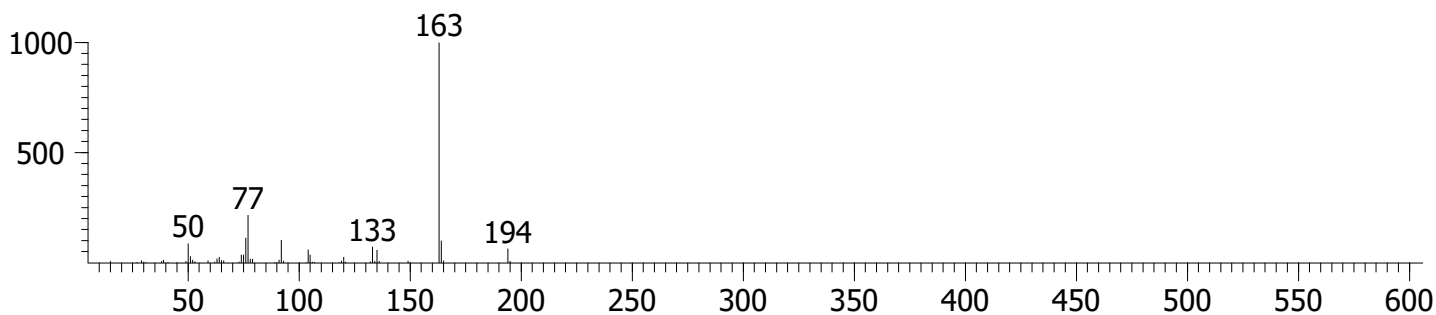
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 2450, at 1200.59 , 2.198 sec , sec (Spec # 109513)



Peak True - sample "INF-C comp 091919 (111419):1", peak 2450, at 1200.59 , 2.198 sec , sec (Spec # 109513)



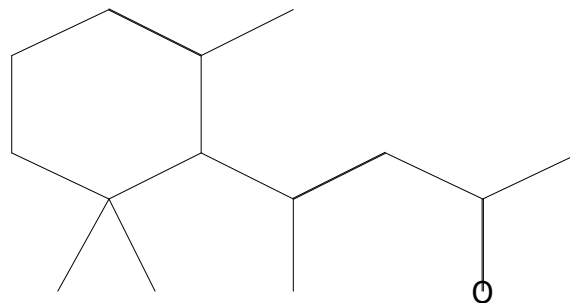
Library Hit - similarity 884, "Dimethyl phthalate"



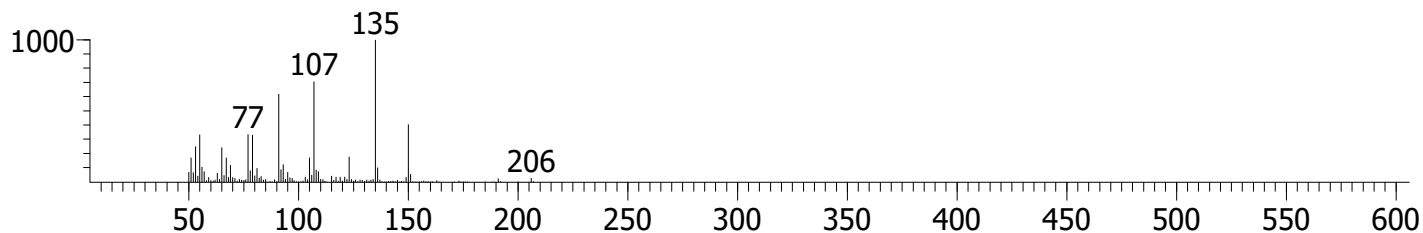
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Dimethyl phthalate	884	4981	131-11-3	mainlib	C10H10O4	194
2	Benzoic acid, 2-(1-oxopropyl)-, methyl ester	820	818	32025-37-9	mainlib	C11H12O3	192
3	Phthalic acid, 3,5-difluorophenyl methyl ester	808	545	0-00-0	mainlib	C15H10F2O4	292
4	Phthalic acid, 3-chlorophenyl methyl ester	807	523	0-00-0	mainlib	C15H11ClO4	290
5	Phthalic acid, 2-bromo-4-fluorophenyl methyl ester	804	462	0-00-0	mainlib	C15H10BrFO4	352

3-Penten-2-one,
4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-

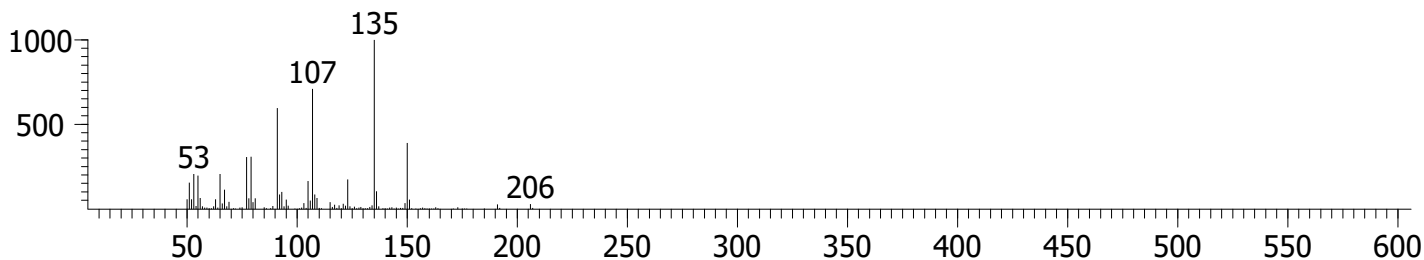
1st Dimension R.T. = 1232.07
 2nd Dimension R.T. = 1.584
 Quant Mass(es) = 135
 S/N = 4501.9
 Area = 1196299
 Height = 139026
 Similarity = 865



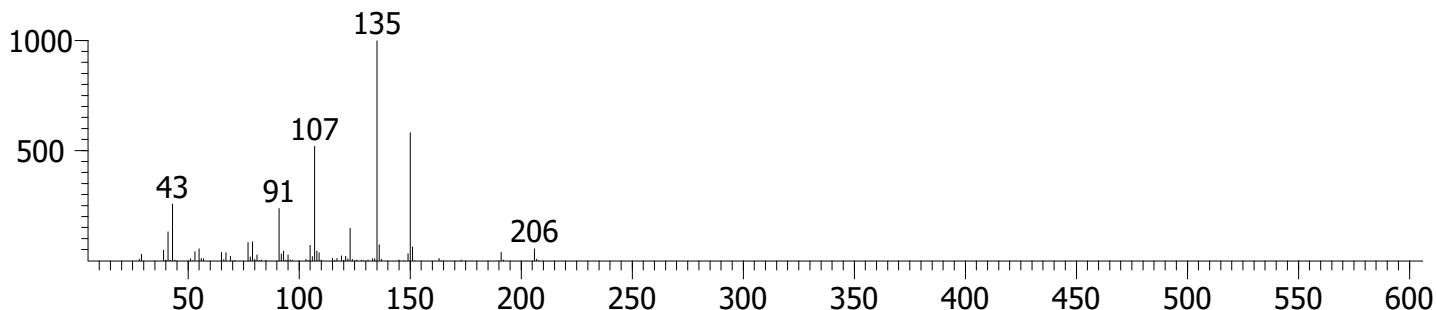
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 2592, at 1232.07 , 1.584 sec , sec (Spec # 114190)



Peak True - sample "INF-C comp 091919 (111419):1", peak 2592, at 1232.07 , 1.584 sec , sec (Spec # 114190)



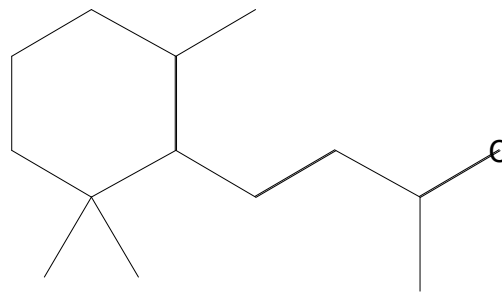
Library Hit - similarity 865, "3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-"



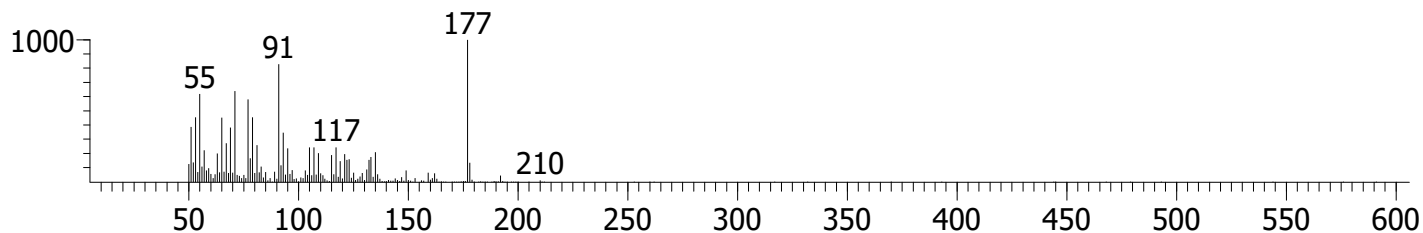
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	865	2926	114933-28-7	mainlib	C14H22O	206
2	Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-	862	2586	24555-40-6	mainlib	C10H14O	150
3	à Isomethyl ionone	843	1255	127-51-5	mainlib	C14H22O	206
4	Phenol, 2-ethyl-4,5-dimethyl-	816	369	2219-78-5	mainlib	C10H14O	150
5	3,5-Heptadienal, 2-ethylidene-6-methyl-	812	312	99172-18-6	mainlib	C10H14O	150

3-Buten-2-one,
4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

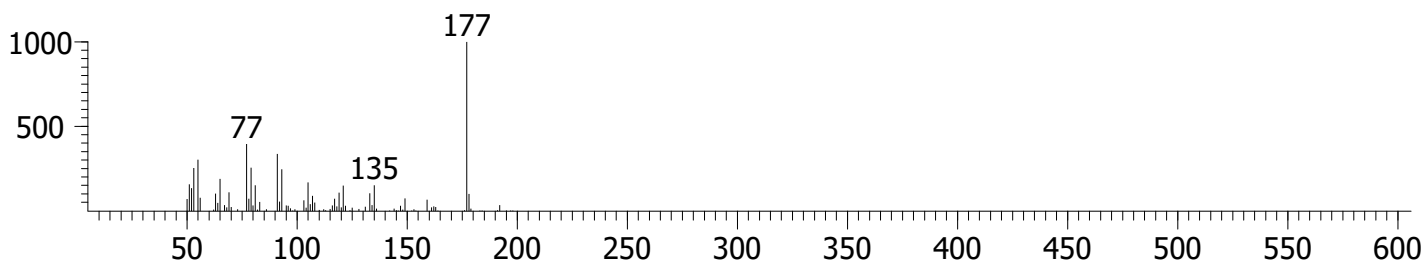
1st Dimension R.T. = 1239.07
 2nd Dimension R.T. = 1.670
 Quant Mass(es) = 177
 S/N = 1806.3
 Area = 238522
 Height = 27388
 Similarity = 846



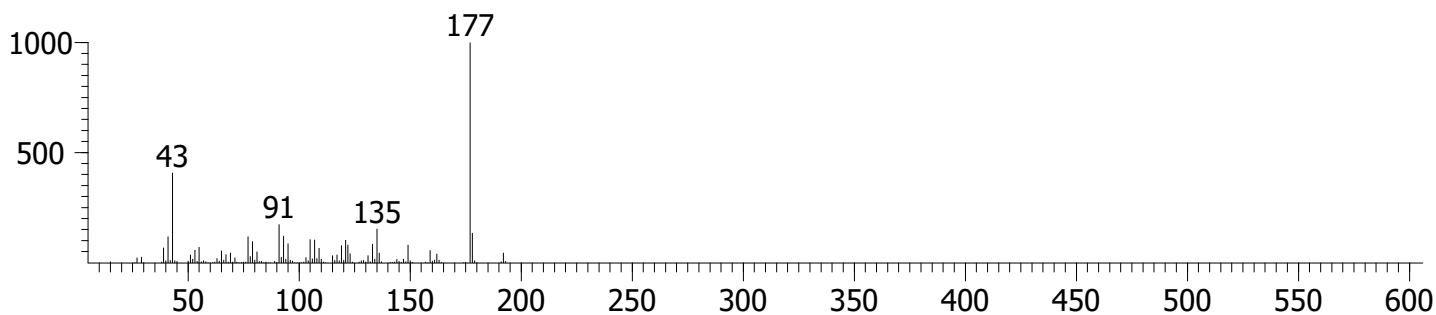
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 2641, at 1239.07 , 1.670 sec , sec (Spec # 1152 63)



Peak True - sample "INF-C comp 091919 (111419):1", peak 2641, at 1239.07 , 1.670 sec , sec (Spec # 11526 3)



Library Hit - similarity 846, "3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	846	3251	14901-07-6	mainlib	C13H20O	192
2	trans-á-Ionone	845	3125	79-77-6	mainlib	C13H20O	192
3	2H-1-Benzopyran, 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-, trans-	834	2143	41678-29-9	mainlib	C13H20O	192
4	á-Oplopenone	766	325	28305-60-4	mainlib	C15H24O	220
5	Edulan II	764	299	41678-30-2	mainlib	C13H20O	192

6,7-Dodecanedione

1st Dimension R.T. = 1305.53

2nd Dimension R.T. = 2.455

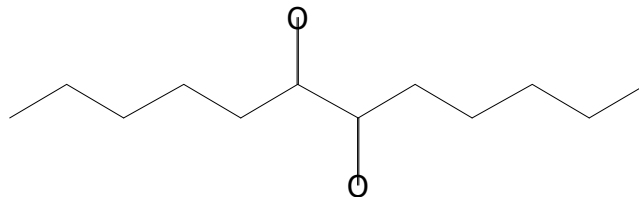
Quant Mass(es) = 99

S/N = 181.74

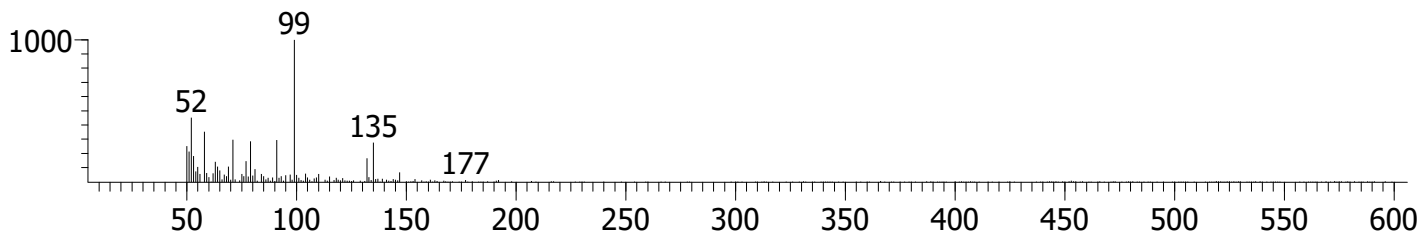
Area = 89275

Height = 8040.5

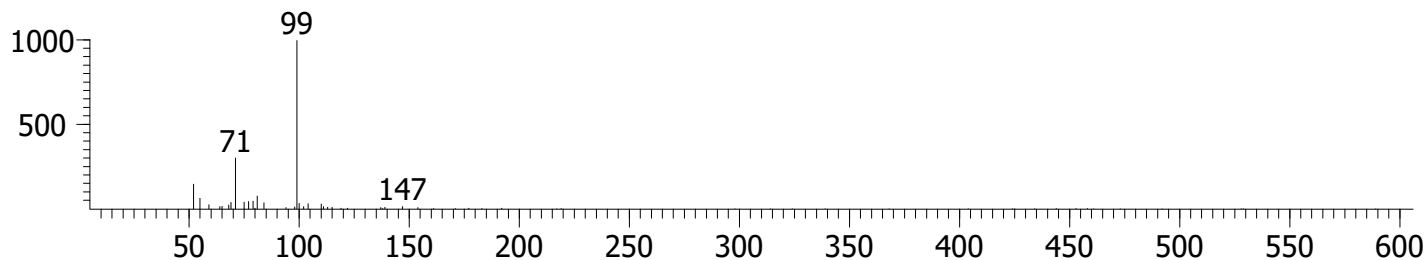
Similarity = 831



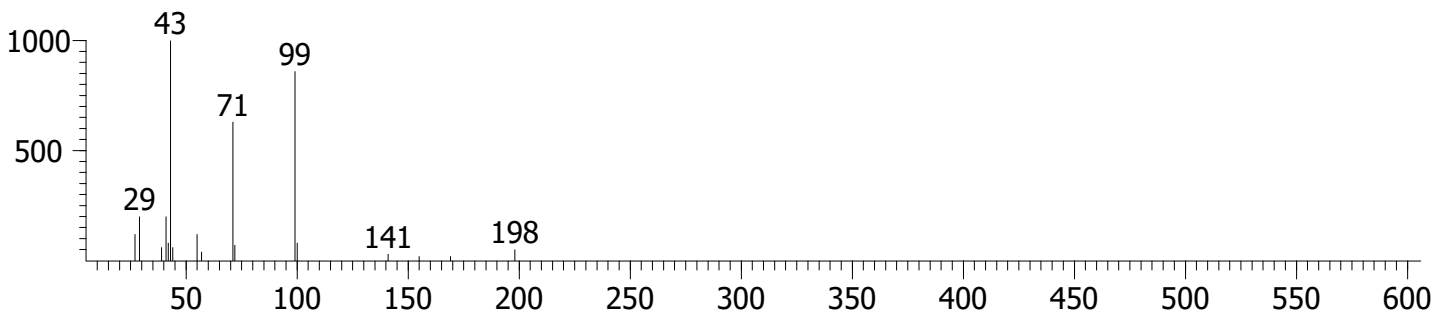
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 3007, at 1305.53 , 2.455 sec , sec (Spec # 1254 52)



Peak True - sample "INF-C comp 091919 (111419):1", peak 3007, at 1305.53 , 2.455 sec , sec (Spec # 12545 2)



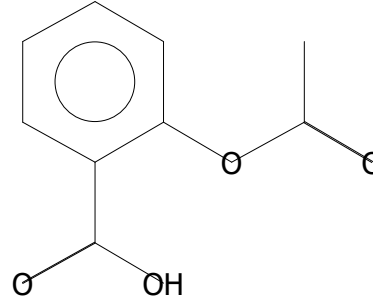
Library Hit - similarity 831, "6,7-Dodecanedione"



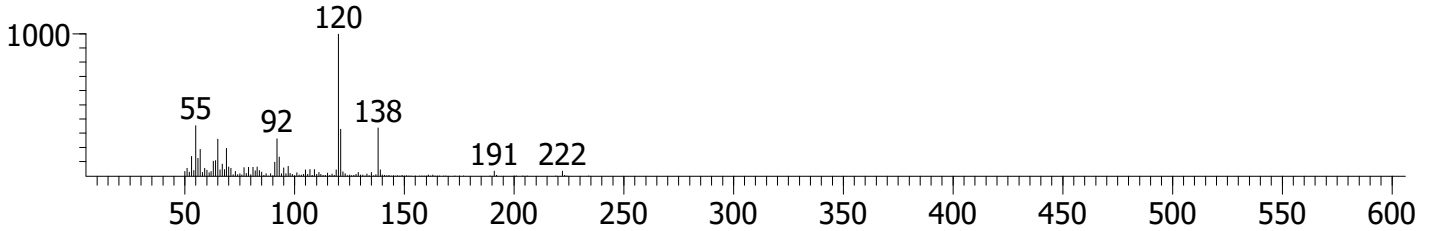
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	6,7-Dodecanedione	831	3946	13757-90-9	mainlib	C12H22O2	198
2	4-Methyl-6-hepten-4-olide	817	2470	0-00-0	mainlib	C8H12O2	140
3	4H-Imidazol-4-one, 2-amino-1,5-dihydro-	796	1050	503-86-6	mainlib	C3H5N3O	99
4	n-Hexyl methylphosphonofluoridate	791	847	113548-89-3	mainlib	C7H16FO2P	182
5	Furan, 2,5-dihydro-2,5-dimethoxy-	788	748	332-77-4	mainlib	C6H10O3	130

Aspirin

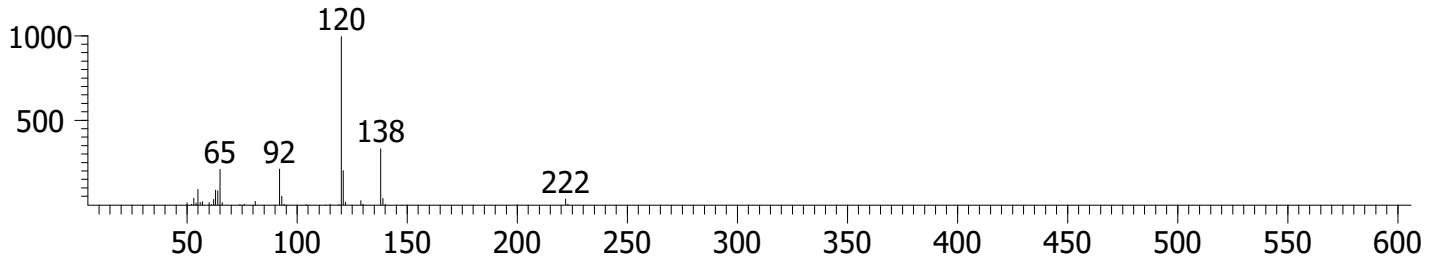
1st Dimension R.T. = 1459.44
2nd Dimension R.T. = 1.670
Quant Mass(es) = 120
S/N = 5360.9
Area = 986298
Height = 105043
Similarity = 868



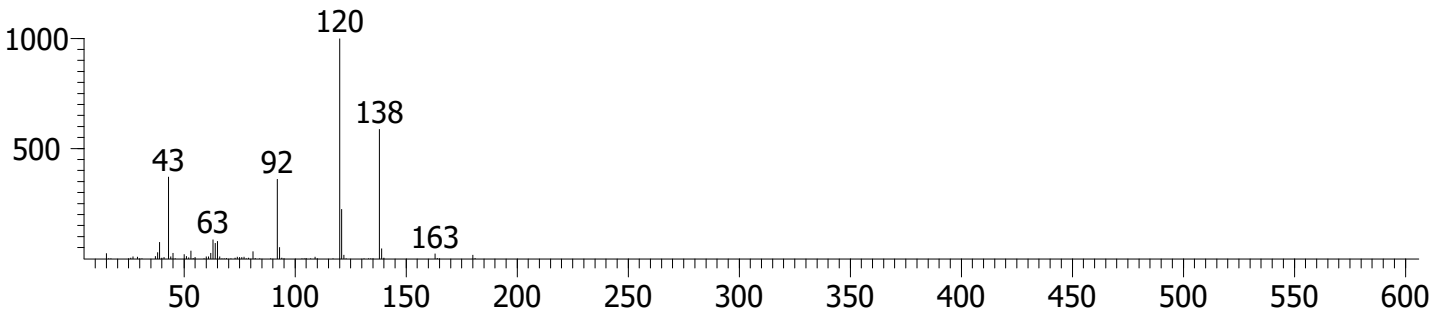
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 3894, at 1459.44 , 1.670 sec , sec (Spec # 148653)



Peak True - sample "INF-C comp 091919 (111419):1", peak 3894, at 1459.44 , 1.670 sec , sec (Spec # 148653)



Library Hit - similarity 868, "Aspirin"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Aspirin	868	1267	50-78-2	mainlib	C9H8O4	180
2	Salicylic acid, 1-methylpropyl ester	868	1267	0-00-0	mainlib	C11H14O3	194
3	Salicylic acid, tert-butyl ester	865	1120	0-00-0	mainlib	C11H14O3	194
4	Benzoic acid, 2-hydroxy-, 2-methylbutyl ester	862	989	51115-63-0	mainlib	C12H16O3	208
5	n-Hexyl salicylate	860	912	6259-76-3	mainlib	C13H18O3	222

2-Octyl benzoate

1st Dimension R.T. = 1490.92

2nd Dimension R.T. = 1.650

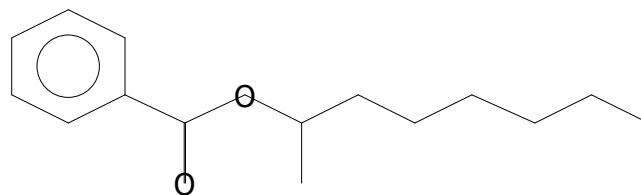
Quant Mass(es) = 105

S/N = 1271.2

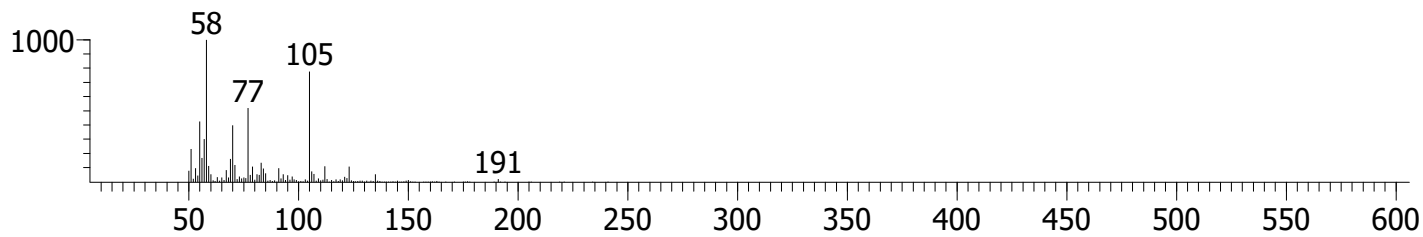
Area = 560290

Height = 54071

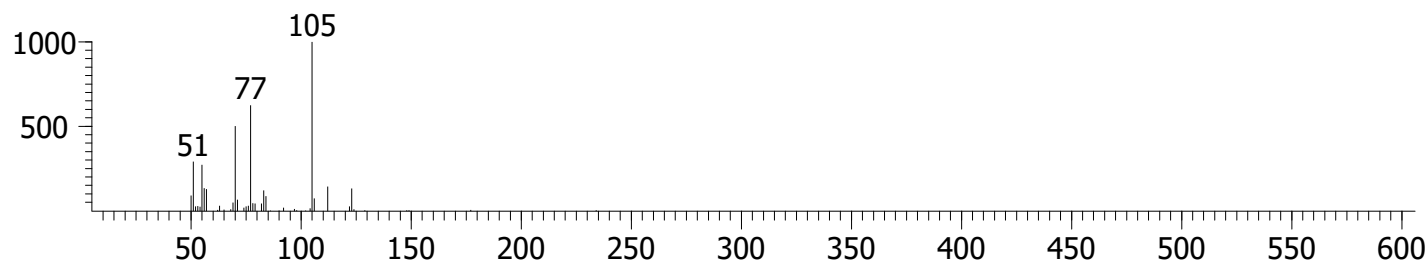
Similarity = 870



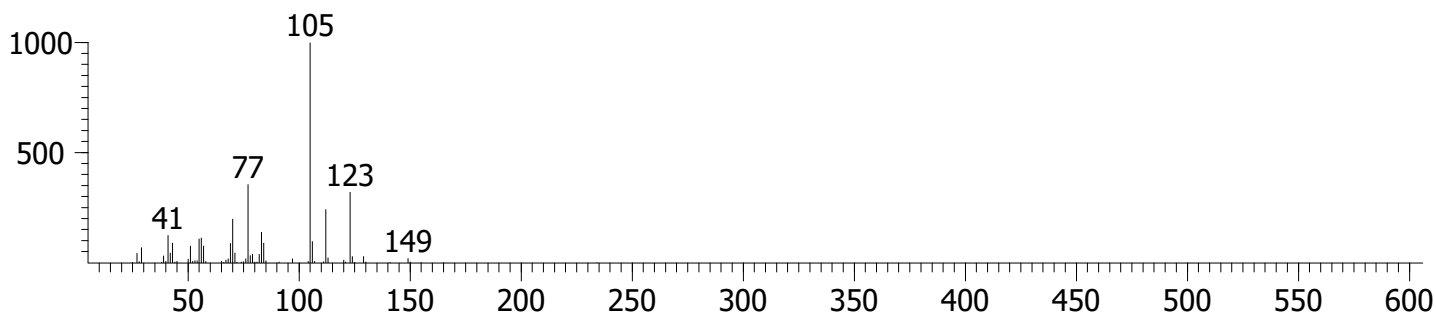
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 4082, at 1490.92 , 1.650 sec , sec (Spec # 153420)



Peak True - sample "INF-C comp 091919 (111419):1", peak 4082, at 1490.92 , 1.650 sec , sec (Spec # 153420)



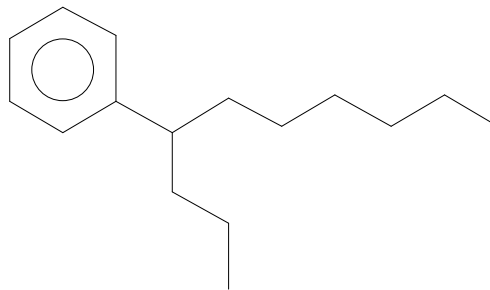
Library Hit - similarity 870, "2-Octyl benzoate"



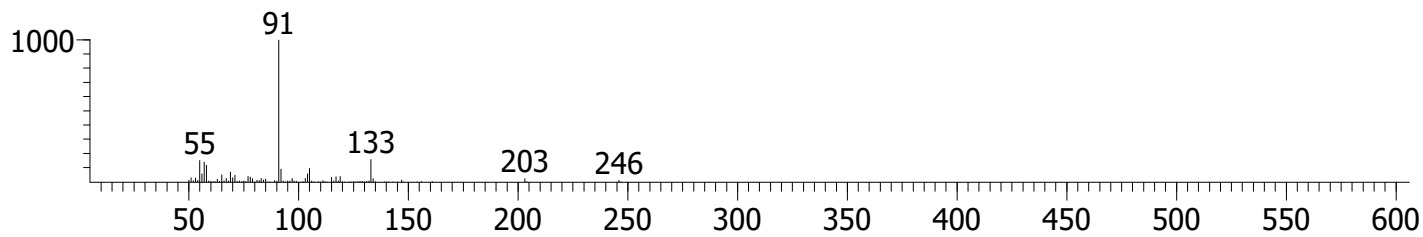
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Octyl benzoate	870	4364	6938-51-8	mainlib	C ₁₅ H ₂₂ O ₂	234
2	Benzoic acid, 2-ethylhexyl ester	868	4026	5444-75-7	mainlib	C ₁₅ H ₂₂ O ₂	234
3	Benzoic acid, 2-methylbutyl ester	794	535	0-00-0	mainlib	C ₁₂ H ₁₆ O ₂	192
4	Benzoic acid, 3-methylbutyl-2 ester	770	179	41757-90-8	mainlib	C ₁₂ H ₁₆ O ₂	192
5	3-tert-Butyl-5-chloro-2-hydroxybenzophenone	763	137	52196-47-1	mainlib	C ₁₇ H ₁₇ ClO ₂	288

Benzene, (1-propylheptyl)-

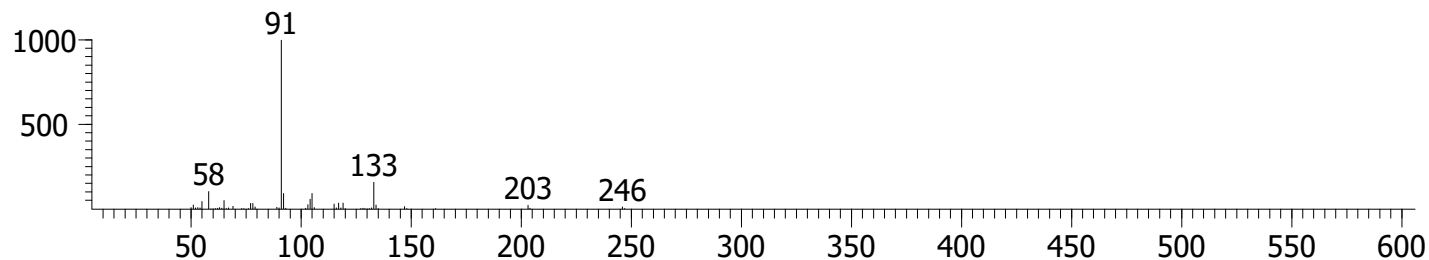
1st Dimension R.T. = 1522.4
2nd Dimension R.T. = 1.432
Quant Mass(es) = 91
S/N = 3399.7
Area = 1920247
Height = 263973
Similarity = 881



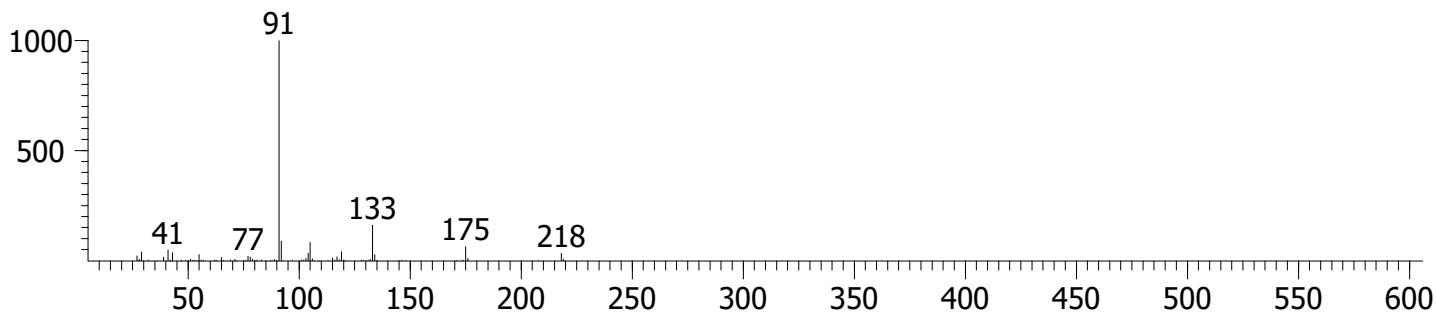
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 4277, at 1522.4 , 1.432 sec , sec (Spec # 158157)



Peak True - sample "INF-C comp 091919 (111419):1", peak 4277, at 1522.4 , 1.432 sec , sec (Spec # 158157)



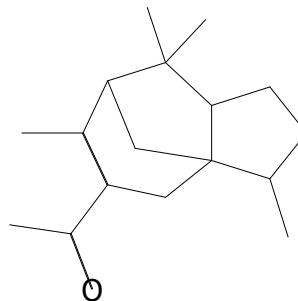
Library Hit - similarity 881, "Benzene, (1-propylheptyl)-"



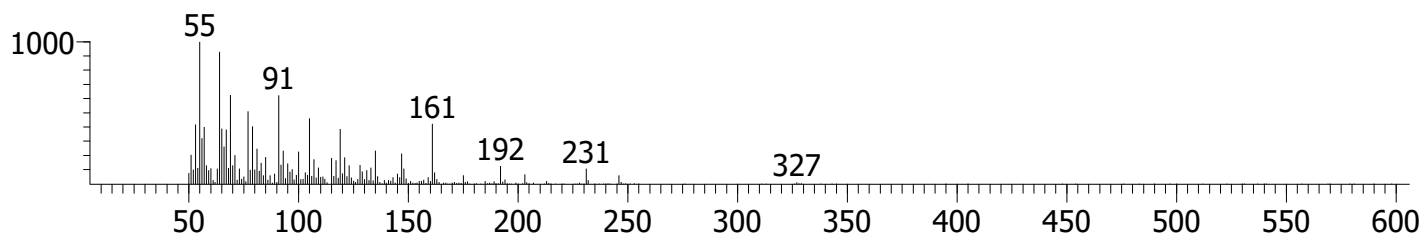
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, (1-propylheptyl)-	881	5072	4537-12-6	mainlib	C16H26	218
2	Benzene, (1-propyldecyl)-	860	2157	4534-51-4	mainlib	C19H32	260
3	Benzene, (1-propyloctyl)-	803	404	4536-86-1	mainlib	C17H28	232
4	S,S'-Methylenebis[benzylsulfone]	802	388	6331-52-8	mainlib	C15H16O4S2	324
5	Methoxyacetic acid, benzyl ester	799	343	32786-24-6	mainlib	C10H12O3	180

Ethanone,
hexahydro-3,6,8,8-tetramethyl-1H-3a,7-meth

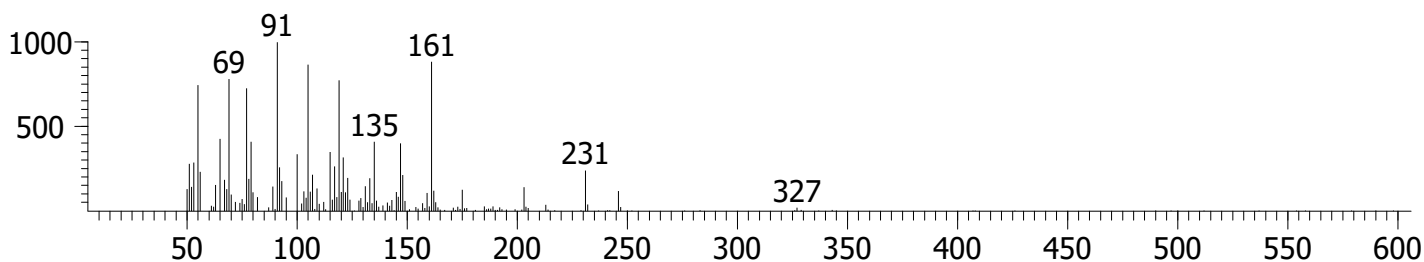
1st Dimension R.T. = 1571.38
2nd Dimension R.T. = 1.742
Quant Mass(es) = 161
S/N = 445.21
Area = 85755
Height = 9451.6
Similarity = 829



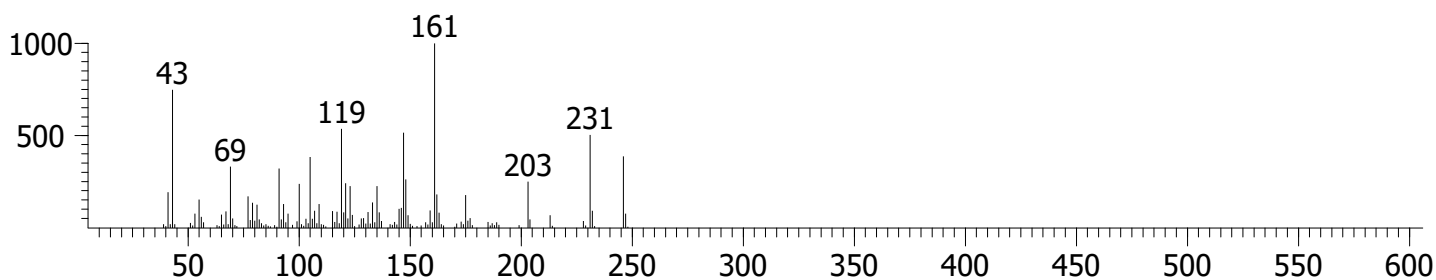
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 4558, at 1571.38 , 1.742 sec , sec (Spec # 165624)



Peak True - sample "INF-C comp 091919 (111419):1", peak 4558, at 1571.38 , 1.742 sec , sec (Spec # 165624)



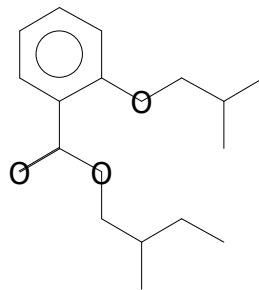
Library Hit - similarity 829, "Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-"



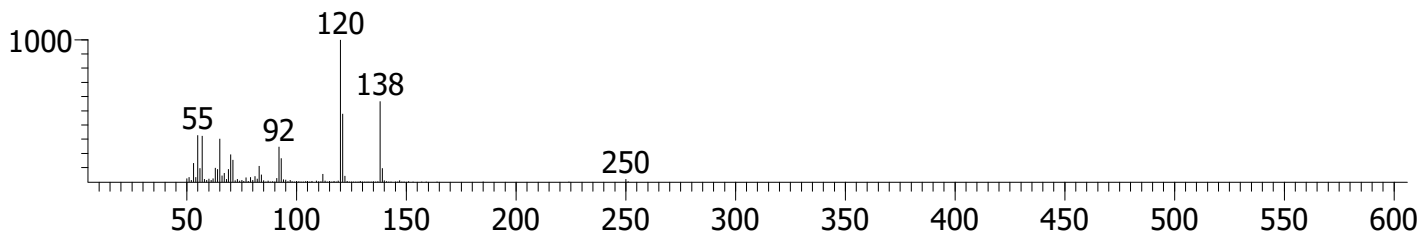
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-	829	4253	68039-35-0	mainlib	C17H26O	246
2	Tetracyclo[6.1.0.0(2,4).0(5,7)]nonane, 3,3,6,6,9,9-hexamethyl-, cis,cis,trans--	733	338	0-00-0	mainlib	C15H24	204
3	Megastigma-4,6(E),8(Z)-triene	729	286	71186-24-8	mainlib	C13H20	176
4	Megastigma-4,6(Z),8(Z)-triene	725	241	71186-25-9	mainlib	C13H20	176
5	Bicyclo[4.1.0]-3-heptene, 2-isopropenyl-5-isopropyl-7,7-dimethyl-	723	223	0-00-0	mainlib	C15H24	204

Salicylic acid, 2-methylbutyl ether,
2-methylbutyl ester

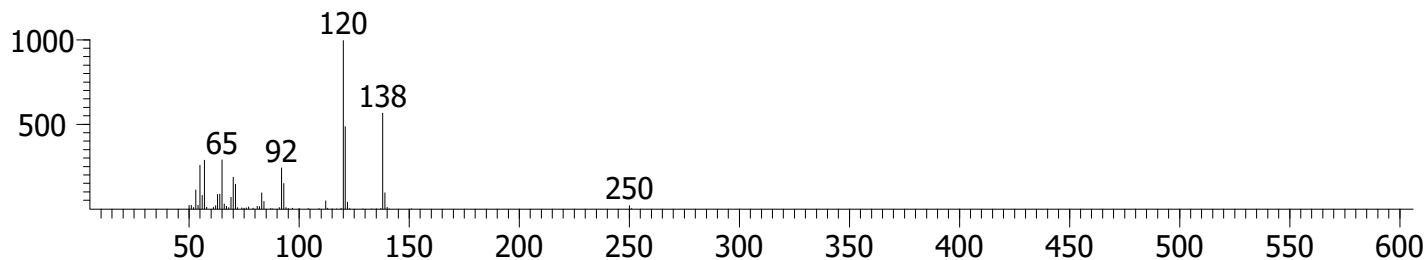
1st Dimension R.T. = 1592.36
2nd Dimension R.T. = 1.617
Quant Mass(es) = 120
S/N = 8713.7
Area = 2739024
Height = 339170
Similarity = 823



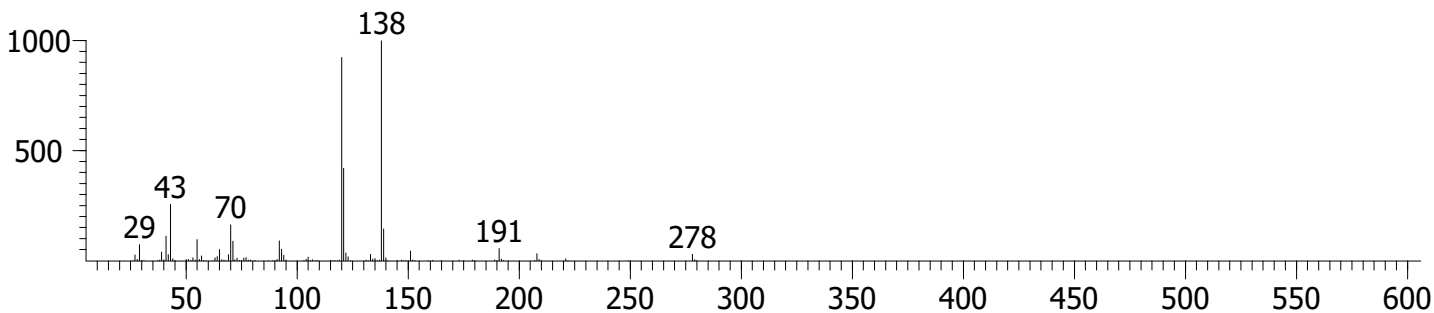
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 4672, at 1592.36 , 1.617 sec , sec (Spec # 168785)



Peak True - sample "INF-C comp 091919 (111419):1", peak 4672, at 1592.36 , 1.617 sec , sec (Spec # 168785)



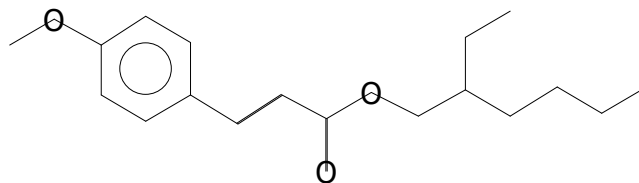
Library Hit - similarity 823, "Salicylic acid, 2-methylbutyl ether, 2-methylbutyl ester"



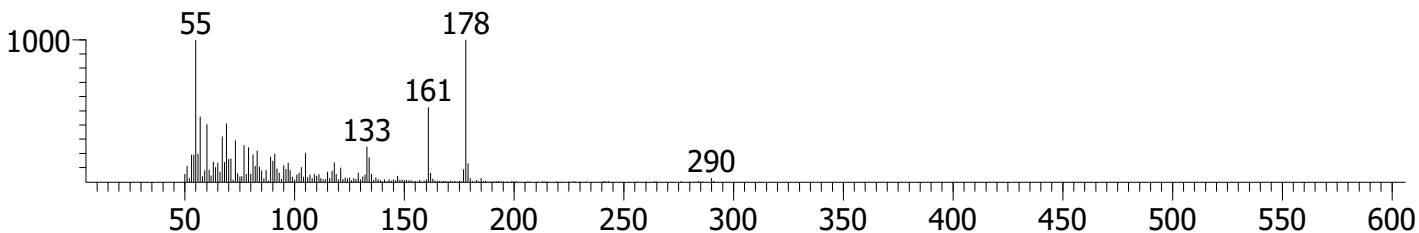
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Salicylic acid, 2-methylbutyl ether, 2-methylbutyl ester	823	1965	0-00-0	mainlib	C17H26O3	278
2	Benzoic acid, 2-hydroxy-, 2-methylbutyl ester	820	1736	51115-63-0	mainlib	C12H16O3	208
3	Salicylic acid, tert.-butyl ester	811	1260	0-00-0	mainlib	C11H14O3	194
4	Benzoic acid, 2-hydroxy-, heptyl ester	811	1260	6259-77-4	mainlib	C14H20O3	236
5	Salicylic acid, 1-methylpropyl ether, 1-methylpropyl ester	797	789	0-00-0	mainlib	C15H22O3	250

2-Propenoic acid, 3-(4-methoxyphenyl)-,
2-ethylhexyl ester

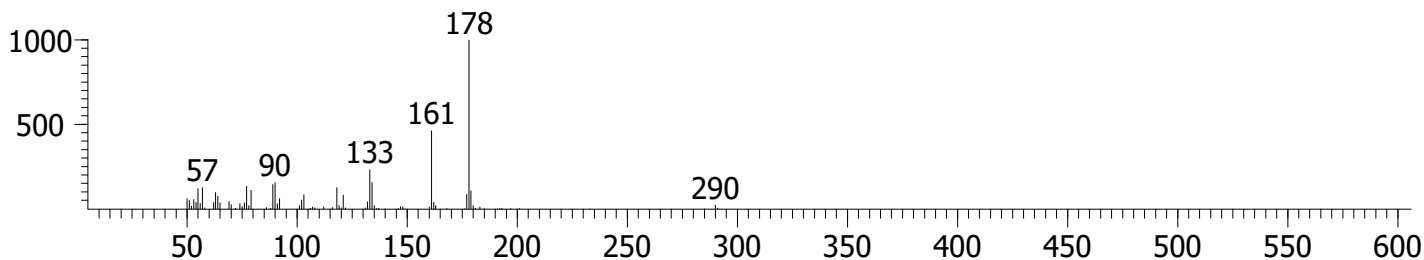
1st Dimension R.T. = 1931.67
 2nd Dimension R.T. = 1.934
 Quant Mass(es) = 178
 S/N = 4643.8
 Area = 763329
 Height = 62066
 Similarity = 878



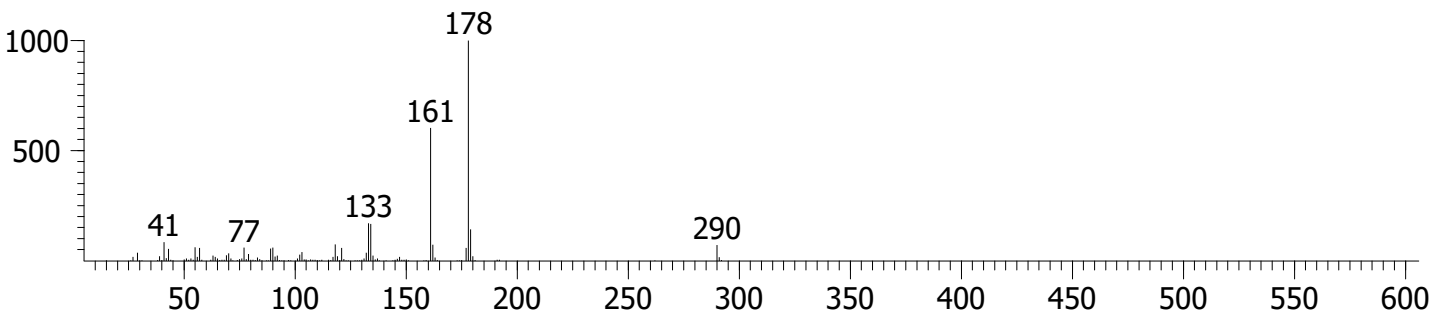
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 6236, at 1931.67 , 1.934 sec , sec (Spec # 2202 43)



Peak True - sample "INF-C comp 091919 (111419):1", peak 6236, at 1931.67 , 1.934 sec , sec (Spec # 22024 3)



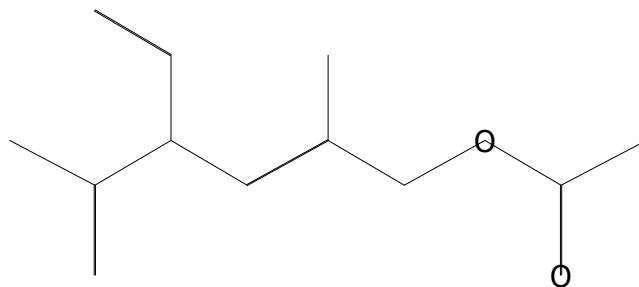
Library Hit - similarity 878, "2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester"



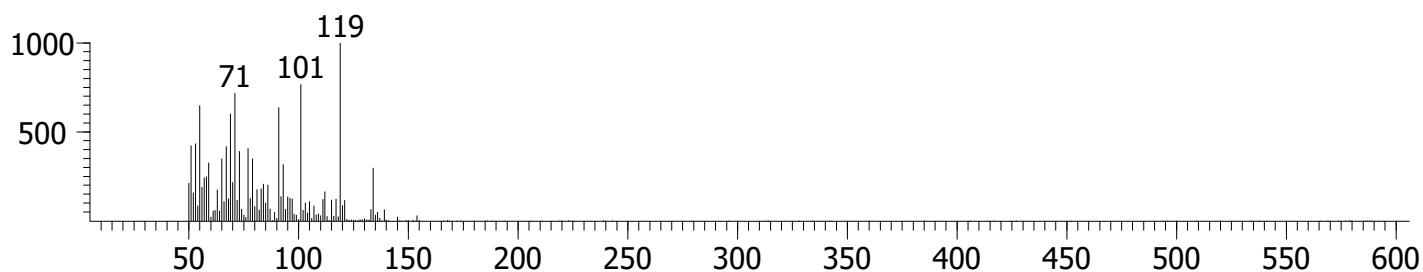
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	878	6918	5466-77-3	mainlib	C18H26O3	290
2	2-Propenoic acid, 3-(4-methoxyphenyl)-, (E)-	810	1049	943-89-5	mainlib	C10H10O3	178
3	2-Ethylhexyl trans-4-methoxycinnamate	798	699	83834-59-7	mainlib	C18H26O3	290
4	2-Propenoic acid, 3-(4-methoxyphenyl)-	792	549	830-09-1	mainlib	C10H10O3	178
5	Cinoxate	787	442	104-28-9	mainlib	C14H18O4	250

(S,E)-2,5-Dimethyl-4-vinylhexa-2,5-dien-1-yl
acetate

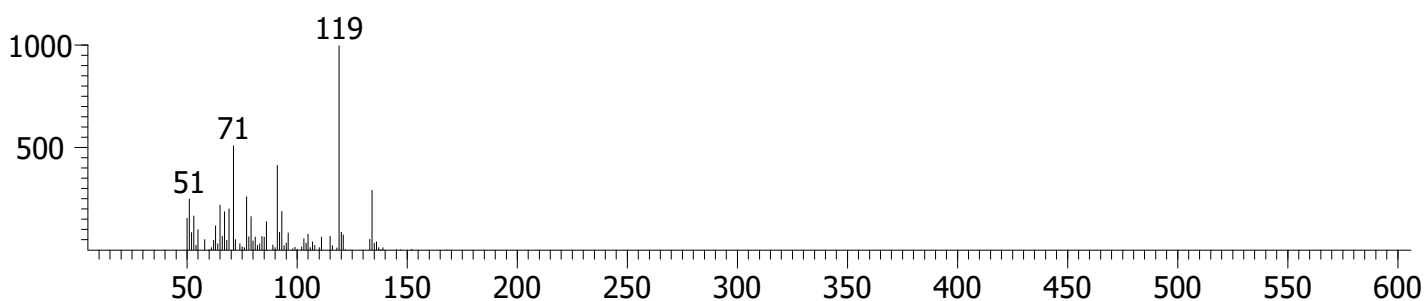
1st Dimension R.T. = 812.31
2nd Dimension R.T. = 1.518
Quant Mass(es) = 119
S/N = 567.54
Area = 145639
Height = 18635
Similarity = 748



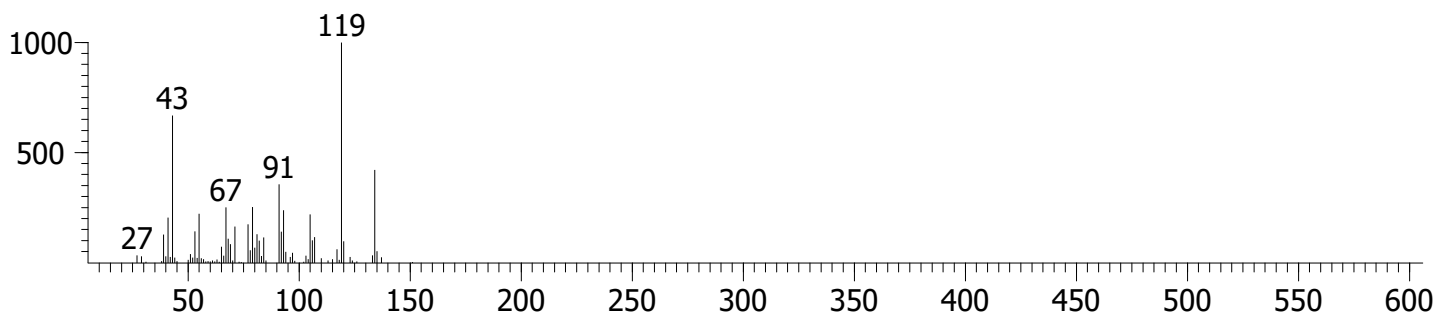
Peak Apex - sample "INF-A comp 092319 (111419):1", peak 738, at 812.31 , 1.518 sec , sec (Spec # 50580)



Peak True - sample "INF-A comp 092319 (111419):1", peak 738, at 812.31 , 1.518 sec , sec (Spec # 50580)



Library Hit - similarity 748, "(S,E)-2,5-Dimethyl-4-vinylhexa-2,5-dien-1-yl acetate"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	(S,E)-2,5-Dimethyl-4-vinylhexa-2,5-dien-1-yl acetate	748	1247	20384-05-8	mainlib	C ₁₂ H ₁₈ O ₂	194
2	(+)-cis-Verbenol, 2-methylpropionate	748	1247	0-00-0	mainlib	C ₁₄ H ₂₂ O ₂	222
3	1,3,8-p-Menthatriene	734	781	18368-95-1	mainlib	C ₁₀ H ₁₄	134
4	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	723	535	460-01-5	mainlib	C ₁₀ H ₁₄	134
5	6,8-Nonadien-2-one, 6-methyl-5-(1-methylethylidene)-	715	399	60714-16-1	mainlib	C ₁₃ H ₂₀ O	192

Tridecanoic acid

1st Dimension R.T. = 1441.95

2nd Dimension R.T. = 1.459

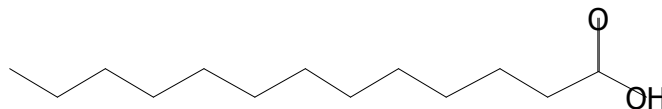
Quant Mass(es) = 60

S/N = 3258.2

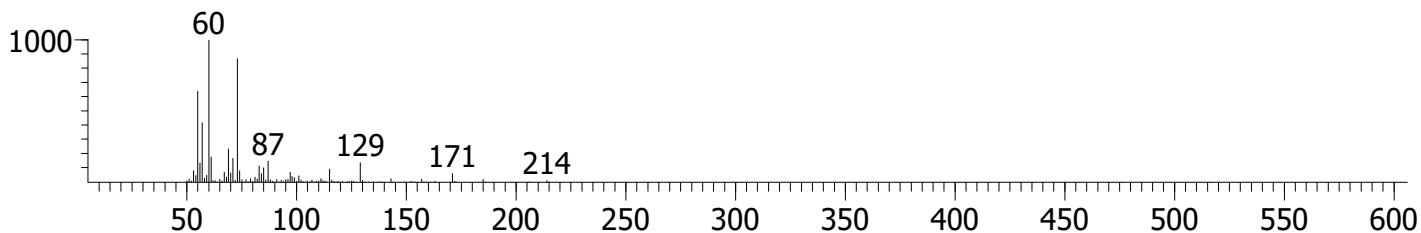
Area = 1589965

Height = 199564

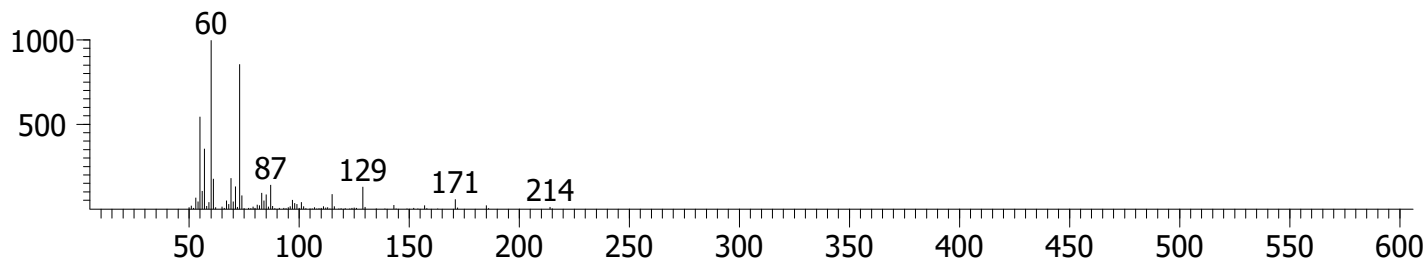
Similarity = 874



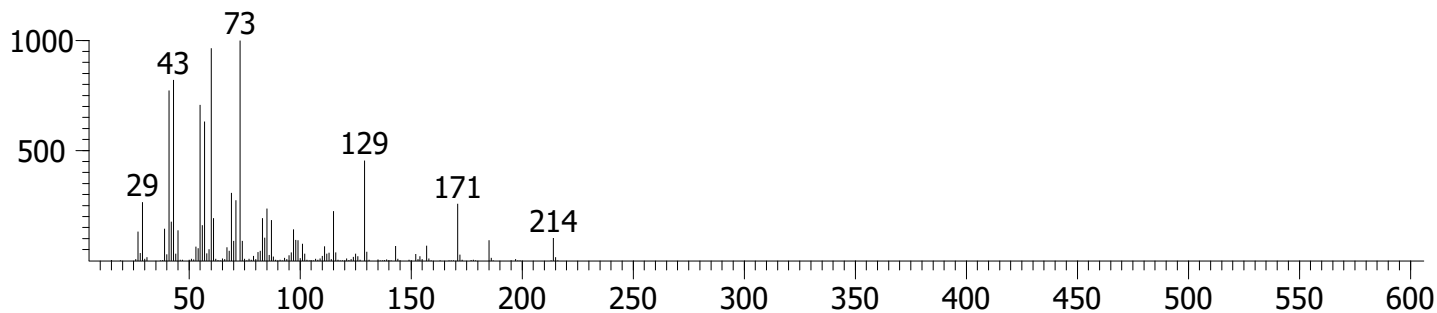
Peak Apex - sample "INF-A comp 092319 (111419):1", peak 3327, at 1441.95 , 1.459 sec , sec (Spec # 145971)



Peak True - sample "INF-A comp 092319 (111419):1", peak 3327, at 1441.95 , 1.459 sec , sec (Spec # 145971)



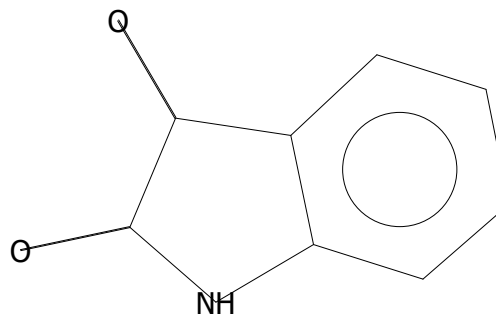
Library Hit - similarity 874, "Tridecanoic acid"



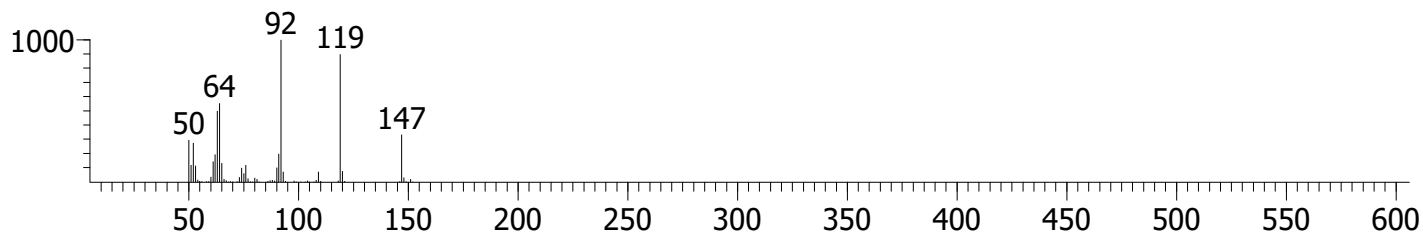
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Tridecanoic acid	874	5380	638-53-9	mainlib	C13H26O2	214
2	n-Hexadecanoic acid	833	1227	57-10-3	mainlib	C16H32O2	256
3	Nonanoic acid	818	744	112-05-0	mainlib	C9H18O2	158
4	Dodecanoic acid	815	657	143-07-7	mainlib	C12H24O2	200
5	Tetradecanoic acid	813	606	544-63-8	mainlib	C14H28O2	228

1H-Indole-2,3-dione

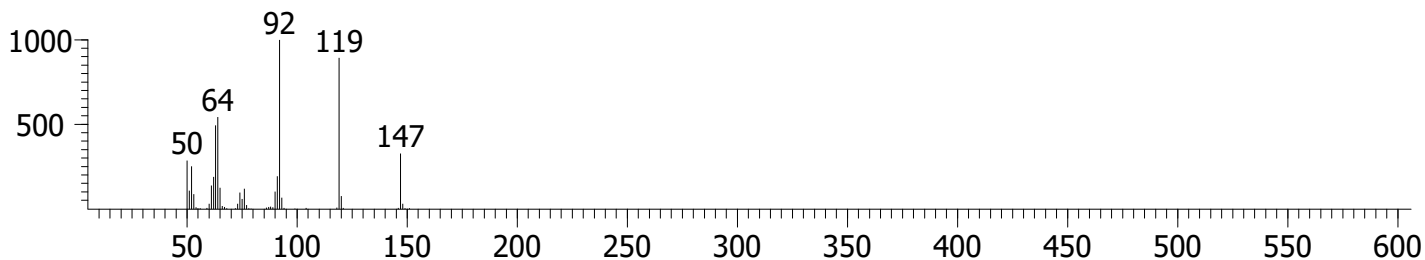
1st Dimension R.T. = 1525.9
2nd Dimension R.T. = 2.812
Quant Mass(es) = 92
S/N = 7820.0
Area = 4923786
Height = 309377
Similarity = 890



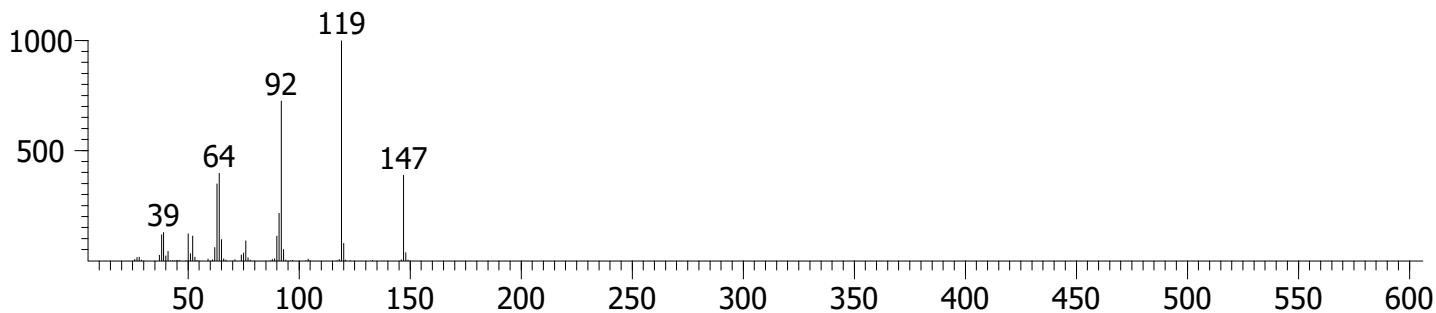
Peak Apex - sample "INF-A comp 092319 (111419):1", peak 3742, at 1525.9 , 2.812 sec , sec (Spec # 158896)



Peak True - sample "INF-A comp 092319 (111419):1", peak 3742, at 1525.9 , 2.812 sec , sec (Spec # 158896)



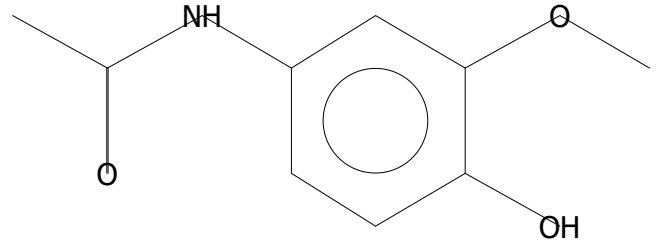
Library Hit - similarity 890, "1H-Indole-2,3-dione"



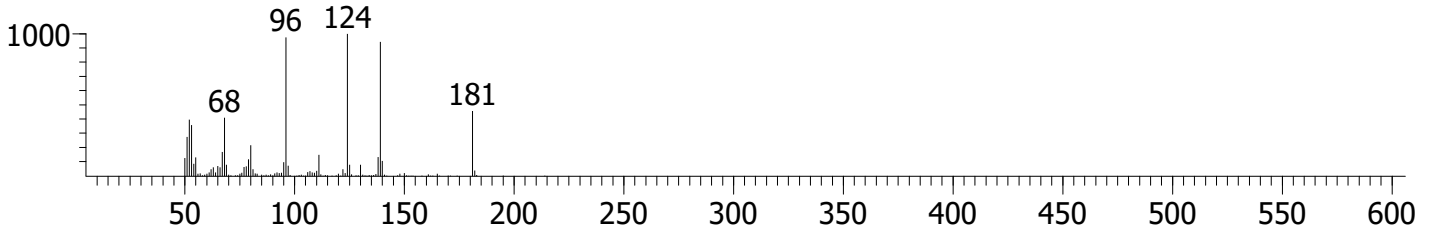
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Indole-2,3-dione	890	7443	91-56-5	mainlib	C8H5NO2	147
2	Indole-2,3-dione, 1-(hydroxymethyl)-	854	1840	50899-59-7	mainlib	C9H7NO3	177
3	Isatoic anhydride	819	461	118-48-9	mainlib	C8H5NO3	163
4	2,1-Benzisoxazole	795	154	271-58-9	mainlib	C7H5NO	119
5	3-Amino-2-cyanopyridine	741	30	42242-11-5	mainlib	C6H5N3	119

3-Methoxyparacetamol

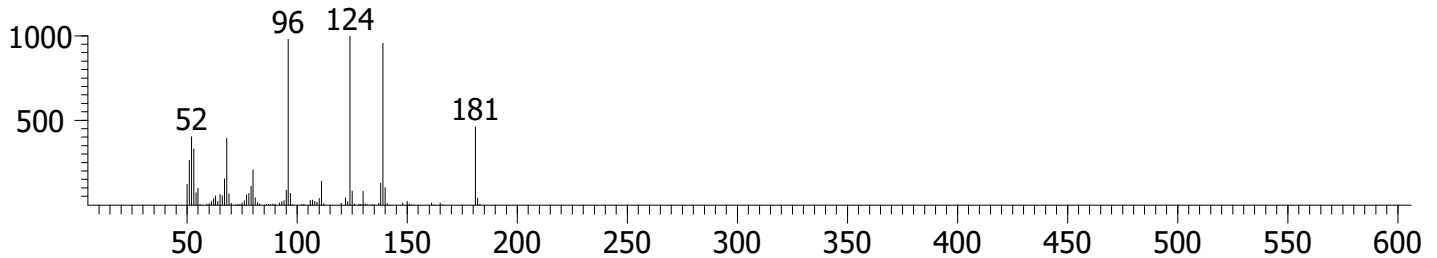
1st Dimension R.T. = 1588.87
2nd Dimension R.T. = 2.515
Quant Mass(es) = 124
S/N = 2960.6
Area = 1068152
Height = 93744
Similarity = 876



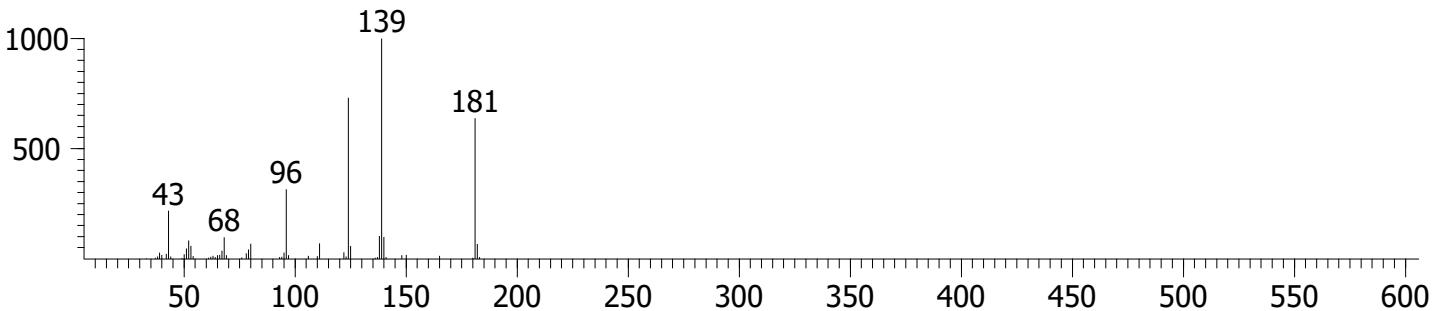
Peak Apex - sample "INF-A comp 092319 (111419):1", peak 4041, at 1588.87 , 2.515 sec , sec (Spec # 1683 91)



Peak True - sample "INF-A comp 092319 (111419):1", peak 4041, at 1588.87 , 2.515 sec , sec (Spec # 16839 1)



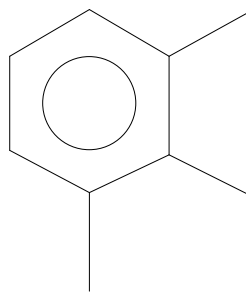
Library Hit - similarity 876, "3-Methoxyparacetamol"



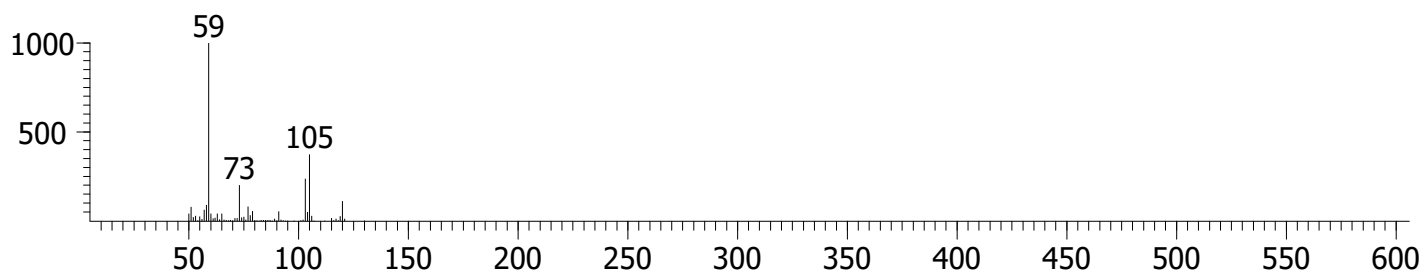
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Methoxyparacetamol	876	8333	3251-55-6	mainlib	C ₉ H ₁₁ NO ₃	181
2	5-Amino-2-methoxyphenol	780	664	1687-53-2	mainlib	C ₇ H ₉ NO ₂	139
3	Phenol, 2-amino-4-methoxy-	766	415	0-00-0	mainlib	C ₇ H ₉ NO ₂	139
4	5-Amino-2-methoxyphenol, N,O-diacetyl-	765	399	0-00-0	mainlib	C ₁₁ H ₁₃ NO ₄	223
5	4-Acetamidophenol	733	106	10352-44-0	mainlib	C ₉ H ₁₁ NOS	181

Benzene, 1,2,3-trimethyl-

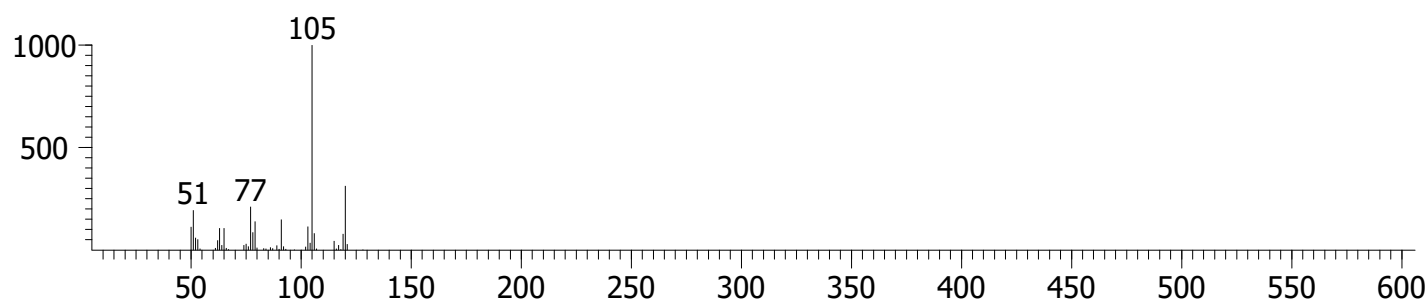
1st Dimension R.T. = 605.928
2nd Dimension R.T. = 1.307
Quant Mass(es) = 105
S/N = 1460.4
Area = 499290
Height = 67882
Similarity = 953



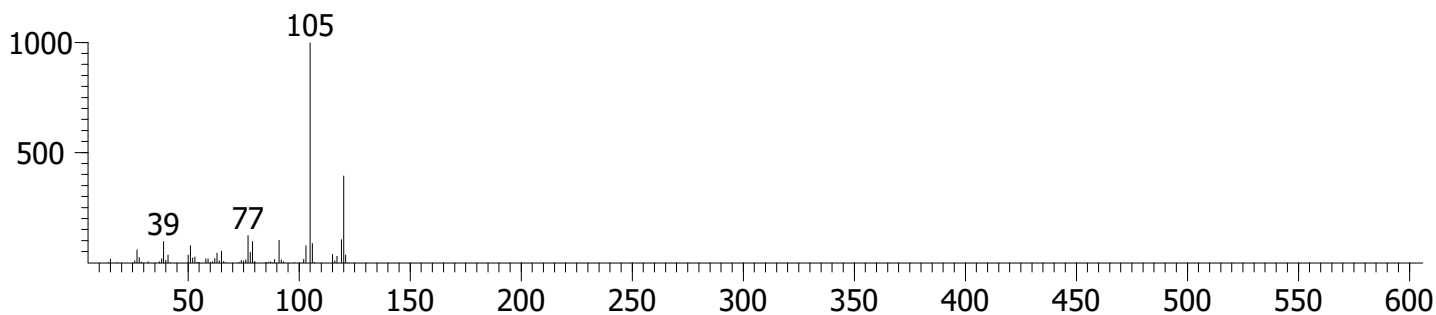
Peak Apex - sample "INF-A grab 100819 (111419):1", peak 245, at 605.928 , 1.307 sec , sec (Spec # 19278)



Peak True - sample "INF-A grab 100819 (111419):1", peak 245, at 605.928 , 1.307 sec , sec (Spec # 19278)



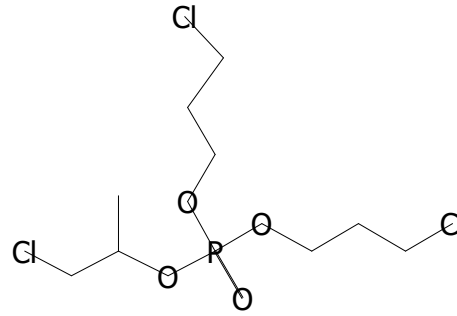
Library Hit - similarity 953, "Benzene, 1,2,3-trimethyl-"



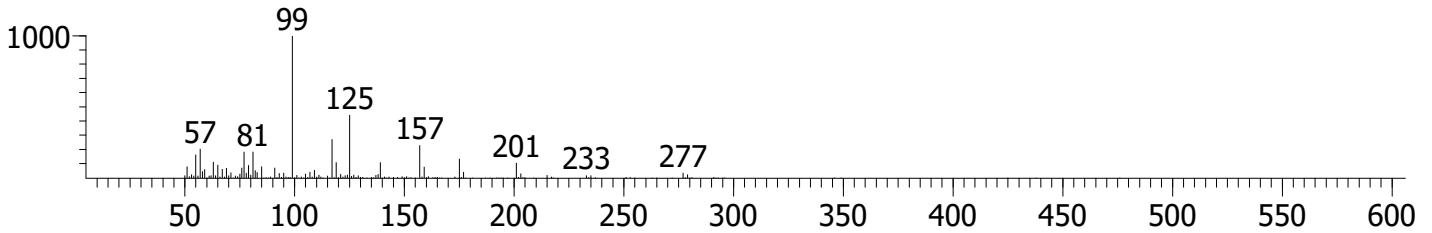
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1,2,3-trimethyl-	953	5171	526-73-8	mainlib	C9H12	120
2	Benzene, 1,2,4-trimethyl-	922	1409	95-63-6	mainlib	C9H12	120
3	2,4-Nonadiyne	907	854	63621-15-8	mainlib	C9H12	120
4	Benzene, 1-ethyl-3-methyl-	893	534	620-14-4	mainlib	C9H12	120
5	Benzene, 1-ethyl-4-methyl-	891	493	622-96-8	mainlib	C9H12	120

(3-chloro-1-propyl)(1-chloro-2-propyl)phosph

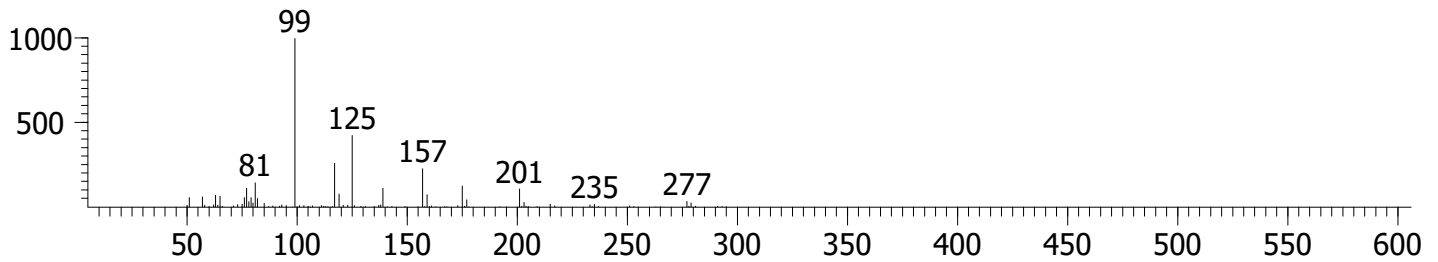
1st Dimension R.T. = 1630.84
2nd Dimension R.T. = 1.848
Quant Mass(es) = 99
S/N = 1027.9
Area = 262401
Height = 24673
Similarity = 734



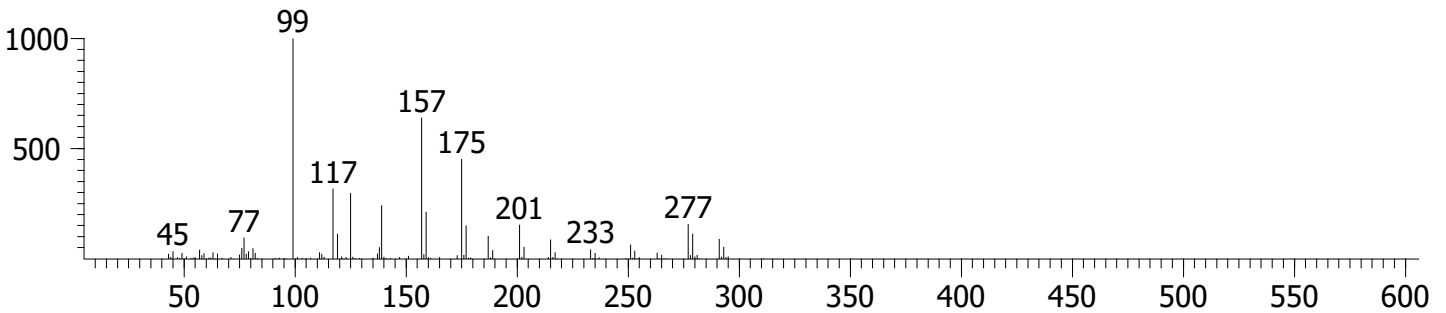
Peak Apex - sample "INF-A grab 100819 (111419):1", peak 3562, at 1630.84 , 1.848 sec , sec (Spec # 174650)



Peak True - sample "INF-A grab 100819 (111419):1", peak 3562, at 1630.84 , 1.848 sec , sec (Spec # 174650)



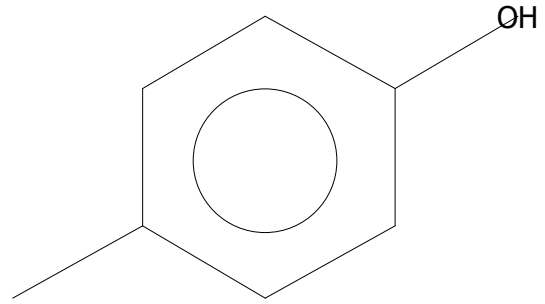
Library Hit - similarity 734, "Bis(3-chloro-1-propyl)(1-chloro-2-propyl)phosphate"



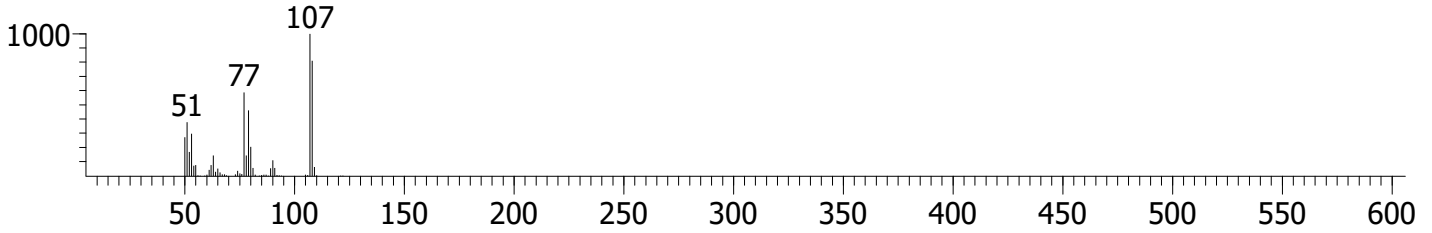
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Bis(3-chloro-1-propyl)(1-chloro-2-propyl)phosphate	734	4328	137888-35-8	mainlib	C9H18Cl3O4P	326
2	Tris(3-chloropropyl) phosphate	732	3992	1067-98-7	mainlib	C9H18Cl3O4P	326
3	Bis(1-chloro-2-propyl)(3-chloro-1-propyl)phosphate	708	1337	137909-40-1	mainlib	C9H18Cl3O4P	326
4	2-Propanol, 1-chloro-, phosphate (3:1)	653	259	13674-84-5	mainlib	C9H18Cl3O4P	326
5	Sarin	586	40	107-44-8	mainlib	C4H10FO2P	140

p-Cresol

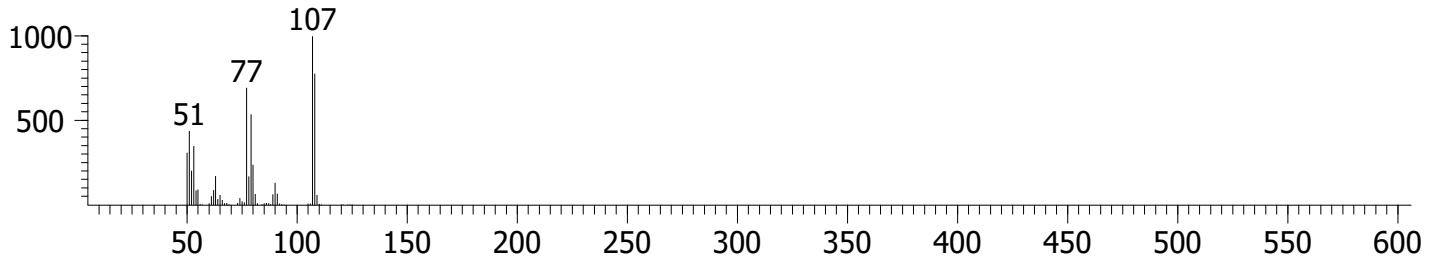
1st Dimension R.T. = 693.378
2nd Dimension R.T. = 1.716
Quant Mass(es) = 107
S/N = 25689
Area = 55944330
Height = 5214309
Similarity = 941



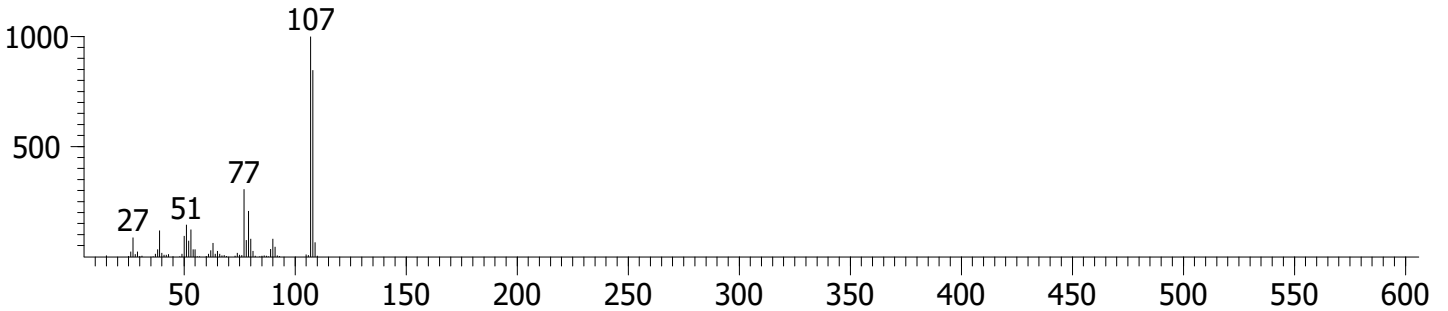
Peak Apex - sample "INF B grab 091919 (20191511):1", peak 342, at 693.378 , 1.716 sec , sec (Spec # 32590)



Peak True - sample "INF B grab 091919 (20191511):1", peak 342, at 693.378 , 1.716 sec , sec (Spec # 32590)



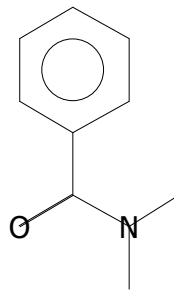
Library Hit - similarity 941, "p-Cresol"



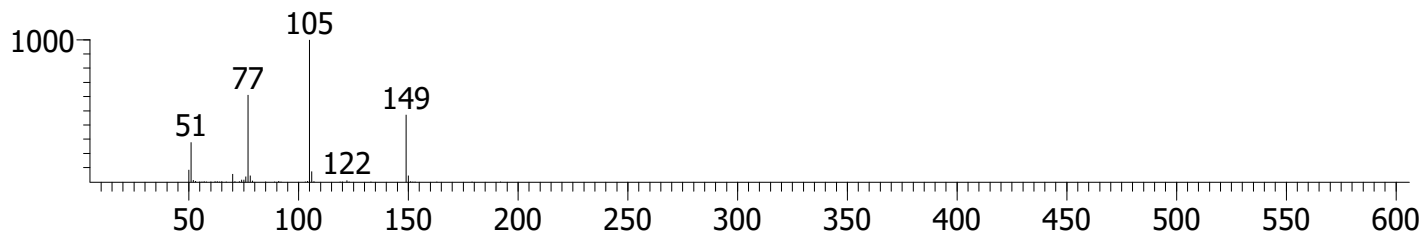
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	p-Cresol	941	6818	106-44-5	mainlib	C7H8O	108
2	Phenol, 3-methyl-	917	2284	108-39-4	mainlib	C7H8O	108
3	Phenol, 3-methyl-	916	3581	108-39-4	replib	C7H8O	108
4	p-Cresol	911	2886	106-44-5	replib	C7H8O	108
5	Phenol, 2-methyl-	907	2438	95-48-7	replib	C7H8O	108

Benzamide, N,N-dimethyl-

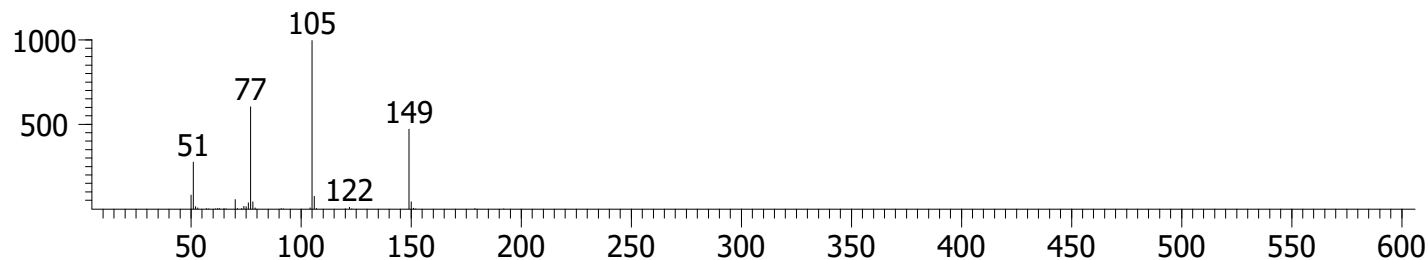
1st Dimension R.T. = 2201.02
2nd Dimension R.T. = 2.501
Quant Mass(es) = 105
S/N = 4211.1
Area = 1712926
Height = 127431
Similarity = 915



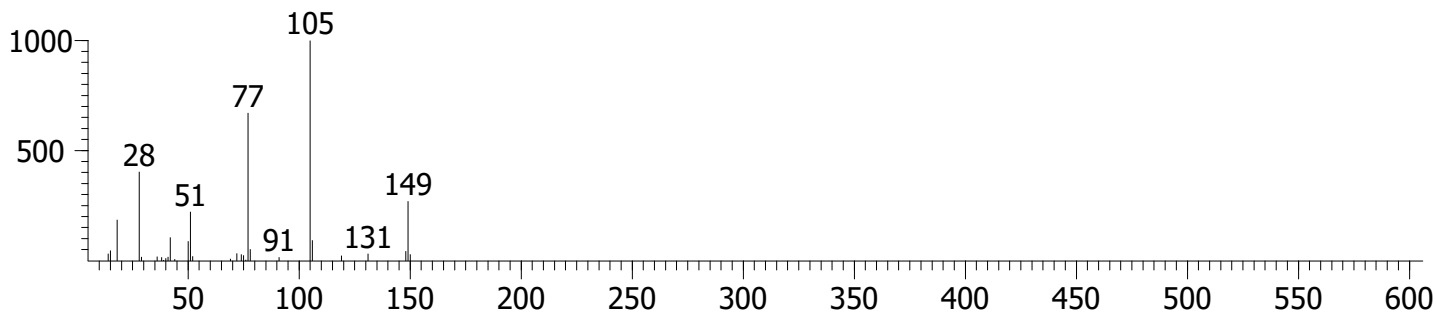
Peak Apex - sample "INF B grab 091919 (20191511):1", peak 3753, at 2201.02 , 2.501 sec , sec (Spec # 261139)



Peak True - sample "INF B grab 091919 (20191511):1", peak 3753, at 2201.02 , 2.501 sec , sec (Spec # 261139)



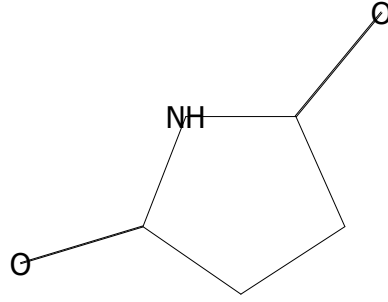
Library Hit - similarity 915, "Benzamide, N,N-dimethyl-"



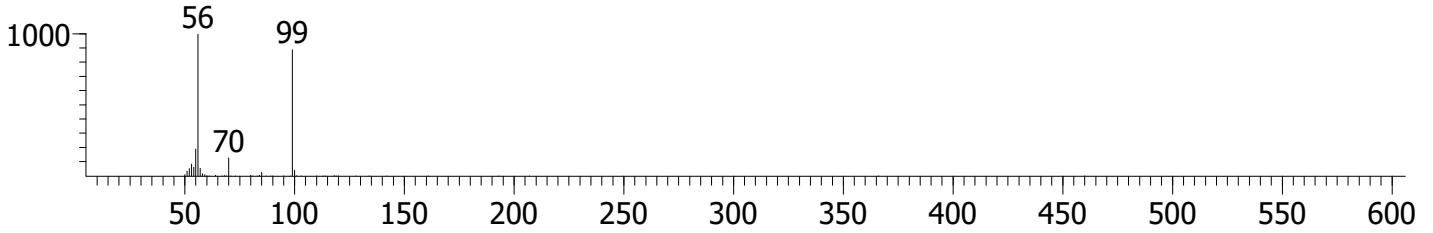
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzamide, N,N-dimethyl-	915	6180	611-74-5	replib	C9H11NO	149
2	2,2'-(Ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl) dibenzoate	855	1413	0-00-0	mainlib	C20H22O6	358
3	Diethylene glycol dibenzoate	844	880	120-55-8	replib	C18H18O5	314
4	2,3-Dimethyl-4a,8a-diphenyl-hexahydro-[1,4]dioxino[2,3-b][1,4]dioxine	843	941	0-00-0	mainlib	C20H22O4	326
5	2-Isopropyl-5-methylphenyl benzoate	838	758	0-00-0	mainlib	C17H18O2	254

Succinimide

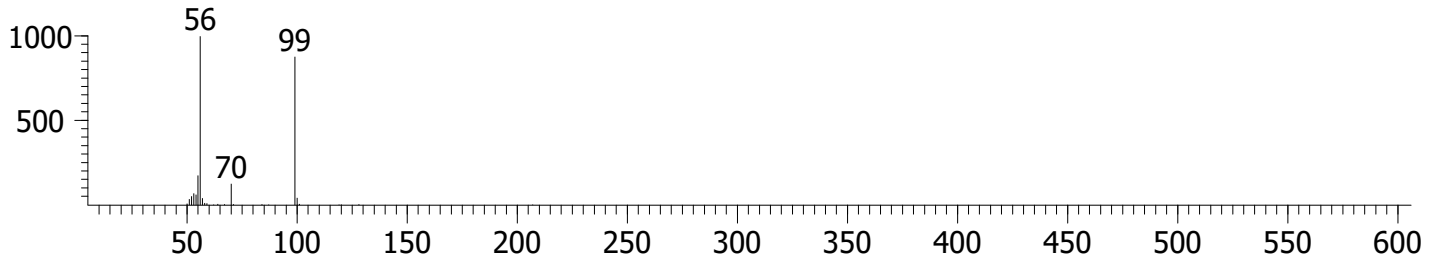
1st Dimension R.T. = 773.832
2nd Dimension R.T. = 2.409
Quant Mass(es) = 99
S/N = 1387.5
Area = 599059
Height = 61901
Similarity = 893



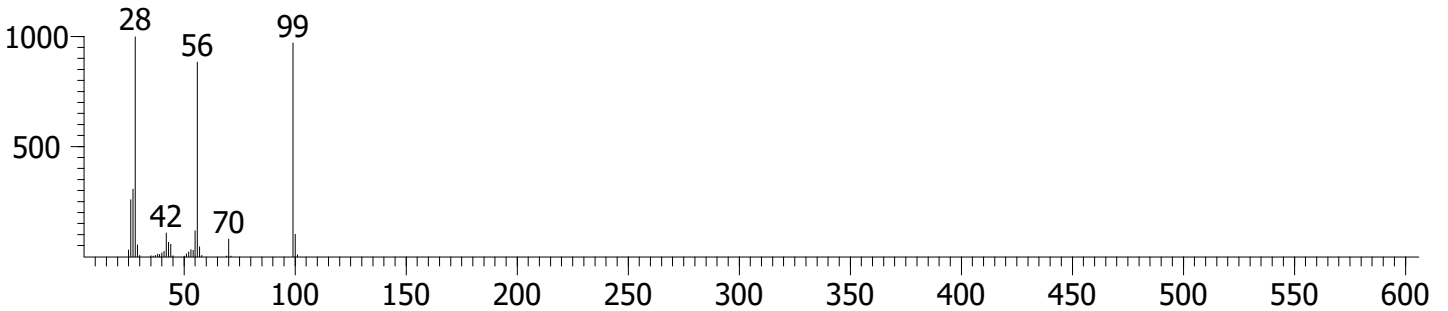
Peak Apex - sample "INF C grab 091919 (20191511):1", peak 542, at 773.832 , 2.409 sec , sec (Spec # 44885)



Peak True - sample "INF C grab 091919 (20191511):1", peak 542, at 773.832 , 2.409 sec , sec (Spec # 44885)



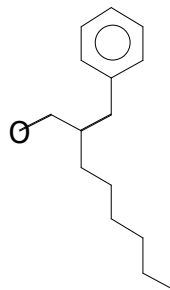
Library Hit - similarity 893, "Succinimide"



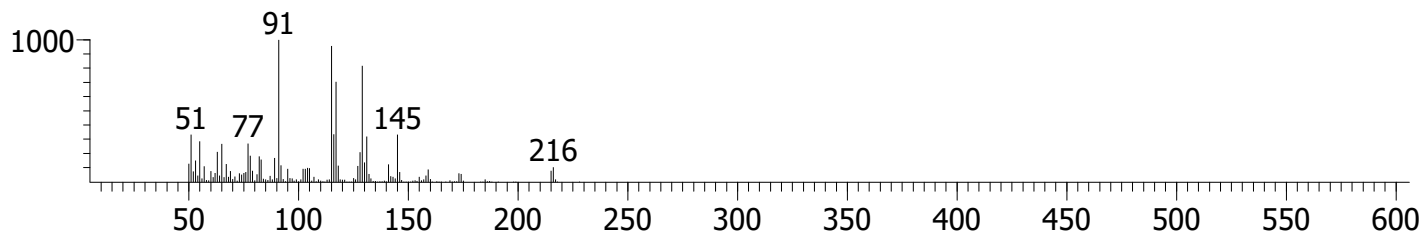
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Succinimide	893	8860	123-56-8	replib	C4H5NO2	99
2	Succinimide	865	8860	123-56-8	replib	C4H5NO2	99
3	Succinimide	849	8860	123-56-8	replib	C4H5NO2	99
4	2,4,6-Triallyloxy-1,3,5-triazine	846	8600	101-37-1	nist_msms	C12H15N3O3	249
5	3-Methyl-2-pyrrolidinone	836	1519	2555-05-7	mainlib	C5H9NO	99

Octanal, 2-(phenylmethylene)-

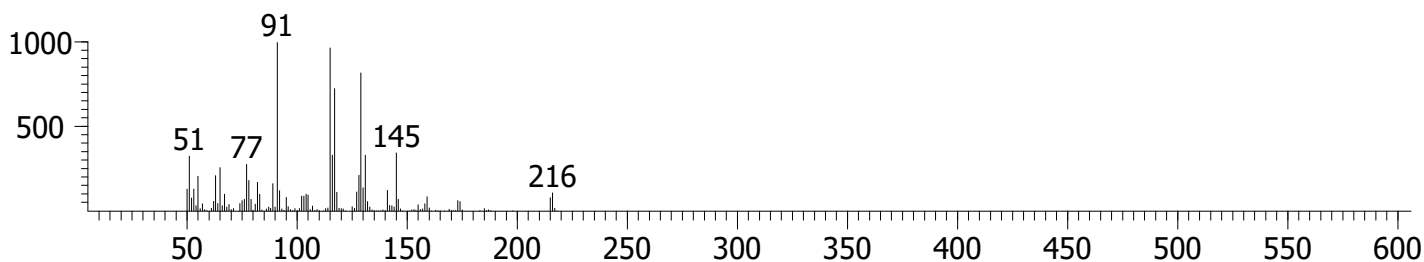
1st Dimension R.T. = 1539.89
2nd Dimension R.T. = 1.769
Quant Mass(es) = 115
S/N = 3565.9
Area = 956405
Height = 102245
Similarity = 932



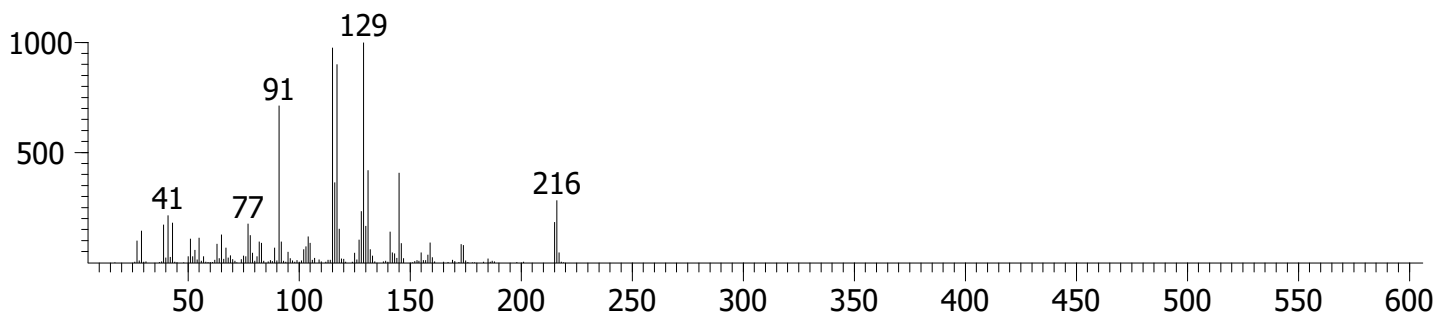
Peak Apex - sample "INF C grab 091919 (20191511):1", peak 2447, at 1539.89 , 1.769 sec , sec (Spec # 160858)



Peak True - sample "INF C grab 091919 (20191511):1", peak 2447, at 1539.89 , 1.769 sec , sec (Spec # 160858)



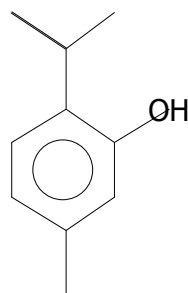
Library Hit - similarity 932, "Octanal, 2-(phenylmethylene)-"



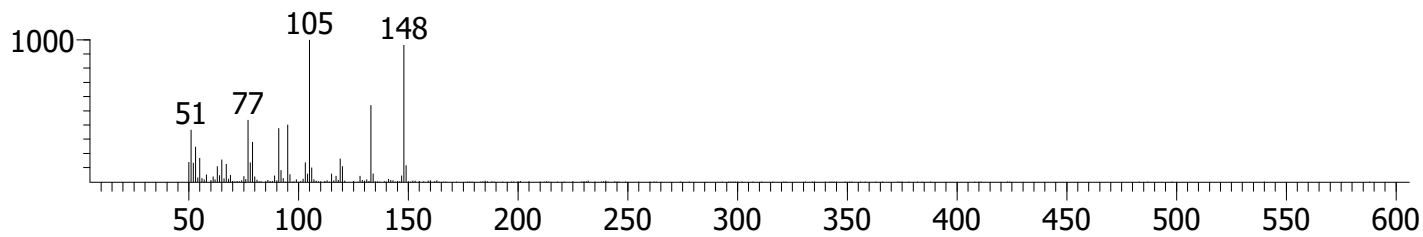
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Octanal, 2-(phenylmethylene)-	932	9068	101-86-0	replib	C15H20O	216
2	Octanal, 2-(phenylmethylene)-	924	9068	101-86-0	replib	C15H20O	216
3	Octanal, 2-(phenylmethylene)-	916	9068	101-86-0	replib	C15H20O	216
4	Octanal, 2-(phenylmethylene)-	857	9068	101-86-0	replib	C15H20O	216
5	Cinnamaldehyde, à-pentyl-	838	742	122-40-7	replib	C14H18O	202

8,9-Dehydrothymol

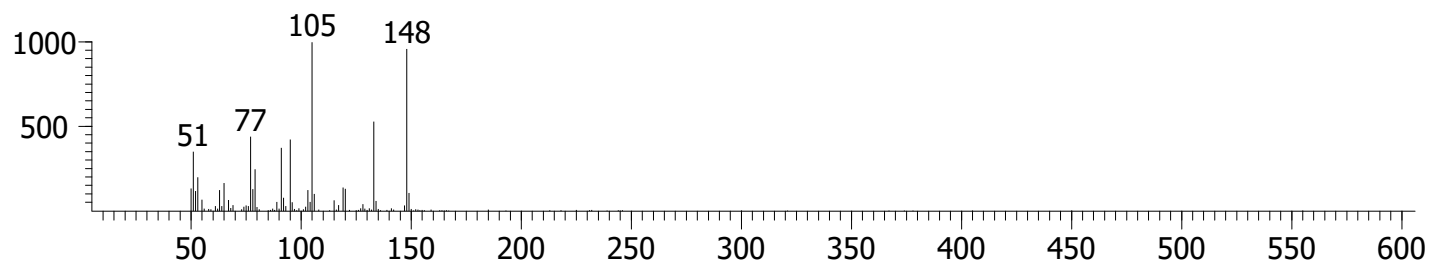
1st Dimension R.T. = 1952.66
2nd Dimension R.T. = 2.554
Quant Mass(es) = 148
S/N = 728.26
Area = 147967
Height = 12096
Similarity = 817



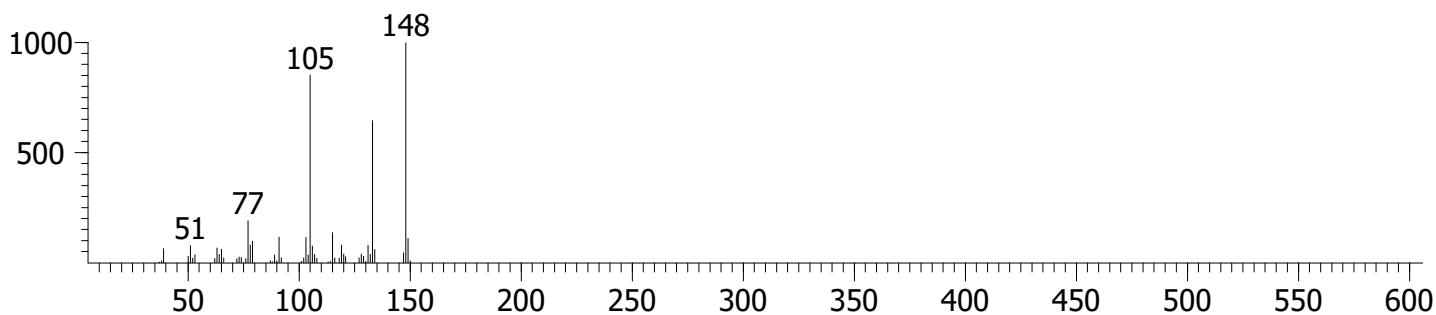
Peak Apex - sample "INF C grab 091919 (20191511):1", peak 3437, at 1952.66 , 2.554 sec , sec (Spec # 223 517)



Peak True - sample "INF C grab 091919 (20191511):1", peak 3437, at 1952.66 , 2.554 sec , sec (Spec # 2235 17)



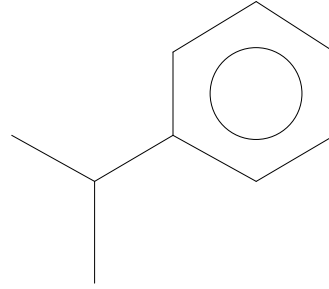
Library Hit - similarity 817, "8,9-Dehydrothymol"



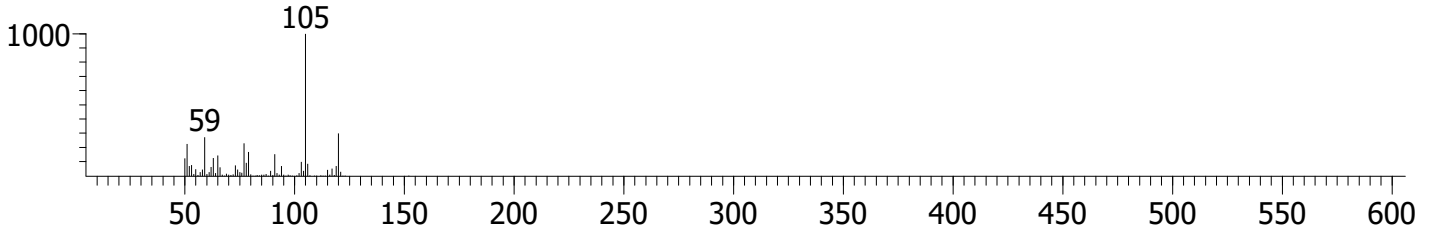
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	8,9-Dehydrothymol	817	2021	18612-99-2	mainlib	C10H12O	148
2	Benzaldehyde, 4-(1-methylethyl)-	815	3712	122-03-2	replib	C10H12O	148
3	3,7,7-Trimethyl-1-penta-1,3-dienyl-2-oxabicyclo[3.2.0]hept-3-ene	802	1225	0-00-0	mainlib	C14H20O	204
4	Benzaldehyde, 4-(1-methylethyl)-	797	3712	122-03-2	replib	C10H12O	148
5	Benzaldehyde, 4-(1-methylethyl)-	795	3712	122-03-2	replib	C10H12O	148

Benzene, (1-methylethyl)-

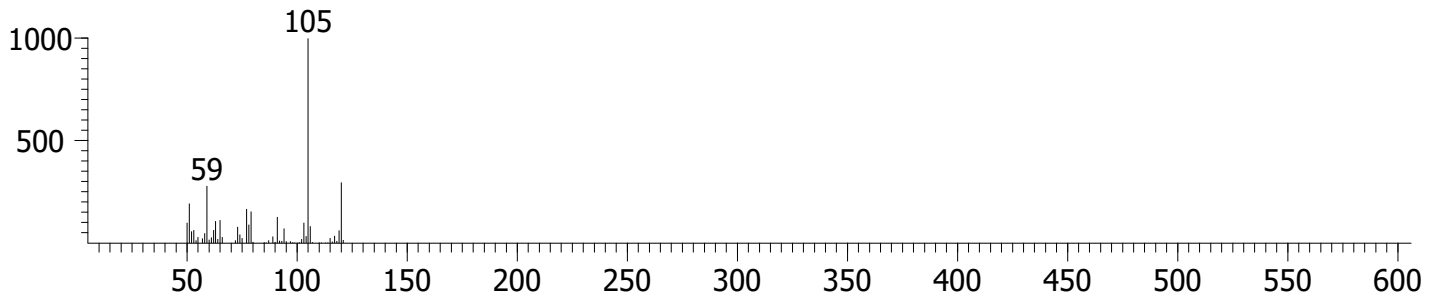
1st Dimension R.T. = 623.418
2nd Dimension R.T. = 1.445
Quant Mass(es) = 105
S/N = 2557.3
Area = 466364
Height = 65029
Similarity = 857



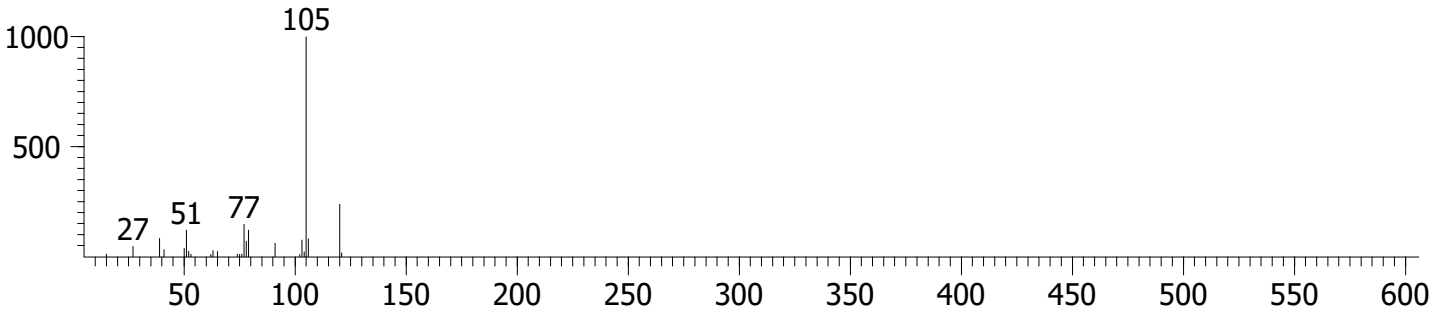
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 298, at 623.418 , 1.445 sec , sec (Spec # 21949)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 298, at 623.418 , 1.445 sec , sec (Spec # 21949)



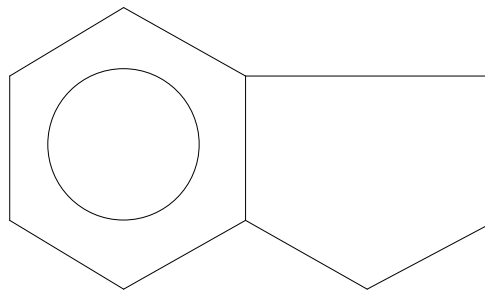
Library Hit - similarity 857, "Benzene, (1-methylethyl)-"



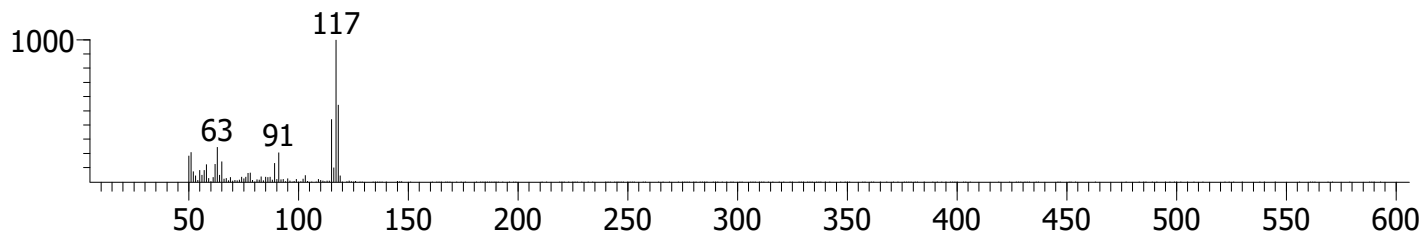
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, (1-methylethyl)-	857	3008	98-82-8	mainlib	C9H12	120
2	2,4-Nonadiyne	846	2063	63621-15-8	mainlib	C9H12	120
3	Benzene, 1,2,3-trimethyl-	839	1580	526-73-8	mainlib	C9H12	120
4	2,3-Heptadien-5-yne, 2,4-dimethyl-	816	577	41898-89-9	mainlib	C9H12	120
5	Benzene, 1-ethyl-2-methyl-	814	532	611-14-3	mainlib	C9H12	120

Indane

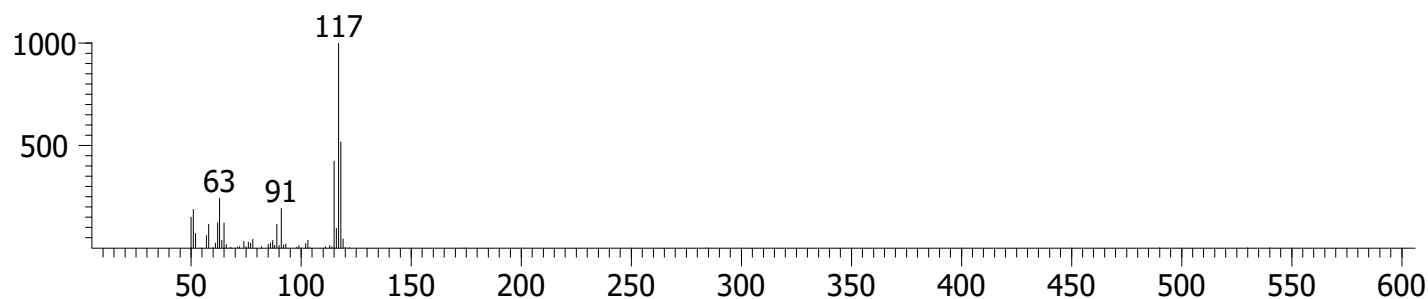
1st Dimension R.T. = 644.406
2nd Dimension R.T. = 1.544
Quant Mass(es) = 117
S/N = 790.90
Area = 109311
Height = 15668
Similarity = 871



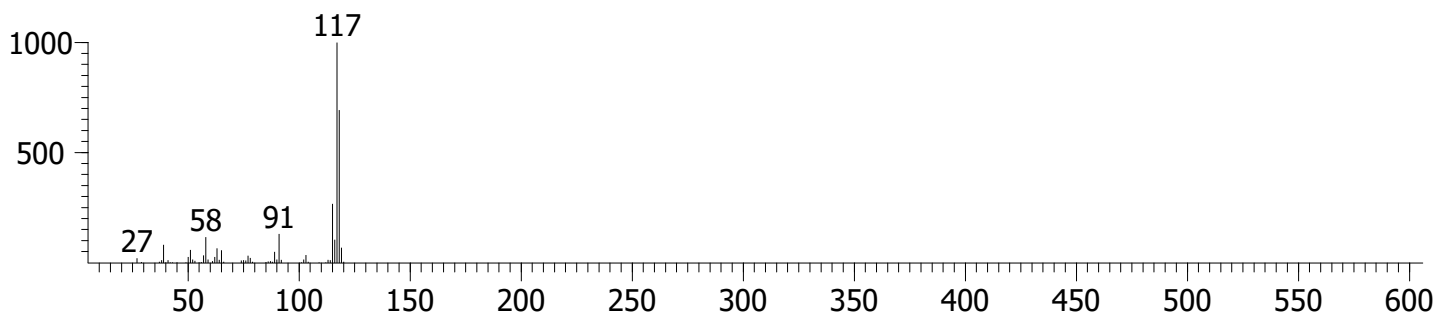
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 340, at 644.406 , 1.544 sec , sec (Spec # 25144)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 340, at 644.406 , 1.544 sec , sec (Spec # 25144)



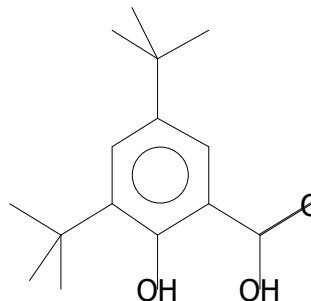
Library Hit - similarity 871, "Indane"



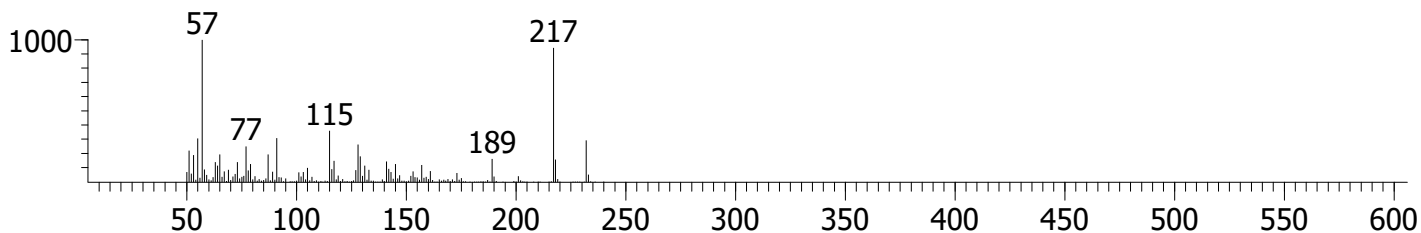
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Indane	871	1570	496-11-7	mainlib	C9H10	118
2	Benzene, 1-ethenyl-2-methyl-	860	1077	611-15-4	mainlib	C9H10	118
3	3-Bromo-1-phenyl-1-propene	859	1035	4392-24-9	mainlib	C9H9Br	196
4	Delta-cyclene	856	914	7785-10-6	mainlib	C9H10	118
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-non-2-ene	852	772	0-00-0	mainlib	C9H10	118

Benzoic acid,
3,5-bis(1,1-dimethylethyl)-2-hydroxy-

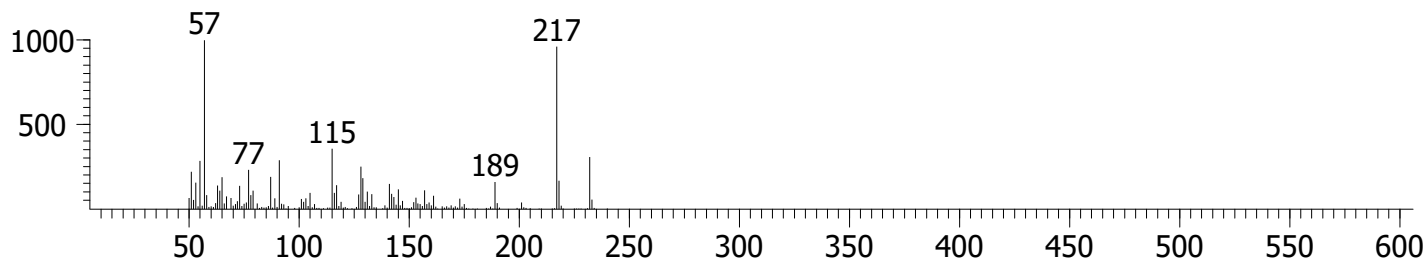
1st Dimension R.T. = 1413.97
2nd Dimension R.T. = 1.610
Quant Mass(es) = 217
S/N = 6293.3
Area = 611256
Height = 83573
Similarity = 701



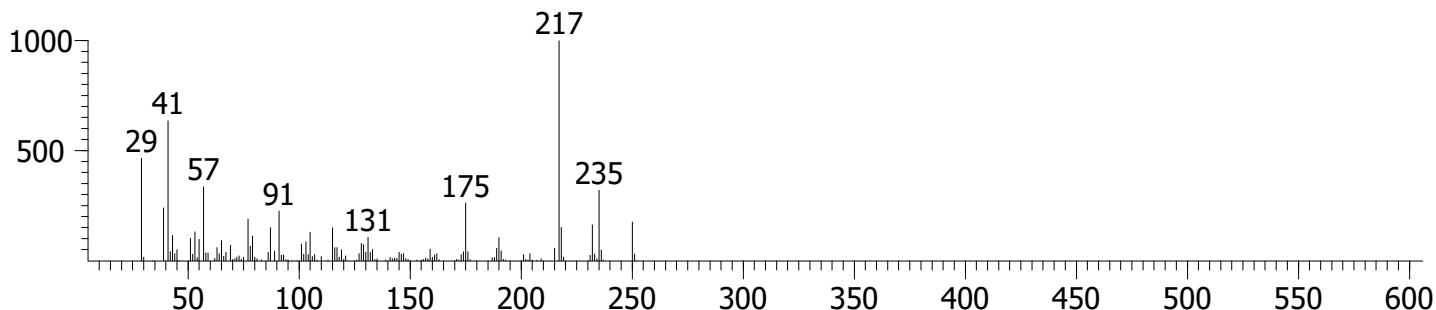
Peak Apex - sample "AerMBR C 091919 (20191119):1", peak 2340, at 1413.97 , 1.610 sec , sec (Spec # 1417 54)



Peak True - sample "AerMBR C 091919 (20191119):1", peak 2340, at 1413.97 , 1.610 sec , sec (Spec # 1417 54)



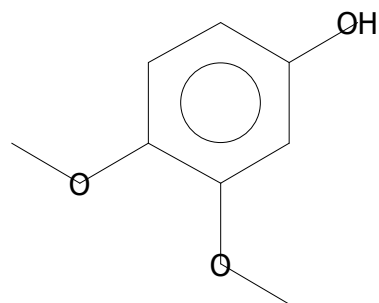
Library Hit - similarity 701, "Benzoic acid, 3,5-bis(1,1-dimethylethyl)-2-hydroxy-"



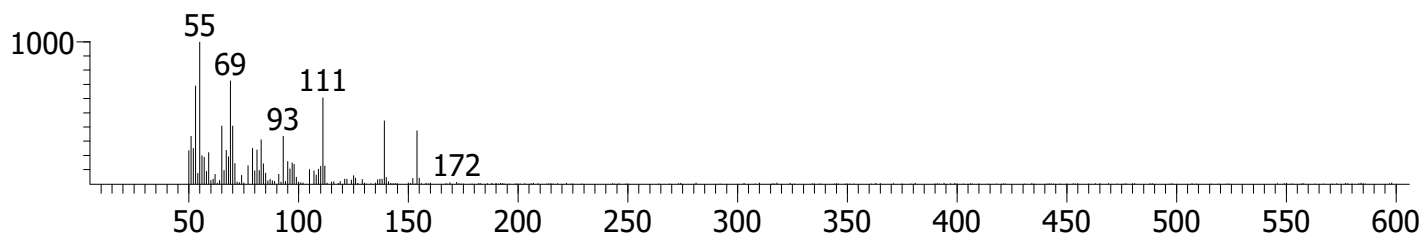
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzoic acid, 3,5-bis(1,1-dimethylethyl)-2-hydroxy-	701	3317	19715-19-6	mainlib	C15H22O3	250
2	Furan, 2-[(2-ethoxy-3,4-dimethyl-2-cyclohexen-1-ylidene) methyl]-	682	1610	55162-49-7	mainlib	C15H20O2	232
3	4-Biphenyl 3,5-di-tert-butylbenzoate	673	1169	293761-63-4	mainlib	C27H30O2	386
4	Benzamide, 3,5-di-tert-butyl-N-(5-methyl-1,3,4-thiadiazol-2-yl)-	659	732	330818-06-9	mainlib	C18H25N3OS	331
5	3,4-Xylyl 3,5-di-tert-butylbenzoate	657	675	293761-66-7	mainlib	C23H30O2	338

Phenol, 3,4-dimethoxy-

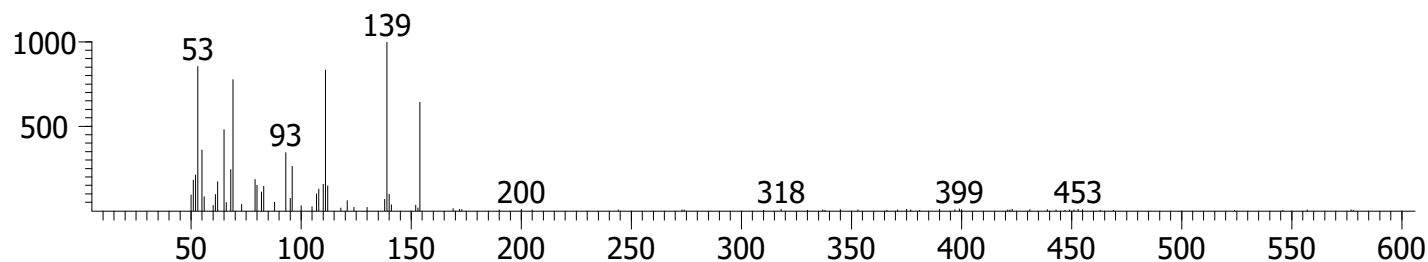
1st Dimension R.T. = 1179.6
2nd Dimension R.T. = 2.132
Quant Mass(es) = 139
S/N = 120.35
Area = 20019
Height = 2300.1
Similarity = 805



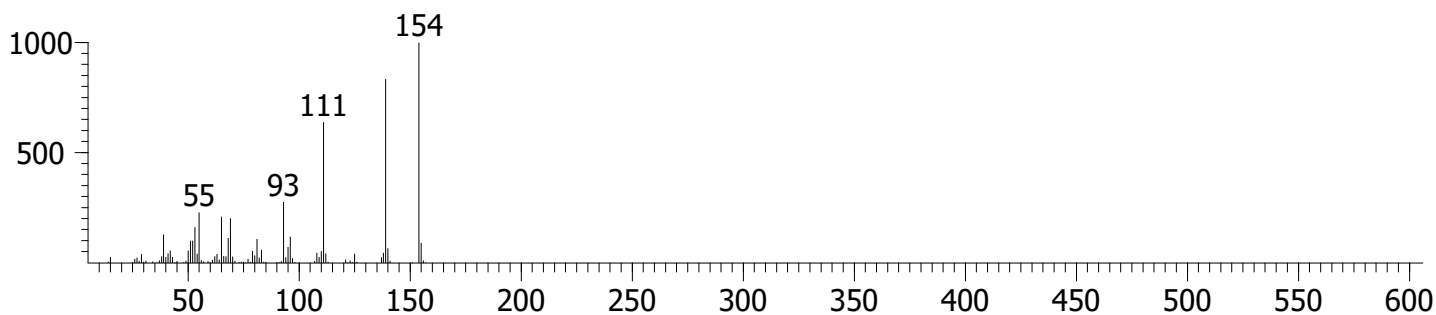
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 1575, at 1179.6 , 2.132 sec , sec (Spec # 10632 3)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 1575, at 1179.6 , 2.132 sec , sec (Spec # 10632 3)



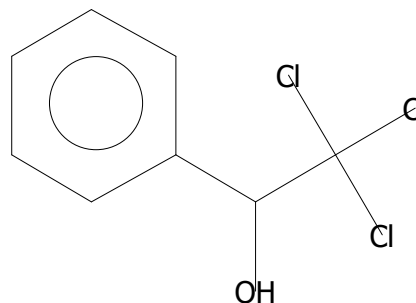
Library Hit - similarity 805, "Phenol, 3,4-dimethoxy-"



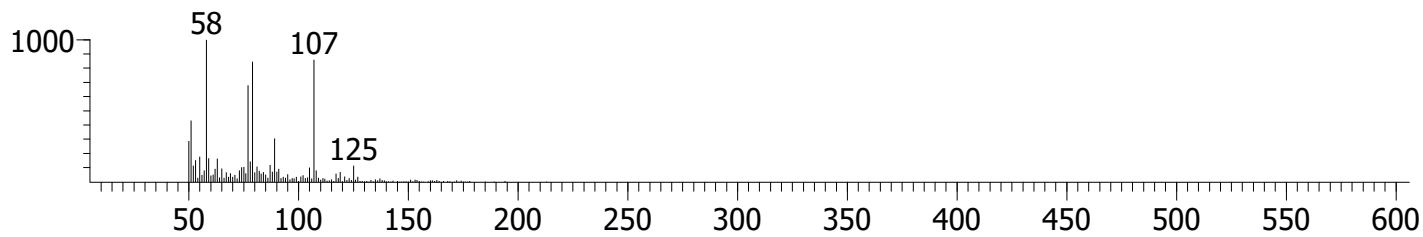
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 3,4-dimethoxy-	805	6300	2033-89-8	mainlib	C ₈ H ₁₀ O ₃	154
2	2,4-Dimethoxyphenol	748	1180	13330-65-9	mainlib	C ₈ H ₁₀ O ₃	154
3	2,3-Dimethoxyphenol	737	810	5150-42-5	mainlib	C ₈ H ₁₀ O ₃	154
4	Phenol, 2,6-dimethoxy-	718	393	91-10-1	mainlib	C ₈ H ₁₀ O ₃	154
5	Phenol, 3,4-dimethoxy-, acetate	701	214	7203-46-5	mainlib	C ₁₀ H ₁₂ O ₄	196

2,2,2-Trichloro-1-phenylethanol

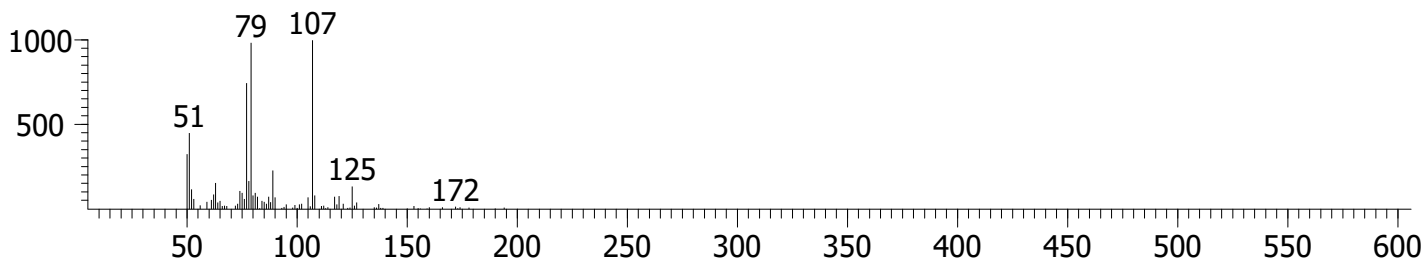
1st Dimension R.T. = 1277.54
2nd Dimension R.T. = 2.086
Quant Mass(es) = 107
S/N = 1337.2
Area = 582339
Height = 60999
Similarity = 893



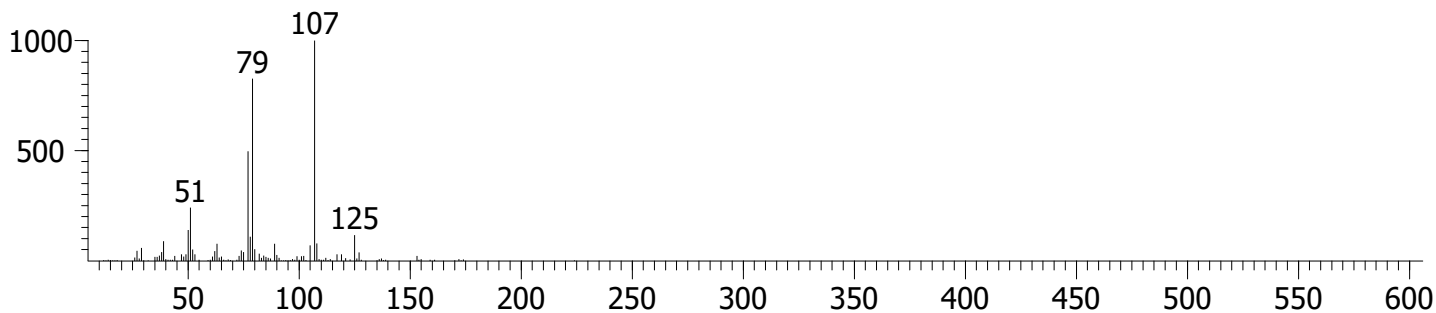
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 3349, at 1277.54 , 2.086 sec , sec (Spec # 121156)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 3349, at 1277.54 , 2.086 sec , sec (Spec # 121156)



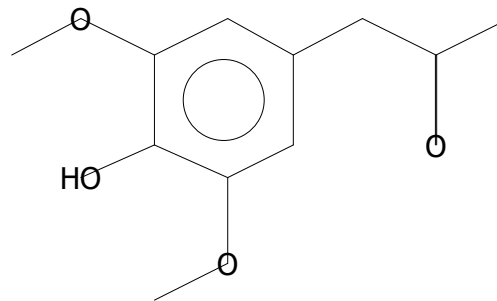
Library Hit - similarity 893, "2,2,2-Trichloro-1-phenylethanol"



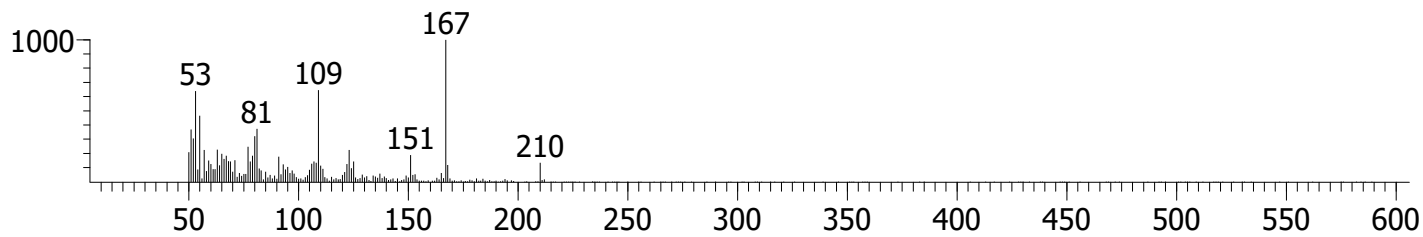
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,2,2-Trichloro-1-phenylethanol	893	6064	2000-43-3	mainlib	C8H7Cl3O	224
2	Mandelamide	778	363	4410-31-5	mainlib	C8H9NO2	151
3	Benzenemethanol, à-ethyl-	766	242	93-54-9	mainlib	C9H12O	136
4	Propionic acid, 2,3-dihydroxy-3-phenyl-	758	180	0-00-0	mainlib	C9H10O4	182
5	Benzenemethanol, à-methyl-	758	180	98-85-1	mainlib	C8H10O	122

Syringylacetone

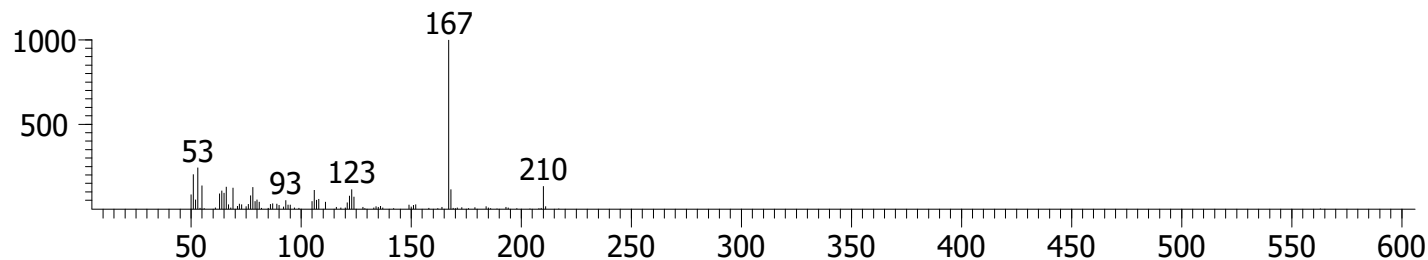
1st Dimension R.T. = 1571.38
 2nd Dimension R.T. = 2.323
 Quant Mass(es) = 167
 S/N = 1160.1
 Area = 163187
 Height = 14945
 Similarity = 784



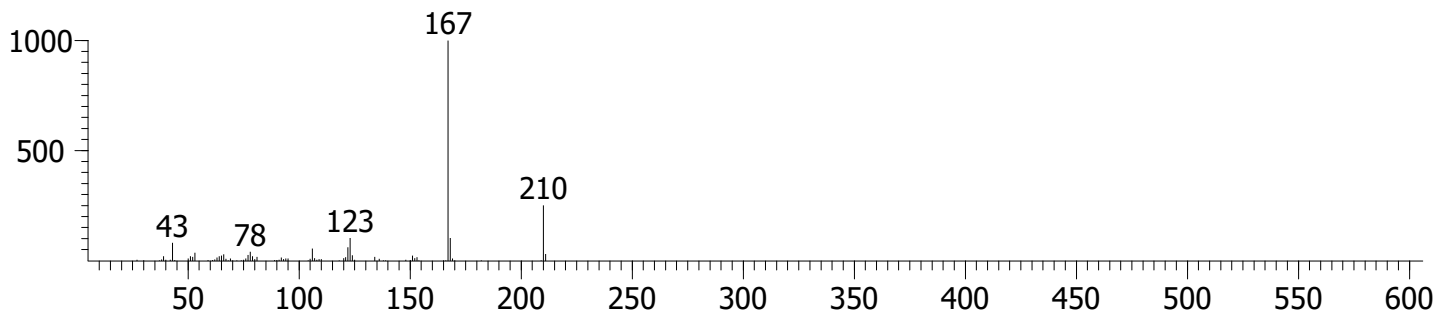
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 5223, at 1571.38 , 2.323 sec , sec (Spec # 165712)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 5223, at 1571.38 , 2.323 sec , sec (Spec # 165712)



Library Hit - similarity 784, "Syringylacetone"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Syringylacetone	784	6282	19037-58-2	mainlib	C ₁₁ H ₁₄ O ₄	210
2	Allylescaline	719	1011	39201-76-8	mainlib	C ₁₃ H ₁₉ NO ₃	237
3	Homosyringaldehyde	702	552	87345-52-6	mainlib	C ₁₀ H ₁₂ O ₄	196
4	2-Pentanone, 1-(2,4,6-trihydroxyphenyl)	702	552	0-00-0	mainlib	C ₁₁ H ₁₄ O ₄	210
5	2,4-Hexadienedioic acid, 3,4-diethyl-, dimethyl ester, (Z,Z)-	682	251	31447-54-8	mainlib	C ₁₂ H ₁₈ O ₄	226

Butanenitrile, 4-(methylthio)-

1st Dimension R.T. = 707.37

2nd Dimension R.T. = 1.973

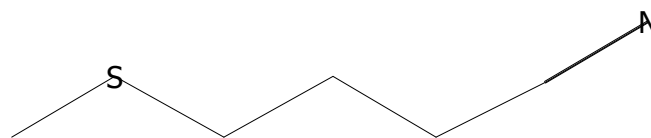
Quant Mass(es) = 61

S/N = 846.53

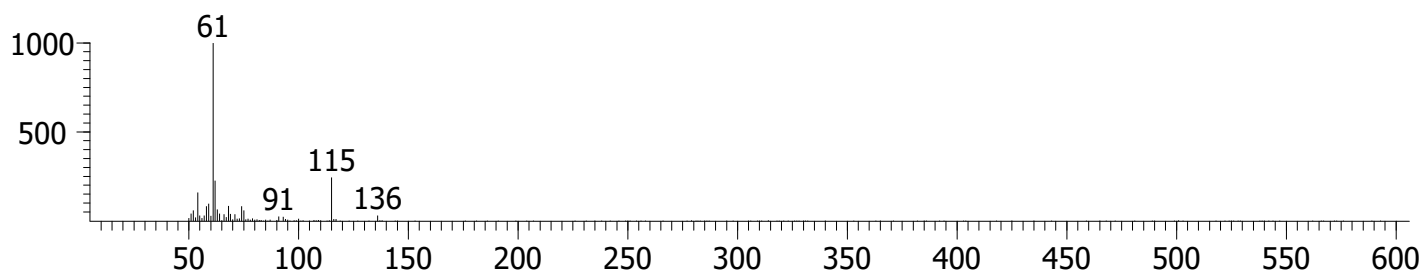
Area = 261659

Height = 30309

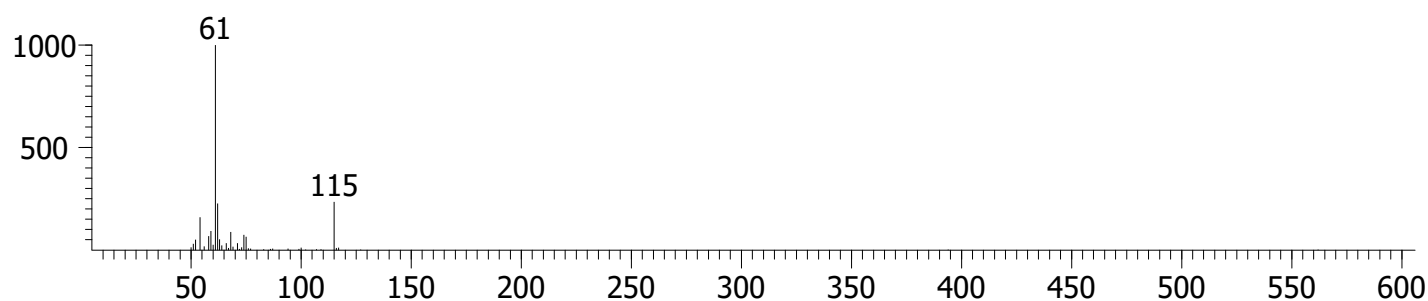
Similarity = 963



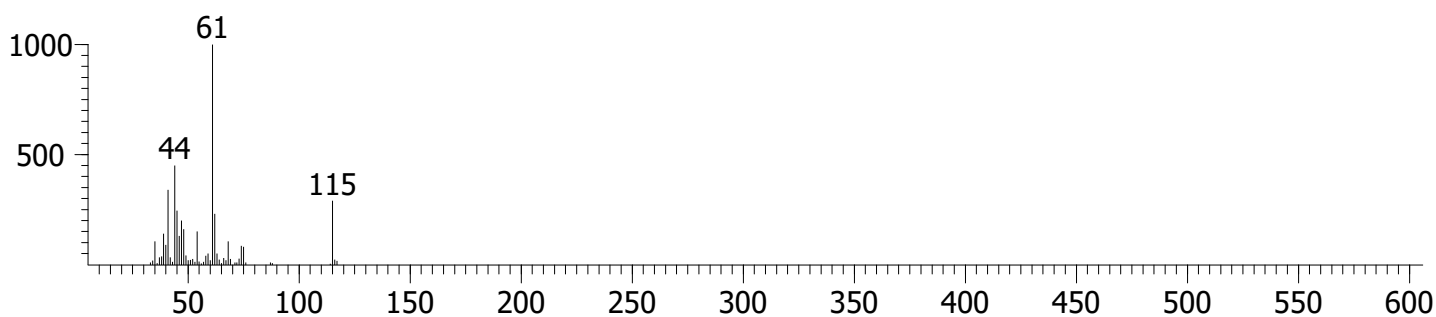
Peak Apex - sample "AnMbr B (20191120):1", peak 511, at 707.37 , 1.973 sec , sec (Spec # 34749)



Peak True - sample "AnMbr B (20191120):1", peak 511, at 707.37 , 1.973 sec , sec (Spec # 34749)



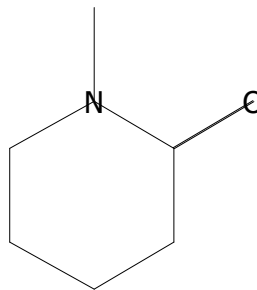
Library Hit - similarity 963, "Butanenitrile, 4-(methylthio)-"



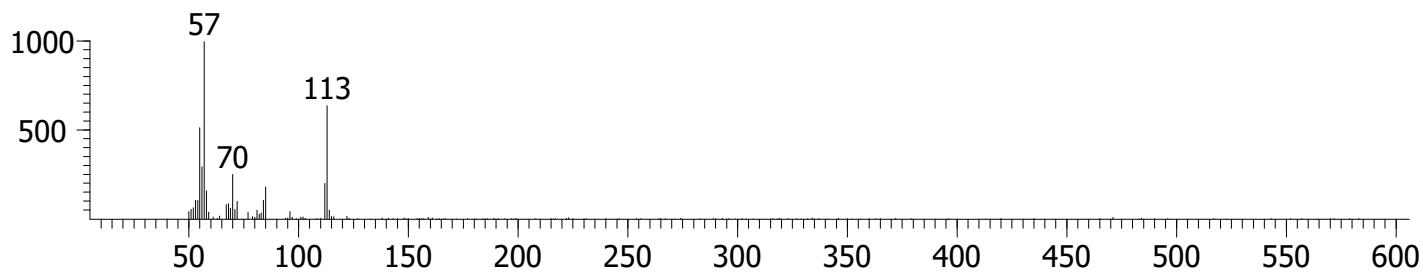
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Butanenitrile, 4-(methylthio)-	963	9483	59121-24-3	mainlib	C5H9NS	115
2	Ethanol, 2-(methylthio)-	574	94	5271-38-5	mainlib	C3H8OS	92
3	Silanol, dimethyl-	560	59	5906-76-3	mainlib	C2H8OSi	76
4	1-Nitro-2-propanol	551	43	3156-73-8	mainlib	C3H7NO3	105
5	Borane-methyl sulfide complex	550	41	13292-87-0	mainlib	C2H9BS	76

2-Piperidinone, 1-methyl-

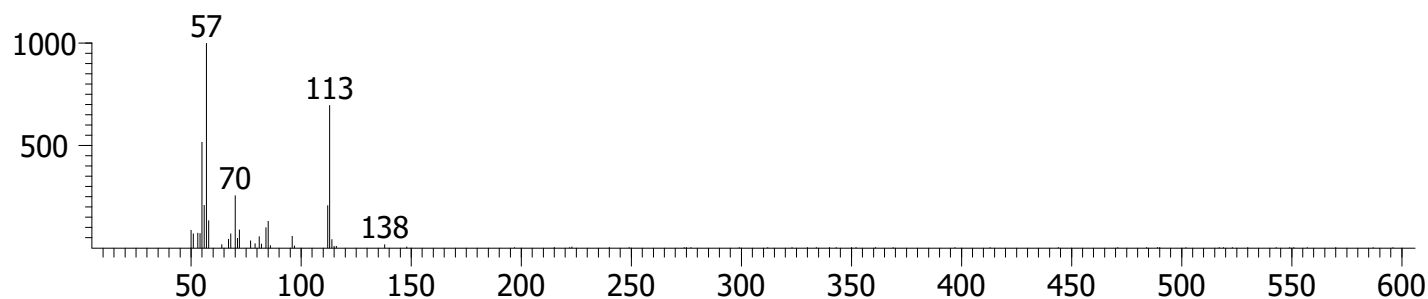
1st Dimension R.T. = 819.306
2nd Dimension R.T. = 2.099
Quant Mass(es) = 113
S/N = 145.82
Area = 25182
Height = 2979.7
Similarity = 833



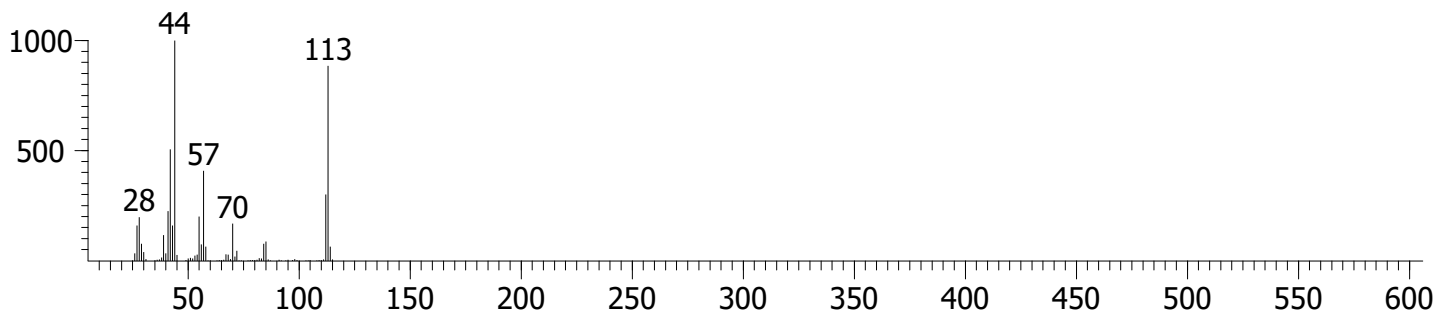
Peak Apex - sample "AnMbr B (20191120):1", peak 900, at 819.306 , 2.099 sec , sec (Spec # 51728)



Peak True - sample "AnMbr B (20191120):1", peak 900, at 819.306 , 2.099 sec , sec (Spec # 51728)



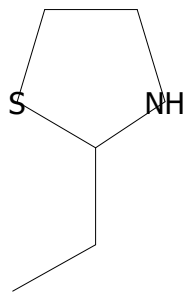
Library Hit - similarity 833, "2-Piperidinone, 1-methyl-"



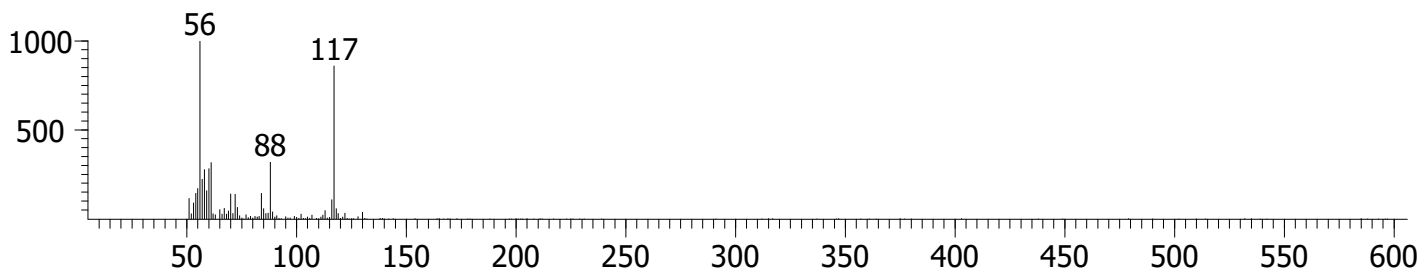
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Piperidinone, 1-methyl-	833	7723	931-20-4	mainlib	C6H11NO	113
2	Cyclohexylamine, N-methyl-4,4-dimethyl-	724	500	45815-91-6	mainlib	C9H19N	141
3	3,3-Dimethylpiperidine	715	363	1193-12-0	mainlib	C7H15N	113
4	3-(Prop-2-enoyloxy)dodecane	693	143	0-00-0	mainlib	C15H28O2	240
5	2-Octanone, 1-nitro-	689	121	16067-01-9	mainlib	C8H15NO3	173

Thiazolidine, 2-ethyl-

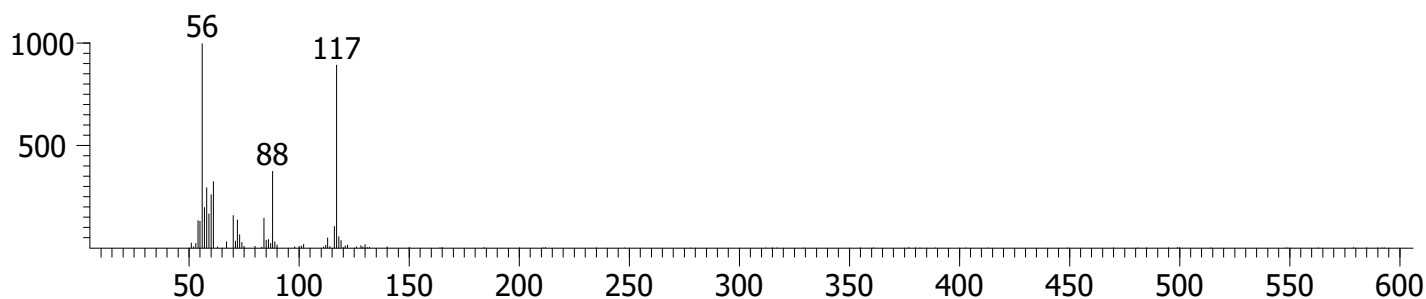
1st Dimension R.T. = 826.302
2nd Dimension R.T. = 2.086
Quant Mass(es) = 117
S/N = 295.79
Area = 45623
Height = 5208.9
Similarity = 681



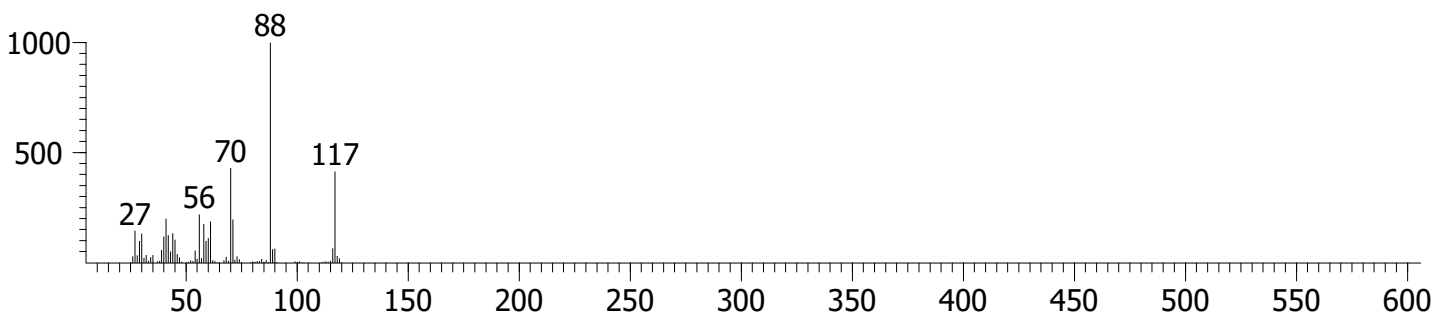
Peak Apex - sample "AnMbr B (20191120):1", peak 924, at 826.302 , 2.086 sec , sec (Spec # 52786)



Peak True - sample "AnMbr B (20191120):1", peak 924, at 826.302 , 2.086 sec , sec (Spec # 52786)



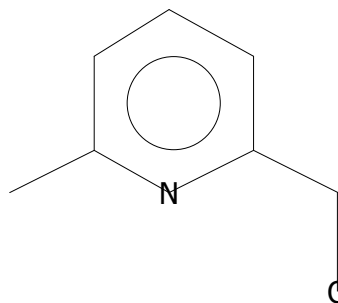
Library Hit - similarity 681, "Thiazolidine, 2-ethyl-"



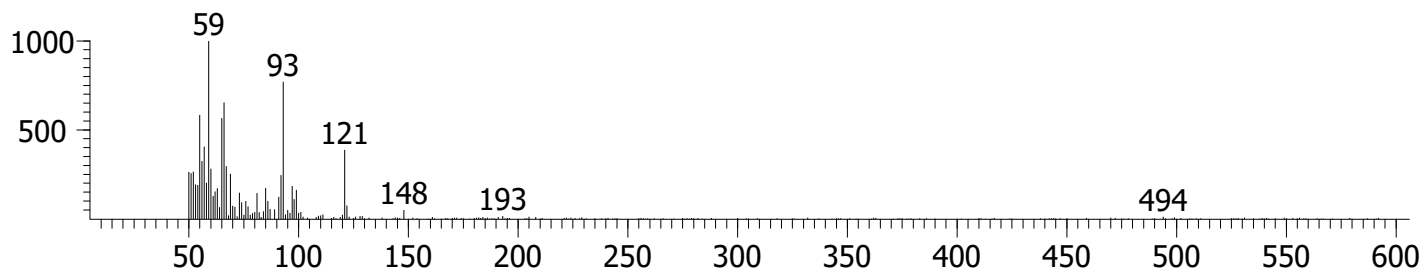
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Thiazolidine, 2-ethyl-	681	3975	24050-09-7	mainlib	C5H11NS	117
2	Tetrahydro-1,3-oxazine-2-thione	664	2169	17374-18-4	mainlib	C4H7NOS	117
3	1-[N-Aziridyl]propane-2-thiol	644	988	0-00-0	mainlib	C5H11NS	117
4	Ethane, 1-isothiocyanato-2-methoxy-	639	796	38663-85-3	mainlib	C4H7NOS	117
5	1,3-Oxathiane, 2,6-dimethyl-	619	362	33709-58-9	mainlib	C6H12OS	132

6-Methyl-2-pyridinecarbaldehyde

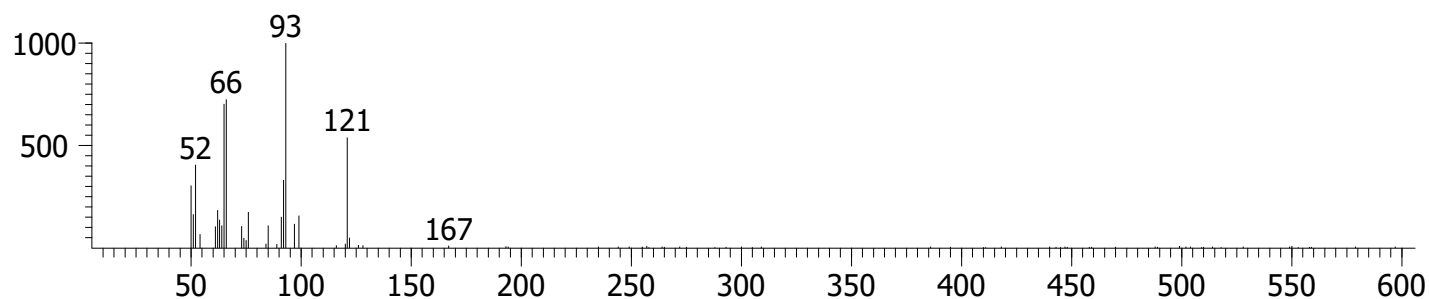
1st Dimension R.T. = 903.258
2nd Dimension R.T. = 2.138
Quant Mass(es) = 121
S/N = 66.192
Area = 9554.9
Height = 1113.2
Similarity = 750



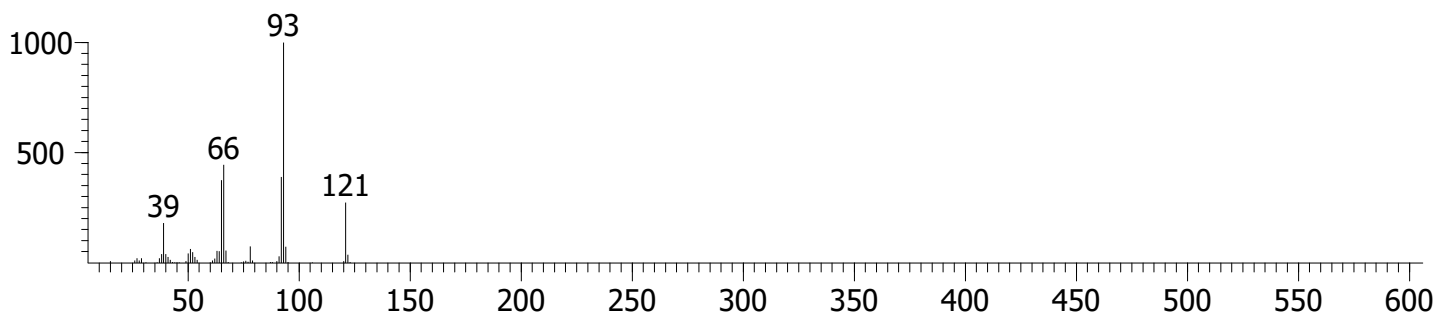
Peak Apex - sample "AnMbr B (20191120):1", peak 1212, at 903.258 , 2.138 sec , sec (Spec # 64454)



Peak True - sample "AnMbr B (20191120):1", peak 1212, at 903.258 , 2.138 sec , sec (Spec # 64454)



Library Hit - similarity 750, "6-Methyl-2-pyridinecarbaldehyde"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	6-Methyl-2-pyridinecarbaldehyde	750	5340	53547-60-7	mainlib	C7H7NO	121
2	Formamide, N-phenyl-	727	1950	103-70-8	mainlib	C7H7NO	121
3	2,4,6-Cycloheptatrien-1-one, 2-amino-	696	531	6264-93-3	mainlib	C7H7NO	121
4	2-Pyridinecarboxylic acid, 6-methyl-	681	322	934-60-1	mainlib	C7H7NO2	137
5	Benzhydrazide, 4-hydroxy-N2-(4,5,6,7-tetrahydro-5-hydroximinobenzofurazan-4-ylideno)-	672	233	0-00-0	mainlib	C13H11N5O4	301

Ethanol, 2-phenoxy-

1st Dimension R.T. = 948.732

2nd Dimension R.T. = 1.762

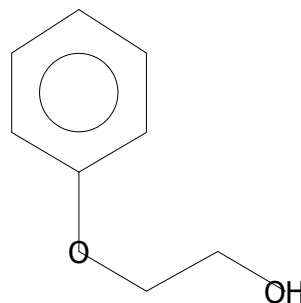
Quant Mass(es) = 138

S/N = 394.50

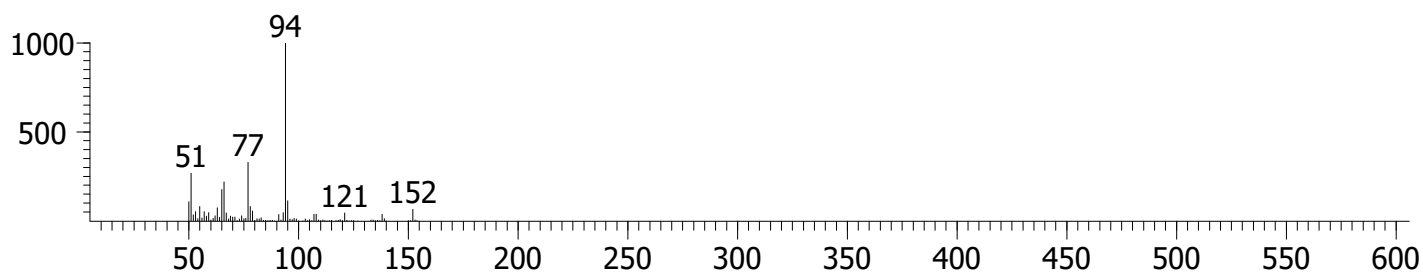
Area = 31913

Height = 3745.9

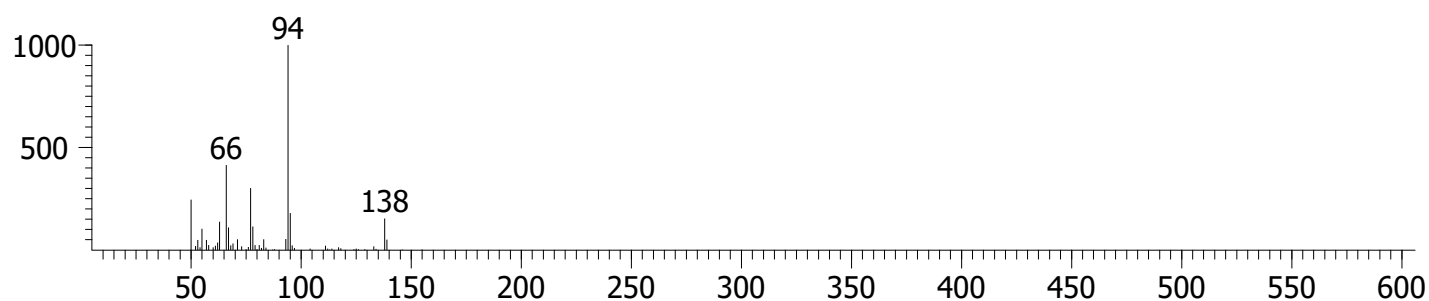
Similarity = 743



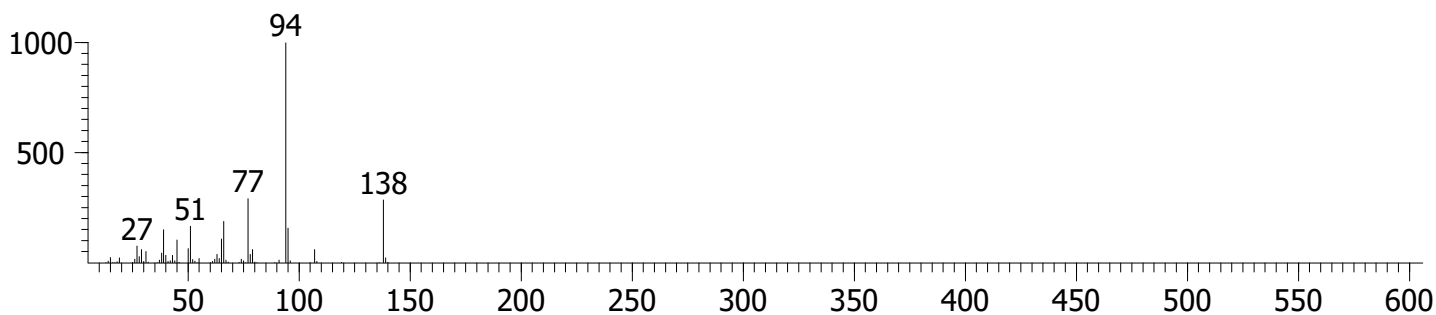
Peak Apex - sample "AnMbr B (20191120):1", peak 1406, at 948.732 , 1.762 sec , sec (Spec # 71287)



Peak True - sample "AnMbr B (20191120):1", peak 1406, at 948.732 , 1.762 sec , sec (Spec # 71287)



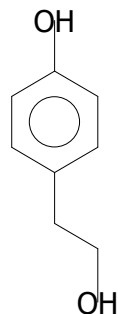
Library Hit - similarity 743, "Ethanol, 2-phenoxy-"



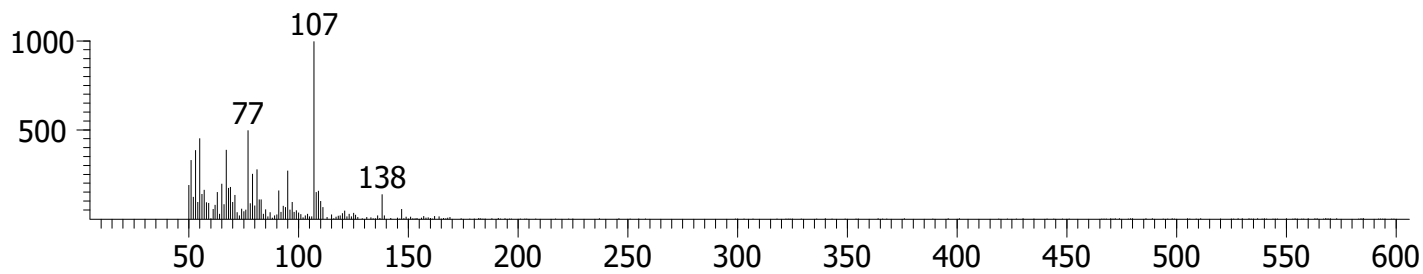
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanol, 2-phenoxy-	743	4231	122-99-6	mainlib	C8H10O2	138
2	Pyrimidine, 5-methyl-	733	2987	2036-41-1	mainlib	C5H6N2	94
3	1H-imidazole, 5-bicyclo[2.2.1]hept-5-en-2-yl-	689	647	0-00-0	mainlib	C10H12N2	160
4	Acetic acid, bromo-, phenyl ester	667	256	620-72-4	mainlib	C8H7BrO2	214
5	Carbamic acid, butylmethyl-, phenyl ester	662	206	54644-61-0	mainlib	C12H17NO2	207

Benzeneethanol, 4-hydroxy-

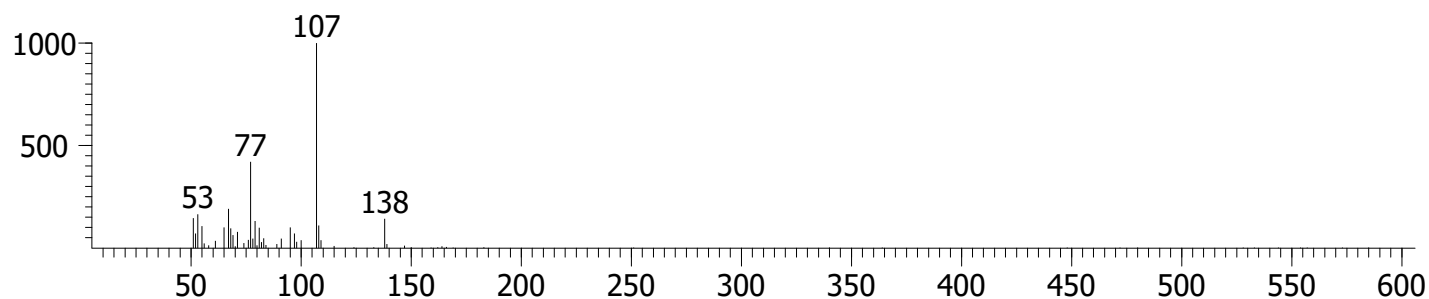
1st Dimension R.T. = 1204.09
2nd Dimension R.T. = 2.066
Quant Mass(es) = 107
S/N = 376.13
Area = 176455
Height = 17334
Similarity = 761



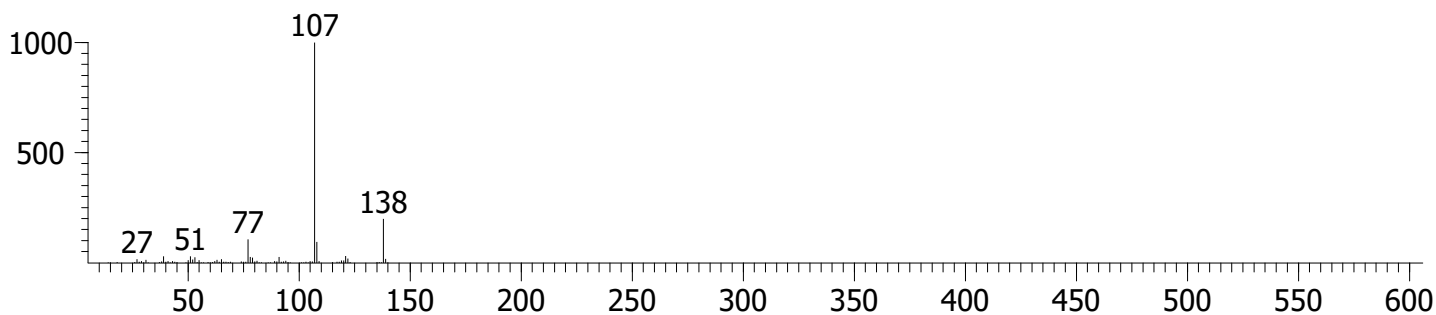
Peak Apex - sample "AnMbr B (20191120):1", peak 2541, at 1204.09 , 2.066 sec , sec (Spec # 110023)



Peak True - sample "AnMbr B (20191120):1", peak 2541, at 1204.09 , 2.066 sec , sec (Spec # 110023)



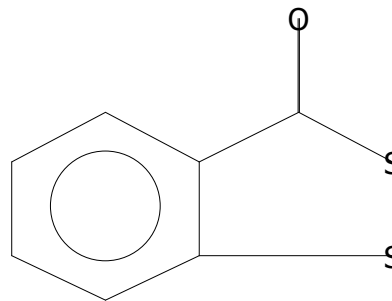
Library Hit - similarity 761, "Benzeneethanol, 4-hydroxy-"



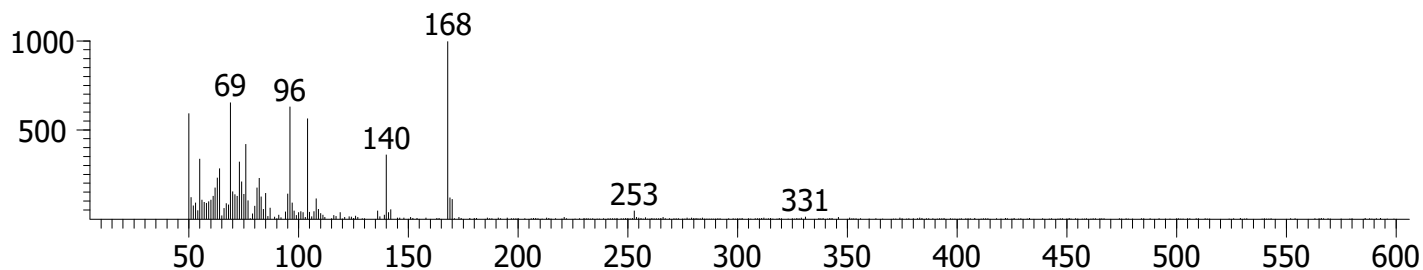
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzeneethanol, 4-hydroxy-	761	6025	501-94-0	mainlib	C ₈ H ₁₀ O ₂	138
2	Hydrazine, 1-(3-hydroxybenzyl)-	736	1837	637-33-2	mainlib	C ₇ H ₁₀ N ₂ O	138
3	5-(4-Hydroxy)-benzyl-2-thioxo-imidazolin-4-one	709	540	0-00-0	mainlib	C ₁₀ H ₁₀ N ₂ O ₂ S	222
4	3-Amino-4-[4-hydroxyphenyl]butanol	684	164	0-00-0	mainlib	C ₁₀ H ₁₅ NO ₂	181
5	9-Oxa-bicyclo[3.3.1]nona-3,6-dien-2-one	684	164	75568-53-5	mainlib	C ₈ H ₈ O ₂	136

3H-1,2-Benzodithiol-3-one

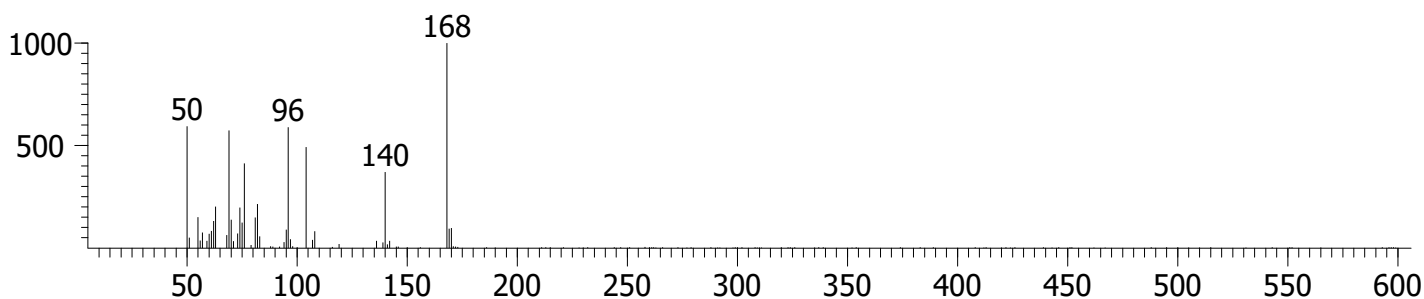
1st Dimension R.T. = 1344.01
2nd Dimension R.T. = 2.449
Quant Mass(es) = 168
S/N = 452.90
Area = 71692
Height = 7498.3
Similarity = 876



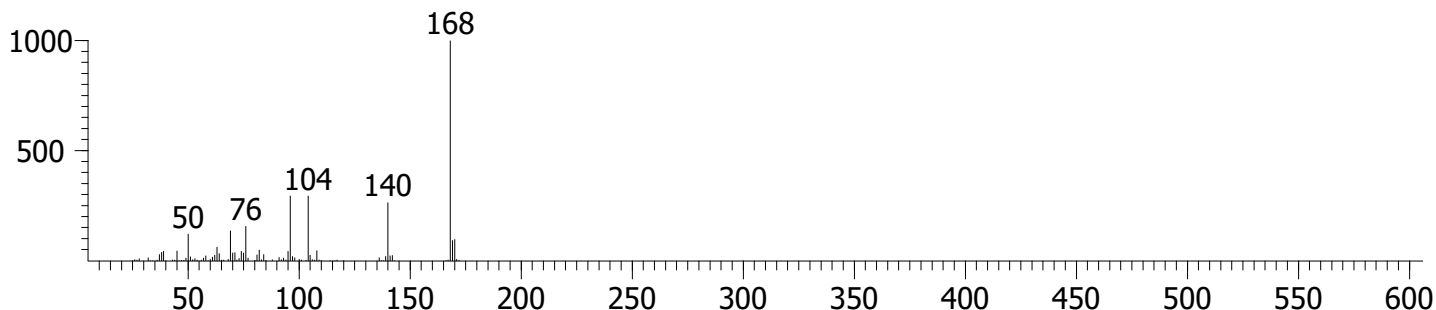
Peak Apex - sample "AnMbr B (20191120):1", peak 3252, at 1344.01 , 2.449 sec , sec (Spec # 131281)



Peak True - sample "AnMbr B (20191120):1", peak 3252, at 1344.01 , 2.449 sec , sec (Spec # 131281)



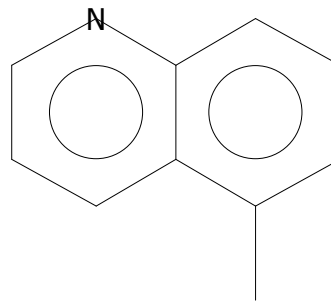
Library Hit - similarity 876, "3H-1,2-Benzodithiol-3-one"



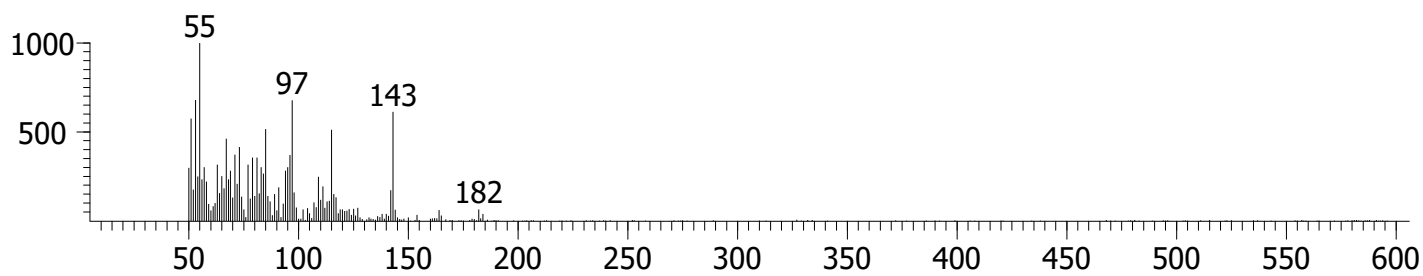
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3H-1,2-Benzodithiol-3-one	876	9758	1677-27-6	mainlib	C7H4OS2	168
2	Quinoline-4-carbonitrile, 2-methyl-	606	97	0-00-0	mainlib	C11H8N2	168
3	Propiohydrazide, 3-(2,3,4,5-tetrahydro-3,5-dioxo-1,2,4-triazin-6-yl)-	582	32	68981-62-4	mainlib	C6H9N5O3	199
4	2-Amino-6-fluorobenzothiazole	561	13	348-40-3	mainlib	C7H5FN2S	168
5	Furan-2-carboxylic acid, 5-[(4-cyclohexylbenzenesulfonylamino)methyl]-, ethyl ester	557	11	0-00-0	mainlib	C20H25NO5S	391

Quinoline, 5-methyl-

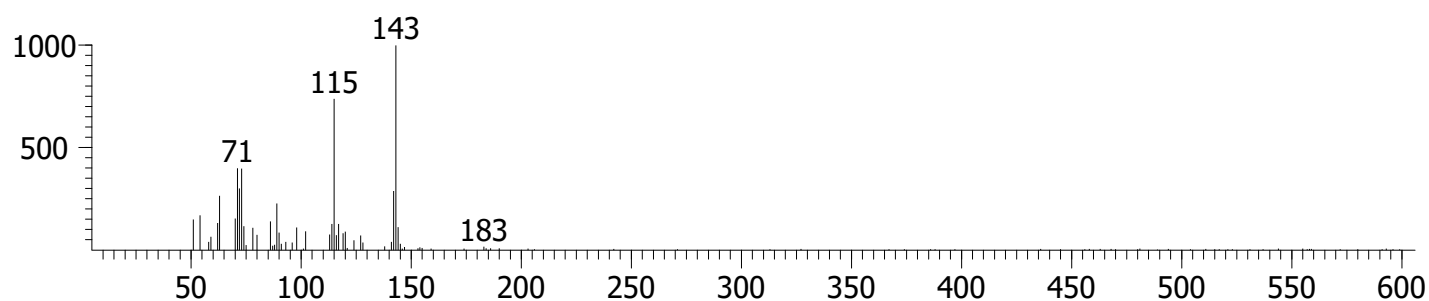
1st Dimension R.T. = 1351
2nd Dimension R.T. = 2.343
Quant Mass(es) = 143
S/N = 198.74
Area = 31514
Height = 3517.0
Similarity = 707



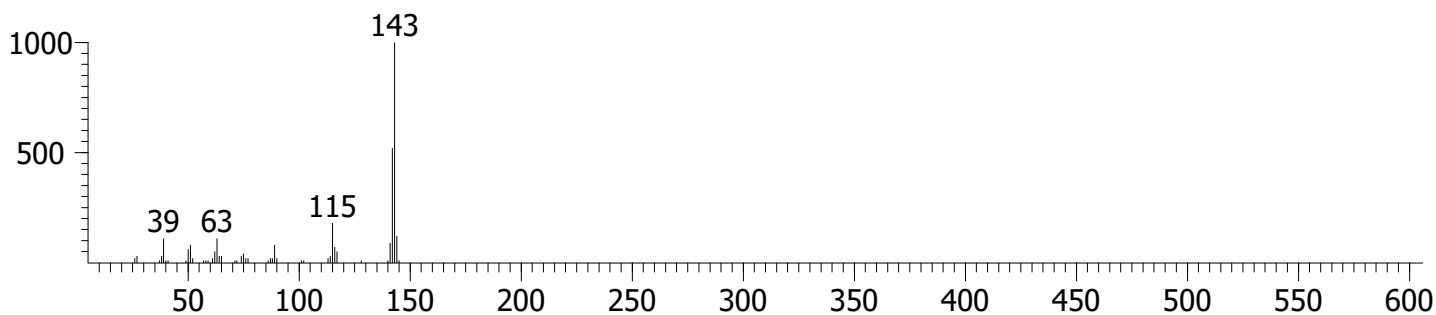
Peak Apex - sample "AnMbr B (20191120):1", peak 3290, at 1351 , 2.343 sec , sec (Spec # 132325)



Peak True - sample "AnMbr B (20191120):1", peak 3290, at 1351 , 2.343 sec , sec (Spec # 132325)



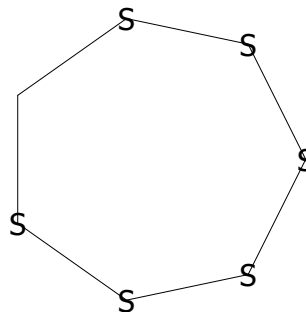
Library Hit - similarity 707, "Quinoline, 5-methyl-"



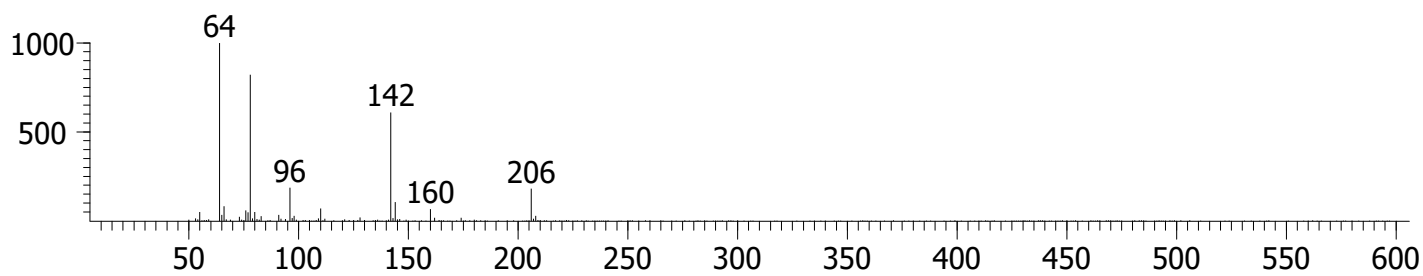
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Quinoline, 5-methyl-	707	1784	7661-55-4	mainlib	C10H9N	143
2	Quinoline, 3-methyl-	703	1507	612-58-8	mainlib	C10H9N	143
3	1H-Pyrrole, 2-phenyl-	696	1154	3042-22-6	mainlib	C10H9N	143
4	Quinoline, 7-methyl-	685	792	612-60-2	mainlib	C10H9N	143
5	Quinoline, 6-methyl-	679	622	91-62-3	mainlib	C10H9N	143

Hexathiepane

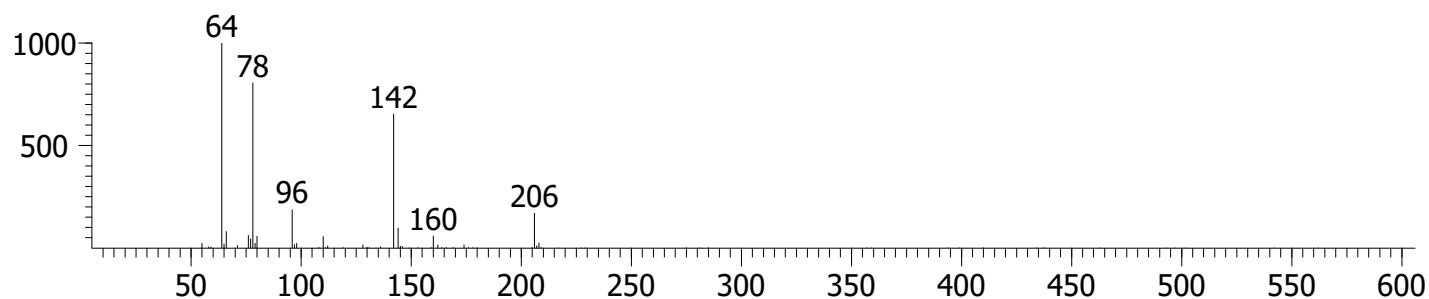
1st Dimension R.T. = 1543.39
2nd Dimension R.T. = 2.937
Quant Mass(es) = 142
S/N = 460.18
Area = 73597
Height = 6718.7
Similarity = 758



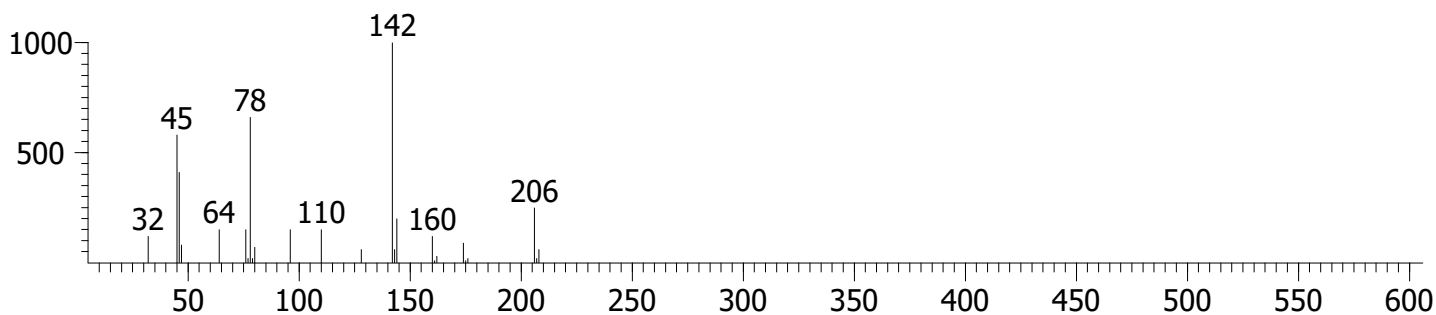
Peak Apex - sample "AnMbr B (20191120):1", peak 4214, at 1543.39 , 2.937 sec , sec (Spec # 161565)



Peak True - sample "AnMbr B (20191120):1", peak 4214, at 1543.39 , 2.937 sec , sec (Spec # 161565)



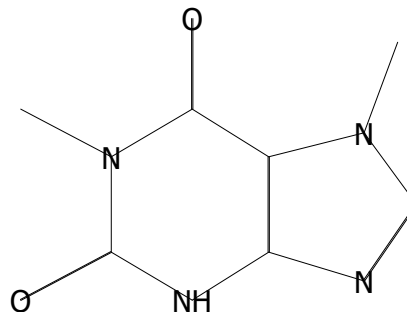
Library Hit - similarity 758, "Hexathiepane"



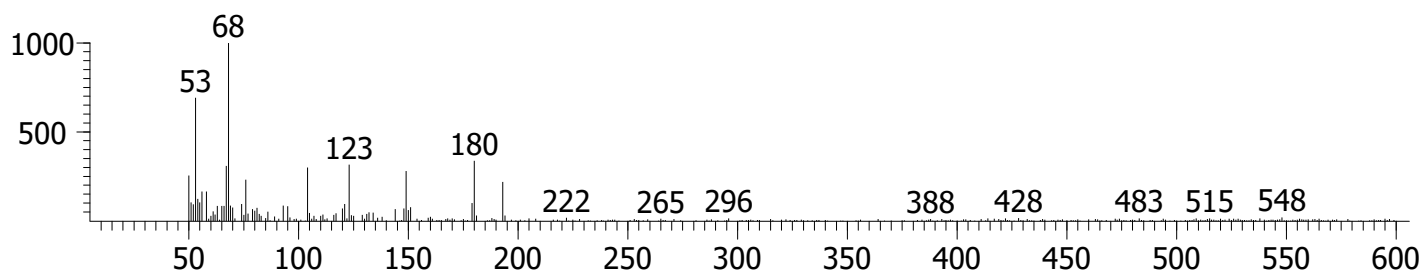
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Hexathiepane	758	9855	17233-71-5	mainlib	CH ₂ S ₆	206
2	Lenthionine	544	98	292-46-6	mainlib	C ₂ H ₄ S ₅	188
3	3,3-Dimercaptoquinuclidine	491	19	4029-14-5	mainlib	C ₇ H ₁₃ NS ₂	175
4	Calconcarboxylic acid	456	4	3737-95-9	mainlib	C ₂₁ H ₁₄ N ₂ O ₇ S	438
5	Cyclohexane-d ₁₂	450	3	1735-17-7	mainlib	C ₆ D ₁₂	96

1,7-Dimethylxanthine

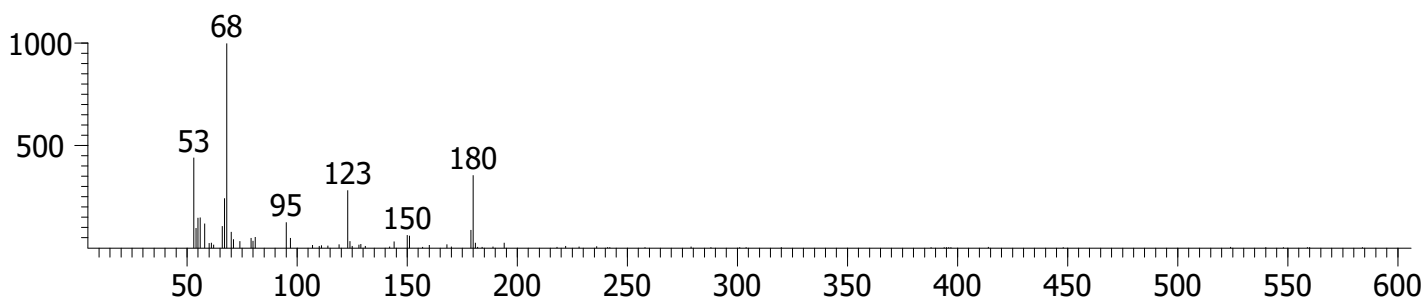
1st Dimension R.T. = 1704.3
2nd Dimension R.T. = 2.779
Quant Mass(es) = 68
S/N = 73.461
Area = 34751
Height = 3117.6
Similarity = 818



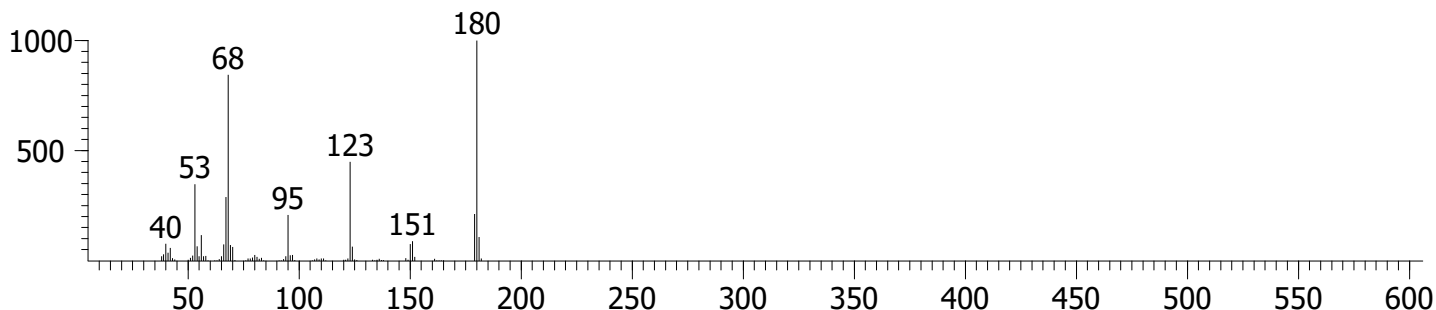
Peak Apex - sample "AnMbr B (20191120):1", peak 4978, at 1704.3 , 2.779 sec , sec (Spec # 185921)



Peak True - sample "AnMbr B (20191120):1", peak 4978, at 1704.3 , 2.779 sec , sec (Spec # 185921)



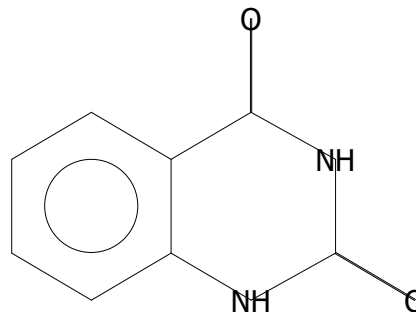
Library Hit - similarity 818, "1,7-Dimethylxanthine"



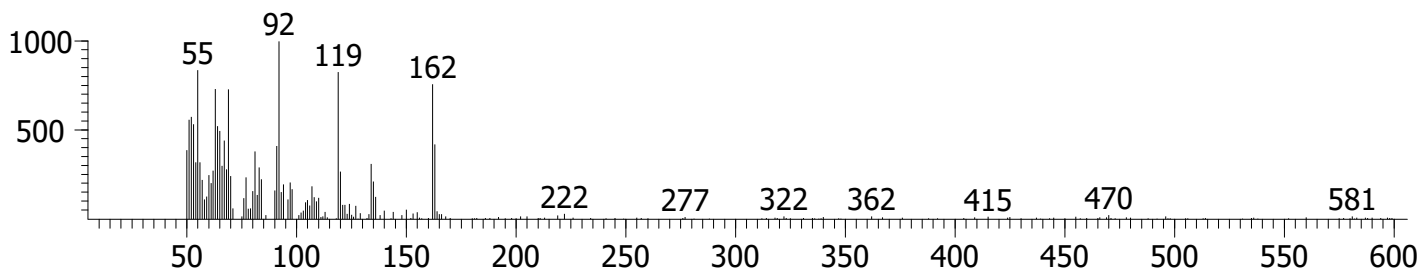
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,7-Dimethylxanthine	818	8189	611-59-6	mainlib	C7H8N4O2	180
2	3-Acetyl-1,7-dimethyl-purine-2,6-dione	757	1426	0-00-0	mainlib	C9H10N4O3	222
3	Theophylline	707	290	58-55-9	mainlib	C7H8N4O2	180
4	7H-Purine-2,6(1H,3H)-dione, 1,3-dimethyl-7-(4-methyl-1,2,5-oxadiazol-3-ylaminomethyl)-	592	17	0-00-0	mainlib	C11H13N7O3	291
5	7-Acetyl-1,3-dimethyl-1H-purine-2,6(3H,7H)-dione	591	16	0-00-0	mainlib	C9H10N4O3	222

2,4(1H,3H)-Quinazolinedione

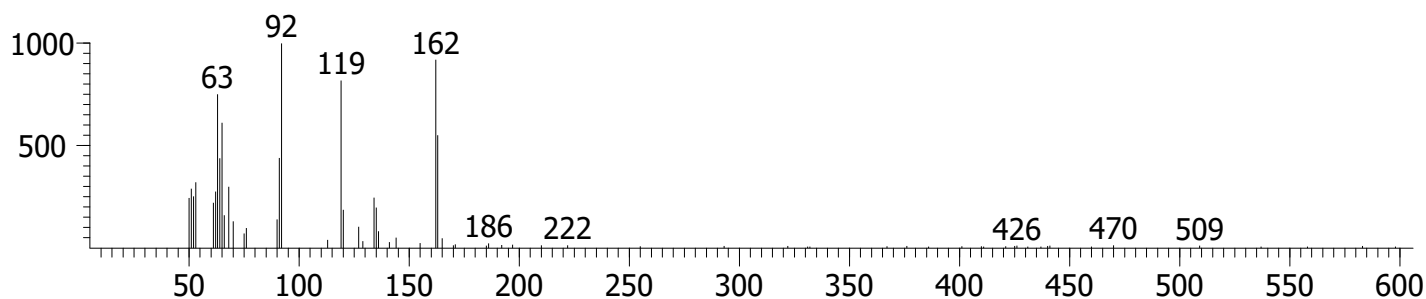
1st Dimension R.T. = 1728.79
2nd Dimension R.T. = 2.785
Quant Mass(es) = 162
S/N = 115.00
Area = 10754
Height = 954.03
Similarity = 696



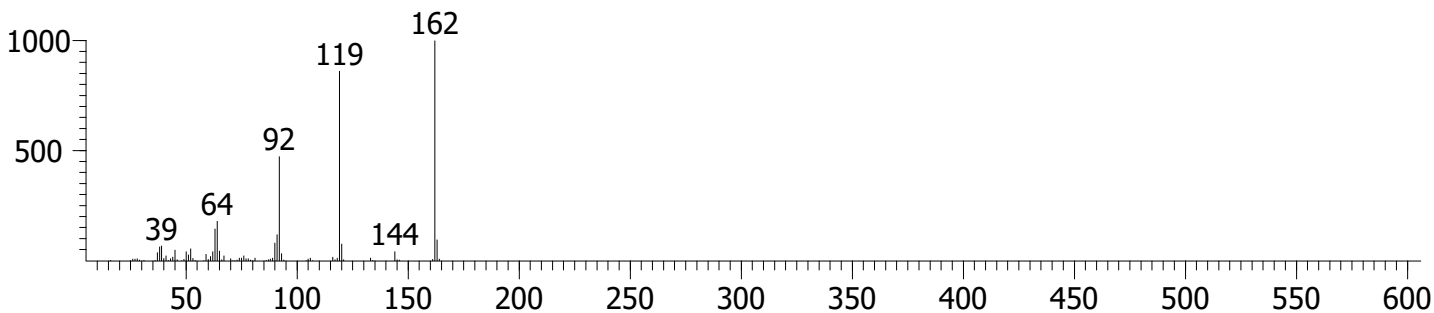
Peak Apex - sample "AnMbr B (20191120):1", peak 5088, at 1728.79 , 2.785 sec , sec (Spec # 189632)



Peak True - sample "AnMbr B (20191120):1", peak 5088, at 1728.79 , 2.785 sec , sec (Spec # 189632)



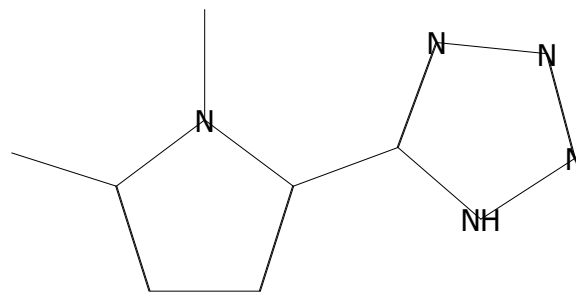
Library Hit - similarity 696, "2,4(1H,3H)-Quinazolinedione"



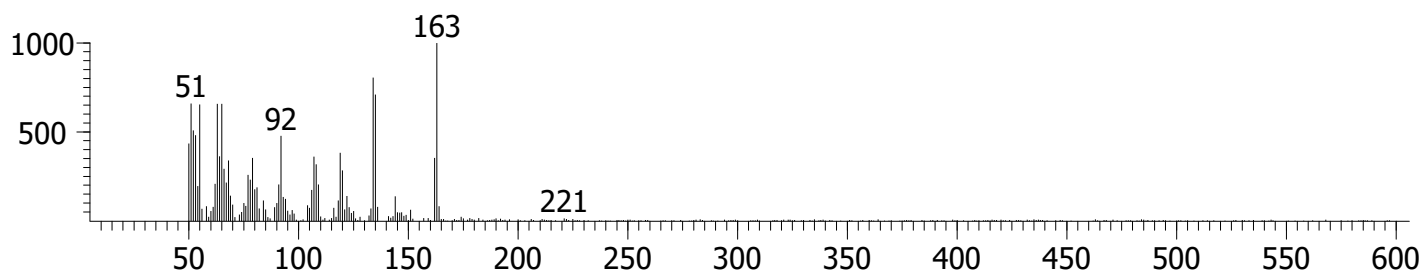
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,4(1H,3H)-Quinazolinedione	696	3387	86-96-4	mainlib	C8H6N2O2	162
2	Urea, 1-(3-methylbenzoyl)-3-(2,4,6-trimethylpyridin-3-yl)-	687	2459	0-00-0	mainlib	C17H19N3O2	297
3	Pyrimidino[2,3-c]pyrrole-5,7(6H)-dione, 2-methyl-	662	749	53636-28-5	mainlib	C8H6N2O2	162
4	Isatoic anhydride	644	386	118-48-9	mainlib	C8H5NO3	163
5	4-Methylquinolinimide	637	296	53636-26-3	mainlib	C8H6N2O2	162

1H-Tetrazole,
5-(1,5-dimethyl-1H-pyrrol-2-yl)-

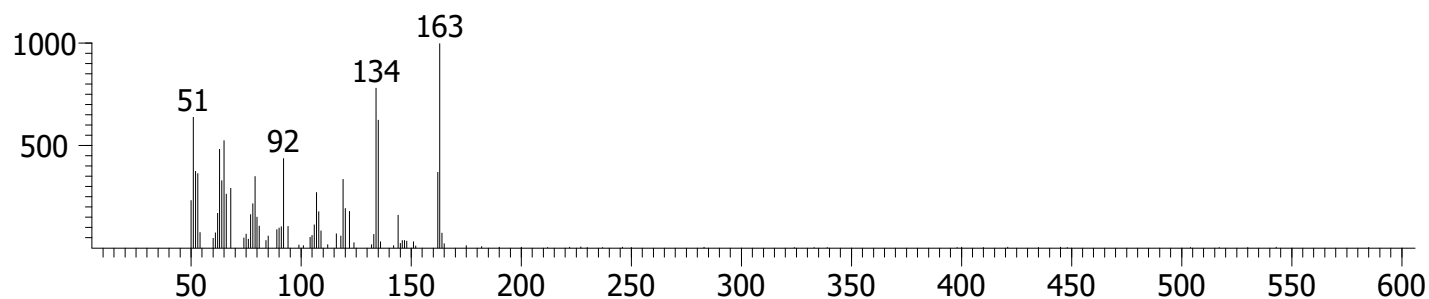
1st Dimension R.T. = 1735.78
 2nd Dimension R.T. = 2.732
 Quant Mass(es) = 163
 S/N = 229.17
 Area = 67736
 Height = 6065.6
 Similarity = 735



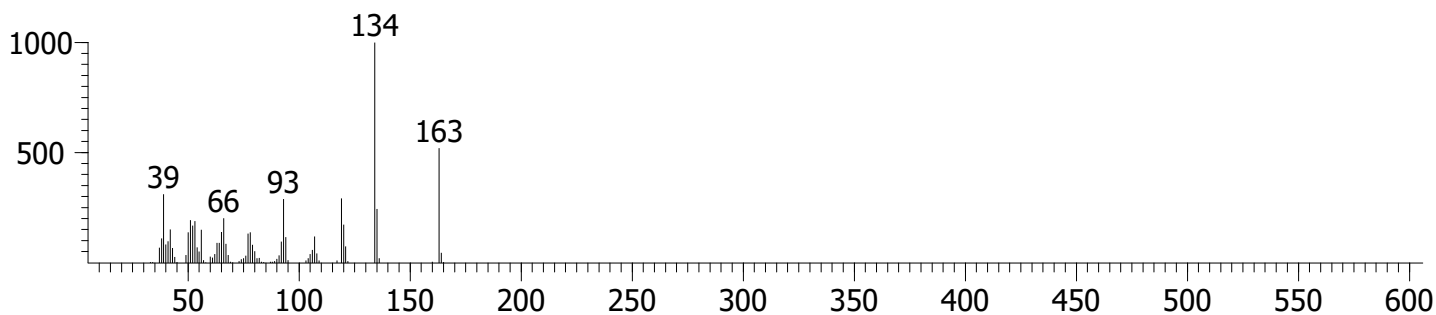
Peak Apex - sample "AnMbr B (20191120):1", peak 5117, at 1735.78 , 2.732 sec , sec (Spec # 190684)



Peak True - sample "AnMbr B (20191120):1", peak 5117, at 1735.78 , 2.732 sec , sec (Spec # 190684)



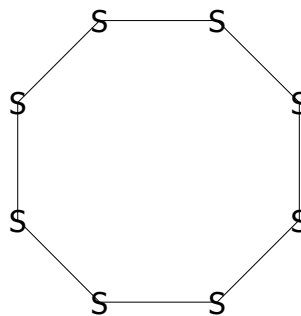
Library Hit - similarity 735, "1H-Tetrazole, 5-(1,5-dimethyl-1H-pyrrol-2-yl)-"



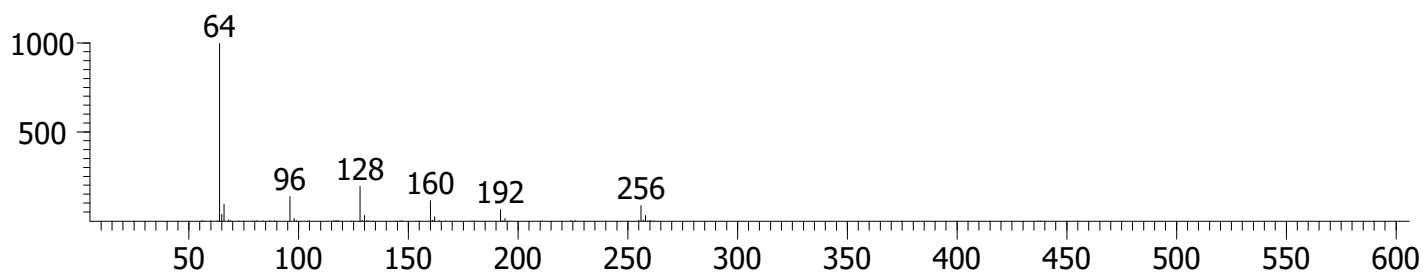
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Tetrazole, 5-(1,5-dimethyl-1H-pyrrol-2-yl)-	735	3658	0-00-0	mainlib	C7H9N5	163
2	1-Amino-4,6-dimethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile	683	730	1562-12-5	mainlib	C8H9N3O	163
3	Phenol, 2-amino-4-(2-methyl-2H-1,2,3,4-tetrazol-5-yl)-	676	559	0-00-0	mainlib	C8H9N5O	191
4	(Chroman-7-yl)methylamine	667	406	0-00-0	mainlib	C10H13NO	163
5	Isoquinoline, 1,2,3,4-tetrahydro-6-methoxy-	664	358	42923-77-3	mainlib	C10H13NO	163

Cyclic octaatomic sulfur

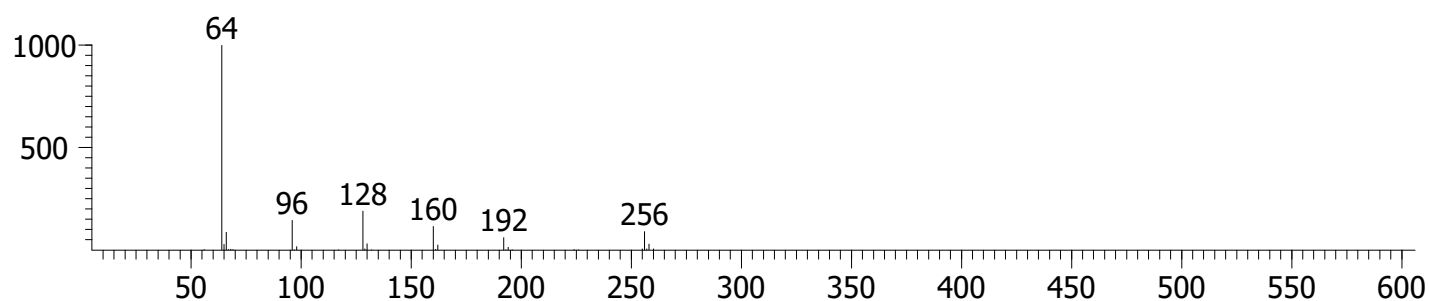
1st Dimension R.T. = 1872.2
2nd Dimension R.T. = 3.175
Quant Mass(es) = 64
S/N = 969.39
Area = 593078
Height = 45705
Similarity = 726



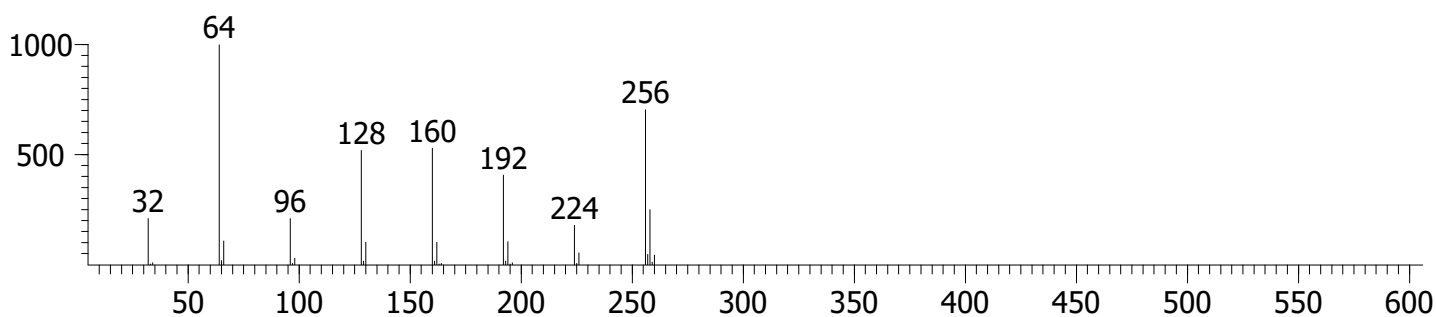
Peak Apex - sample "AnMbr B (20191120):1", peak 5556, at 1872.2 , 3.175 sec , sec (Spec # 211421)



Peak True - sample "AnMbr B (20191120):1", peak 5556, at 1872.2 , 3.175 sec , sec (Spec # 211421)



Library Hit - similarity 726, "Cyclic octaatomic sulfur"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Cyclic octaatomic sulfur	726	9427	10544-50-0	mainlib	S8	256
2	Dibenzo[cd,g]indazole-3-sulfonic acid, 2,6-dihydro-6-oxo-	546	169	293765-87-4	mainlib	C14H8N2O4S	300
3	Hexathiane	546	169	13798-23-7	mainlib	S6	192
4	Methanethiol, N-(p-methoxyphenethyl)amidino-, hydrogen thiosulfate	537	123	40283-94-1	mainlib	C11H16N2O4S2	304
5	Dipentamethylenethiuram hexasulfide	473	20	971-15-3	mainlib	C12H20N2S6	384

1,4-Benzenediamine,
N-(1-methylethyl)-N'-phenyl-

1st Dimension R.T. = 1903.69

2nd Dimension R.T. = 2.317

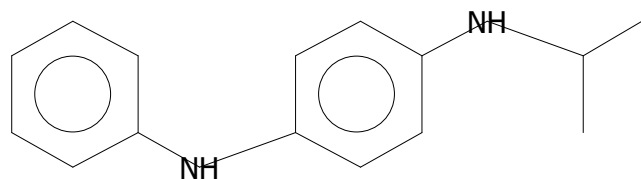
Quant Mass(es) = 211

S/N = 720.17

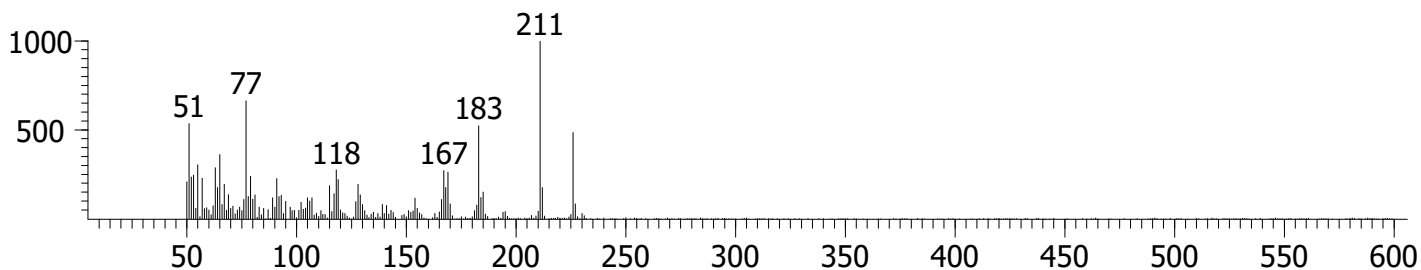
Area = 72790

Height = 6659.1

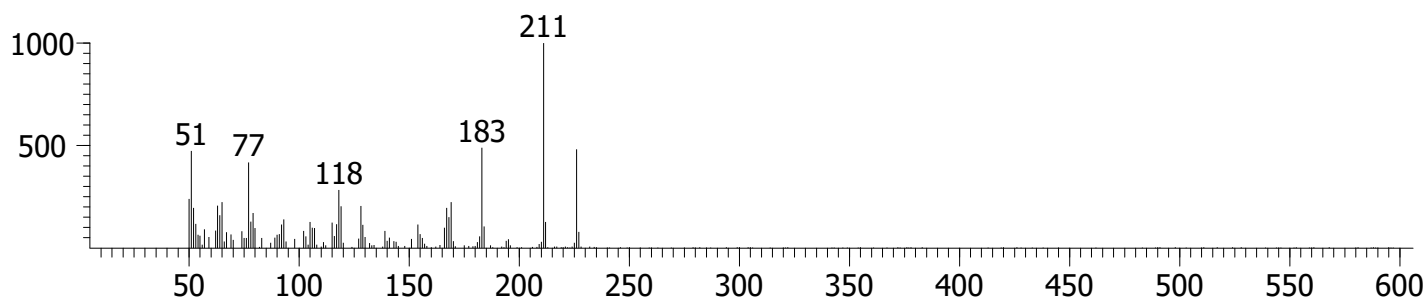
Similarity = 772



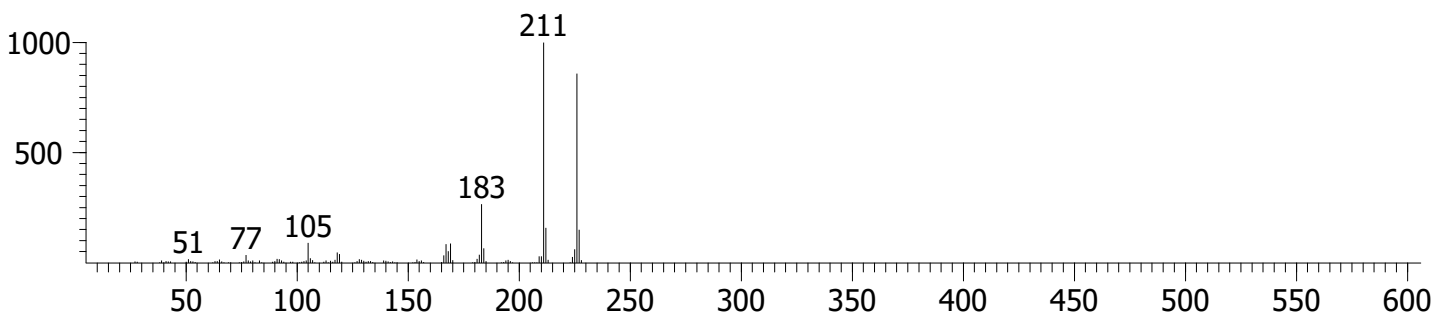
Peak Apex - sample "AnMbr B (20191120):1", peak 5618, at 1903.69 , 2.317 sec , sec (Spec # 216061)



Peak True - sample "AnMbr B (20191120):1", peak 5618, at 1903.69 , 2.317 sec , sec (Spec # 216061)



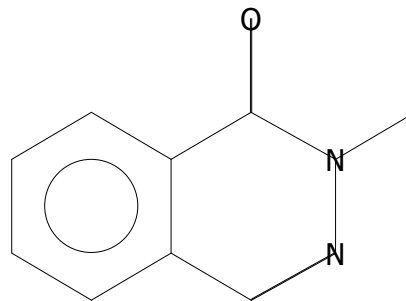
Library Hit - similarity 772, "1,4-Benzenediamine, N-(1-methylethyl)-N'-phenyl-"



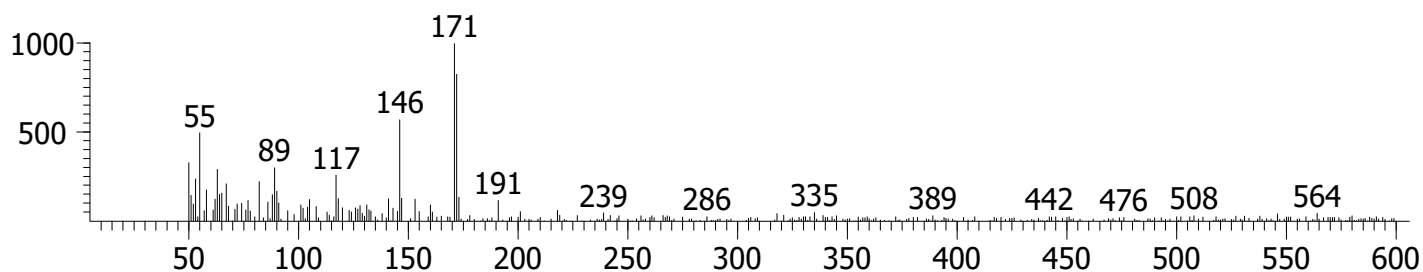
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,4-Benzenediamine, N-(1-methylethyl)-N'-phenyl-	772	5922	101-72-4	mainlib	C15H18N2	226
2	3,8-Dimethyl-2,8-diazatricyclo[8.4.0.0(2,6)]tetradeca-1(10),3,5,11,13-pentaen-9-one	699	806	0-00-0	mainlib	C14H14N2O	226
3	Benzene, 1-(1,1-dimethylethyl)-4-phenoxy-	682	440	5331-28-2	mainlib	C16H18O	226
4	Beta-carboline, 6-methoxy-1,2-dimethyl-	674	328	154505-42-7	mainlib	C14H14N2O	226
5	1,1'-Biphenyl, 3-(1,1-dimethylethoxy)-	673	315	55059-21-7	mainlib	C16H18O	226

Phthalazin-1(2H)-one, 2-ethenyl-

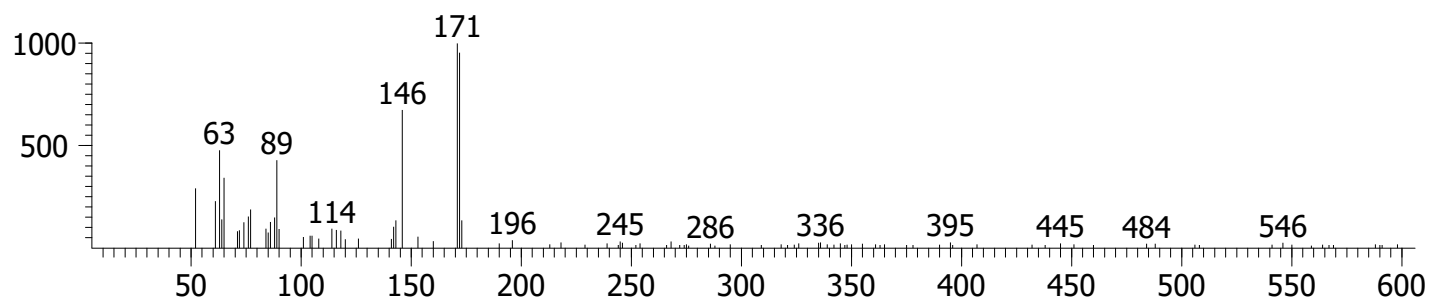
1st Dimension R.T. = 1956.16
2nd Dimension R.T. = 3.188
Quant Mass(es) = 171
S/N = 57.641
Area = 18697
Height = 1314.8
Similarity = 682



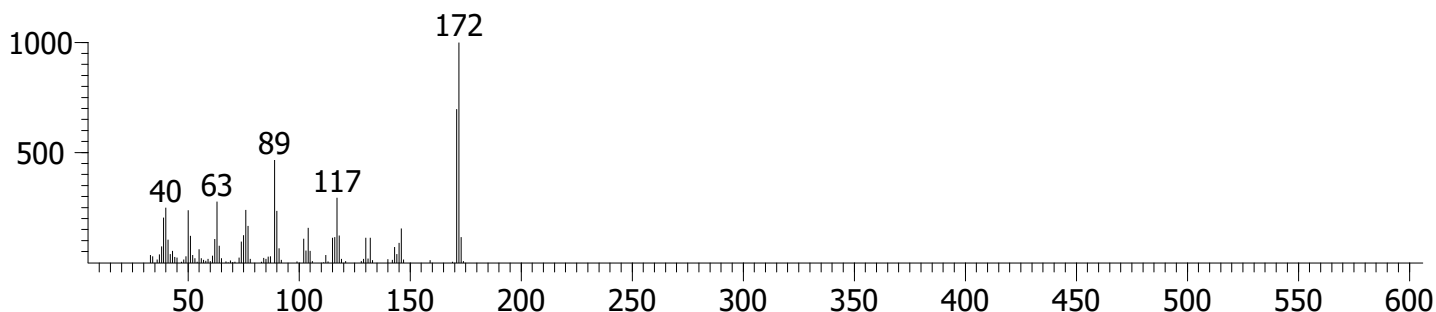
Peak Apex - sample "AnMbr B (20191120):1", peak 5738, at 1956.16 , 3.188 sec , sec (Spec # 224143)



Peak True - sample "AnMbr B (20191120):1", peak 5738, at 1956.16 , 3.188 sec , sec (Spec # 224143)



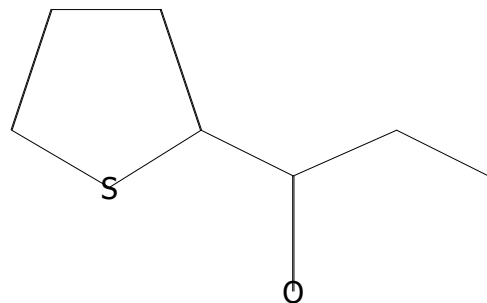
Library Hit - similarity 682, "Phthalazin-1(2H)-one, 2-ethenyl-"



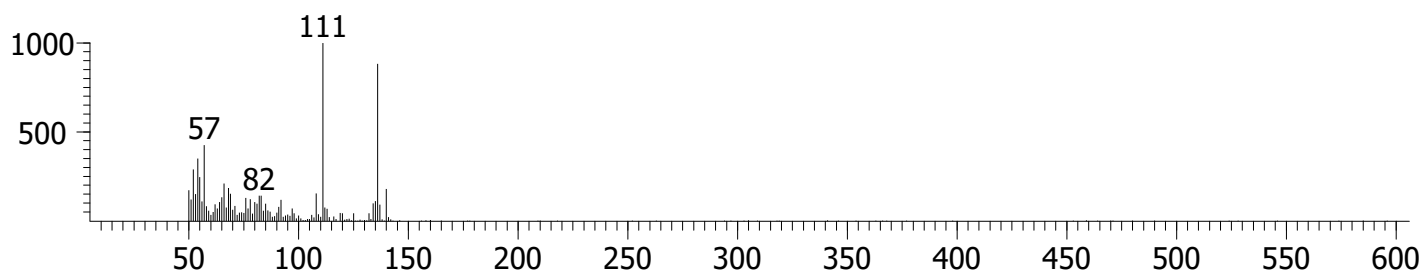
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phthalazin-1(2H)-one, 2-ethenyl-	682	2137	0-00-0	mainlib	C10H8N2O	172
2	4-Hydroxy-1-naphthaldehyde	670	1423	7770-45-8	mainlib	C11H8O2	172
3	3-Phenyl-1H-pyrazole-4-carbaldehyde	663	1090	26033-20-5	mainlib	C10H8N2O	172
4	1,3-Diazatricyclo[6.3.1.0(4,12)]dodeca-4,6,8(12),9-tetraen-2-one	659	921	83848-83-3	mainlib	C10H8N2O	172
5	Imidazole, 1,4-dimethyl-2-phenyl-	654	742	0-00-0	mainlib	C11H12N2	172

1-(2-Thienyl)-1-propanone

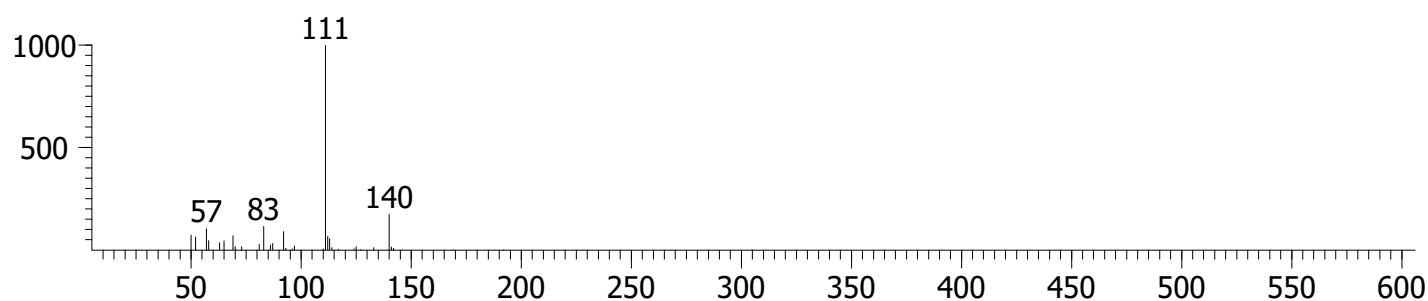
1st Dimension R.T. = 854.286
2nd Dimension R.T. = 1.921
Quant Mass(es) = 111
S/N = 471.09
Area = 82507
Height = 10175
Similarity = 815



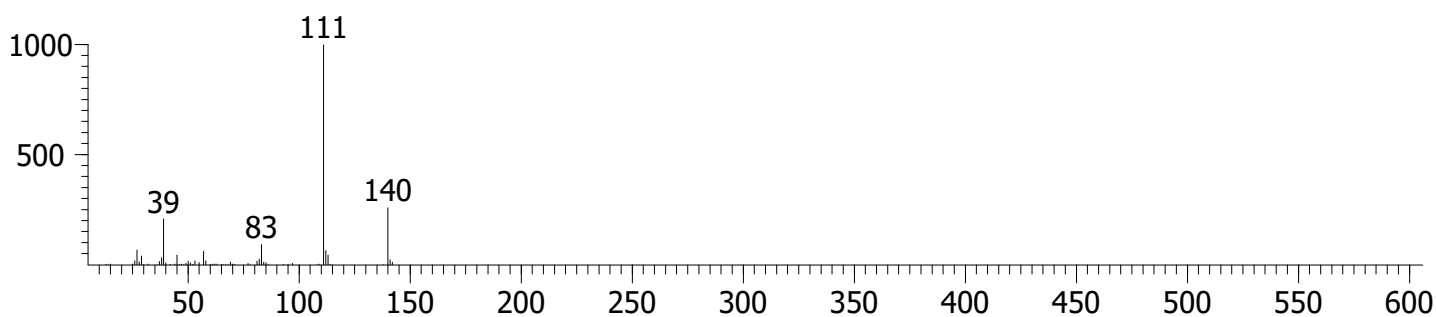
Peak Apex - sample "AnBxr B (20191121):1", peak 1263, at 854.286 , 1.921 sec , sec (Spec # 57001)



Peak True - sample "AnBxr B (20191121):1", peak 1263, at 854.286 , 1.921 sec , sec (Spec # 57001)



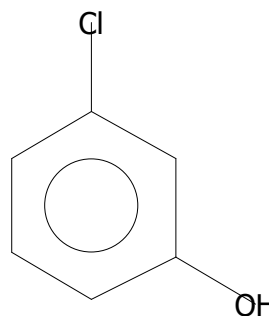
Library Hit - similarity 815, "1-(2-Thienyl)-1-propanone"



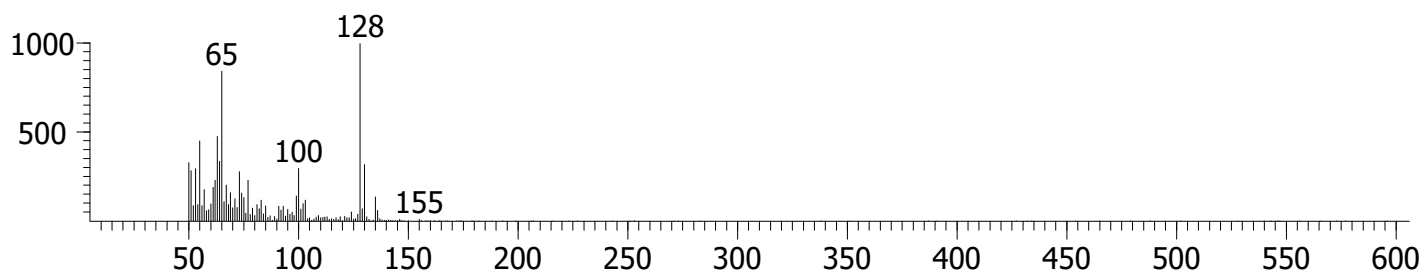
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1-(2-Thienyl)-1-propanone	815	3655	13679-75-9	mainlib	C7H8OS	140
2	1-(2-Thienyl)-1-propanone	814	8267	13679-75-9	replib	C7H8OS	140
3	1-(2-Thienyl)-1-propanone	813	8267	13679-75-9	replib	C7H8OS	140
4	Glycine, N-(2-thienylcarbonyl)-, methyl ester	810	2946	0-00-0	mainlib	C8H9NO3S	199
5	Thiophene, 2-methyl-5-propyl-	778	787	33933-73-2	mainlib	C8H12S	140

Phenol, 3-chloro-

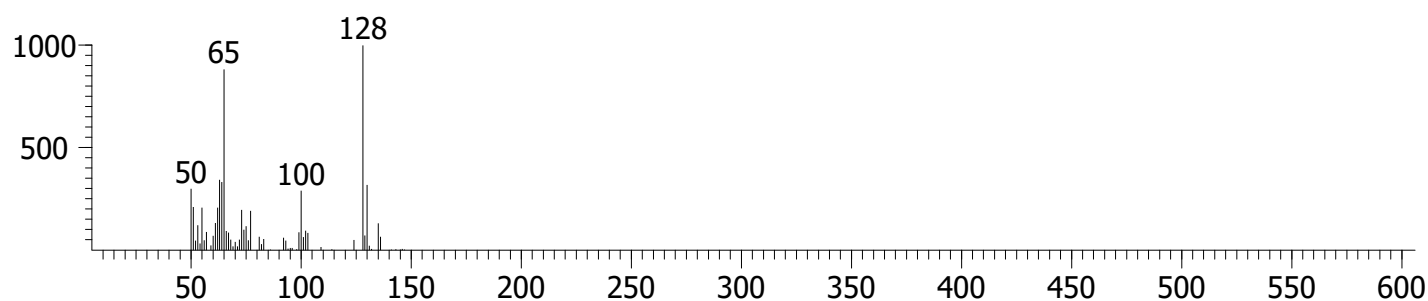
1st Dimension R.T. = 878.772
2nd Dimension R.T. = 1.782
Quant Mass(es) = 128
S/N = 926.37
Area = 328939
Height = 39073
Similarity = 784



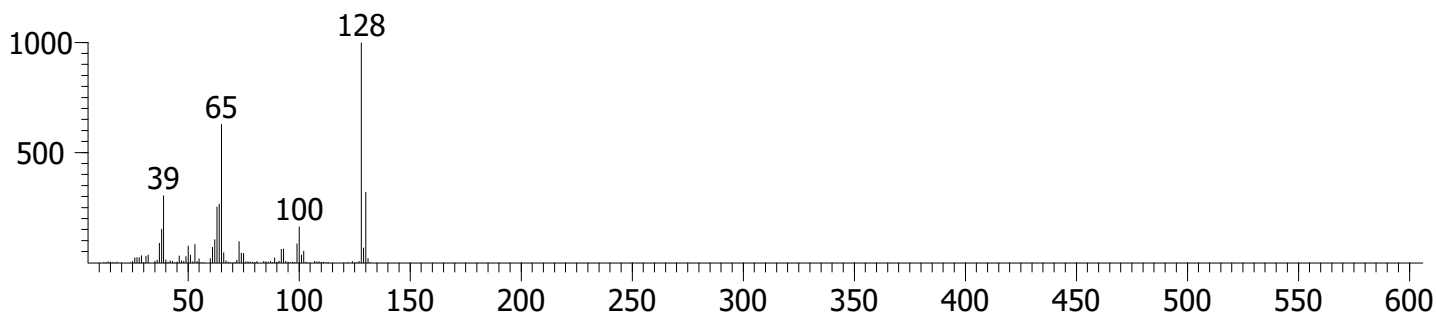
Peak Apex - sample "AnBxr B (20191121):1", peak 1368, at 878.772 , 1.782 sec , sec (Spec # 60690)



Peak True - sample "AnBxr B (20191121):1", peak 1368, at 878.772 , 1.782 sec , sec (Spec # 60690)



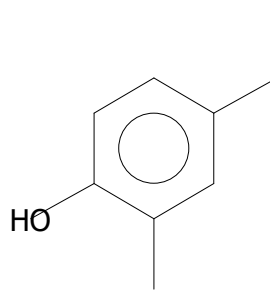
Library Hit - similarity 784, "Phenol, 3-chloro-"



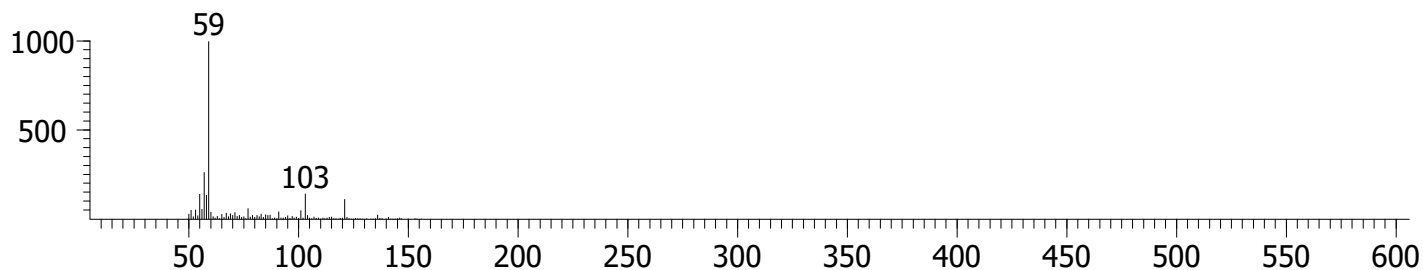
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 3-chloro-	784	4610	108-43-0	replib	C6H5ClO	128
2	Phenol, 3-chloro-	781	4610	108-43-0	replib	C6H5ClO	128
3	Phenol, 4-chloro-	781	4073	106-48-9	replib	C6H5ClO	128
4	Phenol, 4-chloro-	773	4073	106-48-9	replib	C6H5ClO	128
5	Phenol, 4-chloro-	770	2901	106-48-9	mainlib	C6H5ClO	128

Phenol, 4-ethyl-2-methyl-

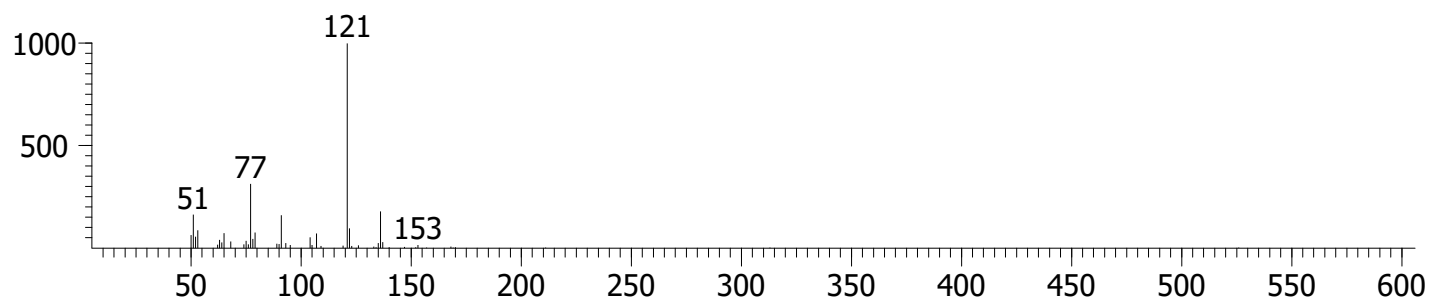
1st Dimension R.T. = 924.246
2nd Dimension R.T. = 1.749
Quant Mass(es) = 121
S/N = 617.25
Area = 114052
Height = 16397
Similarity = 913



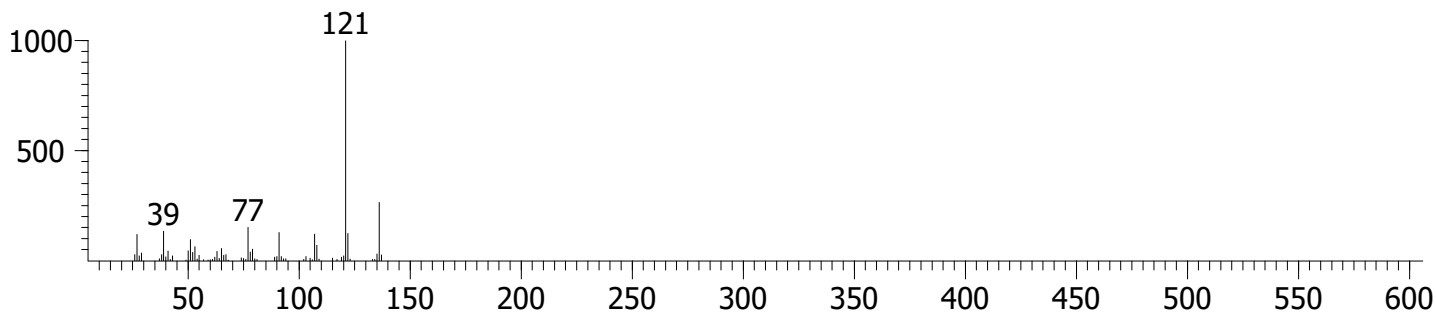
Peak Apex - sample "AnBxr B (20191121):1", peak 1627, at 924.246 , 1.749 sec , sec (Spec # 67575)



Peak True - sample "AnBxr B (20191121):1", peak 1627, at 924.246 , 1.749 sec , sec (Spec # 67575)



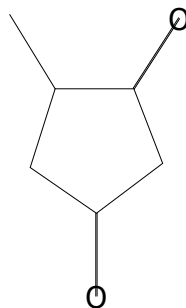
Library Hit - similarity 913, "Phenol, 4-ethyl-2-methyl-"



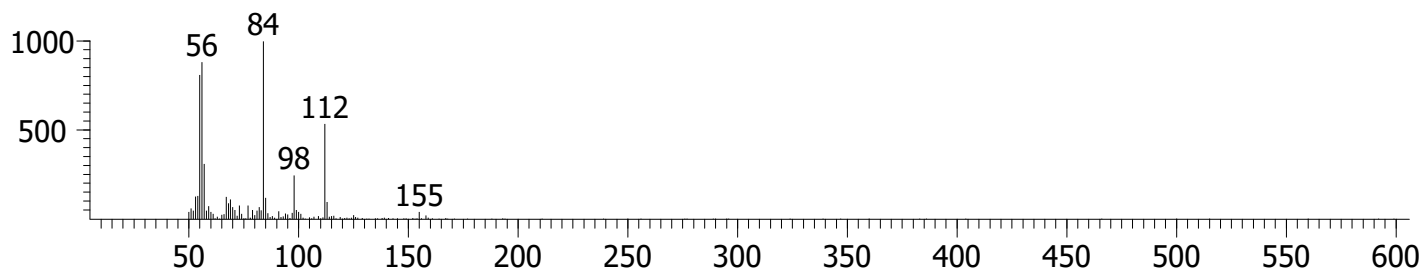
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 4-ethyl-2-methyl-	913	3522	2219-73-0	mainlib	C9H12O	136
2	Phenol, 4-ethyl-3-methyl-	897	2028	1123-94-0	mainlib	C9H12O	136
3	Phenol, 2-ethyl-6-methyl-	894	1792	1687-64-5	mainlib	C9H12O	136
4	Phenol, 2-ethyl-5-methyl-	877	978	1687-61-2	mainlib	C9H12O	136
5	Phenol, 3-ethyl-5-methyl-	865	3969	698-71-5	replib	C9H12O	136

1,3-Cyclopentanedione, 4-methyl-

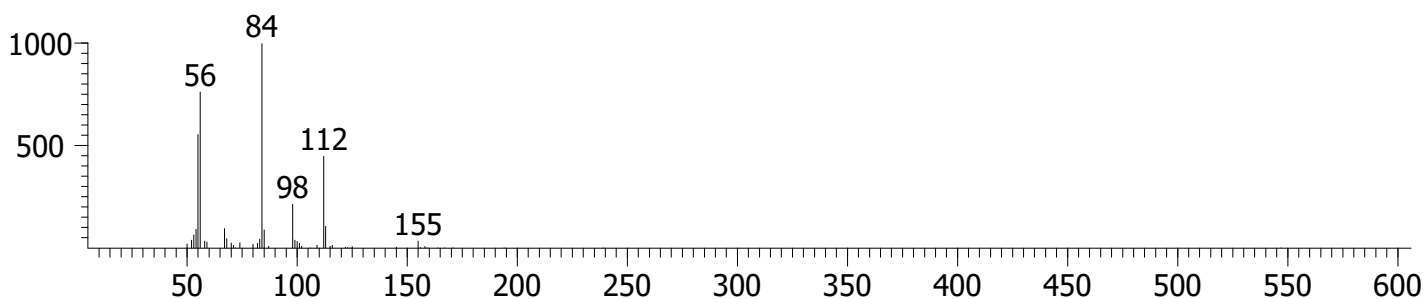
1st Dimension R.T. = 1169.11
2nd Dimension R.T. = 2.363
Quant Mass(es) = 84
S/N = 478.91
Area = 194019
Height = 19059
Similarity = 783



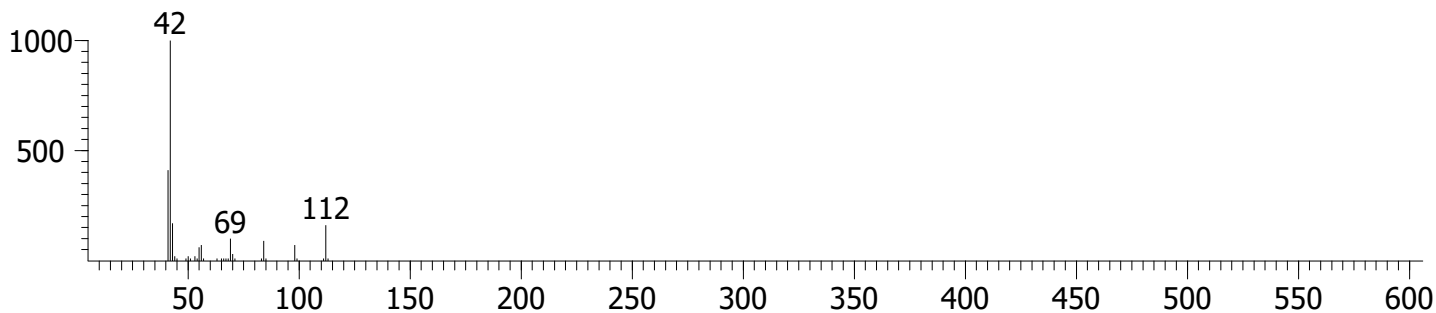
Peak Apex - sample "AnBxr B (20191121):1", peak 3015, at 1169.11 , 2.363 sec , sec (Spec # 104768)



Peak True - sample "AnBxr B (20191121):1", peak 3015, at 1169.11 , 2.363 sec , sec (Spec # 104768)



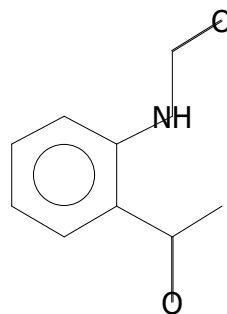
Library Hit - similarity 783, "1,3-Cyclopentanedione, 4-methyl-"



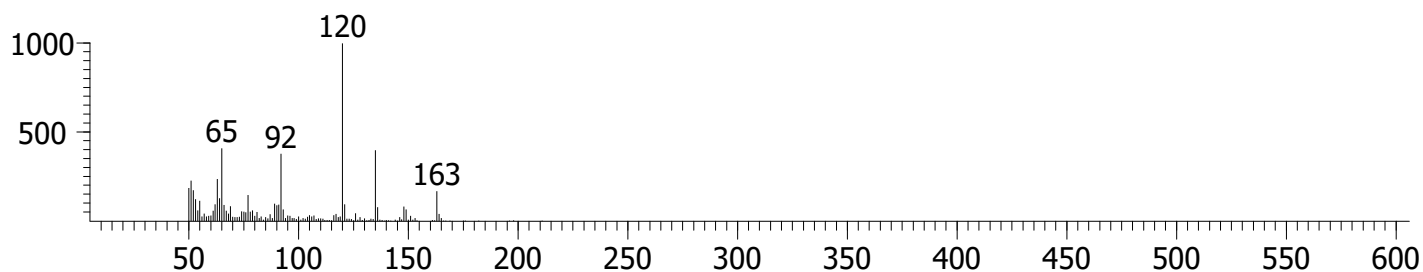
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,3-Cyclopentanedione, 4-methyl-	783	4379	35029-03-9	mainlib	C6H8O2	112
2	2H-Pyran-2,6(3H)-dione	743	1015	5926-95-4	mainlib	C5H4O3	112
3	Aziridine, 1-ethyl-2-methyl-3-(1-methylethyl)-, trans-	730	656	55702-73-3	mainlib	C8H17N	127
4	2-Amino-oxazole	729	630	4570-45-0	mainlib	C3H4N2O	84
5	1,5-Diazocine, octahydro-1,5-dinitroso-	723	495	55556-89-3	mainlib	C6H12N4O2	172

Formamide, N-(2-acetylphenyl)-

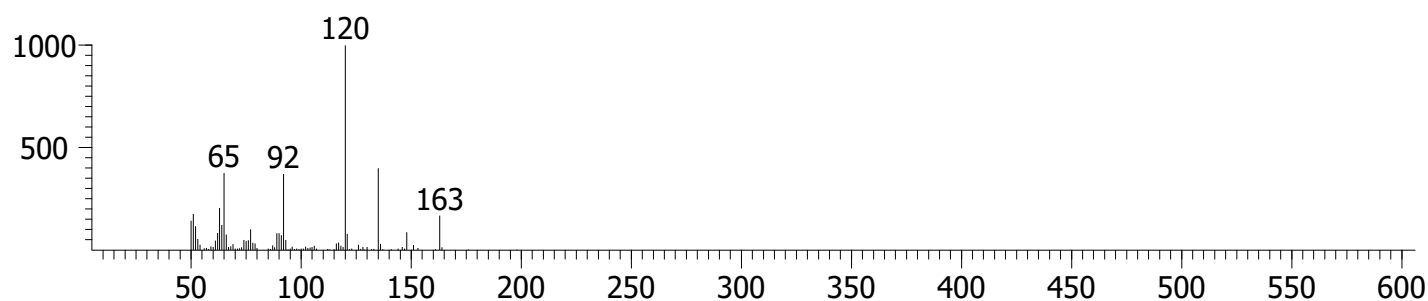
1st Dimension R.T. = 1378.99
2nd Dimension R.T. = 2.449
Quant Mass(es) = 120
S/N = 2685.8
Area = 967479
Height = 92120
Similarity = 884



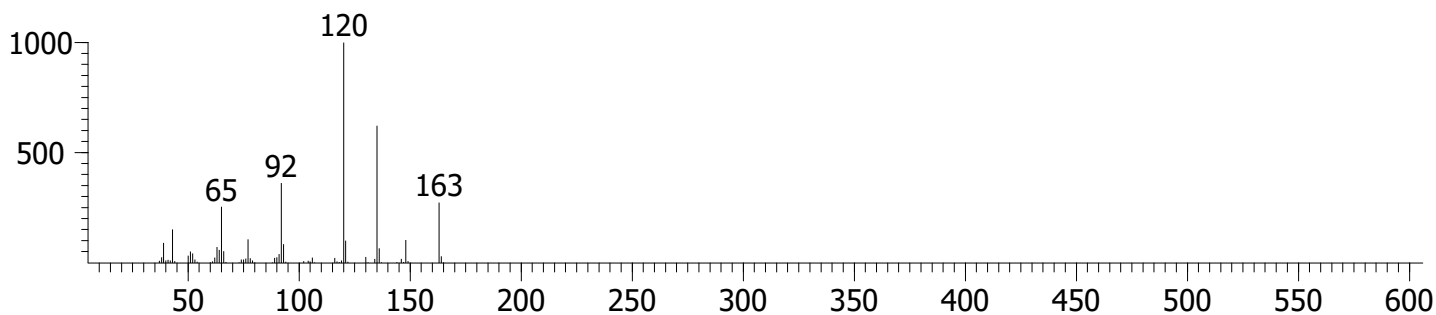
Peak Apex - sample "AnBxr B (20191121):1", peak 4345, at 1378.99 , 2.449 sec , sec (Spec # 136581)



Peak True - sample "AnBxr B (20191121):1", peak 4345, at 1378.99 , 2.449 sec , sec (Spec # 136581)



Library Hit - similarity 884, "Formamide, N-(2-acetylphenyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Formamide, N-(2-acetylphenyl)-	884	6685	5257-06-7	mainlib	C9H9NO2	163
2	Formamide, N-(2-acetylphenyl)-	868	6102	5257-06-7	replib	C9H9NO2	163
3	Acetophenone, 4'-amino-	844	2045	99-92-3	replib	C8H9NO	135
4	Ethanone, 1-(2-aminophenyl)-	833	1347	551-93-9	mainlib	C8H9NO	135
5	Ethanone, 1-(2-aminophenyl)-	827	1116	551-93-9	replib	C8H9NO	135

Benzene.

1,4-dimethyl-2,5-bis(1-methylethyl)-

1st Dimension R.T. = 1494.42

2nd Dimension R.T. = 2.099

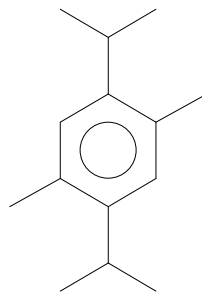
Quant Mass(es) = 175

S/N = 649.04

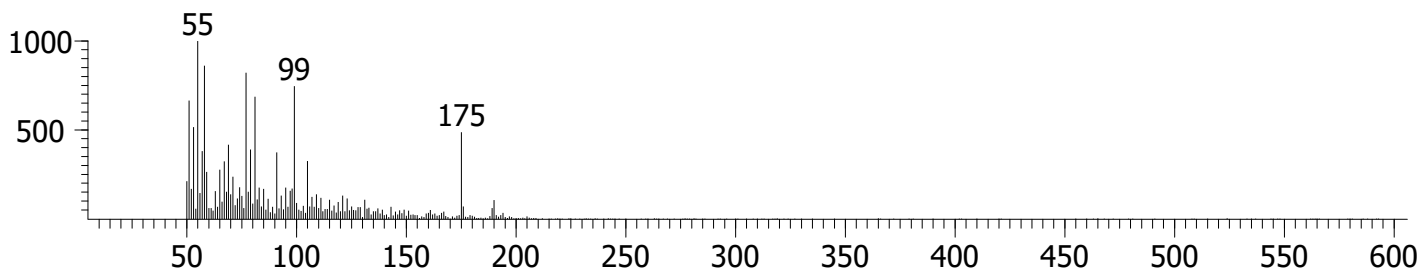
Area = 66684

Height = 6523.3

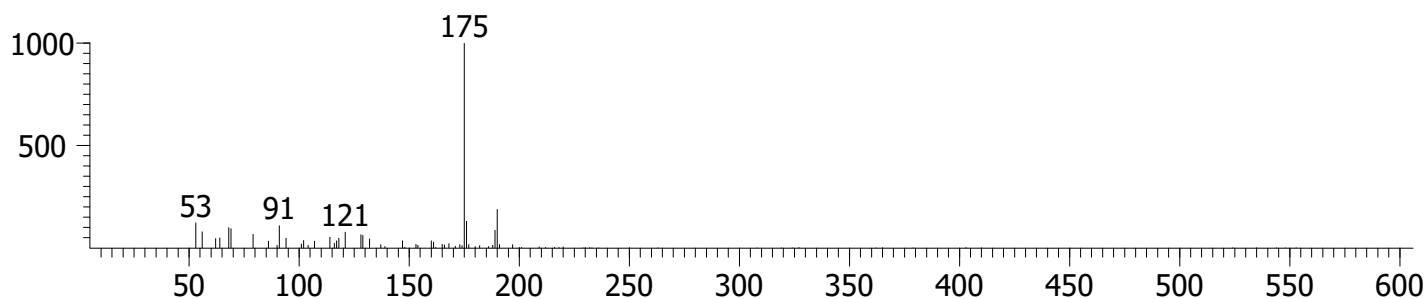
Similarity = 767



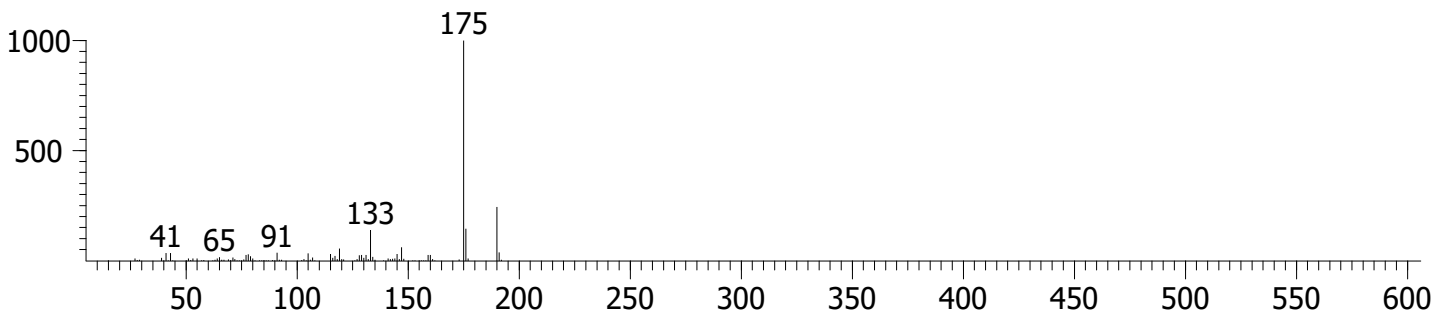
Peak Apex - sample "AnBxr B (20191121):1", peak 5116, at 1494.42 , 2.099 sec , sec (Spec # 154018)



Peak True - sample "AnBxr B (20191121):1", peak 5116, at 1494.42 , 2.099 sec , sec (Spec # 154018)



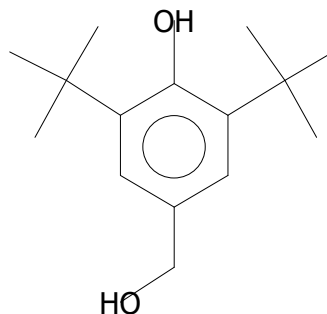
Library Hit - similarity 767, "Benzene, 1,4-dimethyl-2,5-bis(1-methylethyl)-"



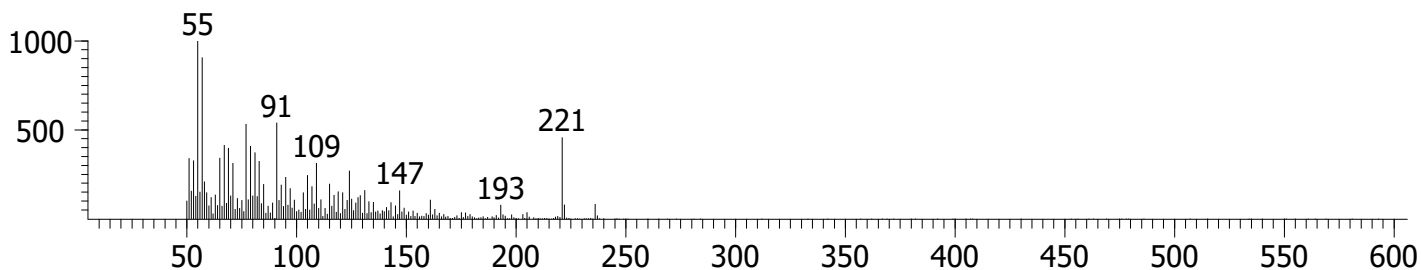
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1,4-dimethyl-2,5-bis(1-methylethyl)-	767	4486	10375-96-9	replib	C14H22	190
2	Precocene I	755	1805	17598-02-6	mainlib	C12H14O2	190
3	Benzene, 1,4-bis(1,1-dimethylethyl)-	753	2808	1012-72-2	replib	C14H22	190
4	1,2,5-Oxadiazole-3-carboxamide, 4-amino-N-[2-[[[(2,3-dihydro-1,3-dimethyl-2-oxo-1H-1,3-benzimidazol-5-yl)methyl]amino]ethyl]-	742	1166	0-00-0	mainlib	C15H19N7O3	345
5	Benzene, 1,5-dimethyl-2,4-bis(1-methylethyl)-	736	916	5186-68-5	mainlib	C14H22	190

3,5-di-tert-Butyl-4-hydroxybenzyl alcohol

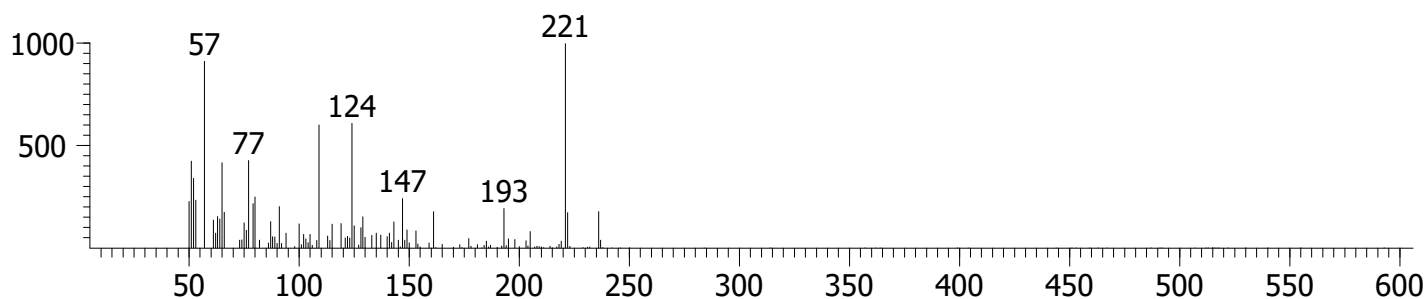
1st Dimension R.T. = 1574.87
2nd Dimension R.T. = 1.861
Quant Mass(es) = 221
S/N = 695.93
Area = 91651
Height = 7184.3
Similarity = 673



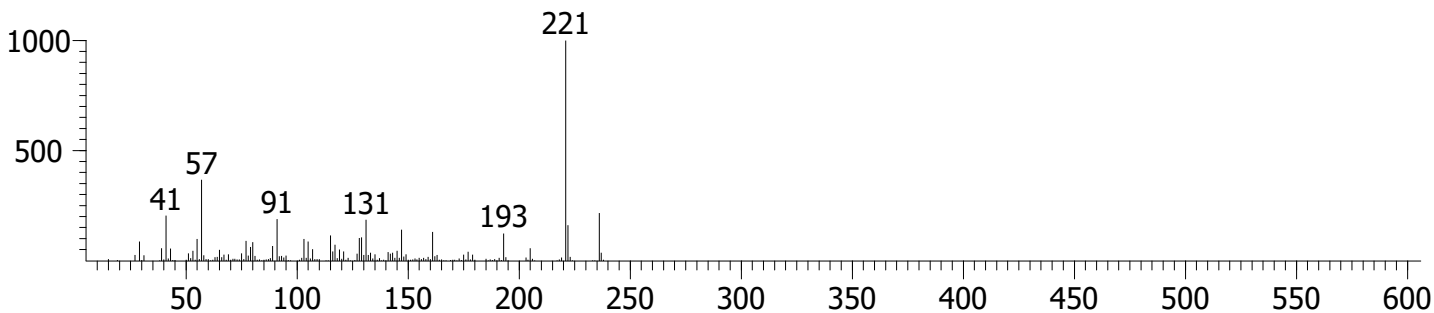
Peak Apex - sample "AnBxr B (20191121):1", peak 5670, at 1574.87 , 1.861 sec , sec (Spec # 166172)



Peak True - sample "AnBxr B (20191121):1", peak 5670, at 1574.87 , 1.861 sec , sec (Spec # 166172)

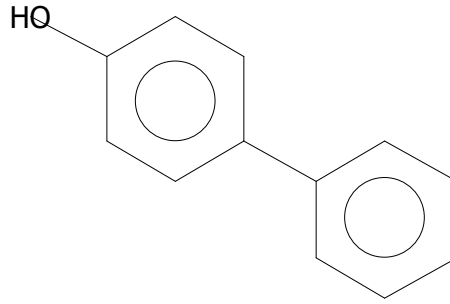


Library Hit - similarity 673, "3,5-di-tert-Butyl-4-hydroxybenzyl alcohol"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3,5-di-tert-Butyl-4-hydroxybenzyl alcohol	673	7859	88-26-6	replib	C15H24O2	236
2	3,5-di-tert-Butyl-4-hydroxybenzyl alcohol	621	7859	88-26-6	replib	C15H24O2	236
3	3,5-di-tert-Butyl-4-hydroxyanisole	613	1395	489-01-0	replib	C15H24O2	236
4	3,5-di-tert-Butyl-4-hydroxybenzyl alcohol	600	1541	88-26-6	mainlib	C15H24O2	236
5	3,5-di-tert-Butyl-4-hydroxyanisole	599	1481	489-01-0	mainlib	C15H24O2	236

p-Hydroxybiphenyl



1st Dimension R.T. = 1585.37

2nd Dimension R.T. = 2.251

Quant Mass(es) = 170

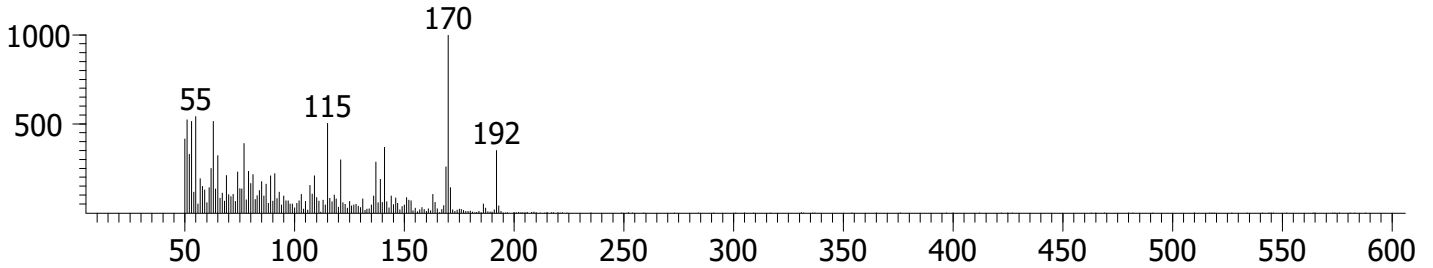
S/N = 2186.2

Area = 336441

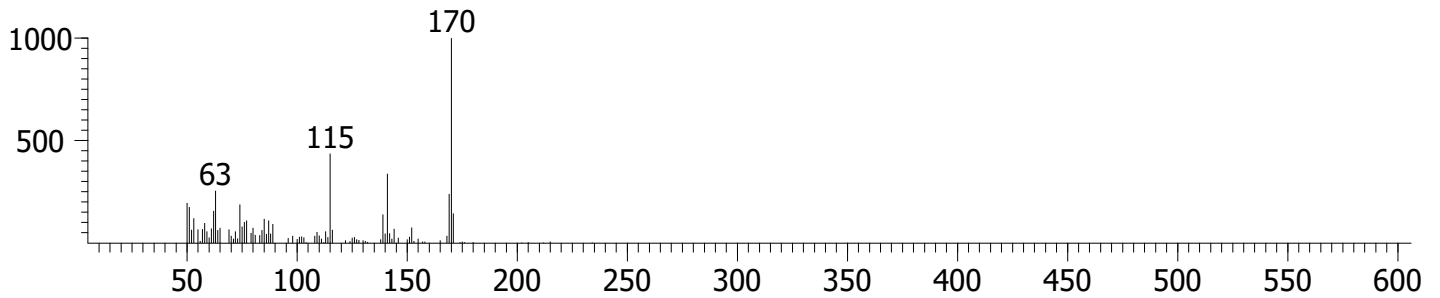
Height = 31627

Similarity = 868

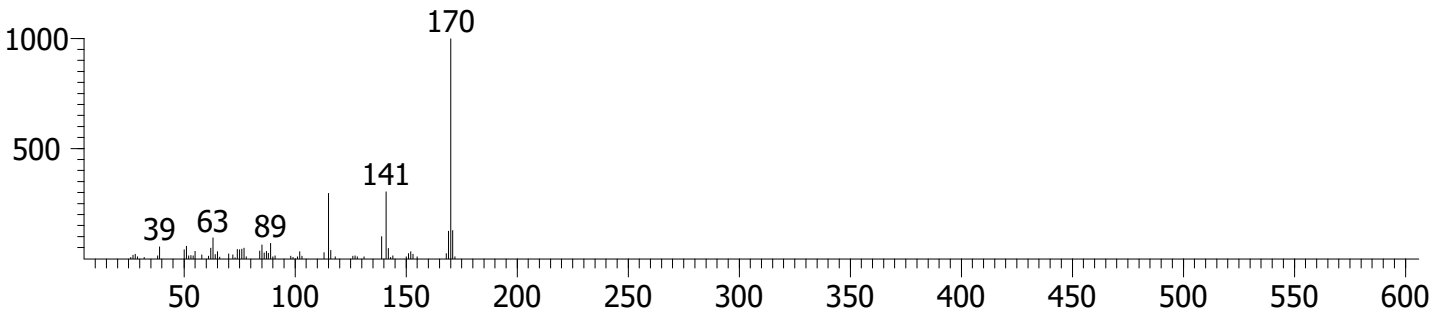
Peak Apex - sample "AnBxr B (20191121):1", peak 5743, at 1585.37 , 2.251 sec , sec (Spec # 167821)



Peak True - sample "AnBxr B (20191121):1", peak 5743, at 1585.37 , 2.251 sec , sec (Spec # 167821)



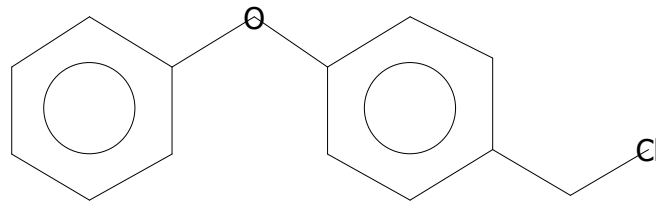
Library Hit - similarity 868, "p-Hydroxybiphenyl"



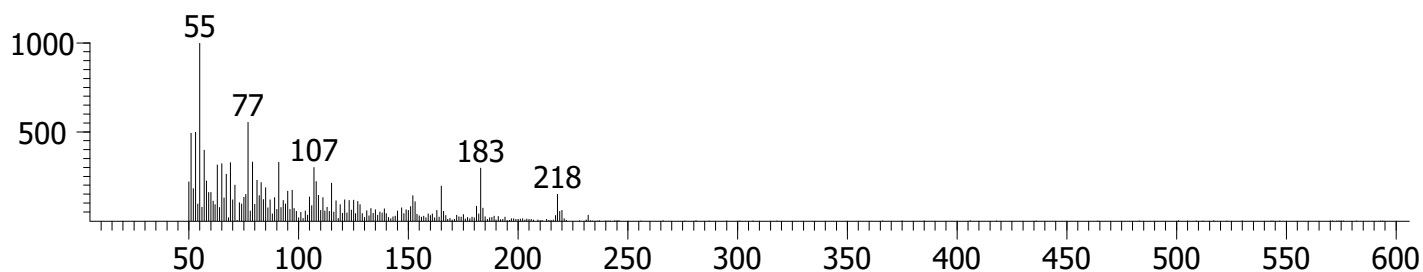
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	p-Hydroxybiphenyl	868	5395	92-69-3	replib	C12H10O	170
2	3-Hydroxybiphenyl	856	3593	580-51-8	replib	C12H10O	170
3	p-Hydroxybiphenyl	820	5395	92-69-3	replib	C12H10O	170
4	o-Hydroxybiphenyl	811	765	90-43-7	replib	C12H10O	170
5	3-Hydroxybiphenyl	808	3593	580-51-8	replib	C12H10O	170

Benzene, 1-(chloromethyl)-3-phenoxy-

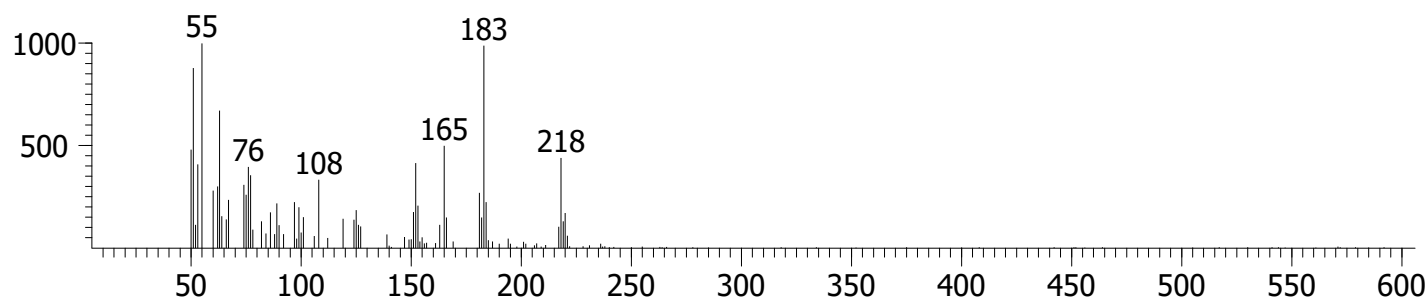
1st Dimension R.T. = 1777.76
2nd Dimension R.T. = 2.323
Quant Mass(es) = 183
S/N = 161.71
Area = 45410
Height = 3907.8
Similarity = 651



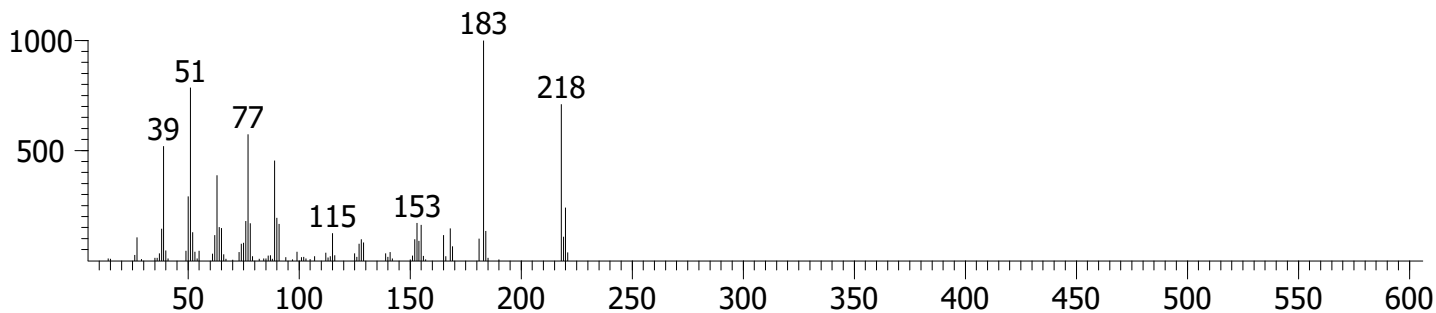
Peak Apex - sample "AnBxr B (20191121):1", peak 6929, at 1777.76 , 2.323 sec , sec (Spec # 196982)



Peak True - sample "AnBxr B (20191121):1", peak 6929, at 1777.76 , 2.323 sec , sec (Spec # 196982)



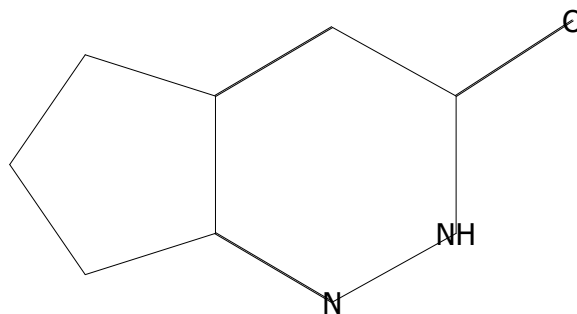
Library Hit - similarity 651, "Benzene, 1-(chloromethyl)-3-phenoxy-"



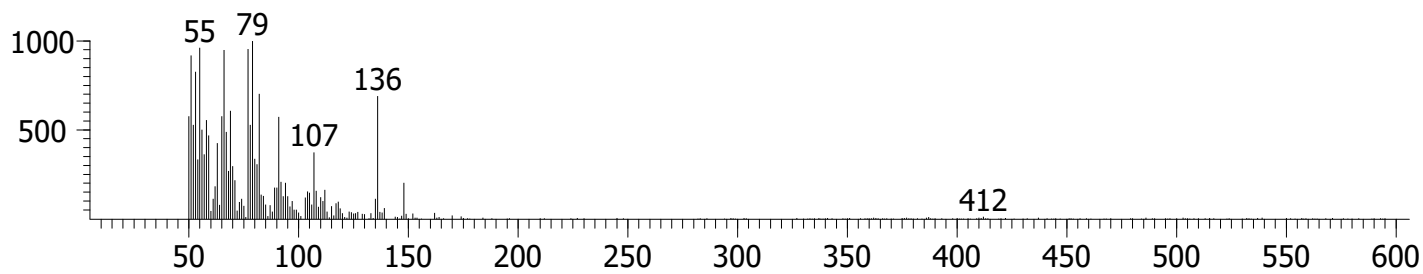
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-(chloromethyl)-3-phenoxy-	651	4367	53874-66-1	mainlib	C13H11ClO	218
2	Clorophene	643	5577	120-32-1	replib	C13H11ClO	218
3	Clorophene	637	5577	120-32-1	replib	C13H11ClO	218
4	Clorophene	630	1858	120-32-1	mainlib	C13H11ClO	218
5	Clorophene	619	5577	120-32-1	replib	C13H11ClO	218

3H-Cyclopenta[c]pyridazin-3-one,
2,5,6,7-tetrahydro-

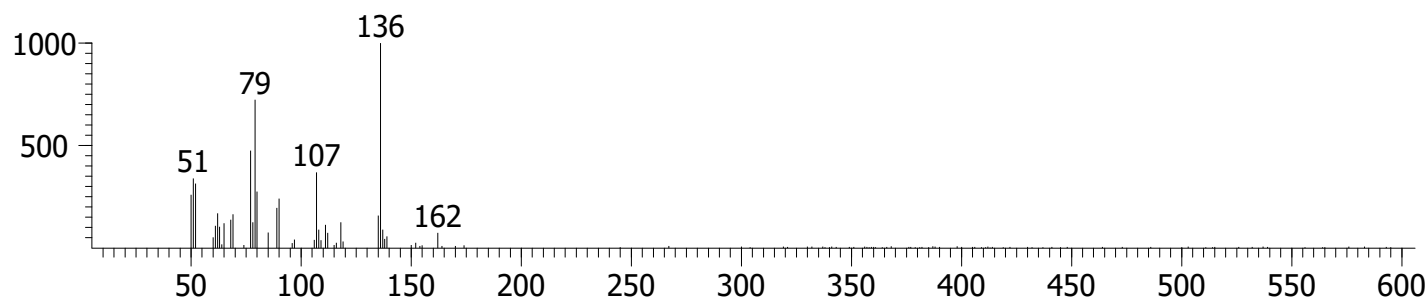
1st Dimension R.T. = 983.712
2nd Dimension R.T. = 2.026
Quant Mass(es) = 136
S/N = 155.51
Area = 22287
Height = 2686.1
Similarity = 706



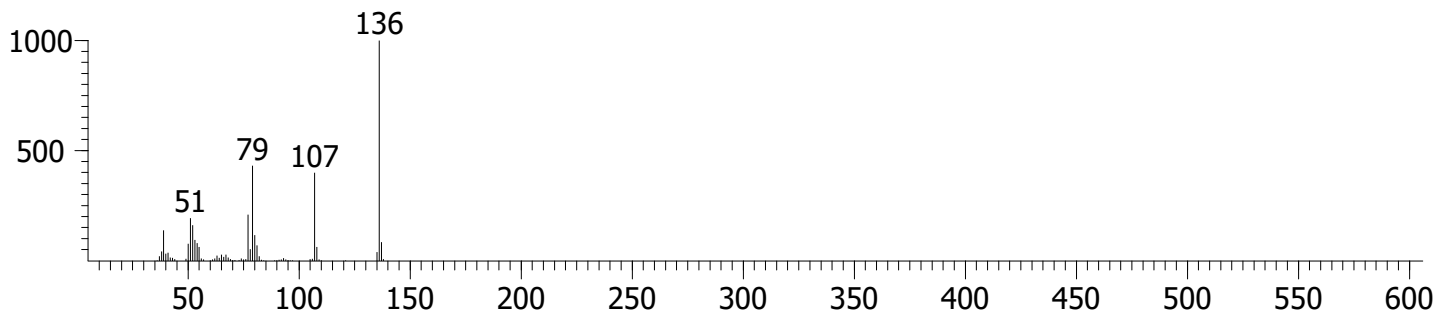
Peak Apex - sample "AnMbr C (20191120):1", peak 1696, at 983.712 , 2.026 sec , sec (Spec # 76627)



Peak True - sample "AnMbr C (20191120):1", peak 1696, at 983.712 , 2.026 sec , sec (Spec # 76627)



Library Hit - similarity 706, "3H-Cyclopenta[c]pyridazin-3-one, 2,5,6,7-tetrahydro-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3H-Cyclopenta[c]pyridazin-3-one, 2,5,6,7-tetrahydro-	706	1938	0-00-0	mainlib	C7H8N2O	136
2	2-Methyl-3(2-furyl)acrolein	696	1368	874-66-8	mainlib	C8H8O2	136
3	3-Hydroxy-2-methylbenzaldehyde	694	1262	90111-15-2	mainlib	C8H8O2	136
4	2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	686	941	0-00-0	mainlib	C8H8O2	136
5	2-Hydroxy-3-methylbenzaldehyde	682	795	824-42-0	mainlib	C8H8O2	136

Trisulfide, methyl propyl

1st Dimension R.T. = 805.314

2nd Dimension R.T. = 1.703

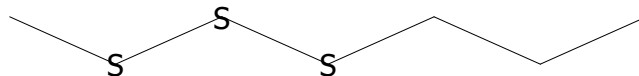
Quant Mass(es) = 154

S/N = 637.09

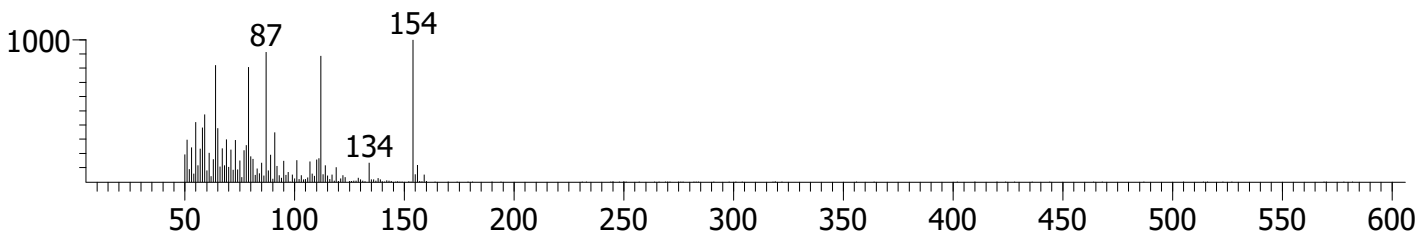
Area = 64834

Height = 9281.7

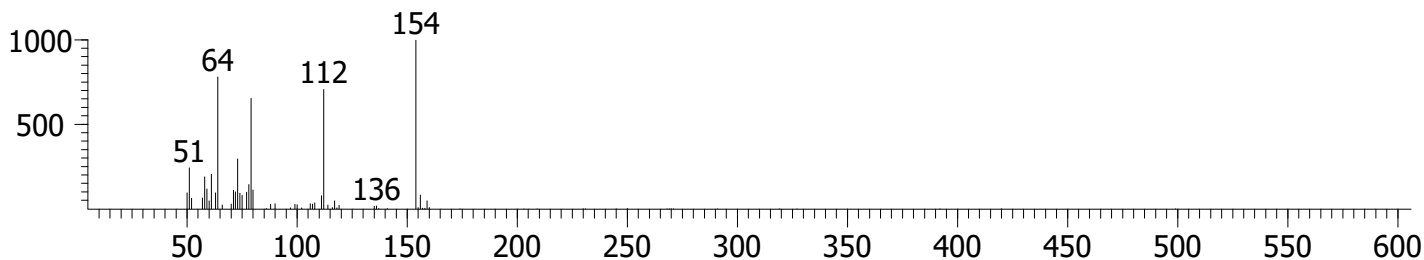
Similarity = 724



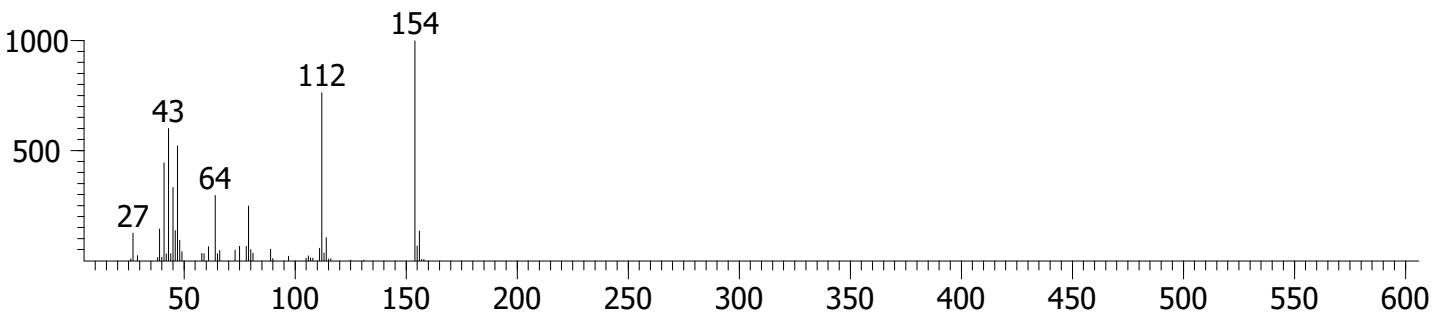
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 924, at 805.314 , 1.703 sec , sec (Spec # 49548)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 924, at 805.314 , 1.703 sec , sec (Spec # 49548)



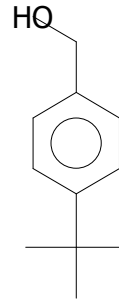
Library Hit - similarity 724, "Trisulfide, methyl propyl"



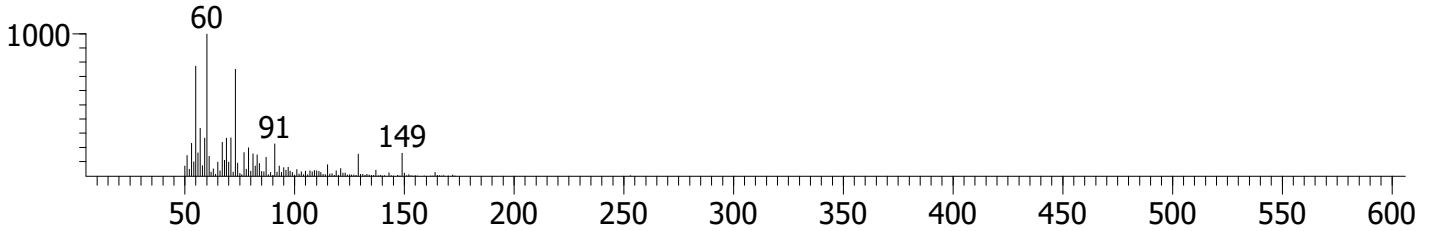
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Trisulfide, methyl propyl	724	9358	17619-36-2	mainlib	C4H10S3	154
2	1,2,4-Triazolo[4,3-b]pyridazine, 6-chloro-	530	132	28593-24-0	mainlib	C5H3ClN4	154
3	1H-Pyrazolo[3,4-d]pyrimidine, 4-chloro-	511	64	0-00-0	mainlib	C5H3ClN4	154
4	2-Thiatricyclo[3.3.1.1(3,7)]decane	509	59	281-25-4	mainlib	C9H14S	154
5	Thiophene-2-carboxamide, N-(2-p-tolyloxyethyl)-	497	39	0-00-0	mainlib	C14H15NO2S	261

Benzenemethanol, 4-(1,1-dimethylethyl)-

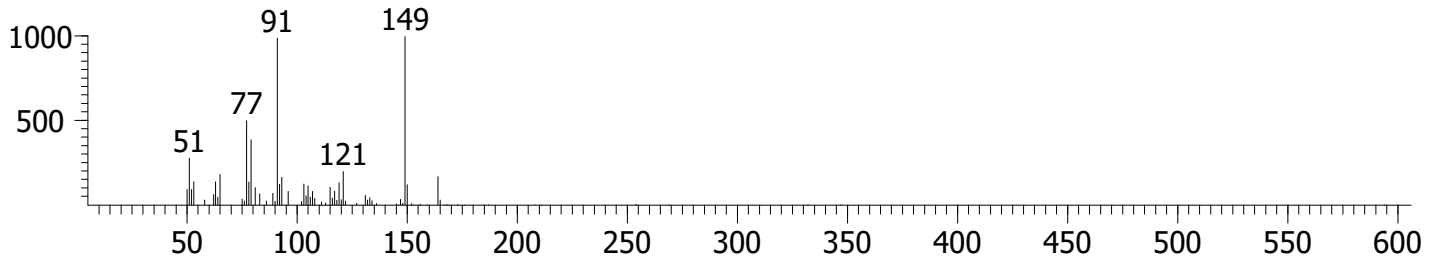
1st Dimension R.T. = 1095.65
2nd Dimension R.T. = 1.749
Quant Mass(es) = 149
S/N = 685.54
Area = 147780
Height = 15173
Similarity = 821



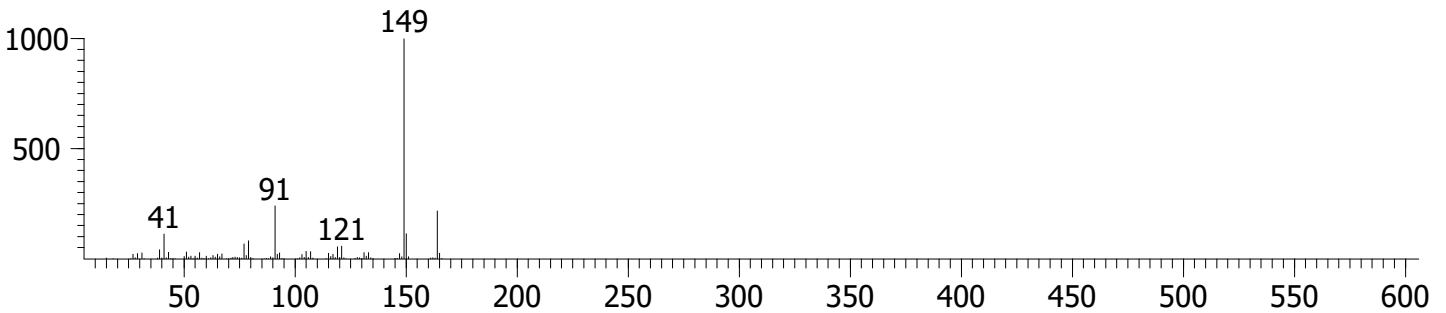
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 2291, at 1095.65 , 1.749 sec , sec (Spec # 93 545)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 2291, at 1095.65 , 1.749 sec , sec (Spec # 935 45)



Library Hit - similarity 821, "Benzenemethanol, 4-(1,1-dimethylethyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzenemethanol, 4-(1,1-dimethylethyl)-	821	4333	877-65-6	mainlib	C11H16O	164
2	Cyclopropane, 1-cyclopropylethynyl-2-methoxy-3,3-dimethyl-	793	1251	0-00-0	mainlib	C11H16O	164
3	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-	779	783	6379-73-3	mainlib	C11H16O	164
4	Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-	767	521	1076-56-8	mainlib	C11H16O	164
5	1,3-Cyclohexadiene, 1,3,5,5,6,6-hexamethyl-	755	347	0-00-0	mainlib	C12H20	164

4-Aminobenzoic acid

1st Dimension R.T. = 1364.99

2nd Dimension R.T. = 2.303

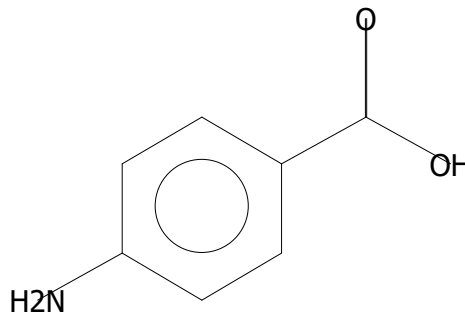
Quant Mass(es) = 120

S/N = 168.04

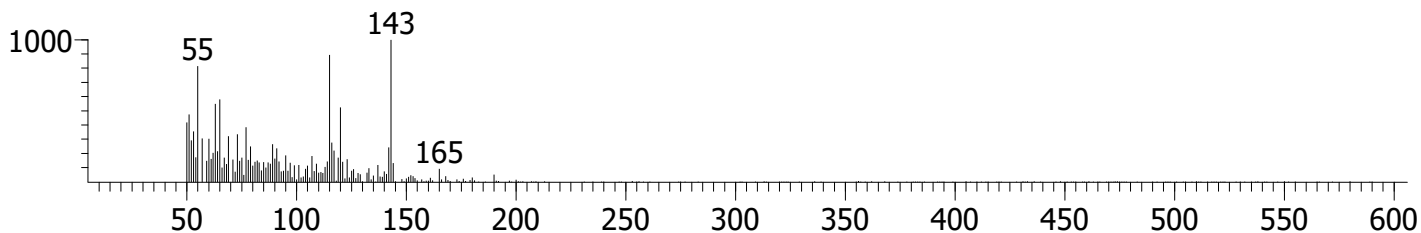
Area = 47269

Height = 4746.6

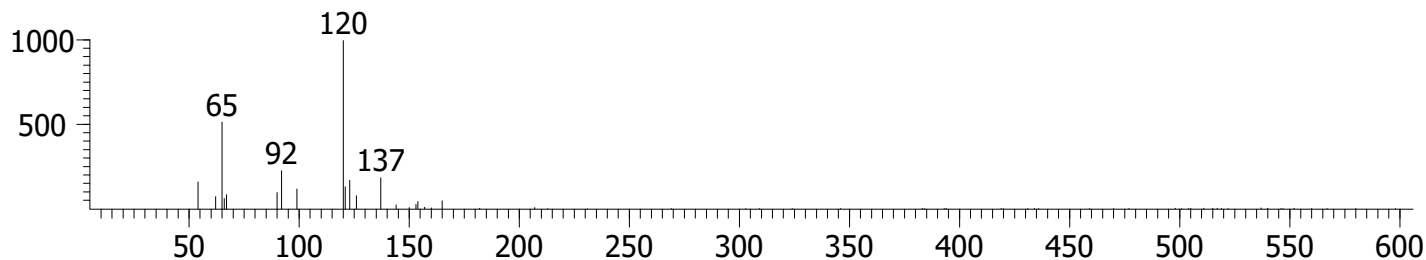
Similarity = 689



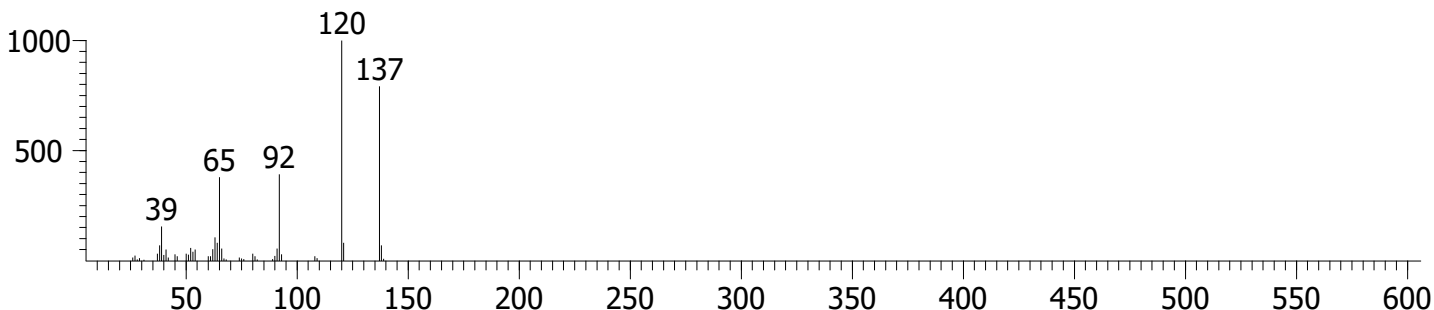
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 3912, at 1364.99 , 2.303 sec , sec (Spec # 134439)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 3912, at 1364.99 , 2.303 sec , sec (Spec # 134439)

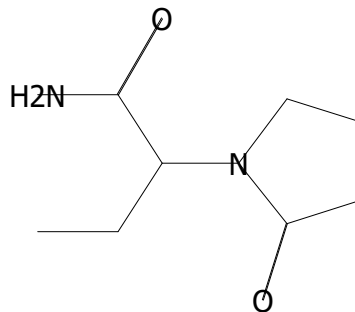


Library Hit - similarity 689, "4-Aminobenzoic acid"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Aminobenzoic acid	689	1975	150-13-0	mainlib	C7H7NO2	137
2	Benzoic acid, 4-amino-, 2,2,6,6-tetramethyl-1-piperidinyl ester	672	1078	0-00-0	mainlib	C16H24N2O2	276
3	Benzoic acid, 4,4'-(hydrazine-1,2-diyl)bis-	667	869	62327-30-4	mainlib	C14H12N2O4	272
4	Salicylamide	665	801	65-45-2	mainlib	C7H7NO2	137
5	Diethyl N-(p-aminobenzoyl)-L-glutamate	645	365	13726-52-8	mainlib	C16H22N2O5	322

Etiracetam



1st Dimension R.T. = 1368.49

2nd Dimension R.T. = 2.482

Quant Mass(es) = 126

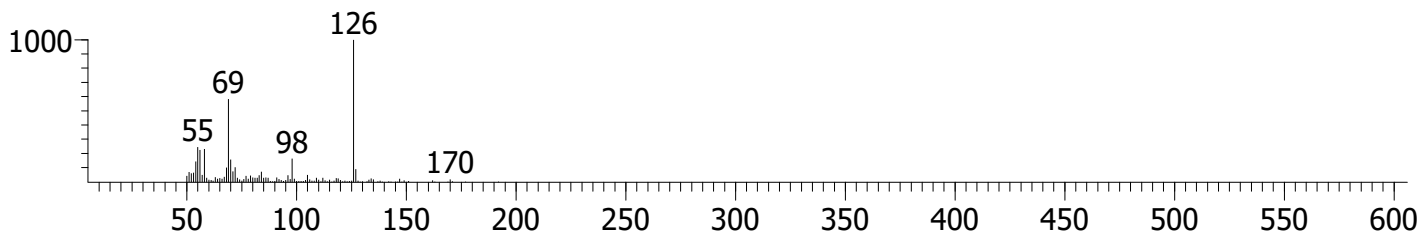
S/N = 3047.7

Area = 659055

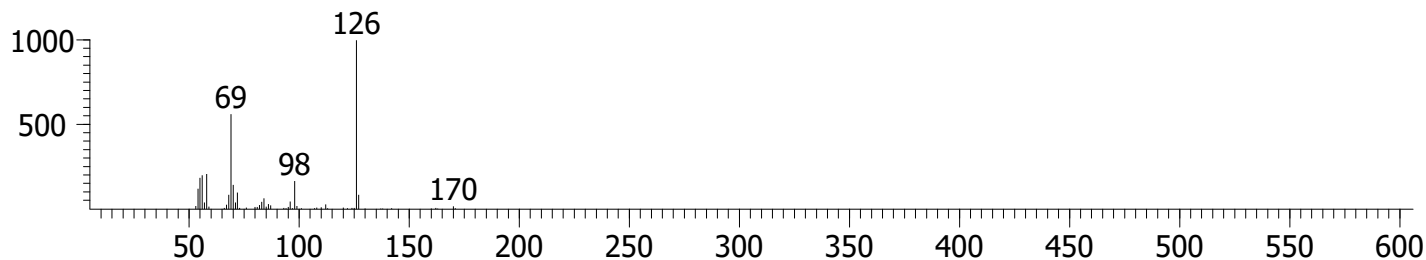
Height = 58394

Similarity = 917

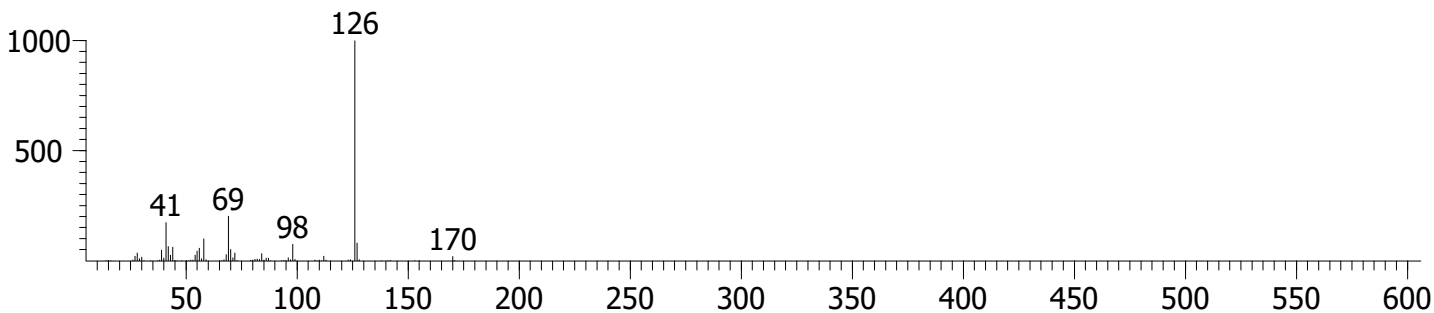
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 3946, at 1368.49 , 2.482 sec , sec (Spec # 134996)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 3946, at 1368.49 , 2.482 sec , sec (Spec # 134996)



Library Hit - similarity 917, "Etiracetam"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Etiracetam	917	4592	33996-58-6	mainlib	C8H14N2O2	170
2	Levetiracetam	916	4414	102767-28-2	mainlib	C8H14N2O2	170
3	4H-Pyran-4-one, 5-hydroxy-2-methyl-	816	328	644-46-2	mainlib	C6H6O3	126
4	2,2-Diethyl-N-ethylpyrrolidine	789	96	89214-92-6	mainlib	C10H21N	155
5	Aziridine, 2-(1,1-dimethylethyl)-1-ethyl-3-methyl-, trans-	785	81	55669-79-9	mainlib	C9H19N	141

Propylparaben

1st Dimension R.T. = 1413.97

2nd Dimension R.T. = 2.020

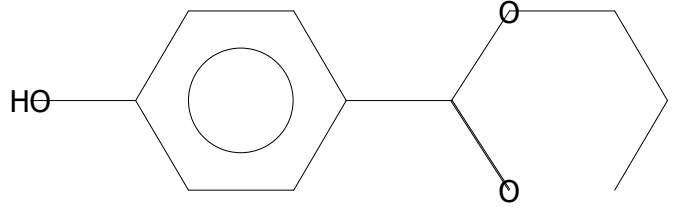
Quant Mass(es) = 121

S/N = 9712.2

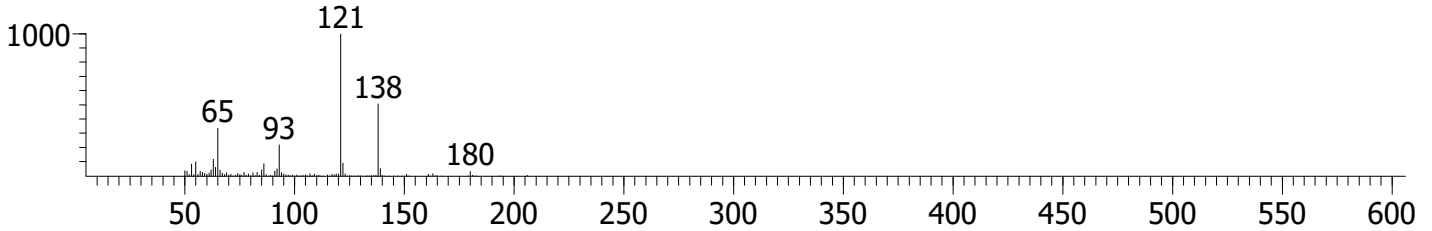
Area = 3314458

Height = 318867

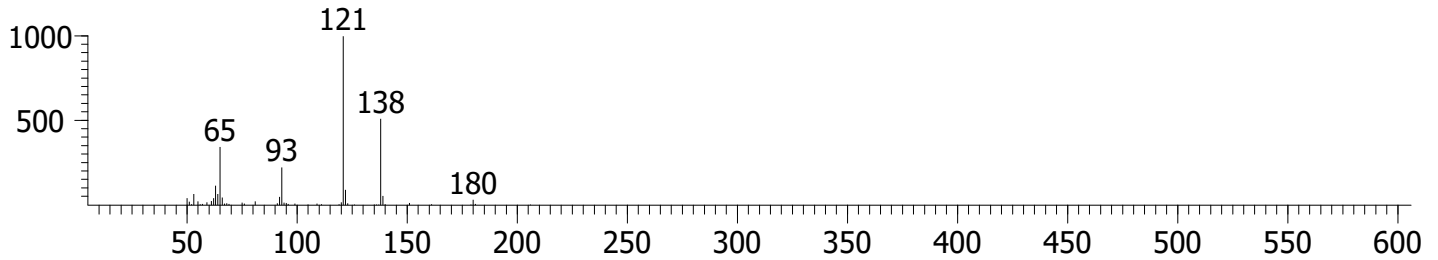
Similarity = 939



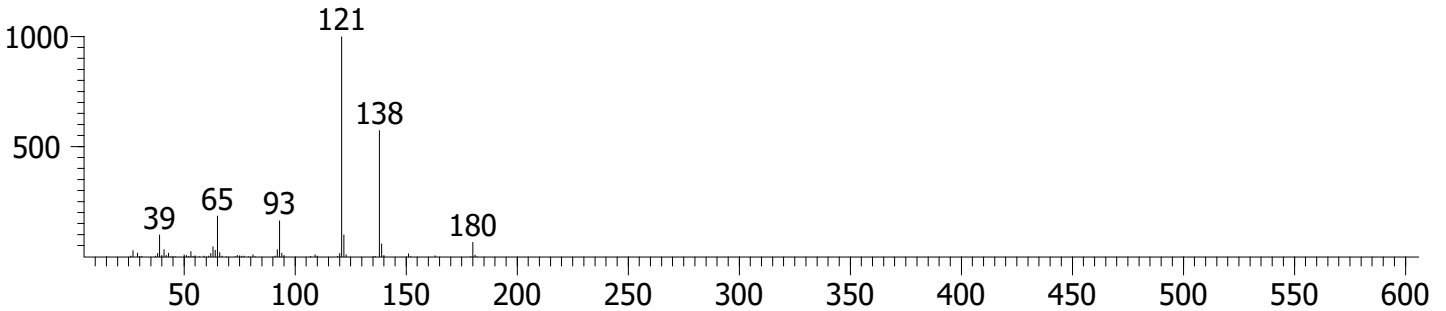
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 4229, at 1413.97 , 2.020 sec , sec (Spec # 141816)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 4229, at 1413.97 , 2.020 sec , sec (Spec # 141816)



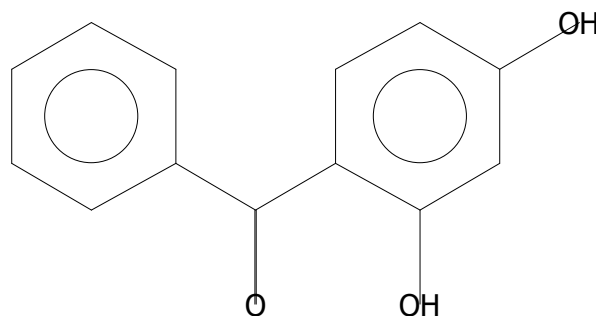
Library Hit - similarity 939, "Propylparaben"



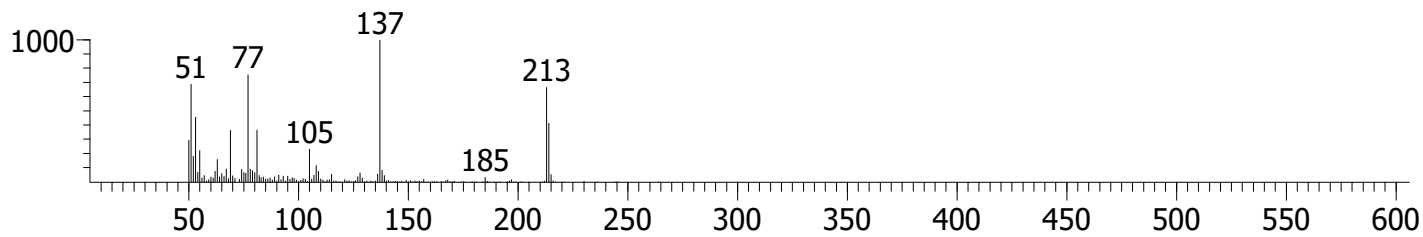
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Propylparaben	939	3041	94-13-3	mainlib	C10H12O3	180
2	Benzoic acid, 4-hydroxy-	928	2086	99-96-7	mainlib	C7H6O3	138
3	Benzoic acid, 3-hydroxy-, 1-methylpropyl ester	911	1138	0-00-0	mainlib	C11H14O3	194
4	4-Hydroxybenzoic acid, O-isopropoxyxycarbonyl-	908	1006	0-00-0	mainlib	C11H12O5	224
5	Isobutyl 4-hydroxybenzoate	905	889	4247-02-3	mainlib	C11H14O3	194

Methanone, (2,4-dihydroxyphenyl)phenyl-

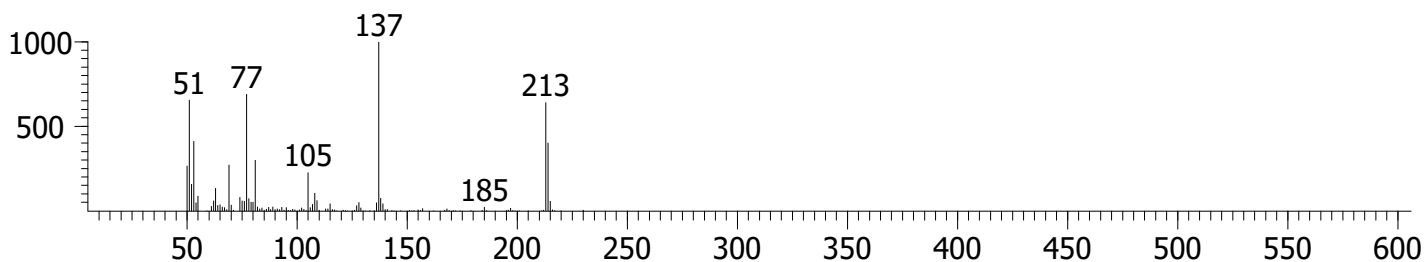
1st Dimension R.T. = 1921.18
2nd Dimension R.T. = 2.528
Quant Mass(es) = 213
S/N = 4720.8
Area = 871379
Height = 72121
Similarity = 868



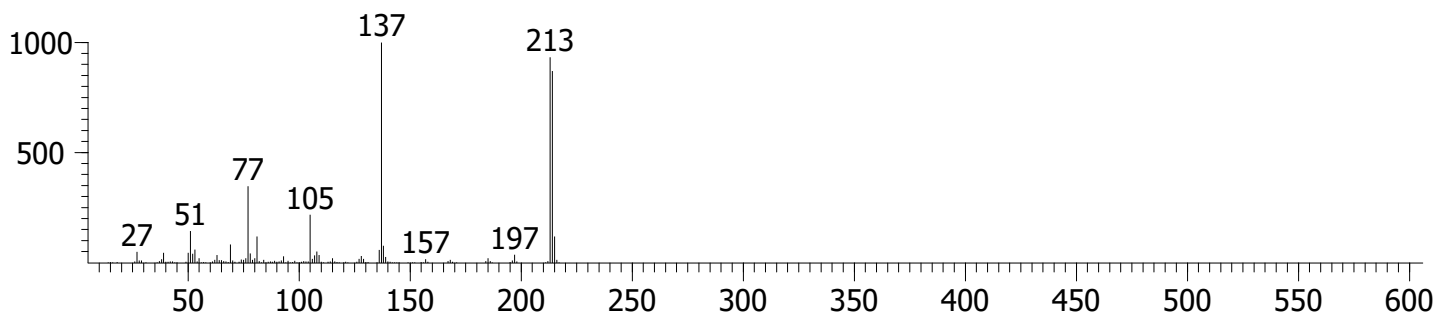
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 7081, at 1921.18 , 2.528 sec , sec (Spec # 218743)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 7081, at 1921.18 , 2.528 sec , sec (Spec # 218743)



Library Hit - similarity 868, "Methanone, (2,4-dihydroxyphenyl)phenyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Methanone, (2,4-dihydroxyphenyl)phenyl-	868	7913	131-56-6	mainlib	C13H10O3	214
2	Phen-1,3-diol, 2-benzoyl-	821	1655	63411-81-4	mainlib	C13H10O3	214
3	2,5-Dihydroxybenzophenone	770	333	2050-37-5	mainlib	C13H10O3	214
4	4-Benzoyl-1,3-phenylene diacetate	715	64	0-00-0	mainlib	C17H14O5	298
5	3,4-Dihydroxybenzophenone	684	17	10425-11-3	mainlib	C13H10O3	214

3H-1,2-Dithiole

1st Dimension R.T. = 493.992

2nd Dimension R.T. = 1.769

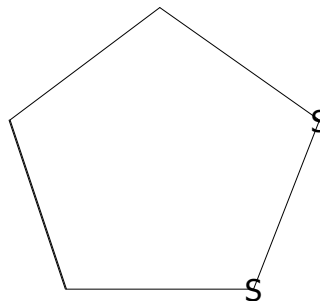
Quant Mass(es) = 103

S/N = 71.245

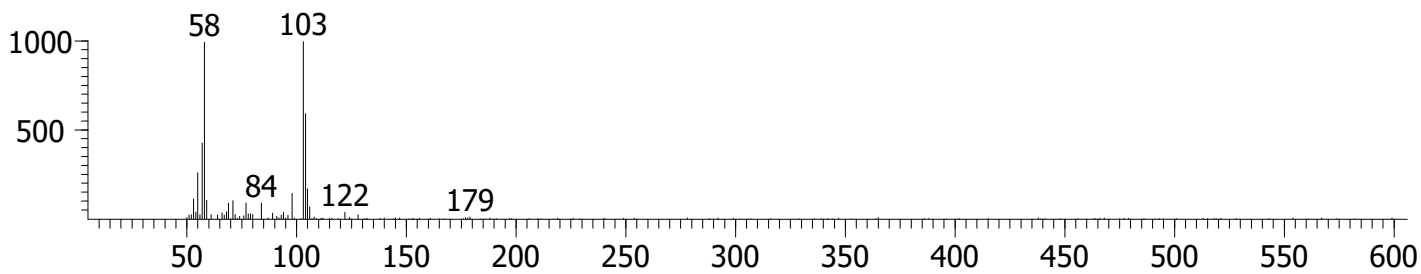
Area = 16726

Height = 2303.3

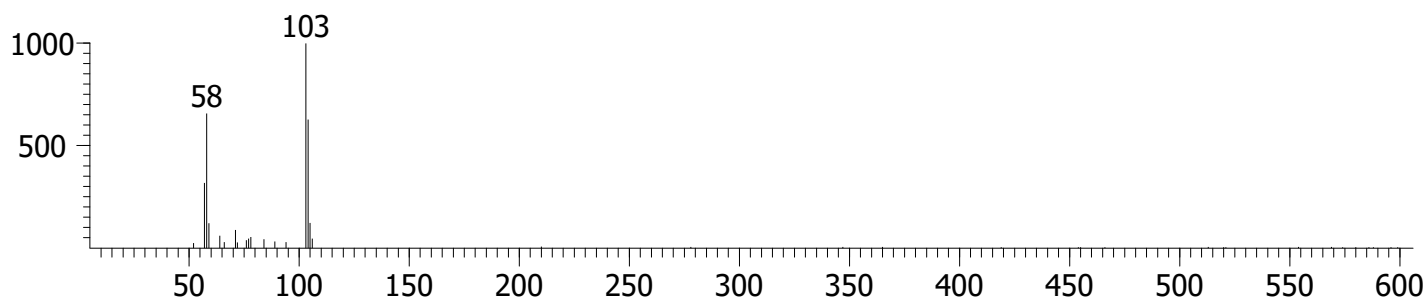
Similarity = 805



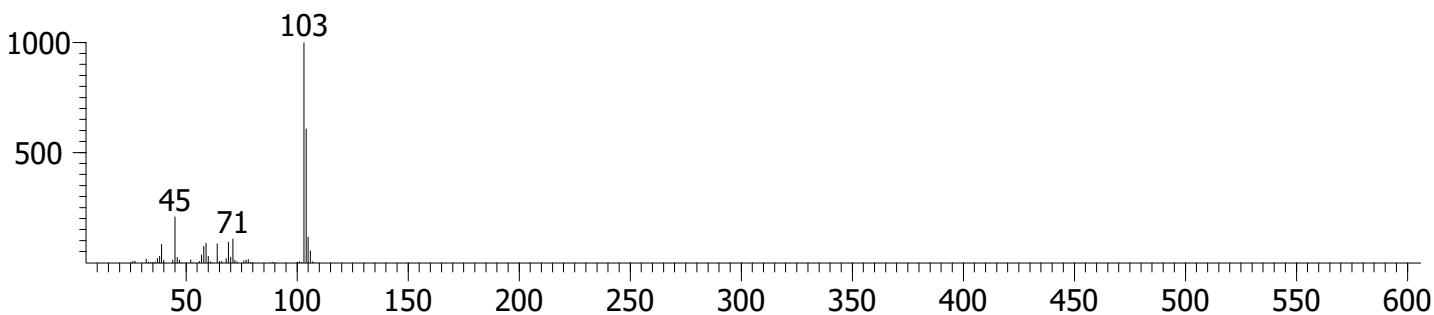
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 21, at 493.992 , 1.769 sec , sec (Spec # 2388)



Peak True - sample "INF-C comp 091919 (111419):1", peak 21, at 493.992 , 1.769 sec , sec (Spec # 2388)



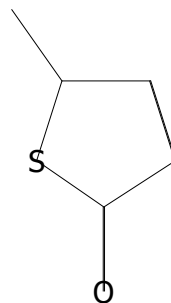
Library Hit - similarity 805, "3H-1,2-Dithiole"



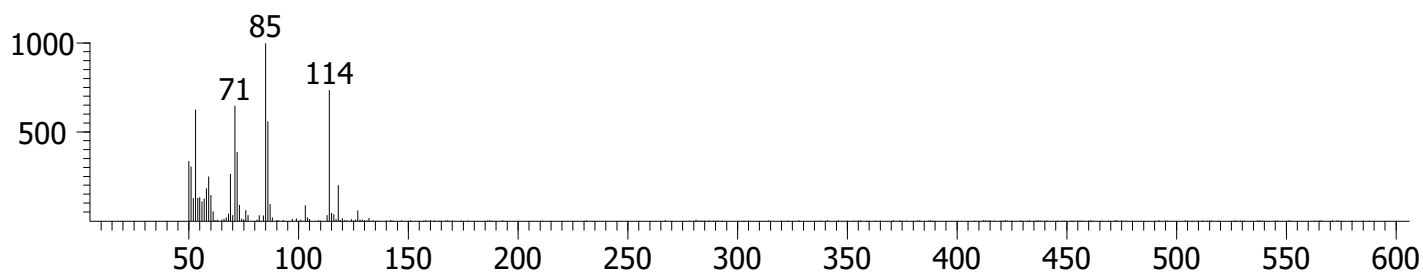
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3H-1,2-Dithiole	805	9217	288-26-6	mainlib	C3H4S2	104
2	Dimethyl diglycolcarbonate	642	224	87292-23-7	mainlib	C8H14O7	222
3	3(2H)-Furanone, dihydro-2,2-dimethyl-5-phenyl-	581	39	63678-00-2	mainlib	C12H14O2	190
4	Butyl 2,5,8,11-tetraoxatridecan-13-oate	575	30	0-00-0	mainlib	C13H26O6	278
5	Butyl 2,5,8,11,14-pentaoxahexadecan-16-oate	575	30	0-00-0	mainlib	C15H30O7	322

2(5H)-Thiophenone, 5-methyl-

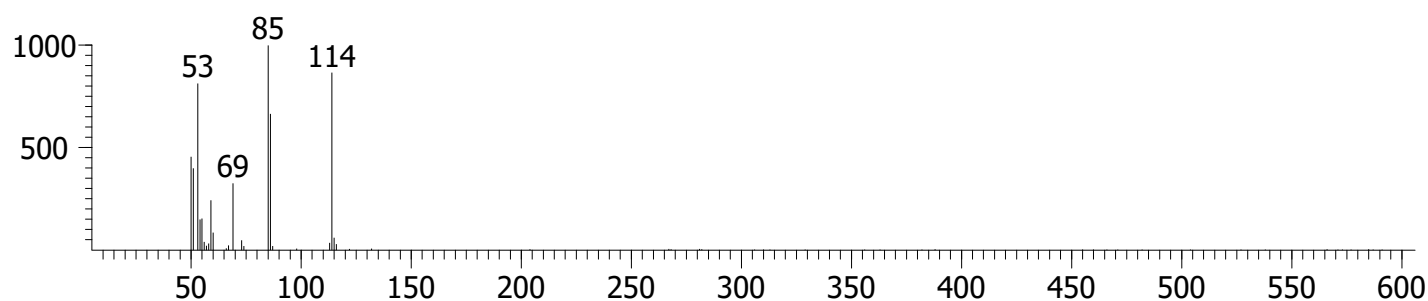
1st Dimension R.T. = 731.856
2nd Dimension R.T. = 2.125
Quant Mass(es) = 114
S/N = 262.88
Area = 33487
Height = 4111.9
Similarity = 694



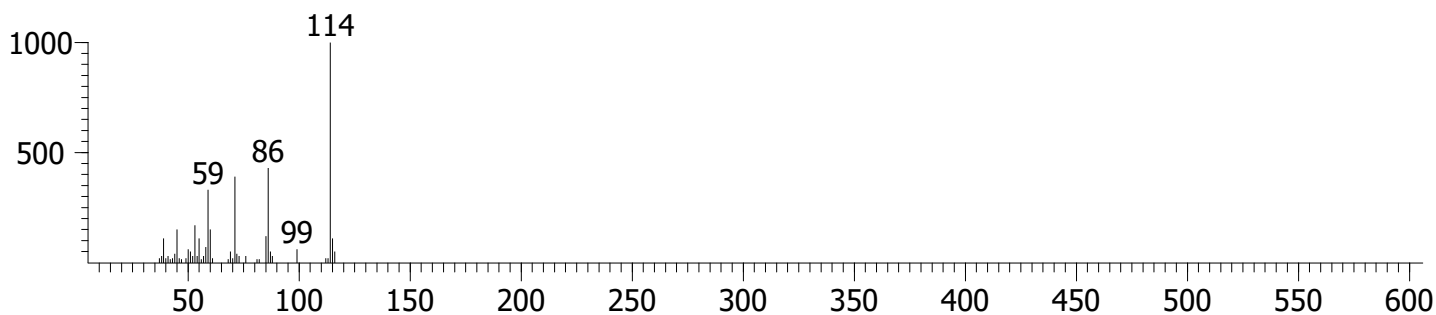
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 653, at 731.856 , 2.125 sec , sec (Spec # 38482)



Peak True - sample "INF-C comp 091919 (111419):1", peak 653, at 731.856 , 2.125 sec , sec (Spec # 38482)



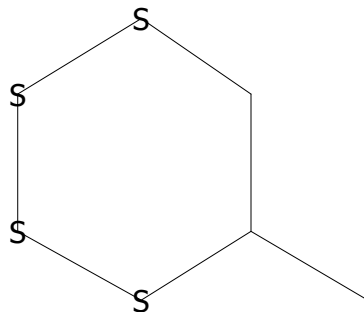
Library Hit - similarity 694, "2(5H)-Thiophenone, 5-methyl-"



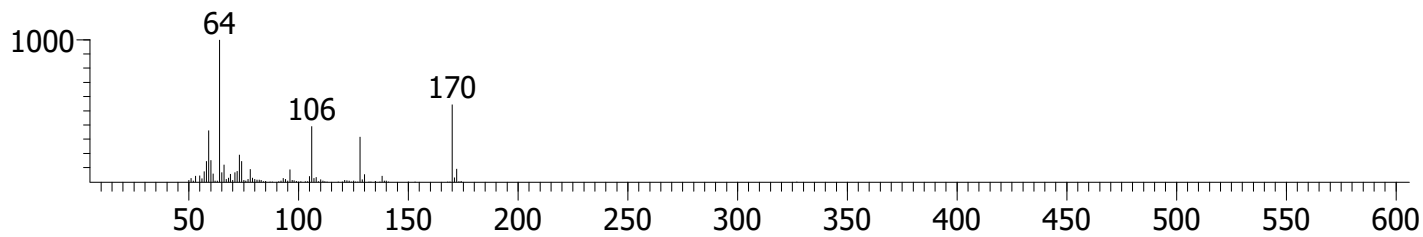
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2(5H)-Thiophenone, 5-methyl-	694	3510	7210-64-2	mainlib	C5H6OS	114
2	Thiirane, ethenyl-	678	2021	5954-75-6	mainlib	C4H6S	86
3	Thiophene, 2-(1,1-dimethylethoxy)-5-methyl-	648	562	54461-04-0	mainlib	C9H14OS	170
4	2-Methyl-3-furanthiol	648	562	28588-74-1	mainlib	C5H6OS	114
5	2,4-Hexanedione	644	474	3002-24-2	mainlib	C6H10O2	114

5-Methyl-1,2,3,4-tetrathiane

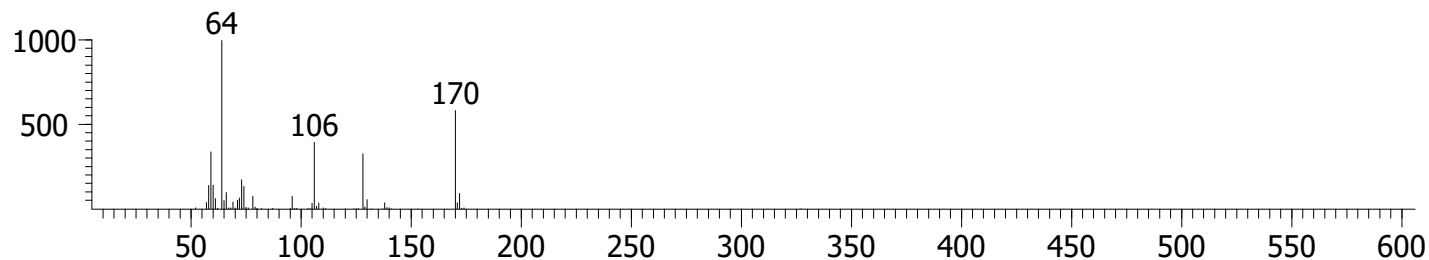
1st Dimension R.T. = 1109.64
2nd Dimension R.T. = 2.330
Quant Mass(es) = 170
S/N = 1798.5
Area = 249536
Height = 27295
Similarity = 950



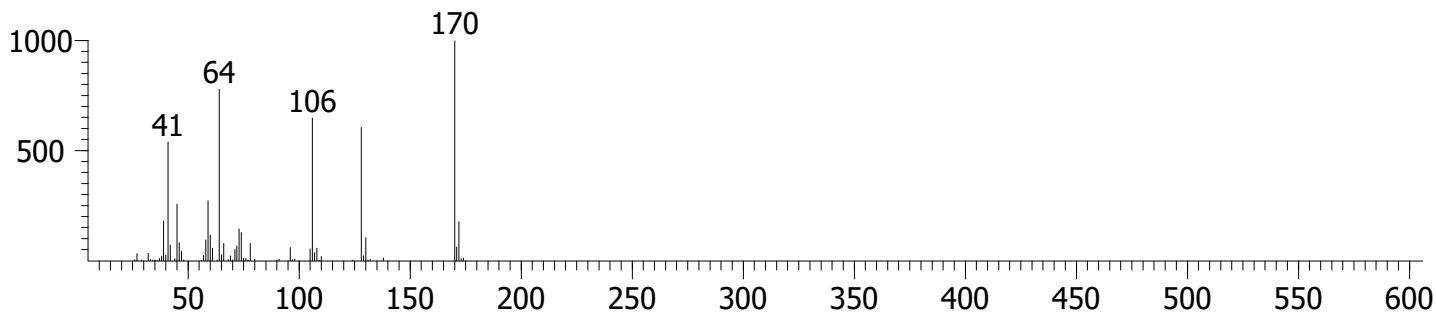
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 2057, at 1109.64 , 2.330 sec , sec (Spec # 95753)



Peak True - sample "INF-C comp 091919 (111419):1", peak 2057, at 1109.64 , 2.330 sec , sec (Spec # 95753)



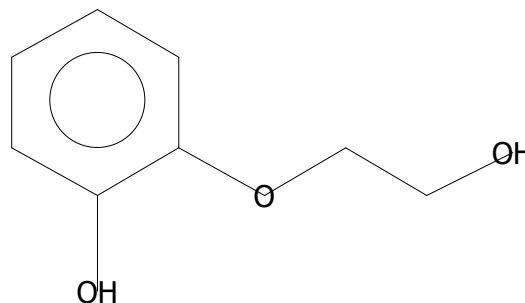
Library Hit - similarity 950, "5-Methyl-1,2,3,4-tetrathiane"



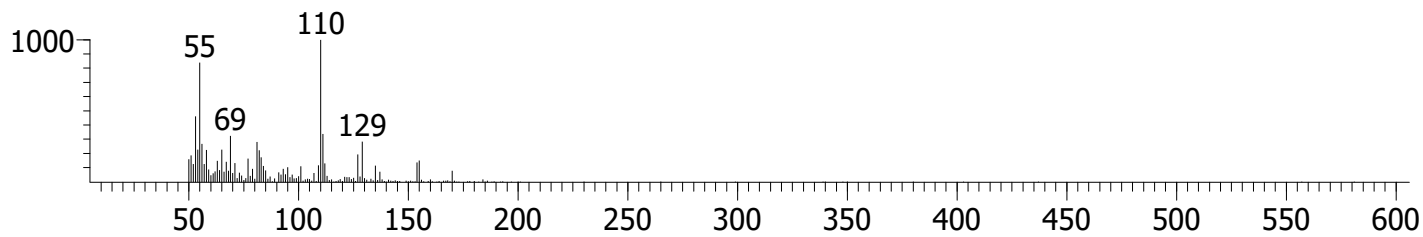
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-Methyl-1,2,3,4-tetrathiane	950	9852	116664-30-3	mainlib	C3H6S4	170
2	4,7-Diethyl-1,2,3,5,6-pentathiepane	632	98	878997-71-8	mainlib	C6H12S5	244
3	1,2-Dithiolane	596	24	557-22-2	mainlib	C3H6S2	106
4	5,7-Diethyl-1,2,3,4,6-pentathiepane	577	11	0-00-0	mainlib	C6H12S5	244
5	5-Chloro-1,2-dithian-4-ol	537	2	0-00-0	mainlib	C4H7ClOS2	170

2-(2-Hydroxyethoxy)phenol

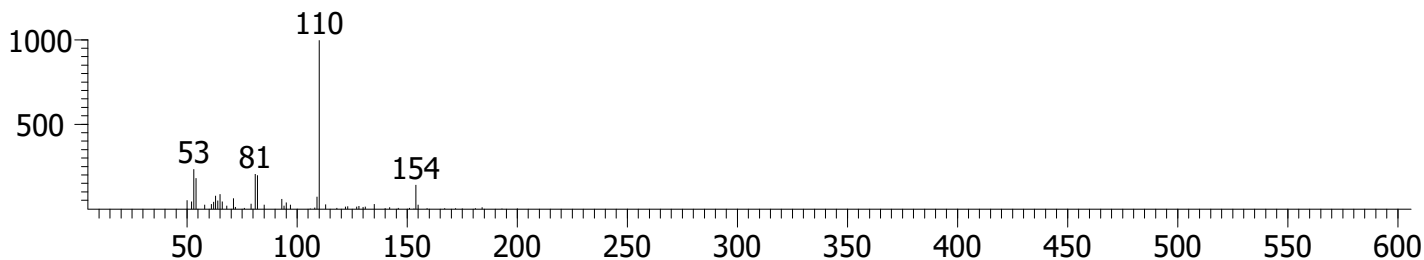
1st Dimension R.T. = 1312.52
2nd Dimension R.T. = 2.204
Quant Mass(es) = 110
S/N = 640.26
Area = 686408
Height = 63103
Similarity = 748



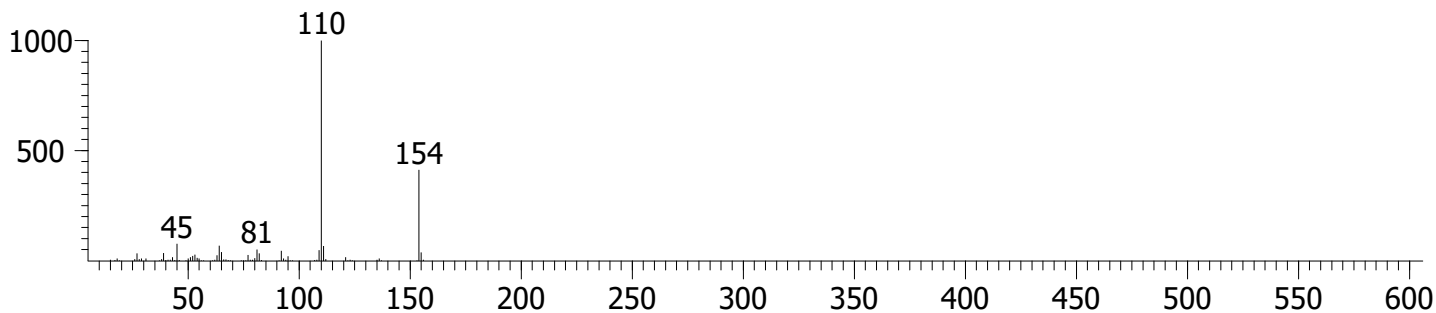
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 3044, at 1312.52 , 2.204 sec , sec (Spec # 126474)



Peak True - sample "INF-C comp 091919 (111419):1", peak 3044, at 1312.52 , 2.204 sec , sec (Spec # 126474)



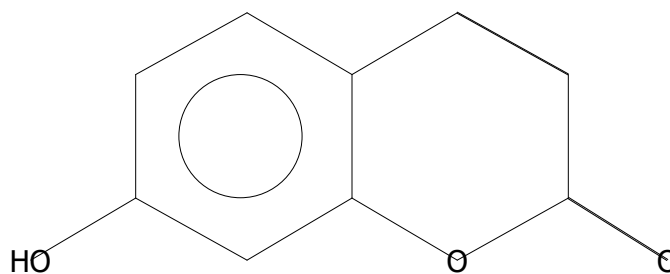
Library Hit - similarity 748, "2-(2-Hydroxyethoxy)phenol"



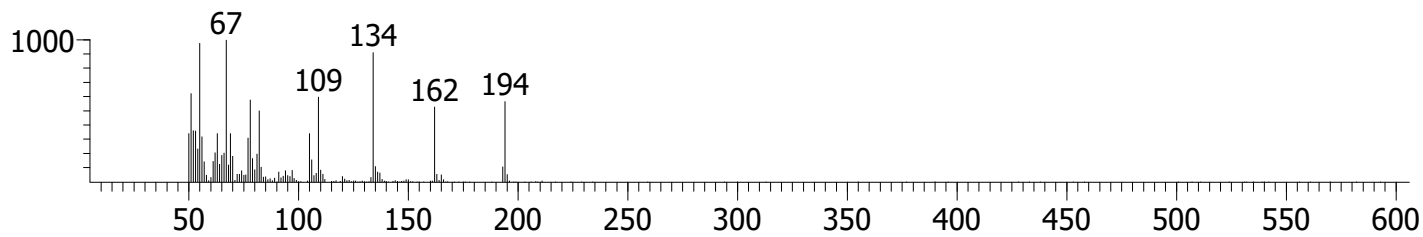
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-(2-Hydroxyethoxy)phenol	748	3483	4792-78-3	mainlib	C ₈ H ₁₀ O ₃	154
2	3-Acetyl-4-hydroxyphenyl acetate	724	1167	21222-04-8	mainlib	C ₁₀ H ₁₀ O ₄	194
3	2-(2-Hydroxyethoxy)phenol, isopropyl ether	712	777	0-00-0	mainlib	C ₁₁ H ₁₆ O ₃	196
4	2-(2-Hydroxyethoxy)phenol, 2-methylpropyl ether	701	533	0-00-0	mainlib	C ₁₂ H ₁₈ O ₃	210
5	4(1H)-Pyrimidinone, 6-methyl-	693	397	3524-87-6	mainlib	C ₅ H ₆ N ₂ O	110

7-Hydroxycoumarin

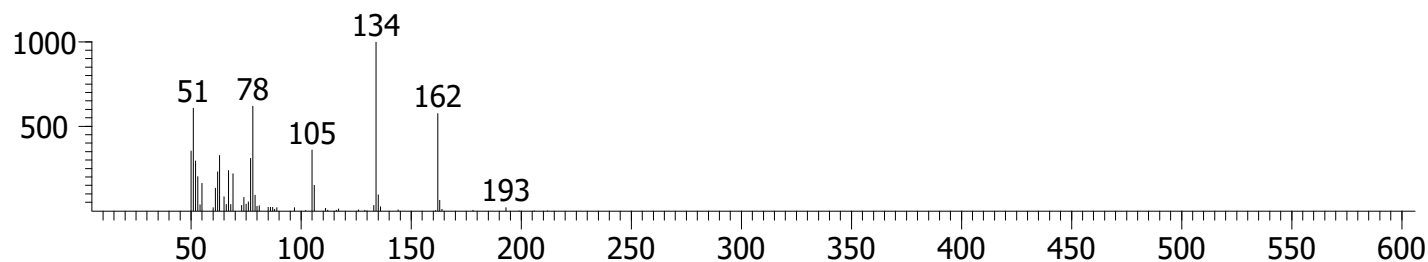
1st Dimension R.T. = 1669.32
2nd Dimension R.T. = 2.666
Quant Mass(es) = 134
S/N = 846.59
Area = 857281
Height = 64930
Similarity = 874



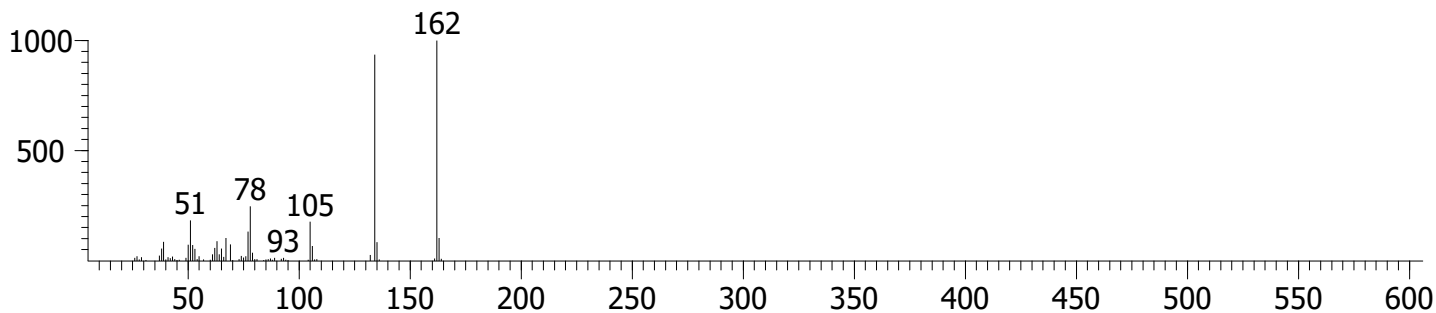
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 5064, at 1669.32 , 2.666 sec , sec (Spec # 180604)



Peak True - sample "INF-C comp 091919 (111419):1", peak 5064, at 1669.32 , 2.666 sec , sec (Spec # 180604)



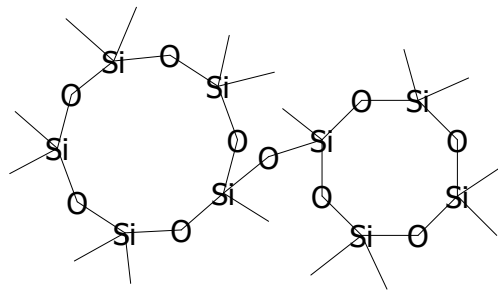
Library Hit - similarity 874, "7-Hydroxycoumarin"



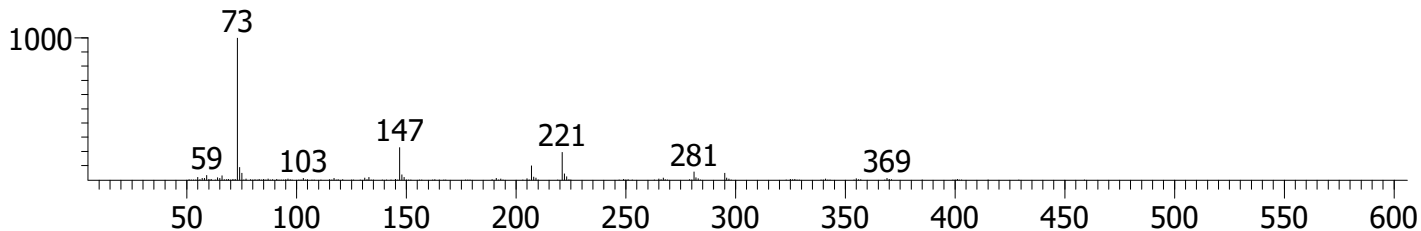
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	7-Hydroxycoumarin	874	3832	93-35-6	mainlib	C ₉ H ₆ O ₃	162
2	2H-1-Benzopyran-2-one, 8-hydroxy-	866	2859	2442-31-1	mainlib	C ₉ H ₆ O ₃	162
3	2H-1-Benzopyran-2-one, 6-hydroxy-	852	1789	6093-68-1	mainlib	C ₉ H ₆ O ₃	162
4	1-Benzofuran-5-ol	814	428	13196-10-6	mainlib	C ₈ H ₆ O ₂	134
5	4H-1-Benzopyran-4-one, 2,3-dihydro-6-methyl-	814	428	39513-75-2	mainlib	C ₁₀ H ₁₀ O ₂	162

yltetrasiloxan-2'-yloxy)-2,4,4,6,6,8,8,10,10-n

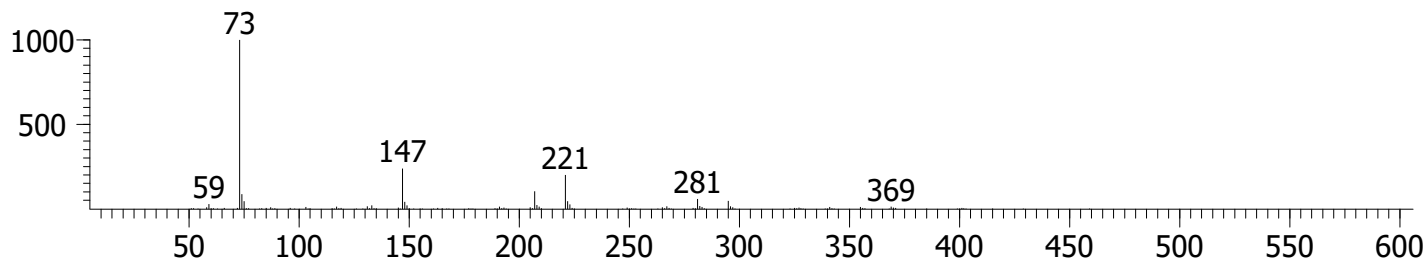
1st Dimension R.T. = 1791.75
 2nd Dimension R.T. = 0.990
 Quant Mass(es) = 221
 S/N = 3165.0
 Area = 302419
 Height = 44688
 Similarity = 726



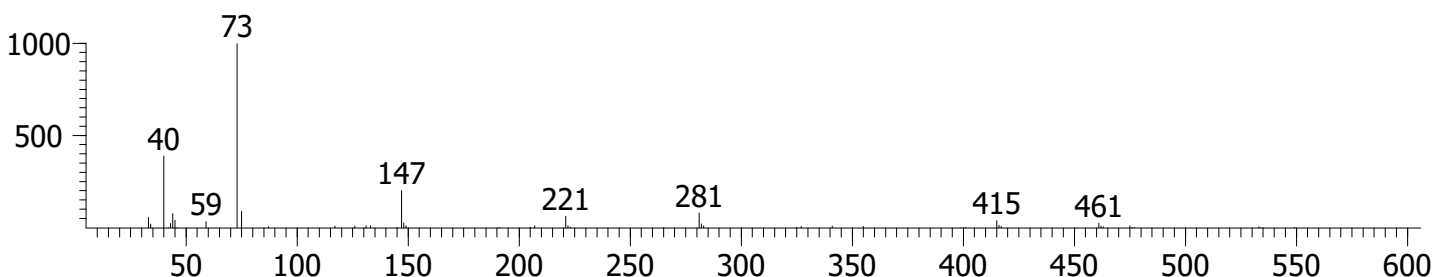
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 5687, at 1791.75 , 0.990 sec , sec (Spec # 198900)



Peak True - sample "INF-C comp 091919 (111419):1", peak 5687, at 1791.75 , 0.990 sec , sec (Spec # 198900)



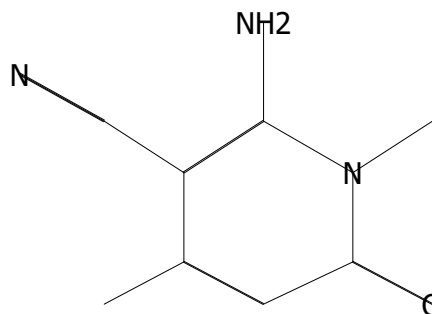
Library Hit - similarity 726, "2-(2',4',4',6',6',8',8'-Heptamethyltetrasiloxan-2'-yloxy)-2,4,4,6,6,8,8,10,10-nonamethylcyclopentasiloxane"



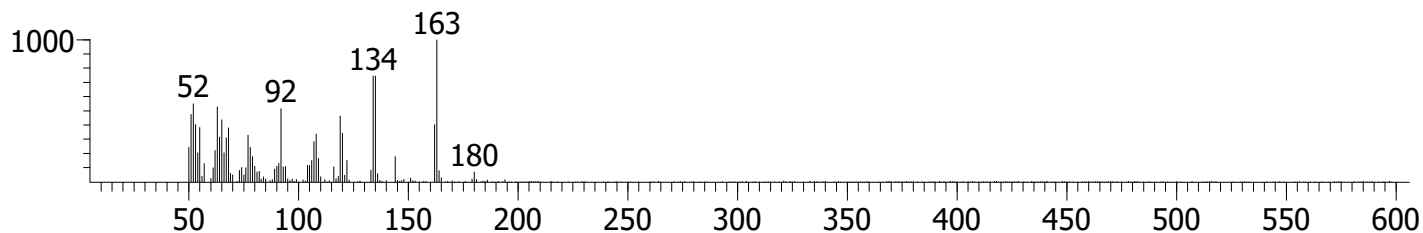
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-(2',4',4',6',6',8',8'-Heptamethyltetrasiloxan-2'-yloxy)-2,4,4,6,6,8,8,10,10-nonamethylcyclopentasiloxane	726	4819	145344-72-5	mainlib	C16H48O10Si9	652
2	Heptasiloxane, hexadecamethyl-	689	1173	541-01-5	mainlib	C16H48O6Si7	532
3	Mercaptoacetic acid, 2TMS derivative	682	898	6398-62-5	mainlib	C8H20O2SSi2	236
4	Suberohydroxamic acid, tetra(tert.-butyldimethylsilyl) derivative	669	580	0-00-0	mainlib	C32H72N2O4Si4	660
5	3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-	663	456	4342-25-0	mainlib	C10H30O2Si4	294

3-pyridinecarbonitrile,
2-amino-1,6-dihydro-1,4-dimethyl-6-oxo-

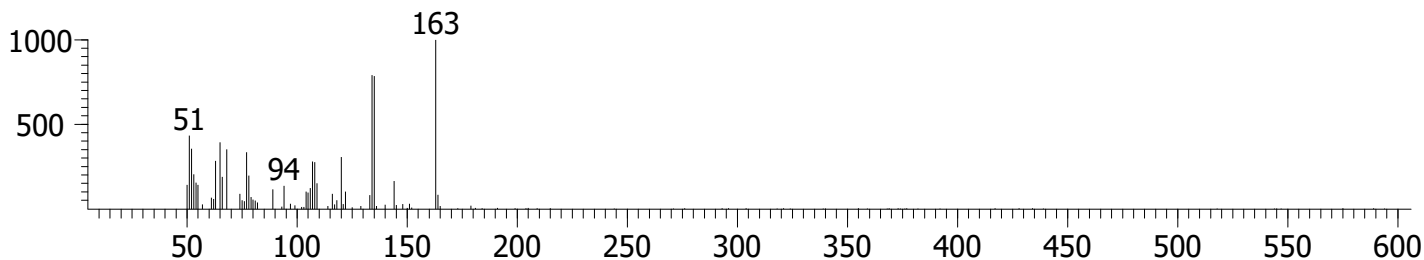
1st Dimension R.T. = 1753.27
 2nd Dimension R.T. = 2.574
 Quant Mass(es) = 134
 S/N = 322.86
 Area = 80134
 Height = 7459.1
 Similarity = 698



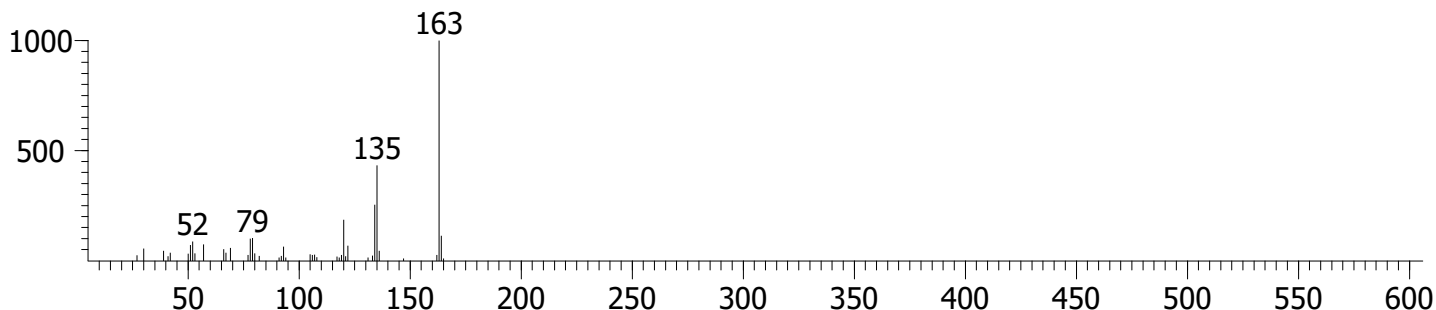
Peak Apex - sample "INF-A grab 100819 (111419):1", peak 3949, at 1753.27 , 2.574 sec , sec (Spec # 193310)



Peak True - sample "INF-A grab 100819 (111419):1", peak 3949, at 1753.27 , 2.574 sec , sec (Spec # 193310)



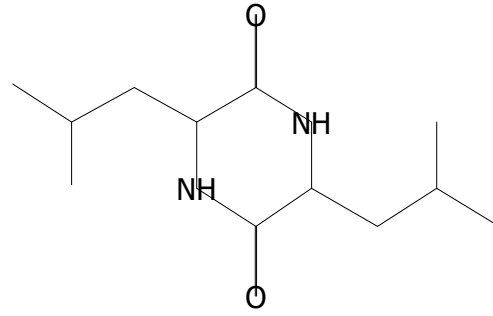
Library Hit - similarity 698, "3-pyridinecarbonitrile, 2-amino-1,6-dihydro-1,4-dimethyl-6-oxo-"



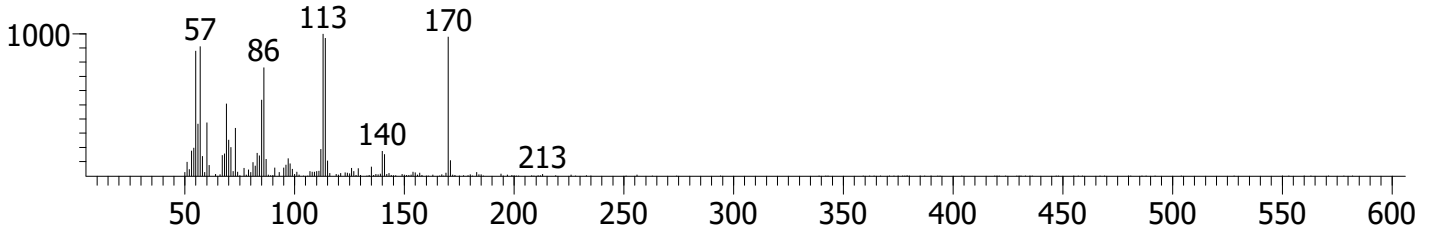
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-pyridinecarbonitrile, 2-amino-1,6-dihydro-1,4-dimethyl-6-oxo-	698	2102	0-00-0	mainlib	C8H9N3O	163
2	2,3-Dihydro-4-methoxyindole-2-one	687	1442	7699-17-4	mainlib	C9H9NO2	163
3	1H-Tetrazole, 5-(1,5-dimethyl-1H-pyrrol-2-yl)-	670	787	0-00-0	mainlib	C7H9N5	163
4	1-Amino-4,6-dimethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile	670	787	1562-12-5	mainlib	C8H9N3O	163
5	2,3-Dihydro-7-methyl-1,4-benzoxazine-3-one	667	695	39522-25-3	mainlib	C9H9NO2	163

2,5-Piperazinedione,
3,6-bis(2-methylpropyl)-

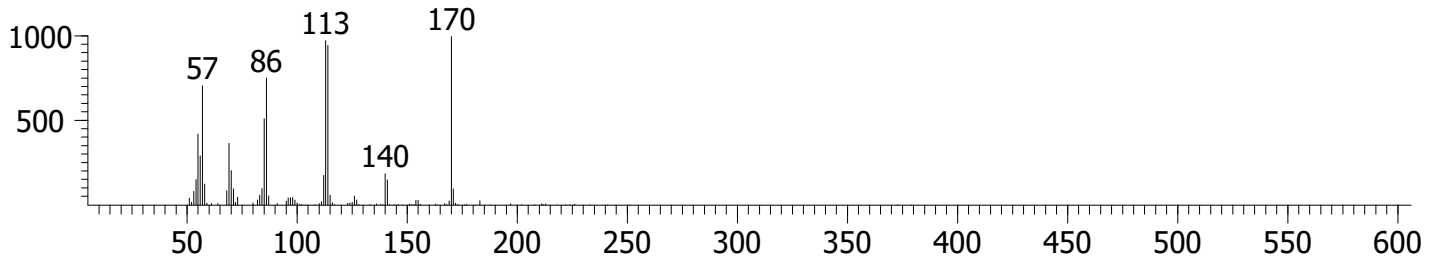
1st Dimension R.T. = 1742.78
2nd Dimension R.T. = 2.237
Quant Mass(es) = 170
S/N = 1453.7
Area = 205628
Height = 19404
Similarity = 813



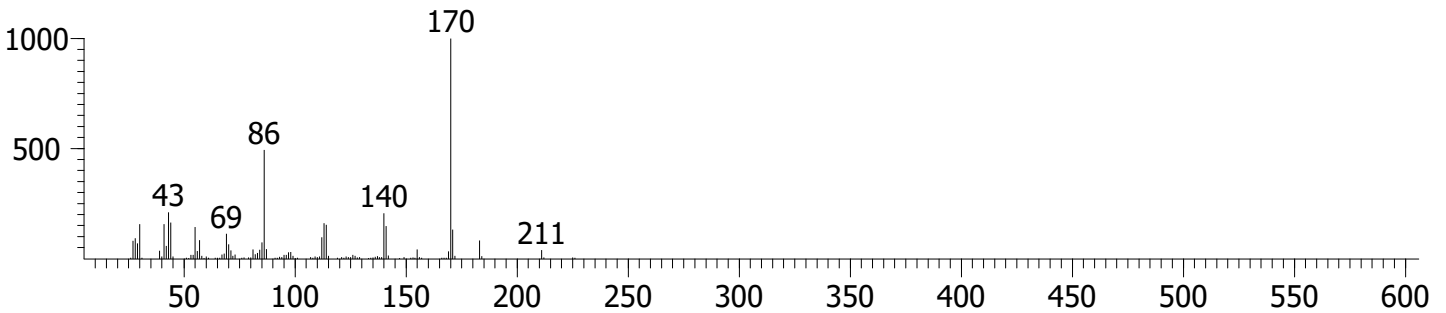
Peak Apex - sample "INF C grab 091919 (20191511):1", peak 3045, at 1742.78 , 2.237 sec , sec (Spec # 191669)



Peak True - sample "INF C grab 091919 (20191511):1", peak 3045, at 1742.78 , 2.237 sec , sec (Spec # 191669)



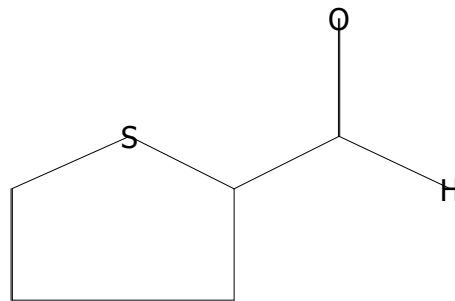
Library Hit - similarity 813, "2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-"



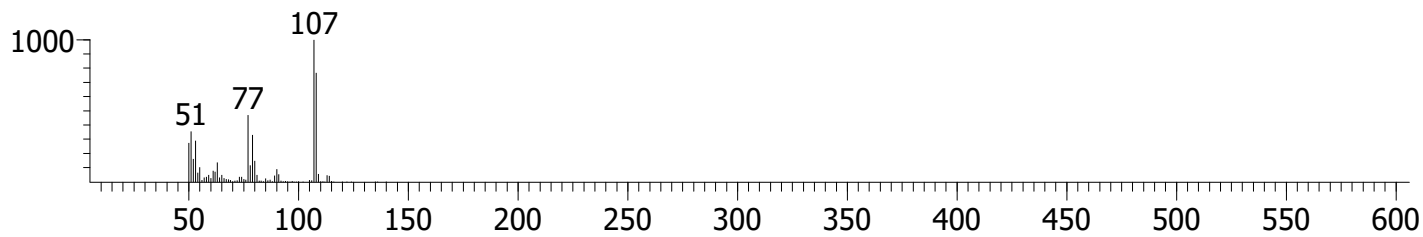
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-	813	8614	1436-27-7	mainlib	C12H22N2O2	226
2	2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-	769	8908	1436-27-7	replib	C12H22N2O2	226
3	l-Leucyl-d-leucine	666	251	17665-02-0	mainlib	C12H24N2O3	244
4	2-(tert-Butylamino)ethyl methacrylate	654	167	3775-90-4	mainlib	C10H19NO2	185
5	Itaconic acid diethyl ester	638	96	2409-52-1	mainlib	C9H14O4	186

Thiophene, 2-formyl-2,3-dihydro-

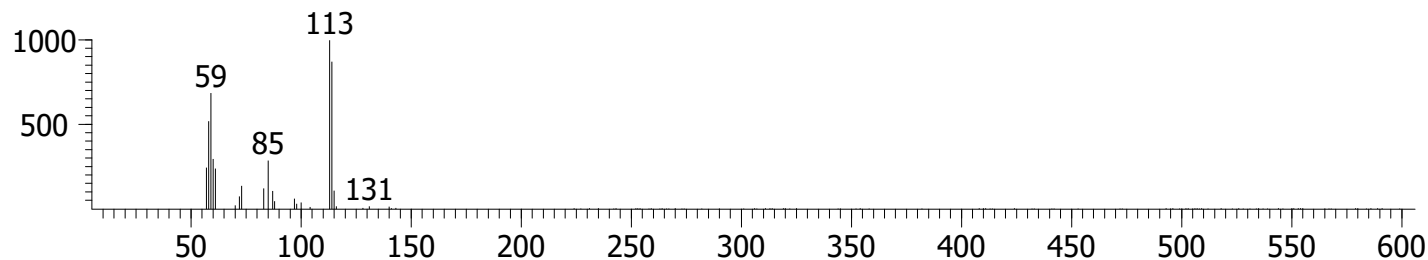
1st Dimension R.T. = 696.876
2nd Dimension R.T. = 1.775
Quant Mass(es) = 113
S/N = 320.15
Area = 47686
Height = 5970.8
Similarity = 814



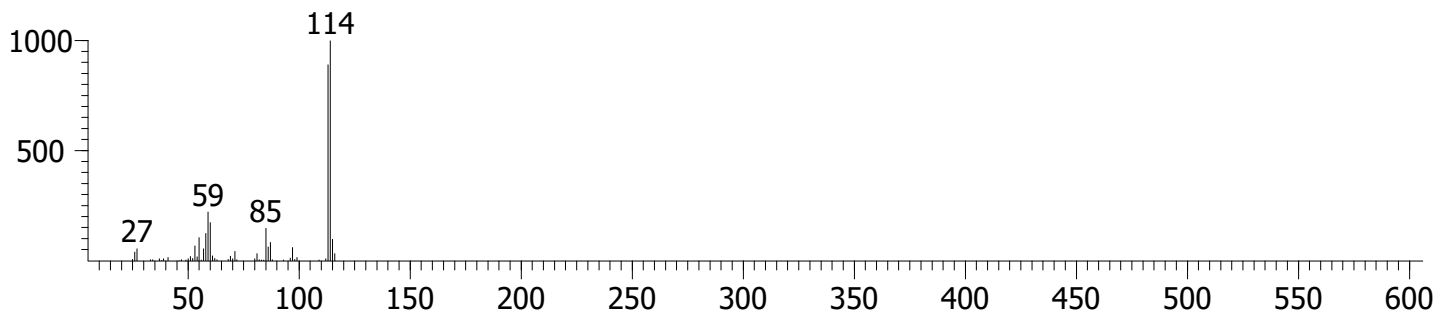
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 569, at 696.876 , 1.775 sec , sec (Spec # 33129)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 569, at 696.876 , 1.775 sec , sec (Spec # 33129)



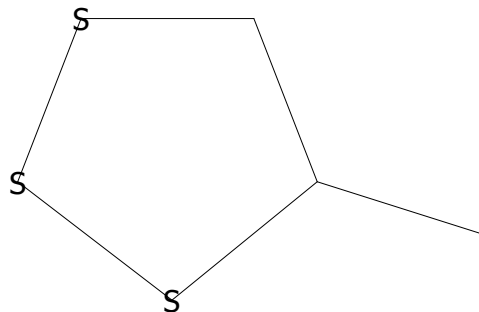
Library Hit - similarity 814, "Thiophene, 2-formyl-2,3-dihydro-"



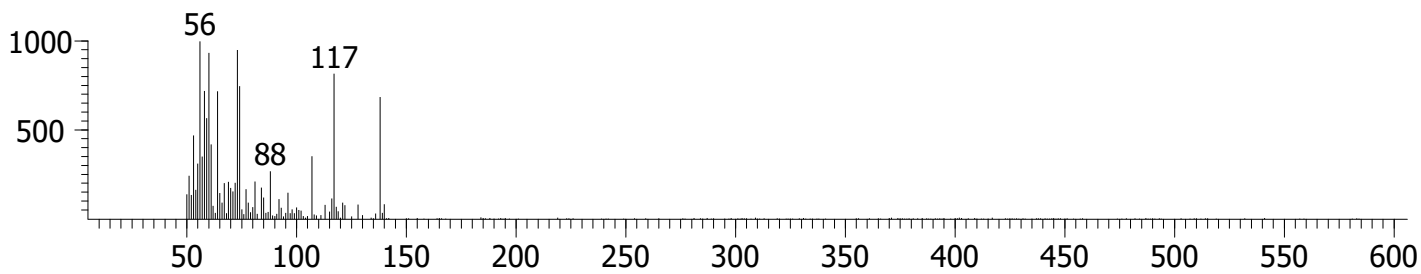
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Thiophene, 2-formyl-2,3-dihydro-	814	8845	290354-70-0	mainlib	C5H6OS	114
2	1-Butoxypropan-2-yl heptanoate	700	537	0-00-0	mainlib	C14H28O3	244
3	Glycyl-D-valine	652	111	10521-49-0	mainlib	C7H14N2O3	174
4	Silane, 1-butenyltrimethyl-	650	102	18291-95-7	mainlib	C7H16Si	128
5	1-(2-methyl-3-furylthio)-ethanethiol	646	86	0-00-0	mainlib	C7H10OS2	174

4-Methyl-1,2,3-trithiolane

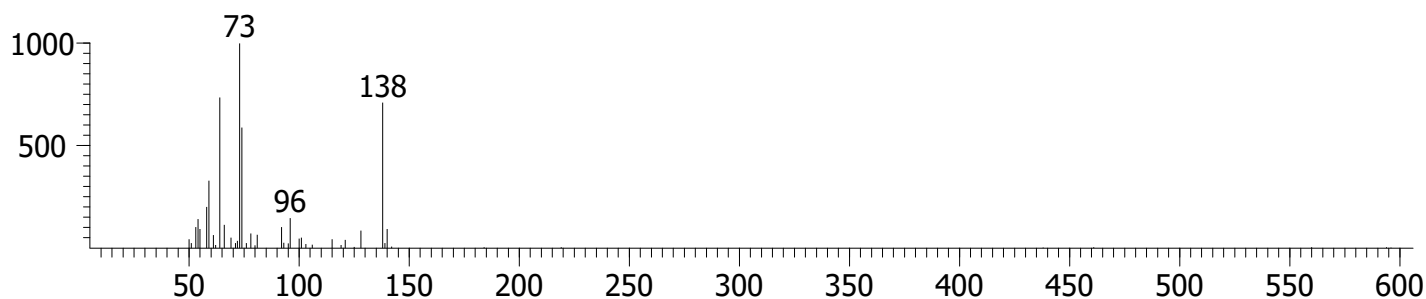
1st Dimension R.T. = 815.808
2nd Dimension R.T. = 2.132
Quant Mass(es) = 138
S/N = 140.73
Area = 29924
Height = 3779.7
Similarity = 811



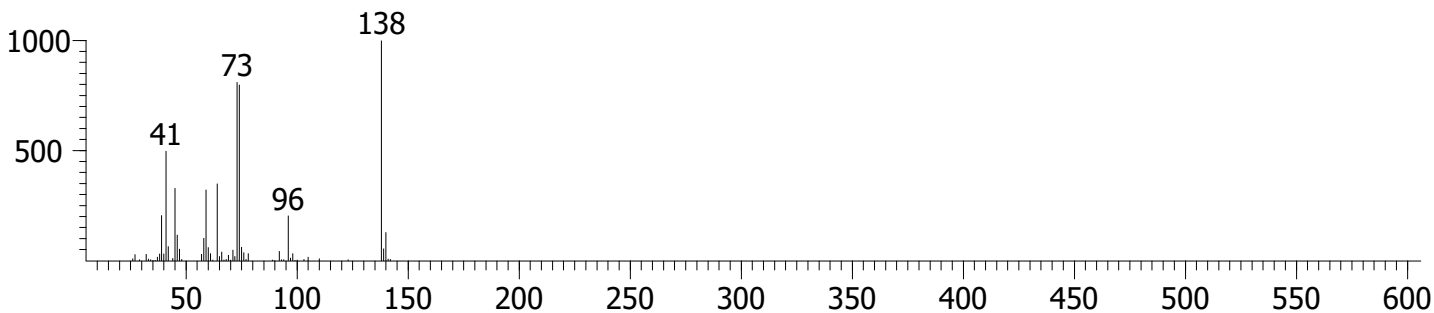
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 904, at 815.808 , 2.132 sec , sec (Spec # 51203)



Peak True - sample "INF-C comp 091919 (111419):1", peak 904, at 815.808 , 2.132 sec , sec (Spec # 51203)



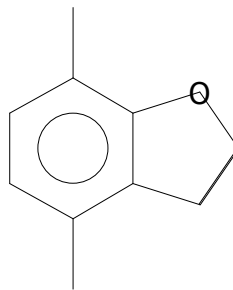
Library Hit - similarity 811, "4-Methyl-1,2,3-trithiolane"



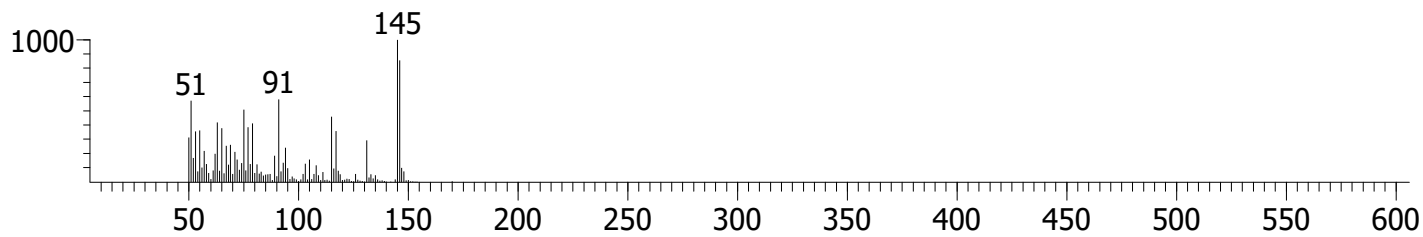
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Methyl-1,2,3-trithiolane	811	9345	116664-29-0	mainlib	C3H6S3	138
2	1,2-Dithiolane, 1,1-dioxide	691	490	18321-16-9	mainlib	C3H6O2S2	138
3	4,6-Diethyl-1,2,3,5-tetrathiolane	587	34	0-00-0	mainlib	C6H12S4	212
4	1,3,5-Trithiane	586	32	291-21-4	mainlib	C3H6S3	138
5	1,4:5,8-dimethano-naphthalene,1,2,4,4a,8,8,8a-octahydro-2-trimethylsilyl-	583	28	0-00-0	mainlib	C15H24Si	232

Benzofuran, 4,7-dimethyl-

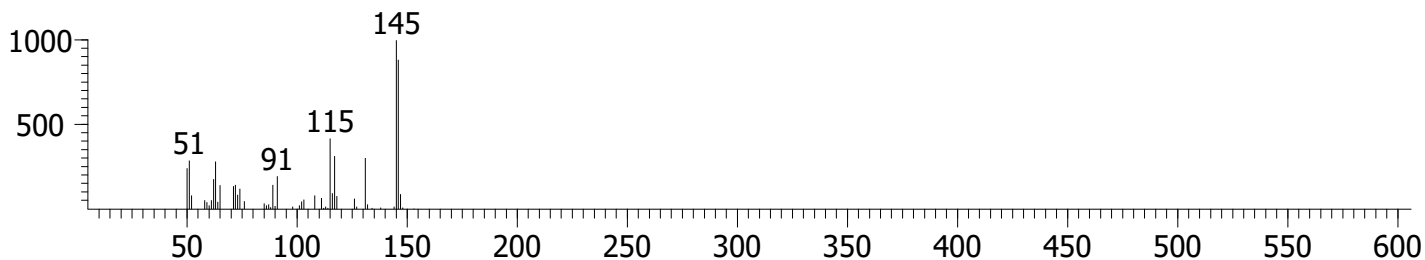
1st Dimension R.T. = 889.266
2nd Dimension R.T. = 1.696
Quant Mass(es) = 146
S/N = 1723.1
Area = 188888
Height = 26164
Similarity = 839



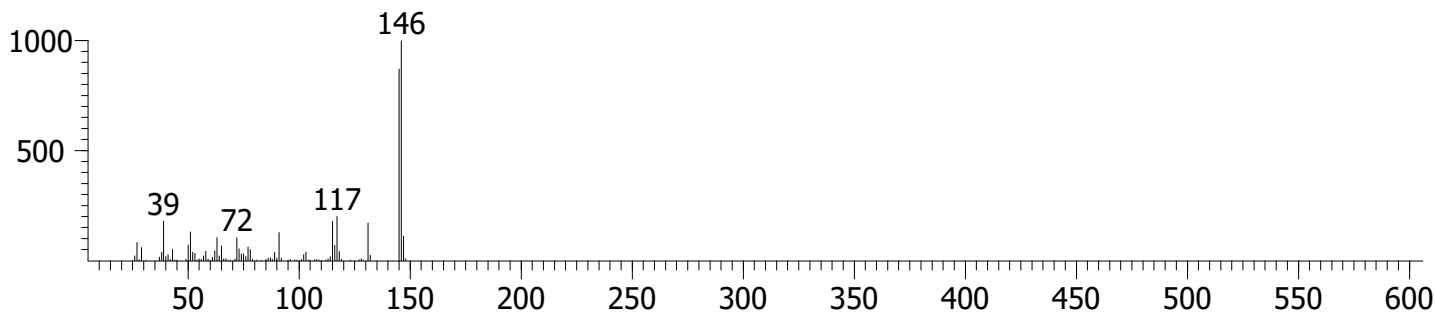
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 1177, at 889.266 , 1.696 sec , sec (Spec # 62267)



Peak True - sample "INF-C comp 091919 (111419):1", peak 1177, at 889.266 , 1.696 sec , sec (Spec # 62267)

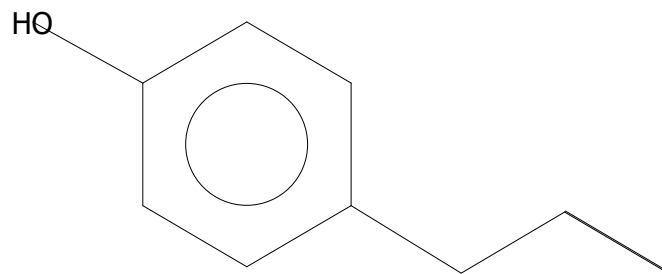


Library Hit - similarity 839, "Benzofuran, 4,7-dimethyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzofuran, 4,7-dimethyl-	839	6901	28715-26-6	mainlib	C10H10O	146
2	Cinnamaldehyde, α -methyl-	794	1469	1196-67-4	mainlib	C10H10O	146
3	1H-Indene-4-carboxaldehyde, 2,3-dihydro-	756	352	51932-70-8	mainlib	C10H10O	146
4	2-Propenal, 2-methyl-3-phenyl-	752	297	101-39-3	mainlib	C10H10O	146
5	2,3-Dimethyl-1H-pyrrolo[2,3-b]pyridine	730	117	10299-69-1	mainlib	C9H10N2	146

Phenol, 4-(2-propenyl)-



1st Dimension R.T. = 945.234

2nd Dimension R.T. = 1.789

Quant Mass(es) = 134

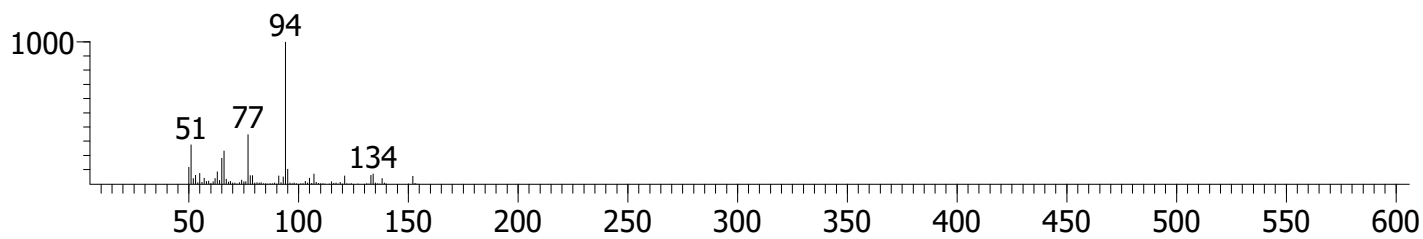
S/N = 858.62

Area = 92265

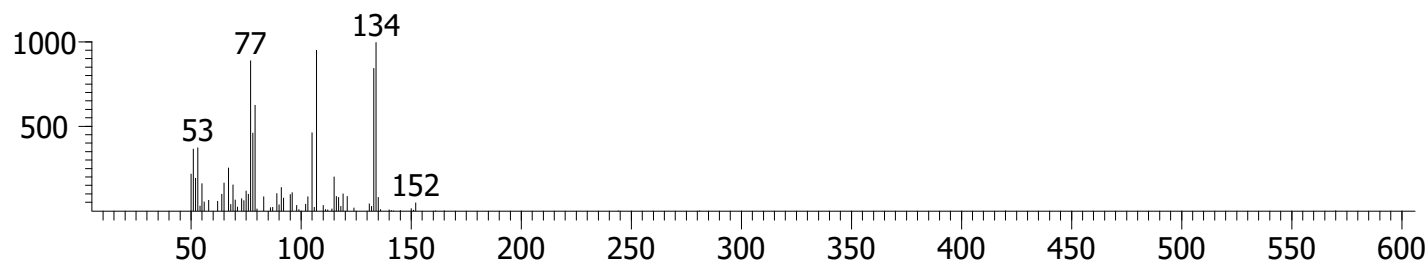
Height = 11809

Similarity = 824

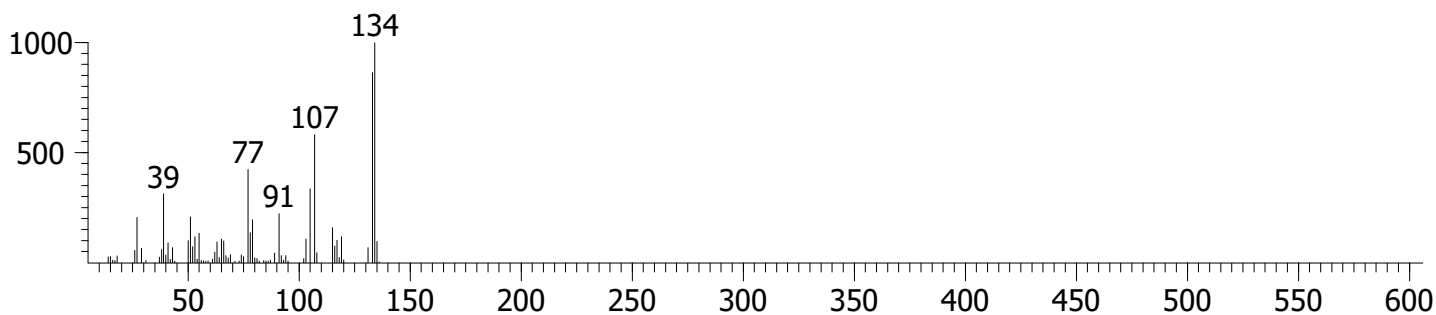
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 1567, at 945.234 , 1.789 sec , sec (Spec # 70761)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 1567, at 945.234 , 1.789 sec , sec (Spec # 70761)



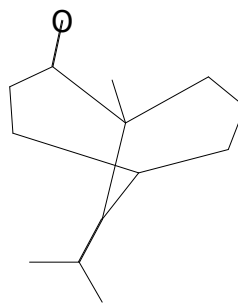
Library Hit - similarity 824, "Phenol, 4-(2-propenyl)-"



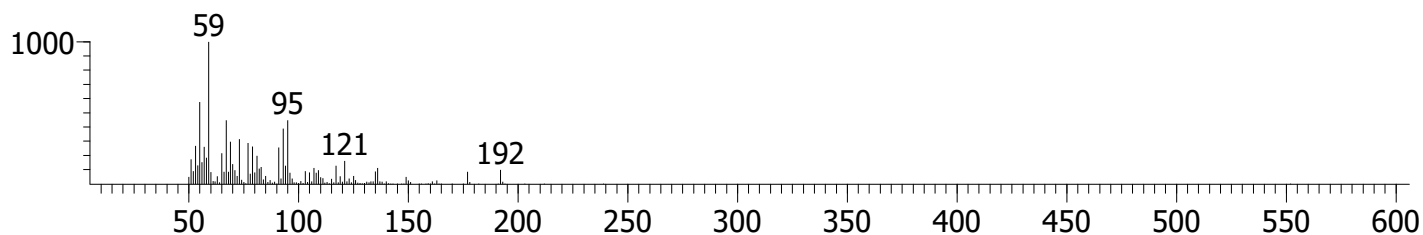
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Phenol, 4-(2-propenyl)-	824	6909	501-92-8	mainlib	C9H10O	134
2	3-(1-Cyclopentenyl)furan	743	732	115754-79-5	mainlib	C9H10O	134
3	Phenol, 4-(2-propenyl)-, acetate	722	311	61499-22-7	mainlib	C11H12O2	176
4	6-APDB	716	244	1281872-58-9	mainlib	C11H15NO	177
5	1-(3-Methyl-2-butenoxy)-4-(1-propenyl)benzene	709	187	78259-41-3	mainlib	C14H18O	202

Bicyclo[3.3.1]nonan-2-one,
1-methyl-9-(1-methylethylidene)-

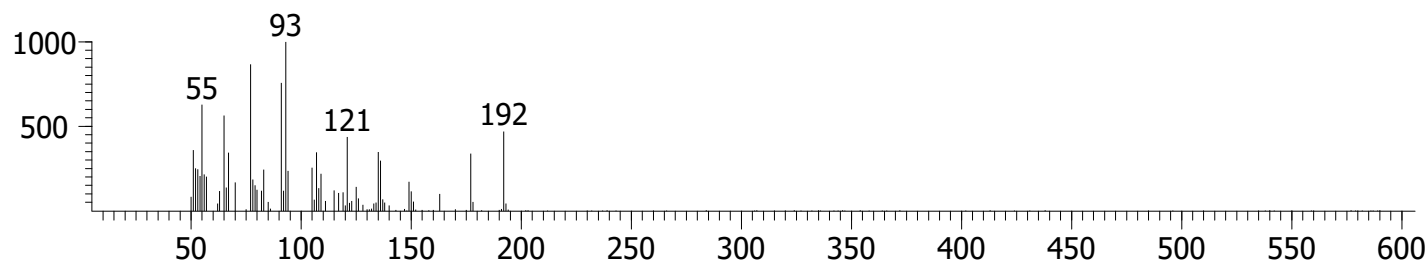
1st Dimension R.T. = 983.712
 2nd Dimension R.T. = 1.498
 Quant Mass(es) = 192
 S/N = 259.60
 Area = 19049
 Height = 2735.4
 Similarity = 747



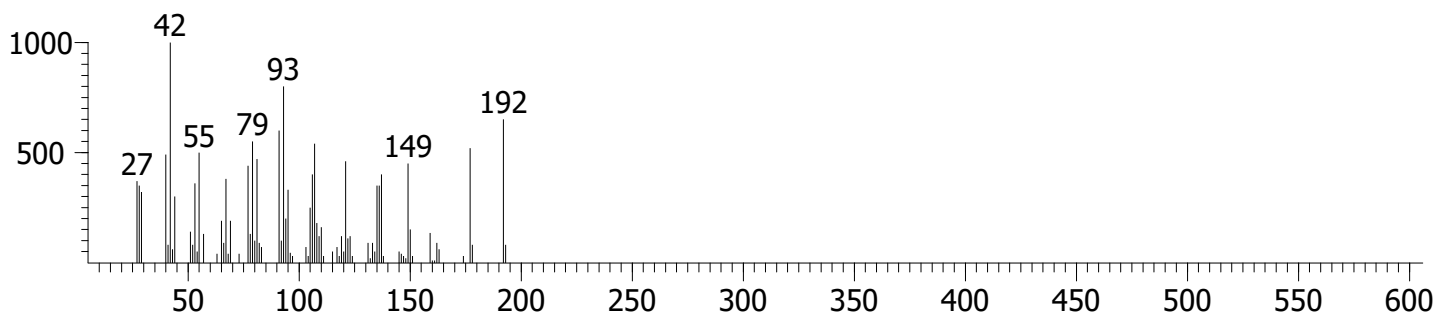
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 1739, at 983.712 , 1.498 sec , sec (Spec # 76 547)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 1739, at 983.712 , 1.498 sec , sec (Spec # 765 47)

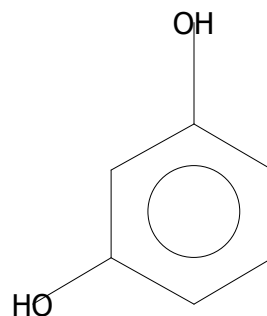


Library Hit - similarity 747, "Bicyclo[3.3.1]nonan-2-one, 1-methyl-9-(1-methylethylidene)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Bicyclo[3.3.1]nonan-2-one, 1-methyl-9-(1-methylethylidene)-	747	2786	56630-95-6	mainlib	C13H20O	192
2	(1R,2R,5R,E)-7-Ethylidene-1,2,8,8-tetramethylbicyclo[3.2.1]octane	722	849	193695-14-6	mainlib	C14H24	192
3	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4a,7,7-trimethyl-, (R)-	719	751	55123-72-3	mainlib	C13H20O	192
4	Ionone	717	692	8013-90-9	mainlib	C13H20O	192
5	2(1H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-1,1,4a-trimethyl-	713	585	4668-61-5	mainlib	C13H20O	192

Resorcinol



1st Dimension R.T. = 1029.19

2nd Dimension R.T. = 1.973

Quant Mass(es) = 110

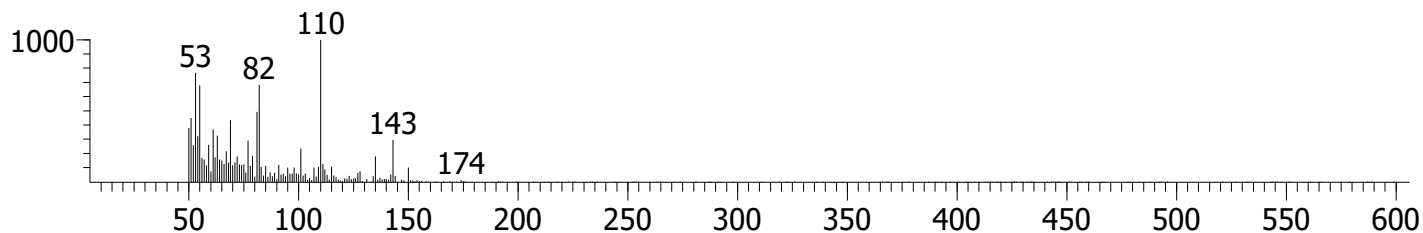
S/N = 73.311

Area = 1152973

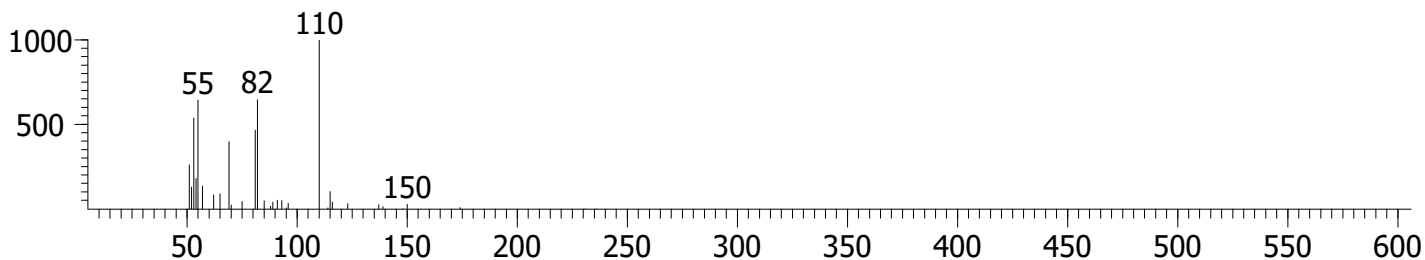
Height = 60605

Similarity = 740

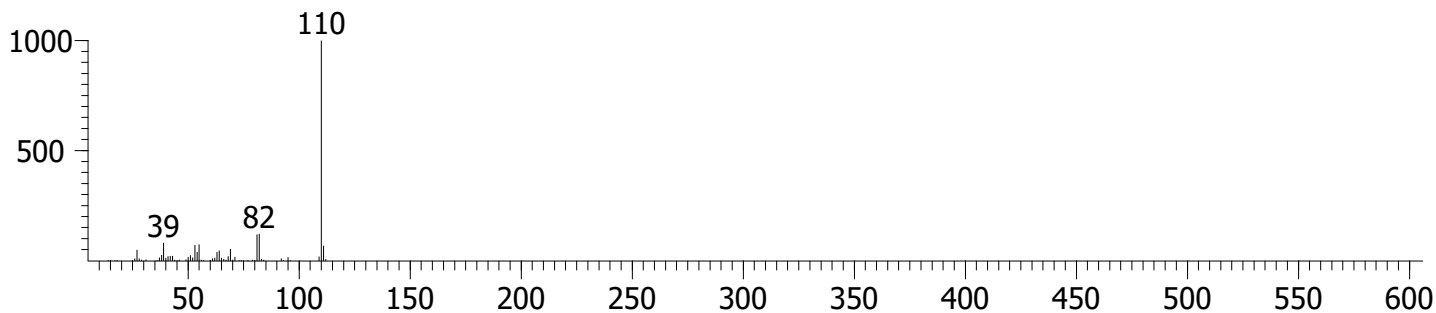
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 1962, at 1029.19 , 1.973 sec , sec (Spec # 83509)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 1962, at 1029.19 , 1.973 sec , sec (Spec # 83509)



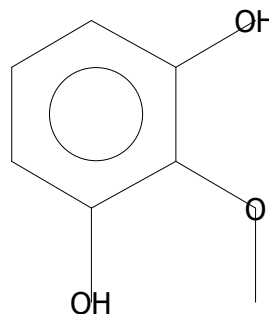
Library Hit - similarity 740, "Resorcinol"



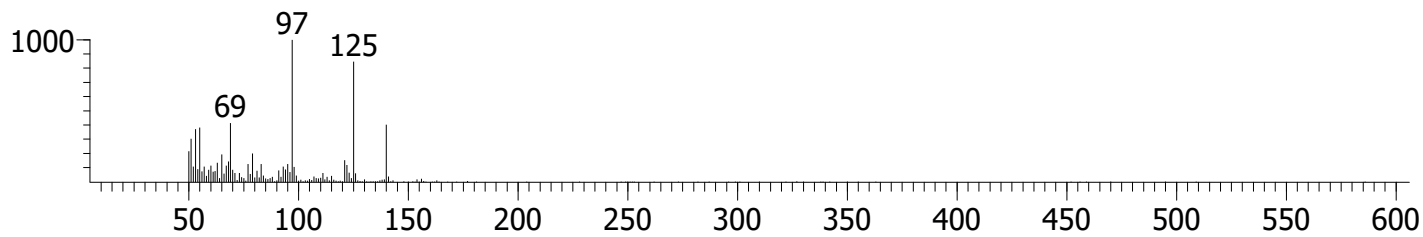
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Resorcinol	740	4702	108-46-3	mainlib	C6H6O2	110
2	4(1H)-Pyrimidinone, 6-methyl-	703	1144	3524-87-6	mainlib	C5H6N2O	110
3	4-(4-Methyl-[1,3,2]dioxaborinan-2-yloxy)-phenol	695	853	0-00-0	mainlib	C10H13BO4	208
4	2(1H)-Pyrimidinone, 5-methyl-	681	534	41398-85-0	mainlib	C5H6N2O	110
5	Resorcinol monoacetate	668	345	102-29-4	mainlib	C8H8O3	152

2-Methoxyresorcinol

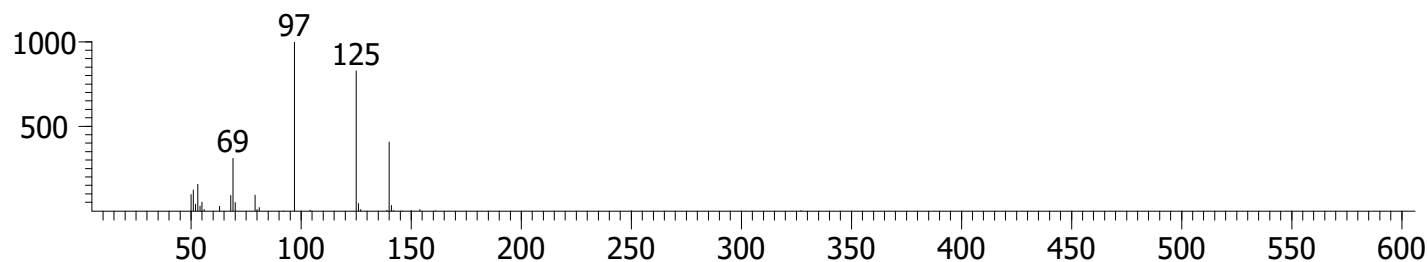
1st Dimension R.T. = 1123.63
2nd Dimension R.T. = 2.086
Quant Mass(es) = 125
S/N = 949.97
Area = 376130
Height = 33557
Similarity = 824



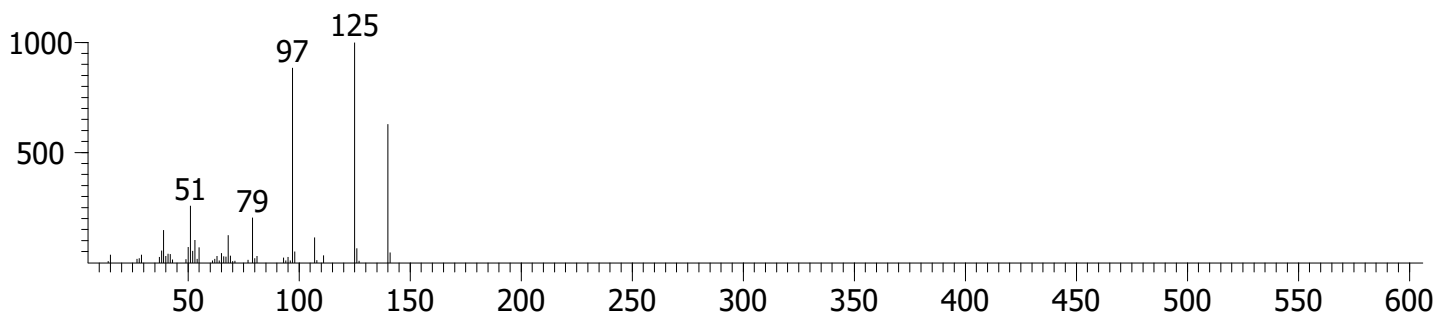
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 2443, at 1123.63 , 2.086 sec , sec (Spec # 97836)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 2443, at 1123.63 , 2.086 sec , sec (Spec # 97836)

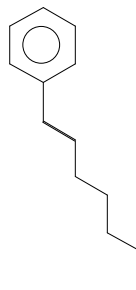


Library Hit - similarity 824, "2-Methoxyresorcinol"



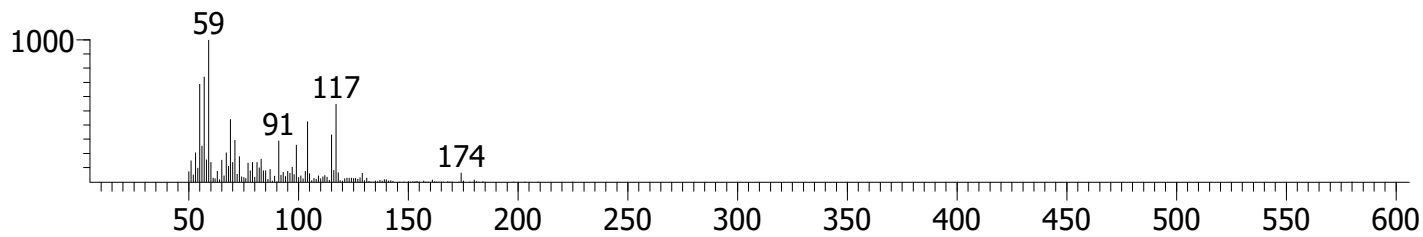
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Methoxyresorcinol	824	5354	29267-67-2	mainlib	C ₇ H ₈ O ₃	140
2	1,4-Benzenediol, 2-methoxy-	800	1794	824-46-4	mainlib	C ₇ H ₈ O ₃	140
3	5-Acetyl-2-furanmethanol	796	1515	55087-82-6	mainlib	C ₇ H ₈ O ₃	140
4	Cyclohexanone, 2-acetyl-	756	351	874-23-7	mainlib	C ₈ H ₁₂ O ₂	140
5	1,2-Benzenediol, 3-methoxy-	746	248	934-00-9	mainlib	C ₇ H ₈ O ₃	140

Benzene, 1-heptenyl-

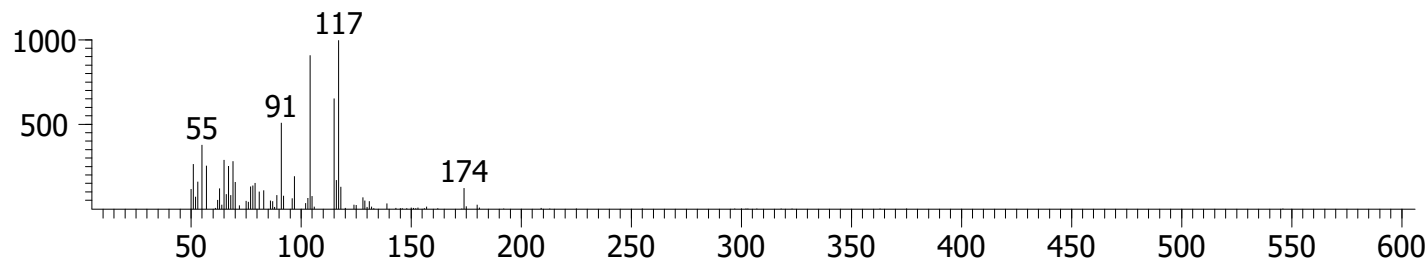


1st Dimension R.T. = 1176.1
2nd Dimension R.T. = 1.525
Quant Mass(es) = 104
S/N = 483.67
Area = 60602
Height = 8512.3
Similarity = 767

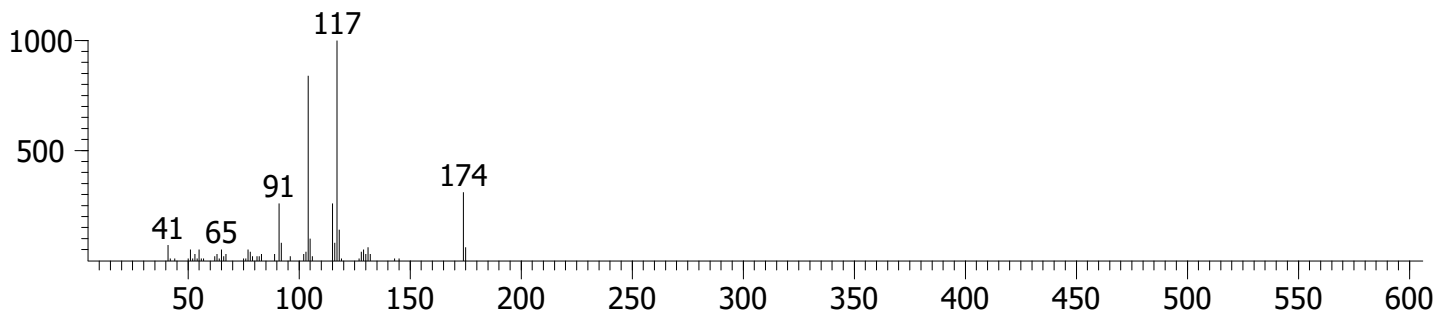
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 2704, at 1176.1 , 1.525 sec , sec (Spec # 105701)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 2704, at 1176.1 , 1.525 sec , sec (Spec # 105701)



Library Hit - similarity 767, "Benzene, 1-heptenyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-heptenyl-	767	3672	829-99-2	mainlib	C13H18	174
2	Benzene, 2-heptenyl-	743	1230	26447-63-2	mainlib	C13H18	174
3	Benzene, 2-heptenyl-, (Z)-	739	1039	54725-18-7	mainlib	C13H18	174
4	1,11-Dimethyltricyclo[9.2.2.14,8]hexadeca-4,6,8(16)triene-12,14-dione	734	837	0-00-0	mainlib	C18H22O2	270
5	Benzene, (5-methyl-1-hexenyl)-	715	406	86761-76-4	mainlib	C13H18	174

4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one

1st Dimension R.T. = 1242.56

2nd Dimension R.T. = 1.690

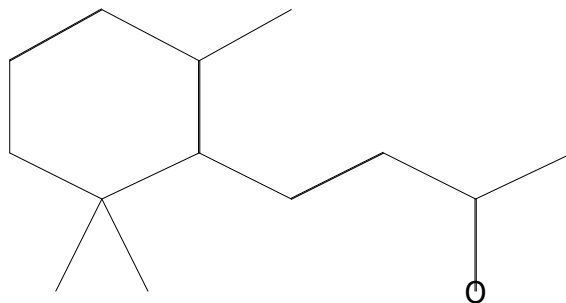
Quant Mass(es) = 175

S/N = 233.33

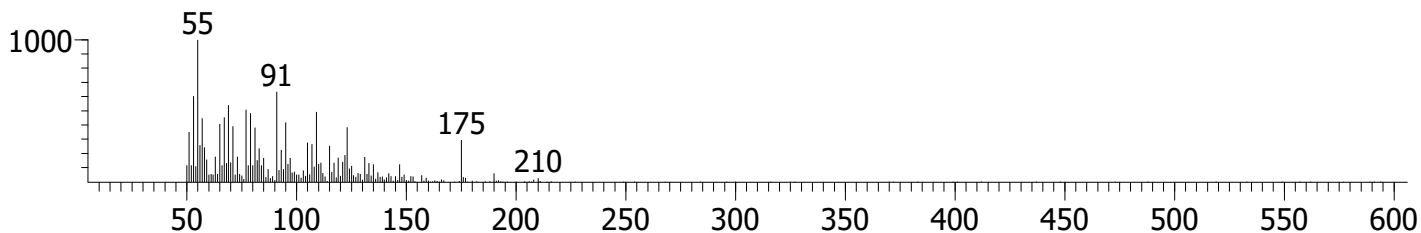
Area = 18666

Height = 2282.7

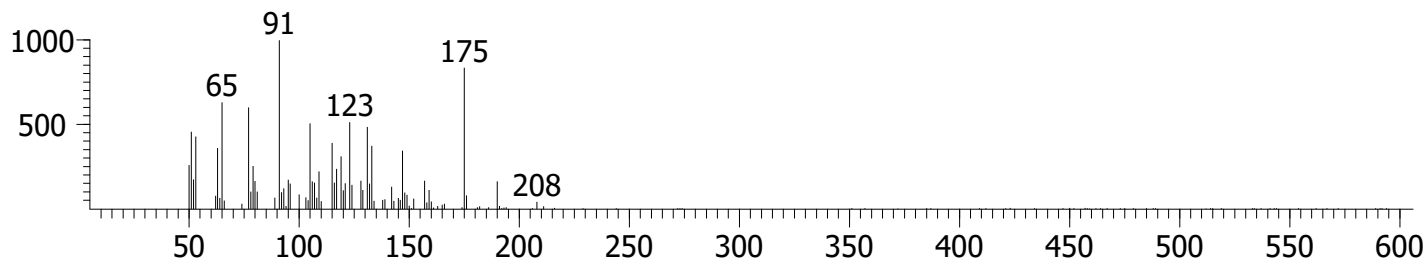
Similarity = 801



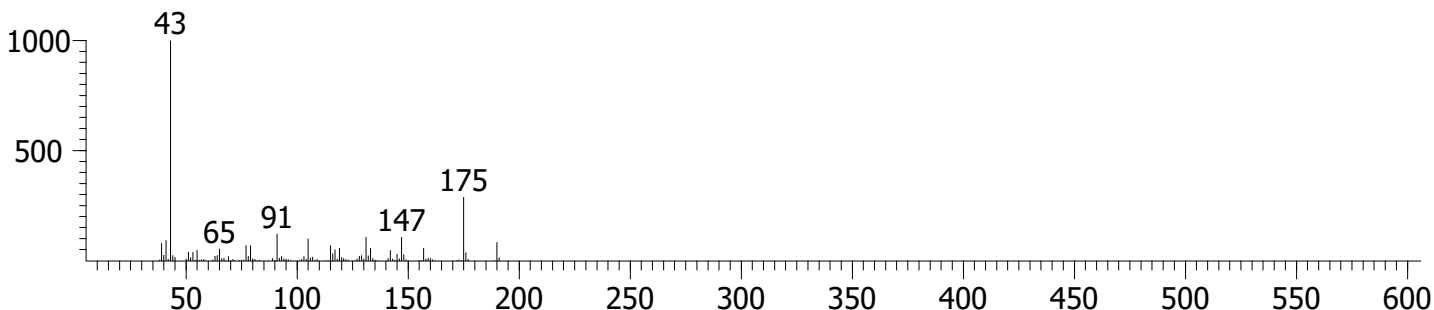
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 3090, at 1242.56 , 1.690 sec , sec (Spec # 115796)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 3090, at 1242.56 , 1.690 sec , sec (Spec # 115796)



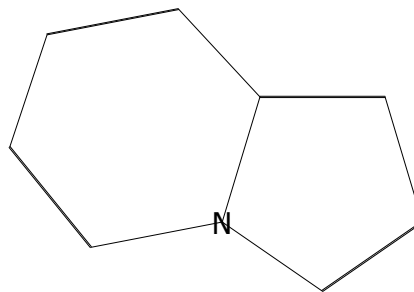
Library Hit - similarity 801, "4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one"



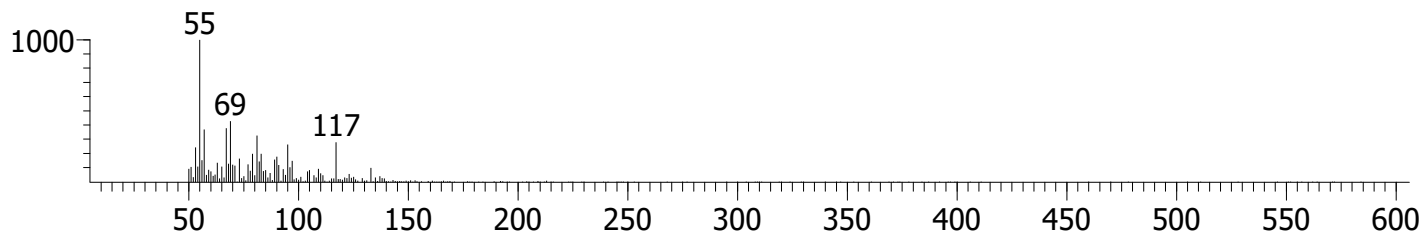
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	801	6274	1203-08-3	mainlib	C13H18O	190
2	4-(2,4,4-Trimethyl-cyclohexa-1,5-dienyl)-but-3-en-2-one	739	1072	0-00-0	mainlib	C13H18O	190
3	3,6-Nonadien-5-one, 2,2,8,8-tetramethyl-	679	190	35845-67-1	mainlib	C13H18O	190
4	syn-Tricyclo[5.1.0.0(2,4)]oct-5-ene, 3,3,5,6,8,8-hexamethyl-	671	141	0-00-0	mainlib	C14H22	190
5	Ylangenal	669	130	41610-68-8	mainlib	C15H22O	218

Indolizine

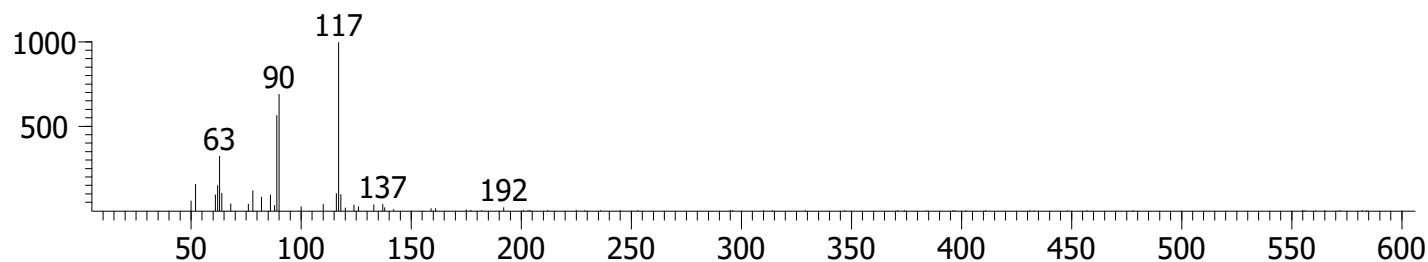
1st Dimension R.T. = 1253.06
2nd Dimension R.T. = 1.478
Quant Mass(es) = 90
S/N = 144.88
Area = 78225
Height = 12362
Similarity = 881



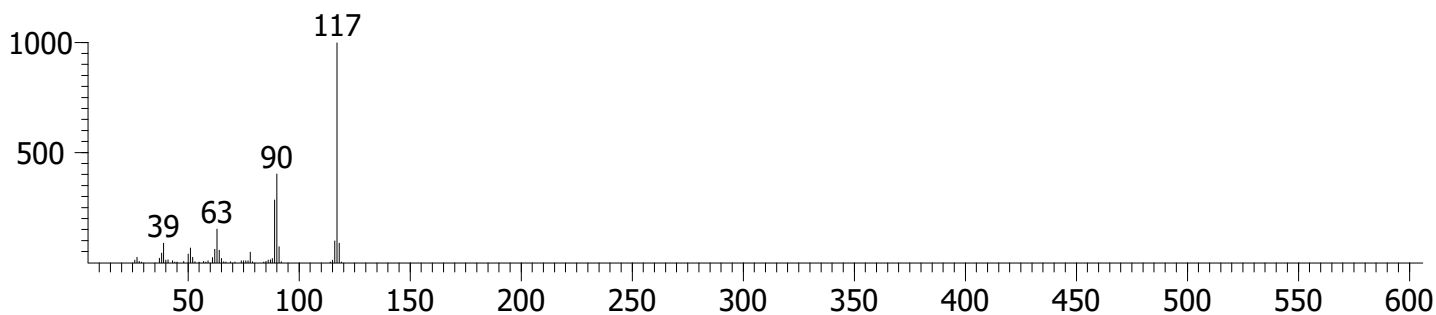
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 3162, at 1253.06 , 1.478 sec , sec (Spec # 117354)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 3162, at 1253.06 , 1.478 sec , sec (Spec # 117354)



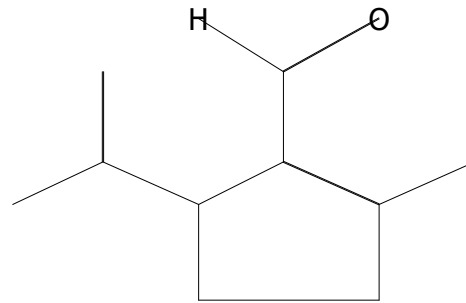
Library Hit - similarity 881, "Indolizine"



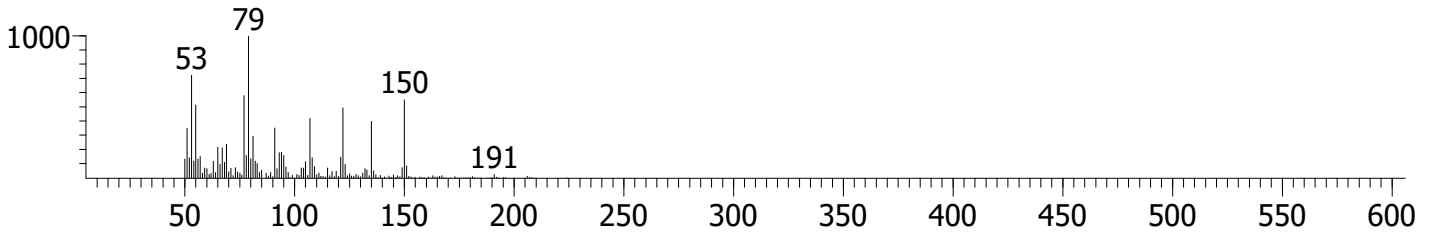
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Indolizine	881	4211	274-40-8	mainlib	C8H7N	117
2	Indole	864	2298	120-72-9	mainlib	C8H7N	117
3	5H-1-Pyridine	858	1806	270-91-7	mainlib	C8H7N	117
4	4-Ethynylaniline	801	338	14235-81-5	mainlib	C8H7N	117
5	Benzyl nitrile	789	225	140-29-4	mainlib	C8H7N	117

ropenyl-2-methylcyclopent-1-enecarboxalde

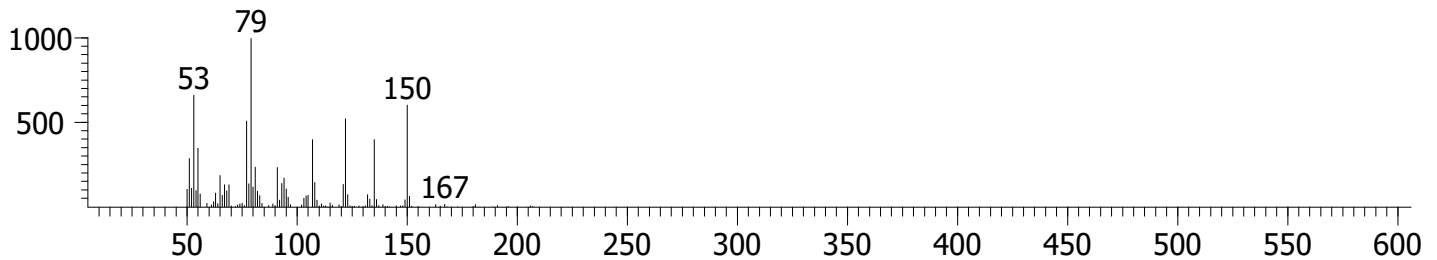
1st Dimension R.T. = 1385.98
2nd Dimension R.T. = 1.940
Quant Mass(es) = 150
S/N = 729.33
Area = 237818
Height = 22477
Similarity = 831



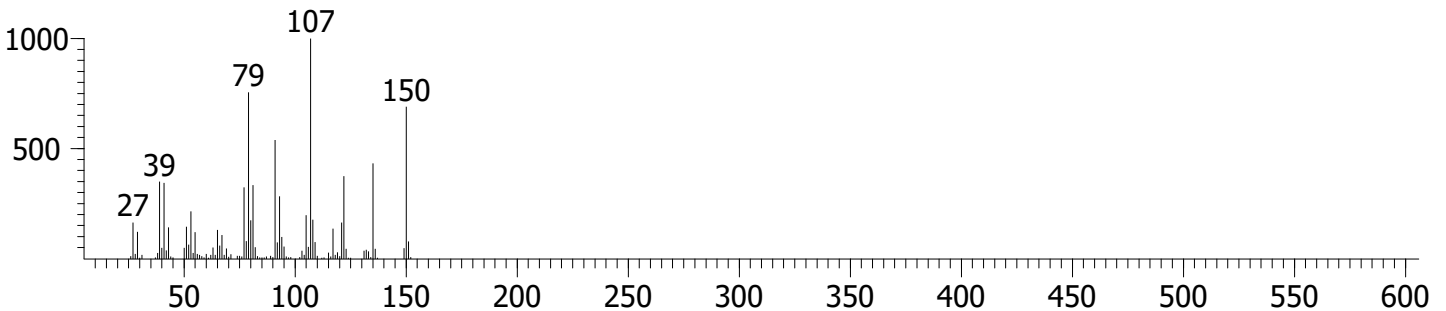
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 3484, at 1385.98 , 1.940 sec , sec (Spec # 137564)



Peak True - sample "INF-C comp 091919 (111419):1", peak 3484, at 1385.98 , 1.940 sec , sec (Spec # 137564)

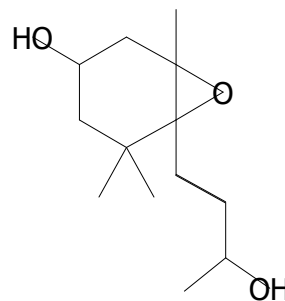


Library Hit - similarity 831, "5-Isopropenyl-2-methylcyclopent-1-enecarboxaldehyde"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-Isopropenyl-2-methylcyclopent-1-enecarboxaldehyde	831	1691	0-00-0	mainlib	C10H14O	150
2	3,9-Epoxy-p-mentha-1,8(10)-diene	814	923	0-00-0	mainlib	C10H14O	150
3	2H-Inden-2-one, 1,4,5,6,7,7a-hexahydro-7a-methyl-, (S)-	805	670	54725-16-5	mainlib	C10H14O	150
4	2-Cyclohexen-1-one, 2-(2-methyl-2-propenyl)-	799	526	18926-98-2	mainlib	C10H14O	150
5	1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethenyl)-	796	465	2111-75-3	mainlib	C10H14O	150

7-Oxabicyclo[4.1.0]heptan-3-ol,
6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-



1st Dimension R.T. = 1473.43

2nd Dimension R.T. = 1.841

Quant Mass(es) = 125

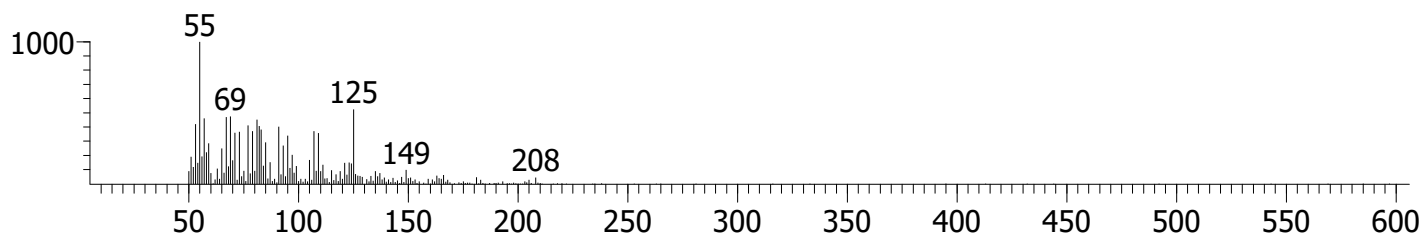
S/N = 493.55

Area = 147921

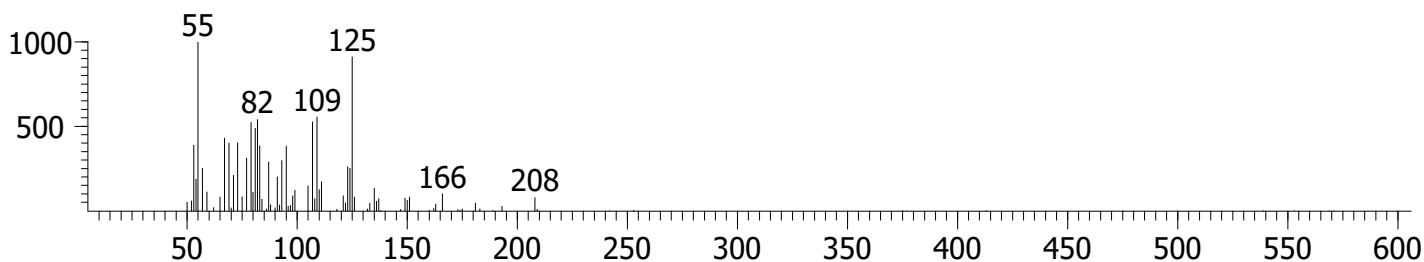
Height = 11990

Similarity = 783

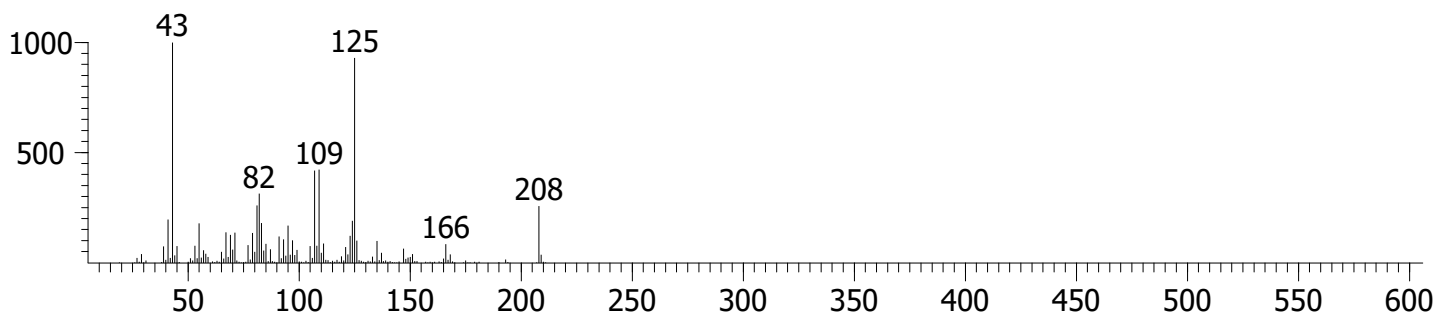
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 4589, at 1473.43 , 1.841 sec , sec (Spec # 15 0799)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 4589, at 1473.43 , 1.841 sec , sec (Spec # 150 799)



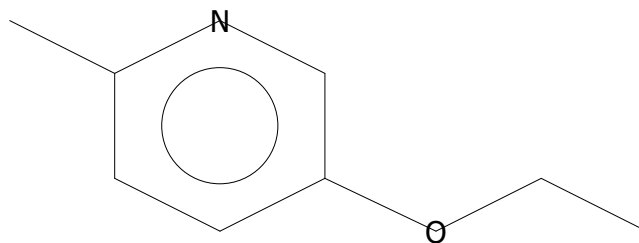
Library Hit - similarity 783, "7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-"



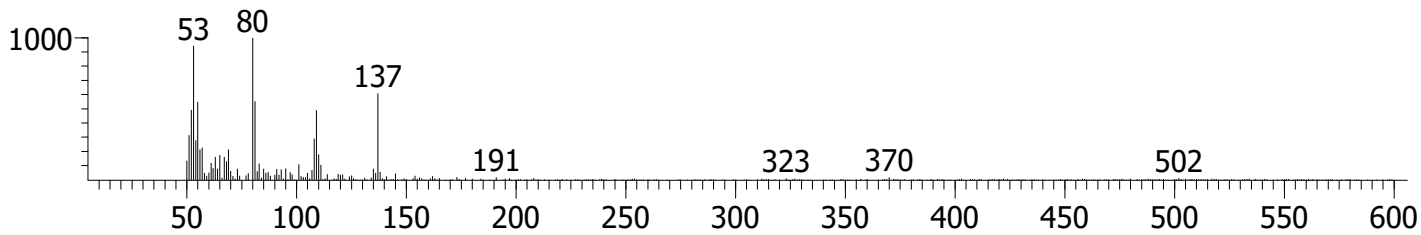
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-	783	5382	72777-88-9	mainlib	C13H22O3	226
2	3-Buten-2-one, 4-(2-hydroxy-2,6,6-trimethylcyclohexyl)-	750	1409	55955-46-9	mainlib	C13H22O2	210
3	Dihydronopol	699	284	0-00-0	mainlib	C11H20O	168
4	3-Buten-2-one, 3-methyl-4-(1,3,3-trimethyl-7-oxabicyclo[4.1.0]heptan-1-yl)-	698	273	97371-44-3	mainlib	C14H22O2	222
5	5-Isopropyl-6-methyl-hepta-3,5-dien-2-ol	690	203	0-00-0	mainlib	C11H20O	168

5-Ethoxy-2-methyl-pyridine

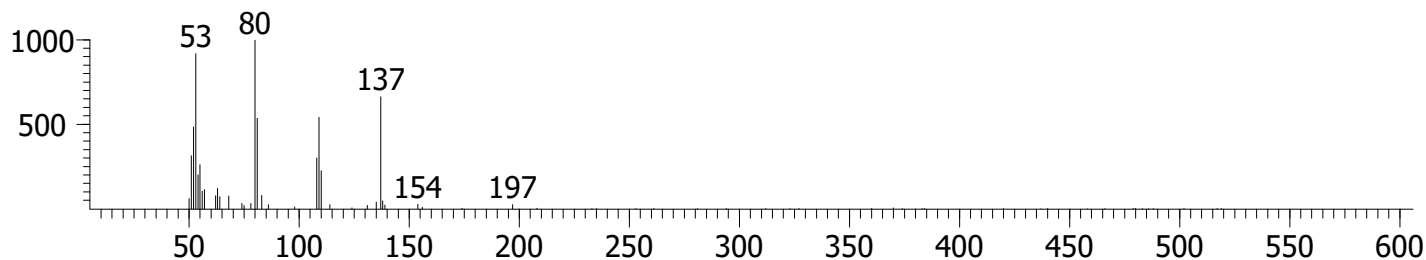
1st Dimension R.T. = 1476.93
2nd Dimension R.T. = 2.495
Quant Mass(es) = 137
S/N = 136.70
Area = 84863
Height = 8751.0
Similarity = 726



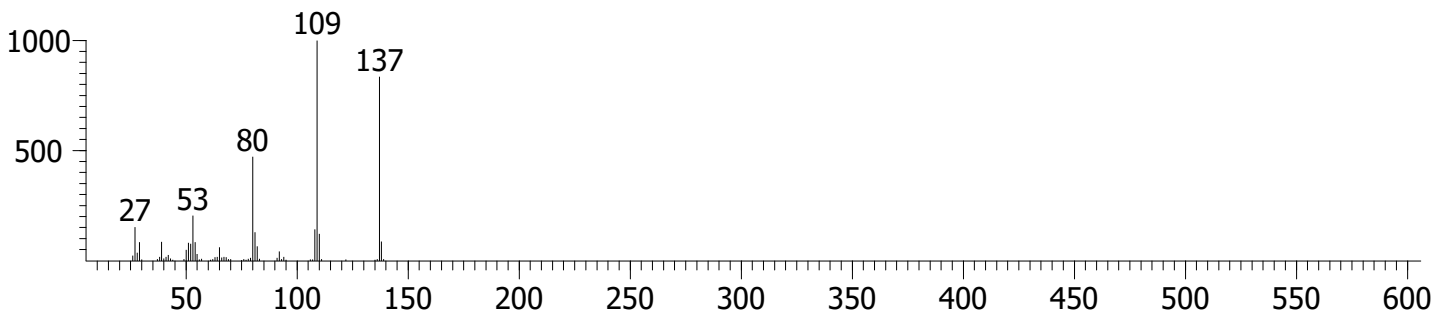
Peak Apex - sample "INF-A comp 092319 (111419):1", peak 3504, at 1476.93 , 2.495 sec , sec (Spec # 151428)



Peak True - sample "INF-A comp 092319 (111419):1", peak 3504, at 1476.93 , 2.495 sec , sec (Spec # 151428)



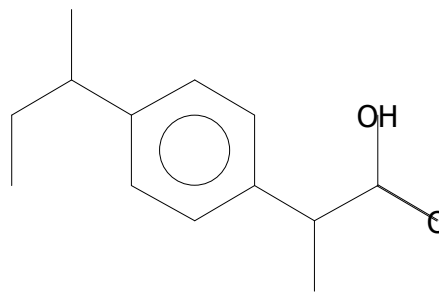
Library Hit - similarity 726, "5-Ethoxy-2-methyl-pyridine"



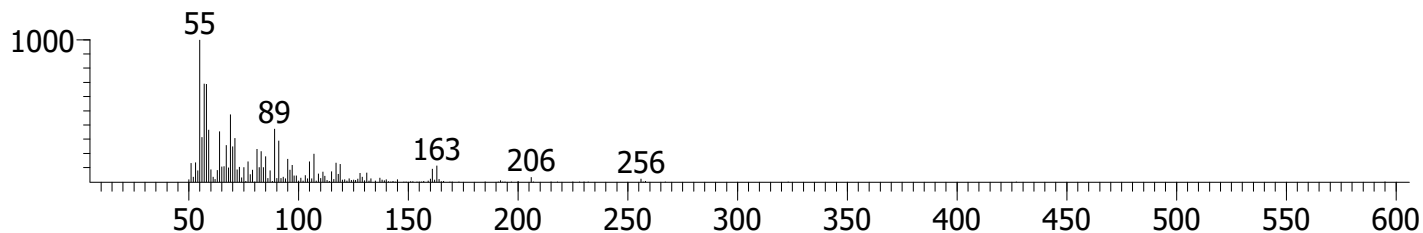
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-Ethoxy-2-methyl-pyridine	726	3738	55270-48-9	mainlib	C8H11NO	137
2	N-Methyl-3-formyl-2(1H)-pyridone	685	853	79138-28-6	mainlib	C7H7NO2	137
3	Benzenamine, 3-ethoxy-	674	585	621-33-0	mainlib	C8H11NO	137
4	5-[3-Methyl-2-furyl]hydantoin	671	517	0-00-0	mainlib	C8H8N2O3	180
5	8-Azabicyclo[3.2.1]oct-2-ene	661	365	5632-85-9	mainlib	C7H11N	109

2-(4-(But-2-yl)phenyl)propanoic acid

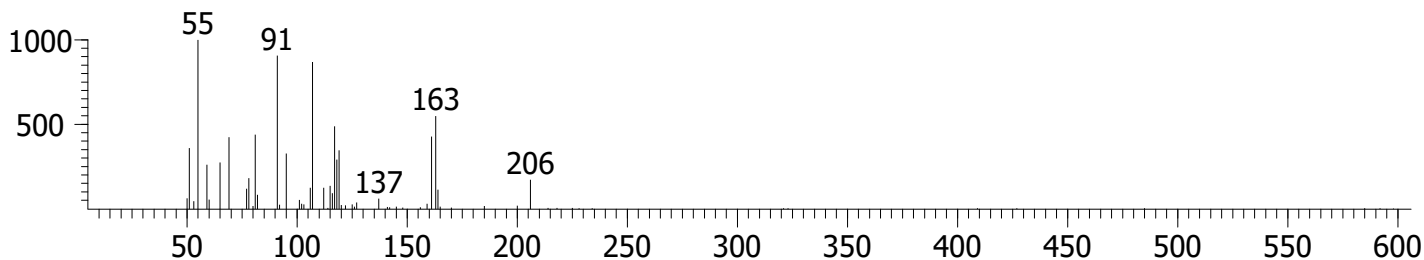
1st Dimension R.T. = 1480.43
2nd Dimension R.T. = 1.564
Quant Mass(es) = 163
S/N = 120.70
Area = 12455
Height = 1833.4
Similarity = 677



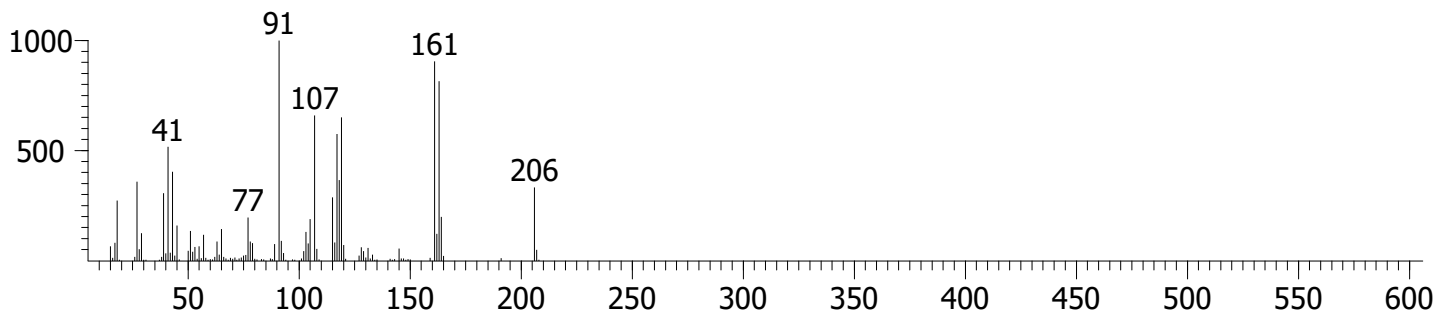
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 4018, at 1480.43 , 1.564 sec , sec (Spec # 151817)



Peak True - sample "INF-C comp 091919 (111419):1", peak 4018, at 1480.43 , 1.564 sec , sec (Spec # 151817)



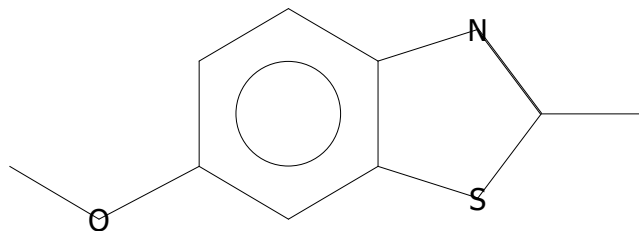
Library Hit - similarity 677, "2-(4-(But-2-yl)phenyl)propanoic acid"



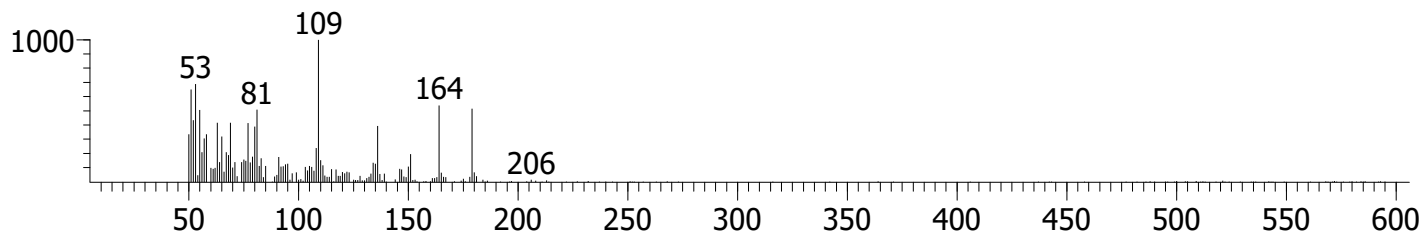
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-(4-(But-2-yl)phenyl)propanoic acid	677	5934	64451-76-9	mainlib	C13H18O2	206
2	Ibuprofen	639	1421	15687-27-1	mainlib	C13H18O2	206
3	2-(3-Isobutylphenyl)propionic acid	625	890	66622-47-7	mainlib	C13H18O2	206
4	1-(3,5-Dimethyl-1-adamantanoyl)semicarbazide	620	717	351327-47-4	mainlib	C14H23N3O2	265
5	Hydrocinnamic acid, à-methyl-, ester with 2-methylacetonitrile	543	87	14025-74-2	mainlib	C14H17NO2	231

Benzothiazole, 6-methoxy-2-methyl-

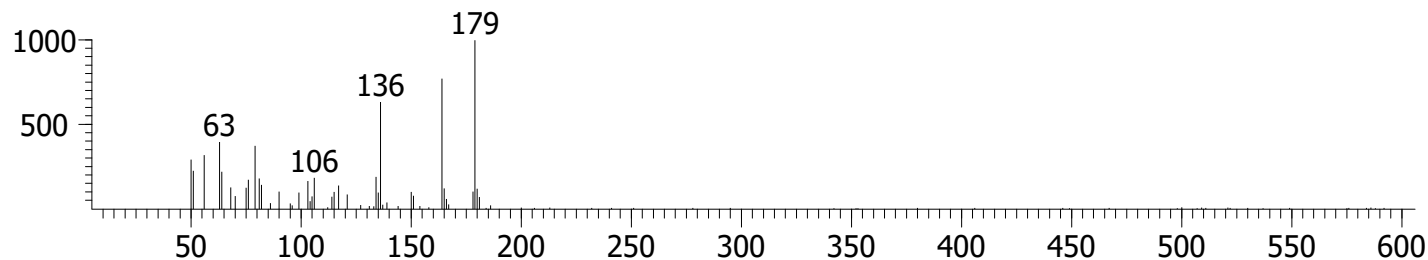
1st Dimension R.T. = 1515.41
2nd Dimension R.T. = 2.508
Quant Mass(es) = 164
S/N = 151.10
Area = 28908
Height = 2395.5
Similarity = 668



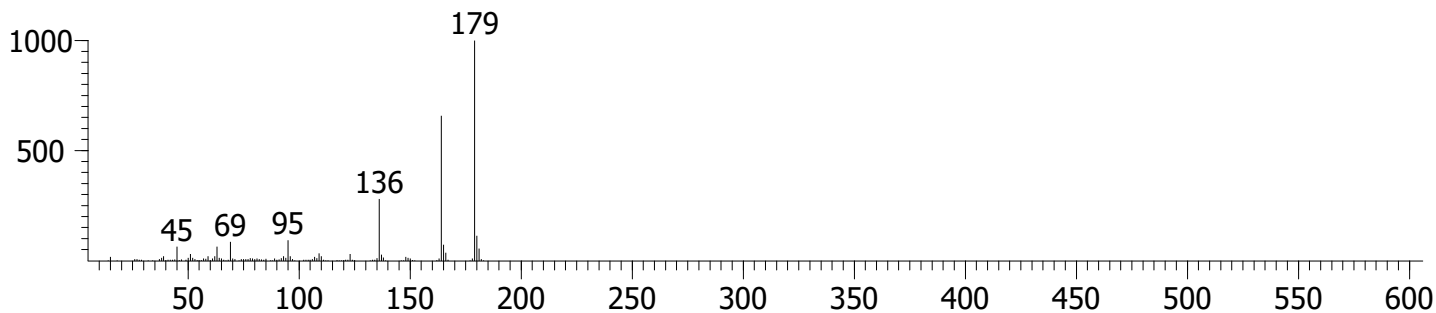
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 4866, at 1515.41 , 2.508 sec , sec (Spec # 157260)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 4866, at 1515.41 , 2.508 sec , sec (Spec # 157260)



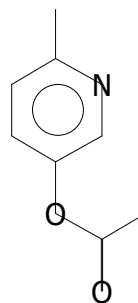
Library Hit - similarity 668, "Benzothiazole, 6-methoxy-2-methyl-"



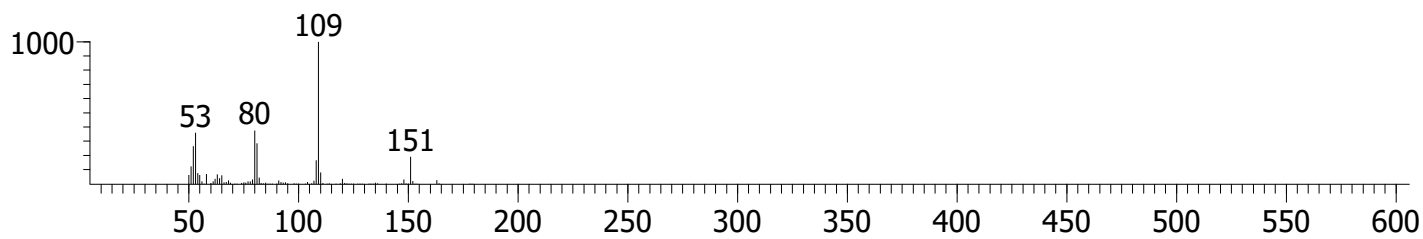
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzothiazole, 6-methoxy-2-methyl-	668	1567	2941-72-2	mainlib	C9H9NOS	179
2	Ethanone, 1-(6-amino-1,3-benzodioxol-5-yl)-	661	1200	28657-75-2	mainlib	C9H9NO3	179
3	benzenamine, N,N-diethyl-3-methoxy-	660	1154	0-00-0	mainlib	C11H17NO	179
4	5-Methoxy-2-methylbenzothiazole	660	1154	0-00-0	mainlib	C9H9NOS	179
5	benzenemethanol, 4-(diethylamino)-	654	907	0-00-0	mainlib	C11H17NO	179

3-Pyridinol, 6-methyl-, acetate (ester)

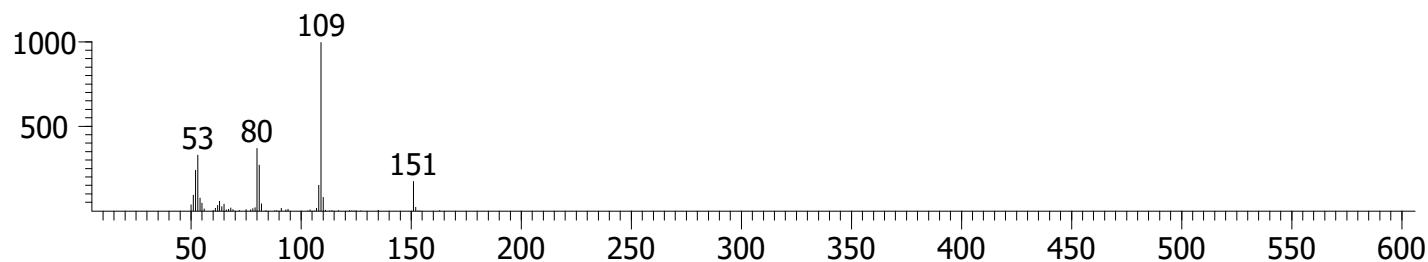
1st Dimension R.T. = 1504.91
2nd Dimension R.T. = 2.620
Quant Mass(es) = 109
S/N = 1747.2
Area = 736881
Height = 55862
Similarity = 874



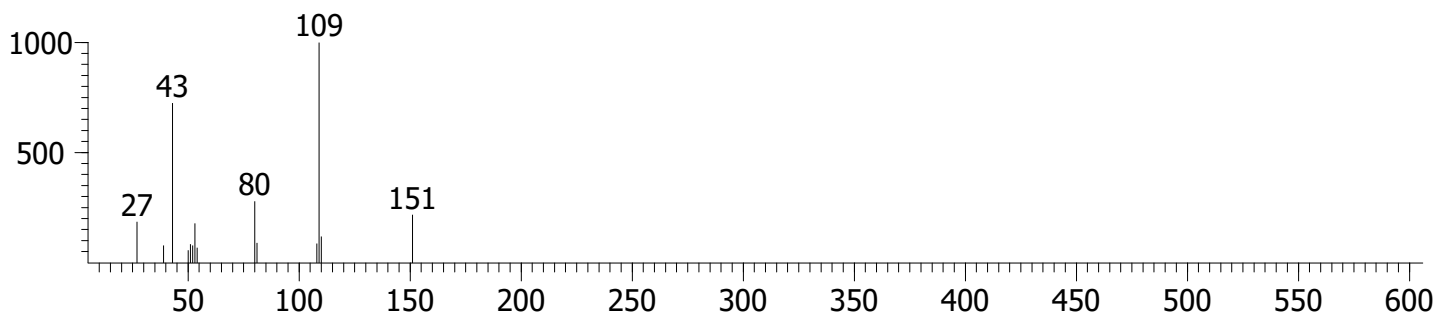
Peak Apex - sample "INF-C comp 091919 (111419):1", peak 4173, at 1504.91 , 2.620 sec , sec (Spec # 155687)



Peak True - sample "INF-C comp 091919 (111419):1", peak 4173, at 1504.91 , 2.620 sec , sec (Spec # 155687)



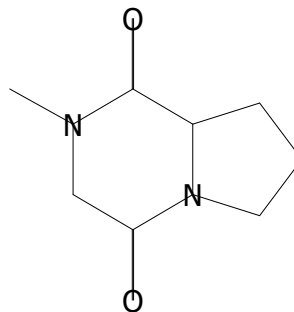
Library Hit - similarity 874, "3-Pyridinol, 6-methyl-, acetate (ester)"



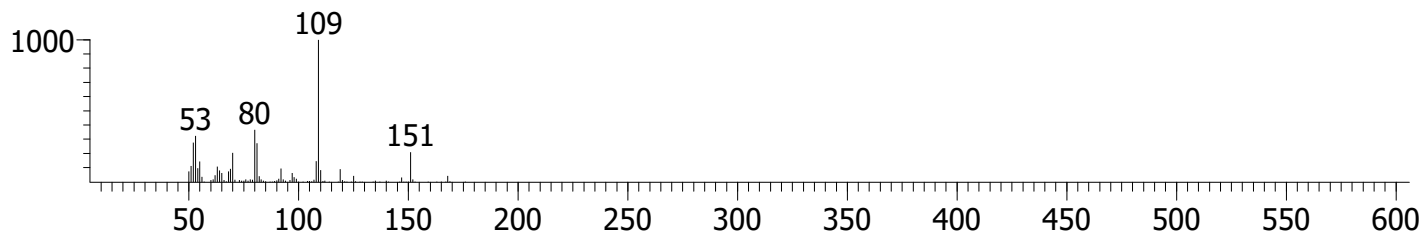
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Pyridinol, 6-methyl-, acetate (ester)	874	2599	4842-89-1	mainlib	C8H9NO2	151
2	Acetaminophen	858	1497	103-90-2	mainlib	C8H9NO2	151
3	Metacetamol	851	1146	621-42-1	mainlib	C8H9NO2	151
4	Acetamide, N-(2-hydroxyphenyl)-	850	1102	614-80-2	mainlib	C8H9NO2	151
5	Phenol, 4-amino-	846	931	123-30-8	mainlib	C6H7NO	109

1,4-diazabicyclo[4.3.0]nonan-2,5-dione,
3-methyl

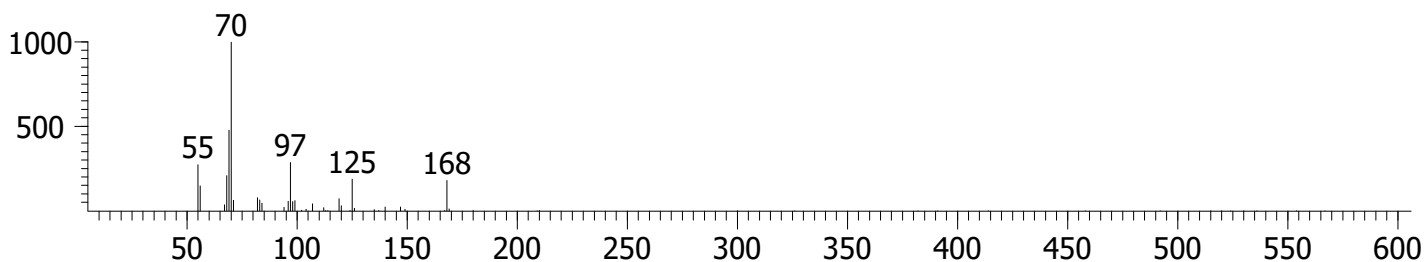
1st Dimension R.T. = 1539.89
2nd Dimension R.T. = 2.752
Quant Mass(es) = 70
S/N = 173.90
Area = 146689
Height = 12608
Similarity = 780



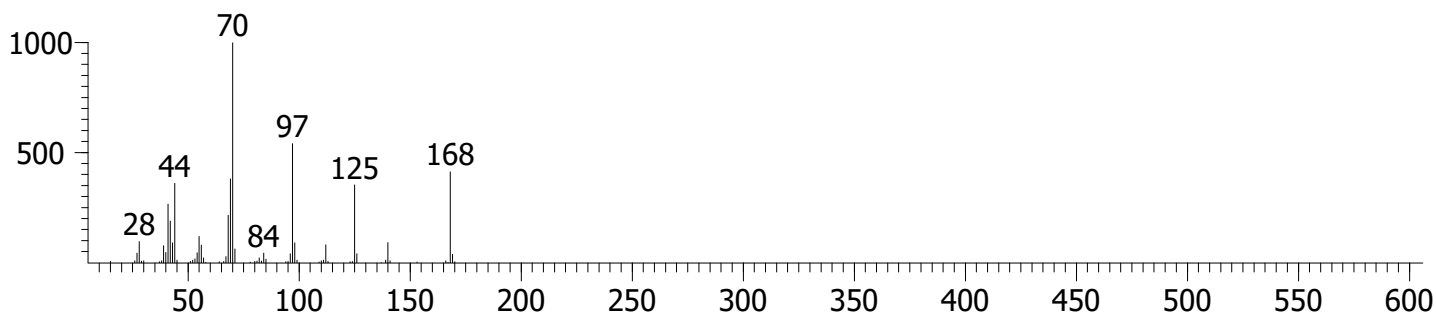
Peak Apex - sample "INF-A grab 100819 (111419):1", peak 3260, at 1539.89 , 2.752 sec , sec (Spec # 161007)



Peak True - sample "INF-A grab 100819 (111419):1", peak 3260, at 1539.89 , 2.752 sec , sec (Spec # 161007)



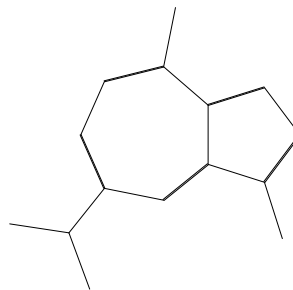
Library Hit - similarity 780, "1,4-diazabicyclo[4.3.0]nonan-2,5-dione, 3-methyl"



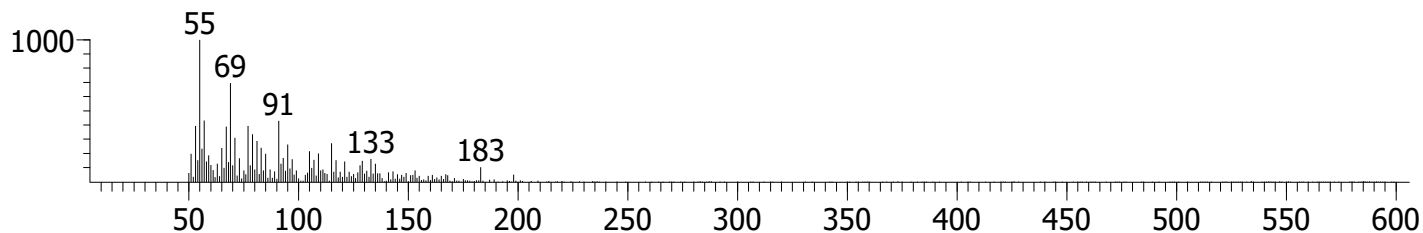
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,4-diazabicyclo[4.3.0]nonan-2,5-dione, 3-methyl	780	5731	0-00-0	mainlib	C8H12N2O2	168
2	3-Pyrrolidin-2-yl-propionic acid	738	1286	0-00-0	mainlib	C7H13NO2	143
3	3-Methyl-1,4-diazabicyclo[4.3.0]nonan-2,5-dione, N-acetyl-	733	1036	0-00-0	mainlib	C10H14N2O3	210
4	Methyl 4,6-decadienyl ether	690	228	0-00-0	mainlib	C11H20O	168
5	2-Acetoxydodecane	671	111	0-00-0	mainlib	C14H28O2	228

Azulene, 1,4-dimethyl-7-(1-methylethyl)-

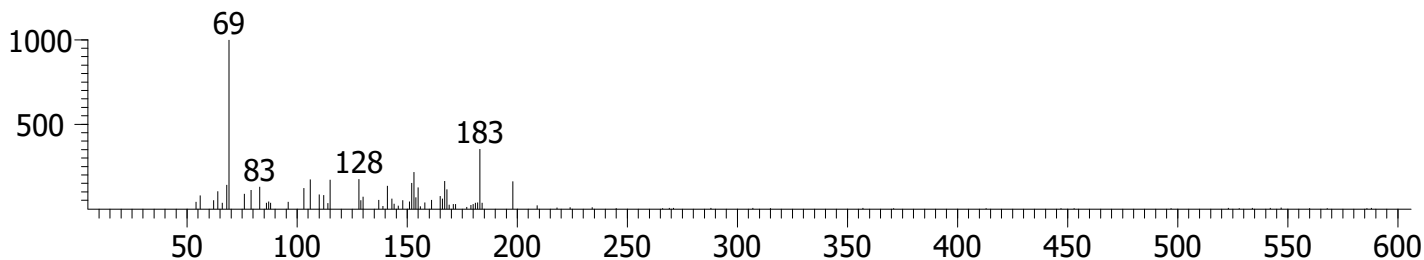
1st Dimension R.T. = 1585.37
2nd Dimension R.T. = 1.901
Quant Mass(es) = 183
S/N = 82.033
Area = 6733.7
Height = 728.57
Similarity = 659



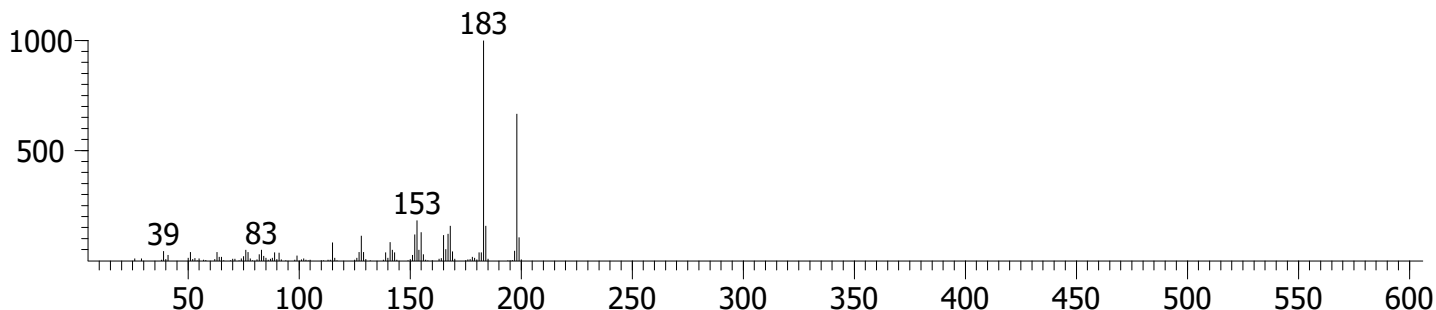
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 5292, at 1585.37 , 1.901 sec , sec (Spec # 167768)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 5292, at 1585.37 , 1.901 sec , sec (Spec # 167768)



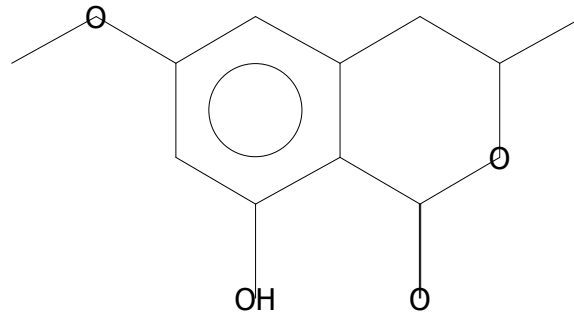
Library Hit - similarity 659, "Azulene, 1,4-dimethyl-7-(1-methylethyl)-"



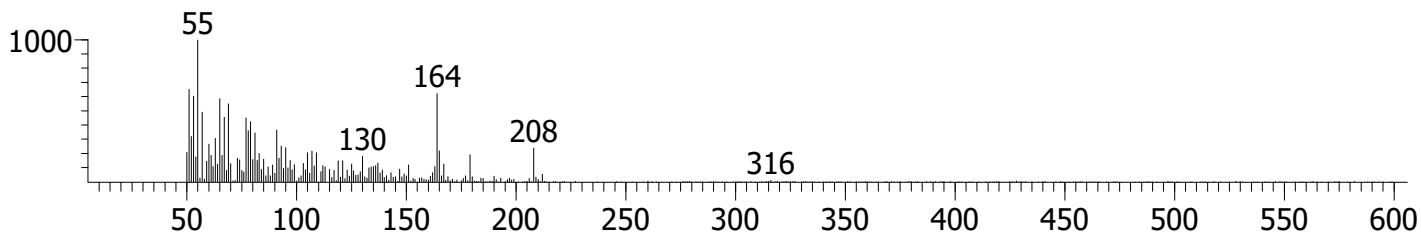
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Azulene, 1,4-dimethyl-7-(1-methylethyl)-	659	5816	489-84-9	mainlib	C15H18	198
2	Cyclopropane, 1,1,2,2-tetramethyl-3-(2-phenylethenylideno)-	618	1327	0-00-0	mainlib	C15H18	198
3	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	612	1043	483-78-3	mainlib	C15H18	198
4	6-Isopropyl-1,4-dimethylnaphthalene	601	715	489-77-0	mainlib	C15H18	198
5	Benzene, 1,1',1'',1'''-(oxydimethylidyne)tetrakis-	563	171	574-42-5	mainlib	C26H22O	350

1H-2-Benzopyran-1-one,
3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-,

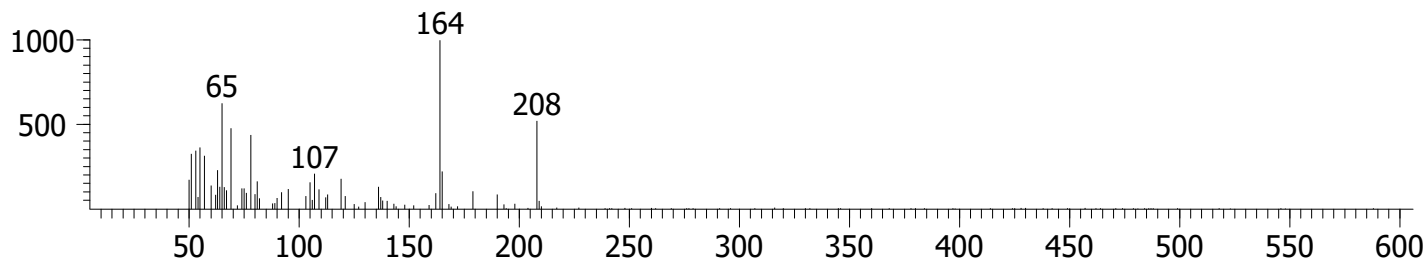
1st Dimension R.T. = 1648.33
 2nd Dimension R.T. = 2.343
 Quant Mass(es) = 164
 S/N = 269.25
 Area = 39544
 Height = 3531.2
 Similarity = 758



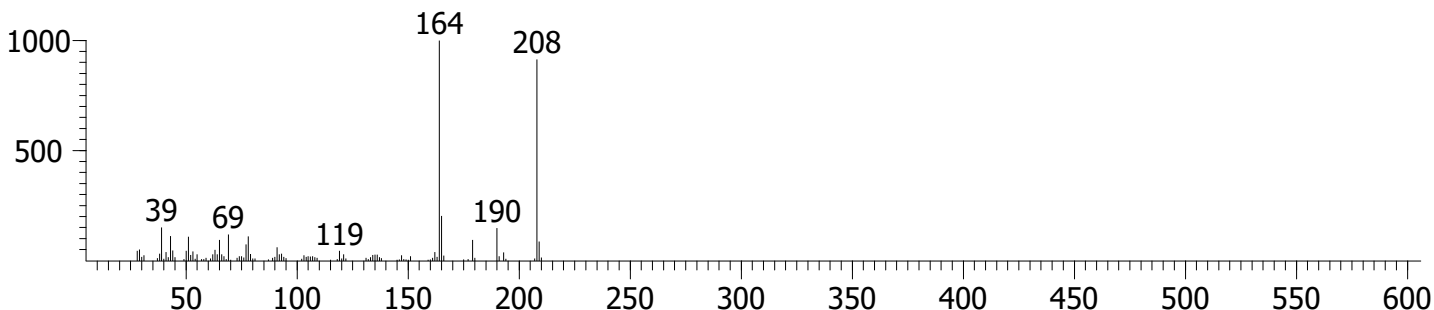
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 5671, at 1648.33 , 2.343 sec , sec (Spec # 17 7375)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 5671, at 1648.33 , 2.343 sec , sec (Spec # 177 375)



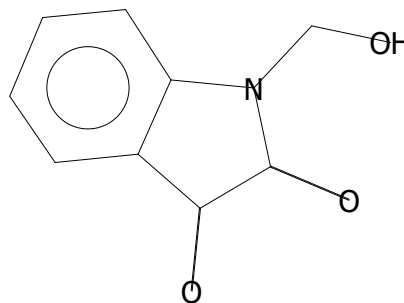
Library Hit - similarity 758, "1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-, (R)-"



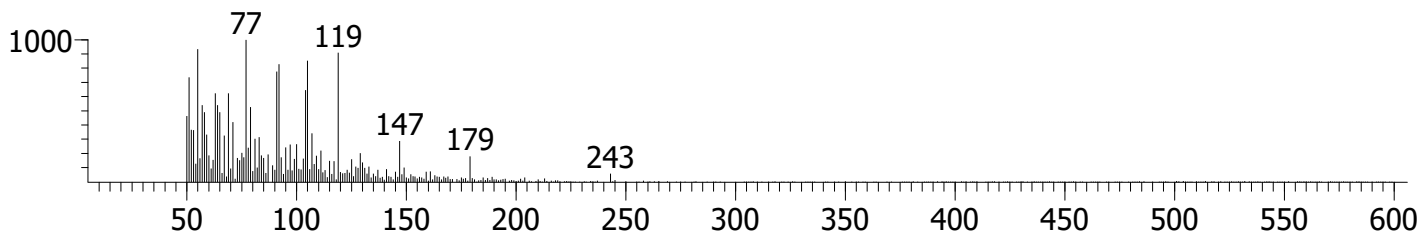
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-, (R)-	758	7901	13410-15-6	mainlib	C11H12O4	208
2	1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-	707	1592	6803-02-7	mainlib	C11H12O4	208
3	7-[3-Chloro-2-hydroxypropyl]guanine	647	282	73100-76-2	mainlib	C8H10ClN5O2	243
4	6,7-Dimethoxy-3-isochromanone	604	62	16135-41-4	mainlib	C11H12O4	208
5	1,3-Dimethyl-3-hydroxy-5-methoxyoxindole	576	18	0-00-0	mainlib	C11H13NO3	207

Indole-2,3-dione, 1-(hydroxymethyl)-

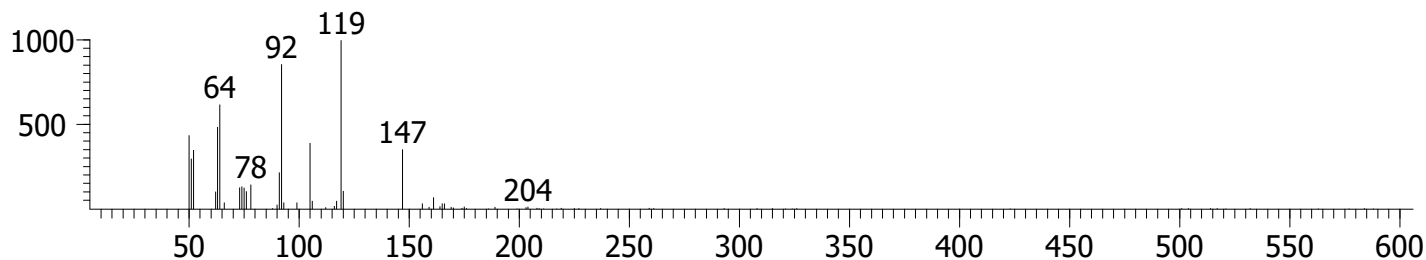
1st Dimension R.T. = 1658.83
2nd Dimension R.T. = 2.145
Quant Mass(es) = 119
S/N = 190.15
Area = 32532
Height = 3615.4
Similarity = 729



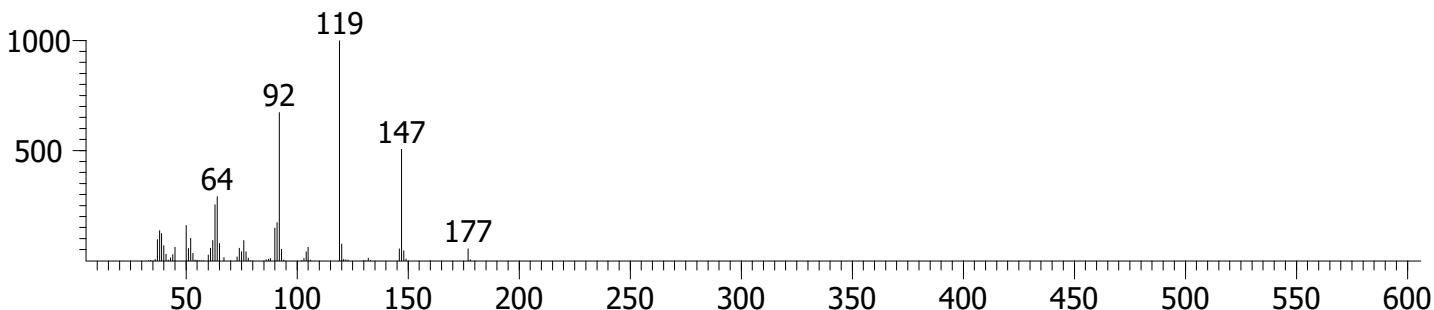
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 5743, at 1658.83 , 2.145 sec , sec (Spec # 178935)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 5743, at 1658.83 , 2.145 sec , sec (Spec # 178935)



Library Hit - similarity 729, "Indole-2,3-dione, 1-(hydroxymethyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Indole-2,3-dione, 1-(hydroxymethyl)-	729	3521	50899-59-7	mainlib	C9H7NO3	177
2	2,1-Benzisoxazole	712	1922	271-58-9	mainlib	C7H5NO	119
3	1H-Indole-2,3-dione	699	1241	91-56-5	mainlib	C8H5NO2	147
4	Isatoic anhydride	684	752	118-48-9	mainlib	C8H5NO3	163
5	Benzonitrile, 4-ethoxy-	678	591	25117-74-2	mainlib	C9H9NO	147

1H-Indole-3-propanoic acid

1st Dimension R.T. = 1788.25

2nd Dimension R.T. = 2.633

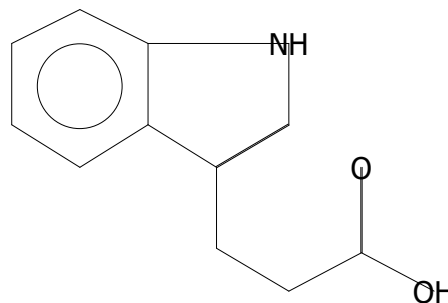
Quant Mass(es) = 130

S/N = 262.14

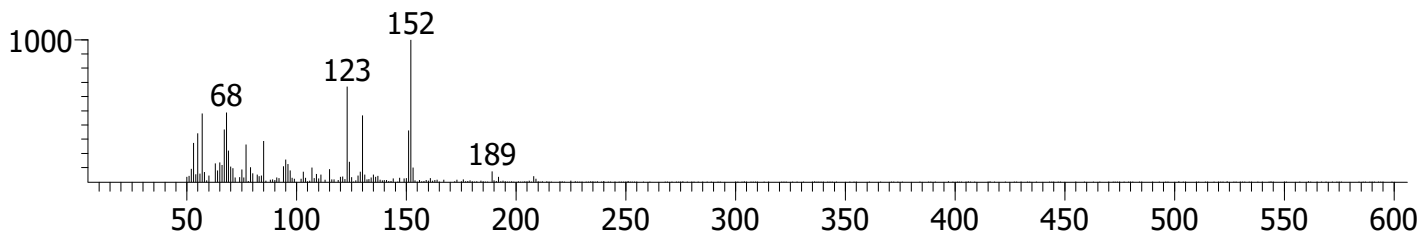
Area = 75565

Height = 5488.3

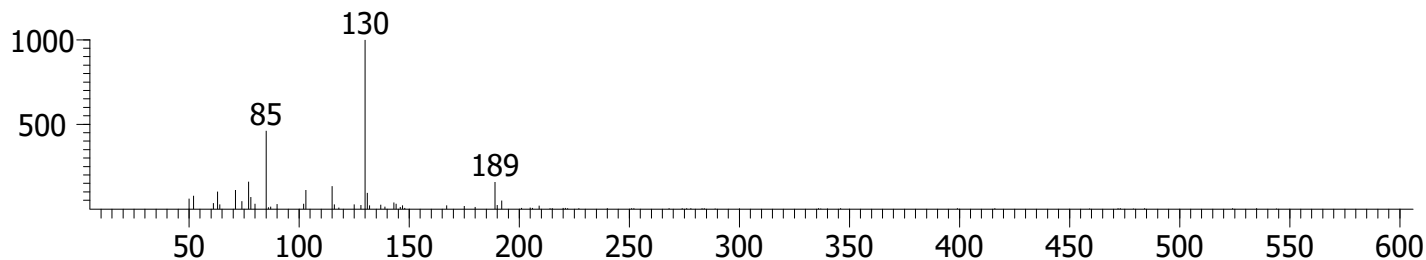
Similarity = 741



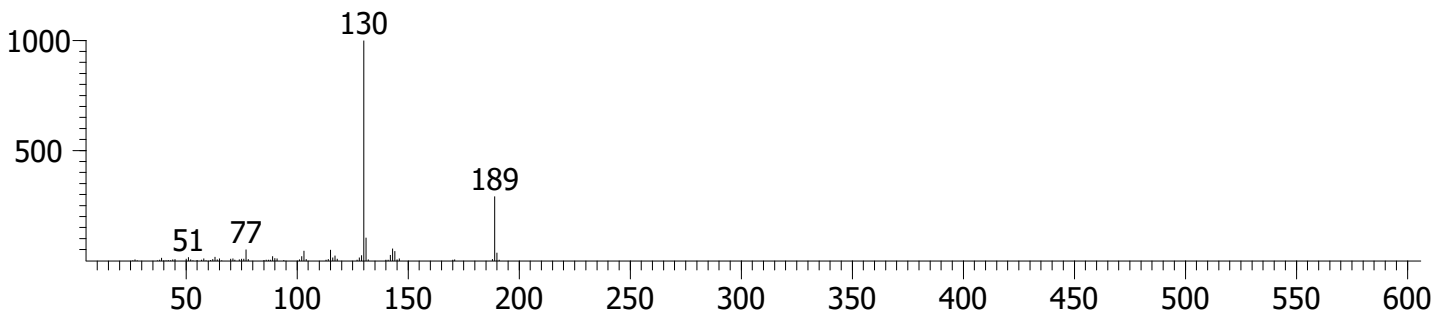
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 6535, at 1788.25 , 2.633 sec , sec (Spec # 198619)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 6535, at 1788.25 , 2.633 sec , sec (Spec # 198619)

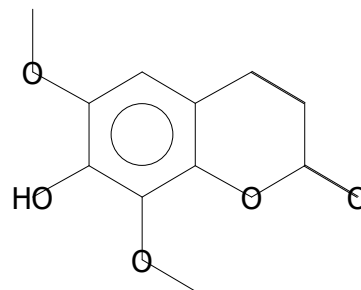


Library Hit - similarity 741, "1H-Indole-3-propanoic acid"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1H-Indole-3-propanoic acid	741	4344	830-96-6	mainlib	C11H11NO2	189
2	1H-Indol-3-ylmethyl acetate #	727	2719	959256-81-6	mainlib	C11H11NO2	189
3	3-[2,2-Dicarbomethoxyethyl]indole	691	672	79782-15-3	mainlib	C14H15NO4	261
4	Propionic acid, 2-[(2-hydroxy-5-nitrobenzylidene)amino]-3-(1H-indol-3-yl)-, methyl ester	663	194	0-00-0	mainlib	C19H17N3O5	367
5	L-Tryptophan, N-(methoxycarbonyl)-, methyl ester	660	171	58635-46-4	mainlib	C14H16N2O4	276

Isofraxidin



1st Dimension R.T. = 1893.19

2nd Dimension R.T. = 2.739

Quant Mass(es) = 222

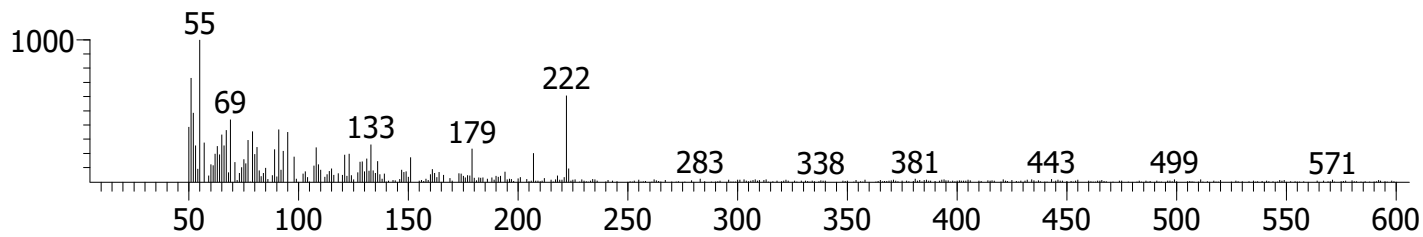
S/N = 85.682

Area = 17270

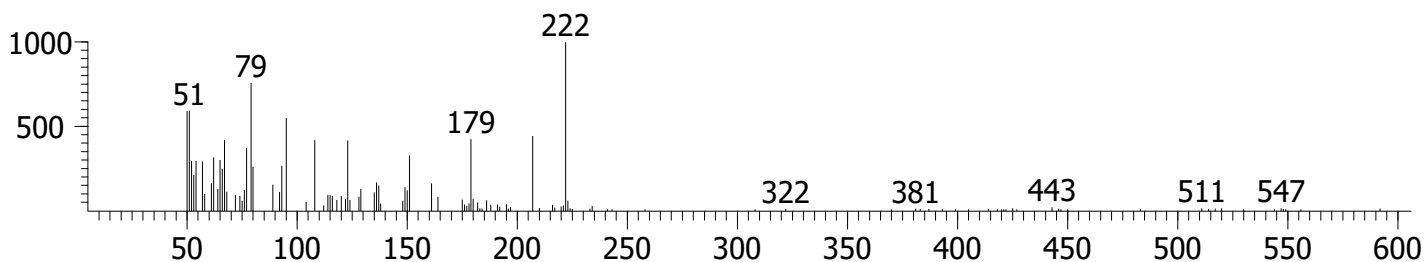
Height = 1547.3

Similarity = 728

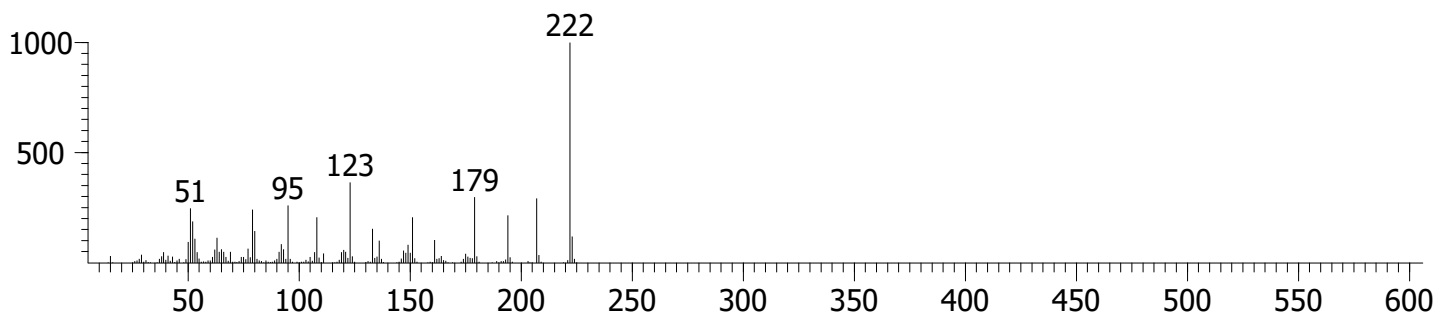
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 6971, at 1893.19 , 2.739 sec , sec (Spec # 214535)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 6971, at 1893.19 , 2.739 sec , sec (Spec # 214535)



Library Hit - similarity 728, "Isofraxidin"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Isofraxidin	728	6611	486-21-5	mainlib	C ₁₁ H ₁₀ O ₅	222
2	Fraxinol	667	1151	486-28-2	mainlib	C ₁₁ H ₁₀ O ₅	222
3	Isofraxidin, acetate	658	836	61195-38-8	mainlib	C ₁₃ H ₁₂ O ₆	264
4	Fraxinol, acetate	633	255	28752-90-1	mainlib	C ₁₃ H ₁₂ O ₆	264
5	(Z)-1-(2,4,5-Trimethoxyphenyl)but-1-ene	632	245	0-00-0	mainlib	C ₁₃ H ₁₈ O ₃	222

2,5-Piperazinedione, 3-(phenylmethyl)-

1st Dimension R.T. = 1980.64

2nd Dimension R.T. = 3.227

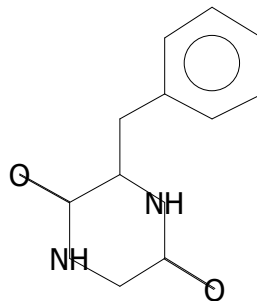
Quant Mass(es) = 91

S/N = 79.384

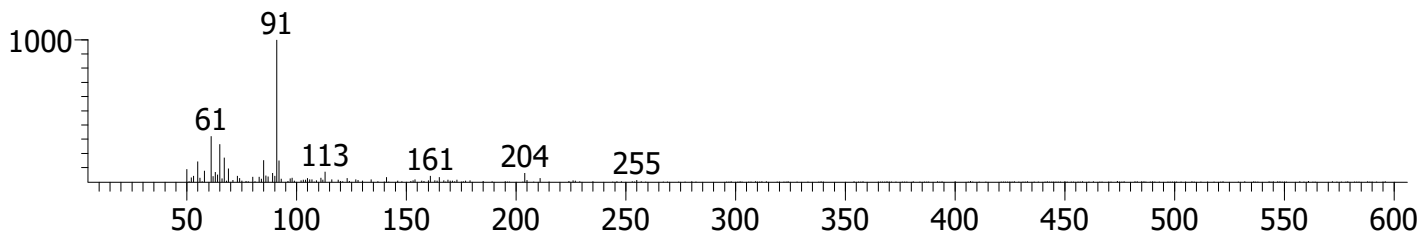
Area = 104924

Height = 7270.1

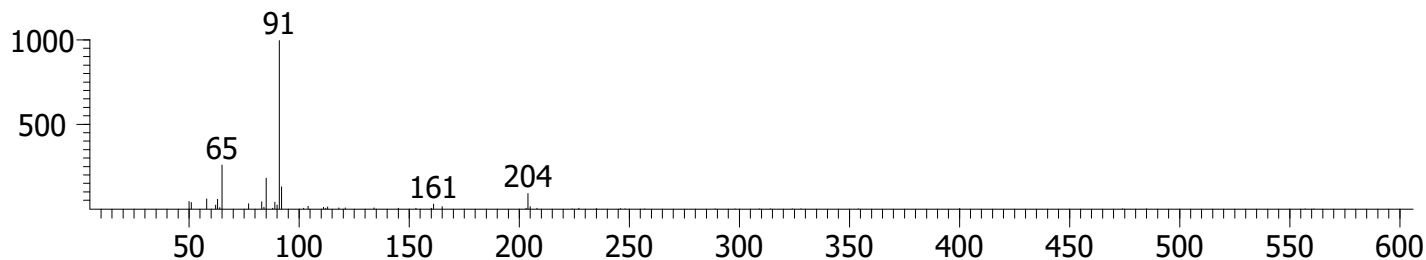
Similarity = 861



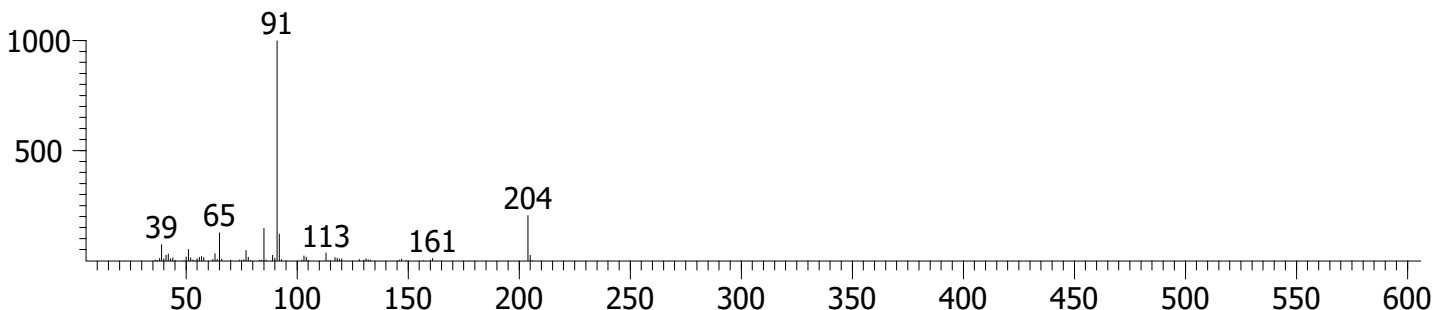
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 7333, at 1980.64 , 3.227 sec , sec (Spec # 227859)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 7333, at 1980.64 , 3.227 sec , sec (Spec # 227859)



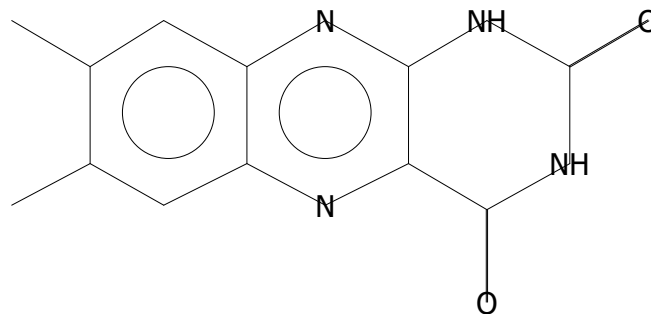
Library Hit - similarity 861, "2,5-Piperazinedione, 3-(phenylmethyl)-"



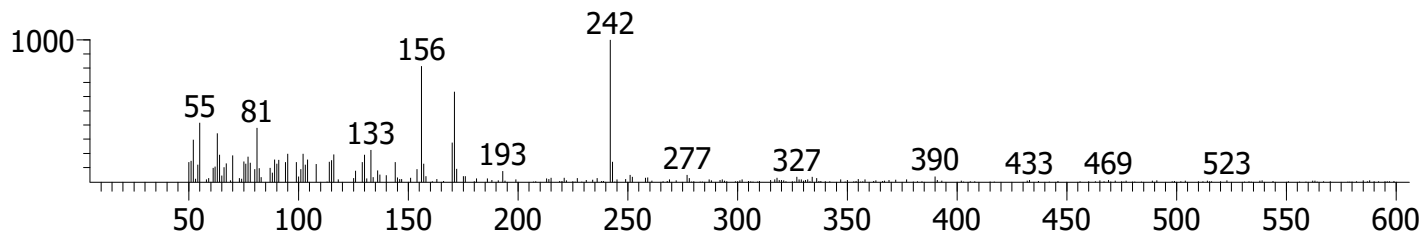
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,5-Piperazinedione, 3-(phenylmethyl)-	861	2533	5037-75-2	mainlib	C11H12N2O2	204
2	2-Benzyloxyethylamine	823	607	38336-04-8	mainlib	C9H13NO	151
3	Benzenoacetic acid, phenylmethyl ester	819	512	102-16-9	mainlib	C15H14O2	226
4	Benzenepropionic acid, 4-benzyloxy-	813	403	50463-48-4	mainlib	C16H16O3	256
5	12-Benzyl-4,9,15-trioxa-3,5,8,10,12,14,16-heptaazatetracyclo[11.3.0.0(2,6).0(7,11)]hexadeca-1(16), 2,5,7,10,13-hexaen-3-one	810	356	1394125-25-7	mainlib	C13H7N7O4	325

Lumichrome

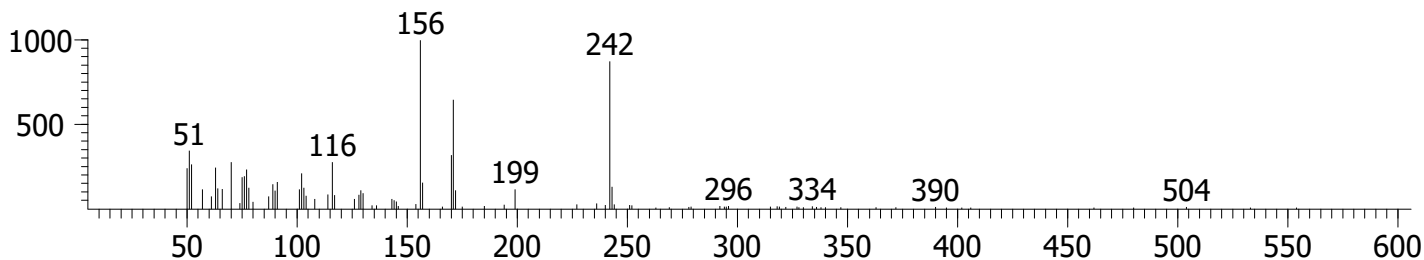
1st Dimension R.T. = 2421.39
 2nd Dimension R.T. = 3.214
 Quant Mass(es) = 242
 S/N = 121.31
 Area = 19795
 Height = 1308.2
 Similarity = 805



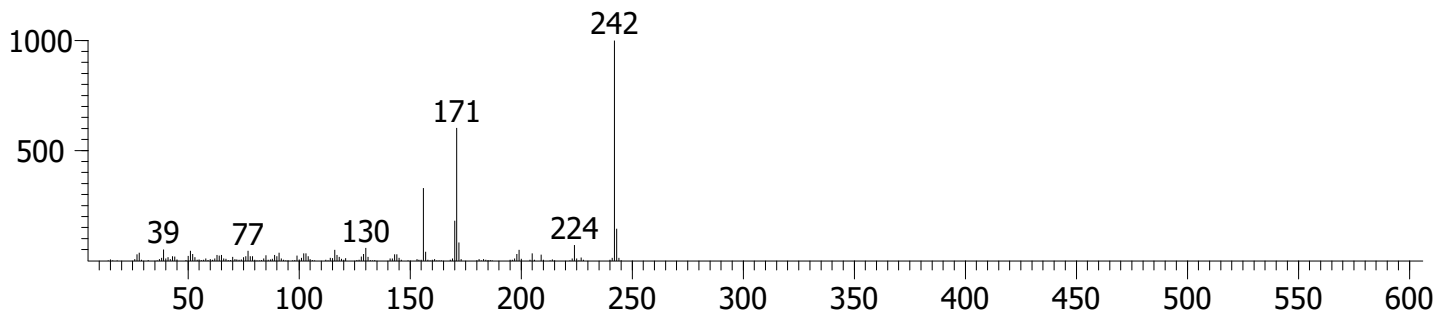
Peak Apex - sample "INF B Comp 091919 (20191122):1", peak 8562, at 2421.39 , 3.214 sec , sec (Spec # 294637)



Peak True - sample "INF B Comp 091919 (20191122):1", peak 8562, at 2421.39 , 3.214 sec , sec (Spec # 294637)



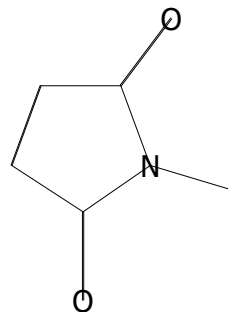
Library Hit - similarity 805, "Lumichrome"



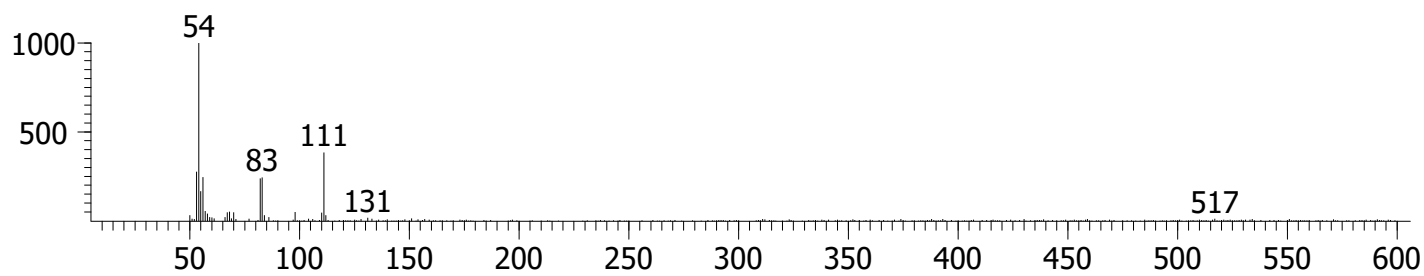
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Lumichrome	805	8751	1086-80-2	mainlib	C ₁₂ H ₁₀ N ₄ O ₂	242
2	Quinoline, 2-(1-methylethyl)-	626	161	17507-24-3	mainlib	C ₁₂ H ₁₃ N	171
3	1,2,3,3a-Tetrahydropentalene, 1,1-dimethyl-3-cyanomethylene-	619	123	0-00-0	mainlib	C ₁₂ H ₁₃ N	171
4	1,4-Dihydro-1,2-dimethylquinolin-4-ylidenemethane	613	96	0-00-0	mainlib	C ₁₂ H ₁₃ N	171
5	(7-Isopropylidenebicyclo[2.2.1]hept-5-en-2-ylidene)acetonitrile	605	72	0-00-0	mainlib	C ₁₂ H ₁₃ N	171

N-Methylmaleimide

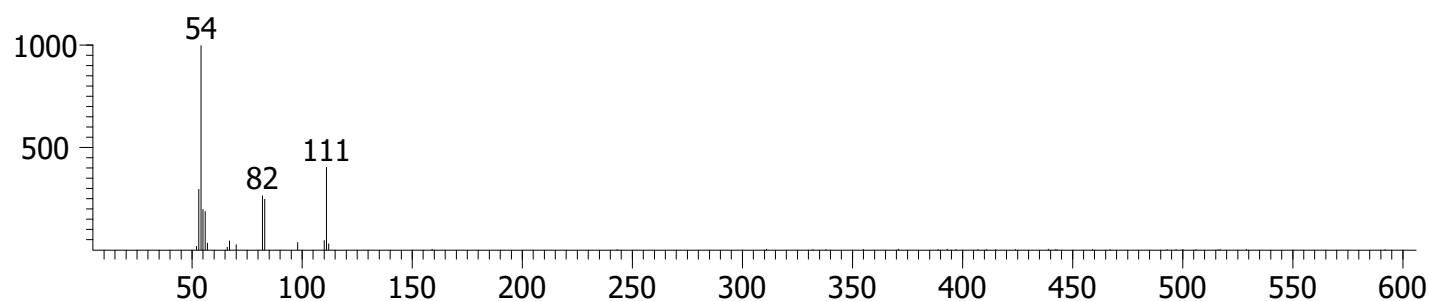
1st Dimension R.T. = 507.984
2nd Dimension R.T. = 1.749
Quant Mass(es) = 54
S/N = 101.03
Area = 19339
Height = 2616.2
Similarity = 858



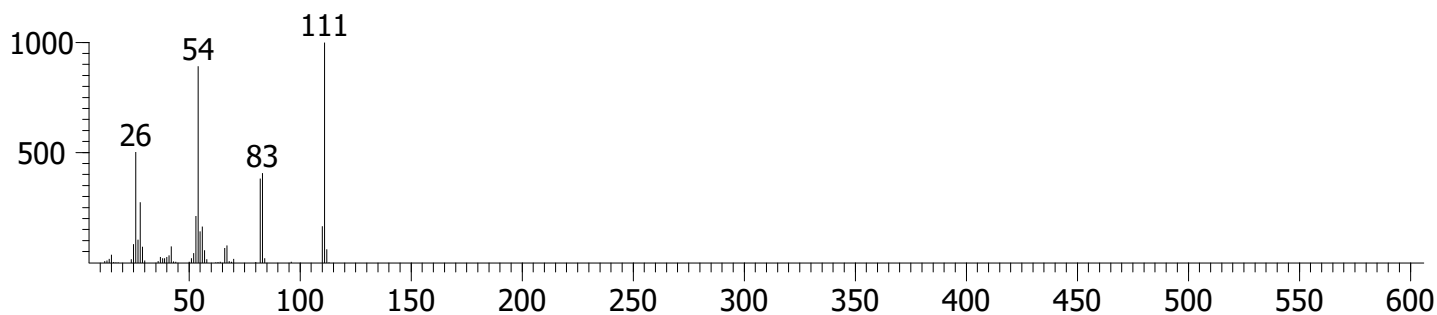
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 62, at 507.984 , 1.749 sec , sec (Spec # 4505)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 62, at 507.984 , 1.749 sec , sec (Spec # 4505)



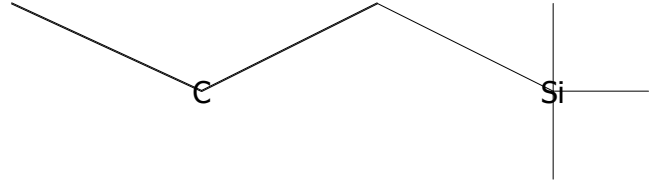
Library Hit - similarity 858, "N-Methylmaleimide"



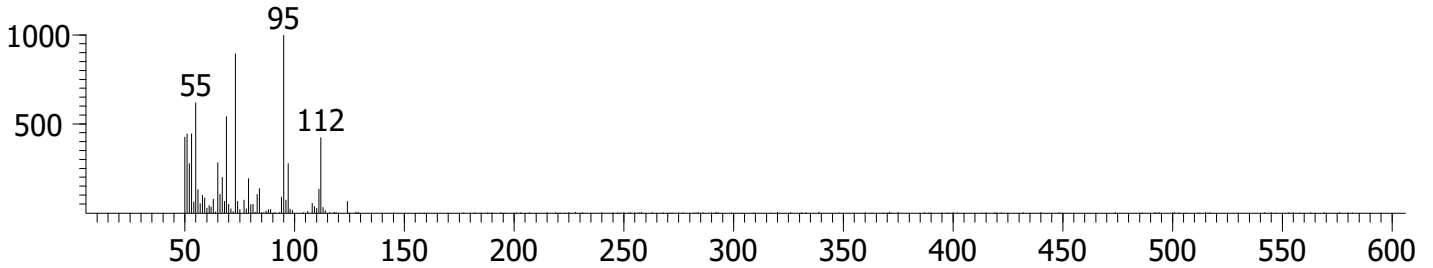
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	N-Methylmaleimide	858	9405	930-88-1	mainlib	C5H5NO2	111
2	4(1H)-Pyridinone, 2,3-dihydro-1-methyl-	644	94	35488-00-7	mainlib	C6H9NO	111
3	2H-Azepin-2-one, 1,5,6,7-tetrahydro-	640	79	2228-79-7	mainlib	C6H9NO	111
4	Cyclohexane, (1-methylpropyl)-	622	40	7058-01-7	mainlib	C10H20	140
5	Diaziridine, 3-cyclopropyl-1,2-diethyl-	617	33	0-00-0	mainlib	C8H16N2	140

Silane, trimethyl-1,2-propadienyl-

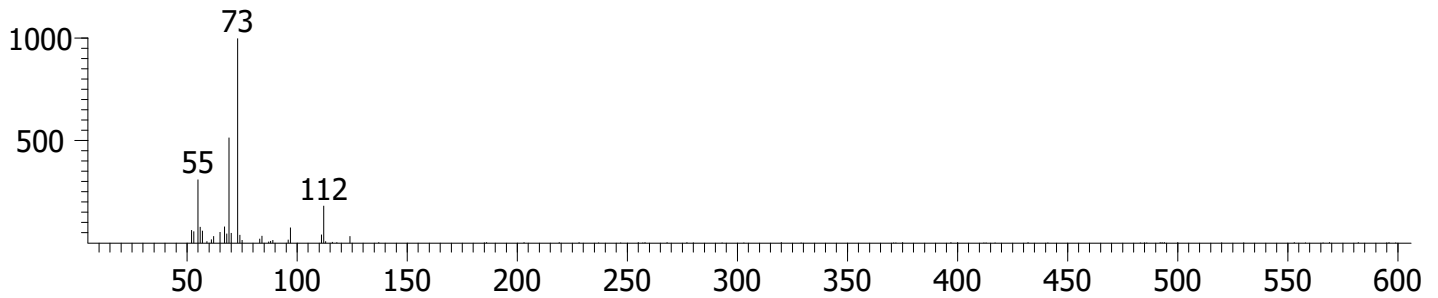
1st Dimension R.T. = 532.47
 2nd Dimension R.T. = 1.505
 Quant Mass(es) = 73
 S/N = 113.22
 Area = 33900
 Height = 3882.0
 Similarity = 776



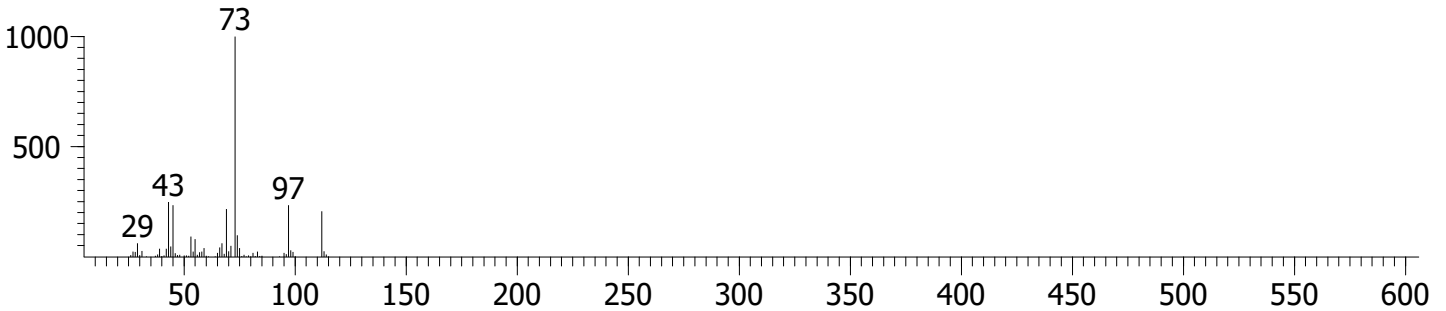
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 110, at 532.47 , 1.505 sec , sec (Spec # 8178)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 110, at 532.47 , 1.505 sec , sec (Spec # 8178)



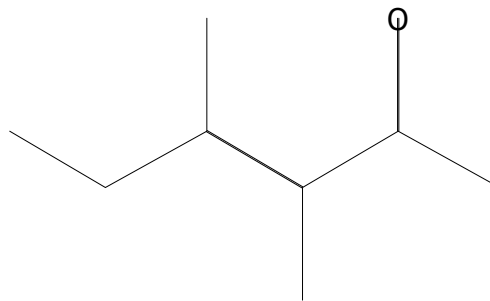
Library Hit - similarity 776, "Silane, trimethyl-1,2-propadienyl-"



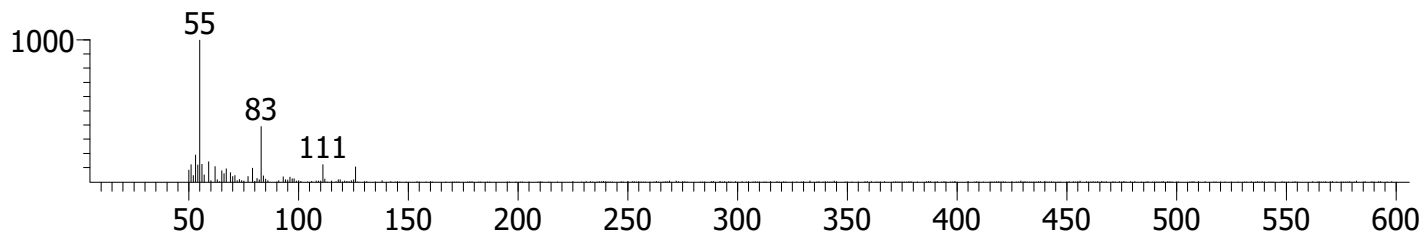
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Silane, trimethyl-1,2-propadienyl-	776	6571	14657-22-8	mainlib	C6H12Si	112
2	Silane, trimethyl-2-propynyl-	743	1720	13361-64-3	mainlib	C6H12Si	112
3	Acetic acid (3-methoxy-3-methyl)butyl ester	657	153	0-00-0	mainlib	C8H16O3	160
4	Octanal, 7-methoxy-3,7-dimethyl-	655	141	3613-30-7	mainlib	C11H22O2	186
5	3-Heptene, 2-methyl-, (E)-	654	135	692-96-6	mainlib	C8H16	112

3-Hexen-2-one, 3,4-dimethyl-

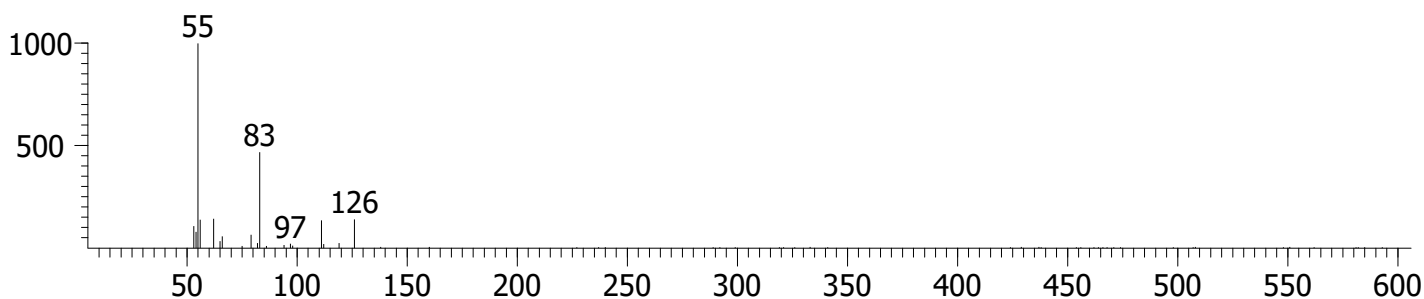
1st Dimension R.T. = 626.916
2nd Dimension R.T. = 1.610
Quant Mass(es) = 83
S/N = 57.756
Area = 8002.5
Height = 1185.8
Similarity = 761



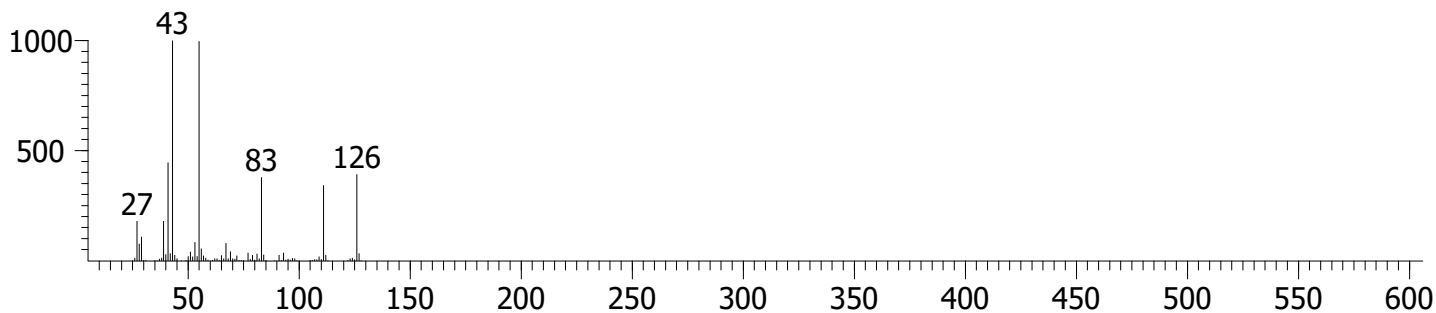
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 321, at 626.916 , 1.610 sec , sec (Spec # 22504)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 321, at 626.916 , 1.610 sec , sec (Spec # 22504)



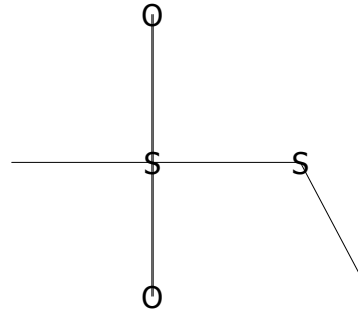
Library Hit - similarity 761, "3-Hexen-2-one, 3,4-dimethyl-"



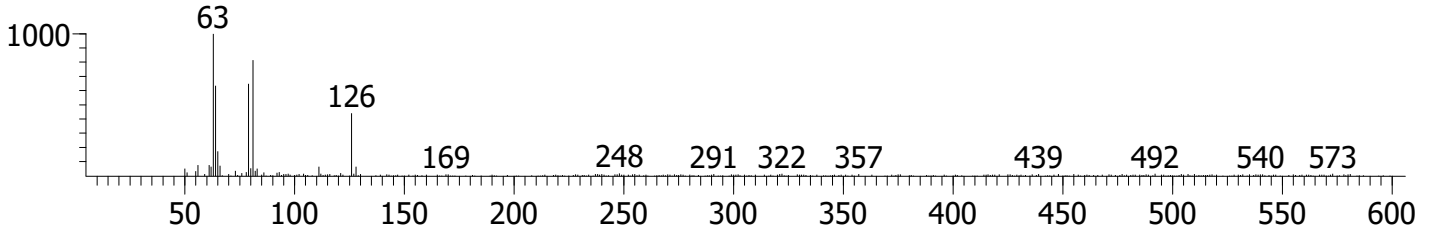
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Hexen-2-one, 3,4-dimethyl-	761	4491	1635-02-5	mainlib	C8H14O	126
2	4-Hexen-2-one, 3,4-dimethyl-	733	1297	53252-21-4	mainlib	C8H14O	126
3	3-Penten-2-one, 3-ethyl-4-methyl-	727	1019	22287-11-2	mainlib	C8H14O	126
4	3,3-Dimethylhex-5-en-2-one	713	638	0-00-0	mainlib	C8H14O	126
5	2-Hexanone, 3-methyl-4-methylene-	705	476	20690-71-5	mainlib	C8H14O	126

S-Methyl methanethiosulphonate

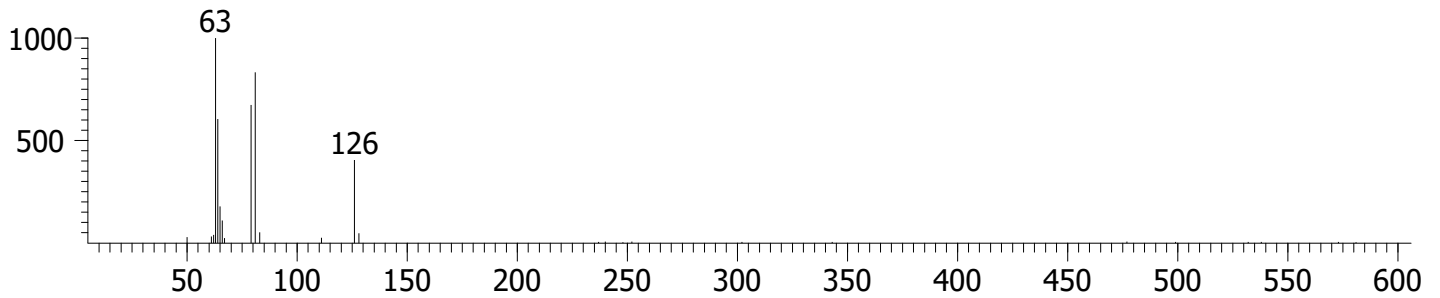
1st Dimension R.T. = 682.884
 2nd Dimension R.T. = 2.290
 Quant Mass(es) = 126
 S/N = 64.627
 Area = 11880
 Height = 1315.4
 Similarity = 853



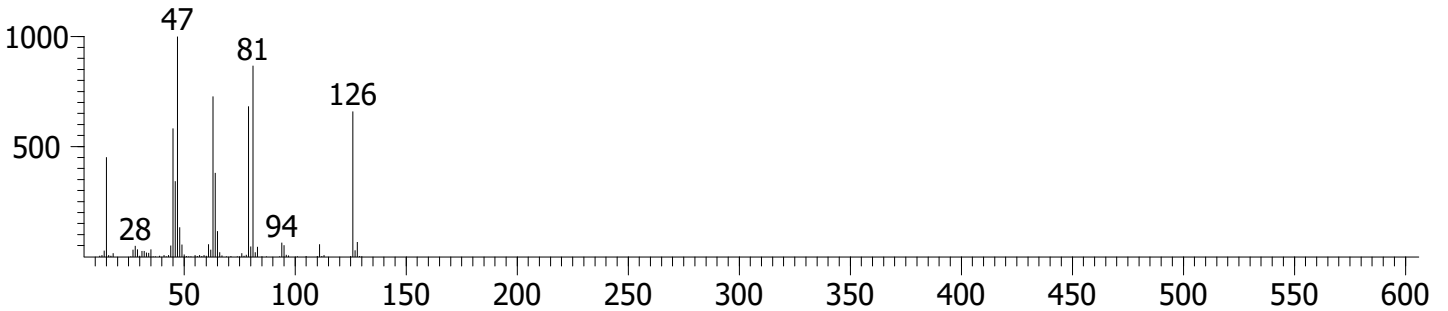
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 450, at 682.884 , 2.290 sec , sec (Spec # 31087)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 450, at 682.884 , 2.290 sec , sec (Spec # 31087)



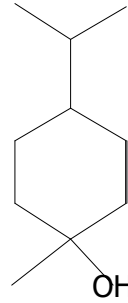
Library Hit - similarity 853, "S-Methyl methanethiosulphonate"



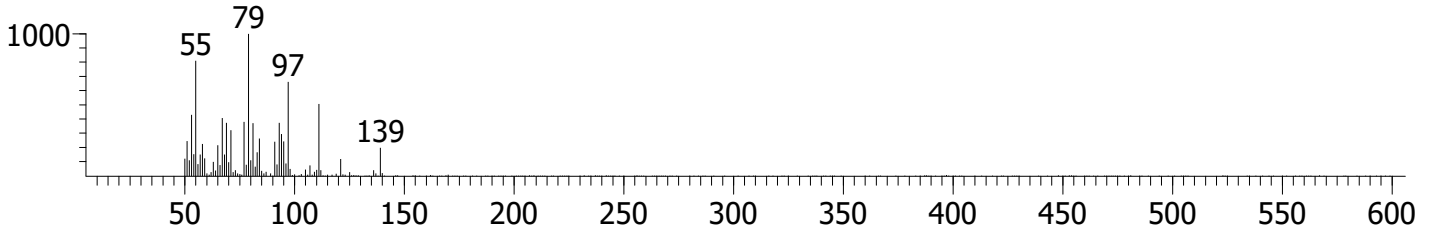
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	S-Methyl methanethiosulphonate	853	9722	2949-92-0	mainlib	C2H6O2S2	126
2	Methylphosphinic acid, ethyl ester	601	97	16391-07-4	mainlib	C3H9O2P	108
3	2-Cyclopentene-1-carboxylic acid, 1-methyl-	600	93	68317-77-1	mainlib	C7H10O2	126
4	2-Methanesulfonylethanol	558	20	15205-66-0	mainlib	C3H8O3S	124
5	2-Propanol, 1-chloro-3-fluoro-	540	10	189937-18-6	mainlib	C3H6ClFO	112

4-Isopropyl-1-methylcyclohex-2-enol

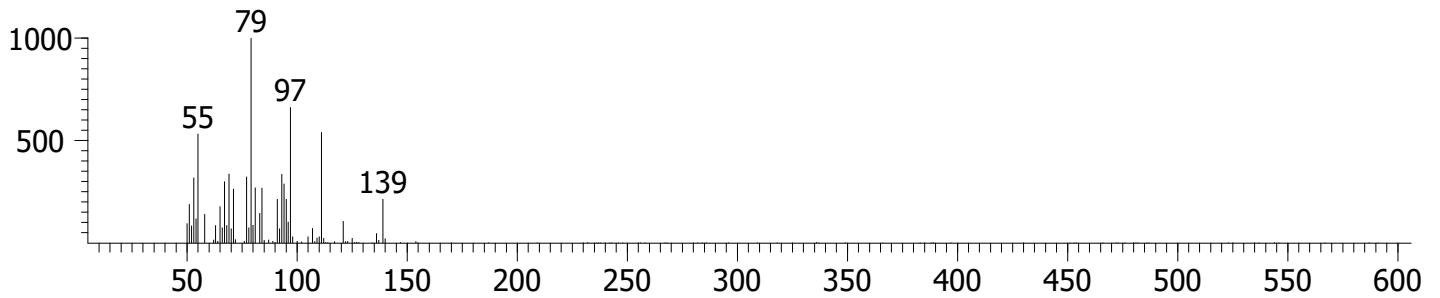
1st Dimension R.T. = 714.366
 2nd Dimension R.T. = 1.379
 Quant Mass(es) = 79
 S/N = 255.45
 Area = 80238
 Height = 9112.3
 Similarity = 829



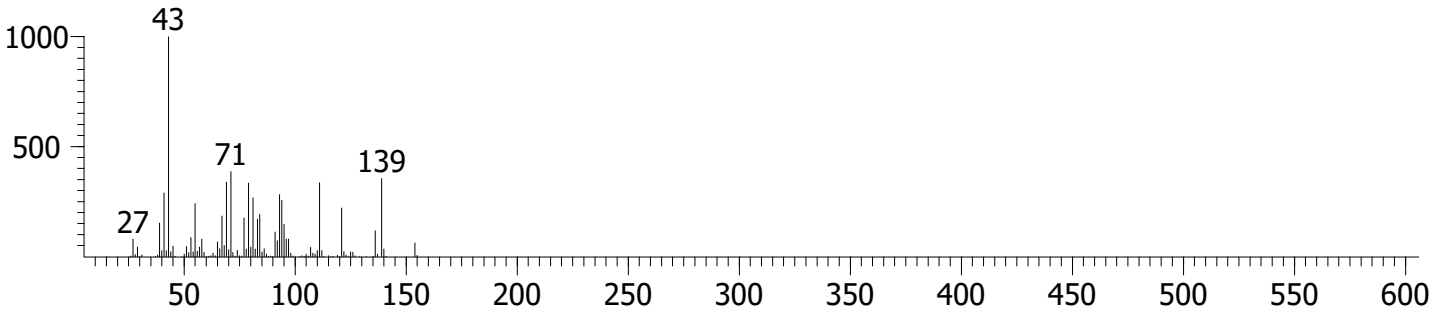
Peak Apex - sample "AerMBR C 091919 (20191119):1", peak 515, at 714.366 , 1.379 sec , sec (Spec # 35719)



Peak True - sample "AerMBR C 091919 (20191119):1", peak 515, at 714.366 , 1.379 sec , sec (Spec # 35719)



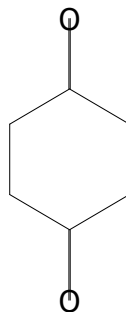
Library Hit - similarity 829, "4-Isopropyl-1-methylcyclohex-2-enol"



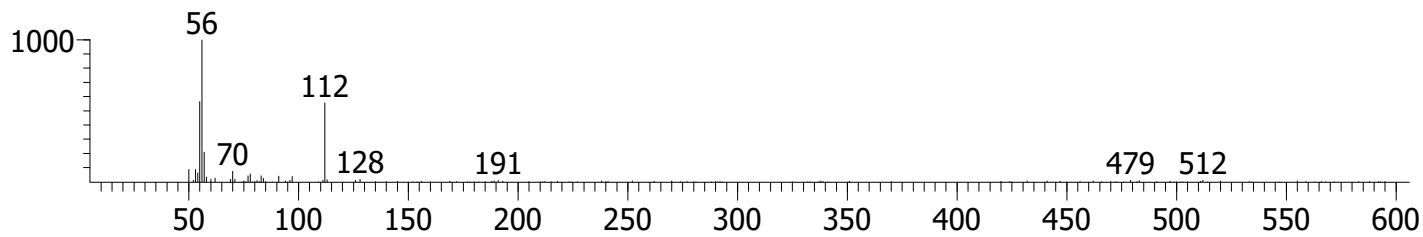
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Isopropyl-1-methylcyclohex-2-enol	829	3811	619-62-5	mainlib	C10H18O	154
2	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, trans-	826	3368	29803-81-4	mainlib	C10H18O	154
3	Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, cis-	791	845	7299-41-4	mainlib	C10H18O	154
4	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, cis-	790	812	29803-82-5	mainlib	C10H18O	154
5	5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol#	761	230	546-79-2	mainlib	C10H18O	154

1,4-Cyclohexanedione

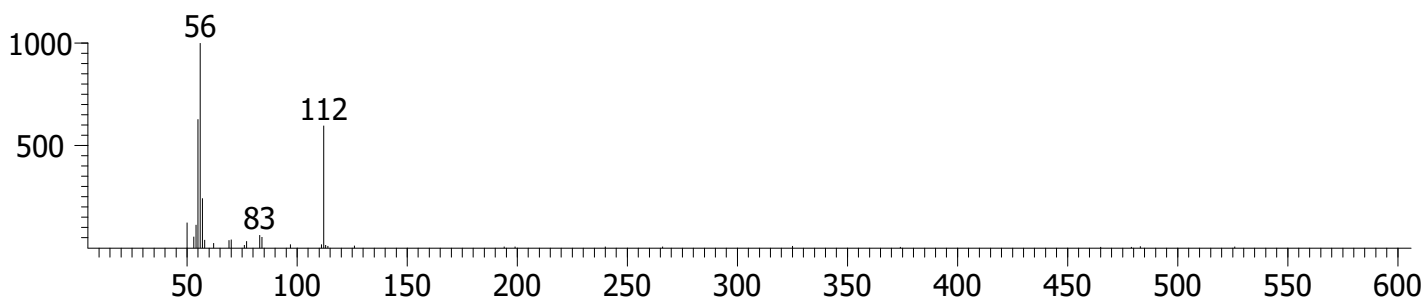
1st Dimension R.T. = 714.366
2nd Dimension R.T. = 2.350
Quant Mass(es) = 112
S/N = 76.629
Area = 10407
Height = 1294.8
Similarity = 840



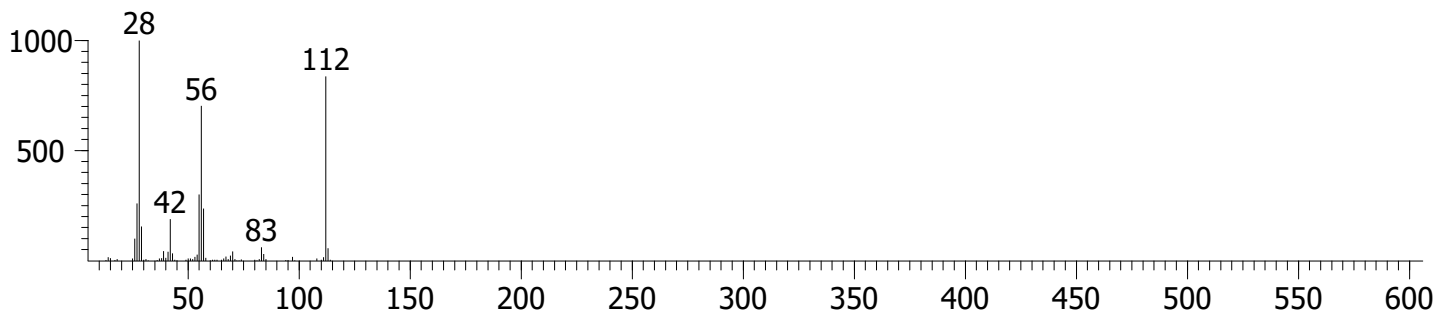
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 525, at 714.366 , 2.350 sec , sec (Spec # 35866)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 525, at 714.366 , 2.350 sec , sec (Spec # 35866)

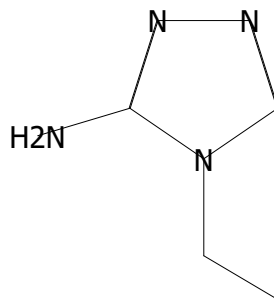


Library Hit - similarity 840, "1,4-Cyclohexanedione"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,4-Cyclohexanedione	840	6542	637-88-7	mainlib	C6H8O2	112
2	3-Methylpyridazin-5-one	795	1393	0-00-0	mainlib	C5H8N2O	112
3	2-Heptene, 5-methyl-	767	402	22487-87-2	mainlib	C8H16	112
4	1,6-Dioxaspiro[4.4]nonane-2,7-dione	764	355	3505-67-7	mainlib	C7H8O4	156
5	1-Hexene, 2,5-dimethyl-	725	83	6975-92-4	mainlib	C8H16	112

4H-1,2,4-Triazol-3-amine, 4-ethyl-



1st Dimension R.T. = 843.792

2nd Dimension R.T. = 1.591

Quant Mass(es) = 112

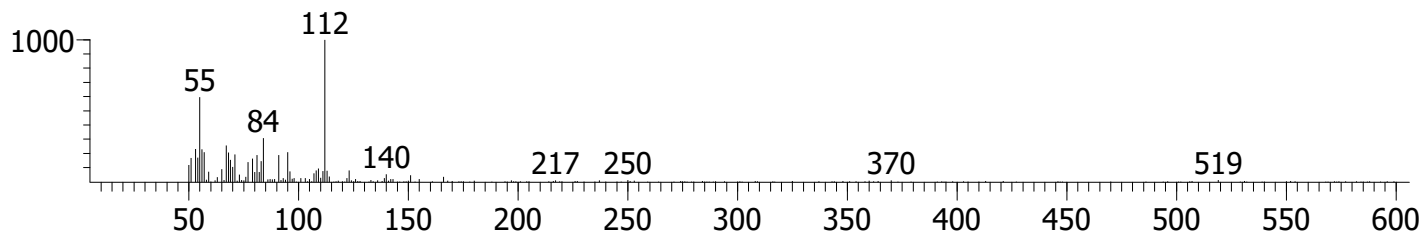
S/N = 198.76

Area = 14993

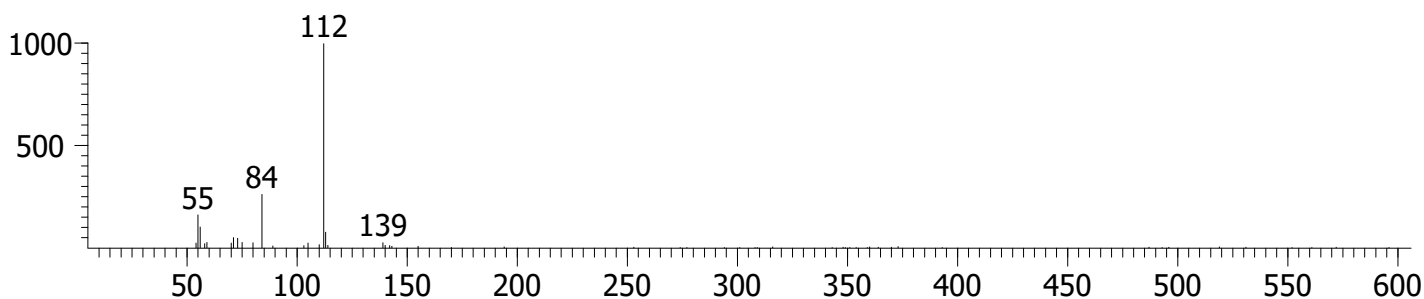
Height = 2101.8

Similarity = 920

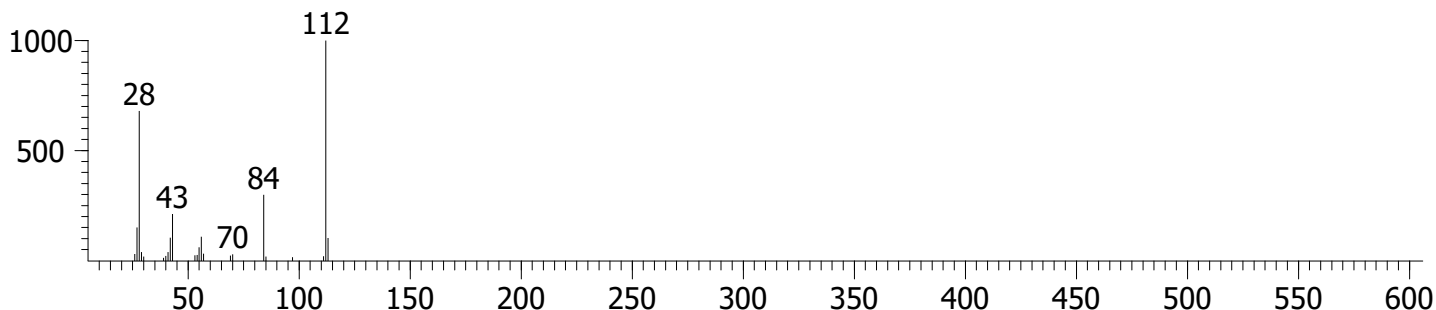
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 768, at 843.792 , 1.591 sec , sec (Spec # 55361)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 768, at 843.792 , 1.591 sec , sec (Spec # 55361)



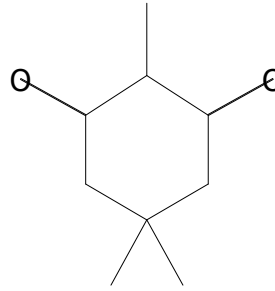
Library Hit - similarity 920, "4H-1,2,4-Triazol-3-amine, 4-ethyl-"



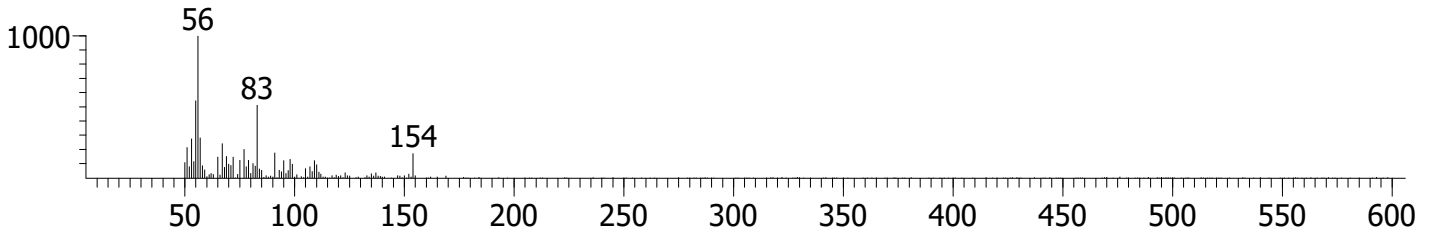
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4H-1,2,4-Triazol-3-amine, 4-ethyl-	920	3941	42786-06-1	mainlib	C4H8N4	112
2	1-Phenethyl-4-piperidone	889	1074	39742-60-4	mainlib	C13H17NO	203
3	2-Pyrrolidinecarboxylic acid, 1,2-dimethyl-5-oxo-, methyl ester	889	1074	56145-23-4	mainlib	C8H13NO3	171
4	2,2-Dimethyl-N-ethylpyrrolidine	883	844	89214-93-7	mainlib	C8H17N	127
5	2H-Benzo[f][oxireno[2,3-E]benzofuran-8(9H)-one, 9-[(hexahydro-1H-azepin-1-yl)methyl]octahydro-2,5a-dimethyl-	870	545	0-00-0	mainlib	C21H33NO3	347

1,3-Cyclohexanedione, 2,5,5-trimethyl-

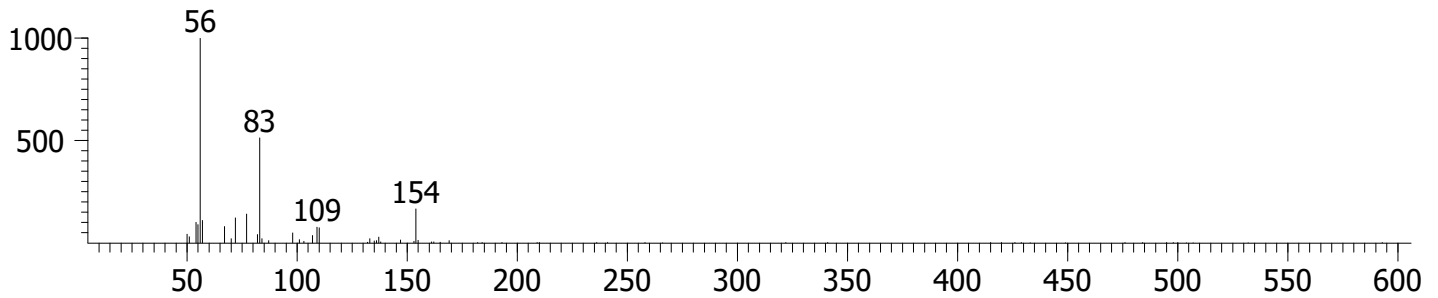
1st Dimension R.T. = 945.234
2nd Dimension R.T. = 1.696
Quant Mass(es) = 56
S/N = 123.91
Area = 35148
Height = 3849.8
Similarity = 642



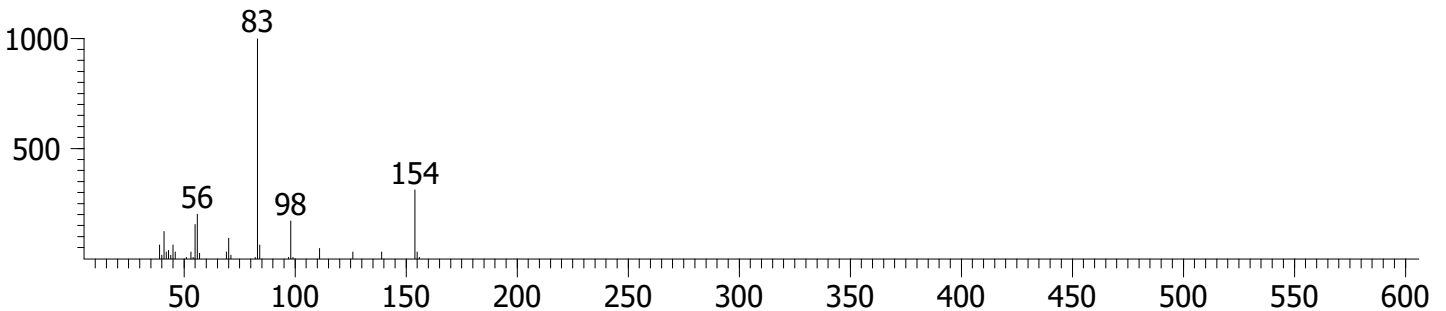
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 946, at 945.234 , 1.696 sec , sec (Spec # 70747)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 946, at 945.234 , 1.696 sec , sec (Spec # 70747)



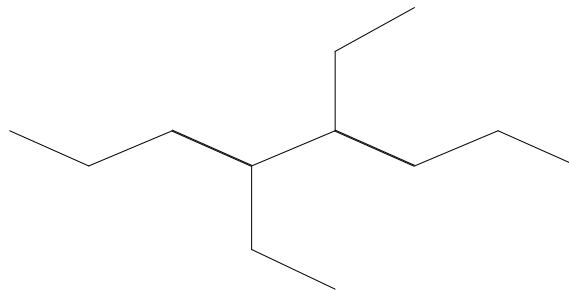
Library Hit - similarity 642, "1,3-Cyclohexanedione, 2,5,5-trimethyl-"



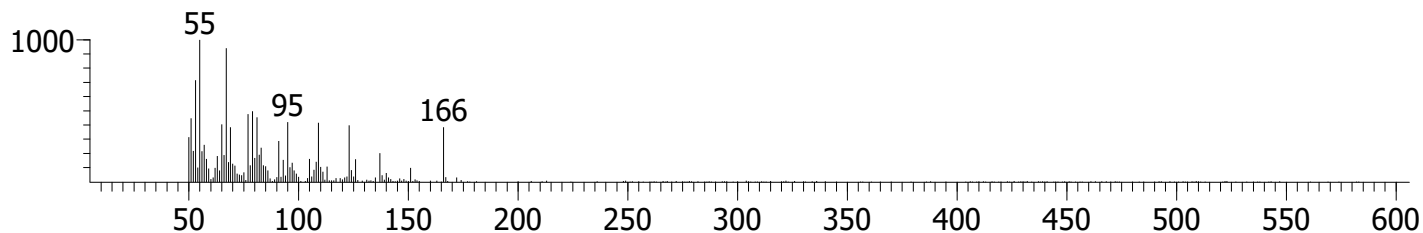
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,3-Cyclohexanedione, 2,5,5-trimethyl-	642	5434	1125-11-7	mainlib	C9H14O2	154
2	Propanenitrile, 2-(dimethylamino)-	616	1628	5350-67-4	mainlib	C5H10N2	98
3	Cyclotridecanamine	551	262	5266-81-9	mainlib	C13H27N	197
4	5-Methyl-6-phenyl-2-(((propan-2-ylidene)amino)oxy)pyridine-3,4-dicarbonitrile	551	262	0-00-0	mainlib	C17H14N4O	290
5	2-Ethylthiolane, S,S-dioxide	549	241	10178-59-3	mainlib	C6H12O2S	148

3,5-Octadiene, 4,5-diethyl-

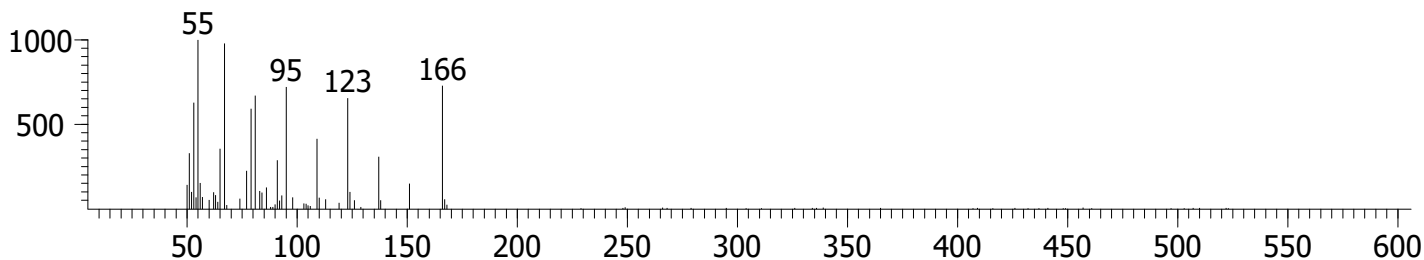
1st Dimension R.T. = 1025.69
2nd Dimension R.T. = 1.855
Quant Mass(es) = 166
S/N = 158.49
Area = 10675
Height = 1352.6
Similarity = 735



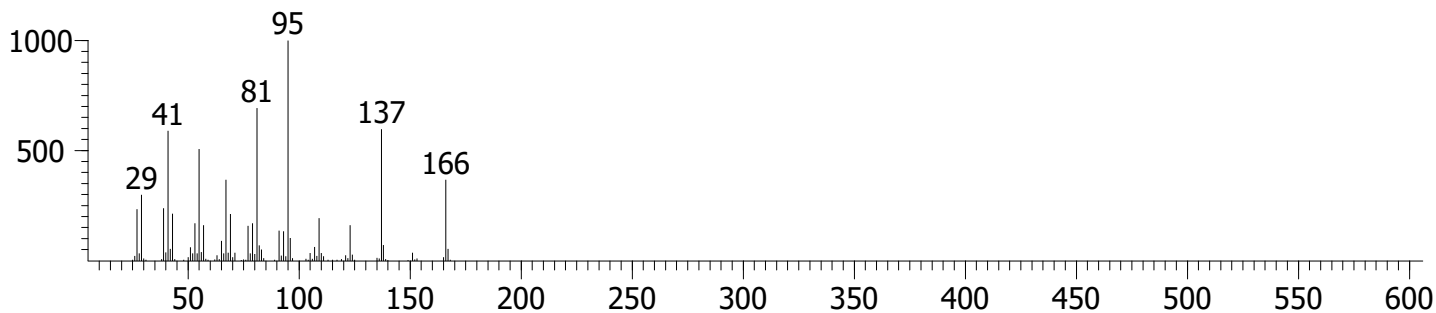
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 1154, at 1025.69 , 1.855 sec , sec (Spec # 8296 1)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 1154, at 1025.69 , 1.855 sec , sec (Spec # 8296 1)



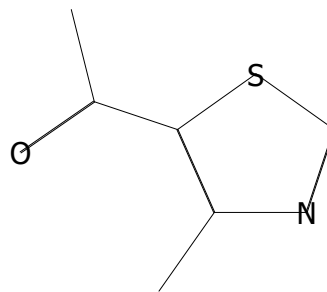
Library Hit - similarity 735, "3,5-Octadiene, 4,5-diethyl-"



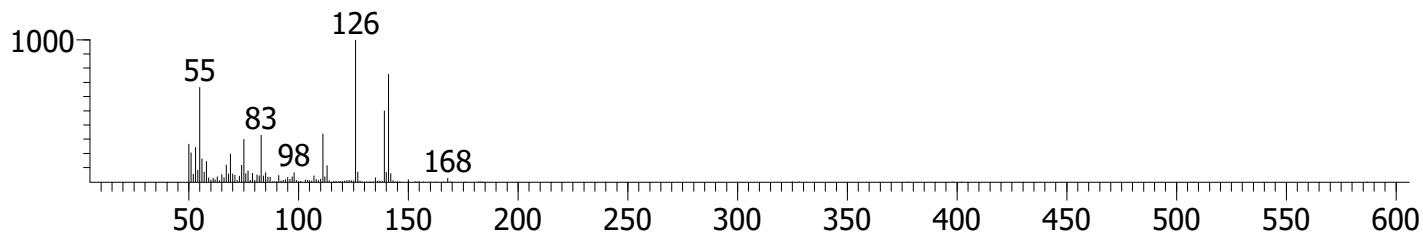
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3,5-Octadiene, 4,5-diethyl-	735	3620	67652-84-0	mainlib	C ₁₂ H ₂₂	166
2	3,5-Octadiene, 4,5-diethyl-, (E,Z)-	714	1540	21293-02-7	mainlib	C ₁₂ H ₂₂	166
3	Cycloheptanone, 2-(2-methylpropylidene)-	692	608	120694-89-5	mainlib	C ₁₁ H ₁₈ O	166
4	trans-Chrysanthamal	678	381	20104-05-6	mainlib	C ₁₀ H ₁₆ O	152
5	Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	670	284	1197-92-8	mainlib	C ₁₁ H ₁₈ O	166

5-Acetyl-4-methylthiazole

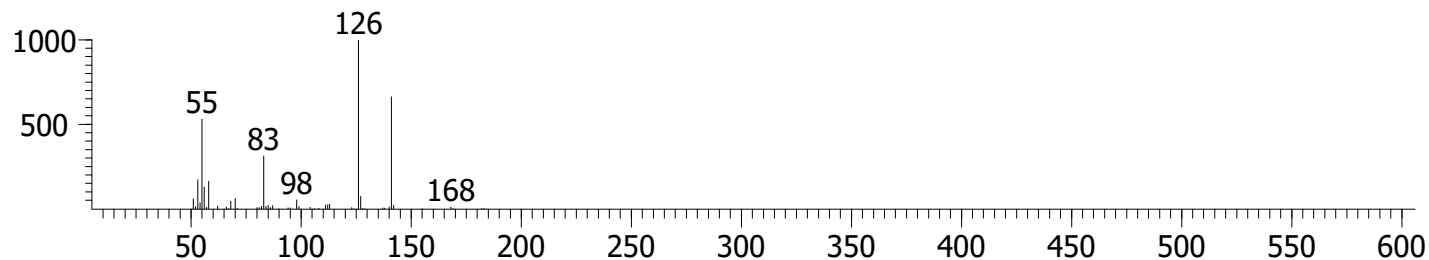
1st Dimension R.T. = 1046.68
 2nd Dimension R.T. = 1.808
 Quant Mass(es) = 126
 S/N = 1476.4
 Area = 341783
 Height = 34916
 Similarity = 723



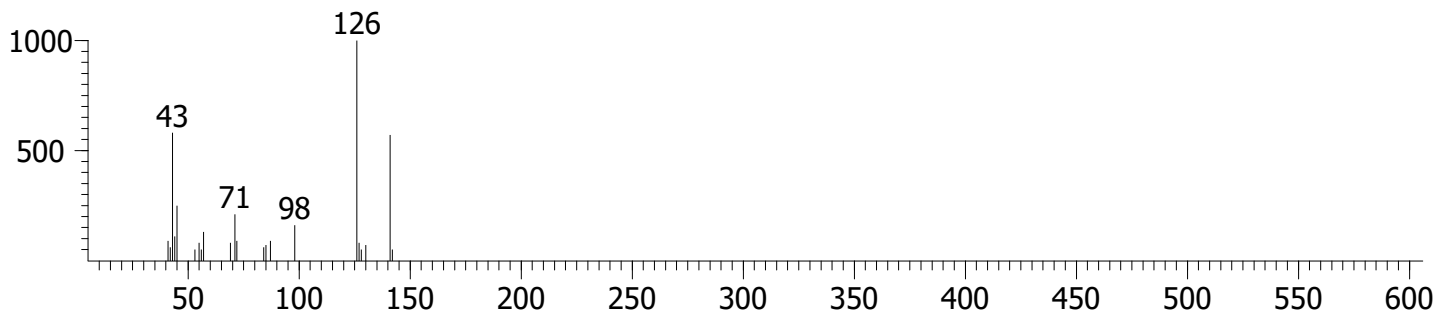
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 1208, at 1046.68 , 1.808 sec , sec (Spec # 8613 4)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 1208, at 1046.68 , 1.808 sec , sec (Spec # 8613 4)



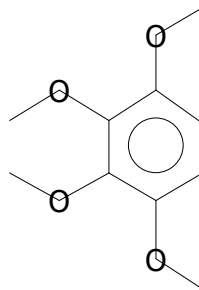
Library Hit - similarity 723, "5-Acetyl-4-methylthiazole"



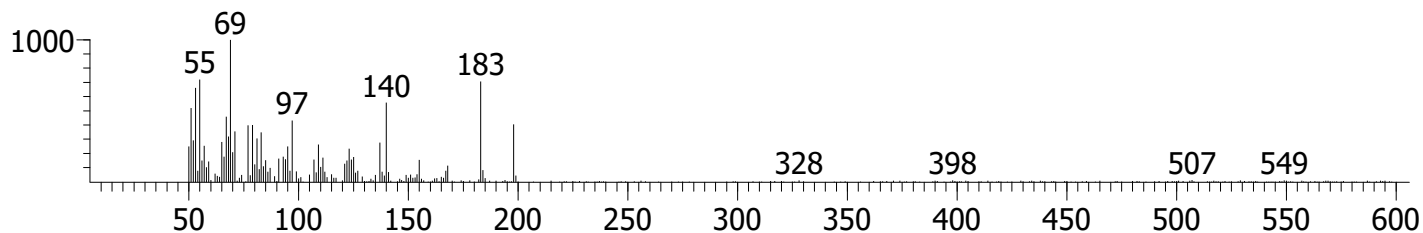
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-Acetyl-4-methylthiazole	723	4984	38205-55-9	mainlib	C6H7NOS	141
2	3H-Pyrazol-3-one, 2,4-dihydro-2,4,5-trimethyl-	668	966	17826-82-3	mainlib	C6H10N2O	126
3	L-Alanine, N-cyclobutylcarbonyl-, hexyl ester	647	411	0-00-0	mainlib	C14H25NO3	255
4	3-Fluoro-p-anisidine	643	347	366-99-4	mainlib	C7H8FNO	141
5	1-[2-(2-Methyl-5-oxo-4-propyl-tetrahydro-furan-2-yl)-2-oxo-ethyl]-1,2-dihydro-pyridazine-3,6-dione	640	307	300701-65-9	mainlib	C14H18N2O5	294

1,2,3,4-Tetramethoxybenzene

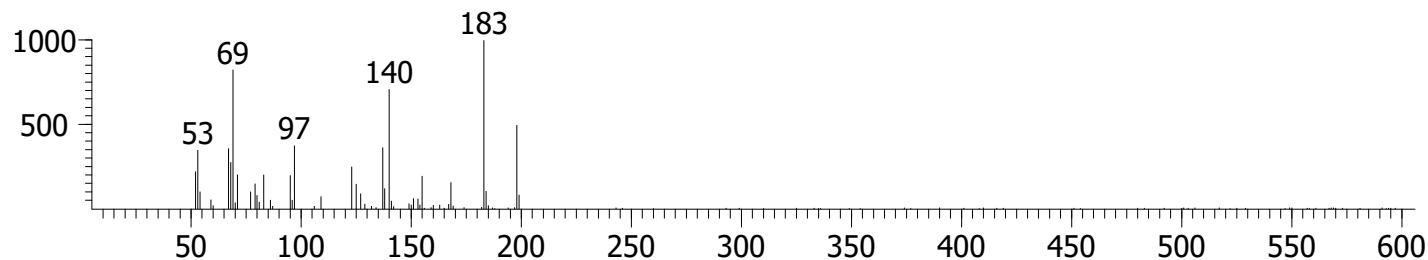
1st Dimension R.T. = 1155.11
2nd Dimension R.T. = 1.855
Quant Mass(es) = 183
S/N = 195.44
Area = 18462
Height = 2155.4
Similarity = 746



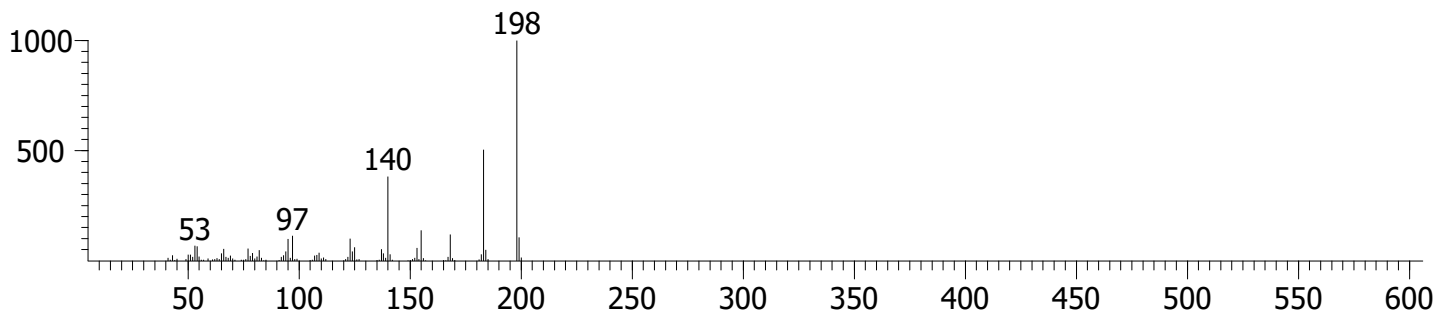
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 1499, at 1155.11 , 1.855 sec , sec (Spec # 1025 71)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 1499, at 1155.11 , 1.855 sec , sec (Spec # 1025 71)



Library Hit - similarity 746, "1,2,3,4-Tetramethoxybenzene"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,2,3,4-Tetramethoxybenzene	746	8288	21450-56-6	mainlib	C10H14O4	198
2	3-Hydroxy-4,5-dimethoxybenzoic acid	632	503	1916-08-1	mainlib	C9H10O5	198
3	Aminoacetic acid, 2-(2-fluoro-4,5-dimethoxybenzoyl)-, ethyl ester	612	229	0-00-0	mainlib	C13H16FNO5	285
4	2,5-dimethoxyphenylethylsulfide	605	175	0-00-0	mainlib	C10H14O2S	198
5	Benzenemethanol, 3,4,5-trimethoxy-	603	162	3840-31-1	mainlib	C10H14O4	198

Pyridine, 2-phenyl-

1st Dimension R.T. = 1221.58

2nd Dimension R.T. = 2.105

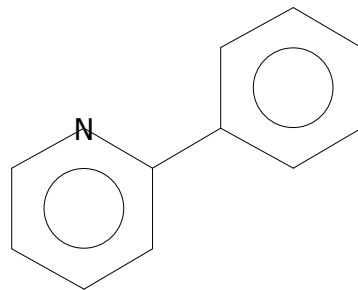
Quant Mass(es) = 155

S/N = 67.412

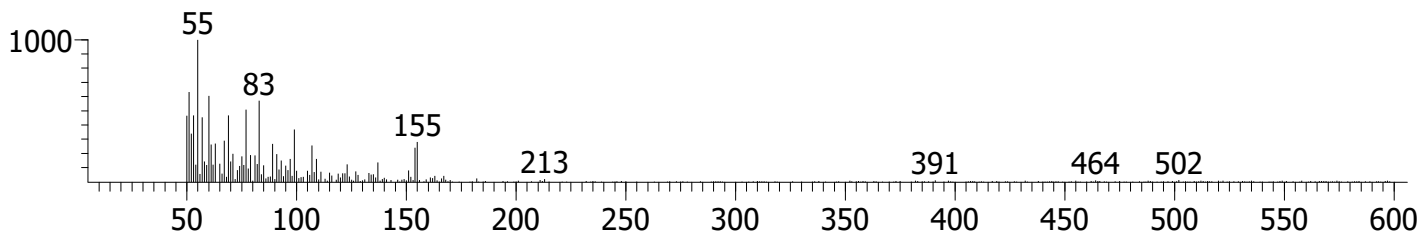
Area = 4985.9

Height = 636.56

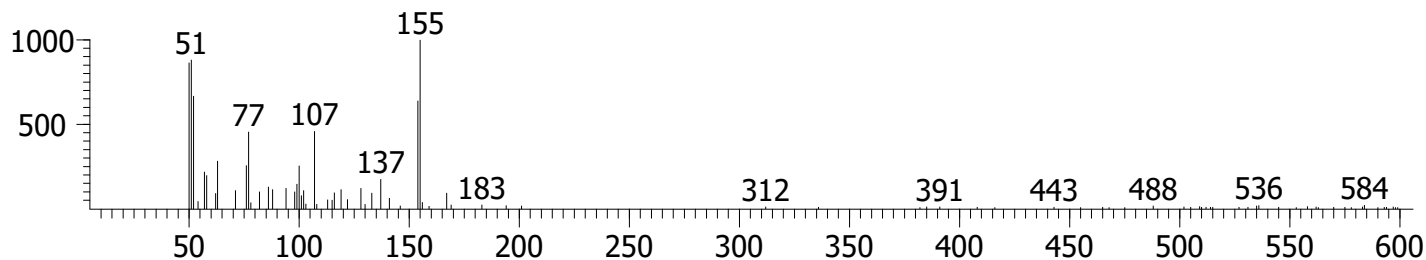
Similarity = 586



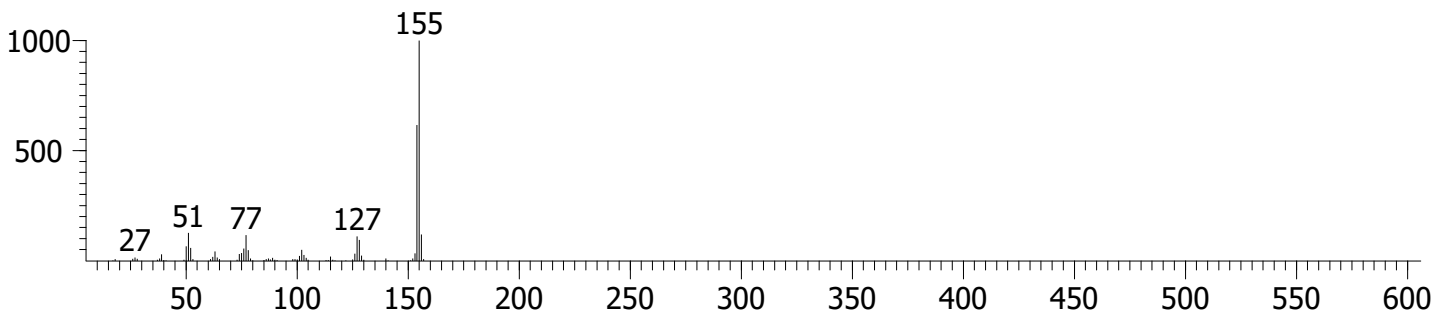
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 1700, at 1221.58 , 2.105 sec , sec (Spec # 1126 79)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 1700, at 1221.58 , 2.105 sec , sec (Spec # 1126 79)



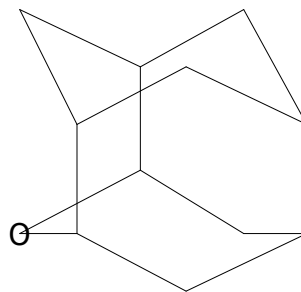
Library Hit - similarity 586, "Pyridine, 2-phenyl-"



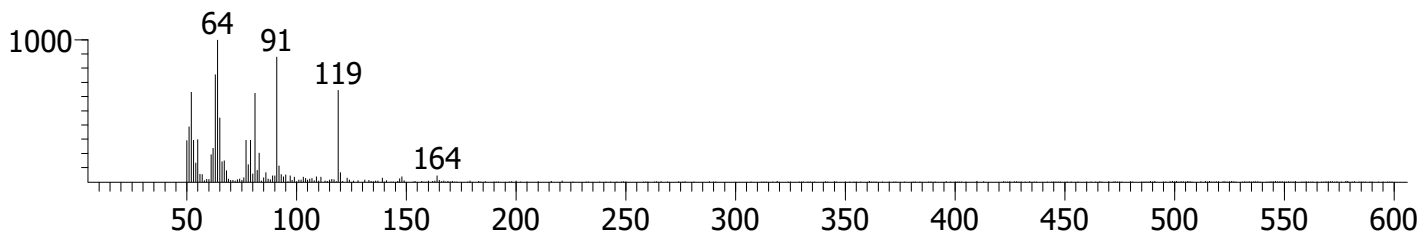
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pyridine, 2-phenyl-	586	2765	1008-89-5	mainlib	C11H9N	155
2	Pyridinium, 1-methyl-2-phenyl-, iodide	565	1176	52806-02-7	mainlib	C12H12IN	297
3	Pyridine, 4-phenyl-	563	1085	939-23-1	mainlib	C11H9N	155
4	Pyridine, 3-phenyl-	559	916	1008-88-4	mainlib	C11H9N	155
5	4-Phenylpyridinium bromide, 1-allylidene-	559	916	57167-61-0	mainlib	C14H14BrN	275

2,7:3,6-Dimethano-2H-1-benzopyran,
octahydro-

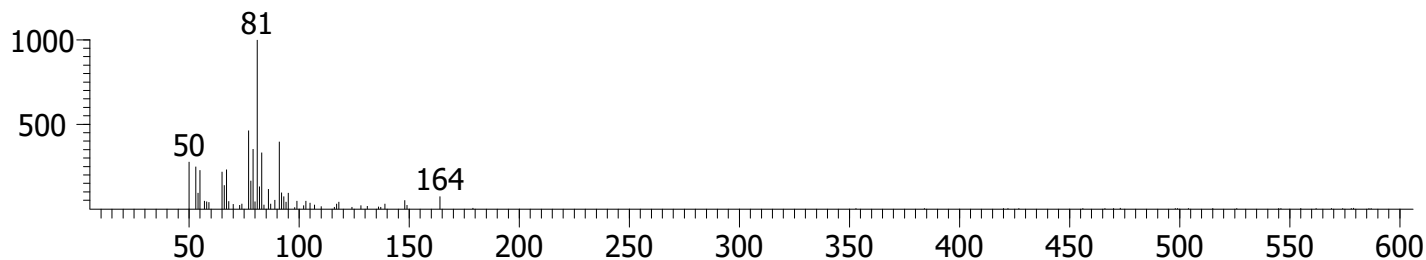
1st Dimension R.T. = 1249.56
2nd Dimension R.T. = 2.303
Quant Mass(es) = 81
S/N = 102.19
Area = 25692
Height = 2469.4
Similarity = 732



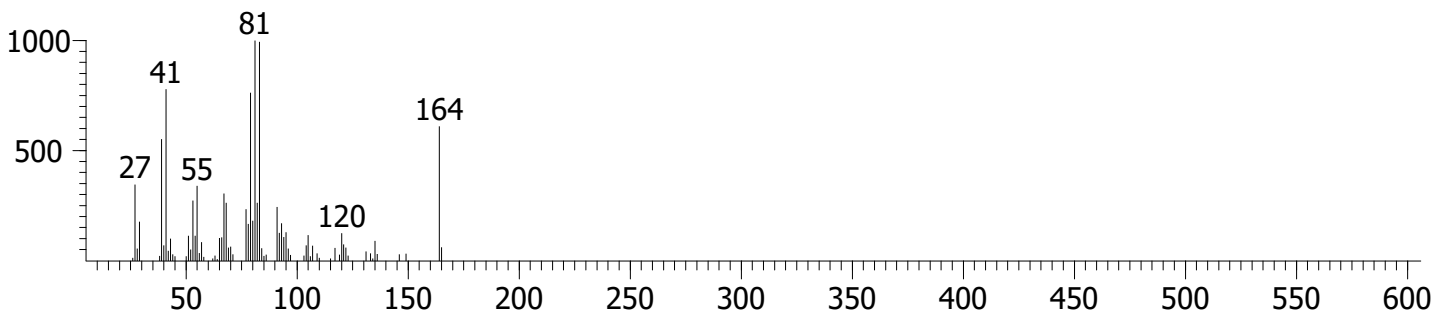
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 1790, at 1249.56 , 2.303 sec , sec (Spec # 1169 49)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 1790, at 1249.56 , 2.303 sec , sec (Spec # 1169 49)



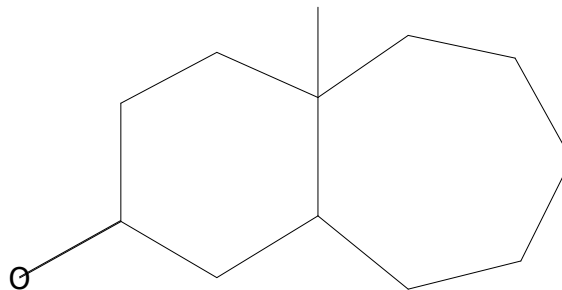
Library Hit - similarity 732, "2,7:3,6-Dimethano-2H-1-benzopyran, octahydro-"



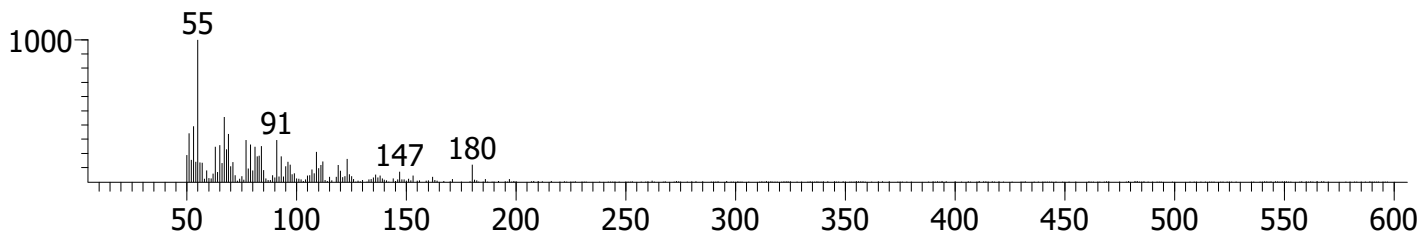
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,7:3,6-Dimethano-2H-1-benzopyran, octahydro-	732	1997	55092-18-7	mainlib	C11H16O	164
2	Dicyclopentadiene diepoxide	727	1609	81-21-0	mainlib	C10H12O2	164
3	2,4-Decadienal, (E,E)-	705	636	25152-84-5	mainlib	C10H16O	152
4	4-Vinylcyclohexene diepoxide (isomer 2)	692	411	0-00-0	mainlib	C8H12O2	140
5	4-Vinylcyclohexene diepoxide (isomer 1)	692	411	0-00-0	mainlib	C8H12O2	140

2H-Benzocyclohepten-2-one,
decahydro-4a-methyl-, trans-

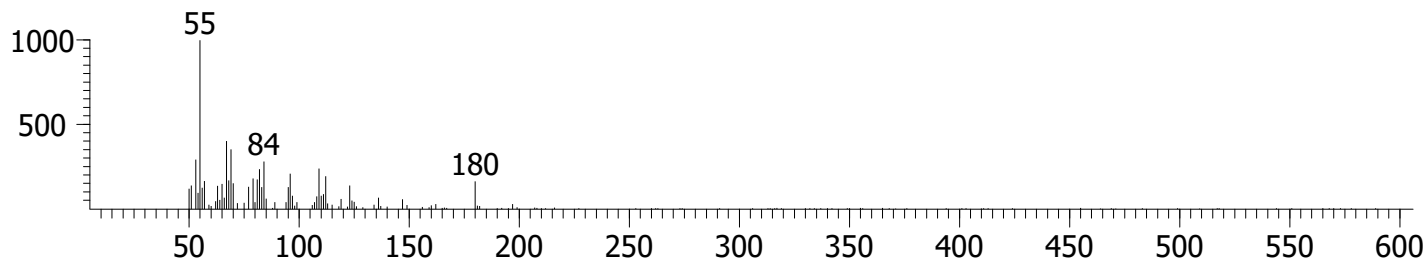
1st Dimension R.T. = 1263.55
2nd Dimension R.T. = 2.165
Quant Mass(es) = 180
S/N = 58.287
Area = 4366.9
Height = 453.01
Similarity = 746



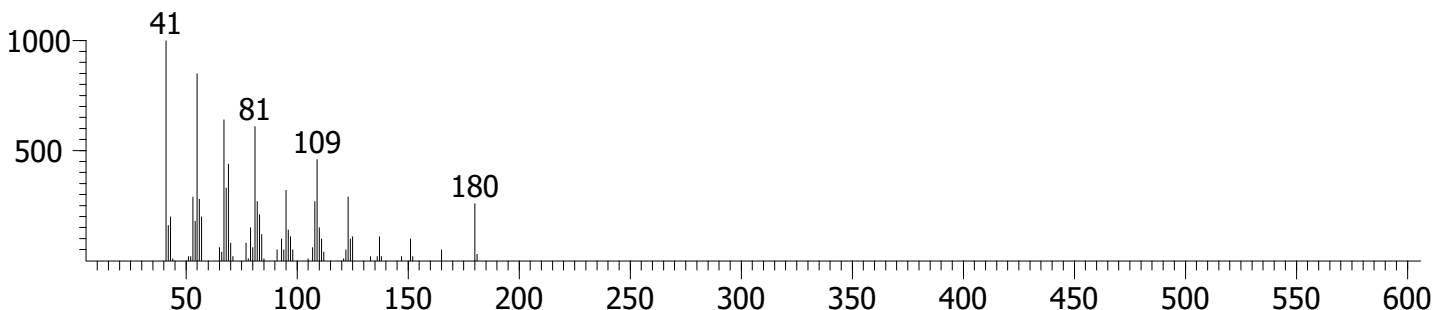
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 1836, at 1263.55 , 2.165 sec , sec (Spec # 1190 48)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 1836, at 1263.55 , 2.165 sec , sec (Spec # 1190 48)



Library Hit - similarity 746, "2H-Benzocyclohepten-2-one, decahydro-4a-methyl-, trans-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2H-Benzocyclohepten-2-one, decahydro-4a-methyl-, trans-	746	1263	55103-64-5	mainlib	C ₁₂ H ₂₀ O	180
2	2(1H)-Naphthalenone, octahydro-1,4a-dimethyl-, (1à,4aà,8aà)-	744	1165	22738-31-4	mainlib	C ₁₂ H ₂₀ O	180
3	2-Methyl-Z,Z-3,13-octadecadienol	718	349	0-00-0	mainlib	C ₁₉ H ₃₆ O	280
4	4-Chloro-3-n-hexyltetrahydropyran	714	295	66555-66-6	mainlib	C ₁₁ H ₂₁ ClO	204
5	E-7-Tetradecenol	711	260	37011-95-3	mainlib	C ₁₄ H ₂₈ O	212

7-Dimethyl-5,6,7,7a-tetrahydrocyclopenta[c]

1st Dimension R.T. = 1291.54

2nd Dimension R.T. = 1.650

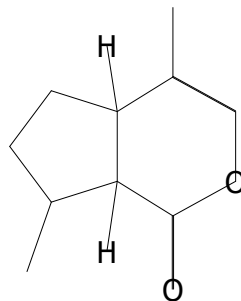
Quant Mass(es) = 166

S/N = 352.71

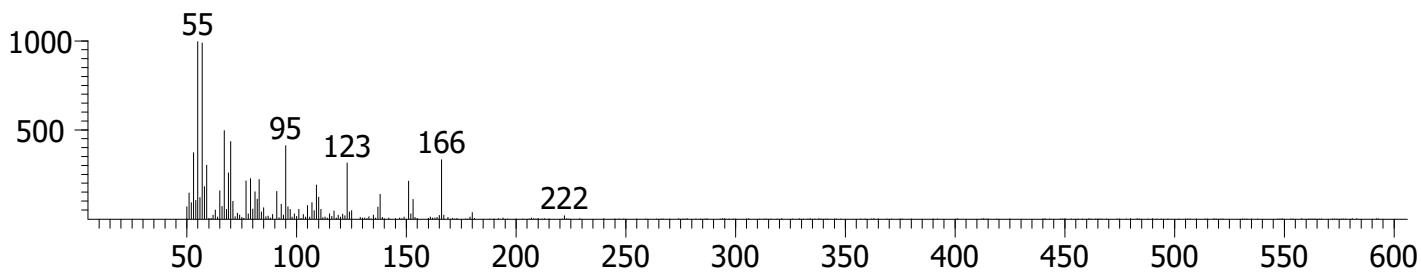
Area = 42024

Height = 5359.0

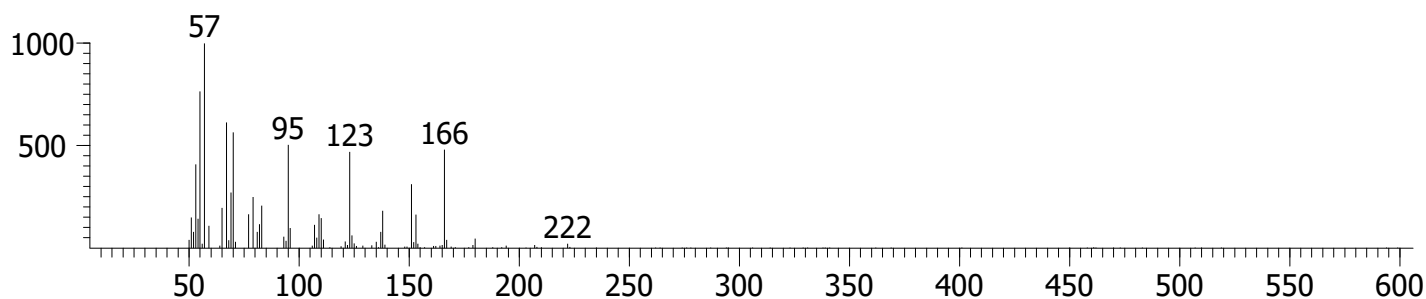
Similarity = 681



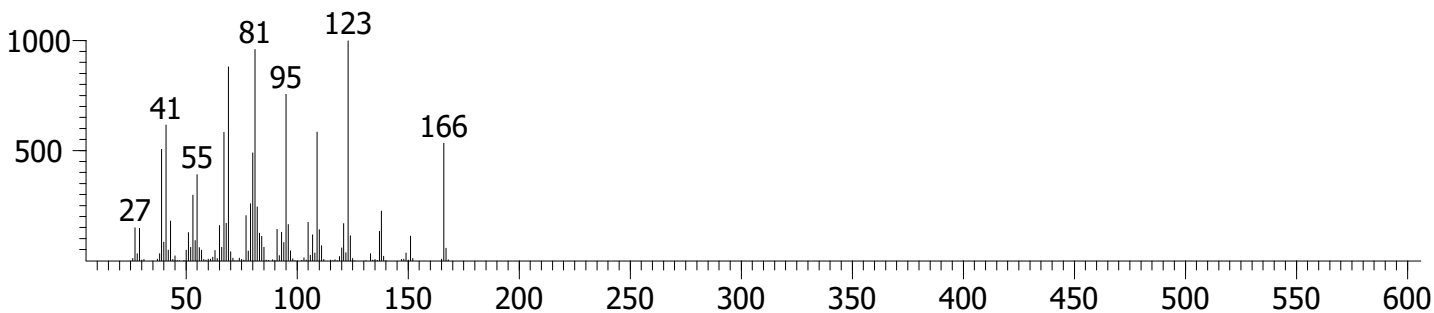
Peak Apex - sample "AerBxr C (20191121):1", peak 2197, at 1291.54 , 1.650 sec , sec (Spec # 123210)



Peak True - sample "AerBxr C (20191121):1", peak 2197, at 1291.54 , 1.650 sec , sec (Spec # 123210)

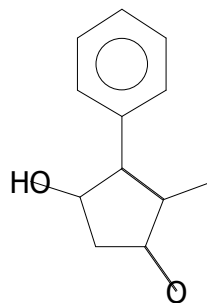


Library Hit - similarity 681, "(4aR,7S,7aS)-4,7-Dimethyl-5,6,7,7a-tetrahydrocyclopenta[c]pyran-1(4aH)-one"



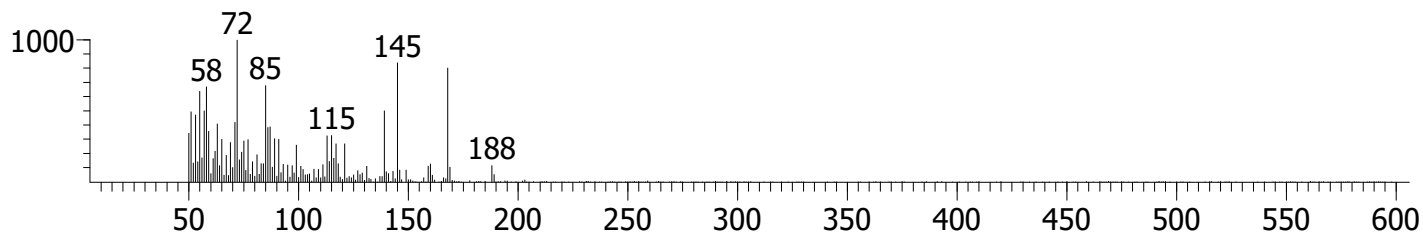
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	(4aR,7S,7aS)-4,7-Dimethyl-5,6,7,7a-tetrahydrocyclopenta[c]pyran-1(4aH)-one	681	1135	21651-53-6	mainlib	C10H14O2	166
2	Cyclodecene, 1,2-dimethyl-, (Z)-	672	824	14113-67-8	mainlib	C12H22	166
3	Cyclohexanone, 2,5-dimethyl-2-(1-methylethenyl)-	667	664	6711-26-8	mainlib	C11H18O	166
4	3,5-Decadiene, 2,2-dimethyl-, (Z,Z)-	658	482	55638-50-1	mainlib	C12H22	166
5	2(5H)-Furanone, 4-(2,3-dimethyl-2-buten-4-yl)-	657	463	0-00-0	mainlib	C10H14O2	166

2-Cyclopenten-1-one,
4-hydroxy-2-methyl-3-phenyl-

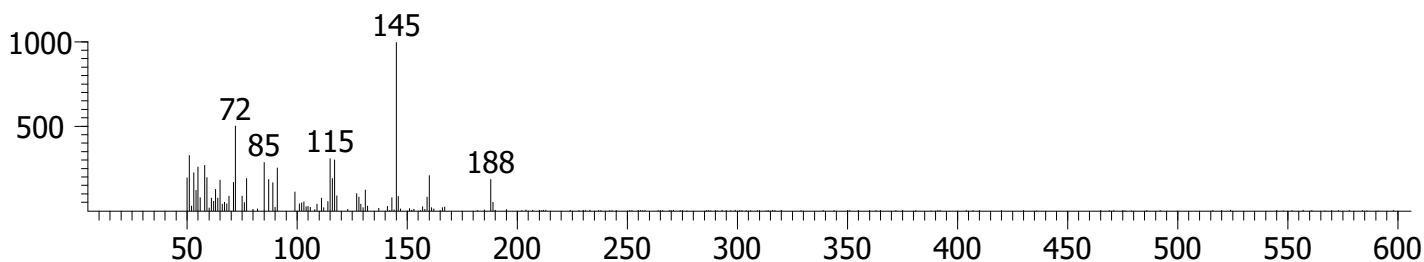


1st Dimension R.T. = 1298.53
2nd Dimension R.T. = 1.973
Quant Mass(es) = 145
S/N = 78.260
Area = 61620
Height = 5551.7
Similarity = 676

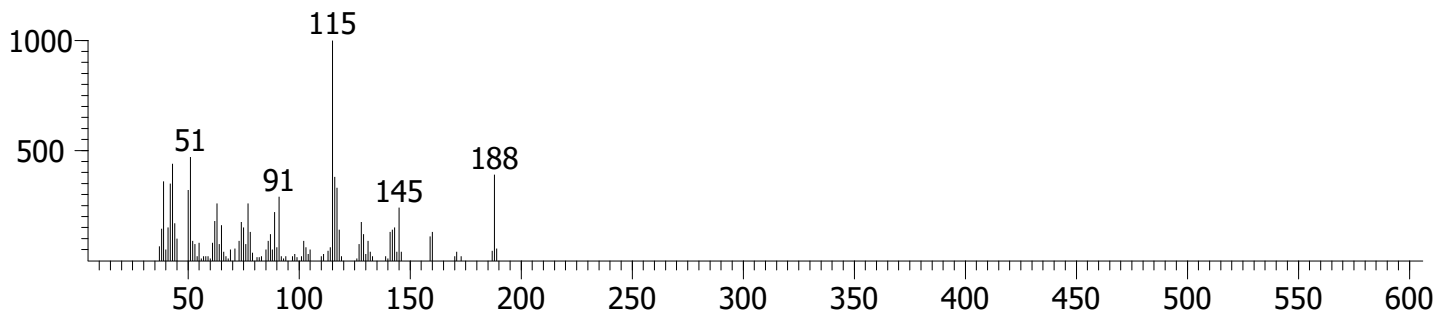
Peak Apex - sample "AerMBR A 092319 (20191119):1", peak 1732, at 1298.53 , 1.973 sec , sec (Spec # 1243 19)



Peak True - sample "AerMBR A 092319 (20191119):1", peak 1732, at 1298.53 , 1.973 sec , sec (Spec # 1243 19)



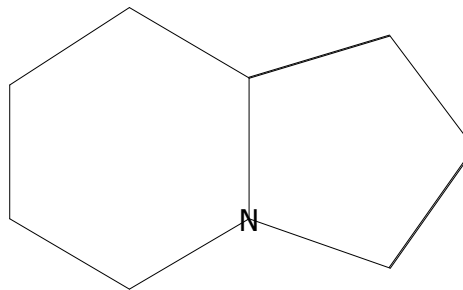
Library Hit - similarity 676, "2-Cyclopenten-1-one, 4-hydroxy-2-methyl-3-phenyl-"



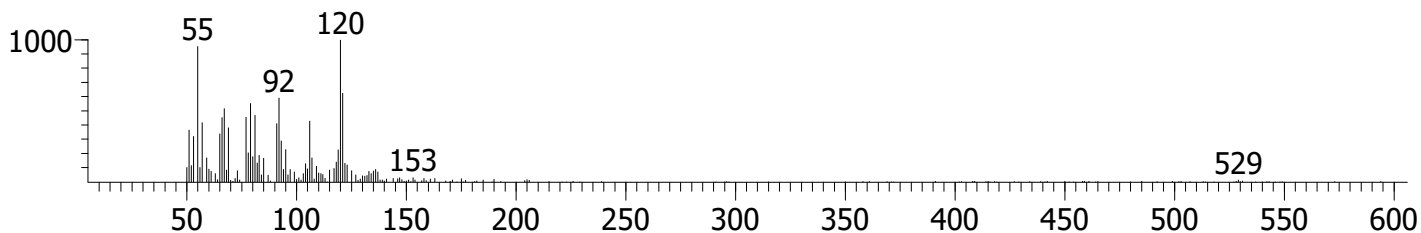
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Cyclopenten-1-one, 4-hydroxy-2-methyl-3-phenyl-	676	1582	69745-73-9	mainlib	C12H12O2	188
2	Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	668	1180	1985-59-7	mainlib	C12H16	160
3	Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	653	715	1129-29-9	mainlib	C12H16	160
4	1H-Inden-1-one, 2,3-dihydro-3,3-dimethyl-	652	687	26465-81-6	mainlib	C11H12O	160
5	Coumarin, 5,7,8-trimethyl-	637	416	40662-19-9	mainlib	C12H12O2	188

5,6,7,8-Tetrahydroindolizine

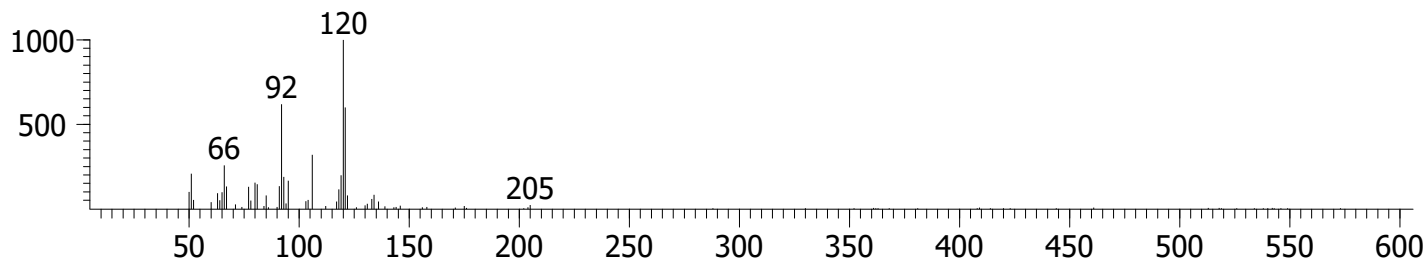
1st Dimension R.T. = 1319.52
2nd Dimension R.T. = 1.617
Quant Mass(es) = 120
S/N = 181.95
Area = 15435
Height = 1905.7
Similarity = 731



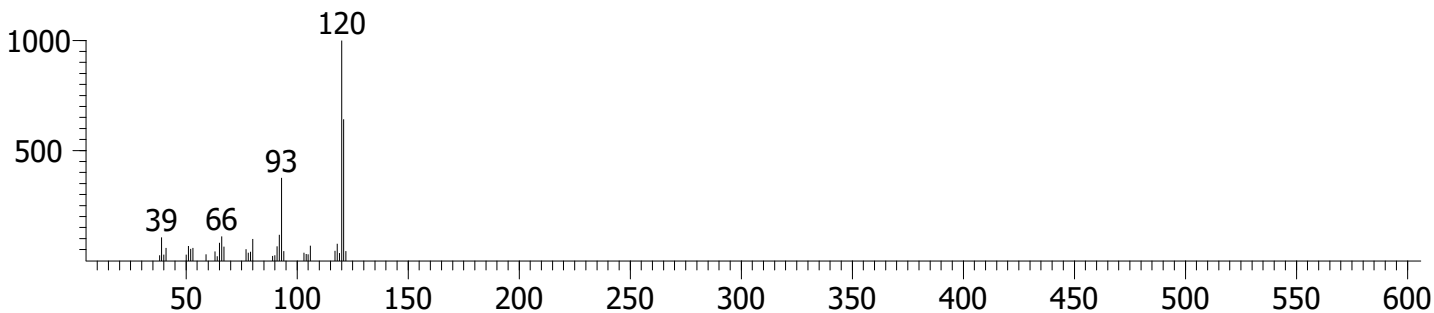
Peak Apex - sample "AerMBR C 091919 (20191119):1", peak 2092, at 1319.52 , 1.617 sec , sec (Spec # 1274 45)



Peak True - sample "AerMBR C 091919 (20191119):1", peak 2092, at 1319.52 , 1.617 sec , sec (Spec # 1274 45)



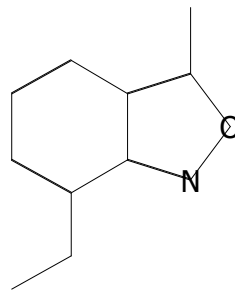
Library Hit - similarity 731, "5,6,7,8-Tetrahydroindolizine"



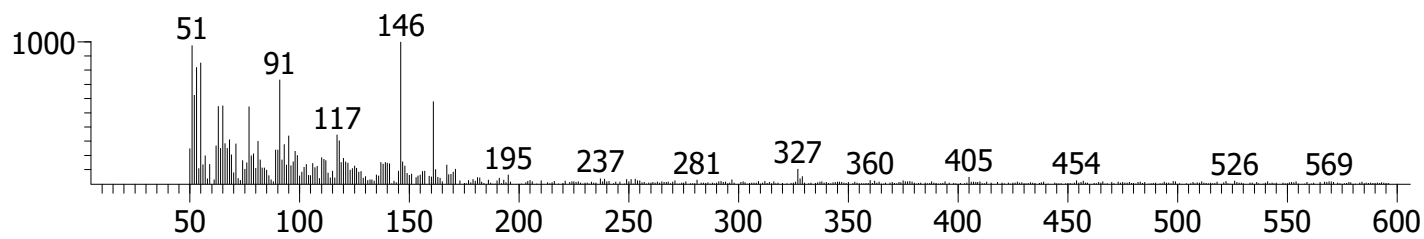
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5,6,7,8-Tetrahydroindolizine	731	3138	13618-88-7	mainlib	C8H11N	121
2	2,2'-Bis[5,6,7,8-tetrahydroindolizine]	724	2404	0-00-0	mainlib	C16H20N2	240
3	Pyridine, 2-ethyl-6-methyl-	682	539	1122-69-6	mainlib	C8H11N	121
4	2-Amino-4-methylpyrrole-3-carbonitrile	669	348	59146-60-0	mainlib	C6H7N3	121
5	3-(Anthraniloylhydrazono)-N-(2-ethylphenyl)butyramide	666	307	350039-69-9	mainlib	C19H22N4O2	338

2,1-Benzisoxazole, 7-ethyl-3-methyl-

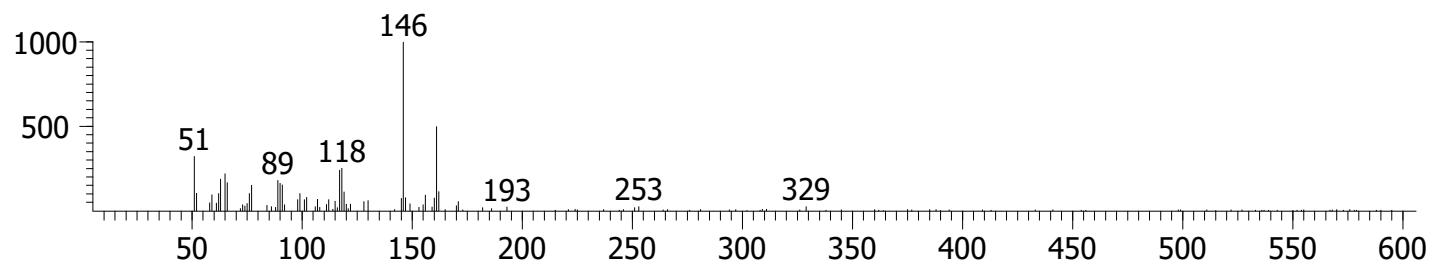
1st Dimension R.T. = 1413.97
2nd Dimension R.T. = 2.356
Quant Mass(es) = 146
S/N = 158.55
Area = 12957
Height = 1383.1
Similarity = 714



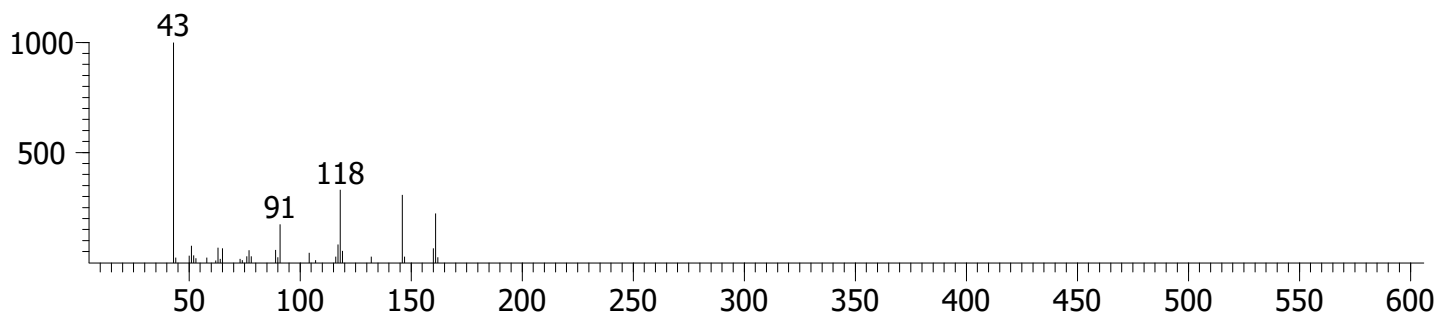
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 2261, at 1413.97 , 2.356 sec , sec (Spec # 1418 67)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 2261, at 1413.97 , 2.356 sec , sec (Spec # 1418 67)



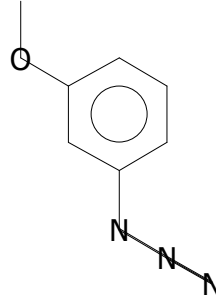
Library Hit - similarity 714, "2,1-Benzisoxazole, 7-ethyl-3-methyl-"



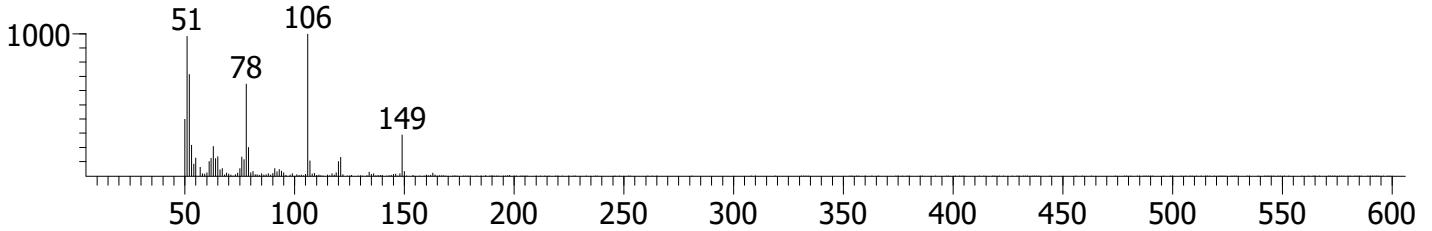
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,1-Benzisoxazole, 7-ethyl-3-methyl-	714	1494	108562-69-2	mainlib	C10H11NO	161
2	1H-isoindol-1-one, 2-ethyl-2,3-dihydro-	708	1174	0-00-0	mainlib	C10H11NO	161
3	1H-Indole, 5-methoxy-2-methyl-	708	1174	1076-74-0	mainlib	C10H11NO	161
4	quinoline, 1-ethyl-1,2,3,4-tetrahydro-	706	1083	0-00-0	mainlib	C11H15N	161
5	2H-Indol-2-one, 1,3-dihydro-3,3-dimethyl-	706	1083	19155-24-9	mainlib	C10H11NO	161

Benzene, 1-azido-3-methoxy-

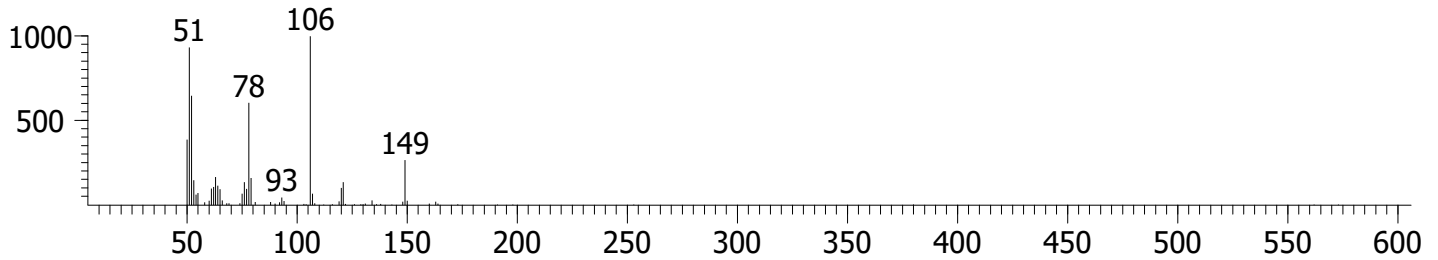
1st Dimension R.T. = 1469.93
2nd Dimension R.T. = 2.495
Quant Mass(es) = 106
S/N = 970.70
Area = 523414
Height = 48607
Similarity = 794



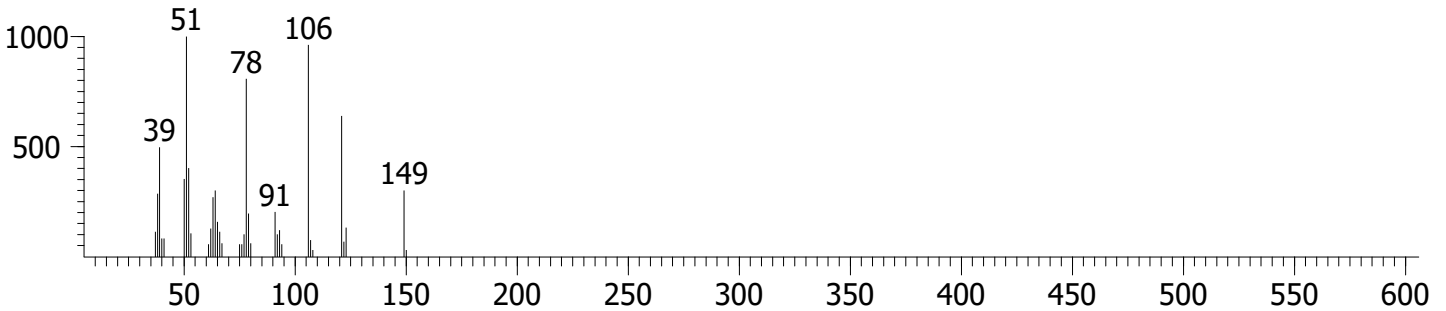
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 2421, at 1469.93 , 2.495 sec , sec (Spec # 1503 68)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 2421, at 1469.93 , 2.495 sec , sec (Spec # 1503 68)



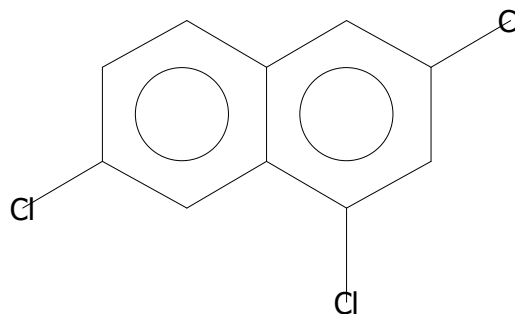
Library Hit - similarity 794, "Benzene, 1-azido-3-methoxy-"



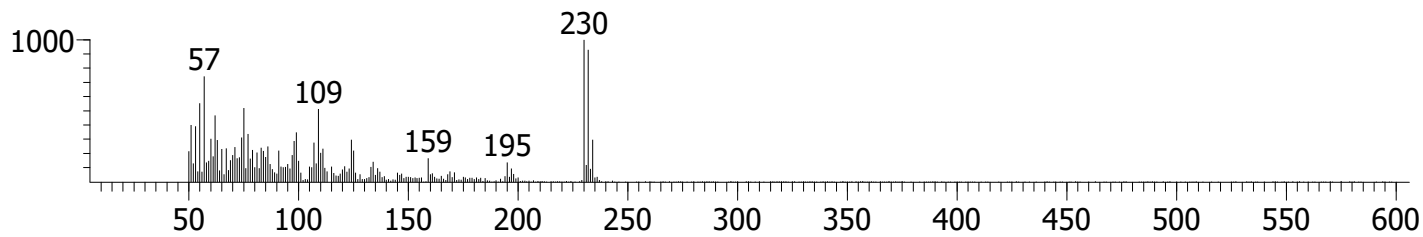
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-azido-3-methoxy-	794	4479	3866-16-8	mainlib	C7H7N3O	149
2	3,5-Dimethyl-5-[2-pyridyl]-1,3,4-thiadiazolidin-2-thione	762	1196	74752-62-8	mainlib	C9H11N3S2	225
3	N-(3-Methoxy-5-tetrazol-1-yl-phenyl)-isonicotinamide	754	892	0-00-0	mainlib	C14H12N6O2	296
4	1H-Benzotriazole, 4-methoxy-	741	576	27799-90-2	mainlib	C7H7N3O	149
5	1-Butanone, 1-(3-pyridinyl)-	738	509	1701-70-8	mainlib	C9H11NO	149

Naphthalene, 1,3,7-trichloro-

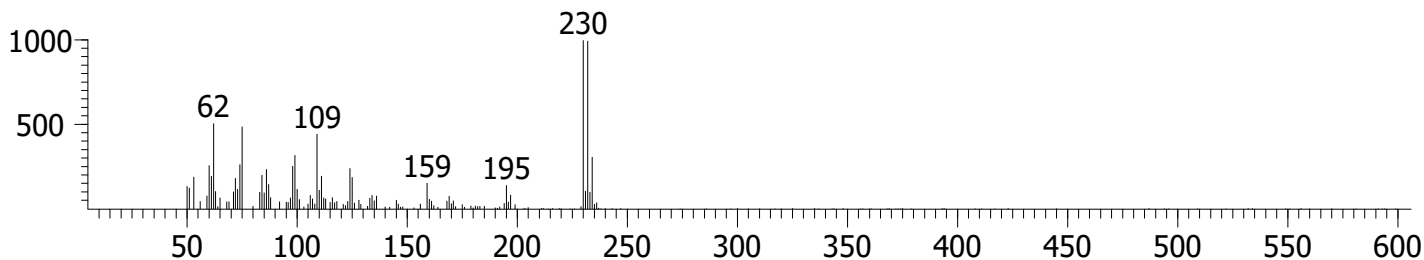
1st Dimension R.T. = 1476.93
2nd Dimension R.T. = 2.198
Quant Mass(es) = 232
S/N = 709.67
Area = 71839
Height = 7646.4
Similarity = 668



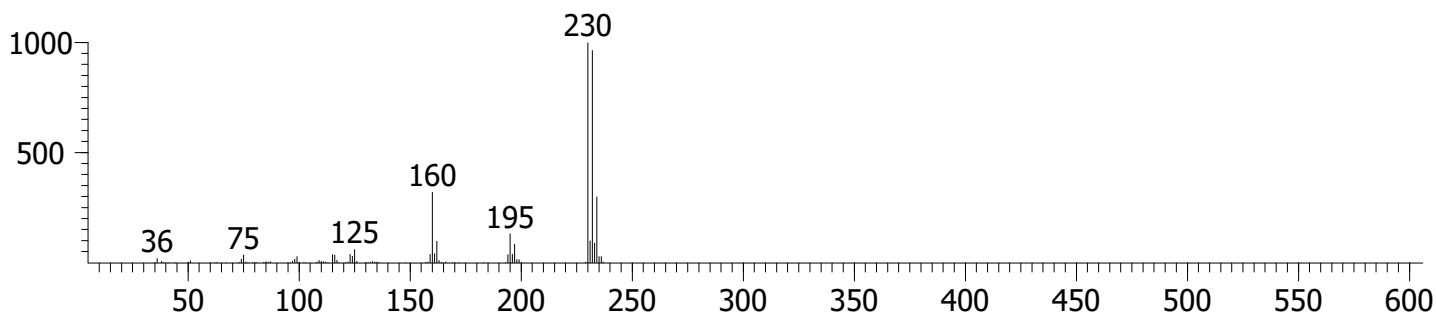
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 2442, at 1476.93 , 2.198 sec , sec (Spec # 1513 83)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 2442, at 1476.93 , 2.198 sec , sec (Spec # 1513 83)



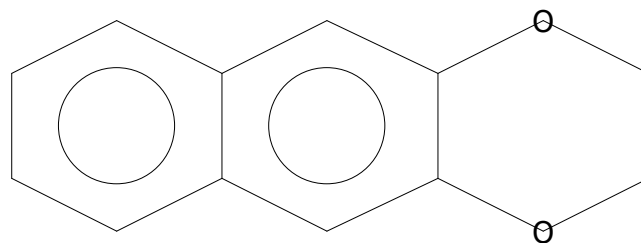
Library Hit - similarity 668, "Naphthalene, 1,3,7-trichloro-"



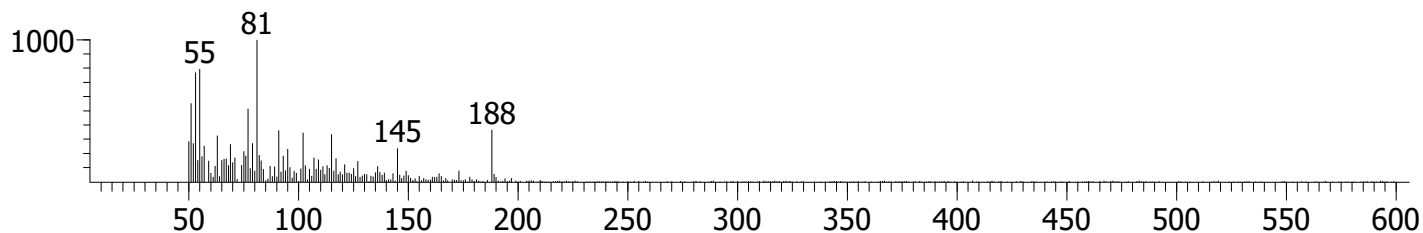
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,4,5,6-Tetrachloro-pyridin-3-ylamine	684	3319	0-00-0	mainlib	C5H2Cl4N2	230
2	Naphthalene, 1,3,7-trichloro-	668	1911	55720-37-1	mainlib	C10H5Cl3	230
3	Naphthalene, 2,3,6-trichloro-	665	1689	55720-40-6	mainlib	C10H5Cl3	230
4	1,3,5-Metheno-1H-cyclopropa[a]pentalene, 1,1a,4,5,5a,6-hexachlorooctahydro-	611	330	69743-71-1	mainlib	C10H6Cl6	336
5	1-Perchloroethenyl-4-ethynylbenzene	601	233	0-00-0	mainlib	C10H5Cl3	230

Naphthalene, 2,3-dimethoxy-

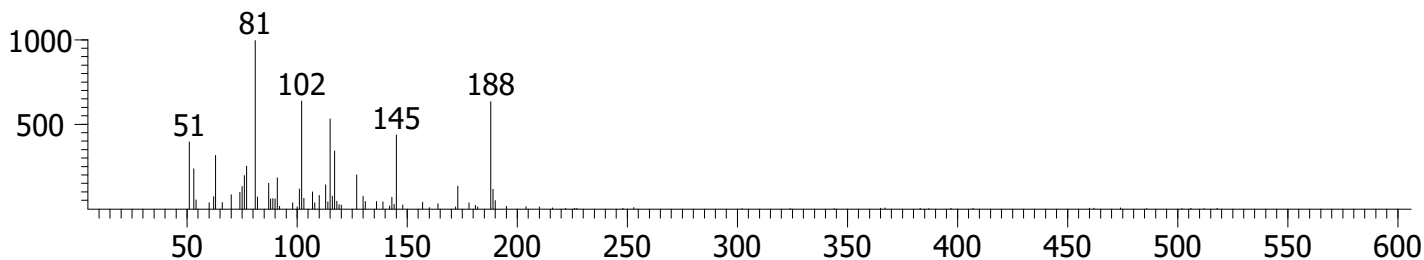
1st Dimension R.T. = 1511.91
2nd Dimension R.T. = 2.224
Quant Mass(es) = 188
S/N = 148.12
Area = 16001
Height = 1655.3
Similarity = 734



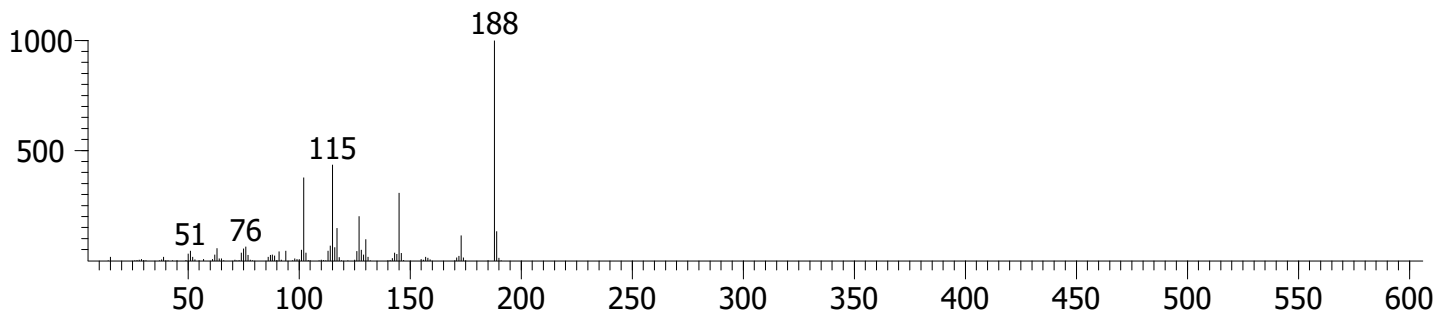
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 2545, at 1511.91 , 2.224 sec , sec (Spec # 1566 87)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 2545, at 1511.91 , 2.224 sec , sec (Spec # 1566 87)



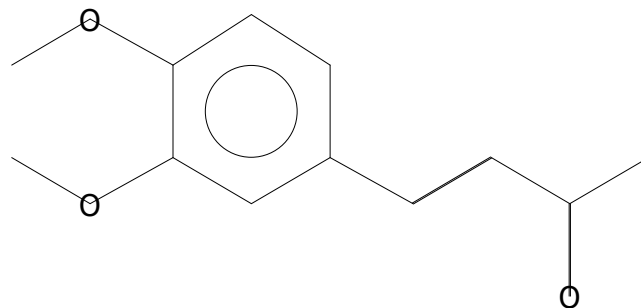
Library Hit - similarity 734, "Naphthalene, 2,3-dimethoxy-"



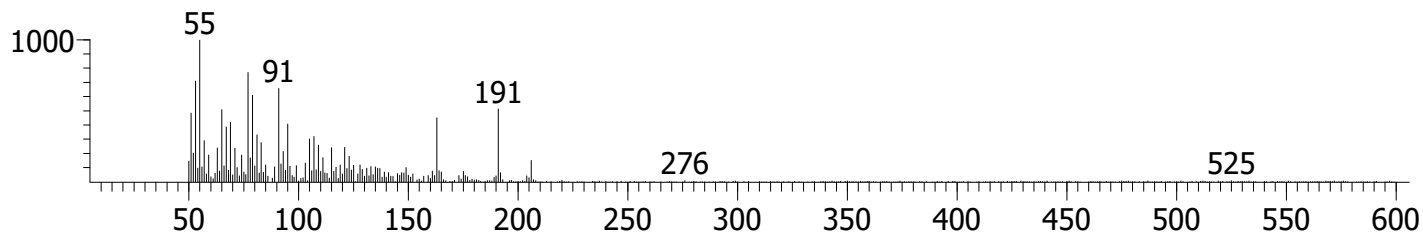
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Naphthalene, 2,3-dimethoxy-	734	7228	10103-06-7	mainlib	C12H12O2	188
2	naphthalene, 1,8-dimethoxy-	663	1029	0-00-0	mainlib	C12H12O2	188
3	Naphthalene, 1,4-dimethoxy-	663	1029	10075-62-4	mainlib	C12H12O2	188
4	1,2-Dimethoxy-5H-benzo[a]cyclohepten-5-one	619	223	0-00-0	mainlib	C13H12O3	216
5	2-Cyclopenten-1-one, 4-hydroxy-3-methyl-2-phenyl-	592	65	69766-87-6	mainlib	C12H12O2	188

3,4-Dimethoxybenzylideneacetone

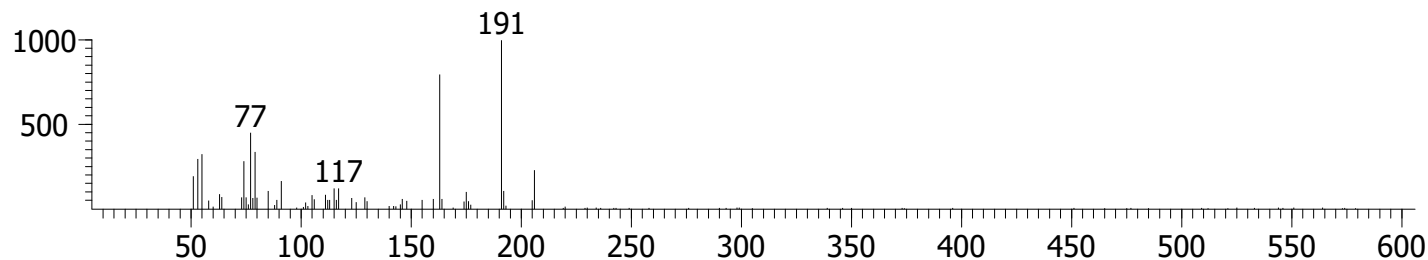
1st Dimension R.T. = 1518.91
2nd Dimension R.T. = 1.967
Quant Mass(es) = 191
S/N = 158.90
Area = 15391
Height = 1505.6
Similarity = 677



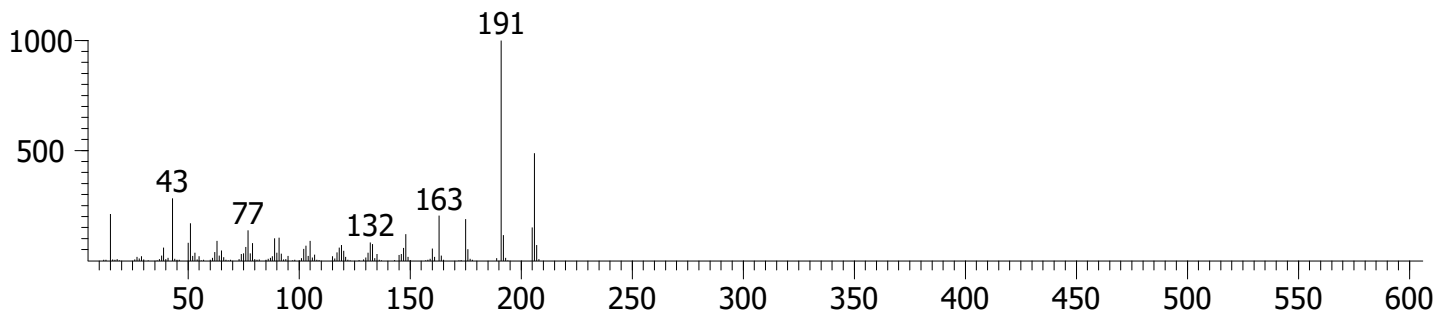
Peak Apex - sample "AerMBR C 091919 (20191119):1", peak 2634, at 1518.91 , 1.967 sec , sec (Spec # 1577 08)



Peak True - sample "AerMBR C 091919 (20191119):1", peak 2634, at 1518.91 , 1.967 sec , sec (Spec # 1577 08)



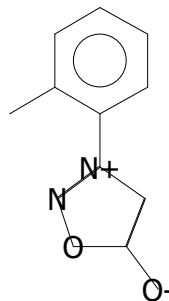
Library Hit - similarity 677, "3,4-Dimethoxybenzylideneacetone"



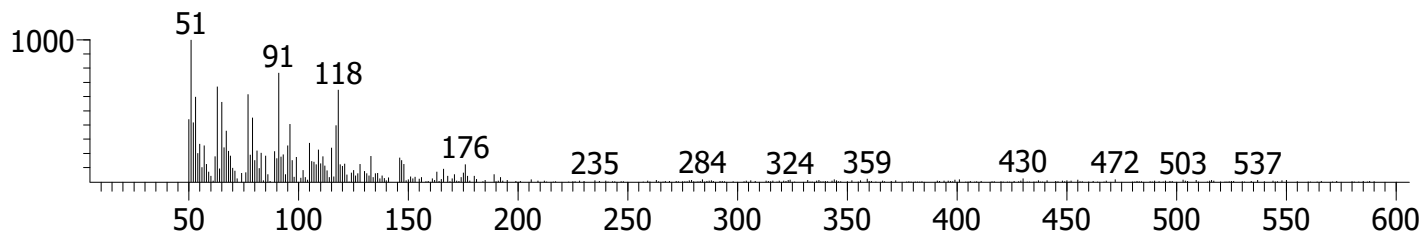
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3,4-Dimethoxybenzylideneacetone	677	2251	15001-27-1	mainlib	C ₁₂ H ₁₄ O ₃	206
2	Phenol, 2,5-bis(1,1-dimethylethyl)-	655	889	5875-45-6	mainlib	C ₁₄ H ₂₂ O	206
3	1H-Inden-1-one, 2,3-dihydro-5,6-dimethoxy-3-methyl-	654	855	4082-25-1	mainlib	C ₁₂ H ₁₄ O ₃	206
4	Phenol, 2,6-bis(1,1-dimethylethyl)-	647	655	128-39-2	mainlib	C ₁₄ H ₂₂ O	206
5	2,4-Di-tert-butylphenol	645	604	96-76-4	mainlib	C ₁₄ H ₂₂ O	206

Sydnone, 3-(2-methylphenyl)-

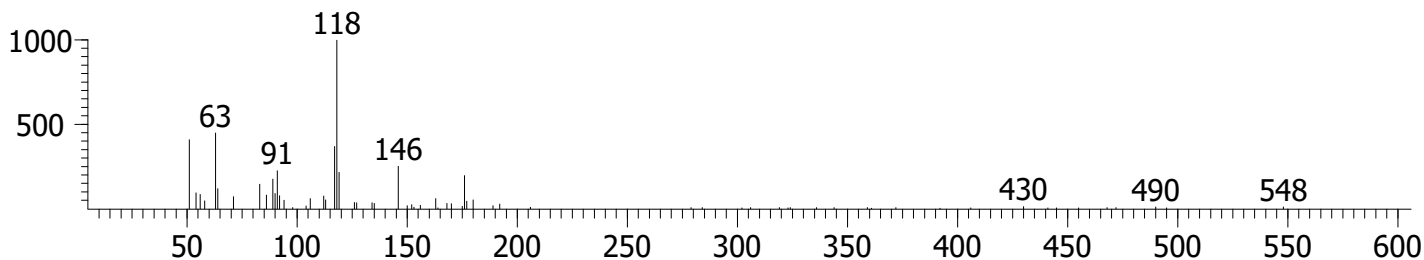
1st Dimension R.T. = 1529.4
2nd Dimension R.T. = 2.409
Quant Mass(es) = 118
S/N = 89.468
Area = 9917.5
Height = 919.05
Similarity = 696



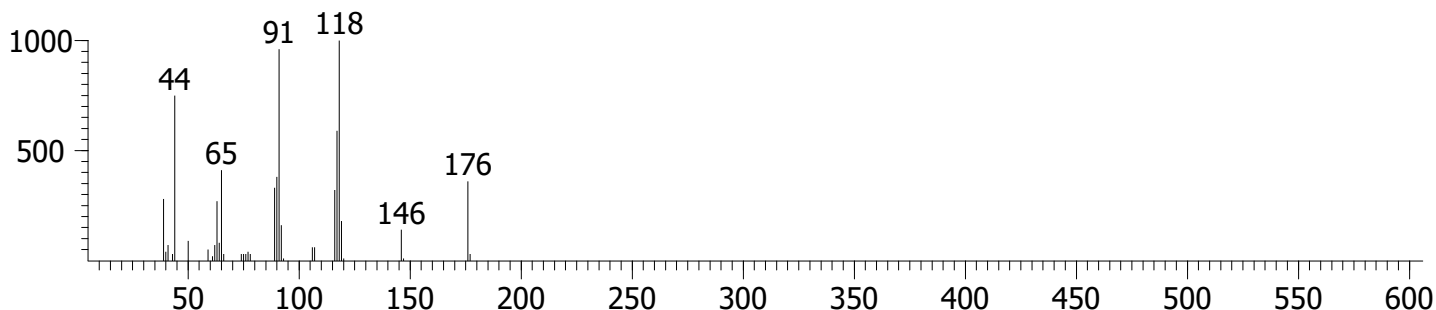
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 2603, at 1529.4 , 2.409 sec , sec (Spec # 15936 5)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 2603, at 1529.4 , 2.409 sec , sec (Spec # 15936 5)



Library Hit - similarity 696, "Sydnone, 3-(2-methylphenyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Sydnone, 3-(2-methylphenyl)-	696	2677	3483-18-9	mainlib	C9H8N2O2	176
2	4-Butylbenzoic acid, 3-phenylpropyl ester	629	414	0-00-0	mainlib	C20H24O2	296
3	Quinazoline-4-carboxylic acid, 1,2-dihydro-2-oxo-	627	382	99066-77-0	mainlib	C9H6N2O3	190
4	2-Propenoic acid, 3-(di-2-propynylamino)-, methyl ester	622	308	50838-16-9	mainlib	C10H11NO2	177
5	2-[5-(4-Aminophenyl)-1,2,3,4-tetrazol-2-yl]ethanol	621	296	0-00-0	mainlib	C9H11N5O	205

3-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)pher

1st Dimension R.T. = 1774.26

2nd Dimension R.T. = 1.815

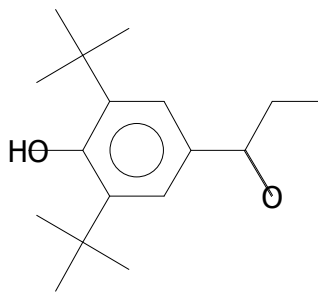
Quant Mass(es) = 233

S/N = 946.26

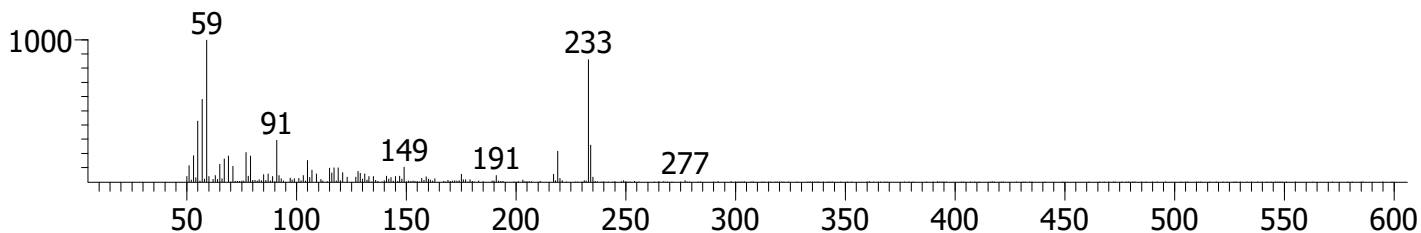
Area = 97976

Height = 10407

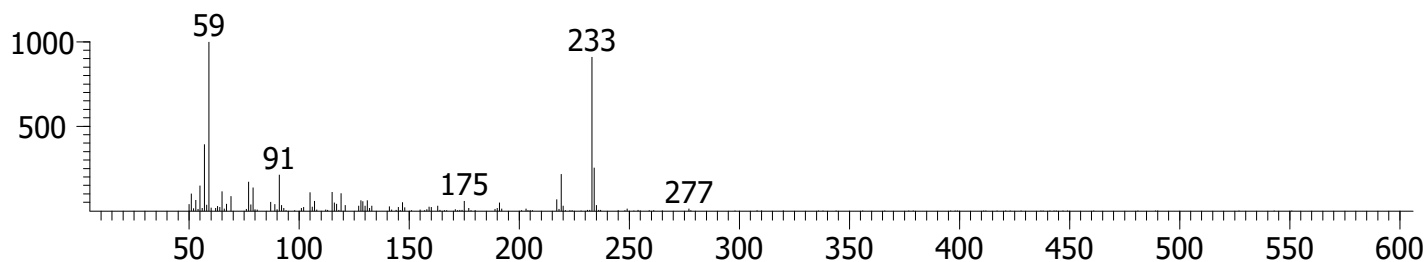
Similarity = 730



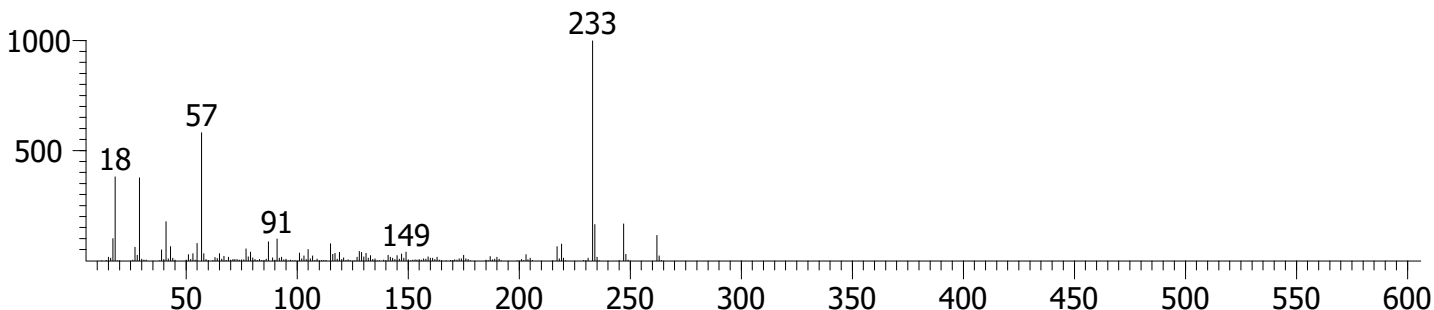
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3368, at 1774.26 , 1.815 sec , sec (Spec # 1963 75)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3368, at 1774.26 , 1.815 sec , sec (Spec # 1963 75)



Library Hit - similarity 730, "2,6-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)phenol"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,6-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)phenol	730	7944	14035-34-8	mainlib	C17H26O2	262
2	1-(3,5-Di-tert-butyl-4-hydroxyphenyl)-2-bromethanone	640	679	14386-64-2	mainlib	C16H23BrO2	326
3	2,4-Pentanedione, 1-(7-acetyl-4,6-dihydroxy-3,5-dimethyl-2-benzofuranyl)-	624	391	21402-79-9	mainlib	C17H18O6	318
4	2H-1-benzopyran-6-ol, 3,4-dihydro-2,2,4-trimethyl-7-(1,1,3,3-tetramethylbutyl)-	613	268	0-00-0	mainlib	C20H32O2	304
5	Succinic acid, di(2-tert-butylphenyl) ester	604	194	0-00-0	mainlib	C24H30O4	382

4-(4-Chlorophenyl)-2-pyrrolidinone

1st Dimension R.T. = 1777.76

2nd Dimension R.T. = 2.739

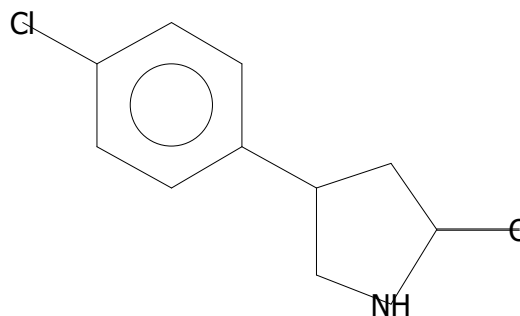
Quant Mass(es) = 138

S/N = 248.32

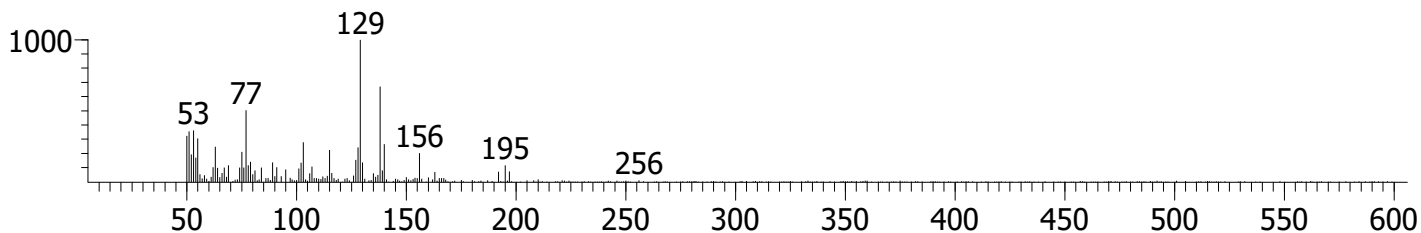
Area = 41692

Height = 3688.4

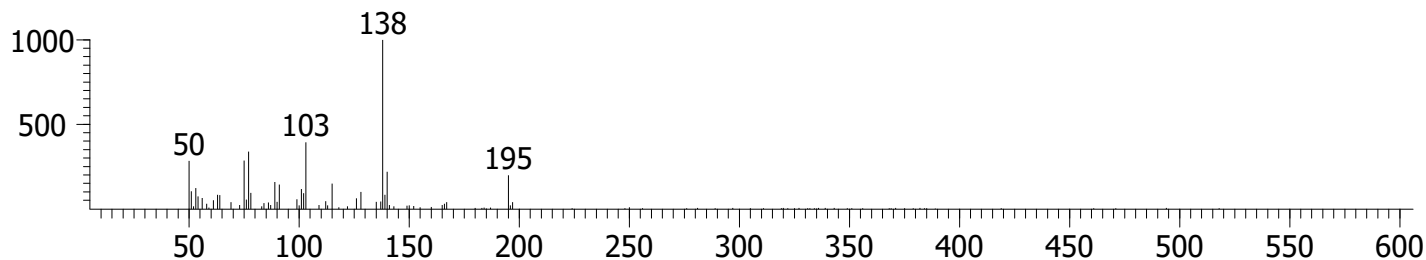
Similarity = 760



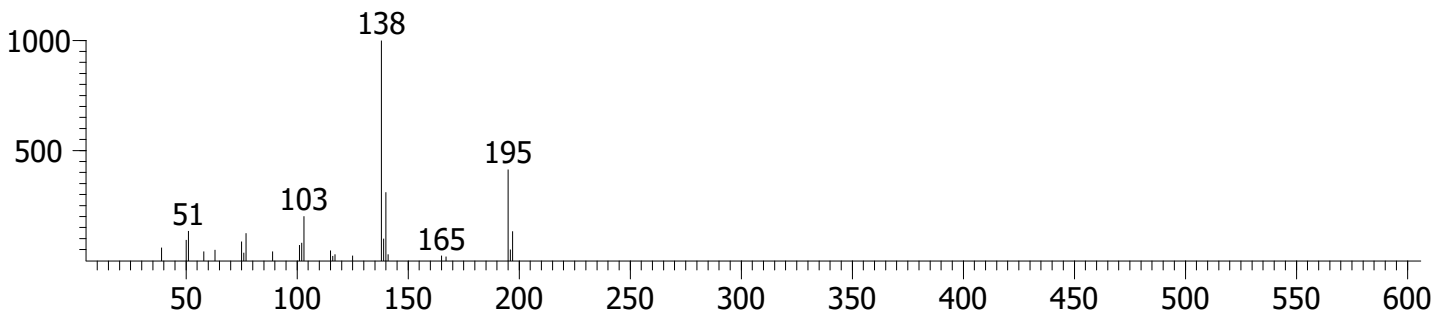
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3389, at 1777.76 , 2.739 sec , sec (Spec # 1970 45)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3389, at 1777.76 , 2.739 sec , sec (Spec # 1970 45)



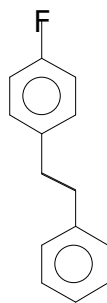
Library Hit - similarity 760, "4-(4-Chlorophenyl)-2-pyrrolidinone"



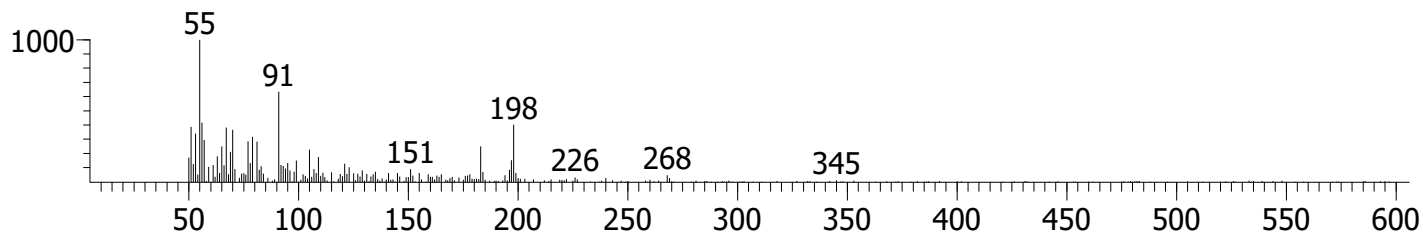
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-(4-Chlorophenyl)-2-pyrrolidinone	760	5500	22518-27-0	mainlib	C10H10ClNO	195
2	Baclofen	733	1618	1134-47-0	mainlib	C10H12ClNO2	213
3	4-(4-Chlorophenyl)-5,5-dimethyldihydrofuran-2-one	709	542	63507-00-6	mainlib	C12H13ClO2	224
4	Benzene, 1-chloro-4-ethenyl-	692	295	1073-67-2	mainlib	C8H7Cl	138
5	Benzene, 1-chloro-4-(4-methyl-4-pentenyl)-	692	295	74672-11-0	mainlib	C12H15Cl	194

Benzene, 1-fluoro-4-(2-phenylethenyl)-, (E)-

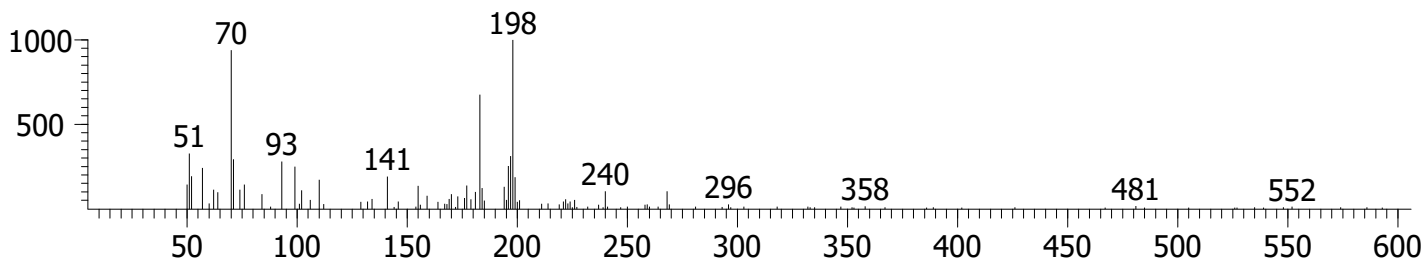
1st Dimension R.T. = 1854.71
2nd Dimension R.T. = 2.171
Quant Mass(es) = 198
S/N = 77.111
Area = 9094.8
Height = 881.62
Similarity = 701



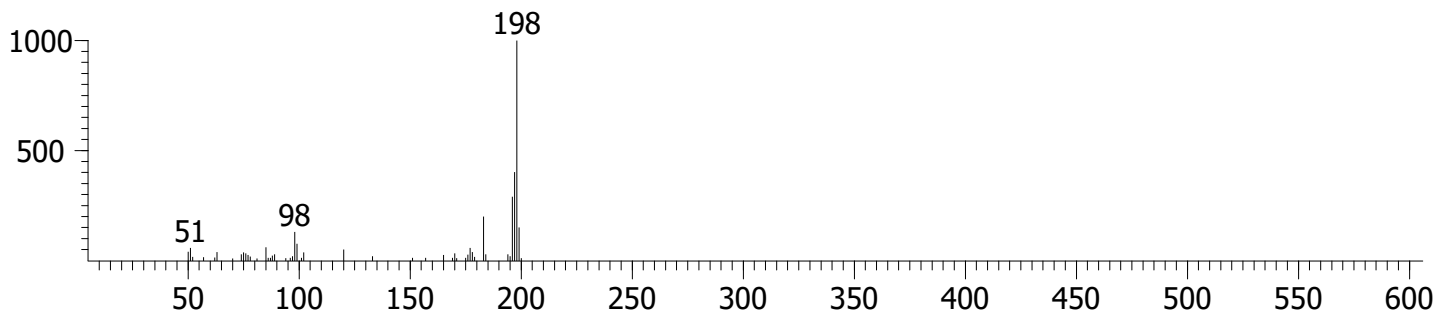
Peak Apex - sample "AerMBR C 091919 (20191119):1", peak 3423, at 1854.71 , 2.171 sec , sec (Spec # 2086 19)



Peak True - sample "AerMBR C 091919 (20191119):1", peak 3423, at 1854.71 , 2.171 sec , sec (Spec # 2086 19)



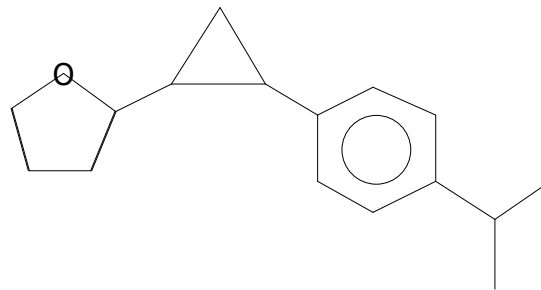
Library Hit - similarity 701, "Benzene, 1-fluoro-4-(2-phenylethenyl)-, (E)-"



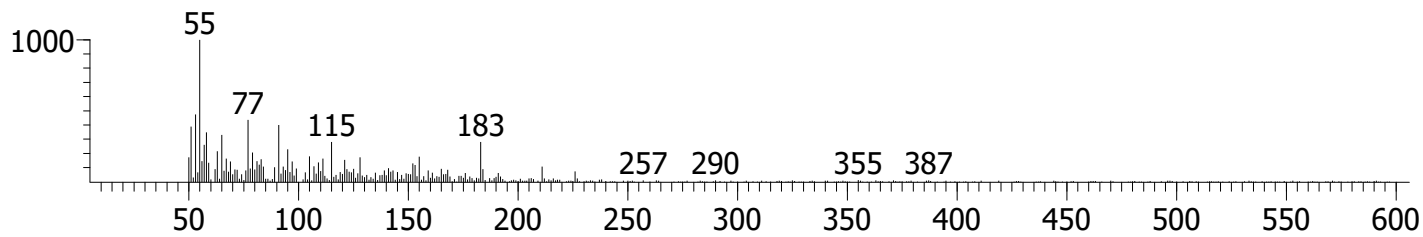
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzene, 1-fluoro-4-(2-phenylethenyl)-, (E)-	701	6432	718-25-2	mainlib	C14H11F	198
2	Benzene, 1-fluoro-3-(2-phenylethenyl)-, (E)-	670	1753	3041-81-4	mainlib	C14H11F	198
3	Benzene, 1,1'-(1-fluoro-1,2-ethenediyl)bis-, (E)-	629	400	671-19-2	mainlib	C14H11F	198
4	2,5-Dimethyl-4-(4-aminophenyl)pyridine	629	400	71153-40-7	mainlib	C13H14N2	198
5	Benzene, 1-fluoro-4-(2-phenylethenyl)-	626	353	17404-69-2	mainlib	C14H11F	198

:-1-(4-Isopropylphenyl)-3-(2-furyl)cyclopropa

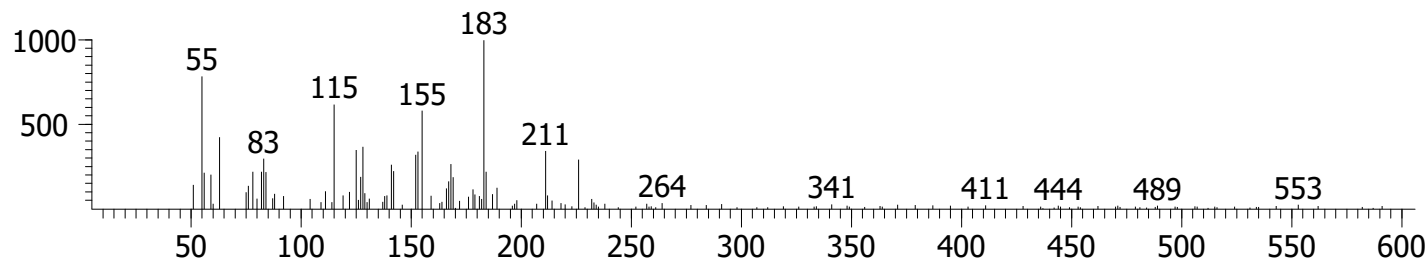
1st Dimension R.T. = 1868.71
2nd Dimension R.T. = 2.303
Quant Mass(es) = 183
S/N = 116.12
Area = 10252
Height = 890.27
Similarity = 631



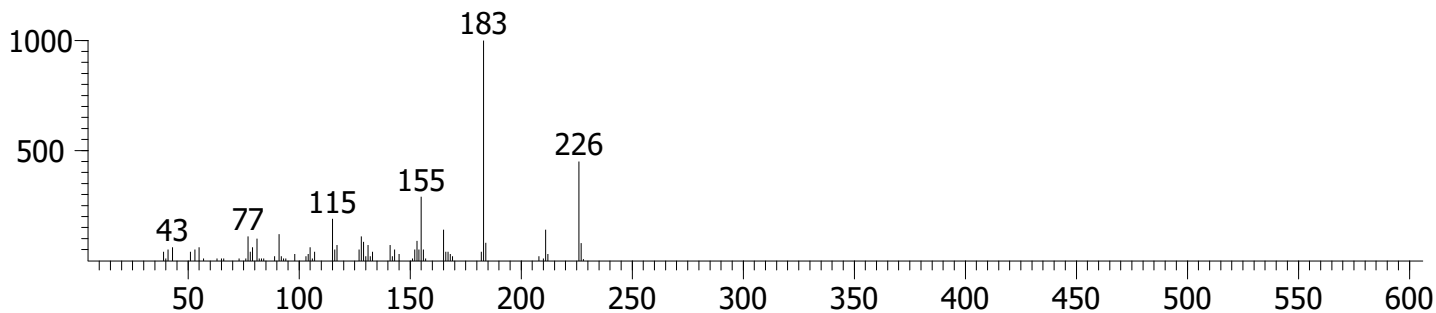
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3574, at 1868.71 , 2.303 sec , sec (Spec # 2107 59)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3574, at 1868.71 , 2.303 sec , sec (Spec # 2107 59)



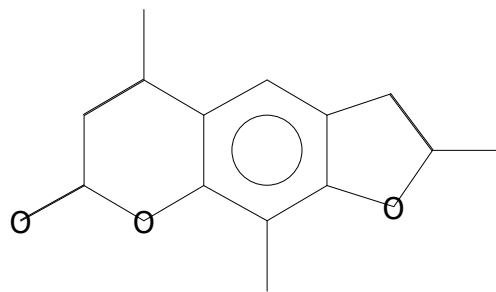
Library Hit - similarity 631, "cis-1-(4-Isopropylphenyl)-3-(2-furyl)cyclopropane"



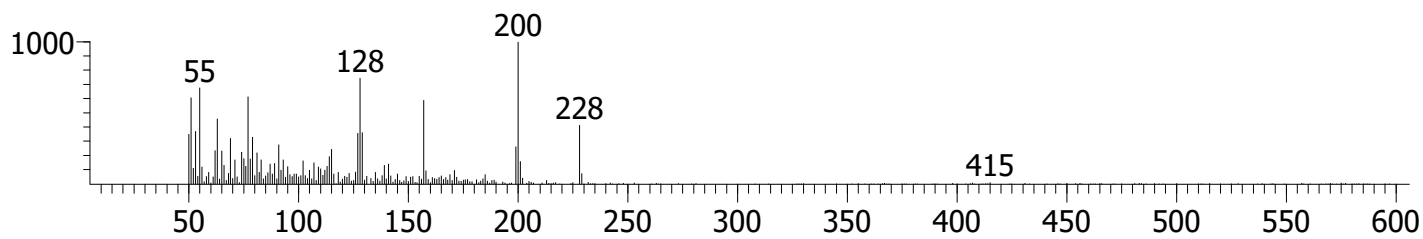
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	cis-1-(4-Isopropylphenyl)-3-(2-furyl)cyclopropane	631	3856	84922-05-4	mainlib	C16H18O	226
2	Cyclopropane, 1,1,2,2-tetramethyl-3-(2-phenylethenylideno)-	607	1292	0-00-0	mainlib	C15H18	198
3	Azulene, 1,4-dimethyl-7-(1-methylethyl)-	606	1242	489-84-9	mainlib	C15H18	198
4	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	596	876	483-78-3	mainlib	C15H18	198
5	[1,1'-Biphenyl]-2-ol, 3-(1,1-dimethylethyl)-	567	248	2416-98-0	mainlib	C16H18O	226

Trioxsalen

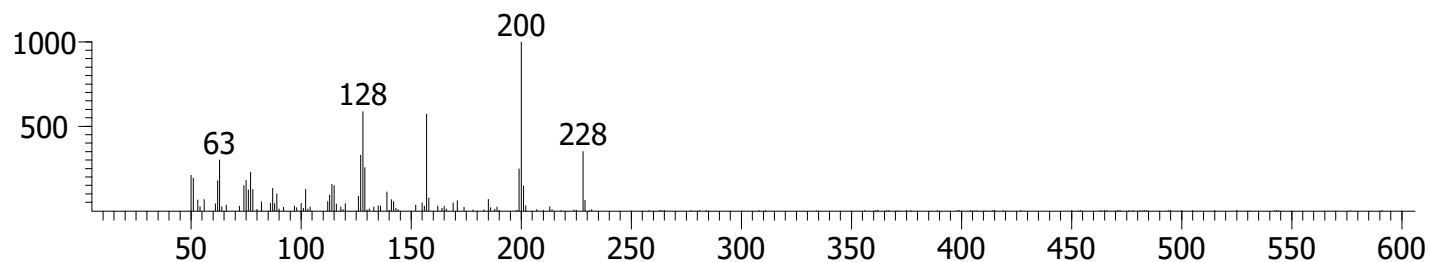
1st Dimension R.T. = 1875.7
2nd Dimension R.T. = 2.383
Quant Mass(es) = 200
S/N = 516.87
Area = 39733
Height = 3441.0
Similarity = 701



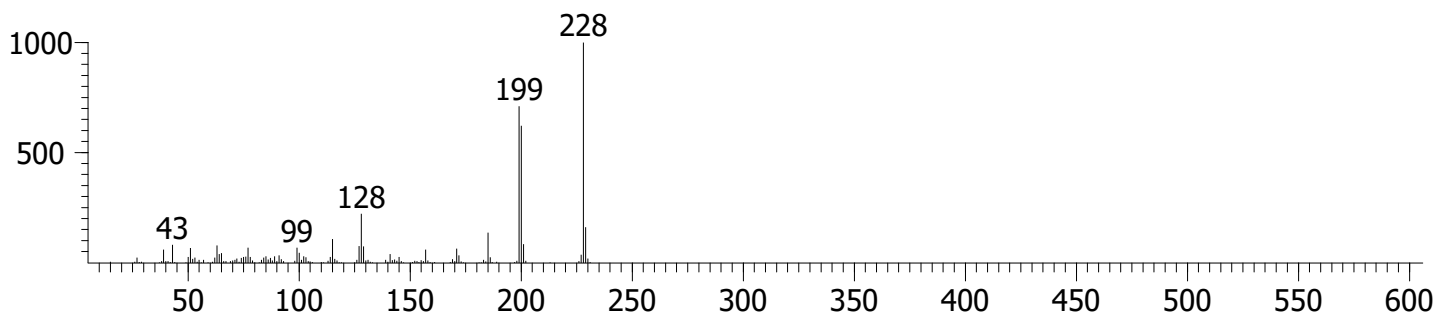
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3585, at 1875.7 , 2.383 sec , sec (Spec # 21183 1)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3585, at 1875.7 , 2.383 sec , sec (Spec # 21183 1)



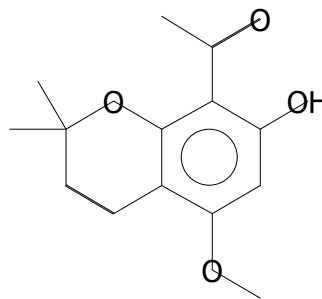
Library Hit - similarity 701, "Trioxsalen"



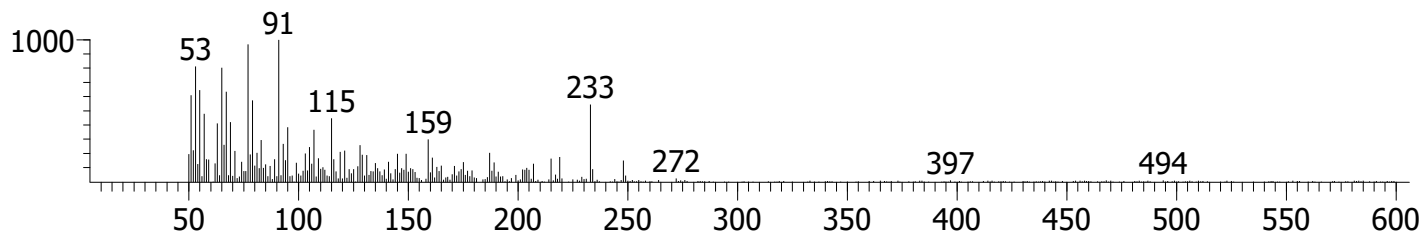
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Trioxsalen	701	1880	3902-71-4	mainlib	C14H12O3	228
2	2-(2-Methoxyphenyl)phenol	698	1661	3594-88-5	mainlib	C13H12O2	200
3	7H-Furo[3,2-g][1]benzopyran-7-one, 2,3,5-trimethyl-	692	1306	13008-11-2	mainlib	C14H12O3	228
4	Naphtho[1,2-b]furan-4,5-dione, 2,3-dihydro-3,6-dimethyl-	685	1000	23473-44-1	mainlib	C14H12O3	228
5	4-Phenyl-2-(2-oxopropyl)furan	669	576	0-00-0	mainlib	C13H12O2	200

Ethanone,
roxy-5-methoxy-2,2-dimethyl-2H-1-benzopyr

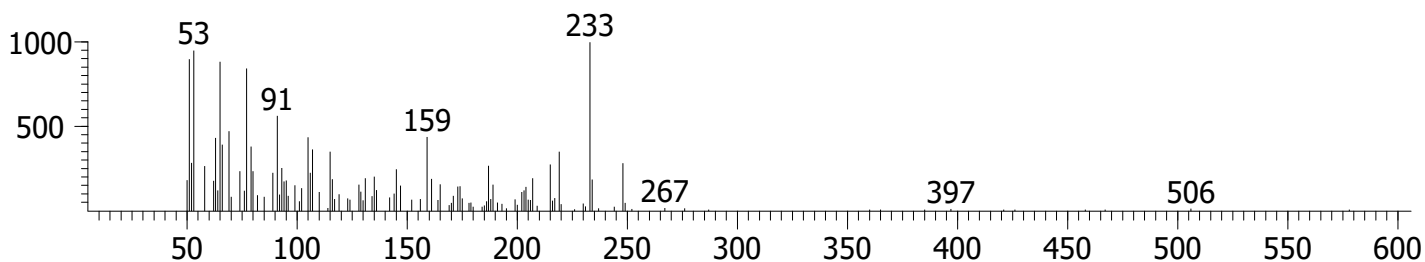
1st Dimension R.T. = 1896.69
2nd Dimension R.T. = 2.204
Quant Mass(es) = 233
S/N = 132.74
Area = 12996
Height = 1385.3
Similarity = 679



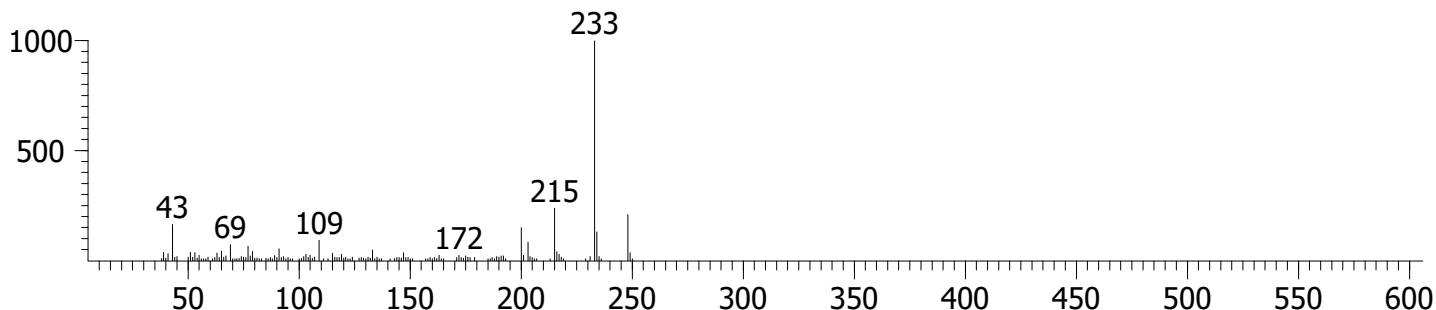
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3615, at 1896.69 , 2.204 sec , sec (Spec # 2149 84)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3615, at 1896.69 , 2.204 sec , sec (Spec # 2149 84)



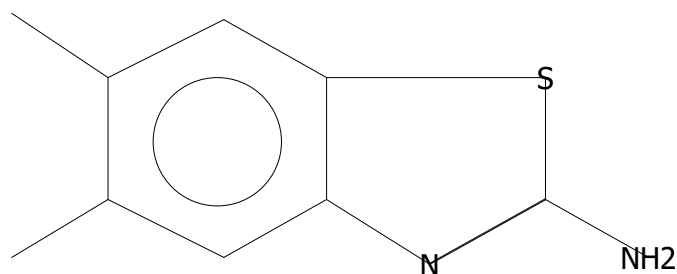
Library Hit - similarity 679, "Ethanone, 1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzopyran-8-yl)-"



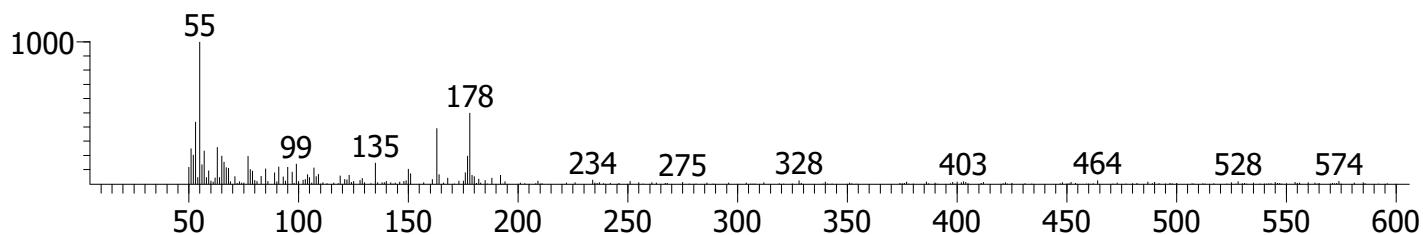
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanone, 1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzopyran-8-yl)-	679	4444	484-18-4	mainlib	C ₁₄ H ₁₆ O ₄	248
2	2,4,6-Triisopropylbenzoic acid	623	847	49623-71-4	mainlib	C ₁₆ H ₂₄ O ₂	248
3	4-(Trimethylsilyloxy)-6-methylcoumarin	612	581	0-00-0	mainlib	C ₁₃ H ₁₆ O ₃ Si	248
4	Powelline, 6-hydroxy-	595	317	31128-98-0	mainlib	C ₁₇ H ₁₉ NO ₅	317
5	1-(3,5-Di-tert-butyl-4-hydroxyphenyl)-2-bromethanone	593	292	14386-64-2	mainlib	C ₁₆ H ₂₃ BrO ₂	326

2-Benzothiazolamine, 5,6-dimethyl-

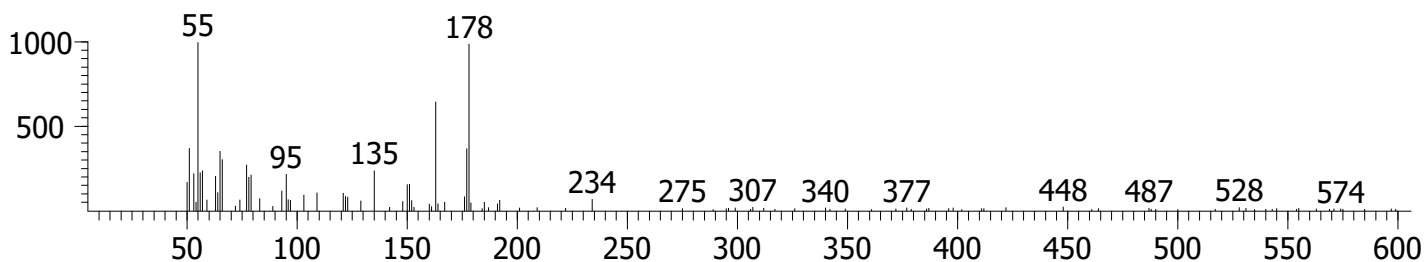
1st Dimension R.T. = 1959.65
2nd Dimension R.T. = 2.904
Quant Mass(es) = 178
S/N = 77.319
Area = 8052.9
Height = 649.93
Similarity = 645



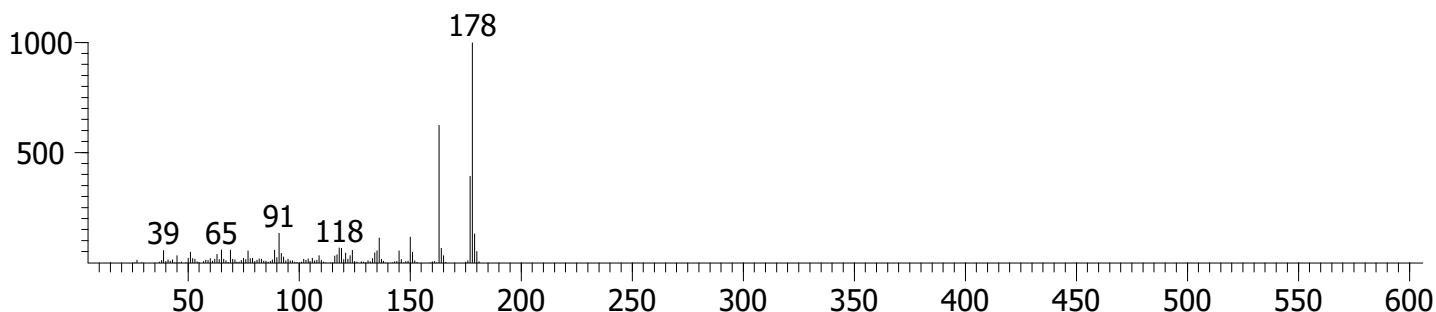
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3729, at 1959.65 , 2.904 sec , sec (Spec # 2246 30)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3729, at 1959.65 , 2.904 sec , sec (Spec # 2246 30)



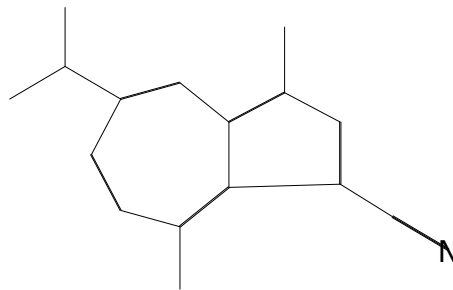
Library Hit - similarity 645, "2-Benzothiazolamine, 5,6-dimethyl-"



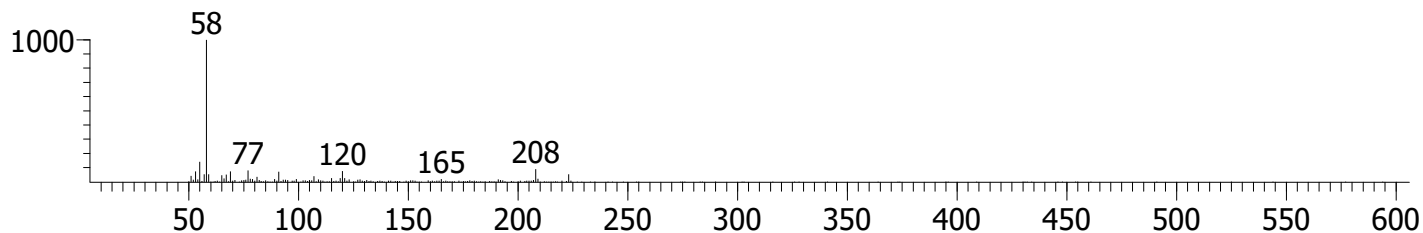
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-Benzothiazolamine, 5,6-dimethyl-	645	2293	29927-08-0	mainlib	C9H10N2S	178
2	6-Methoxy-1-methyl-1,2,3,4-tetrahydroisoquinolin-7-ol	608	558	4593-97-9	mainlib	C11H15NO2	193
3	2-Benzothiazolamine, 4,6-dimethyl-	602	438	64036-71-1	mainlib	C9H10N2S	178
4	2-Isopropylidene-5,6,7,8-tetrahydro-2H-imidazo[1,2-a]pyridin-3-one	601	421	172882-45-0	mainlib	C10H14N2O	178
5	Pyridine, 2,6-epidioxo-5-ethyl-3-iminomethyl-4-methyl-	600	405	0-00-0	mainlib	C9H10N2O2	178

i-Isopropyl-3,8-dimethylazulene-1-carbonitril

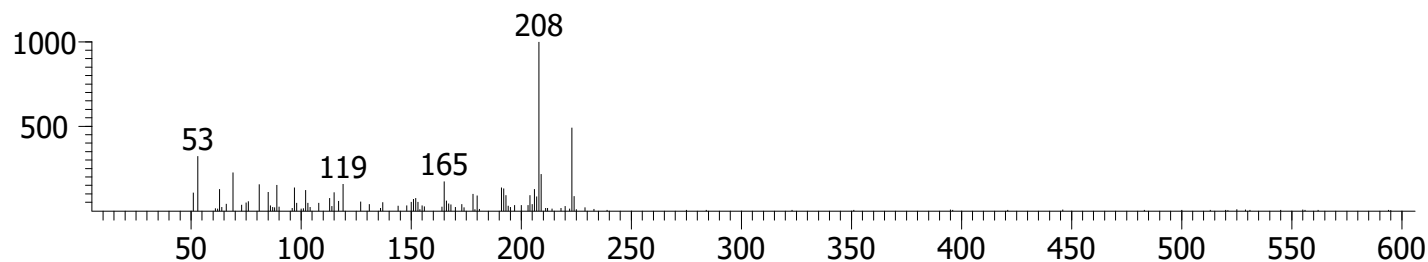
1st Dimension R.T. = 1991.14
2nd Dimension R.T. = 2.198
Quant Mass(es) = 208
S/N = 161.49
Area = 14723
Height = 1534.4
Similarity = 724



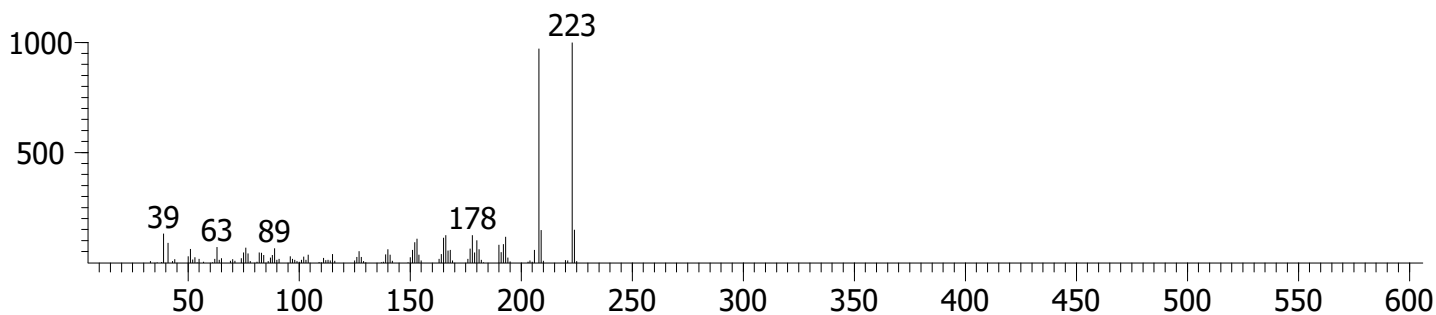
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3781, at 1991.14 , 2.198 sec , sec (Spec # 2292 93)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3781, at 1991.14 , 2.198 sec , sec (Spec # 2292 93)



Library Hit - similarity 724, "5-Isopropyl-3,8-dimethylazulene-1-carbonitrile"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-Isopropyl-3,8-dimethylazulene-1-carbonitrile	724	4733	93007-54-6	mainlib	C16H17N	223
2	Acridine, 9,10-dihydro-9,9,10-trimethyl-	707	2583	25308-77-4	mainlib	C16H17N	223
3	4-Ethyl-10H-acridin-9-one	660	540	142726-22-5	mainlib	C15H13NO	223
4	3-Acetyl-9-methylcarbazole	641	262	1484-05-5	mainlib	C15H13NO	223
5	2'-Hydroxy-6'-methoxyacetophenone, TMS derivative	628	169	0-00-0	mainlib	C12H18O3Si	238

Danthron

1st Dimension R.T. = 2005.13

2nd Dimension R.T. = 2.501

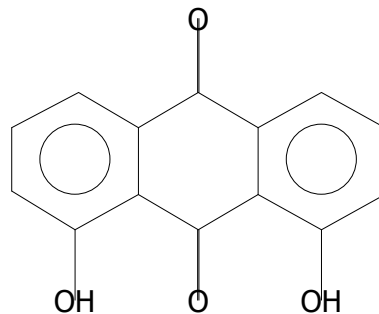
Quant Mass(es) = 240

S/N = 147.55

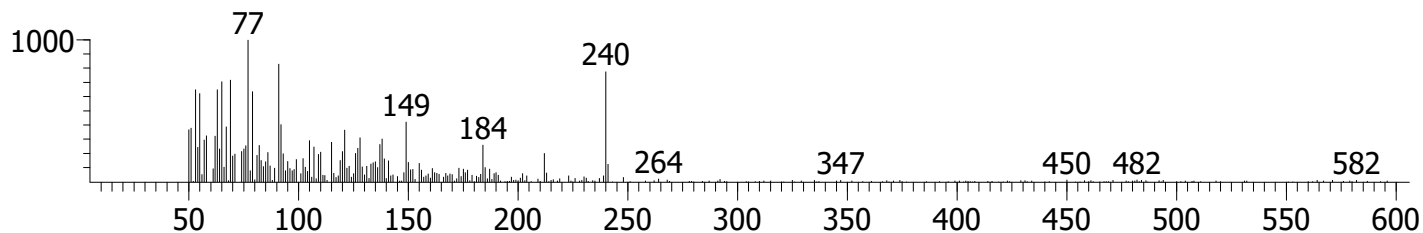
Area = 8649.8

Height = 926.39

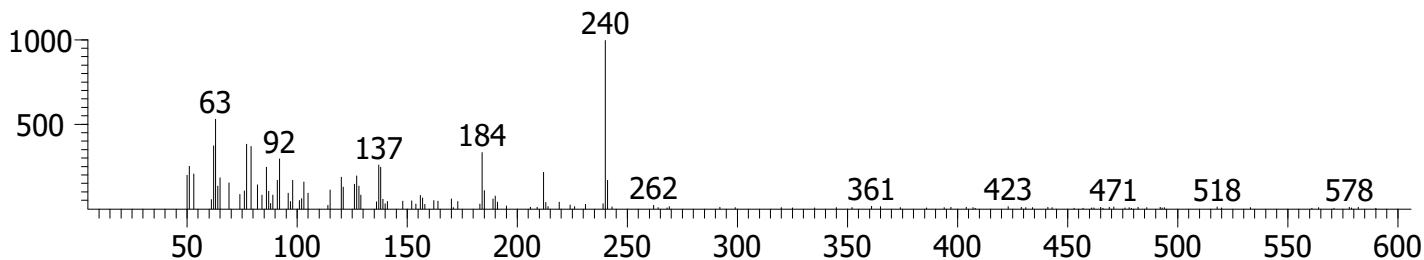
Similarity = 730



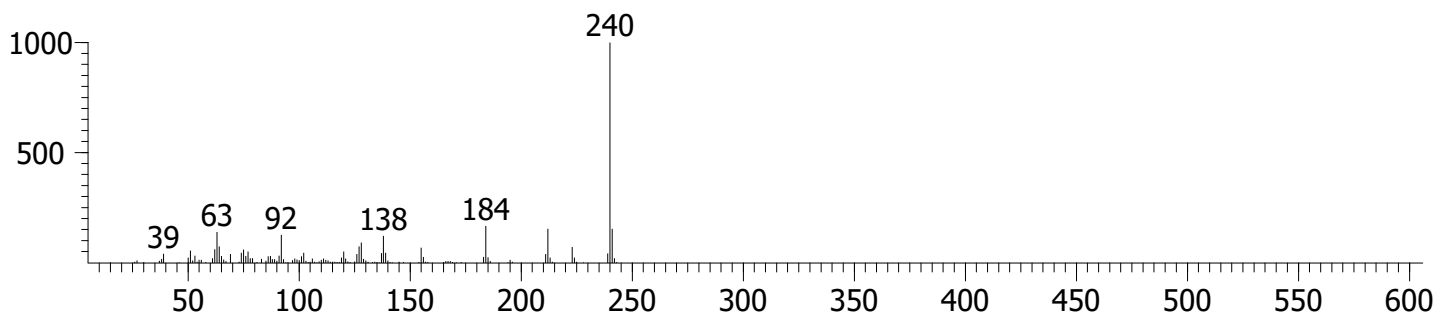
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 3802, at 2005.13 , 2.501 sec , sec (Spec # 2314 59)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 3802, at 2005.13 , 2.501 sec , sec (Spec # 2314 59)



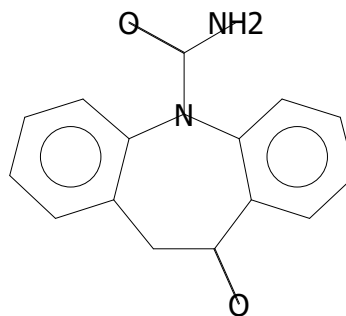
Library Hit - similarity 730, "Danthron"



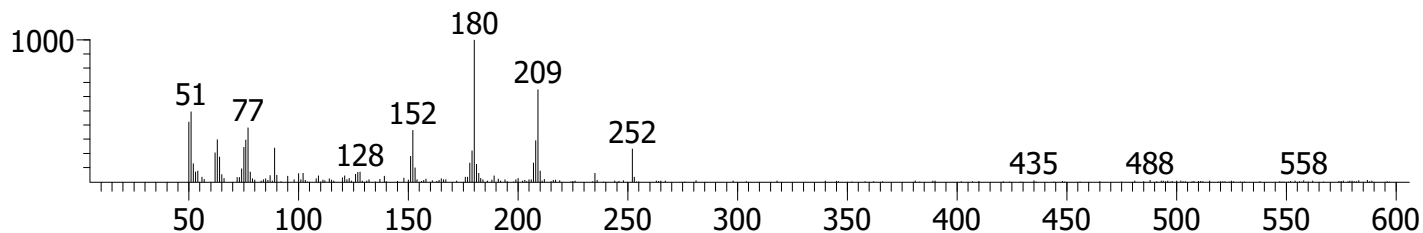
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Danthron	730	7244	117-10-2	mainlib	C14H8O4	240
2	9,10-Anthracenedione, 1,5-dihydroxy-	671	1309	117-12-4	mainlib	C14H8O4	240
3	Alizarin	644	385	72-48-0	mainlib	C14H8O4	240
4	Phenol, 2-[5-(2-furanyl)pyrazol-3-yl]-5-methyl-	626	198	84637-15-0	mainlib	C14H12N2O2	240
5	2-(4,6-Bis-ethylamino-[1,3,5]triazin-2-ylsulfanyl)-N-(2,4-dimethyl-phenyl)-acetamide	611	120	0-00-0	mainlib	C17H24N6OS	360

Oxcarbazepine

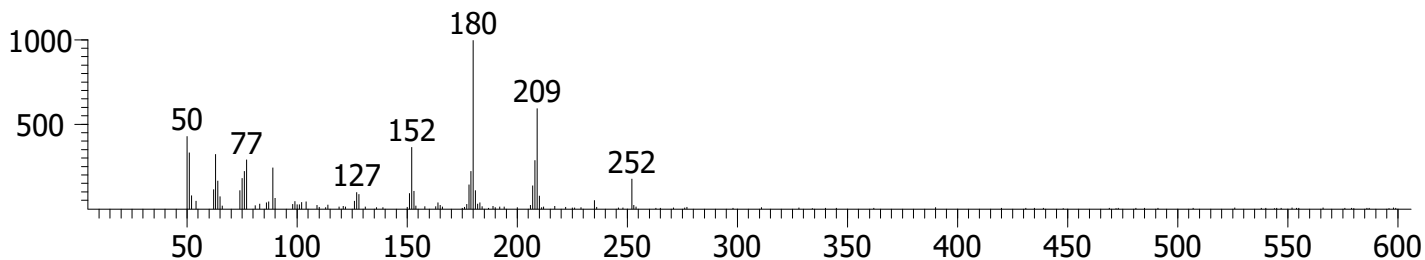
1st Dimension R.T. = 2204.51
2nd Dimension R.T. = 3.300
Quant Mass(es) = 180
S/N = 183.48
Area = 34896
Height = 2339.6
Similarity = 911



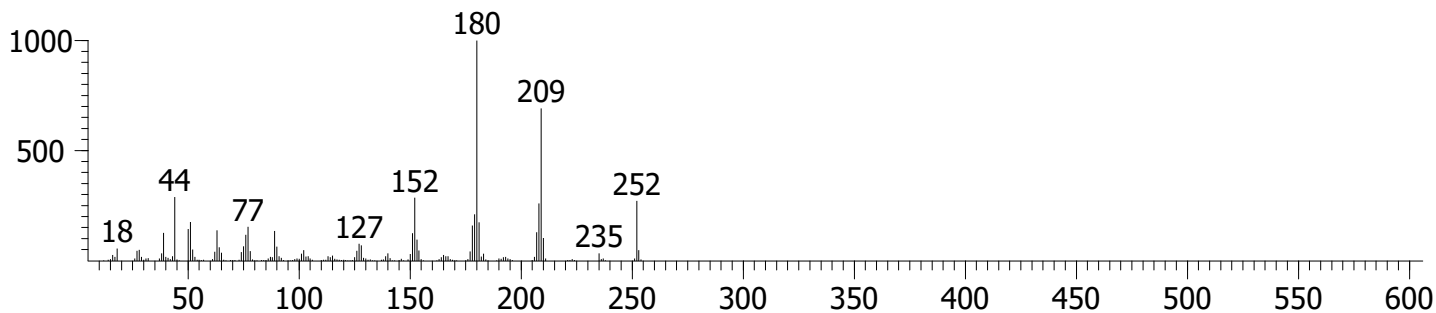
Peak Apex - sample "AerMBR B 091919 (20191119):1", peak 4079, at 2204.51 , 3.300 sec , sec (Spec # 2617 90)



Peak True - sample "AerMBR B 091919 (20191119):1", peak 4079, at 2204.51 , 3.300 sec , sec (Spec # 2617 90)



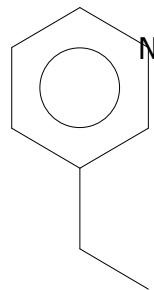
Library Hit - similarity 911, "Oxcarbazepine"



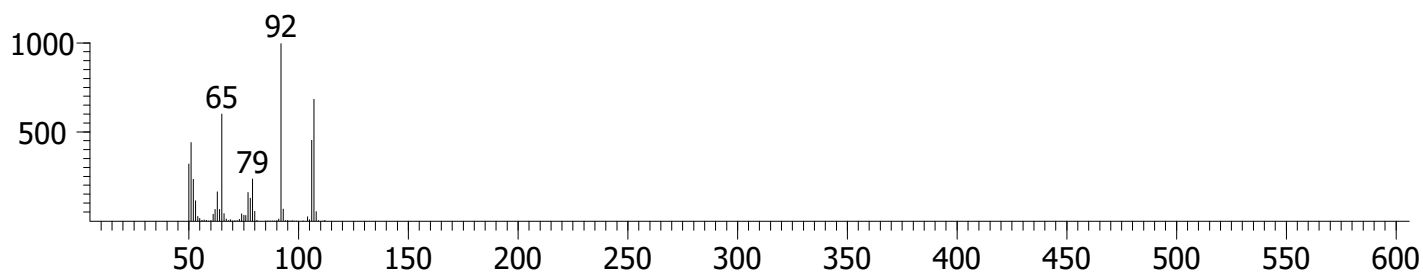
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Oxcarbazepine	911	8547	28721-07-5	mainlib	C ₁₅ H ₁₂ N ₂ O ₂	252
2	5,11-Dihydro-10H-dibenzo[b,f]azepin-10-one	827	803	21737-58-6	mainlib	C ₁₄ H ₁₁ NO	209
3	4-(2-(4-Formylphenyl)ethenyl)pyridine	797	223	74401-03-9	mainlib	C ₁₄ H ₁₁ NO	209
4	2-Methyl-acridone	783	139	23864-43-9	mainlib	C ₁₄ H ₁₁ NO	209
5	4-Methyl-acridone	775	104	68506-36-5	mainlib	C ₁₄ H ₁₁ NO	209

Pyridine, 3-ethyl-

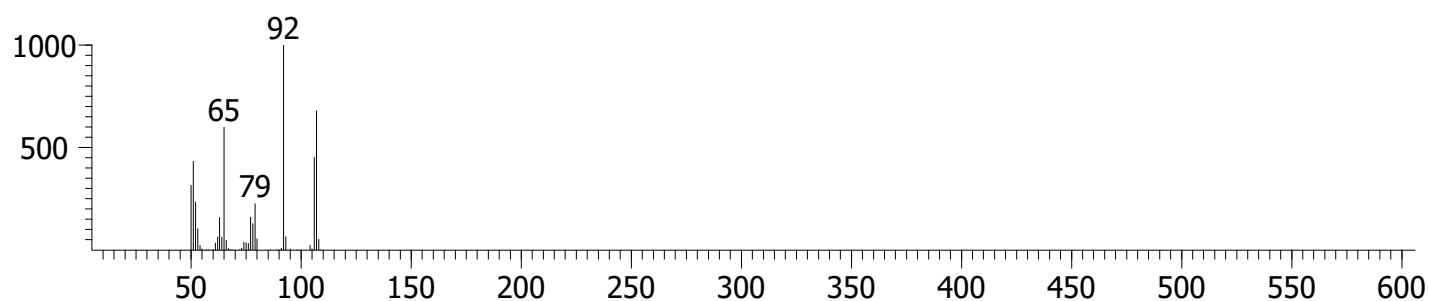
1st Dimension R.T. = 542.964
2nd Dimension R.T. = 1.492
Quant Mass(es) = 92
S/N = 4342.3
Area = 1557986
Height = 197197
Similarity = 961



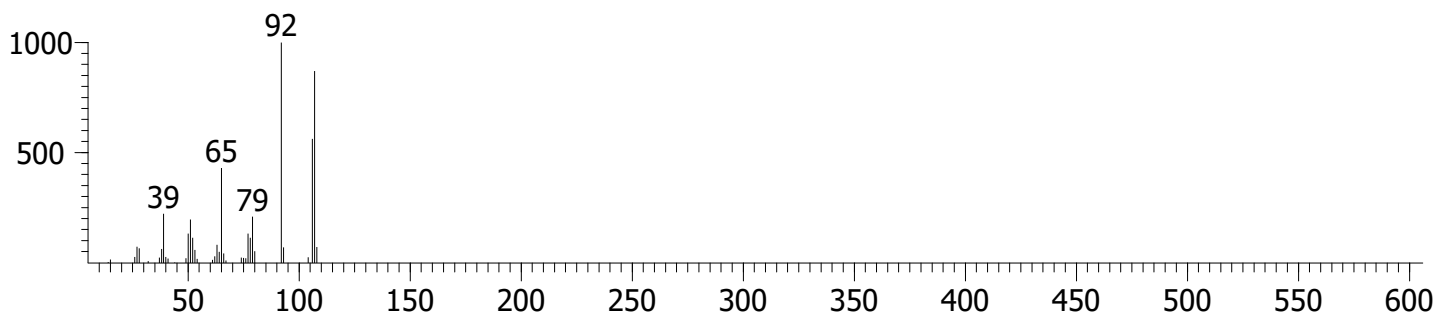
Peak Apex - sample "AnMbr C (20191120):1", peak 140, at 542.964 , 1.492 sec , sec (Spec # 9766)



Peak True - sample "AnMbr C (20191120):1", peak 140, at 542.964 , 1.492 sec , sec (Spec # 9766)



Library Hit - similarity 961, "Pyridine, 3-ethyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pyridine, 3-ethyl-	961	9150	536-78-7	mainlib	C7H9N	107
2	Pyridine, 4-ethyl-	835	405	536-75-4	mainlib	C7H9N	107
3	1,4-Dimethyl-pyridinium chloride	820	245	0-00-0	mainlib	C7H10CIN	143
4	Pyridine, 3,5-dimethyl-	776	53	591-22-0	mainlib	C7H9N	107
5	Pyridine, 3,4-dimethyl-	759	29	583-58-4	mainlib	C7H9N	107

Ethanone, 1-(3-pyridinyl)-

1st Dimension R.T. = 745.848

2nd Dimension R.T. = 1.960

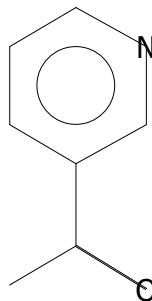
Quant Mass(es) = 106

S/N = 82.822

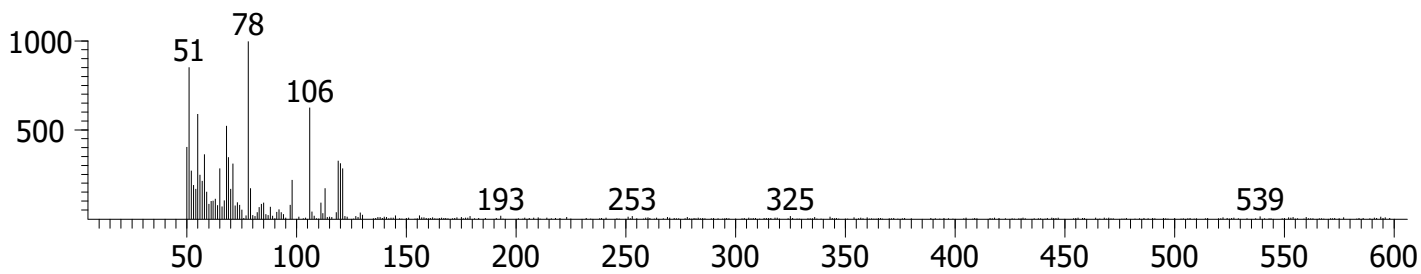
Area = 16703

Height = 2095.8

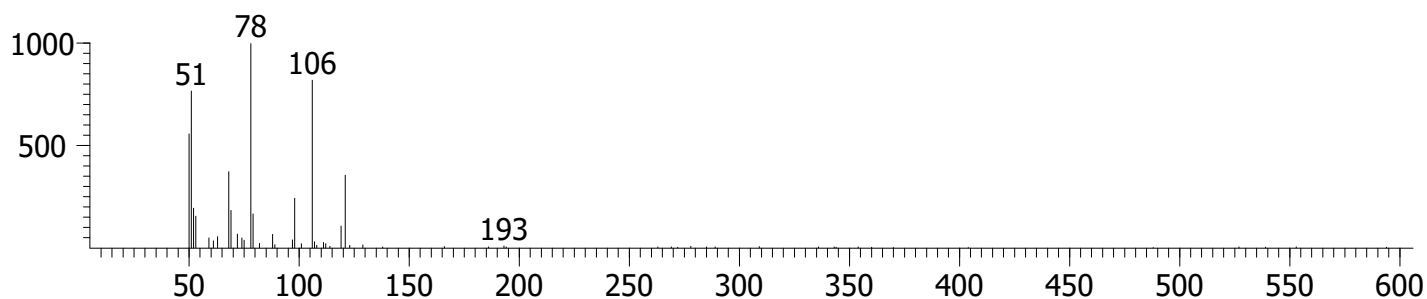
Similarity = 754



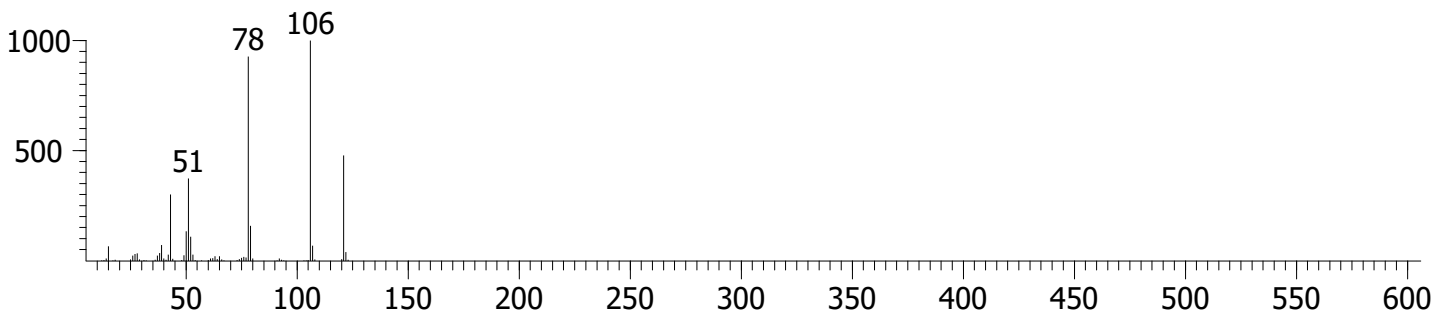
Peak Apex - sample "AnMbr C (20191120):1", peak 711, at 745.848 , 1.960 sec , sec (Spec # 40577)



Peak True - sample "AnMbr C (20191120):1", peak 711, at 745.848 , 1.960 sec , sec (Spec # 40577)



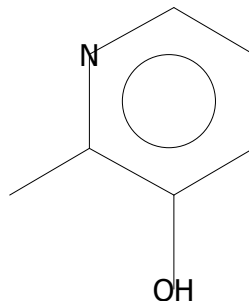
Library Hit - similarity 754, "Ethanone, 1-(3-pyridinyl)-"



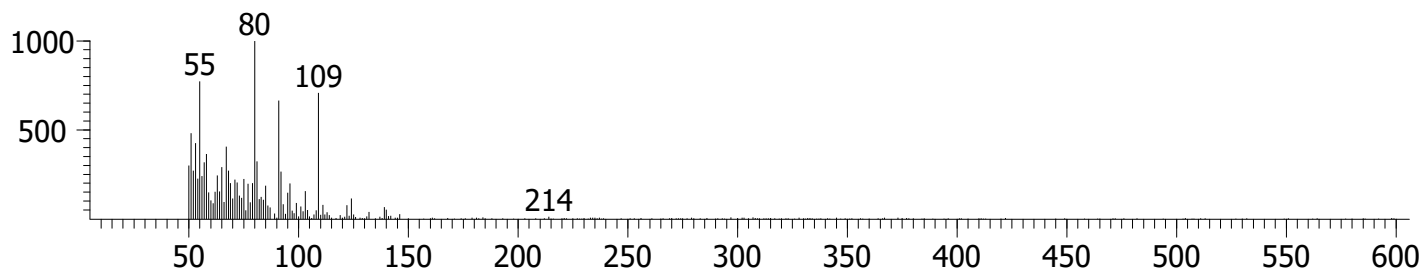
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Ethanone, 1-(3-pyridinyl)-	754	6834	350-03-8	mainlib	C7H7NO	121
2	N'-(3,4-Dihydroxybenzylidene)-3-pyridinohydrazide	683	973	315207-10-4	mainlib	C13H11N3O3	257
3	3-Pyridinecarboxamide, N-[5-phenyl-4-(trifluoromethyl)-2-thiazolyl]-	657	291	0-00-0	mainlib	C16H10F3N3OS	349
4	Butanoic acid, 2-acetyl-4,4,4-trifluoro-3-trifluoromethyl-3-(3-pyridylcarbonylamino)-	647	205	0-00-0	mainlib	C15H14F6N2O4	400
5	N-(3-Methoxy-5-tetrazol-1-yl-phenyl)-isonicotinamide	640	157	0-00-0	mainlib	C14H12N6O2	296

3-Pyridinol, 2-methyl-

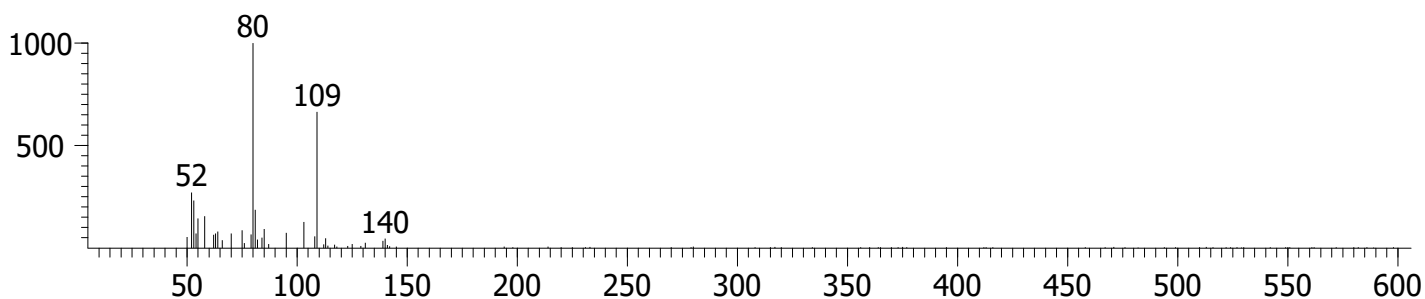
1st Dimension R.T. = 777.33
2nd Dimension R.T. = 1.769
Quant Mass(es) = 80
S/N = 130.57
Area = 64125
Height = 7156.2
Similarity = 746



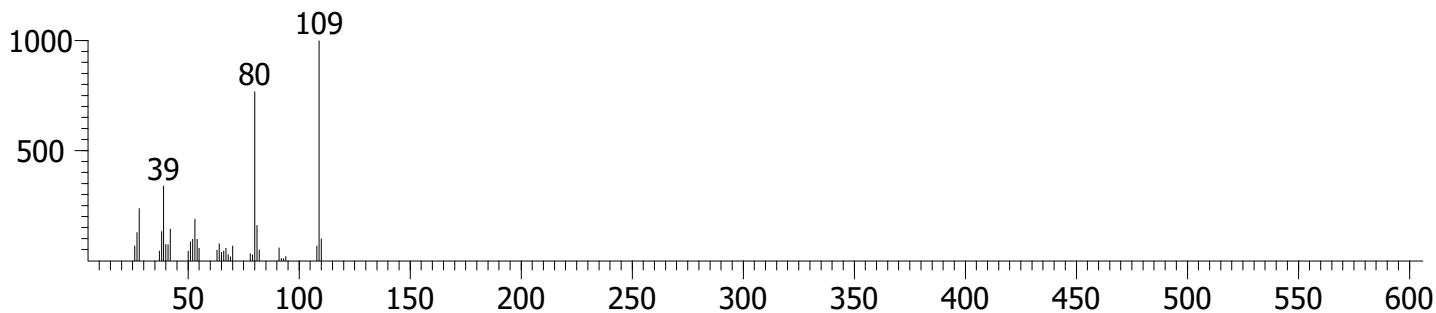
Peak Apex - sample "AnMbr C (20191120):1", peak 798, at 777.33 , 1.769 sec , sec (Spec # 45318)



Peak True - sample "AnMbr C (20191120):1", peak 798, at 777.33 , 1.769 sec , sec (Spec # 45318)



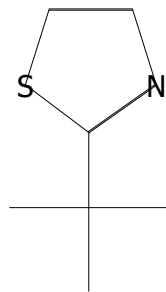
Library Hit - similarity 746, "3-Pyridinol, 2-methyl-"



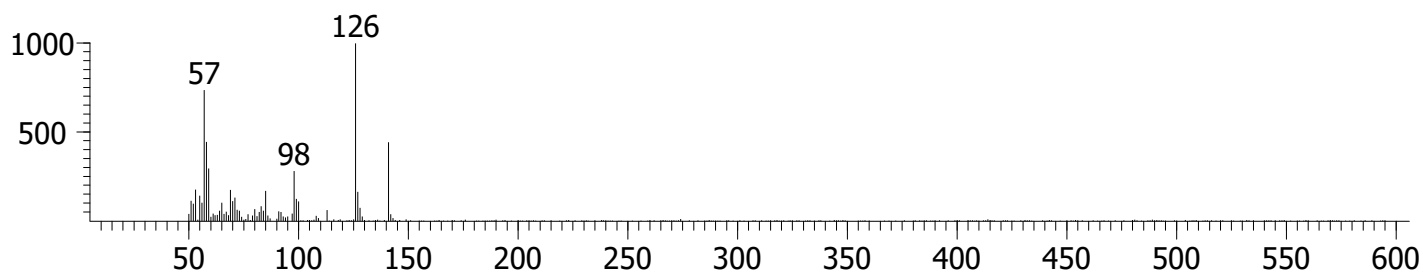
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	3-Pyridinol, 2-methyl-	746	4612	1121-25-1	mainlib	C6H7NO	109
2	2(1H)-Pyridinone, 3-methyl-	723	1684	1003-56-1	mainlib	C6H7NO	109
3	2(1H)-Pyridinone, 5-methyl-	717	1323	1003-68-5	mainlib	C6H7NO	109
4	Phenol, 4-amino-	698	642	123-30-8	mainlib	C6H7NO	109
5	3-Pyridinol, 6-methyl-	691	492	1121-78-4	mainlib	C6H7NO	109

2-tert-Butylthiazole

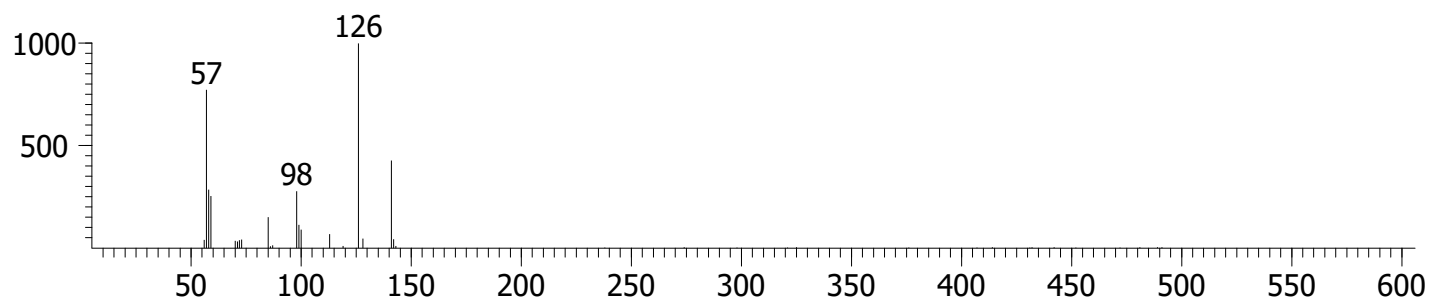
1st Dimension R.T. = 780.828
2nd Dimension R.T. = 1.881
Quant Mass(es) = 126
S/N = 346.15
Area = 35224
Height = 4054.0
Similarity = 636



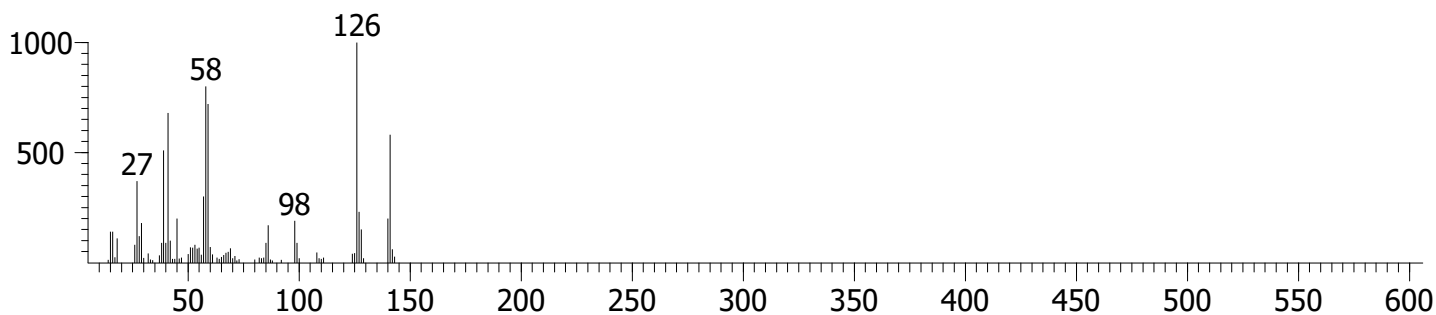
Peak Apex - sample "AnMbr C (20191120):1", peak 811, at 780.828 , 1.881 sec , sec (Spec # 45865)



Peak True - sample "AnMbr C (20191120):1", peak 811, at 780.828 , 1.881 sec , sec (Spec # 45865)



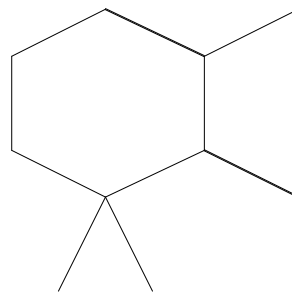
Library Hit - similarity 636, "2-tert-Butylthiazole"



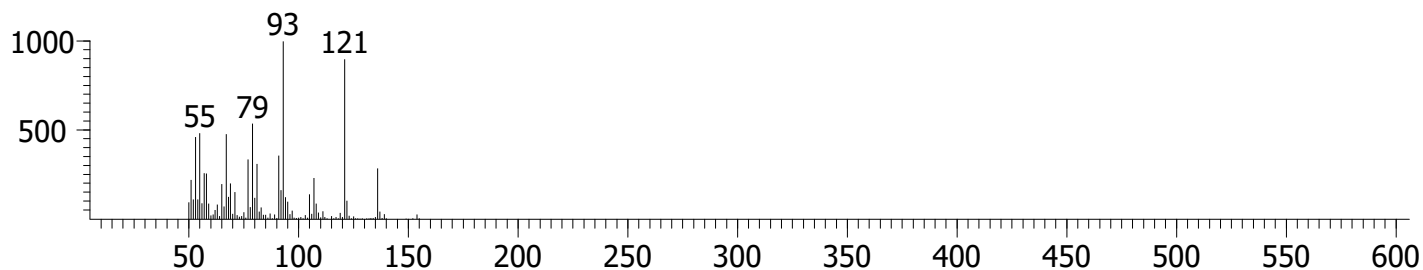
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-tert-Butylthiazole	636	2556	13623-12-6	mainlib	C7H11NS	141
2	3-Fluoro-p-anisidine	618	1318	366-99-4	mainlib	C7H8FNO	141
3	1,6-Heptadien-4-ol, (3-cyanopropyl)dimethylsilyl ether	604	825	0-00-0	mainlib	C13H23NOSi	237
4	Thiazole, 2-methyl-4-(1-methylethyl)-	603	793	32272-52-9	mainlib	C7H11NS	141
5	3-Fluoro-o-anisidine	594	575	437-83-2	mainlib	C7H8FNO	141

1,5,5-Trimethyl-6-methylene-cyclohexene

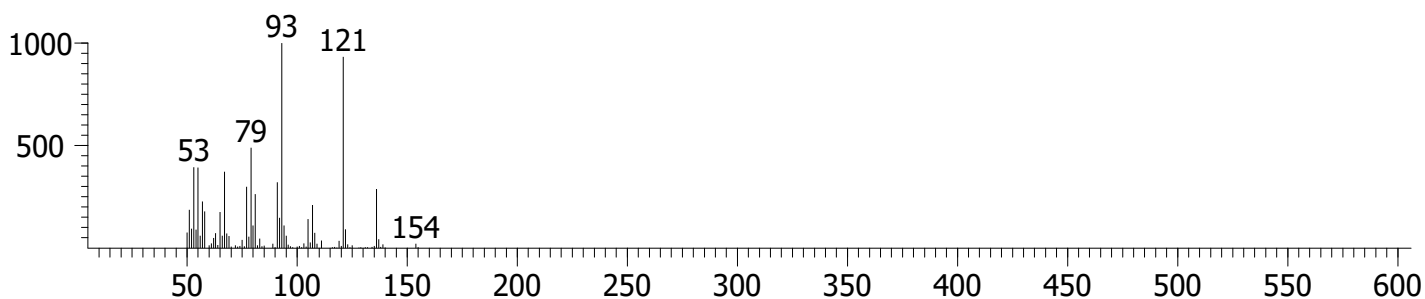
1st Dimension R.T. = 868.278
2nd Dimension R.T. = 1.525
Quant Mass(es) = 121
S/N = 4487.1
Area = 953005
Height = 121471
Similarity = 870



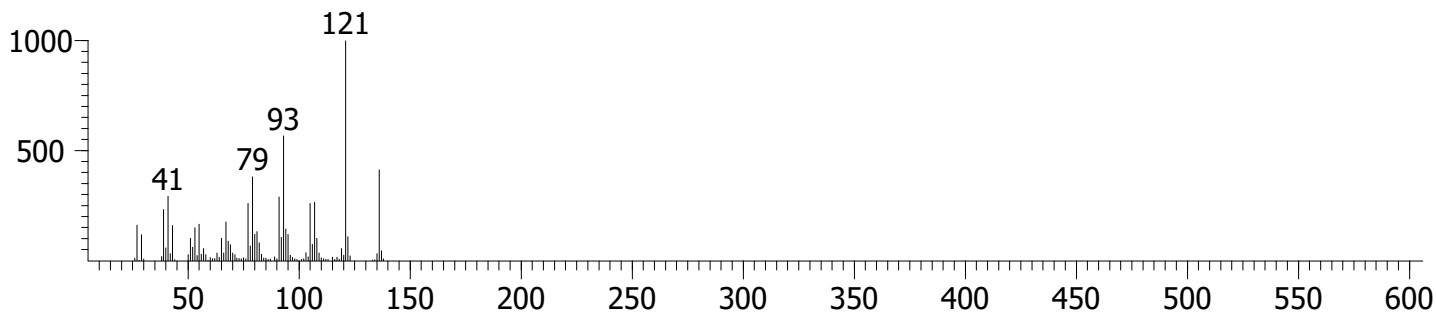
Peak Apex - sample "AnMbr C (20191120):1", peak 1145, at 868.278 , 1.525 sec , sec (Spec # 59061)



Peak True - sample "AnMbr C (20191120):1", peak 1145, at 868.278 , 1.525 sec , sec (Spec # 59061)



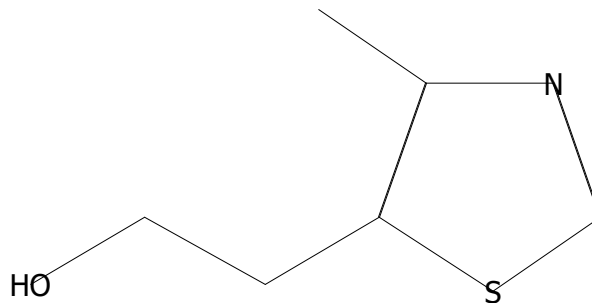
Library Hit - similarity 870, "1,5,5-Trimethyl-6-methylene-cyclohexene"



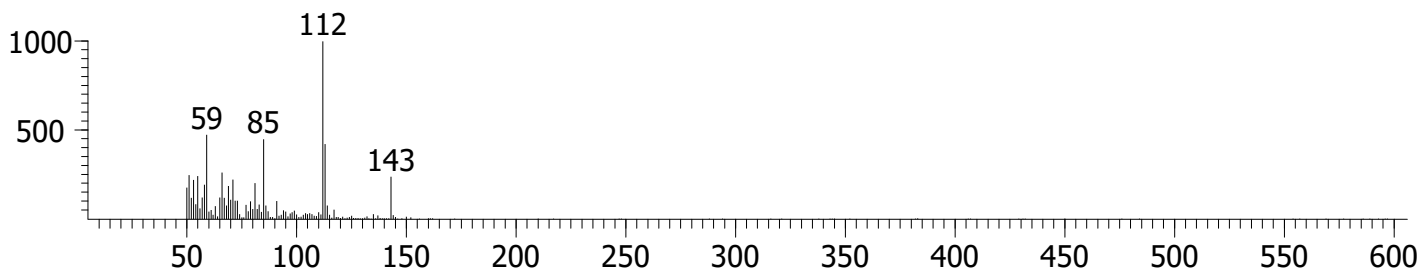
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	1,5,5-Trimethyl-6-methylene-cyclohexene	870	1131	514-95-4	mainlib	C10H16	136
2	Bicyclo[3.1.0]hexane, 6-isopropylidene-1-methyl-	869	1087	24524-57-0	mainlib	C10H16	136
3	Camphene	860	789	79-92-5	mainlib	C10H16	136
4	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, (1S)-	843	430	5794-04-7	mainlib	C10H16	136
5	(1R,3S,4R,5S)-1-Isopropyl-4-methylbicyclo[3.1.0]hexan-3-yl acetate-rel-	841	397	62181-91-3	mainlib	C12H20O2	196

5-Thiazoleethanol, 4-methyl-

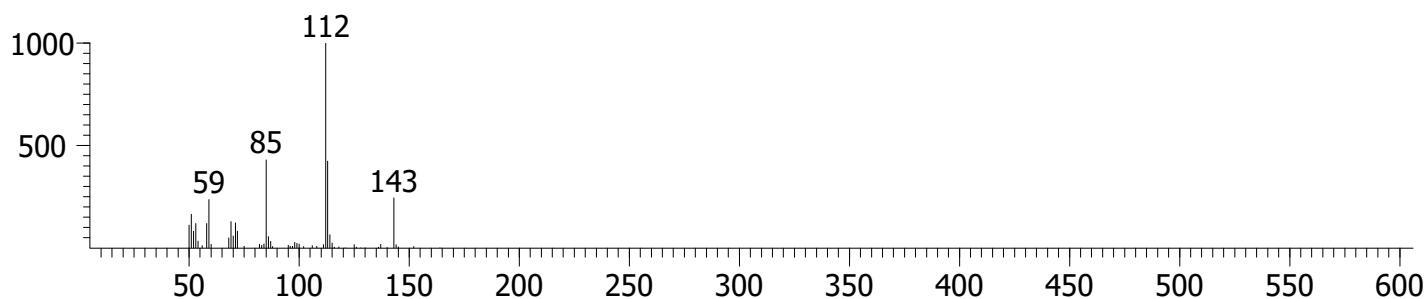
1st Dimension R.T. = 997.704
2nd Dimension R.T. = 2.059
Quant Mass(es) = 112
S/N = 1351.2
Area = 605519
Height = 62086
Similarity = 882



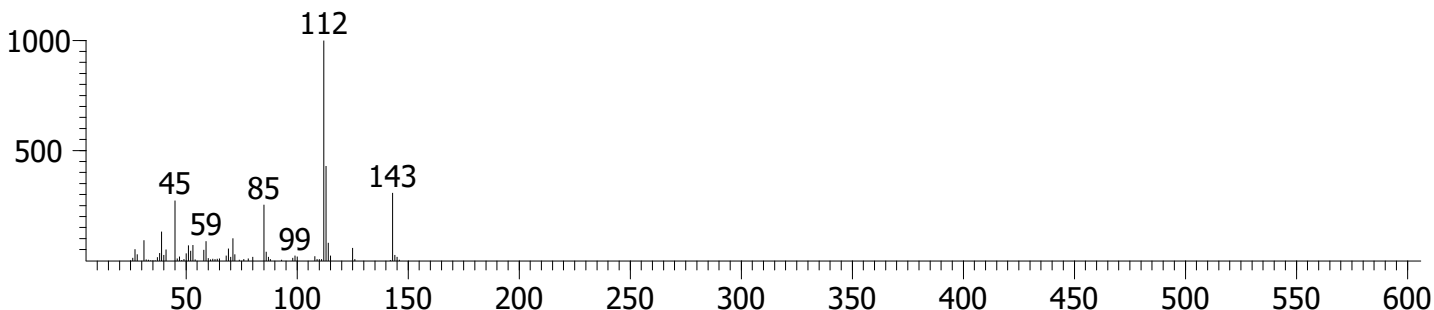
Peak Apex - sample "AnMbr C (20191120):1", peak 1776, at 997.704 , 2.059 sec , sec (Spec # 78752)



Peak True - sample "AnMbr C (20191120):1", peak 1776, at 997.704 , 2.059 sec , sec (Spec # 78752)



Library Hit - similarity 882, "5-Thiazoleethanol, 4-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-Thiazoleethanol, 4-methyl-	882	9434	137-00-8	mainlib	C6H9NOS	143
2	5-Thiazoleacetaldehyde, 4-methyl-	754	404	18764-34-6	mainlib	C6H7NOS	141
3	4-(Chloromethyl)-5-methyl-1,3-thiazole	668	36	0-00-0	mainlib	C5H6ClNS	147
4	5-Methylthiophen-3-ylamine	667	34	0-00-0	mainlib	C5H7NS	113
5	2-Thiophenemethanamine	662	27	27757-85-3	mainlib	C5H7NS	113

(R)-(+)-Citronellic acid

1st Dimension R.T. = 1015.19

2nd Dimension R.T. = 1.505

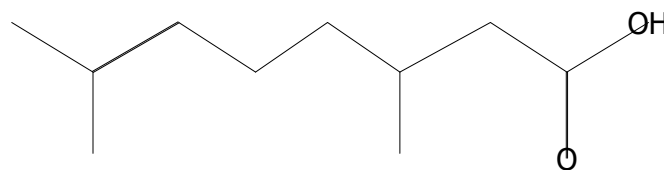
Quant Mass(es) = 69

S/N = 816.33

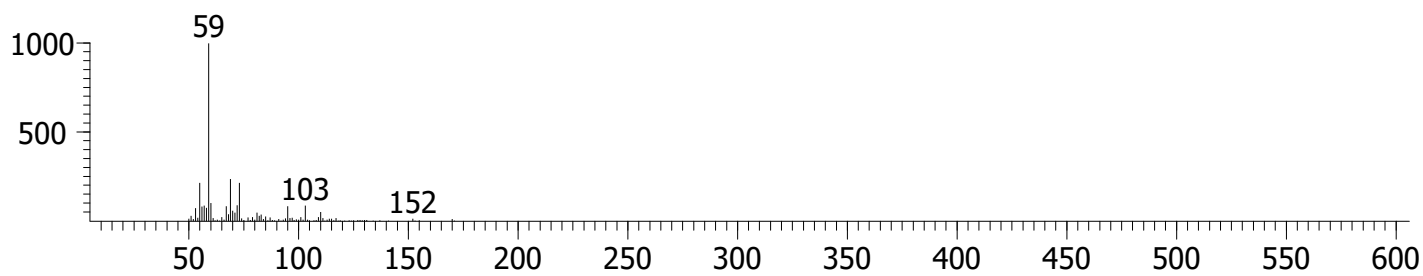
Area = 1334122

Height = 105735

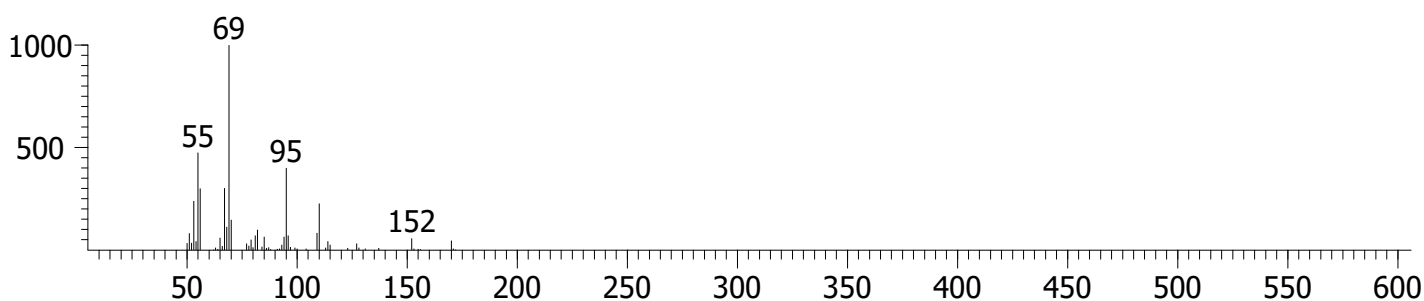
Similarity = 834



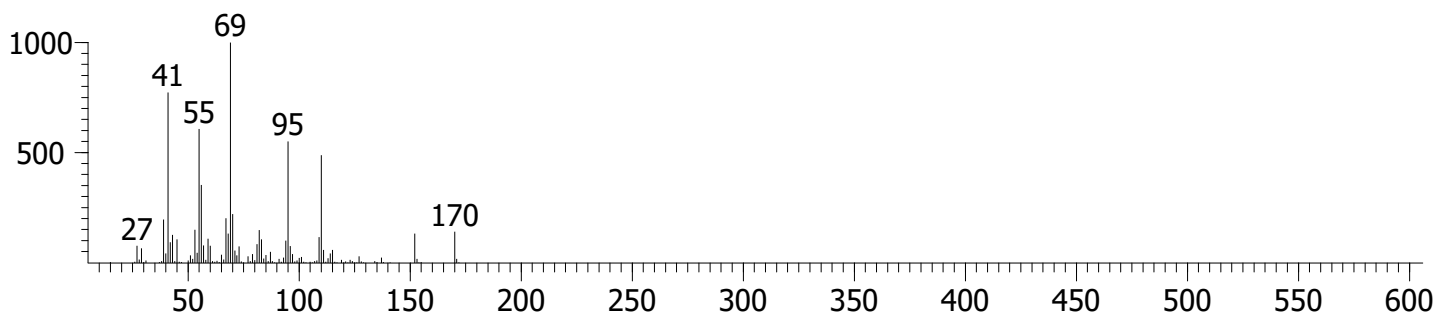
Peak Apex - sample "AnMbr C (20191120):1", peak 1854, at 1015.19 , 1.505 sec , sec (Spec # 81318)



Peak True - sample "AnMbr C (20191120):1", peak 1854, at 1015.19 , 1.505 sec , sec (Spec # 81318)



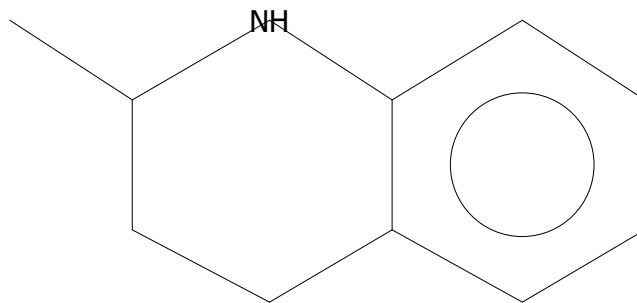
Library Hit - similarity 834, "(R)-(+)-Citronellic acid"



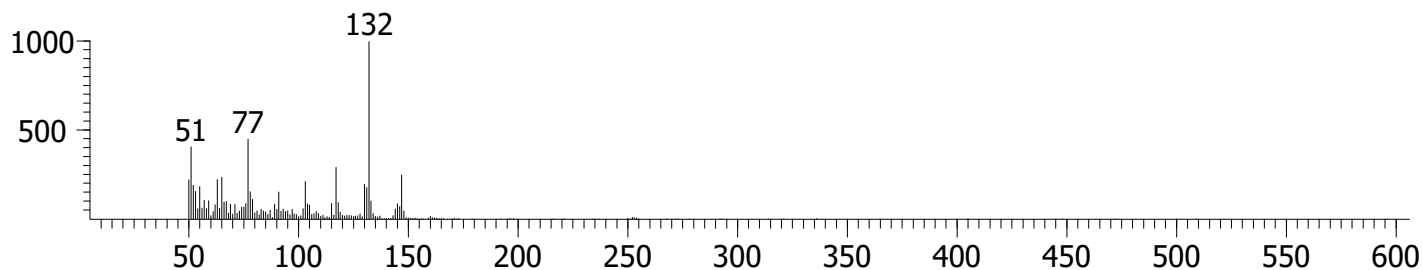
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	(R)-(+)-Citronellic acid	834	3426	18951-85-4	mainlib	C10H18O2	170
2	6-Octenoic acid, 3,7-dimethyl-	831	3027	502-47-6	mainlib	C10H18O2	170
3	6-Octenoic acid, 3,7-dimethyl-, methyl ester	752	345	2270-60-2	mainlib	C11H20O2	184
4	1,5-Heptadiene, 2,3,6-trimethyl-	736	198	33501-88-1	mainlib	C10H18	138
5	2-Octene, 2-methyl-6-methylene-	736	198	10054-09-8	mainlib	C10H18	138

Quinoline, 1,2,3,4-tetrahydro-2-methyl-

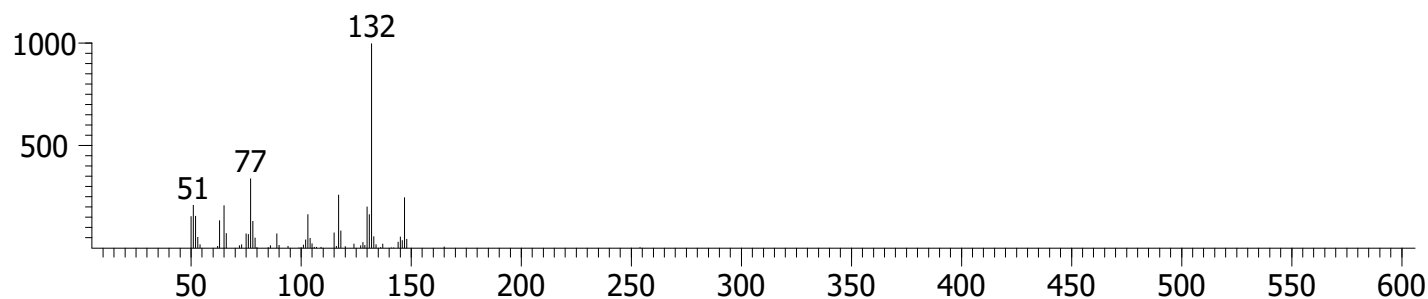
1st Dimension R.T. = 1088.65
2nd Dimension R.T. = 1.927
Quant Mass(es) = 132
S/N = 1847.6
Area = 224373
Height = 26873
Similarity = 795



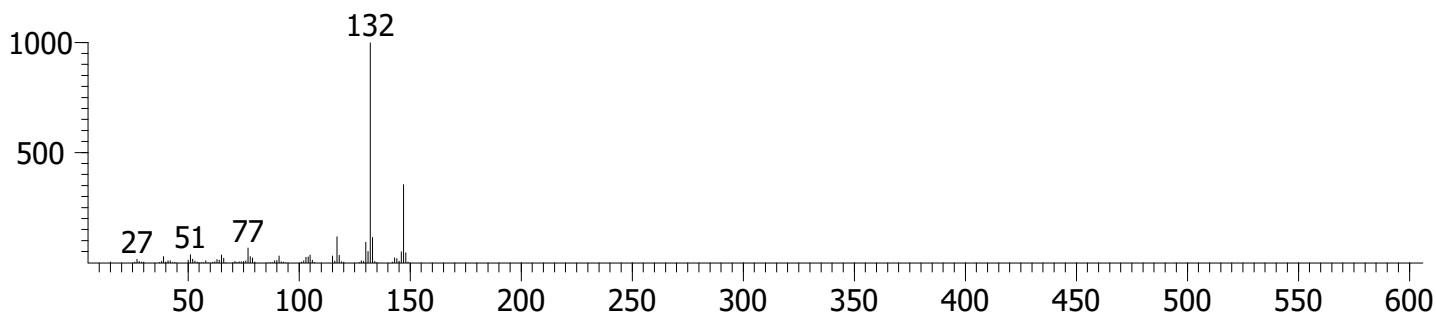
Peak Apex - sample "AnMbr C (20191120):1", peak 2249, at 1088.65 , 1.927 sec , sec (Spec # 92512)



Peak True - sample "AnMbr C (20191120):1", peak 2249, at 1088.65 , 1.927 sec , sec (Spec # 92512)

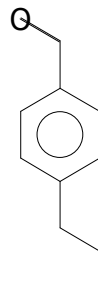


Library Hit - similarity 795, "Quinoline, 1,2,3,4-tetrahydro-2-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Quinoline, 1,2,3,4-tetrahydro-2-methyl-	795	4340	1780-19-4	mainlib	C10H13N	147
2	Isoquinoline, 1,2,3,4-tetrahydro-1-methyl-	766	1230	4965-09-7	mainlib	C10H13N	147
3	1H-Indole, 2,3-dihydro-1,2-dimethyl-	747	597	26216-93-3	mainlib	C10H13N	147
4	2-(1-Methylcyclopropyl)aniline	731	344	71759-33-6	mainlib	C10H13N	147
5	Sulfone, (1,2,3,4-tetrahydroquinol-1-yl)(4-nitrophenyl)-	730	330	0-00-0	mainlib	C15H14N2O4S	318

Benzaldehyde, 4-propyl-



1st Dimension R.T. = 1239.07

2nd Dimension R.T. = 2.310

Quant Mass(es) = 119

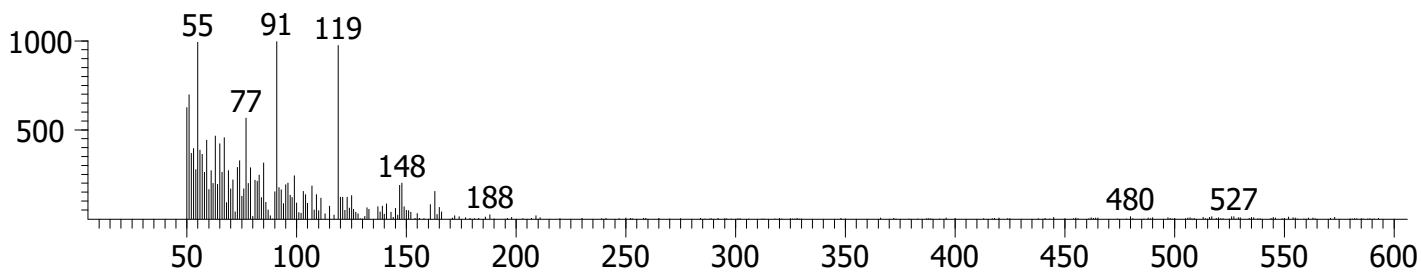
S/N = 84.279

Area = 14563

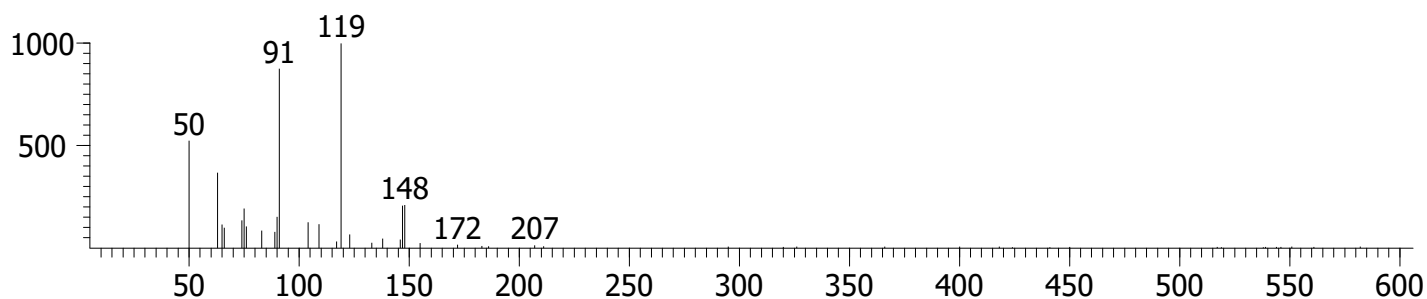
Height = 1483.5

Similarity = 706

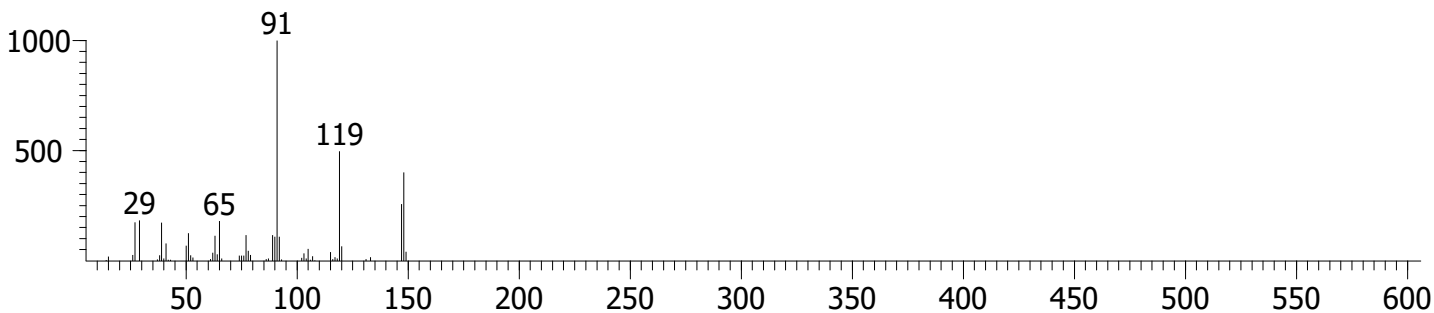
Peak Apex - sample "AnMbr C (20191120):1", peak 3109, at 1239.07 , 2.310 sec , sec (Spec # 115360)



Peak True - sample "AnMbr C (20191120):1", peak 3109, at 1239.07 , 2.310 sec , sec (Spec # 115360)



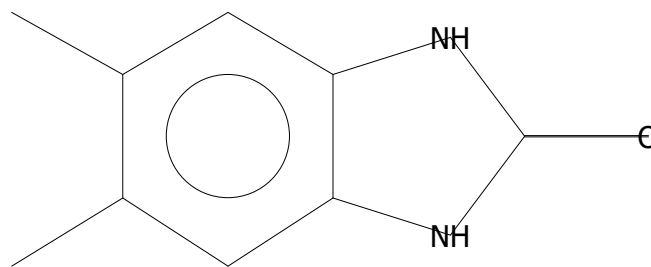
Library Hit - similarity 706, "Benzaldehyde, 4-propyl-"



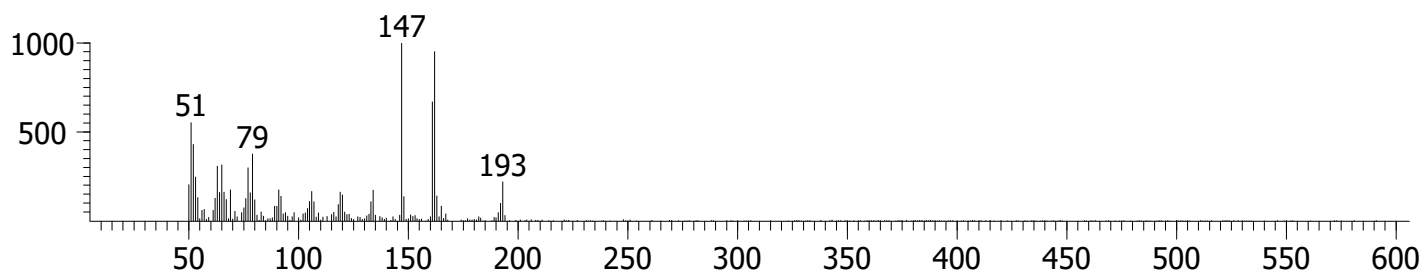
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Benzaldehyde, 4-propyl-	706	3888	28785-06-0	mainlib	C10H12O	148
2	1(3H)-Isobenzofuranone, 5-methyl-	681	1185	54120-64-8	mainlib	C9H8O2	148
3	4-Methylphthalaldehyde	668	766	15158-36-8	mainlib	C9H8O2	148
4	benz[d]isoxazole, 3-ethyl-	647	325	66033-77-0	mainlib	C9H9NO	147
5	Propiophenone, 2'-methyl-	636	223	2040-14-4	mainlib	C10H12O	148

5,6-Dimethyl-2-benzimidazolinone

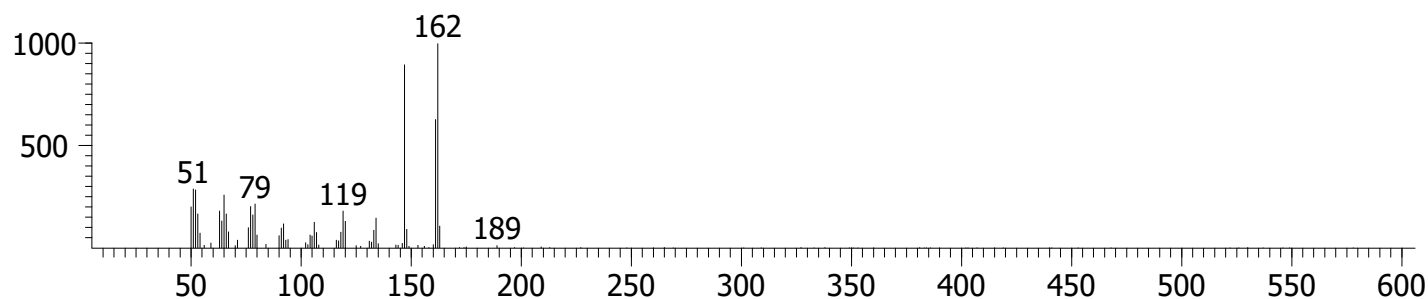
1st Dimension R.T. = 1798.75
2nd Dimension R.T. = 2.660
Quant Mass(es) = 162
S/N = 304.06
Area = 233498
Height = 19304
Similarity = 908



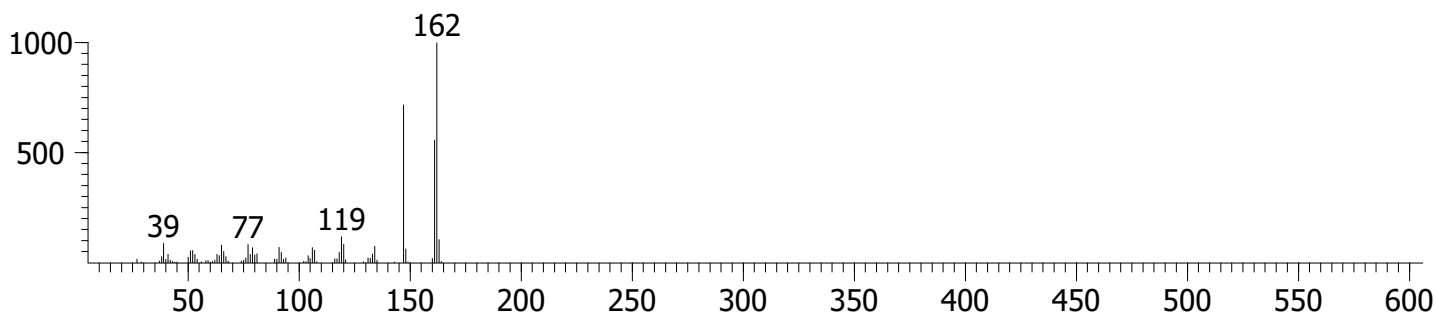
Peak Apex - sample "AnMbr C (20191120):1", peak 6214, at 1798.75 , 2.660 sec , sec (Spec # 200213)



Peak True - sample "AnMbr C (20191120):1", peak 6214, at 1798.75 , 2.660 sec , sec (Spec # 200213)



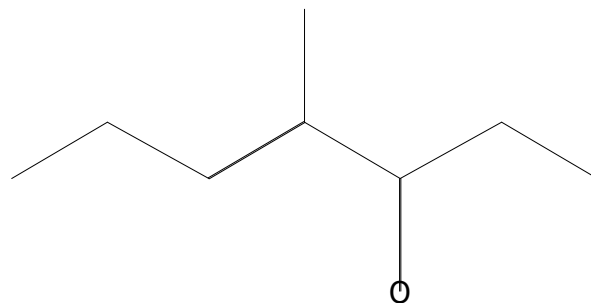
Library Hit - similarity 908, "5,6-Dimethyl-2-benzimidazolinone"



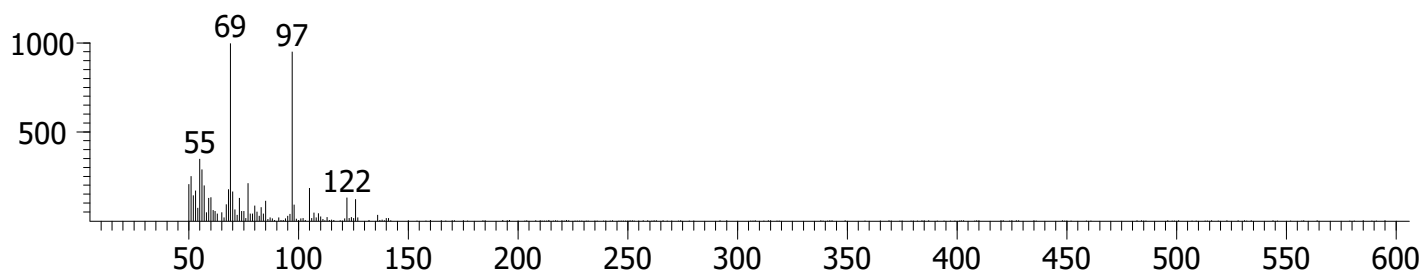
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5,6-Dimethyl-2-benzimidazolinone	908	8184	2033-30-9	mainlib	C9H10N2O	162
2	3-(1-Methylethyl)(1H)pyrazolo[3,4-b]pyrazine	774	316	0-00-0	mainlib	C8H10N4	162
3	Pyrazine, trimethyl-1-propenyl-, (E)-	769	255	55138-79-9	mainlib	C10H14N2	162
4	Pyrazine, trimethyl-1-propenyl-, (Z)-	753	147	55138-75-5	mainlib	C10H14N2	162
5	5-Hydroxy-3-methyl-1-indanone	753	147	57878-30-5	mainlib	C10H10O2	162

4-Hepten-3-one, 4-methyl-

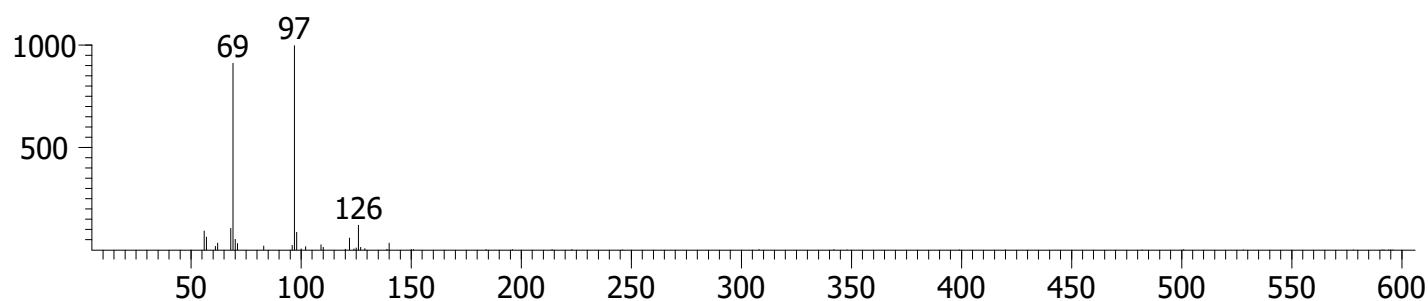
1st Dimension R.T. = 829.8
2nd Dimension R.T. = 2.013
Quant Mass(es) = 97
S/N = 174.87
Area = 52435
Height = 6411.6
Similarity = 828



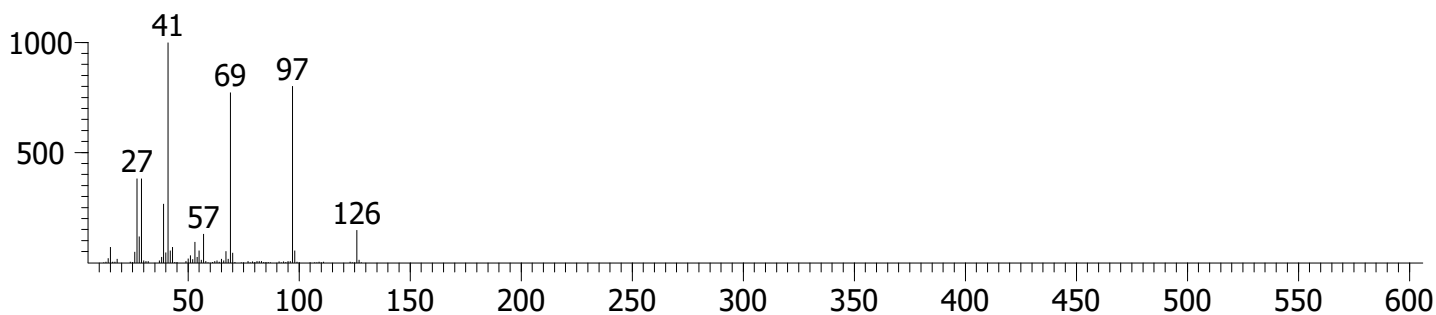
Peak Apex - sample "AnBxr B (20191121):1", peak 1155, at 829.8 , 2.013 sec , sec (Spec # 53305)



Peak True - sample "AnBxr B (20191121):1", peak 1155, at 829.8 , 2.013 sec , sec (Spec # 53305)



Library Hit - similarity 828, "4-Hepten-3-one, 4-methyl-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4-Hepten-3-one, 4-methyl-	828	5111	22319-31-9	mainlib	C ₈ H ₁₄ O	126
2	1-(Cyclopentylcarbonyl)-4-piperidinamine	827	5700	926234-06-2	nist_msms	C ₁₁ H ₂₀ N ₂ O	196
3	4-Hexen-3-one, 4,5-dimethyl-	803	1558	17325-90-5	mainlib	C ₈ H ₁₄ O	126
4	1-(Cyclopentylcarbonyl)-4-piperidinamine	796	5700	926234-06-2	nist_msms	C ₁₁ H ₂₀ N ₂ O	196
5	1H-Pyrazole, 4,5-dihydro-3-methyl-1-propyl-	793	1100	26964-49-8	mainlib	C ₇ H ₁₄ N ₂	126

Carbonic acid, monoamide, N-butyl-, allyl ester

1st Dimension R.T. = 871.776

2nd Dimension R.T. = 1.617

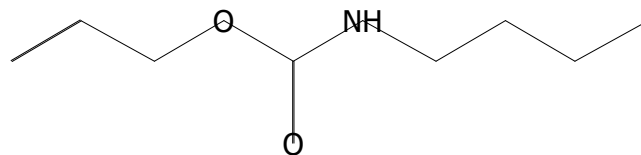
Quant Mass(es) = 114

S/N = 926.29

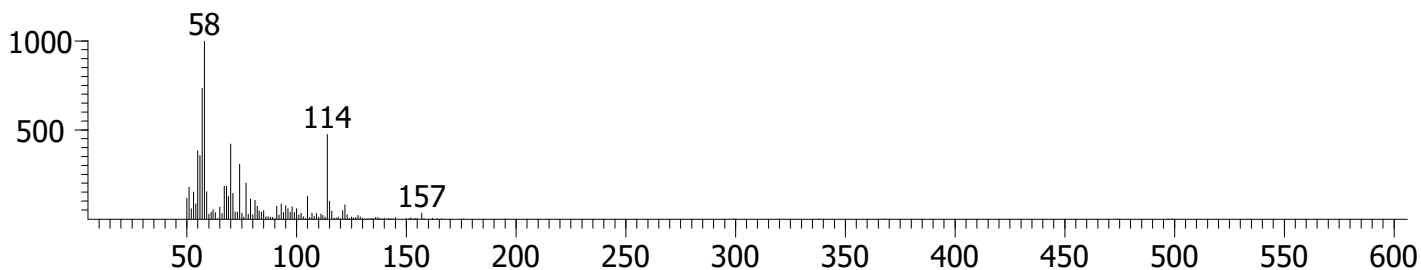
Area = 147105

Height = 19408

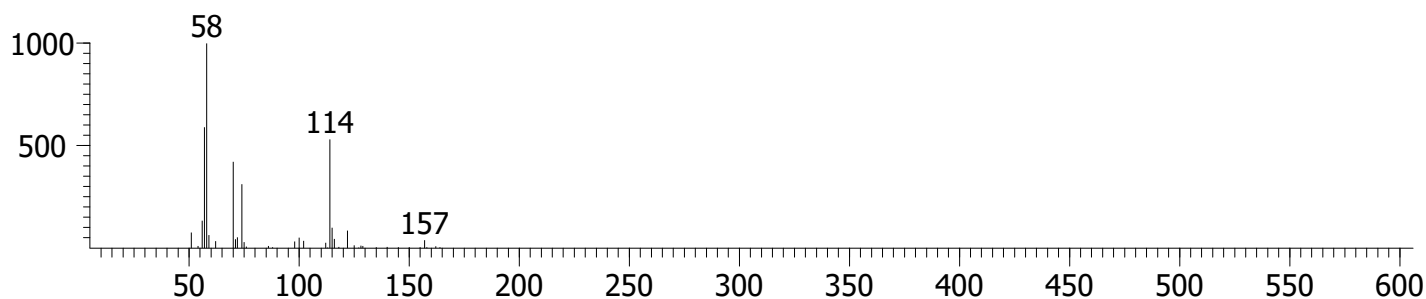
Similarity = 809



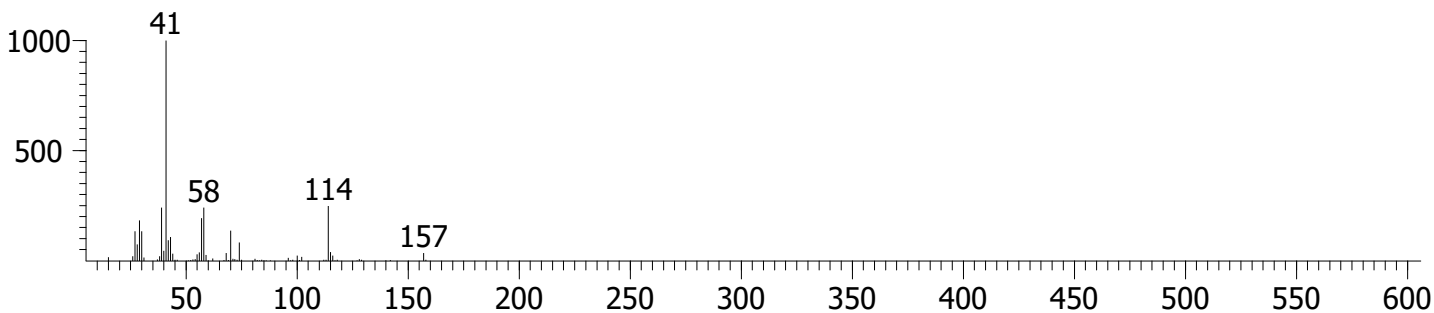
Peak Apex - sample "AnBxr B (20191121):1", peak 1327, at 871.776 , 1.617 sec , sec (Spec # 59605)



Peak True - sample "AnBxr B (20191121):1", peak 1327, at 871.776 , 1.617 sec , sec (Spec # 59605)



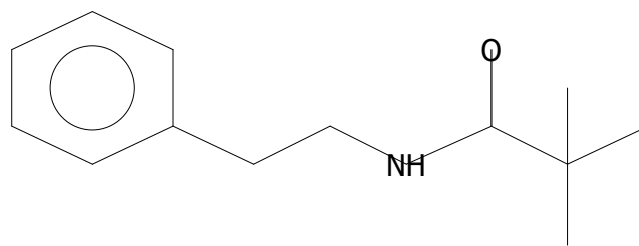
Library Hit - similarity 809, "Carbonic acid, monoamide, N-butyl-, allyl ester"



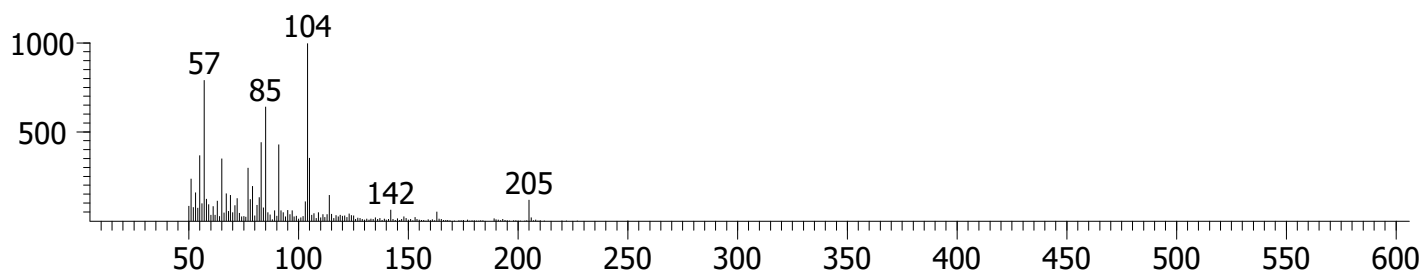
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Carbonic acid, monoamide, N-butyl-, allyl ester	809	3991	0-00-0	mainlib	C8H15NO2	157
2	Carbonic acid, monoamide, N-heptyl-, allyl ester	809	3991	0-00-0	mainlib	C11H21NO2	199
3	Carbonic acid, monoamide, N-isobutyl-, allyl ester	754	774	0-00-0	mainlib	C8H15NO2	157
4	Carbonic acid, monoamide, N-hexyl-, allyl ester	739	469	0-00-0	mainlib	C10H19NO2	185
5	Carbonic acid, monoamide, N-octyl-, allyl ester	717	185	0-00-0	mainlib	C12H23NO2	213

2,2-Dimethyl-N-phenethylpropionamide

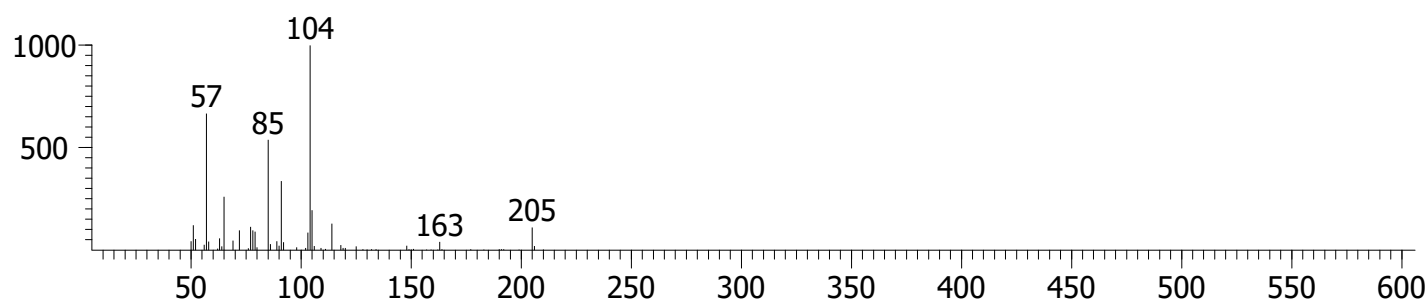
1st Dimension R.T. = 1518.91
2nd Dimension R.T. = 2.033
Quant Mass(es) = 104
S/N = 4070.0
Area = 826728
Height = 71963
Similarity = 828



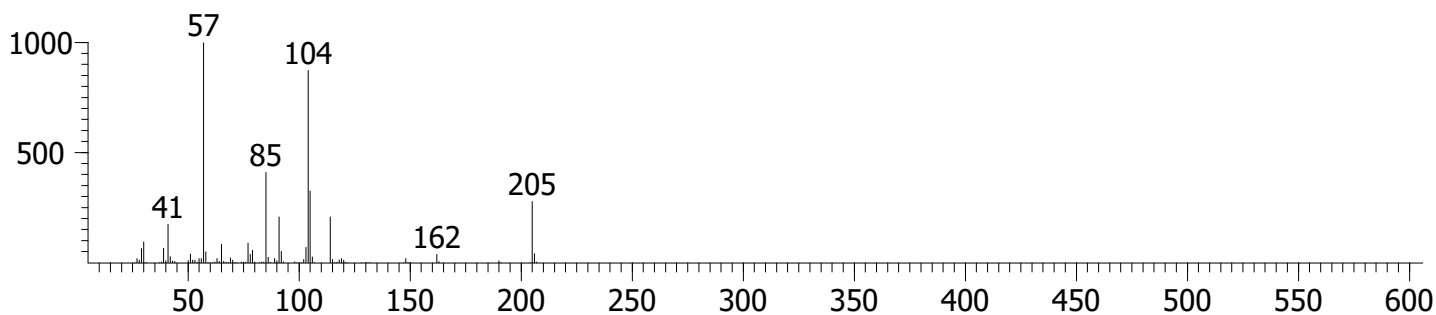
Peak Apex - sample "AnBxr B (20191121):1", peak 5280, at 1518.91 , 2.033 sec , sec (Spec # 157718)



Peak True - sample "AnBxr B (20191121):1", peak 5280, at 1518.91 , 2.033 sec , sec (Spec # 157718)



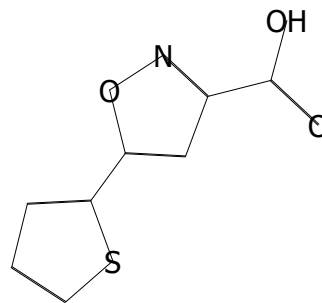
Library Hit - similarity 828, "2,2-Dimethyl-N-phenethylpropionamide"



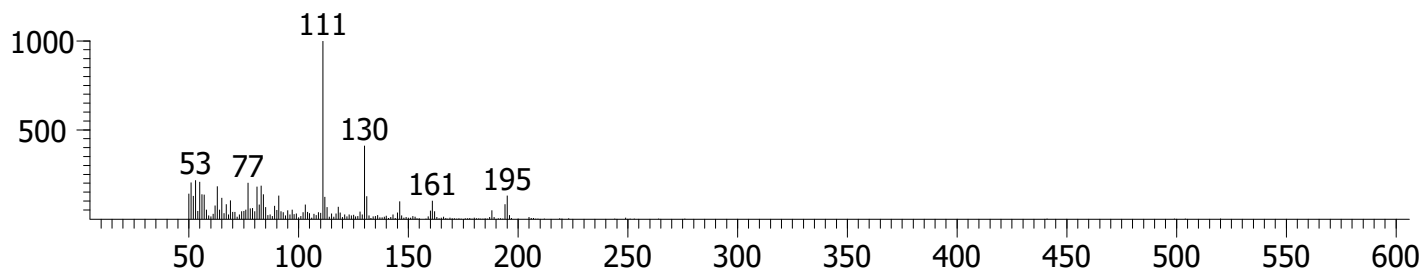
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2,2-Dimethyl-N-phenethylpropionamide	828	6348	62056-54-6	replib	C13H19NO	205
2	Butanoic acid, 3-methyl-, 2-phenylethyl ester	794	1627	140-26-1	replib	C13H18O2	206
3	Pentanoic acid, 2-phenylethyl ester	783	1116	7460-74-4	replib	C13H18O2	206
4	2,2-Dimethyl-N-phenethylpropionamide	777	2962	62056-54-6	mainlib	C13H19NO	205
5	Butanoic acid, 3-methyl-, 2-phenylethyl ester	763	1854	140-26-1	mainlib	C13H18O2	206

5-(Thiophen-2-yl)-1,2-oxazole-3-carboxylic acid

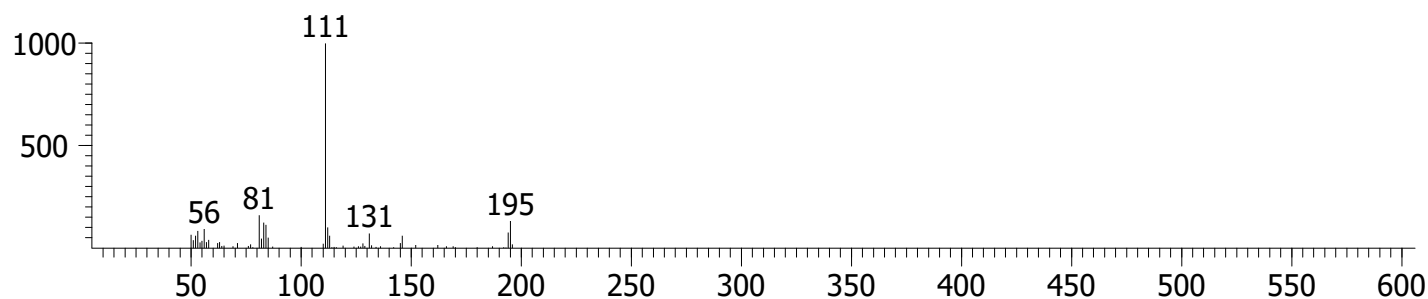
1st Dimension R.T. = 1564.38
 2nd Dimension R.T. = 2.455
 Quant Mass(es) = 111
 S/N = 1461.7
 Area = 413393
 Height = 31807
 Similarity = 710



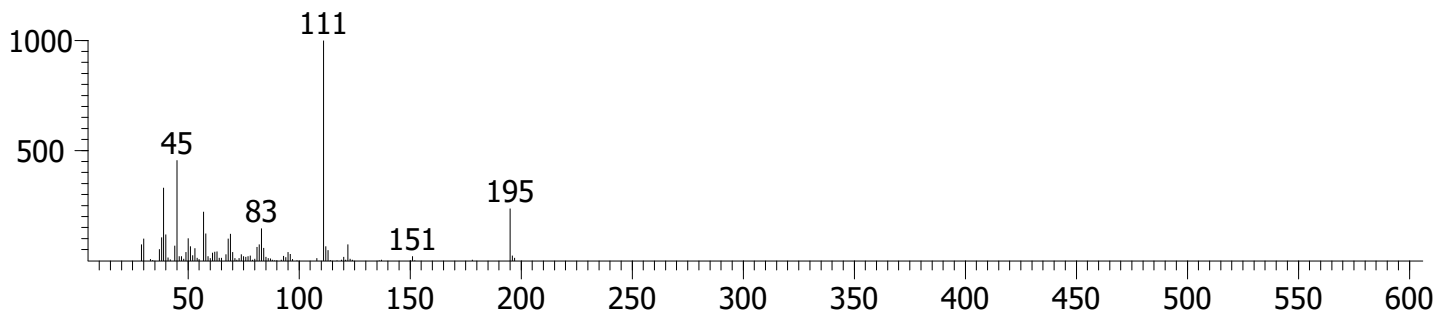
Peak Apex - sample "AnBxr B (20191121):1", peak 5609, at 1564.38 , 2.455 sec , sec (Spec # 164672)



Peak True - sample "AnBxr B (20191121):1", peak 5609, at 1564.38 , 2.455 sec , sec (Spec # 164672)

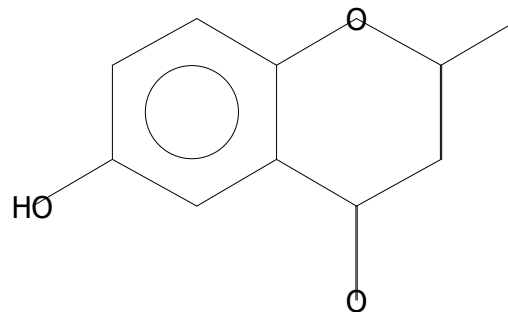


Library Hit - similarity 710, "5-(Thiophen-2-yl)-1,2-oxazole-3-carboxylic acid"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	5-(Thiophen-2-yl)-1,2-oxazole-3-carboxylic acid	710	2178	0-00-0	mainlib	C8H5NO3S	195
2	4-Amino-6-hydroxypyrimidine	695	6021	1193-22-2	replib	C4H5N3O	111
3	5-(Thiophen-3-yl)-1,2-oxazole-3-carboxylic acid	692	1123	0-00-0	mainlib	C8H5NO3S	195
4	2-Thiophenecarboxylic acid, 3-fluoro-6-nitrophenyl ester	680	748	0-00-0	mainlib	C11H6FNO4S	267
5	Dimetilan	669	4069	644-64-4	nist_msms	C10H16N4O3	240

4H-1-Benzopyran-4-one,
6-hydroxy-2-methyl-



1st Dimension R.T. = 1581.87

2nd Dimension R.T. = 2.501

Quant Mass(es) = 136

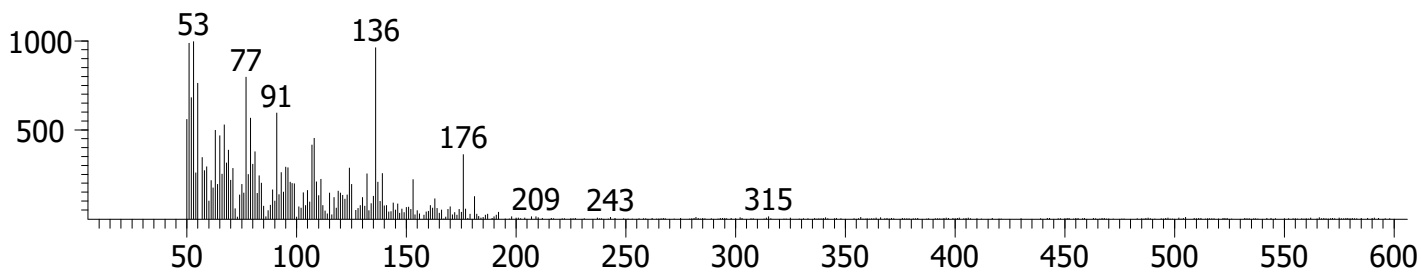
S/N = 206.48

Area = 30641

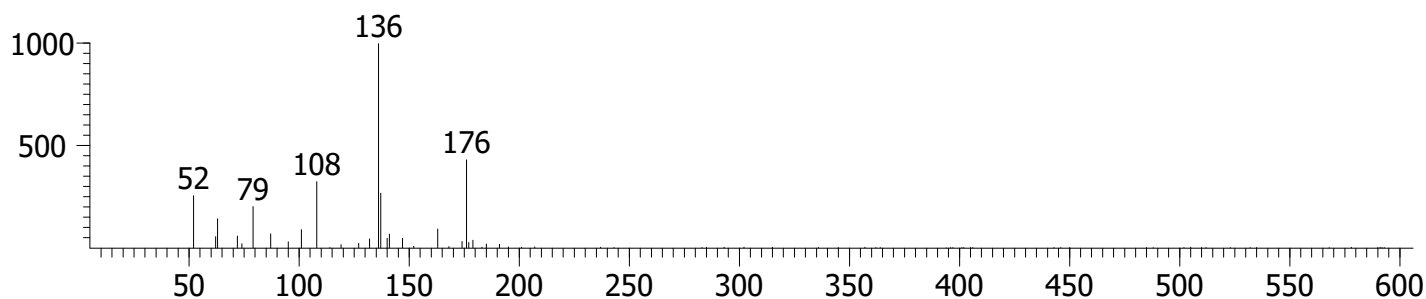
Height = 2721.9

Similarity = 677

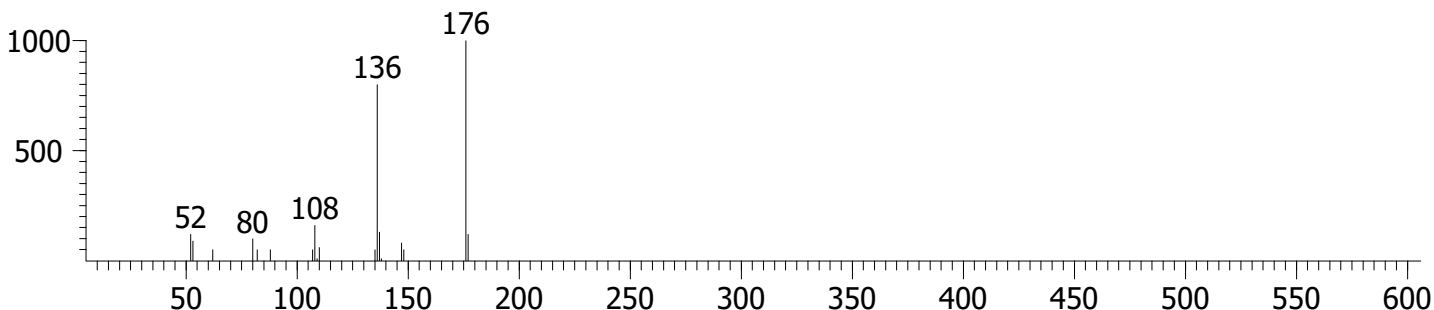
Peak Apex - sample "AnBxr B (20191121):1", peak 5720, at 1581.87 , 2.501 sec , sec (Spec # 167329)



Peak True - sample "AnBxr B (20191121):1", peak 5720, at 1581.87 , 2.501 sec , sec (Spec # 167329)



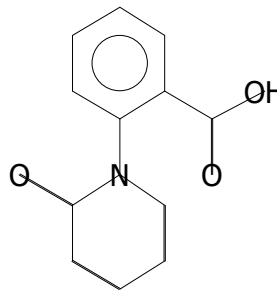
Library Hit - similarity 677, "4H-1-Benzopyran-4-one, 6-hydroxy-2-methyl-"



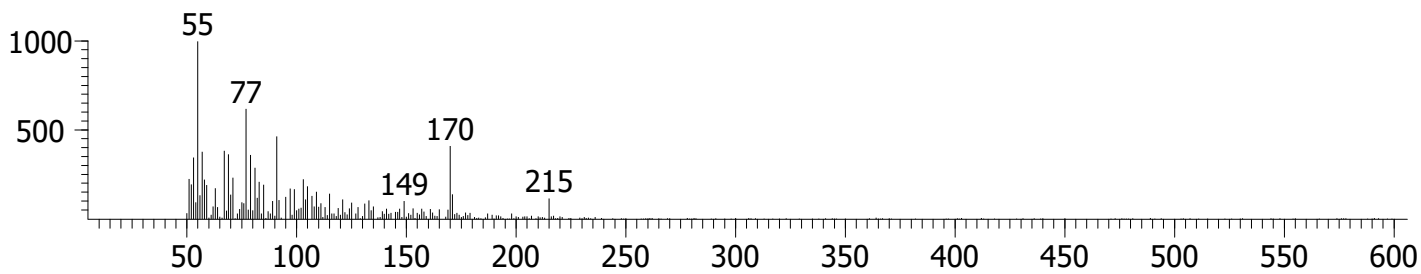
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4H-1-Benzopyran-4-one, 6-hydroxy-2-methyl-	677	5249	22105-12-0	mainlib	C10H8O3	176
2	Ethylvanillin	619	2705	121-32-4	nist_msms	C9H10O3	166
3	Benzofuroxan	617	5077	480-96-6	replib	C6H4N2O2	136
4	3-Hydroxyanthranilic acid	612	2072	548-93-6	nist_msms	C7H7NO3	153
5	Benzoic acid, 2-hydroxy-4-[[2-[[[(4-methylphenyl)sulfonyl]oxy]acetyl]amino]-	606	1628	501919-59-1	nist_msms	C16H15NO7S	365

2-(2-Oxo-2H-pyridin-1-yl)benzoic acid

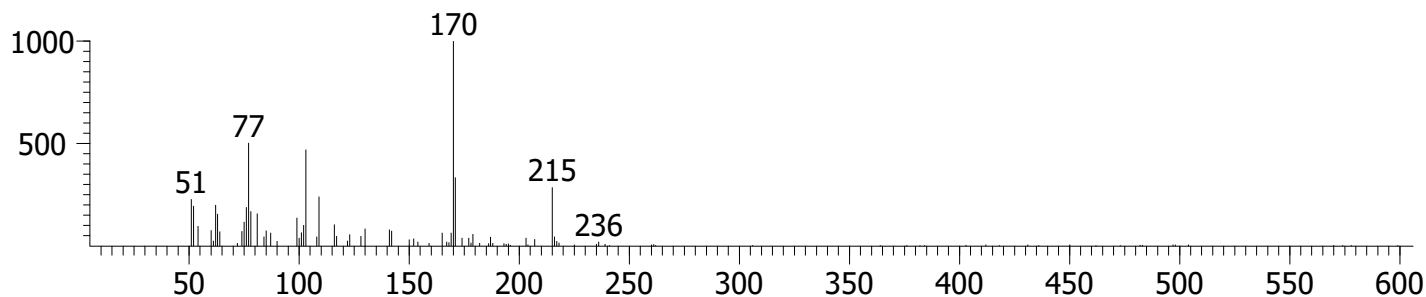
1st Dimension R.T. = 1889.69
2nd Dimension R.T. = 2.376
Quant Mass(es) = 170
S/N = 221.22
Area = 31840
Height = 2893.3
Similarity = 643



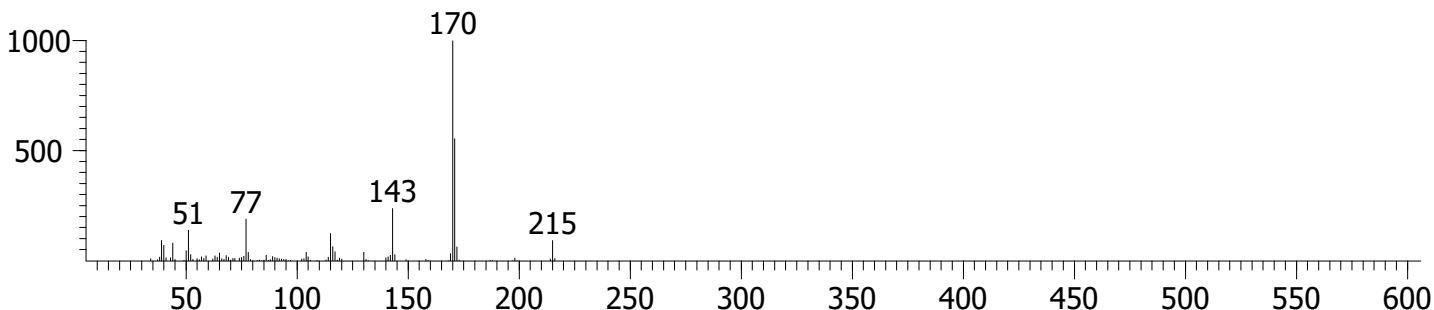
Peak Apex - sample "AnBxr B (20191121):1", peak 7407, at 1889.69 , 2.376 sec , sec (Spec # 213950)



Peak True - sample "AnBxr B (20191121):1", peak 7407, at 1889.69 , 2.376 sec , sec (Spec # 213950)



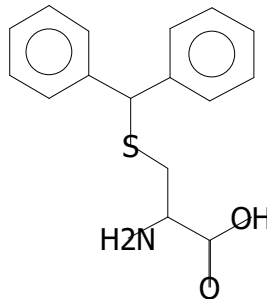
Library Hit - similarity 643, "2-(2-Oxo-2H-pyridin-1-yl)benzoic acid"



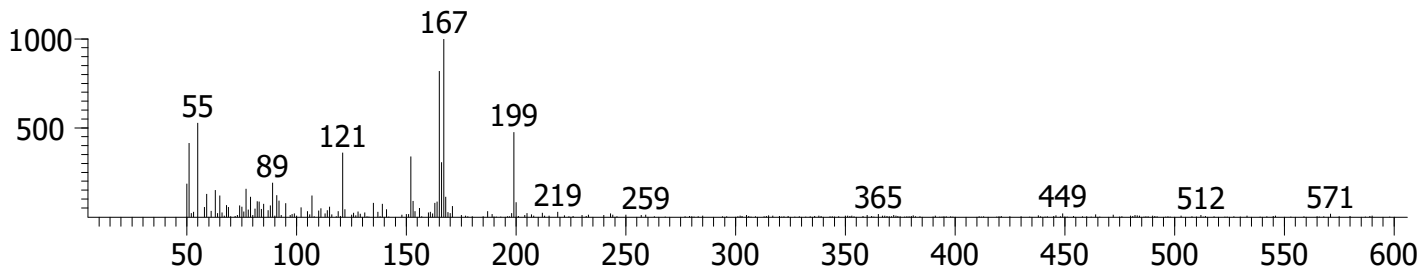
Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	2-(2-Oxo-2H-pyridin-1-yl)benzoic acid	643	4204	0-00-0	mainlib	C12H9NO3	215
2	N-Methyl-2-(2-oxo-2H-pyridin-1-yl)benzamide	624	2041	0-00-0	mainlib	C13H12N2O2	228
3	2-{5-Methyl-7-nitro-2-phenylimidazo[1,5-a][1,3]diazol-1-yl}ethanol	589	512	0-00-0	mainlib	C14H14N4O3	286
4	8aH-pyrazolo[1,5-a]benzimidazole, 2-methyl-	581	382	0-00-0	mainlib	C10H9N3	171
5	1-(2-Acetylphenyl)-1H-pyridin-2-one	572	277	0-00-0	mainlib	C13H11NO2	213

L-Cysteine, S-(diphenylmethyl)-

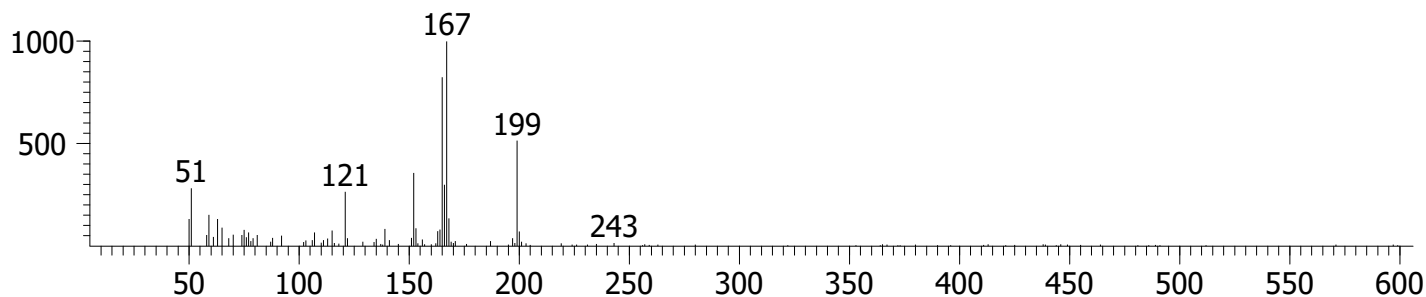
1st Dimension R.T. = 2124.06
2nd Dimension R.T. = 3.010
Quant Mass(es) = 167
S/N = 181.32
Area = 34255
Height = 2527.8
Similarity = 788



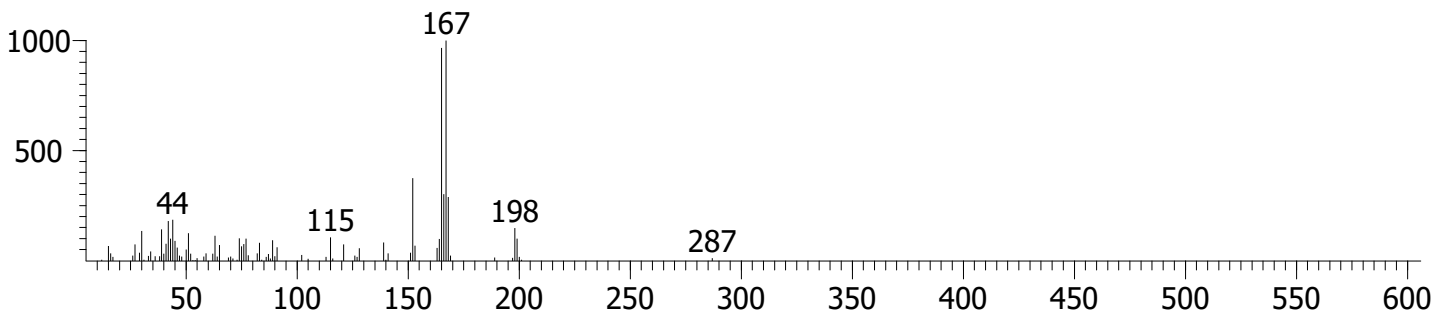
Peak Apex - sample "AnBxr B (20191121):1", peak 8184, at 2124.06 , 3.010 sec , sec (Spec # 249556)



Peak True - sample "AnBxr B (20191121):1", peak 8184, at 2124.06 , 3.010 sec , sec (Spec # 249556)



Library Hit - similarity 788, "L-Cysteine, S-(diphenylmethyl)-"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	L-Cysteine, S-(diphenylmethyl)-	788	1698	5191-80-0	mainlib	C16H17NO2S	287
2	1,1'-[[[(2-bromoethyl)sulfanyl]methanediyl]dibenzene	780	1267	0-00-0	mainlib	C15H15BrS	306
3	Benzene, 1,1'-(bromomethylene)bis-	779	1946	776-74-9	replib	C13H11Br	246
4	2,2-Diphenylethylamine	771	1452	3963-62-0	replib	C14H15N	197
5	Benzene, 1,1'-(bromomethylene)bis-	770	1946	776-74-9	replib	C13H11Br	246

4,8,12,16-tetraoxaeicosan-1-ol

1st Dimension R.T. = 2288.47

2nd Dimension R.T. = 1.610

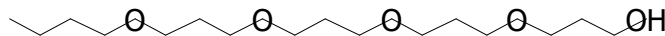
Quant Mass(es) = 59

S/N = 184.38

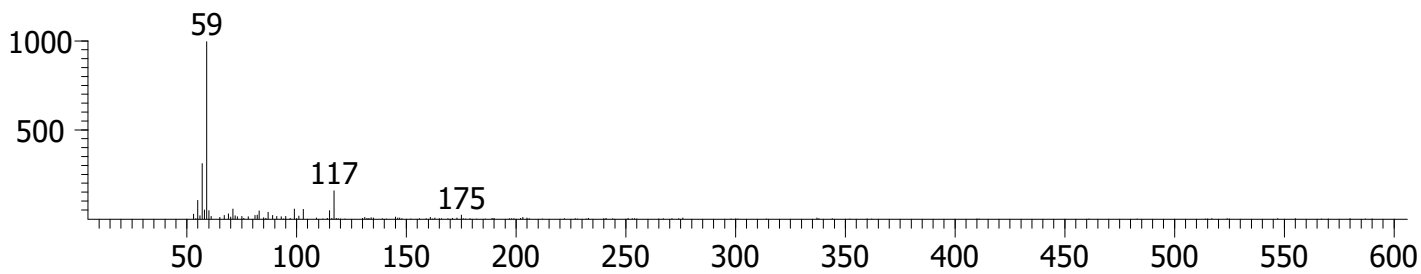
Area = 317655

Height = 21693

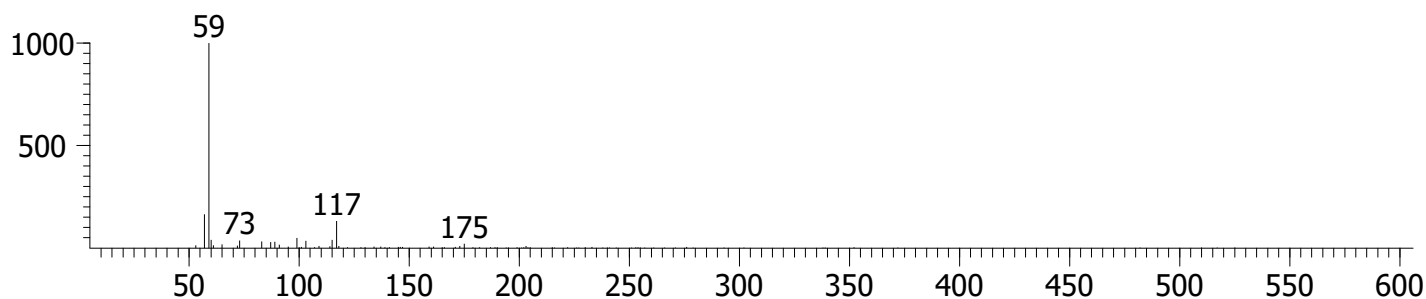
Similarity = 919



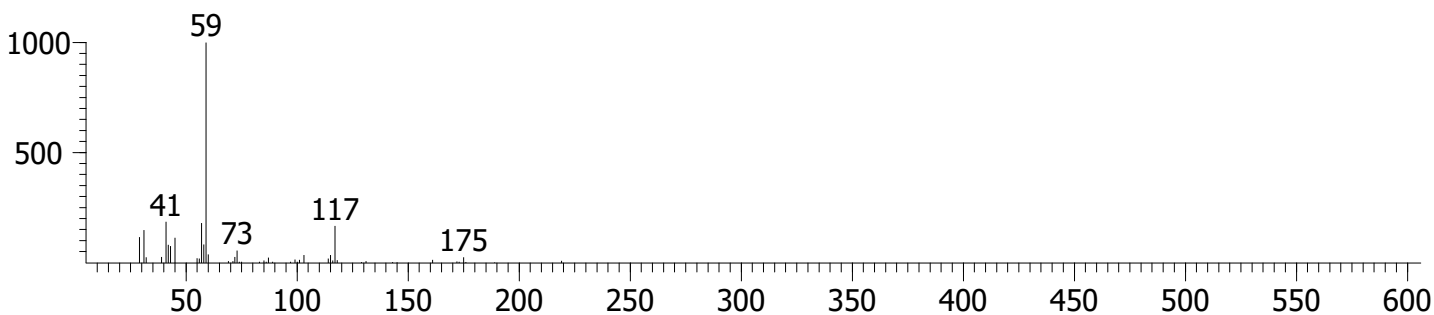
Peak Apex - sample "AnMbr C (20191120):1", peak 7302, at 2288.47 , 1.610 sec , sec (Spec # 274254)



Peak True - sample "AnMbr C (20191120):1", peak 7302, at 2288.47 , 1.610 sec , sec (Spec # 274254)



Library Hit - similarity 919, "4,8,12,16-tetraoxaeicosan-1-ol"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	4,8,12,16-tetraoxaeicosan-1-ol	919	5965	0-00-0	mainlib	C16H34O5	306
2	s-Trioxane, 2,4,6-triethyl-	872	1247	2396-42-1	mainlib	C9H18O3	174
3	2-Butanol	871	1199	78-92-2	mainlib	C4H10O	74
4	3-Methyl-oxirane-2-carboxylic acid, methyl ester	856	726	0-00-0	mainlib	C5H8O3	116
5	Propanol, [(butoxymethylethoxy)methylethoxy]-	831	221	55934-93-5	mainlib	C13H28O4	248

Pentadecanoic acid

1st Dimension R.T. = 1609.85

2nd Dimension R.T. = 1.426

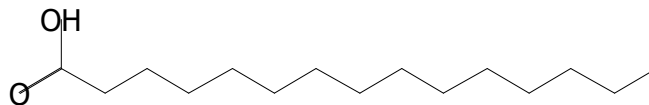
Quant Mass(es) = 60

S/N = 649.02

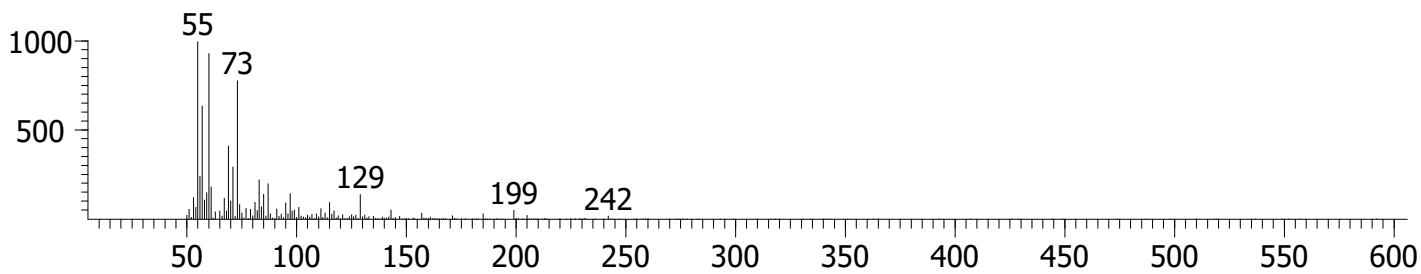
Area = 244157

Height = 27378

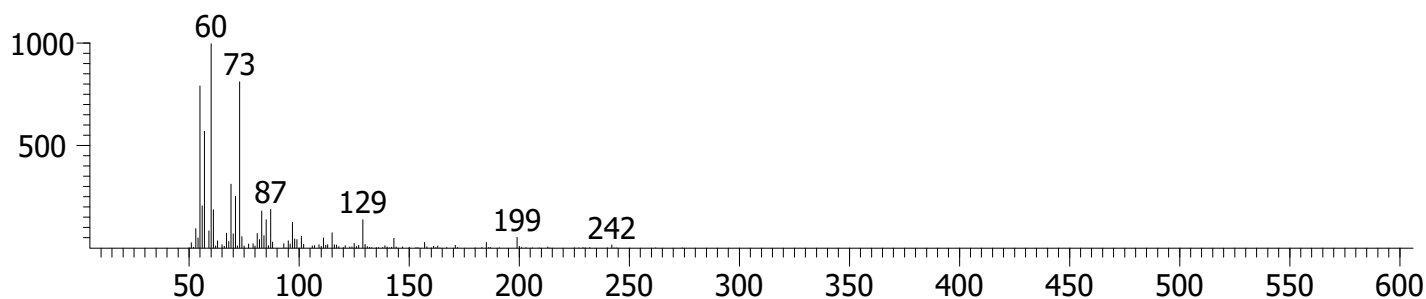
Similarity = 878



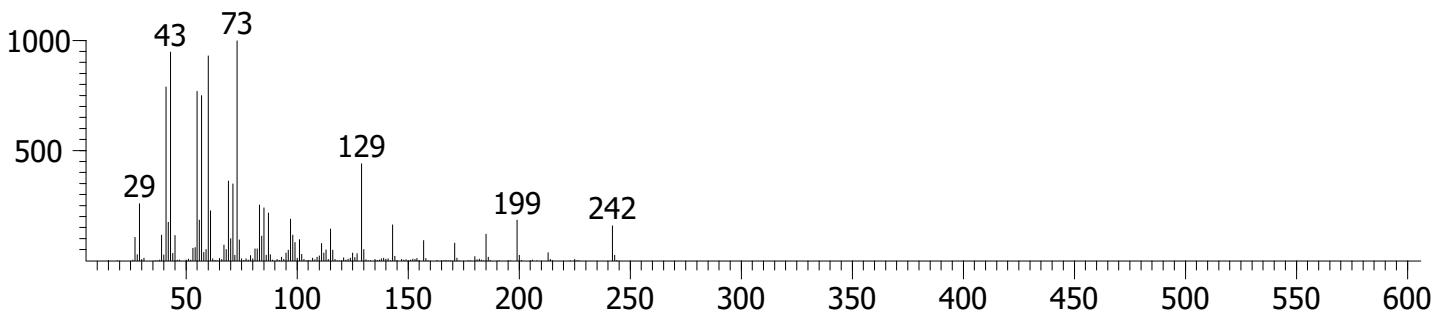
Peak Apex - sample "AnMbr C (20191120):1", peak 5229, at 1609.85 , 1.426 sec , sec (Spec # 171406)



Peak True - sample "AnMbr C (20191120):1", peak 5229, at 1609.85 , 1.426 sec , sec (Spec # 171406)



Library Hit - similarity 878, "Pentadecanoic acid"



Hit	Name	Similarity	Probability	CAS	Library	Formula	Weight
1	Pentadecanoic acid	878	5245	1002-84-2	mainlib	C15H30O2	242
2	Tetradecanoic acid	831	1097	544-63-8	mainlib	C14H28O2	228
3	n-Hexadecanoic acid	824	840	57-10-3	mainlib	C16H32O2	256
4	8-Methylnonanoic acid	816	627	5963-14-4	mainlib	C10H20O2	172
5	Dodecanoic acid	803	405	143-07-7	mainlib	C12H24O2	200