

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
 Data File : BF124876.D
 Acq On : 30 Jul 2021 15:05
 Operator : JU/CG
 Sample : M3217-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 280

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124876.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	6	10	14	rBB2	6666	7595	2.94%	0.483%
2	5.110	511	514	518	rBB	2903	3525	1.36%	0.224%
3	5.493	574	579	582	rBV	188479	198403	76.80%	12.618%
4	6.504	745	751	754	rBV	186802	206554	79.96%	13.136%
5	6.869	810	813	816	rBB	45950	33776	13.07%	2.148%
6	7.439	905	910	913	rBV	149507	140088	54.23%	8.909%
7	8.051	1012	1014	1018	rBV	13289	10415	4.03%	0.662%
8	8.151	1028	1031	1035	rBB	61914	49005	18.97%	3.117%
9	9.233	1210	1215	1218	rBV	275819	258331	100.00%	16.429%
10	9.910	1326	1330	1333	rBV	75507	60231	23.32%	3.830%
11	10.704	1460	1465	1468	rBV	208317	184123	71.27%	11.710%
12	11.398	1579	1583	1585	rBV	77752	61752	23.90%	3.927%
13	11.422	1585	1587	1589	rVB	7006	4737	1.83%	0.301%
14	11.916	1669	1671	1674	rBB	12403	10005	3.87%	0.636%
15	12.610	1786	1789	1792	rBB	10685	8440	3.27%	0.537%
16	12.839	1825	1828	1831	rVB	9307	7408	2.87%	0.471%
17	12.986	1849	1853	1856	rBV	264005	226986	87.87%	14.436%
18	13.551	1947	1949	1954	rVB2	2583	3208	1.24%	0.204%
19	13.880	2002	2005	2013	rBB	9184	14797	5.73%	0.941%
20	14.039	2028	2032	2034	rBV	35646	34681	13.43%	2.206%
21	14.498	2107	2110	2112	rBV2	2579	2887	1.12%	0.184%
22	14.521	2112	2114	2120	rVB3	2081	3102	1.20%	0.197%
23	15.080	2206	2209	2211	rBV	2467	3070	1.19%	0.195%
24	15.145	2217	2220	2223	rVB	2892	3015	1.17%	0.192%
25	15.380	2257	2260	2265	rBB	1983	2920	1.13%	0.186%
26	15.515	2278	2283	2288	rBB	26710	30686	11.88%	1.952%
27	15.733	2317	2320	2324	rVB2	1583	2669	1.03%	0.170%

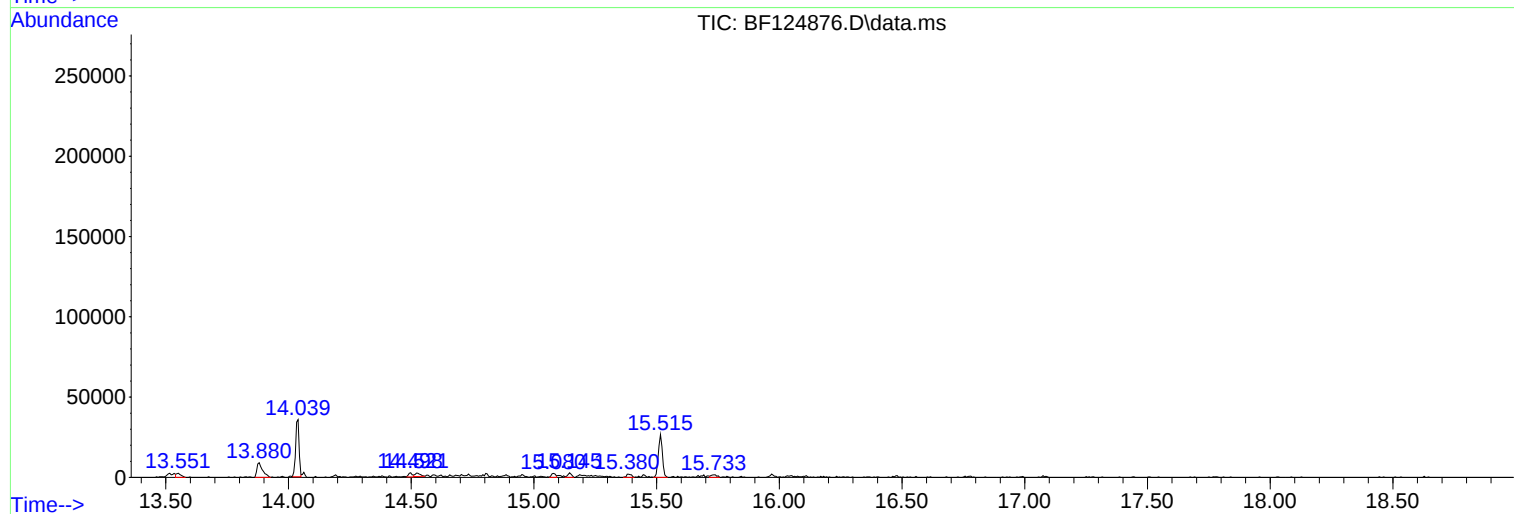
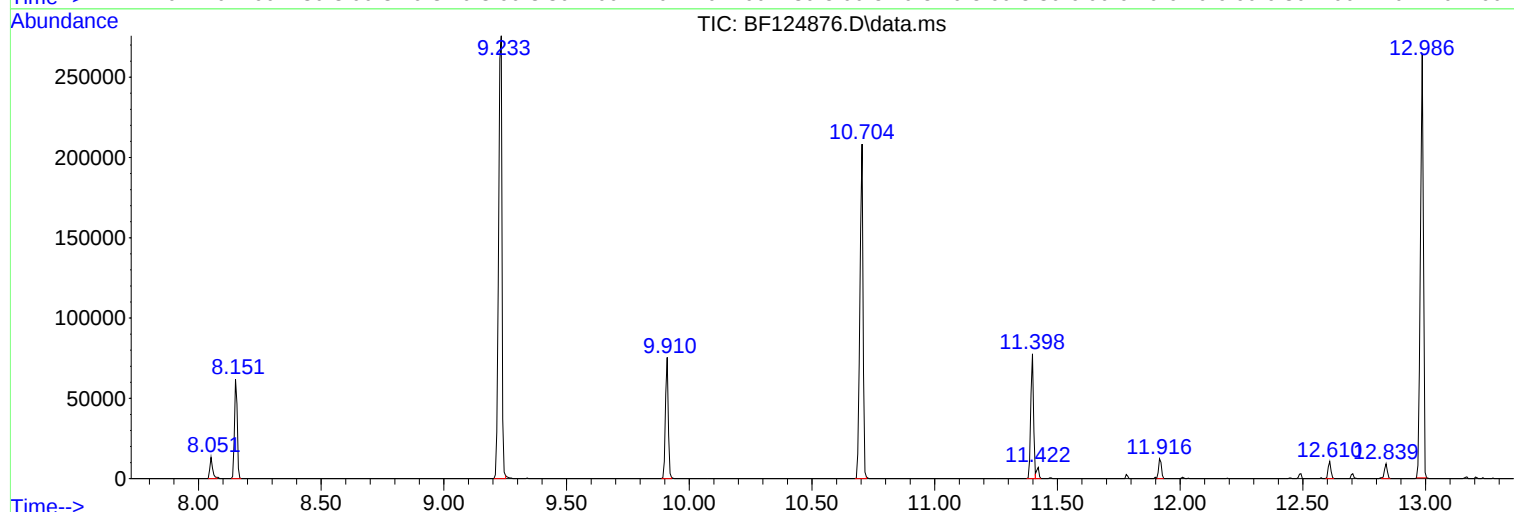
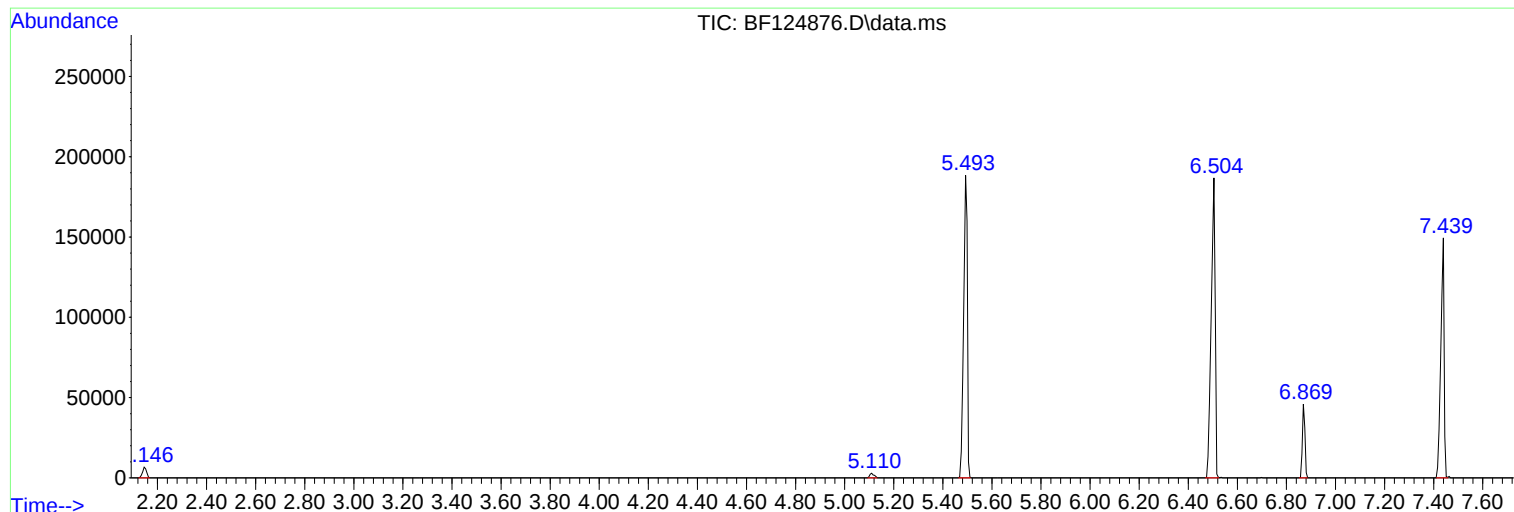
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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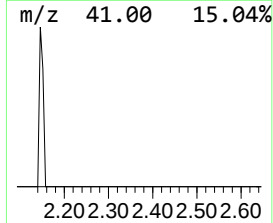
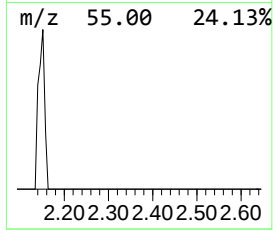
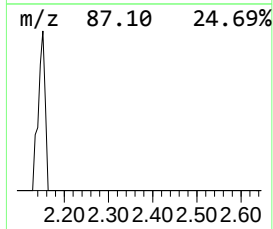
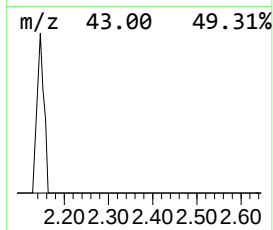
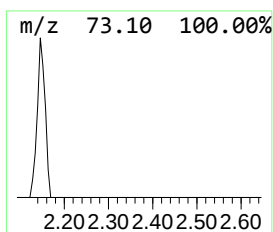
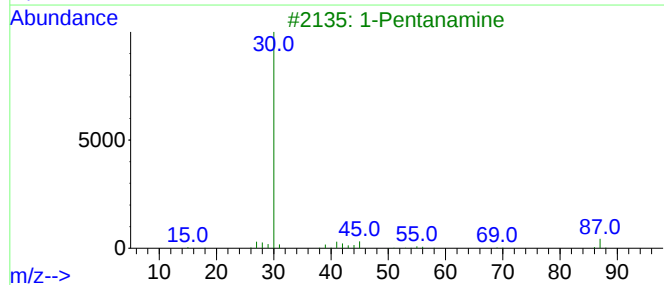
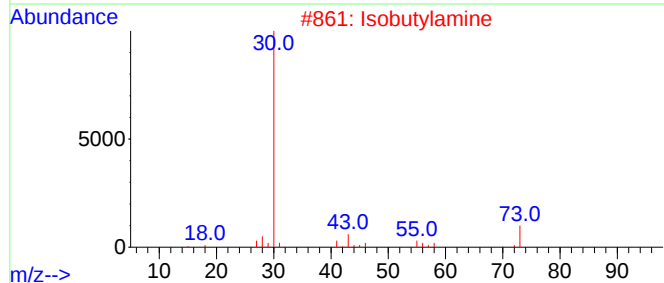
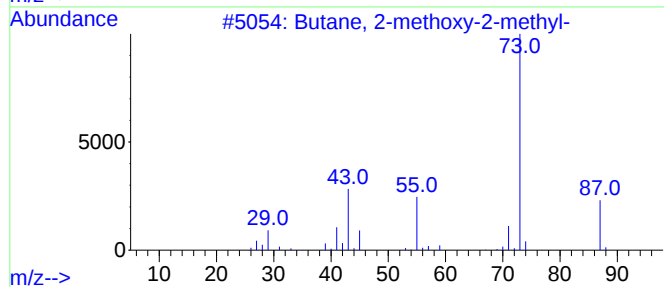
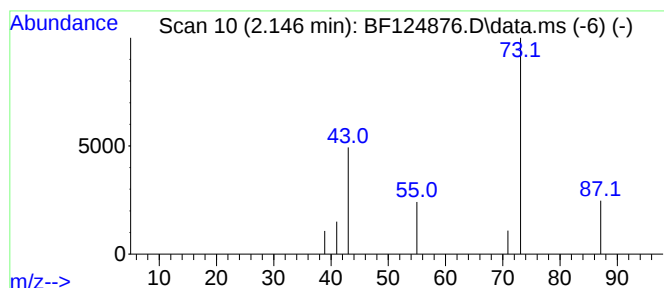
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Peak Number 1 unknown2.146 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	4.50 ng	7595	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2			Isobutylamine	73	C4H11N	000078-81-9	4
3			1-Pentanamine	87	C5H13N	000110-58-7	3
4			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
5			N-Ethylformamide	73	C3H7NO	000627-45-2	3



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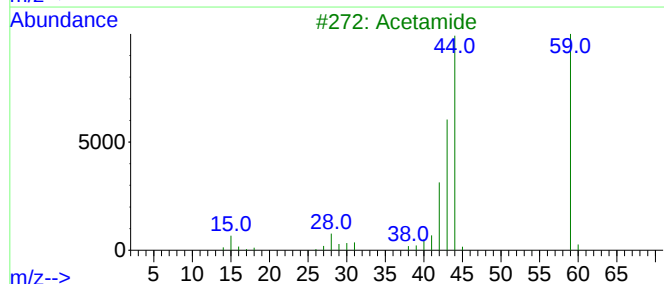
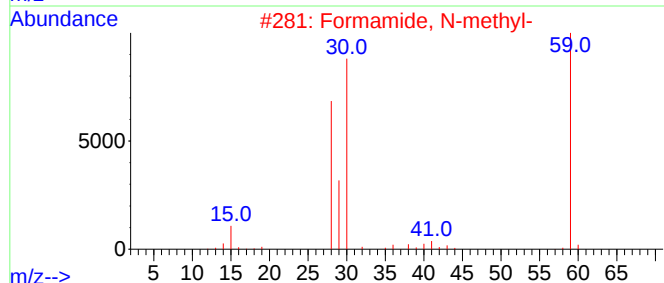
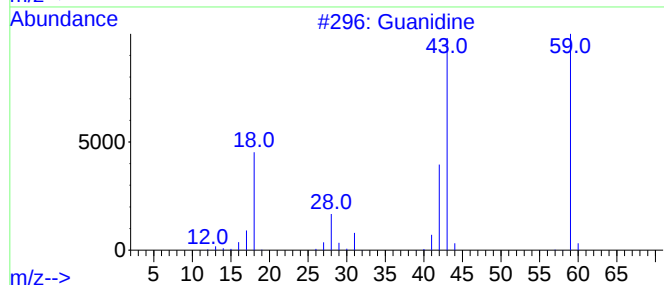
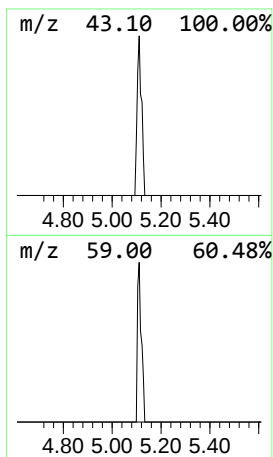
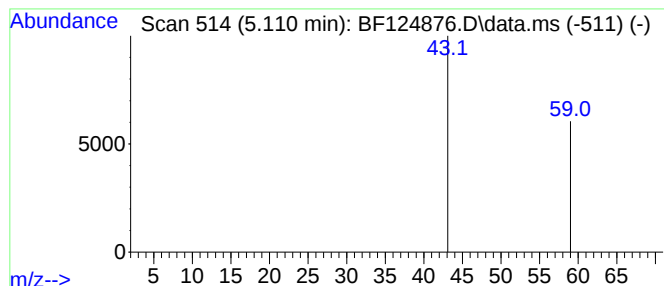
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.110 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	2.09 ng	3525	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Guanidine	59	CH5N3	000113-00-8	2
2			Formamide, N-methyl-	59	C2H5NO	000123-39-7	2
3			Acetamide	59	C2H5NO	000060-35-5	2
4			Acetaldoxime	59	C2H5NO	000107-29-9	2
5			Propylamine	59	C3H9N	000107-10-8	1



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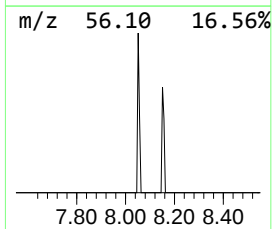
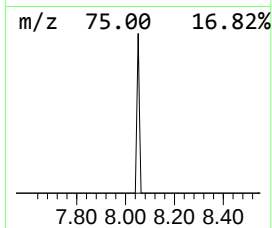
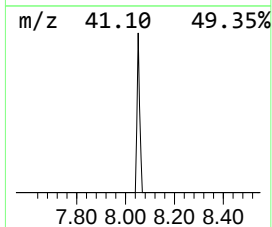
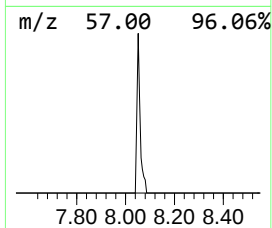
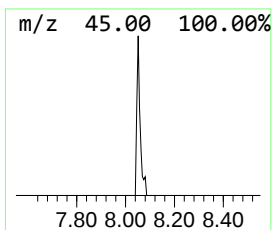
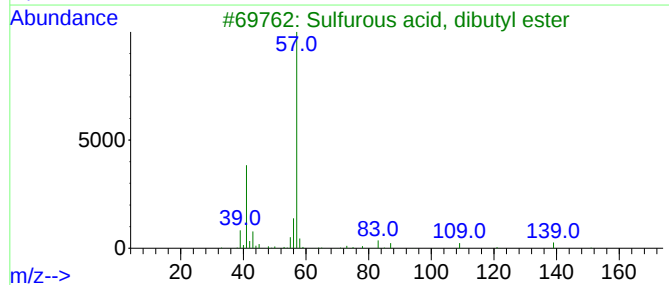
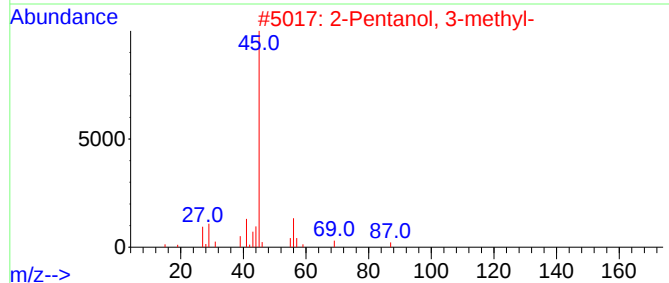
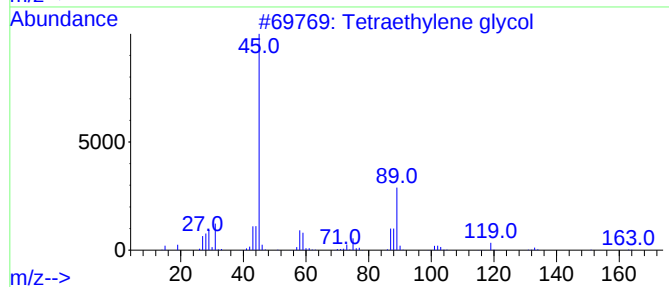
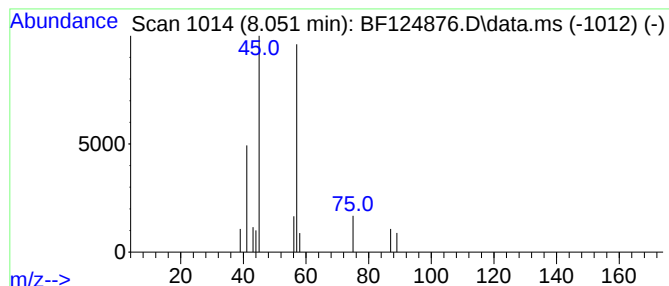
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Peak Number 3 unknown8.051 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	4.25 ng	10415	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetraethylene glycol	194	C8H18O5	000112-60-7	9
2			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	9
3			Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	9
4			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	9
5			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9



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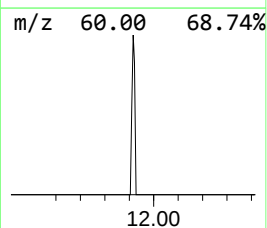
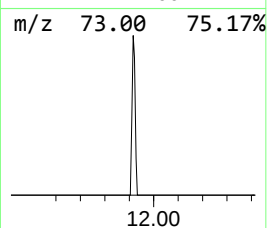
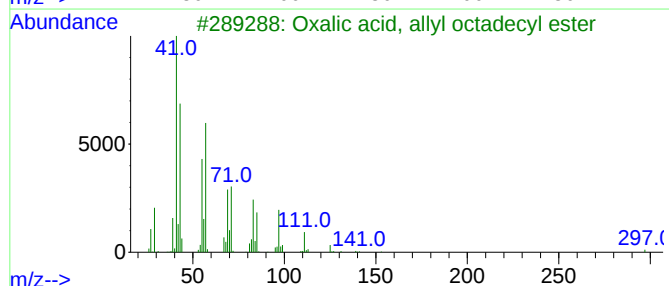
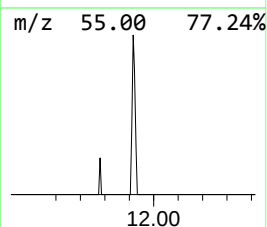
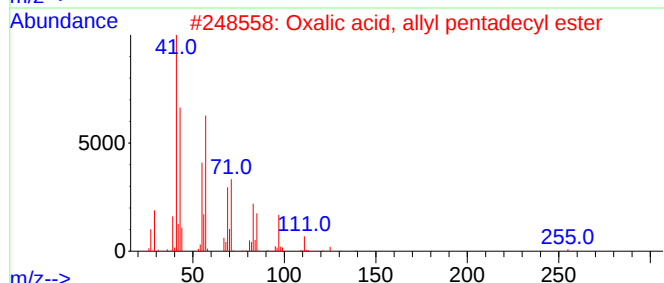
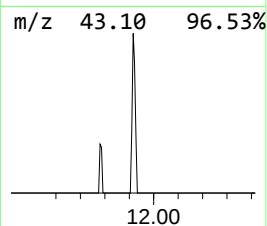
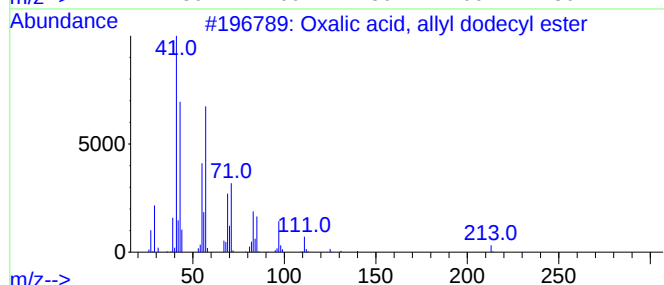
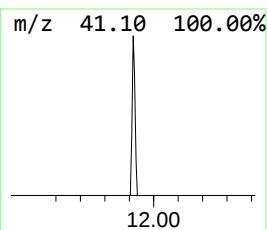
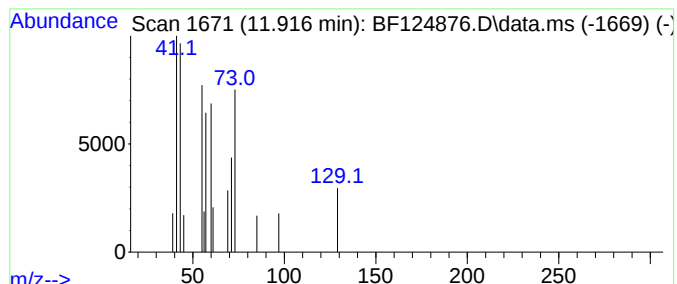
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Peak Number 4 unknown11.916 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.24 ng	10005	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	25
2			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	25
3			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	25
4			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	25
5			1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	25



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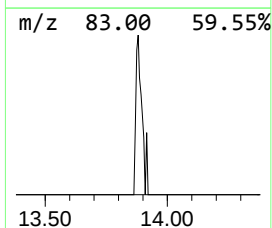
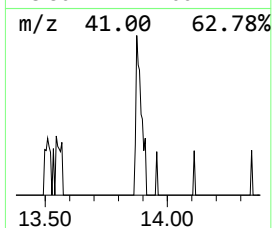
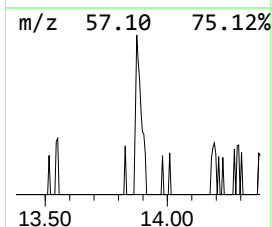
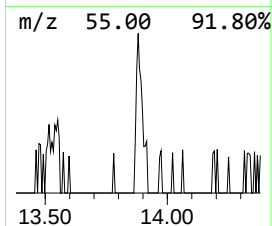
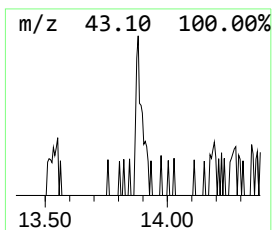
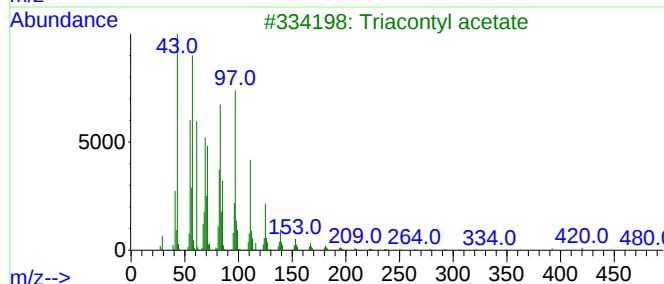
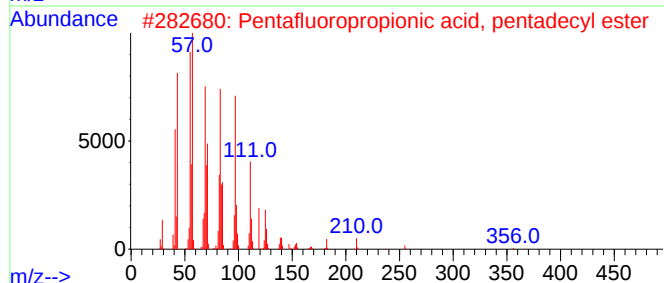
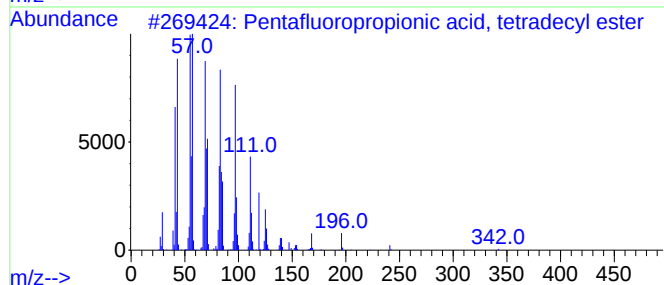
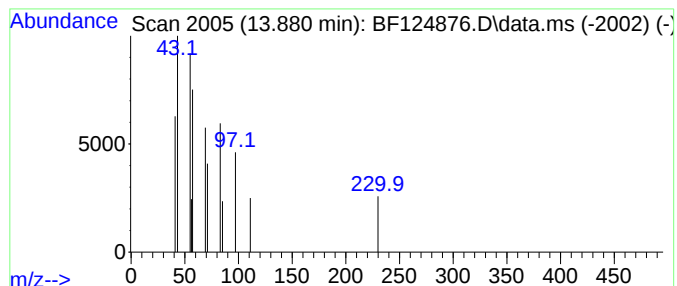
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	8.53 ng	14797	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	86
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	78
3			Triacontyl acetate	480	C32H64O2	041755-58-2	78
4			17-Pentatriacontene	491	C35H70	006971-40-0	78
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown5.110	5.110	2.1	ng	3525	1	6.869	33776	20.0
unknown8.051	8.051	4.3	ng	10415	2	8.151	49005	20.0
unknown11.916	11.916	3.2	ng	10005	4	11.398	61752	20.0
Pentafluoroprop...	13.880	8.5	ng	14797	5	14.039	34681	20.0