

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
 Data File : BF096617.D
 Acq On : 10 Jul 2017 22:43
 Operator : SJ/JU
 Sample : I4061-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-B

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	469	474	487	rBV	330305	445235	15.92%	1.704%
2	5.298	541	546	549	rBV	2819423	2796520	100.00%	10.704%
3	6.328	715	721	724	rBV	2441885	2794992	99.95%	10.698%
4	6.451	738	742	746	rBV	2568790	2714790	97.08%	10.391%
5	6.681	778	781	785	rBV	834116	722305	25.83%	2.765%
6	6.840	804	808	812	rBV	2314132	2059747	73.65%	7.884%
7	7.245	871	877	880	rBV	1808373	1770046	63.29%	6.775%
8	7.963	995	999	1003	rBV	1102607	973932	34.83%	3.728%
9	9.045	1177	1183	1186	rBV	2702460	2751583	98.39%	10.532%
10	9.433	1246	1249	1252	rBV	242439	185026	6.62%	0.708%
11	9.716	1292	1297	1300	rBV	1040309	962190	34.41%	3.683%
12	9.745	1300	1302	1306	rVB	163707	121399	4.34%	0.465%
13	9.916	1326	1331	1335	rVB	50968	45619	1.63%	0.175%
14	10.163	1370	1373	1375	rVB	35084	28091	1.00%	0.108%
15	10.257	1386	1389	1392	rVB	90241	69863	2.50%	0.267%
16	10.498	1425	1430	1434	rBV	1466437	1371501	49.04%	5.250%
17	10.633	1450	1453	1460	rBV	54958	64414	2.30%	0.247%
18	11.080	1521	1529	1533	rBV4	50859	92062	3.29%	0.352%
19	11.192	1544	1548	1550	rBV	876367	767720	27.45%	2.939%
20	11.216	1550	1552	1555	rVV	349463	263220	9.41%	1.008%
21	11.263	1555	1560	1564	rVB	93036	95161	3.40%	0.364%
22	11.422	1584	1587	1592	rVB	34060	36883	1.32%	0.141%
23	11.504	1596	1601	1607	rBV5	24090	53015	1.90%	0.203%
24	11.722	1635	1638	1643	rVB2	34684	43837	1.57%	0.168%
25	11.804	1648	1652	1654	rBV	55842	53232	1.90%	0.204%
26	12.398	1749	1753	1757	rBV	404781	334397	11.96%	1.280%
27	12.621	1786	1791	1795	rBV2	276276	321003	11.48%	1.229%
28	12.774	1813	1817	1821	rVB	1698676	1753365	62.70%	6.711%
29	12.957	1845	1848	1852	rVB	48518	48223	1.72%	0.185%
30	13.021	1857	1859	1861	rVB	47422	34250	1.22%	0.131%
31	13.569	1948	1952	1955	rBV3	32321	42341	1.51%	0.162%
32	13.680	1968	1971	1977	rVB	131564	150990	5.40%	0.578%
33	13.821	1990	1995	1997	rBV2	743420	815438	29.16%	3.121%
34	13.845	1997	1999	2002	rVB	119859	95359	3.41%	0.365%

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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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.674	2137	2140	2144	rVB2	54269	61613	2.20%	0.236%
36	14.821	2162	2165	2174	rVB	113820	230941	8.26%	0.884%
37	15.098	2209	2212	2218	rVB	59265	75315	2.69%	0.288%
38	15.157	2219	2222	2227	rVB	87947	94032	3.36%	0.360%
39	15.215	2227	2232	2239	rBV	552960	679362	24.29%	2.600%
40	16.539	2453	2457	2462	rBV2	34156	60425	2.16%	0.231%
41	17.292	2581	2585	2590	rVB8	24963	46593	1.67%	0.178%

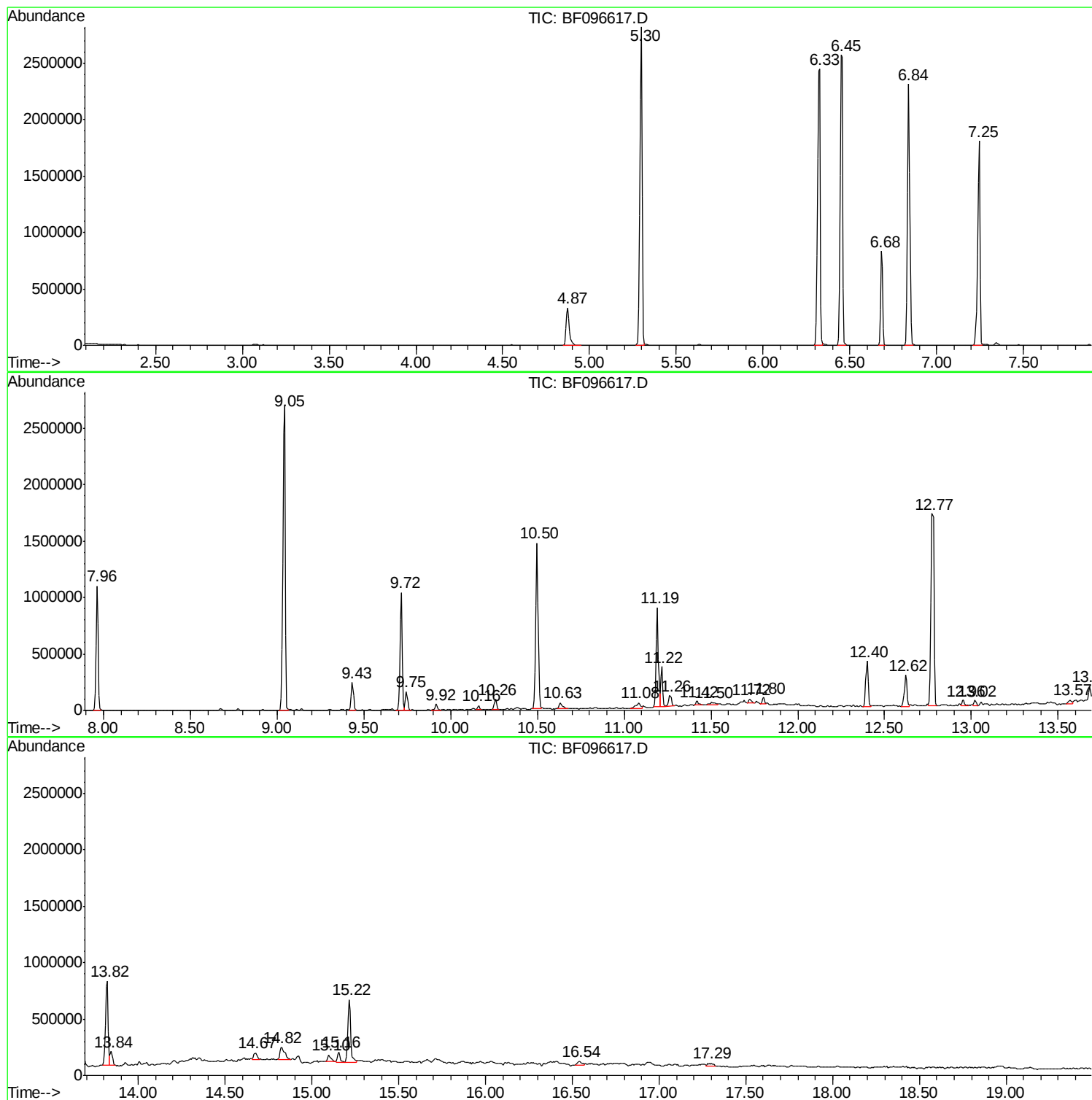
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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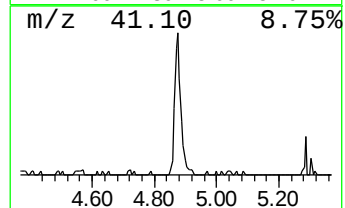
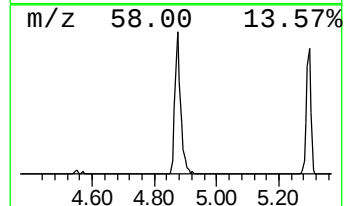
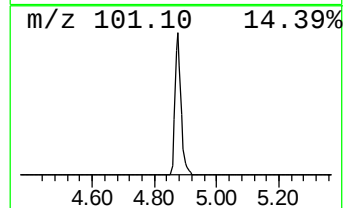
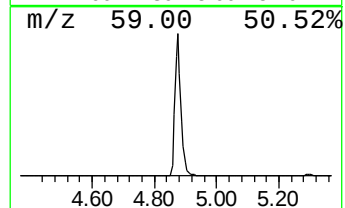
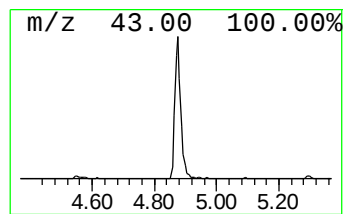
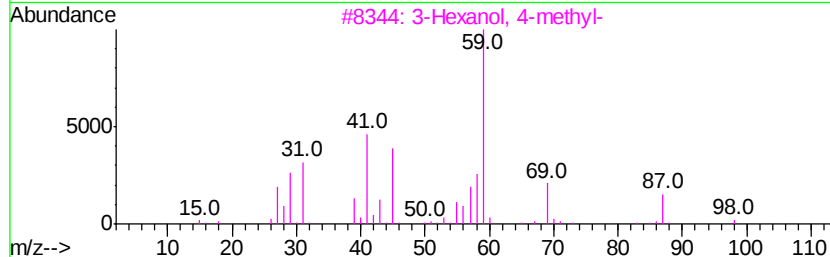
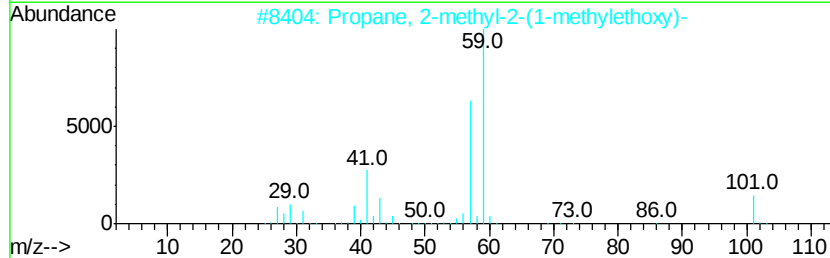
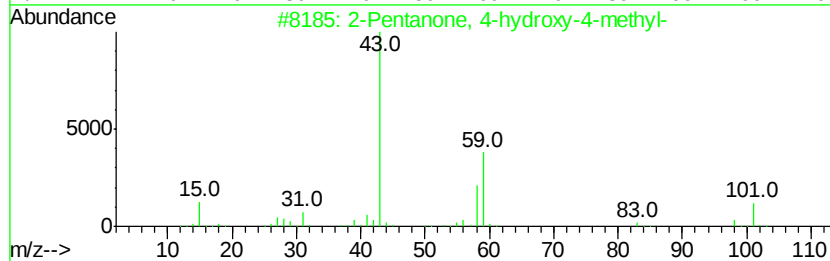
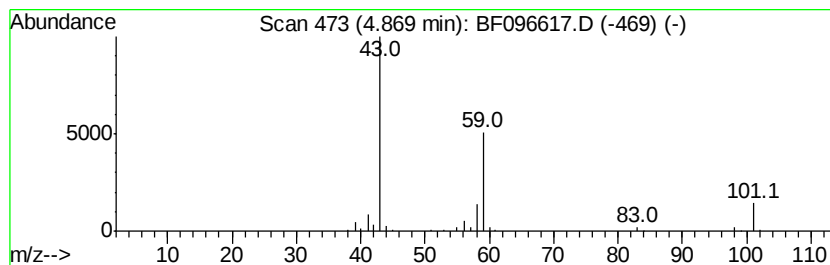
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	12.33 ng	445235	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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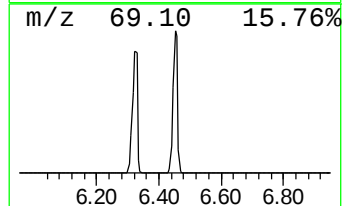
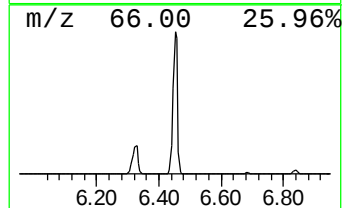
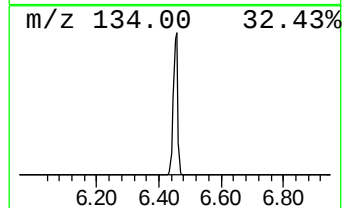
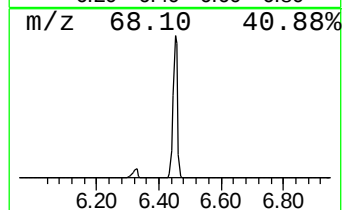
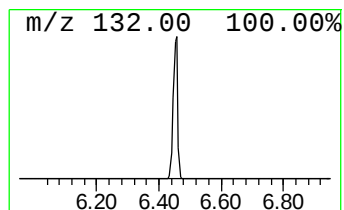
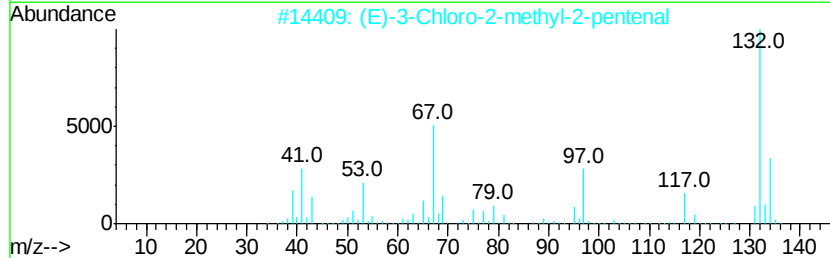
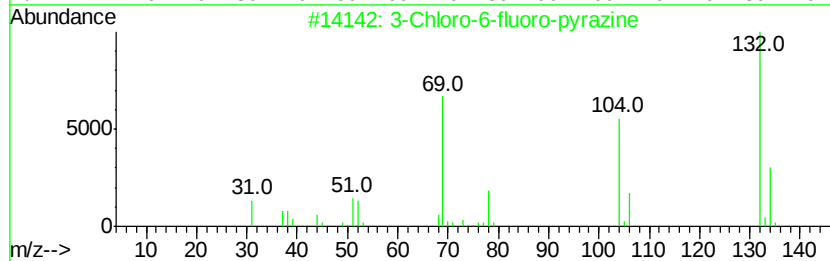
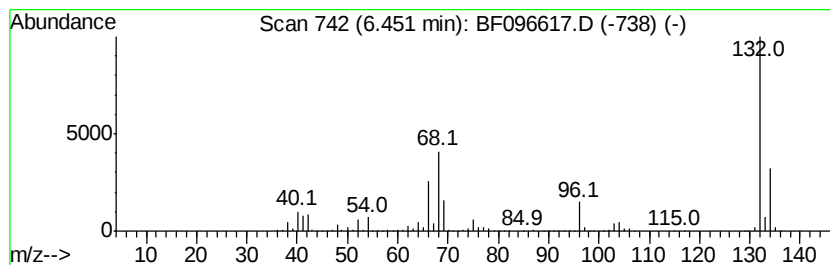
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	75.17 ng	2714790	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
3	5-Aminoindole	132	C8H8N2	005192-03-0	12	
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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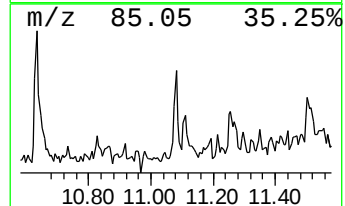
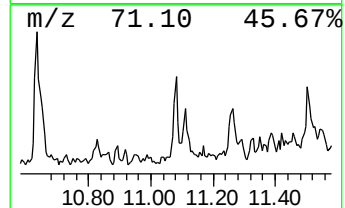
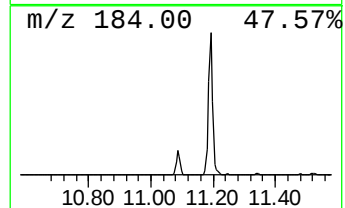
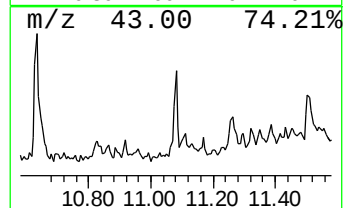
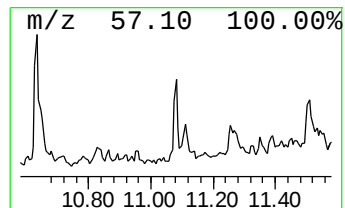
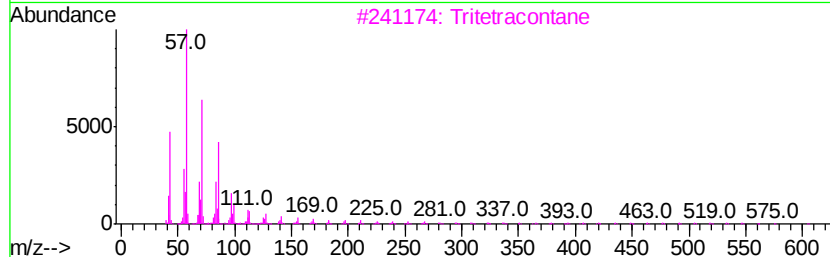
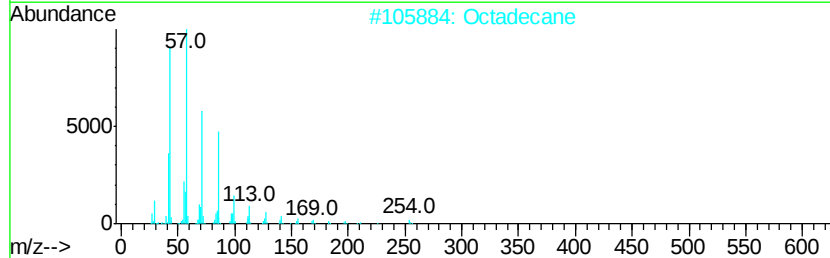
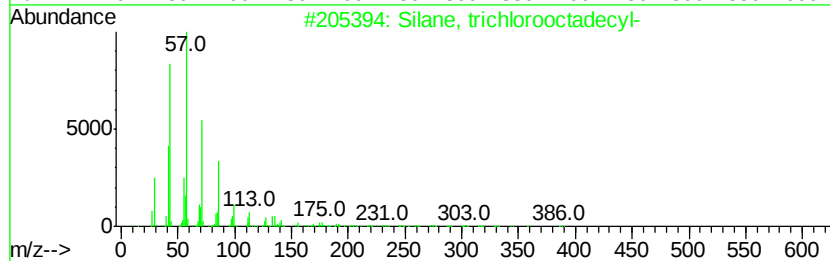
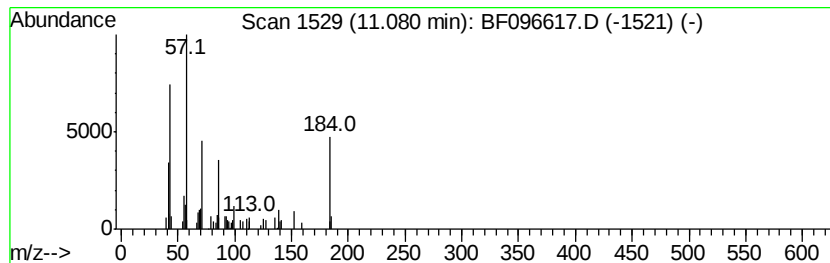
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown11.08 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	2.40 ng	92062	Phenanthrene-d10	11.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	49
2		Octadecane	254	C18H38	000593-45-3	49
3		Tritetracontane	605	C43H88	007098-21-7	46
4		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	46
5		Heptadecane	240	C17H36	000629-78-7	46



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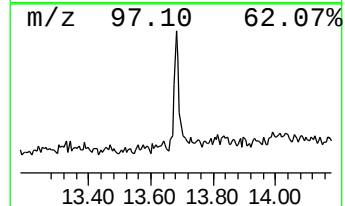
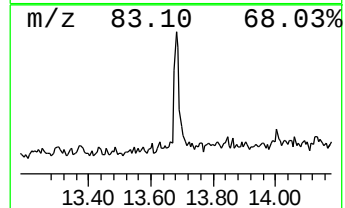
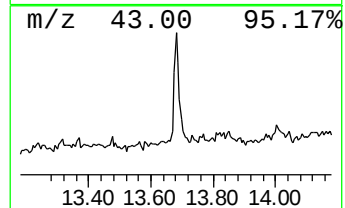
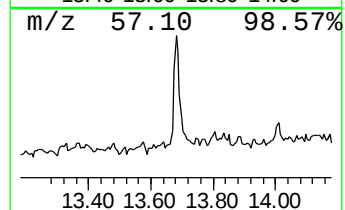
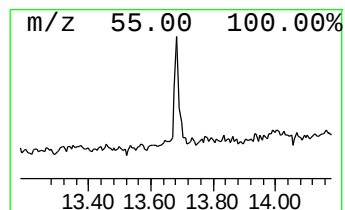
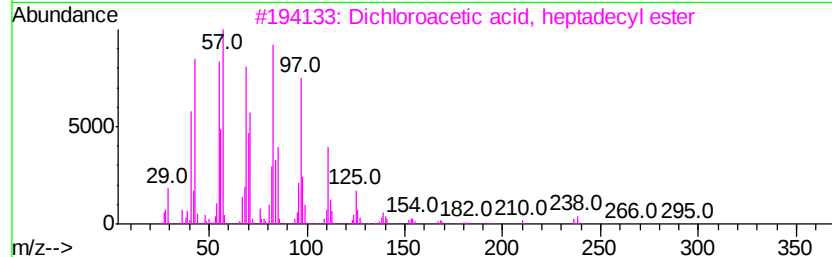
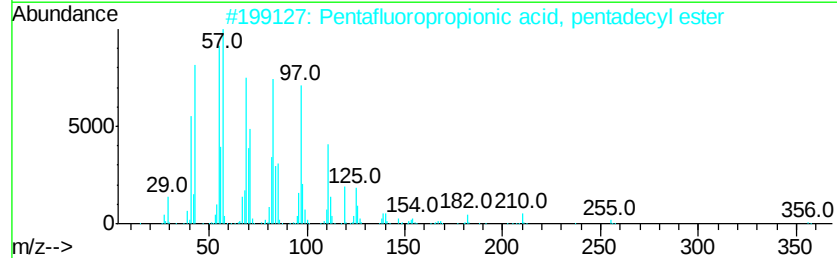
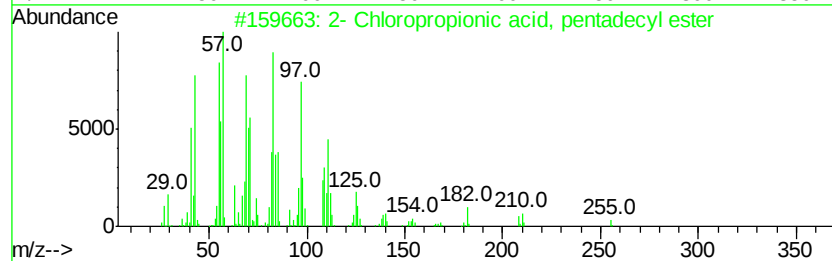
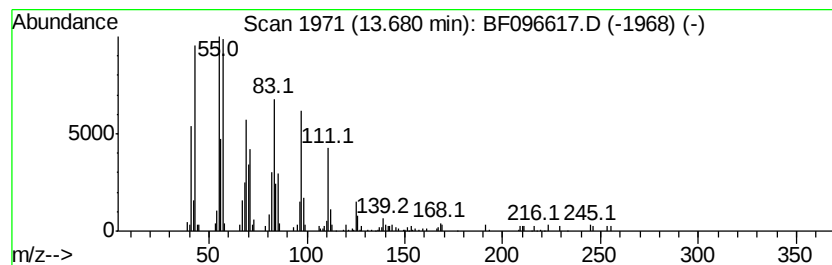
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 2- Chloropropionic acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.70 ng	150990	Chrysene-d12	13.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	94
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	12.3	ng	445235	1	6.68	722305	20.0
unknown6.45	6.45	75.2	ng	2714790	1	6.68	722305	20.0
unknown11.08	11.08	2.4	ng	92062	4	11.19	767720	20.0
2- Chloropropioni...	13.68	3.7	ng	150990	5	13.82	815438	20.0