

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
 Data File : BF096639.D
 Acq On : 11 Jul 2017 12:49
 Operator : SJ/JU
 Sample : I4113-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4(10.0-10.5)

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	2.410	50	55	60	rVB	23190	31194	1.26%	0.137%
2	4.875	469	474	485	rVB	357757	485783	19.65%	2.131%
3	5.298	541	546	550	rBV	2297316	2389812	96.69%	10.486%
4	6.328	716	721	724	rBV	2368567	2412666	97.62%	10.586%
5	6.457	738	743	746	rBV	2542675	2354828	95.28%	10.332%
6	6.687	778	782	785	rBV	699758	611843	24.76%	2.685%
7	6.757	790	794	804	rBV	240089	201215	8.14%	0.883%
8	6.840	804	808	812	rBV	1887828	1805348	73.04%	7.921%
9	7.245	872	877	880	rBV	1590853	1505311	60.90%	6.605%
10	7.963	995	999	1003	rBV	877433	842308	34.08%	3.696%
11	9.045	1177	1183	1186	rBV	2615892	2471573	100.00%	10.844%
12	9.433	1245	1249	1253	rBV	279004	222496	9.00%	0.976%
13	9.716	1292	1297	1301	rBV2	1048546	947044	38.32%	4.155%
14	10.163	1370	1373	1376	rVB	46209	35830	1.45%	0.157%
15	10.504	1426	1431	1434	rBV	1542897	1484178	60.05%	6.512%
16	10.633	1450	1453	1466	rVB	64739	67417	2.73%	0.296%
17	11.080	1526	1529	1532	rBV2	31200	27510	1.11%	0.121%
18	11.192	1544	1548	1552	rBV	1006204	911258	36.87%	3.998%
19	11.733	1635	1640	1644	rBV	70080	66415	2.69%	0.291%
20	12.516	1770	1773	1778	rBV3	28168	32401	1.31%	0.142%
21	12.780	1813	1818	1821	rBV	2199993	2157093	87.28%	9.465%
22	13.680	1968	1971	1978	rBV	140704	151523	6.13%	0.665%
23	13.821	1991	1995	1999	rBV	805698	711588	28.79%	3.122%
24	14.157	2049	2052	2056	rBV	187414	158028	6.39%	0.693%
25	14.674	2137	2140	2145	rVB	29474	31709	1.28%	0.139%
26	15.221	2228	2233	2238	rBV	457864	516022	20.88%	2.264%
27	15.668	2305	2309	2313	rBV3	20101	27362	1.11%	0.120%
28	16.127	2383	2387	2393	rVB2	26401	45234	1.83%	0.198%
29	16.668	2475	2479	2486	rBV5	19057	44598	1.80%	0.196%
30	17.309	2581	2588	2595	rBV5	16319	41576	1.68%	0.182%

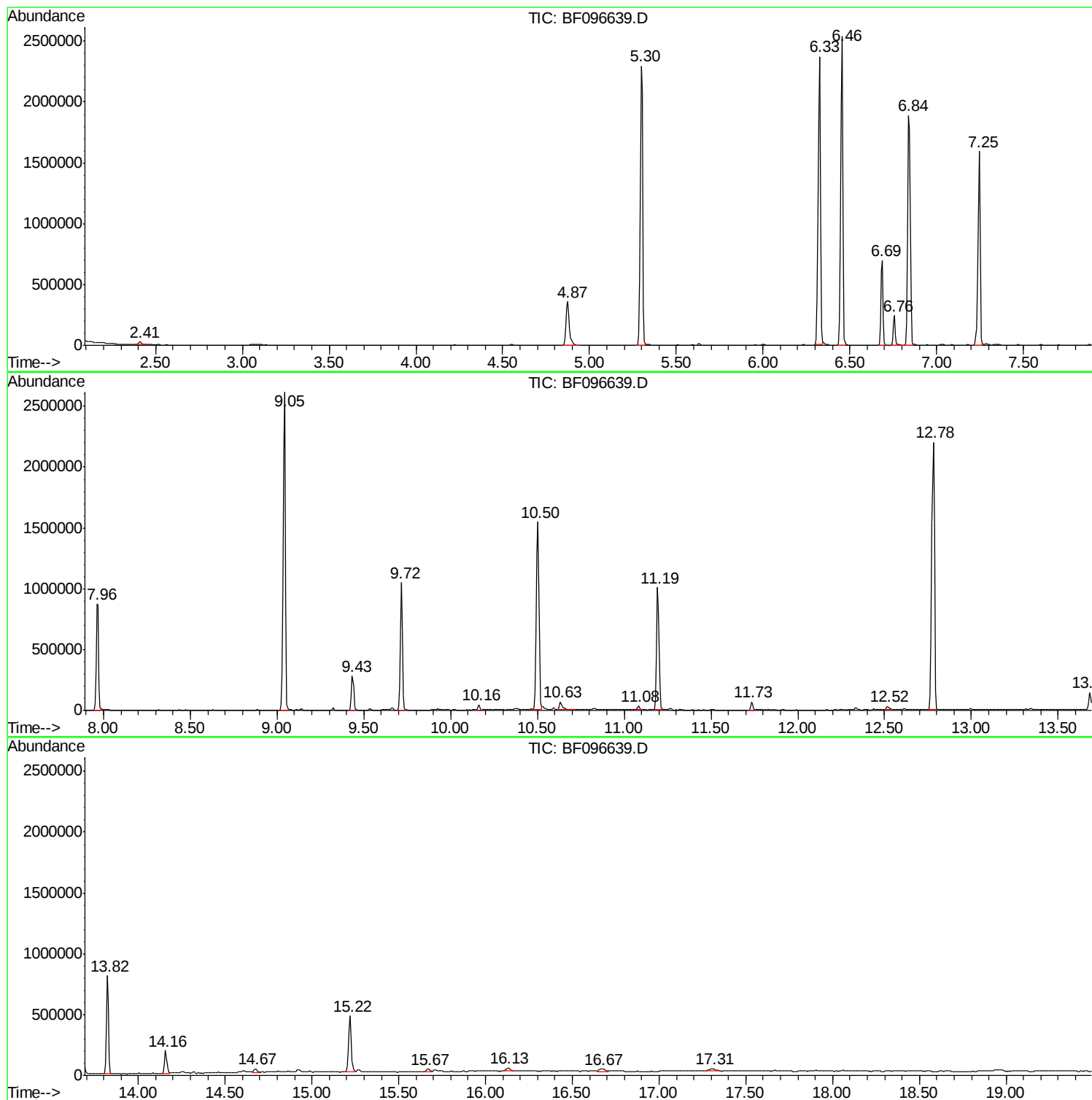
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SB-4(10.0-10.5)

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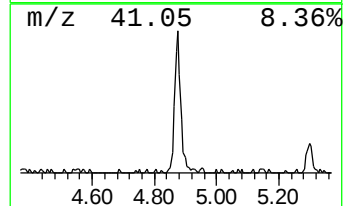
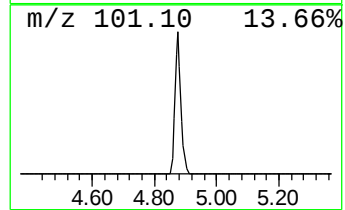
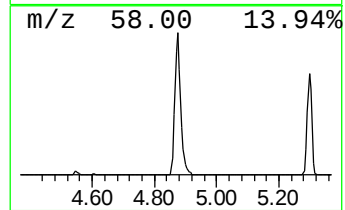
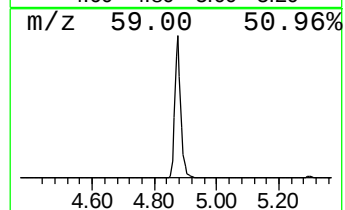
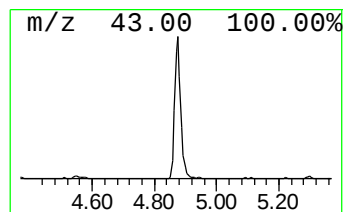
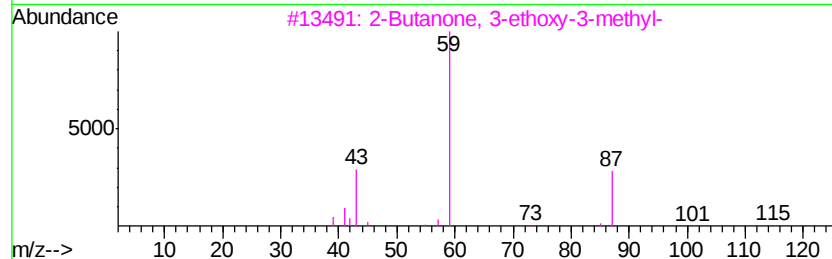
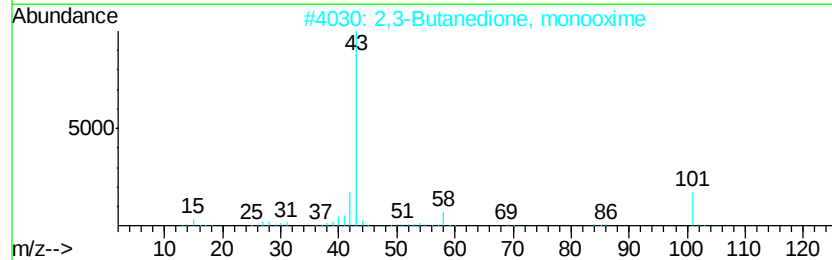
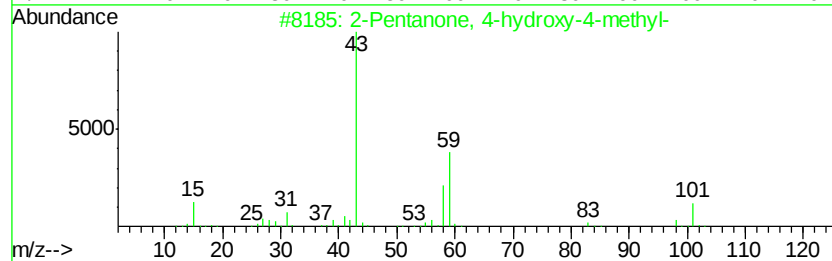
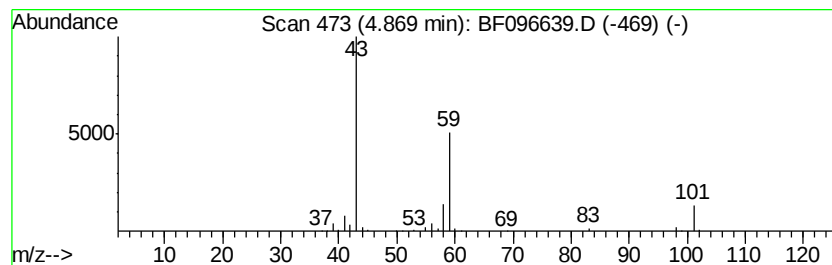
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	15.88 ng	485783	1,4-Dichlorobenzene-d4	6.69

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9
4		Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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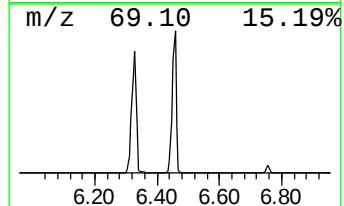
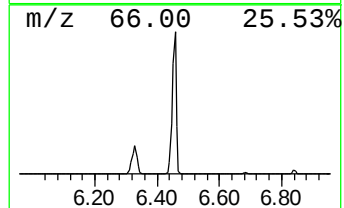
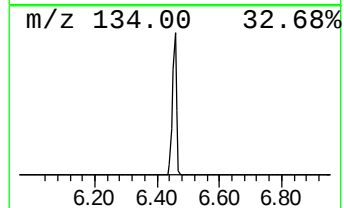
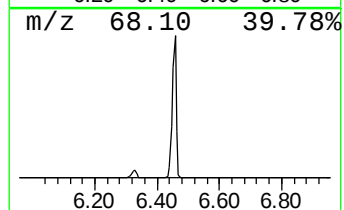
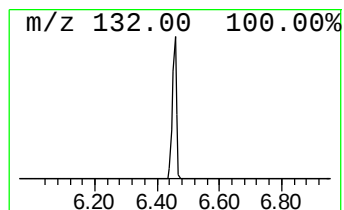
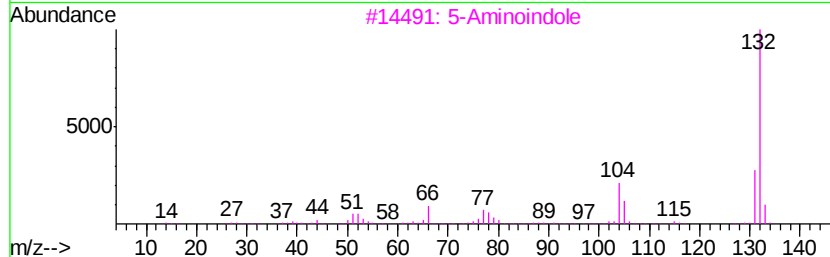
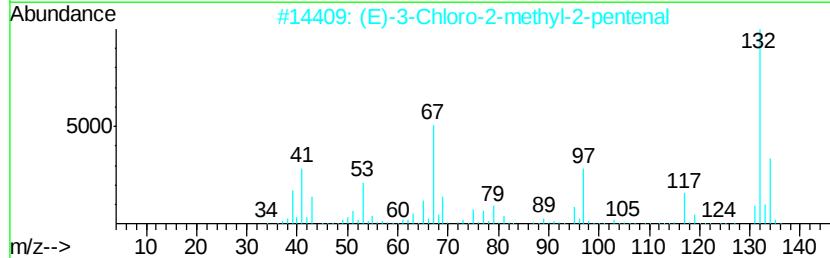
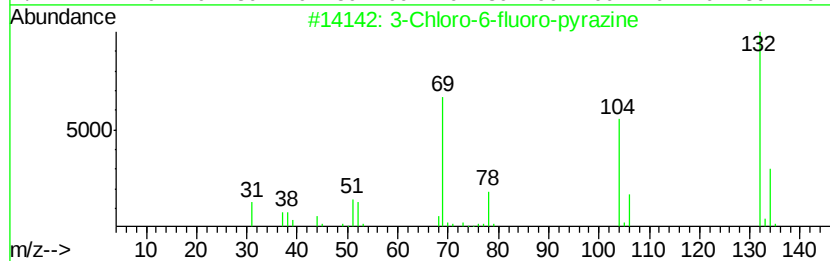
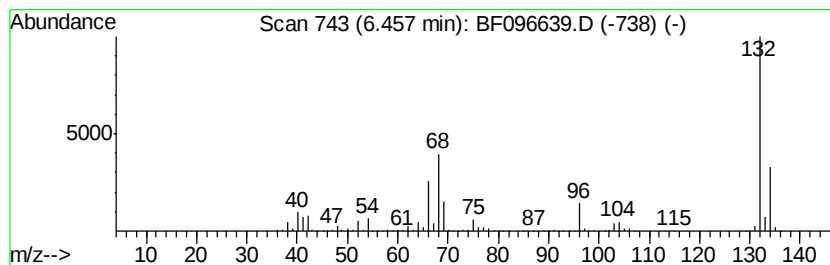
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Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	76.97 ng	2354830	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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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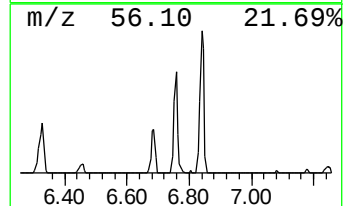
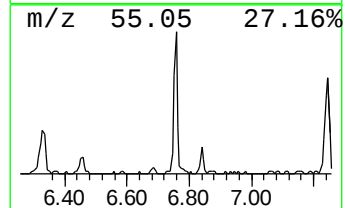
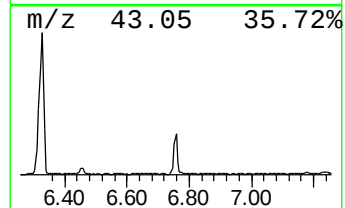
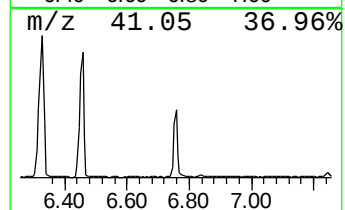
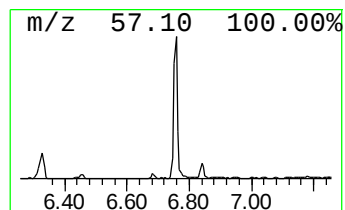
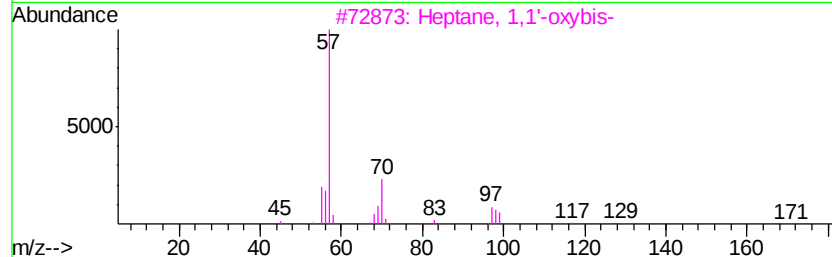
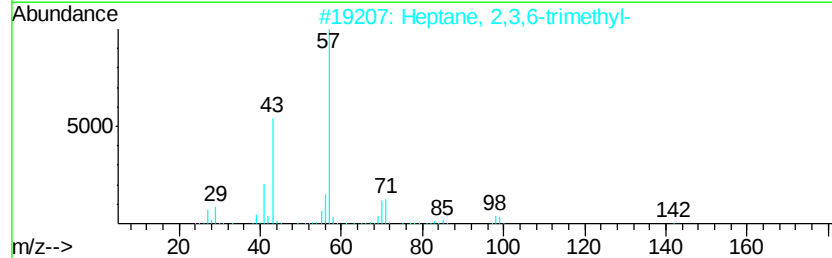
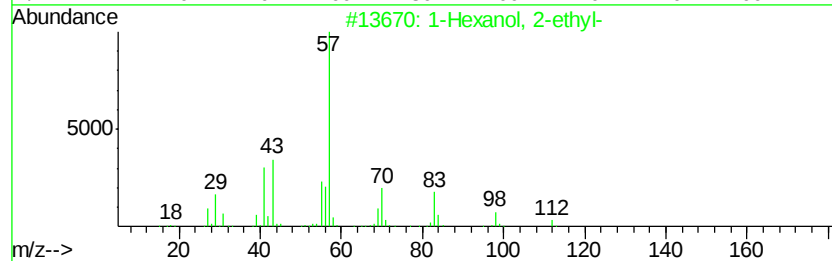
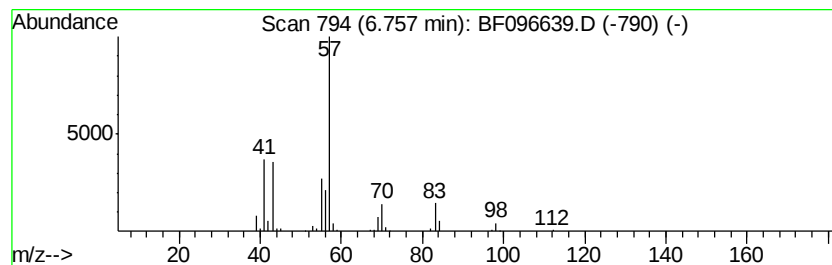
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	6.58 ng	201215	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
5			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	47



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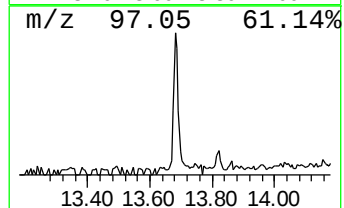
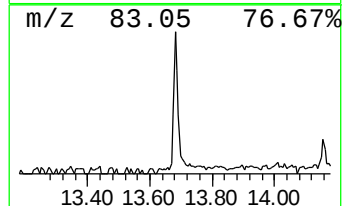
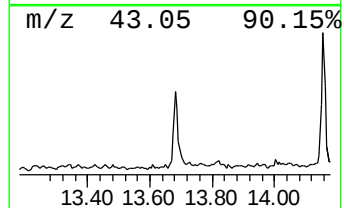
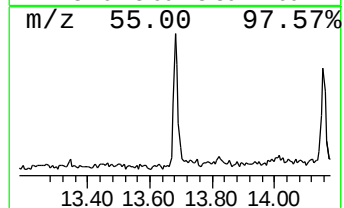
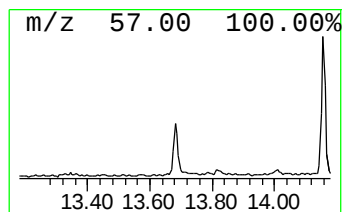
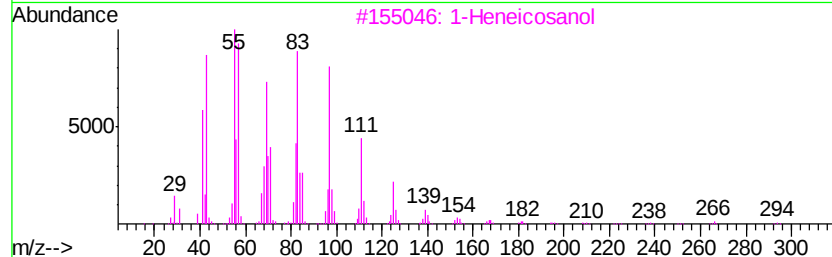
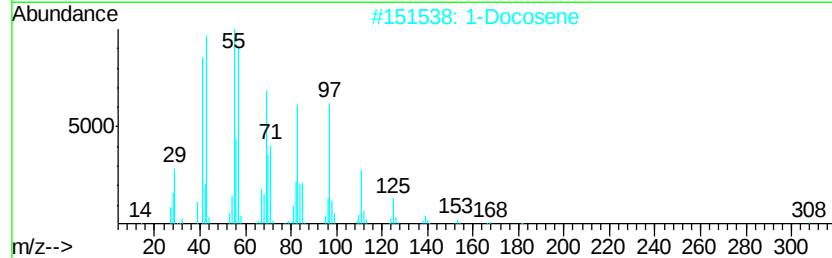
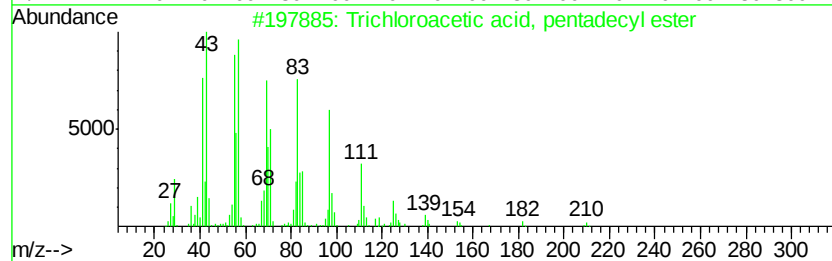
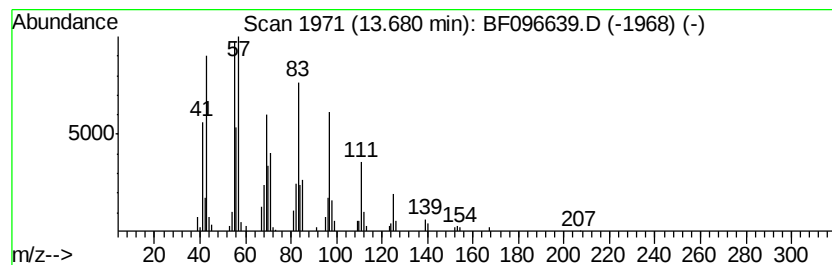
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Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	4.26 ng	151523	Chrysene-d12	13.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
2		1-Docosene	308	C22H44	001599-67-3	91
3		1-Heneicosanol	312	C21H44O	015594-90-8	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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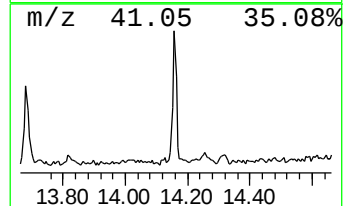
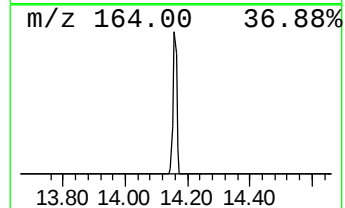
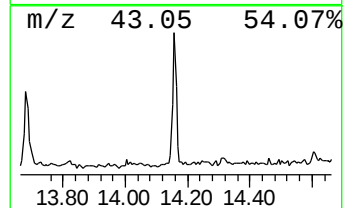
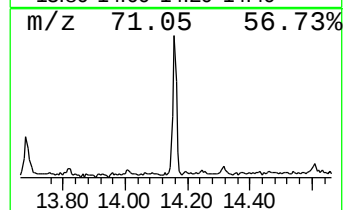
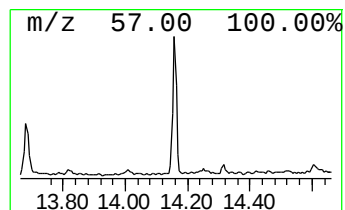
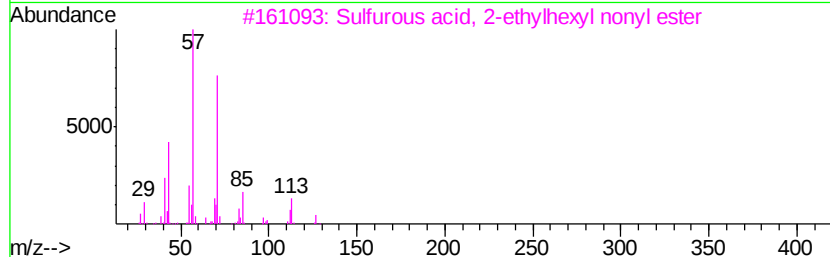
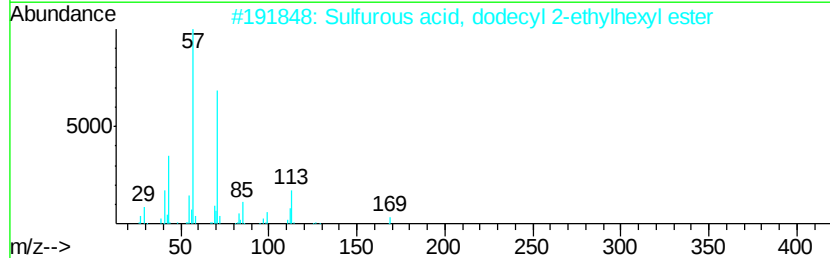
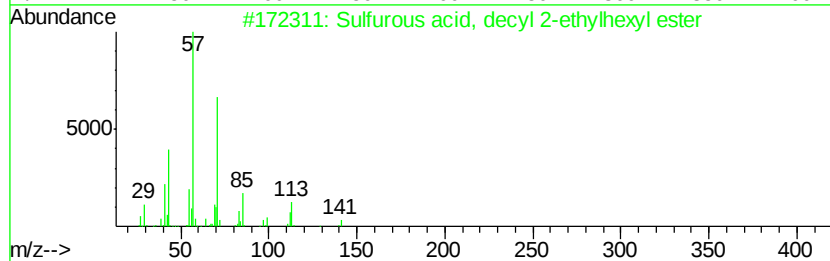
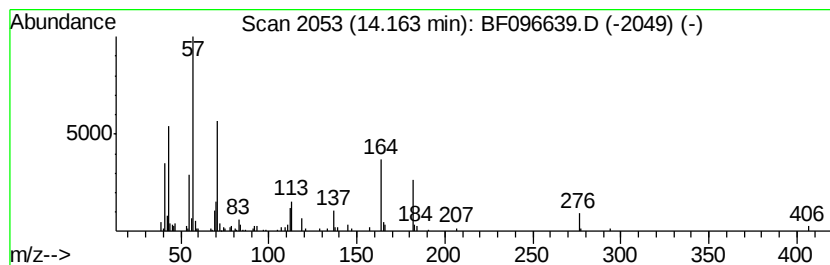
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Peak Number 6 unknown14.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	4.44 ng	158028	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	46
2		Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	46
3		Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	46
4		Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	43
5		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	15.9	ng	485783	1	6.69	611843	20.0
unknown6.46	6.46	77.0	ng	2354830	1	6.69	611843	20.0
1-Hexanol, 2-ethyl-	6.76	6.6	ng	201215	1	6.69	611843	20.0
Trichloroacetic a...	13.68	4.3	ng	151523	5	13.82	711588	20.0
unknown14.16	14.16	4.4	ng	158028	5	13.82	711588	20.0