

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
 Data File : BF097808.D
 Acq On : 18 Aug 2017 1:37
 Operator : SJ/JU
 Sample : I4761-03
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RUSB-03

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-BF081517.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	4.975	486	491	502	rVB	444391	561320	18.14%	2.323%
2	5.387	556	561	564	rBV	2985237	2931597	94.76%	12.132%
3	6.410	729	735	741	rBV	2738900	3093656	100.00%	12.803%
4	6.545	753	758	761	rBV	2989545	2859885	92.44%	11.836%
5	6.775	793	797	801	rVB	1047300	807651	26.11%	3.342%
6	6.934	820	824	827	rBV	2499543	2125683	68.71%	8.797%
7	7.339	888	893	896	rBV	1867827	1710174	55.28%	7.078%
8	8.057	1011	1015	1019	rBV	1165646	946448	30.59%	3.917%
9	9.133	1194	1198	1202	rBV	2639983	2483732	80.28%	10.279%
10	9.527	1261	1265	1269	rBV	338917	253524	8.19%	1.049%
11	9.810	1306	1313	1317	rBV2	940814	813571	26.30%	3.367%
12	10.251	1386	1388	1390	rVB	48445	32806	1.06%	0.136%
13	10.469	1420	1425	1428	rBV	49761	75297	2.43%	0.312%
14	10.598	1442	1447	1450	rBV	1312634	1131636	36.58%	4.683%
15	10.739	1465	1471	1477	rBV2	90723	154219	4.99%	0.638%
16	11.204	1547	1550	1552	rVB	64175	59761	1.93%	0.247%
17	11.292	1562	1565	1569	rBV	819565	712979	23.05%	2.951%
18	12.880	1831	1835	1839	rBV	2148535	1950364	63.04%	8.072%
19	13.780	1985	1988	1996	rVB	100303	116716	3.77%	0.483%
20	13.927	2009	2013	2017	rBV	881069	763545	24.68%	3.160%
21	14.851	2167	2170	2176	rBV6	31743	38187	1.23%	0.158%
22	15.357	2251	2256	2262	rBV	468638	540628	17.48%	2.237%

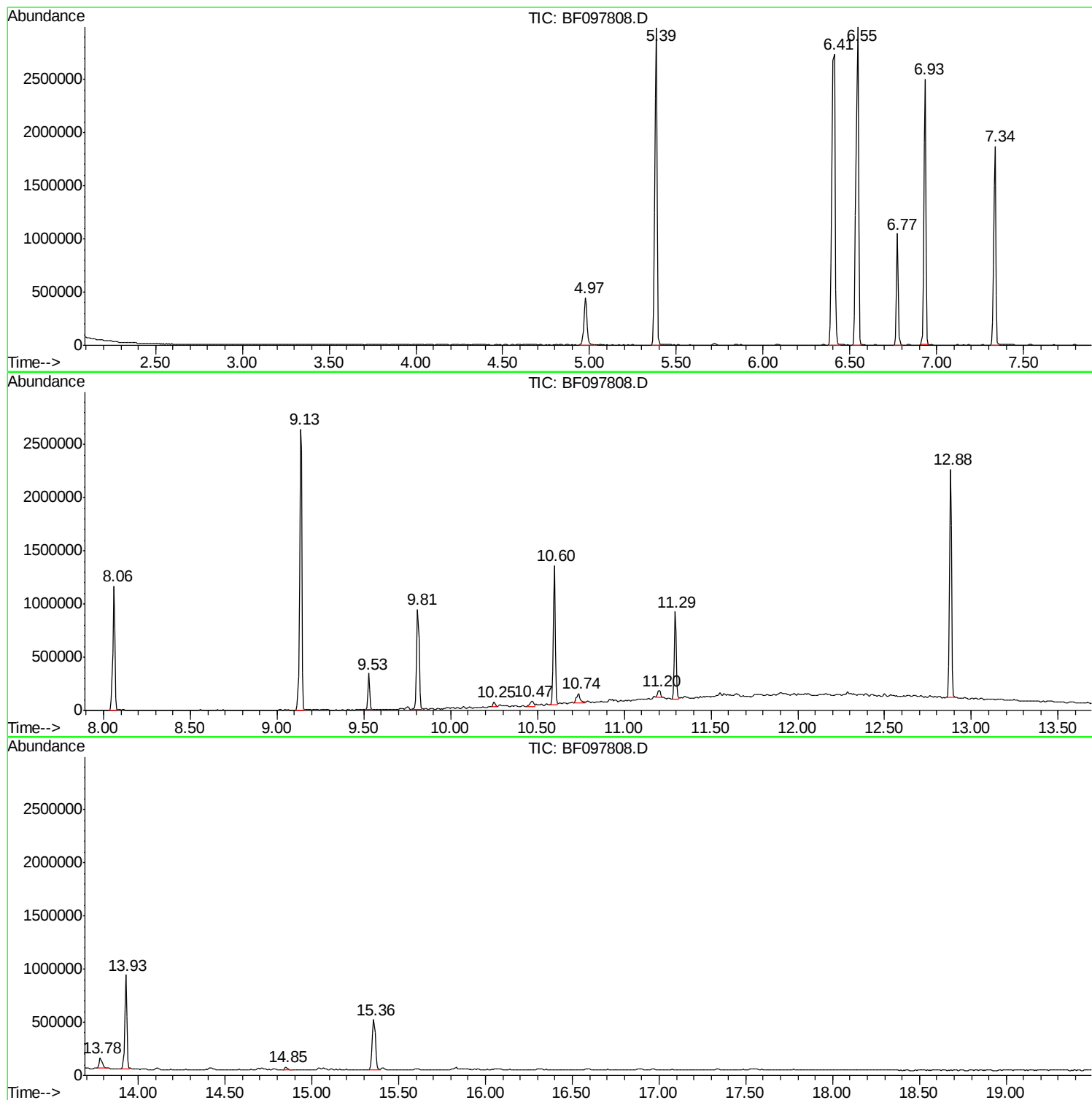
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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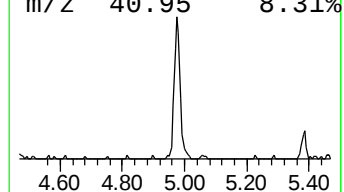
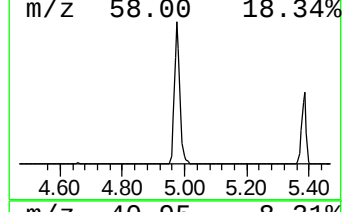
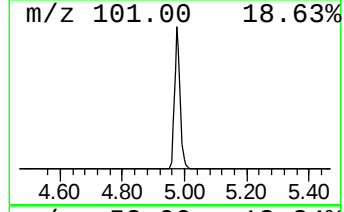
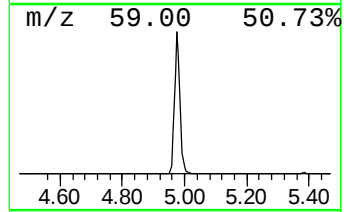
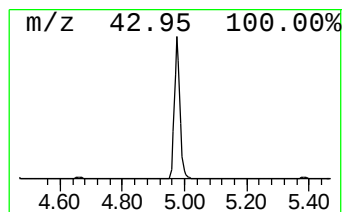
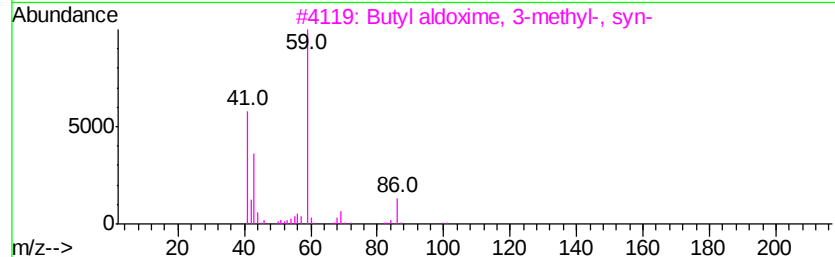
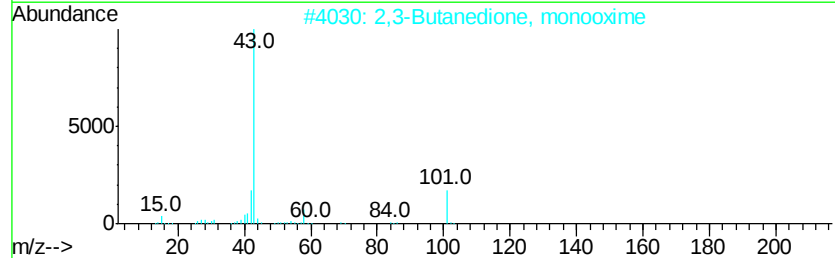
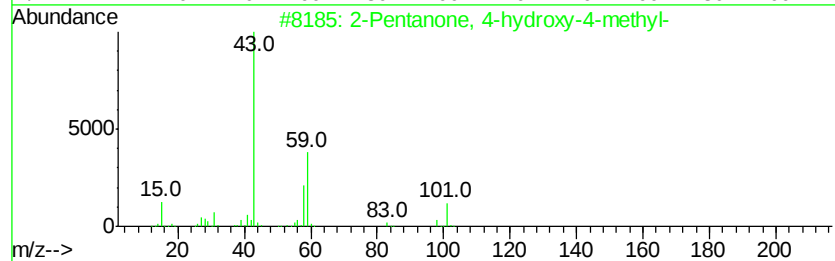
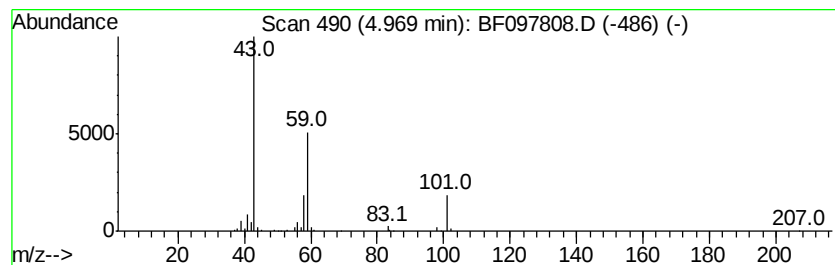
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.97	13.90 ng	561320	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		
4	Acetone	58	C3H6O	000067-64-1	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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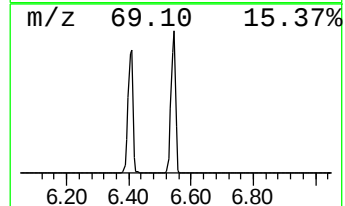
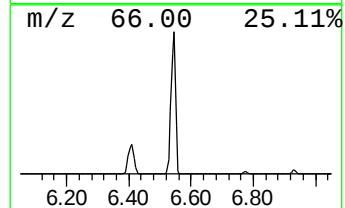
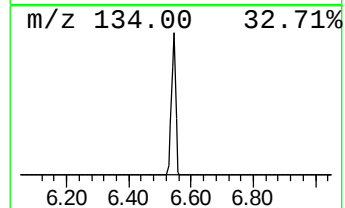
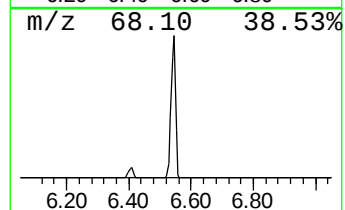
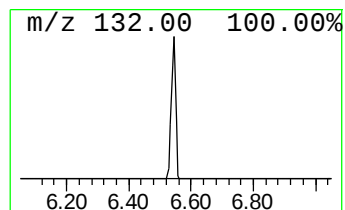
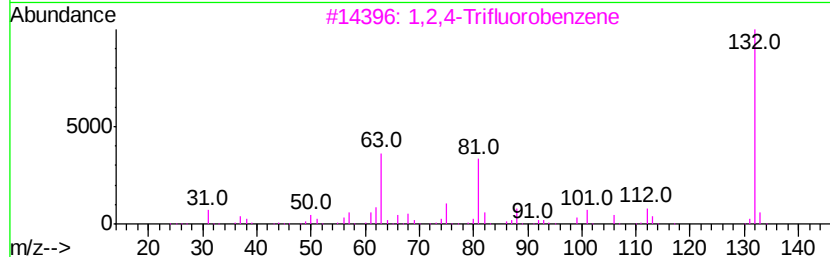
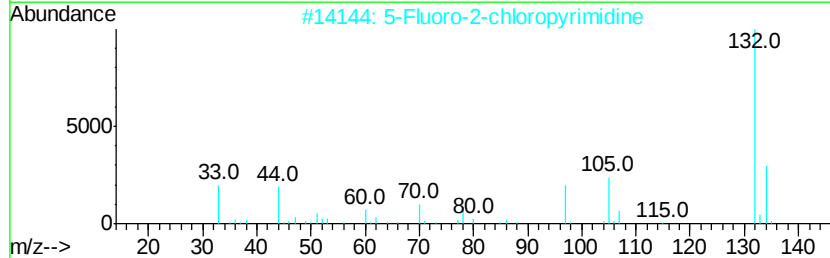
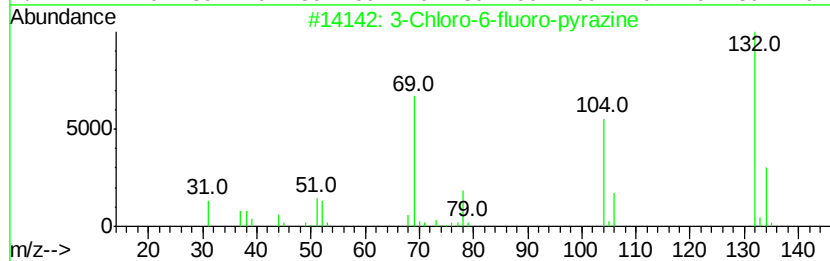
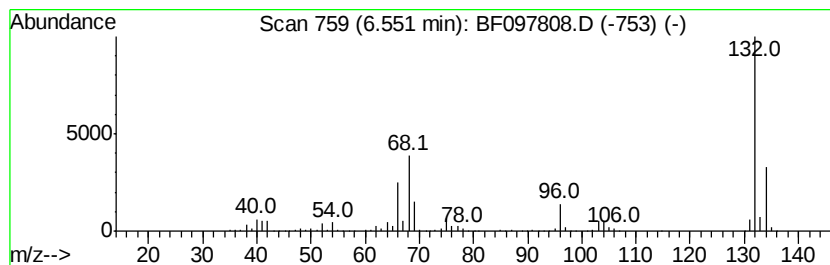
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	70.82 ng	2859890	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3			1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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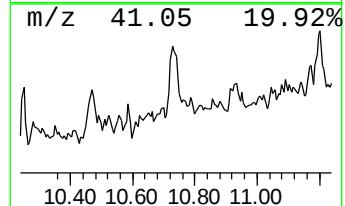
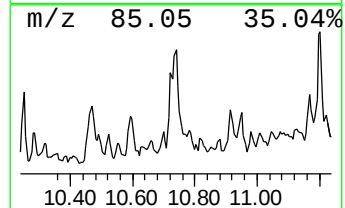
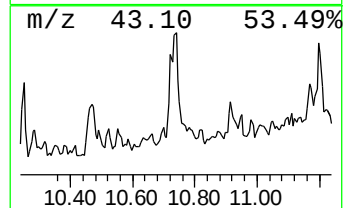
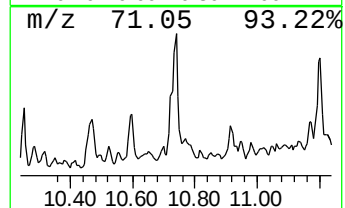
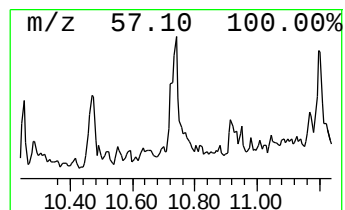
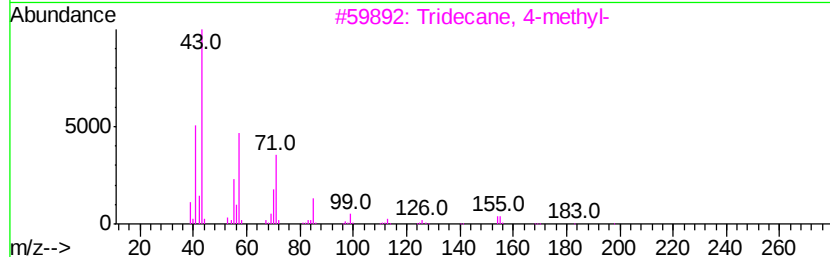
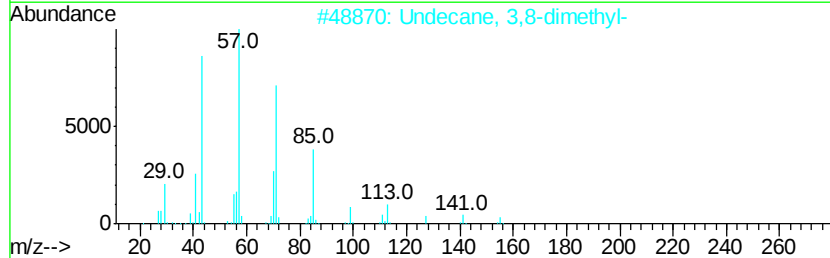
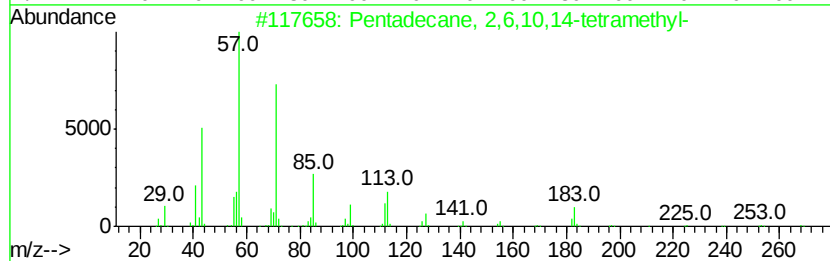
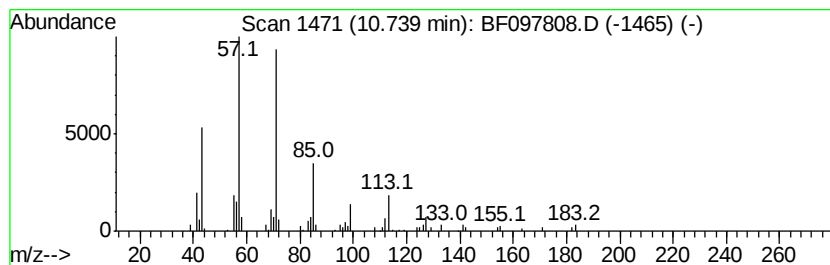
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Peak Number 4 Pentadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.74	4.33 ng	154219	Phenanthrene-d10	11.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	83
2		Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	83
3		Tridecane, 4-methyl-	198	C14H30	026730-12-1	80
4		Decane, 5-propyl-	184	C13H28	017312-62-8	78
5		Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	78



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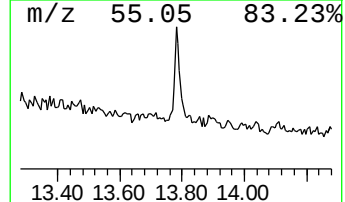
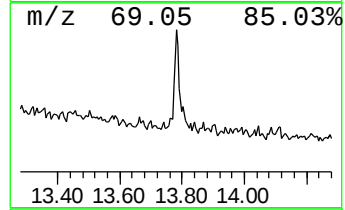
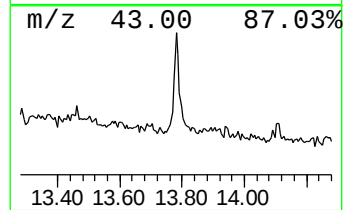
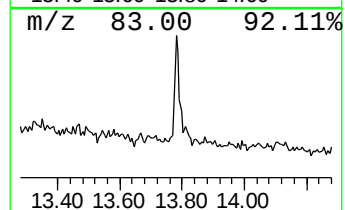
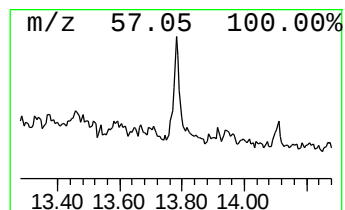
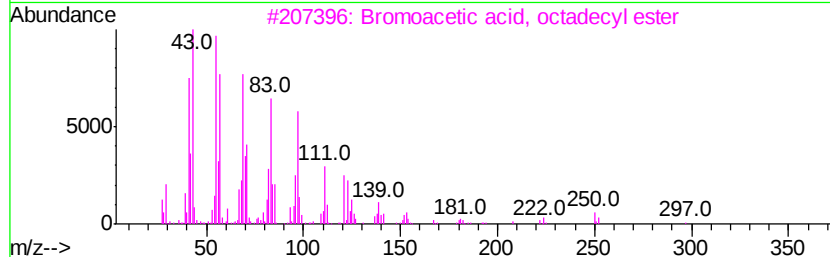
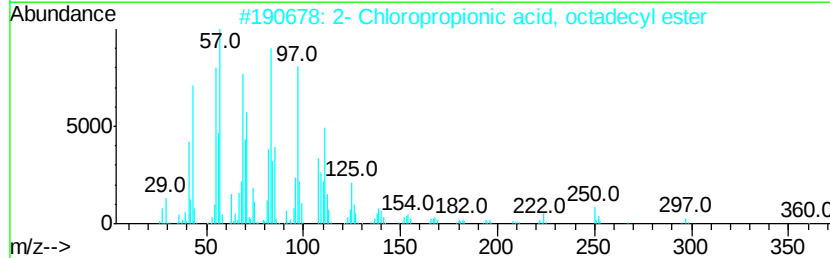
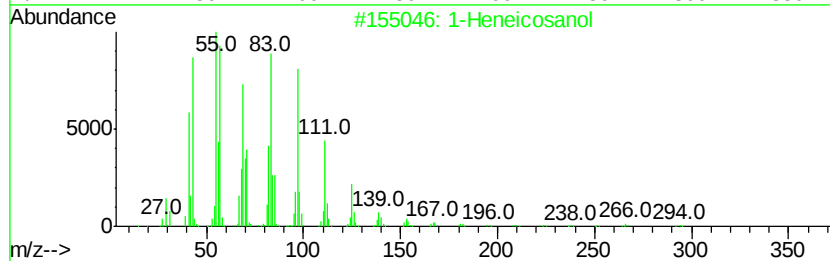
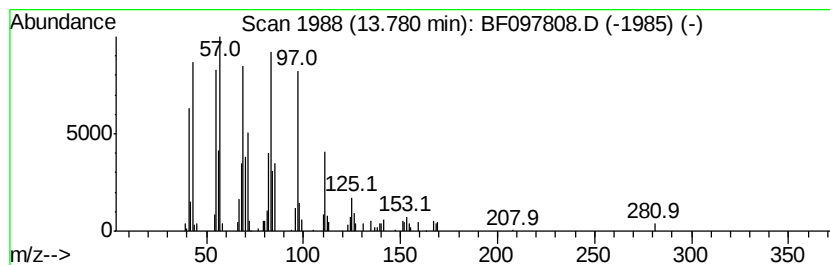
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.78	3.06 ng	116716	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
4	11-Tricosene	322	C23H46	052078-56-5	87
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	13.9	ng	561320	1	6.77	807651	20.0
unknown6.55	6.55	70.8	ng	2859890	1	6.77	807651	20.0
Pentadecane, 2,6,...	10.74	4.3	ng	154219	4	11.29	712979	20.0
1-Heneicosanol	13.78	3.1	ng	116716	5	13.93	763545	20.0