

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080117\
 Data File : BF097244.D
 Acq On : 1 Aug 2017 21:05
 Operator : SJ/JU
 Sample : I4512-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HDD-PILWC4

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-BF072517.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	2.634	124	127	140	rBV	153634	293919	10.49%	1.374%
2	4.604	458	462	476	rBV	307964	533660	19.05%	2.495%
3	5.075	538	542	560	rBV	2510516	2801897	100.00%	13.099%
4	6.140	718	723	736	rBV	2497557	2654530	94.74%	12.410%
5	6.240	736	740	753	rVB	2612459	2574366	91.88%	12.035%
6	6.463	775	778	786	rBV	767456	642888	22.94%	3.005%
7	6.622	801	805	808	rBV	2196574	2039858	72.80%	9.536%
8	7.034	870	875	878	rBV	1903994	1735399	61.94%	8.113%
9	7.181	897	900	905	rBV	28361	32160	1.15%	0.150%
10	7.675	981	984	992	rBV	47763	63442	2.26%	0.297%
11	7.745	992	996	1001	rBV	956309	803089	28.66%	3.754%
12	8.828	1175	1180	1183	rBV	2228921	2029912	72.45%	9.490%
13	9.228	1244	1248	1251	rBV	470309	418195	14.93%	1.955%
14	9.492	1289	1293	1302	rVB	769490	643586	22.97%	3.009%
15	9.945	1368	1370	1374	rVB	43694	33334	1.19%	0.156%
16	10.280	1423	1427	1434	rBV	1025594	959239	34.24%	4.484%
17	10.416	1447	1450	1457	rBV	54000	61139	2.18%	0.286%
18	10.863	1522	1526	1529	rBV	34584	29957	1.07%	0.140%
19	10.963	1540	1543	1547	rBV	566585	495676	17.69%	2.317%
20	11.522	1635	1638	1646	rBV4	21663	28555	1.02%	0.133%
21	12.551	1808	1813	1816	rBV	1373602	1324507	47.27%	6.192%
22	13.468	1963	1969	1977	rBV2	76624	122367	4.37%	0.572%
23	13.586	1985	1989	1998	rBV	587434	587107	20.95%	2.745%
24	14.351	2116	2119	2122	rBV	70740	70204	2.51%	0.328%
25	14.933	2214	2218	2223	rBV	387696	411735	14.69%	1.925%

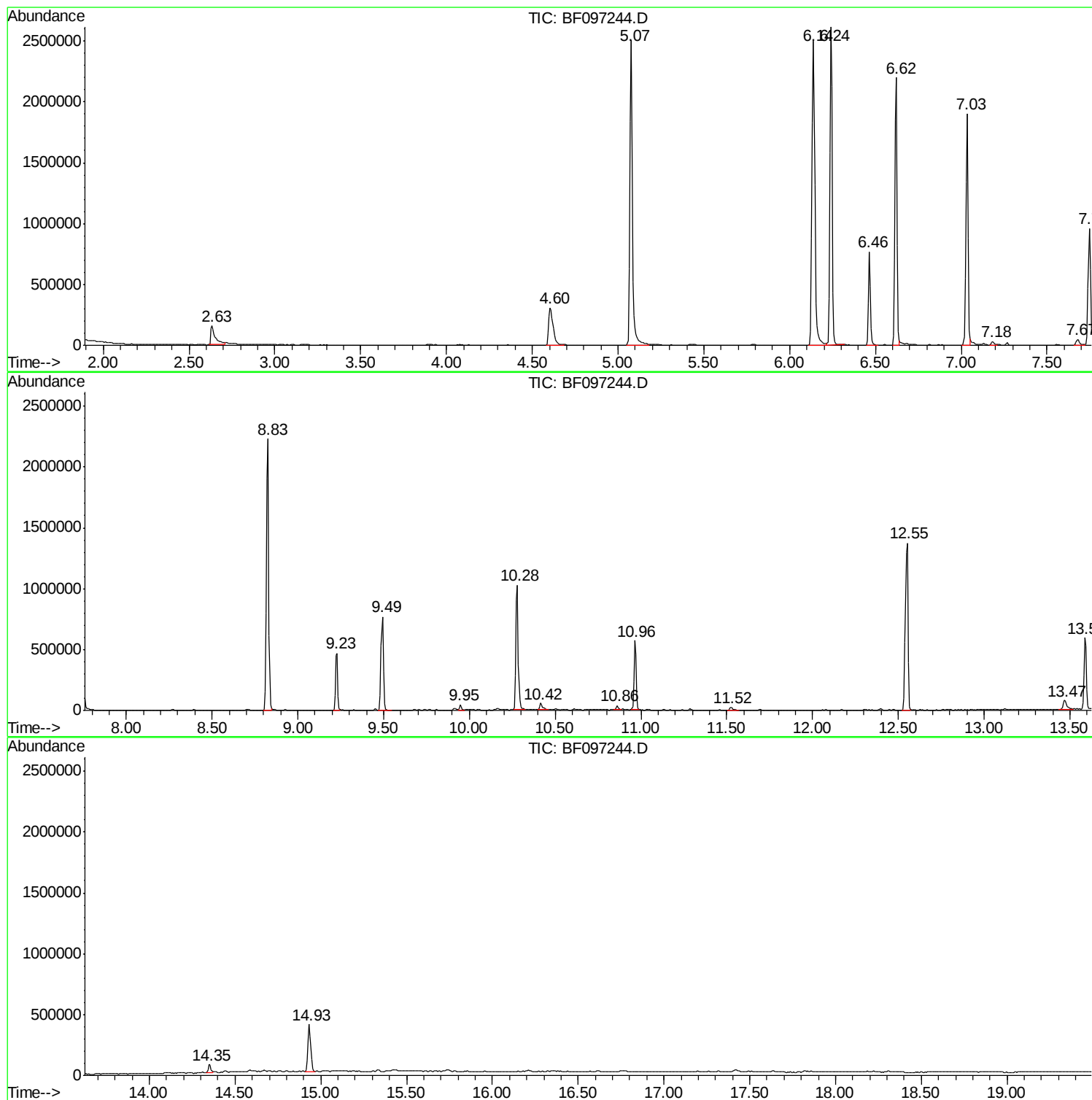
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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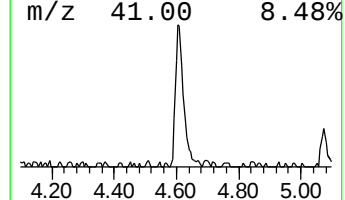
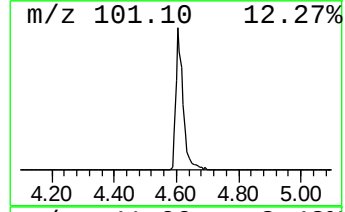
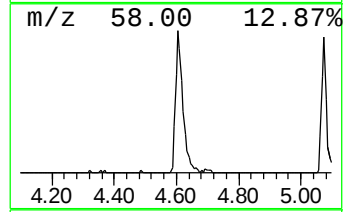
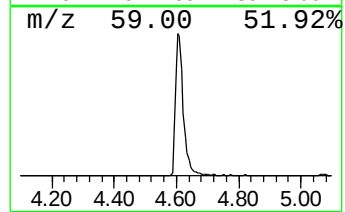
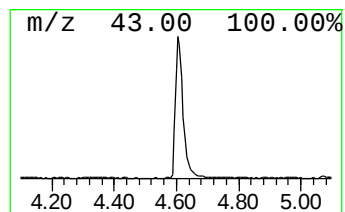
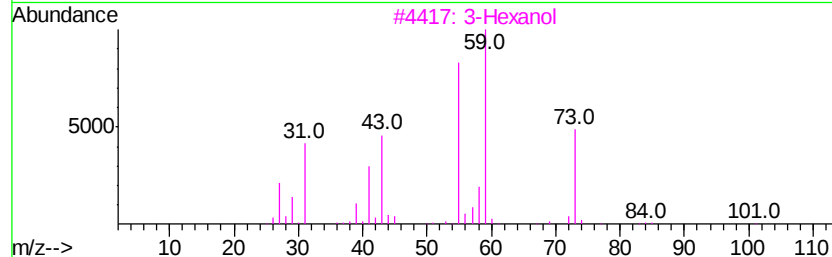
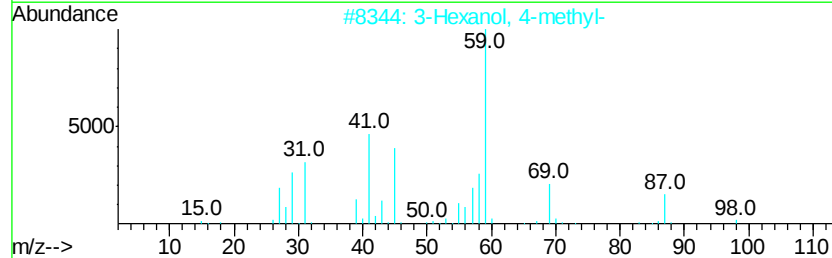
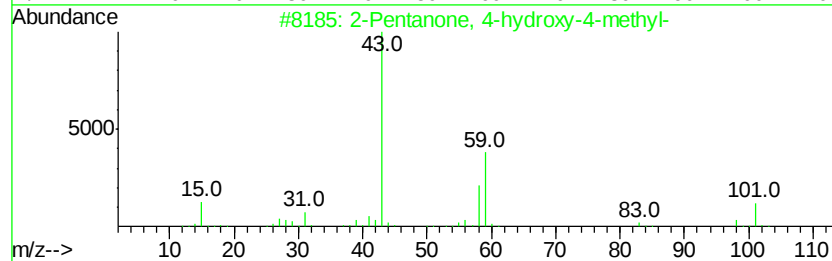
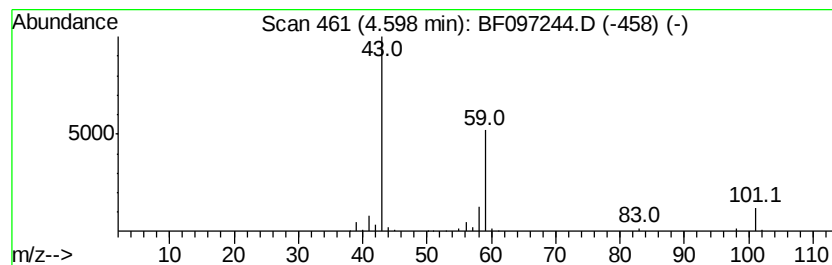
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.60	16.60 ng	533660	1,4-Dichlorobenzene-d4	6.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	33
3	3-Hexanol	102	C6H14O		000623-37-0	33
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	25



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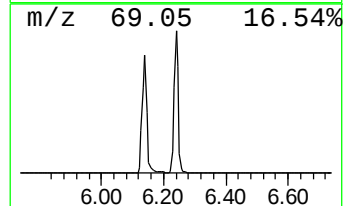
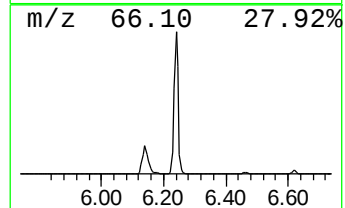
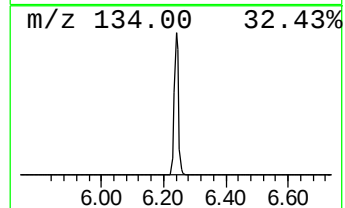
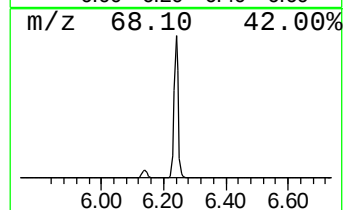
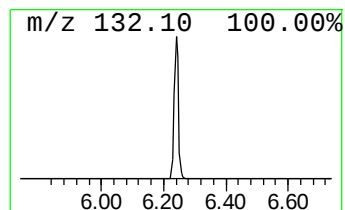
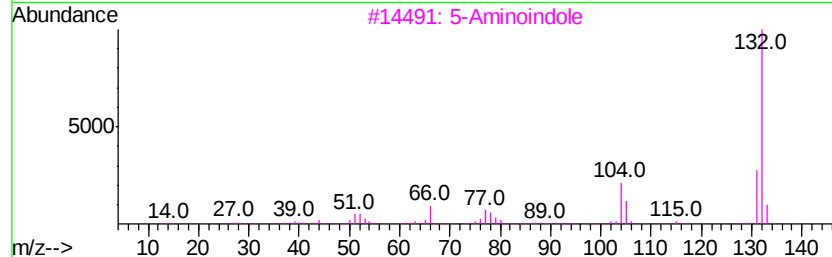
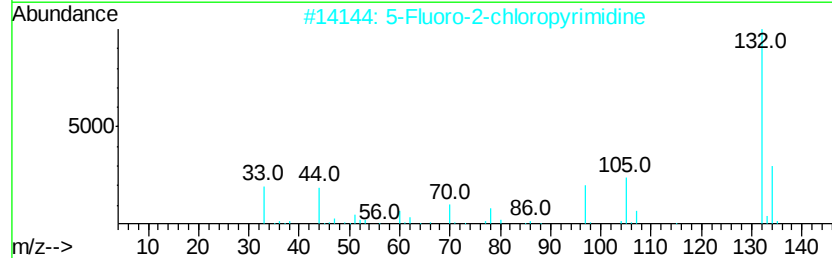
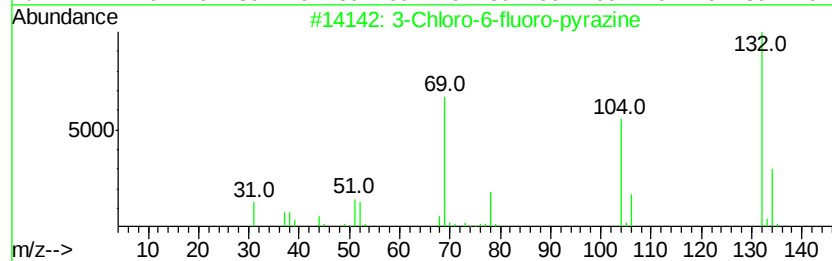
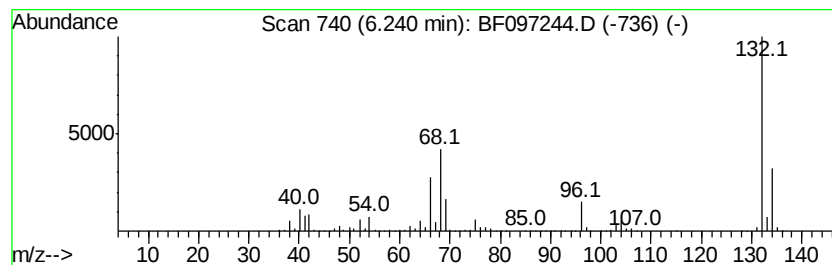
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Peak Number 3 unknown6.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	80.09 ng	2574370	1,4-Dichlorobenzene-d4	6.46

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	5-Aminoindole	132	C8H8N2	005192-03-0	12		
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10		
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9		



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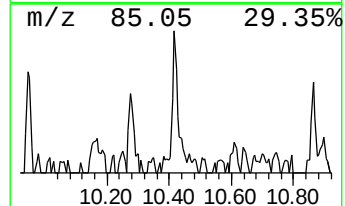
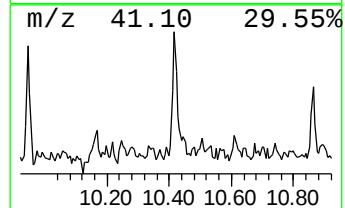
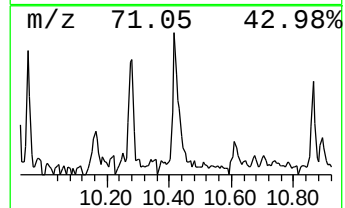
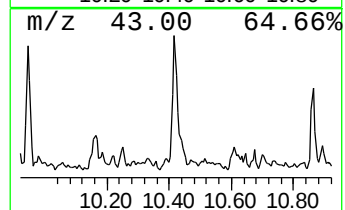
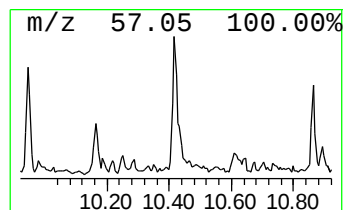
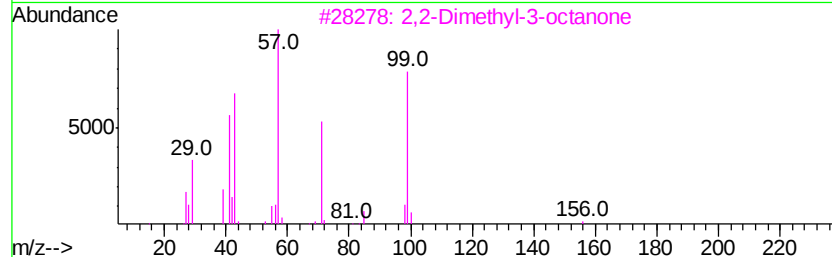
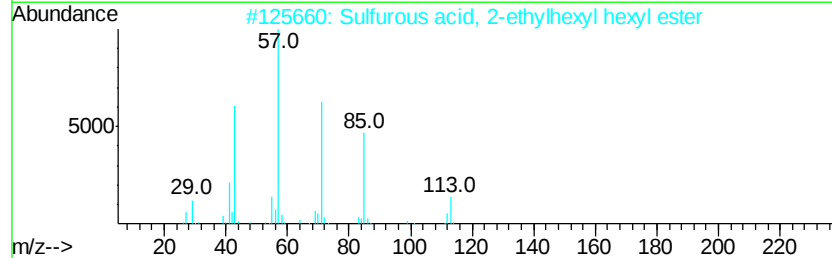
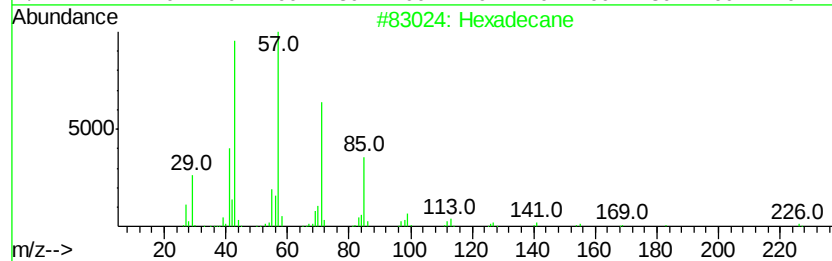
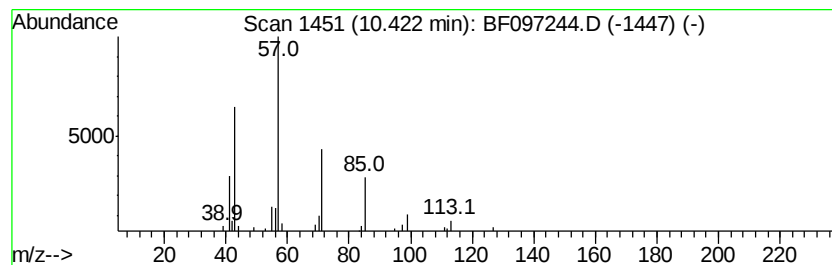
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.42	2.47 ng	61139	Phenanthrene-d10	10.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	78
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
3	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	59
4	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	50
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	47



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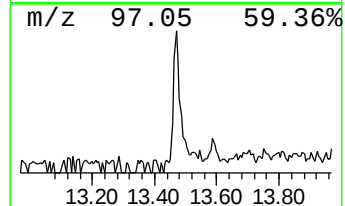
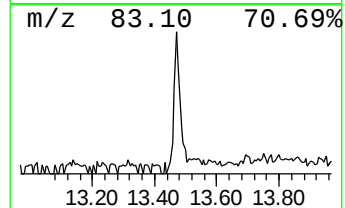
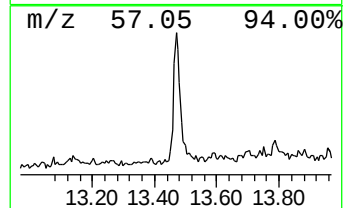
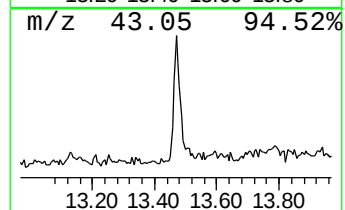
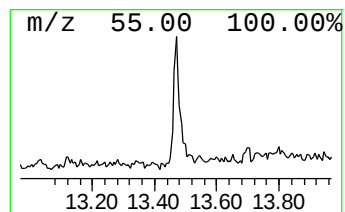
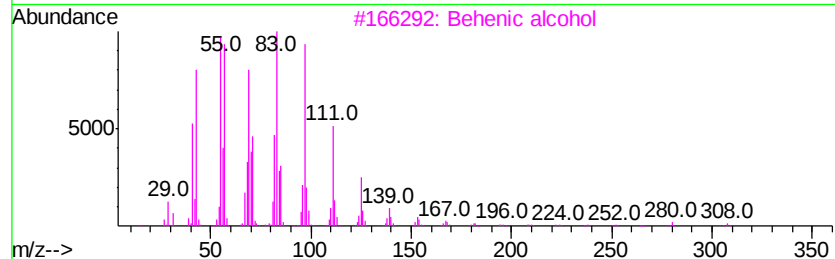
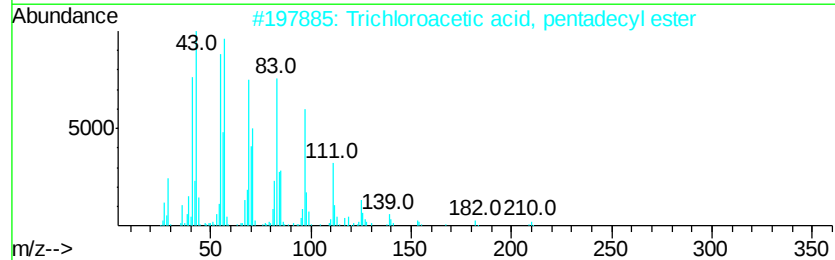
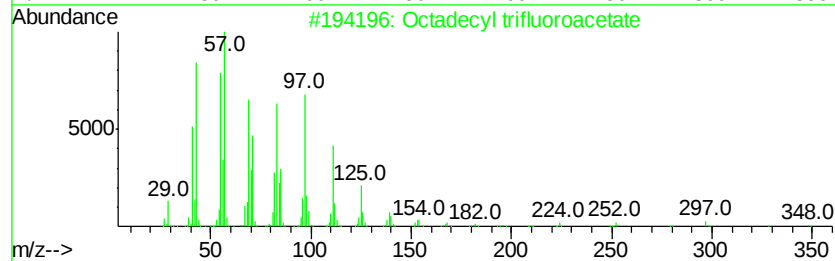
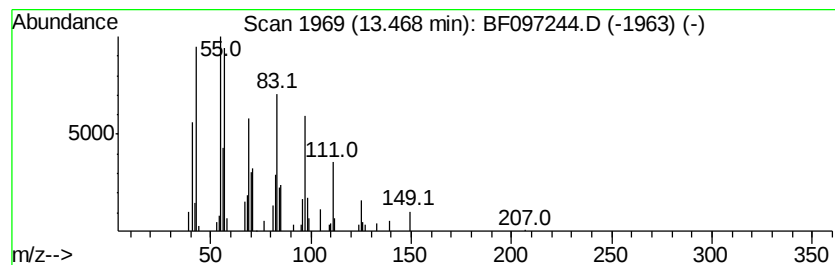
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Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	4.17 ng	122367	Chrysene-d12	13.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3		Behenic alcohol	326	C22H46O	000661-19-8	87
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
5		11-Tricosene	322	C23H46	052078-56-5	87



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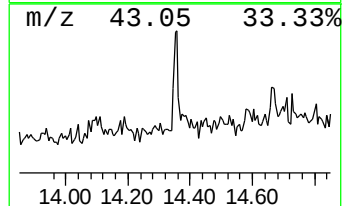
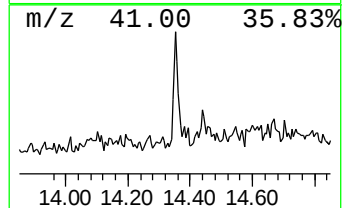
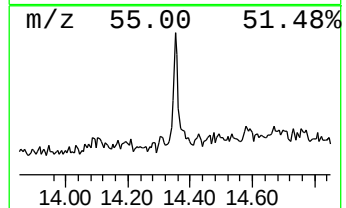
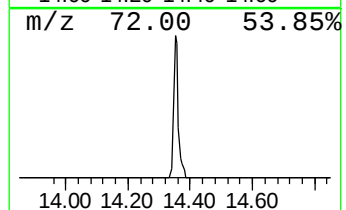
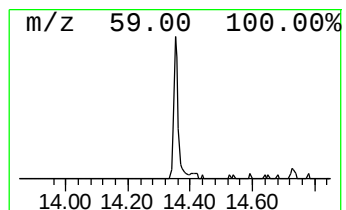
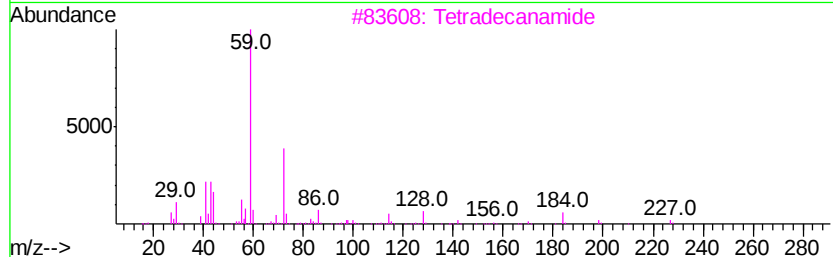
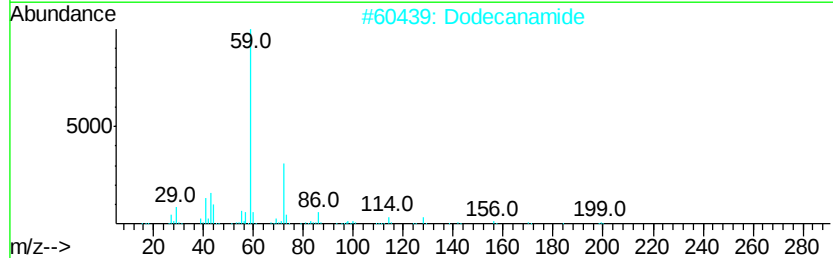
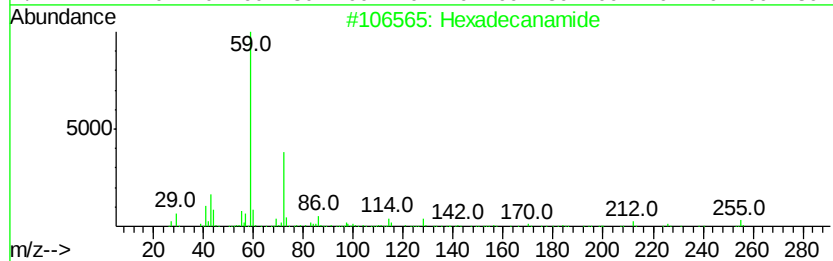
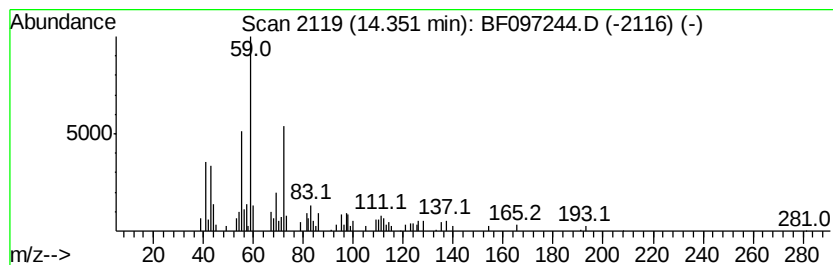
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Peak Number 7 Hexadecanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.41 ng	70204	Perylene-d12	14.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide		255	C16H33NO	000629-54-9	72
2	Dodecanamide		199	C12H25NO	001120-16-7	59
3	Tetradecanamide		227	C14H29NO	000638-58-4	59
4	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	52
5	7-Nonenamide		155	C9H17NO	090949-53-4	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.60	16.6	ng	533660	1	6.46	642888	20.0
unknown6.24	6.24	80.1	ng	2574370	1	6.46	642888	20.0
Hexadecane	10.42	2.5	ng	61139	4	10.96	495676	20.0
Octadecyl trifluo...	13.47	4.2	ng	122367	5	13.59	587107	20.0
Hexadecanamide	14.35	3.4	ng	70204	6	14.93	411735	20.0