

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
 Data File : BF097799.D
 Acq On : 17 Aug 2017 21:23
 Operator : SJ/JU
 Sample : I4808-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-TP106-I(0-5)COMP

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:\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	4.987	488	493	505	rVB	368177	525209	13.47%	1.749%
2	5.393	556	562	565	rBV	3594039	3810226	97.75%	12.690%
3	6.410	729	735	738	rBV	3459601	3897911	100.00%	12.982%
4	6.545	753	758	761	rBV	3684531	3648312	93.60%	12.150%
5	6.775	794	797	801	rBV	1107129	860590	22.08%	2.866%
6	6.934	820	824	827	rBV	3140874	2796380	71.74%	9.313%
7	7.340	888	893	896	rBV	2316872	2284922	58.62%	7.610%
8	8.057	1011	1015	1019	rBV	1217314	1019845	26.16%	3.397%
9	9.139	1193	1199	1202	rBV	3463673	3214498	82.47%	10.706%
10	9.528	1261	1265	1269	rBV	396587	305398	7.83%	1.017%
11	9.810	1309	1313	1317	rBV	964420	870310	22.33%	2.898%
12	10.598	1442	1447	1450	rBV	1762131	1573586	40.37%	5.241%
13	11.292	1561	1565	1568	rBV	854004	752230	19.30%	2.505%
14	12.504	1768	1771	1775	rVB	49236	41342	1.06%	0.138%
15	12.727	1804	1809	1812	rBV	49459	55512	1.42%	0.185%
16	12.880	1831	1835	1839	rBV	2550818	2408159	61.78%	8.020%
17	13.780	1985	1988	1994	rBV2	109289	124130	3.18%	0.413%
18	13.927	2009	2013	2016	rBV	903353	805508	20.67%	2.683%
19	14.692	2139	2143	2150	rBV	387901	483195	12.40%	1.609%
20	15.357	2252	2256	2261	rBV	479070	549020	14.08%	1.828%

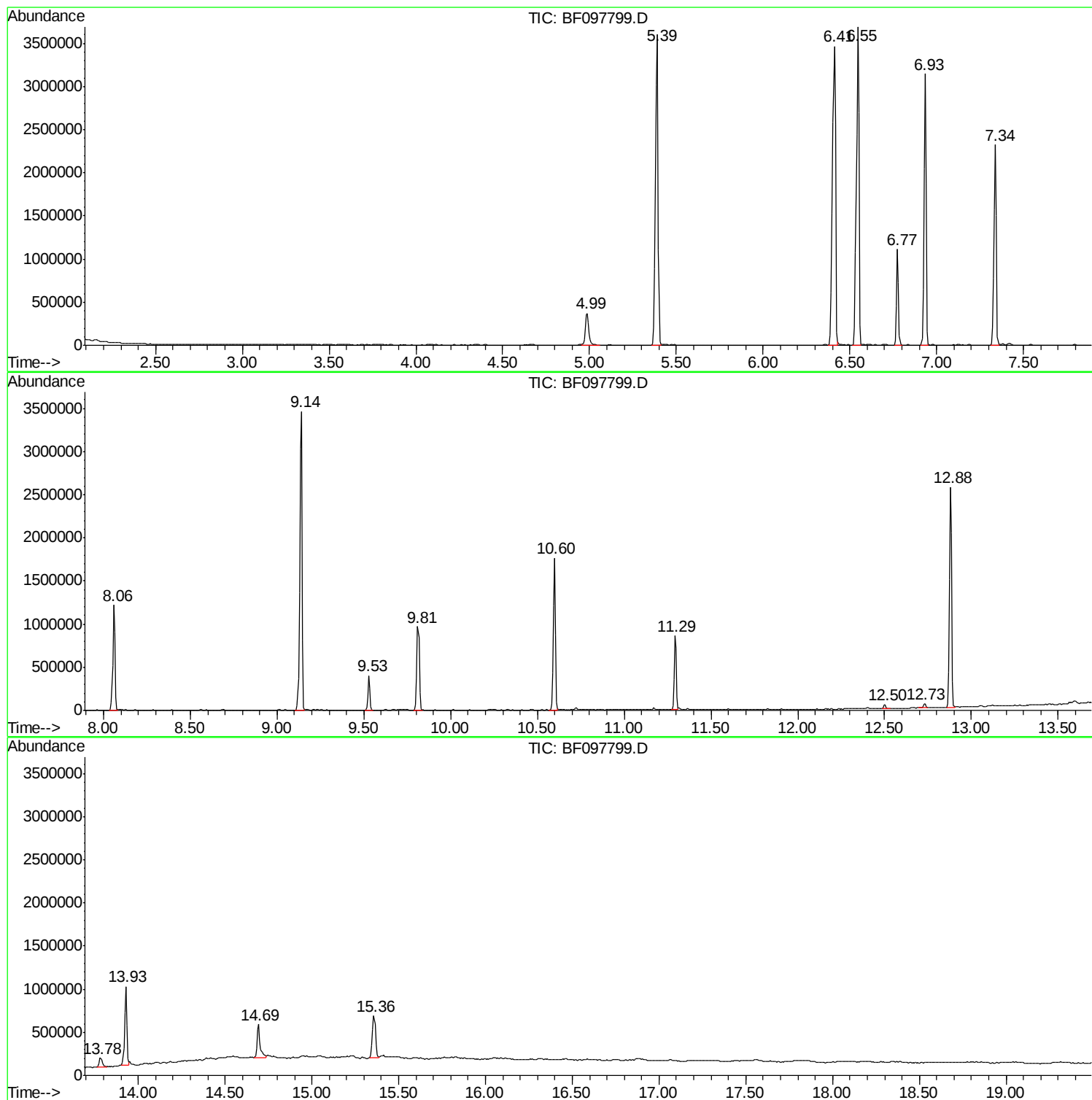
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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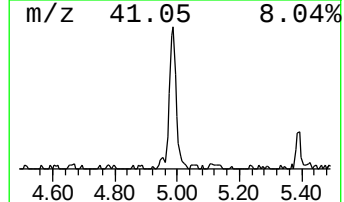
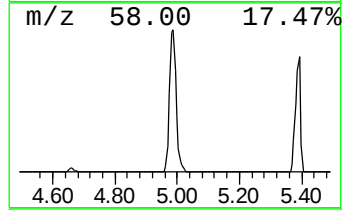
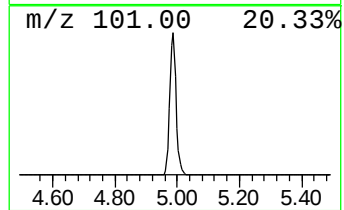
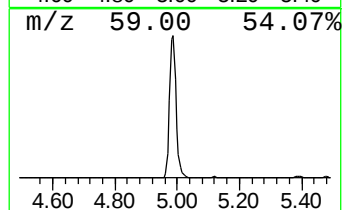
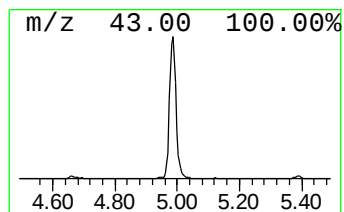
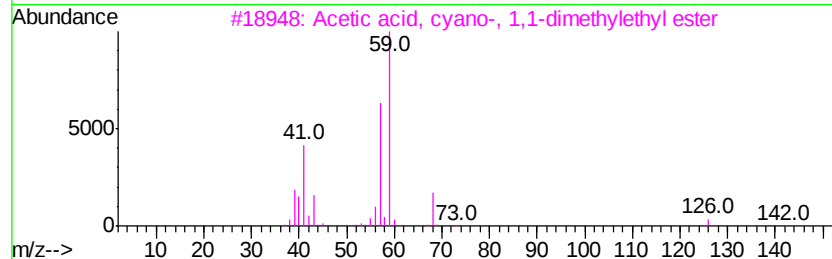
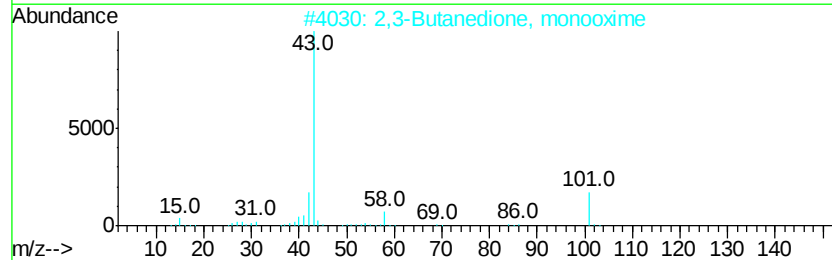
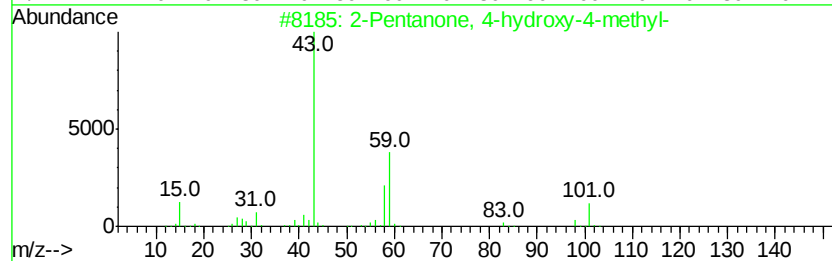
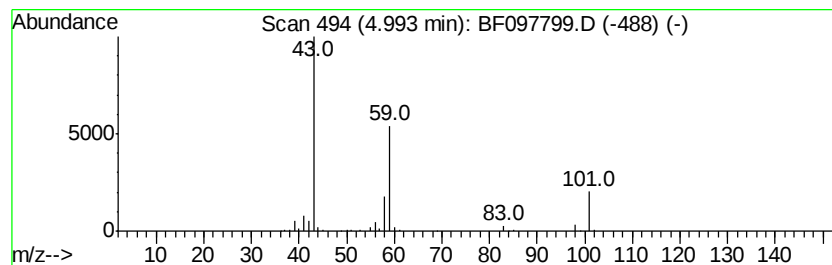
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	12.21 ng	525209	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Butane	58	C4H10	000106-97-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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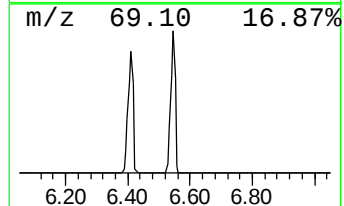
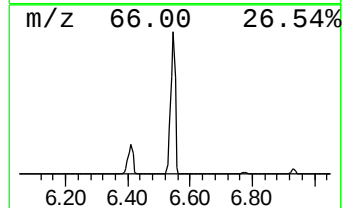
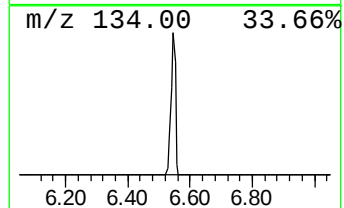
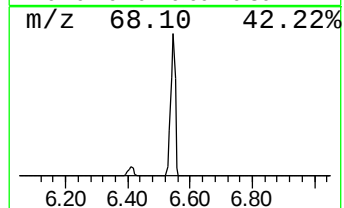
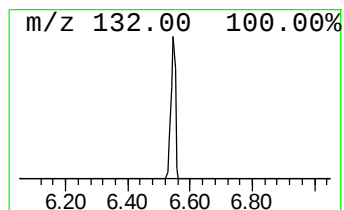
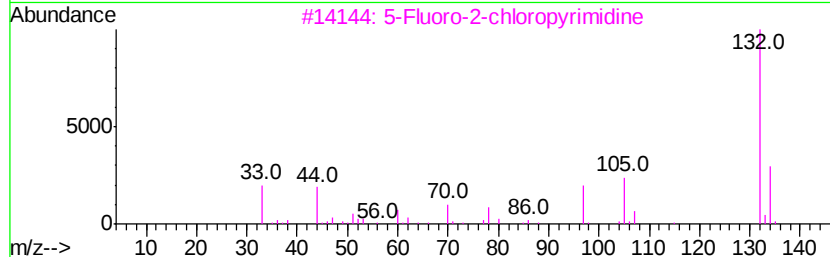
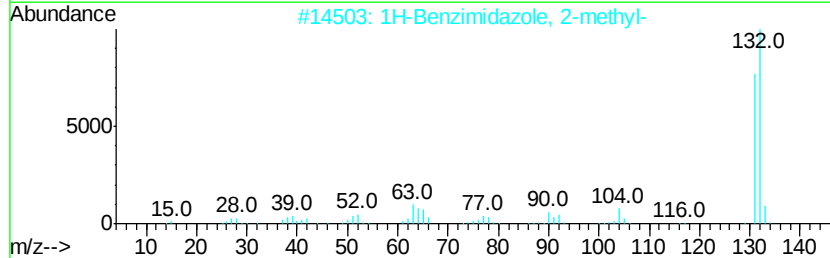
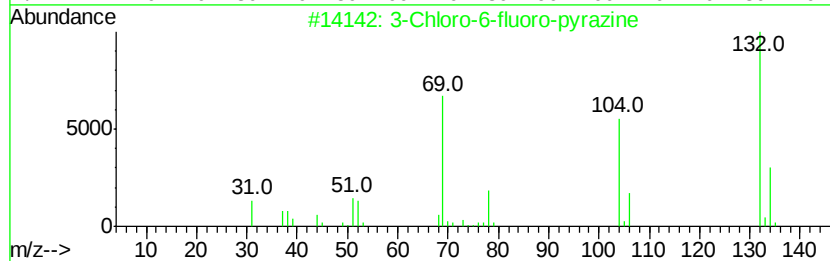
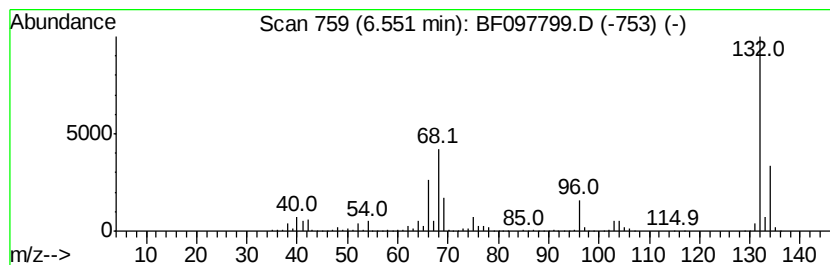
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	84.79 ng	3648310	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H	Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5	Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Cyclopropanamine, 1-phenyl-		133	C9H11N	1000351-26-2	10
5	(E)-3-Chloro-2-methyl-2-pentenal		132	C6H9ClO	031357-76-3	9



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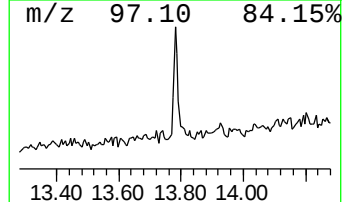
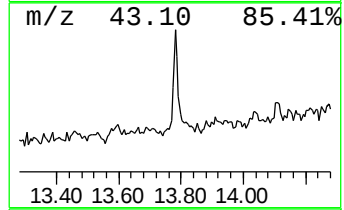
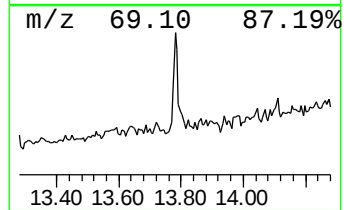
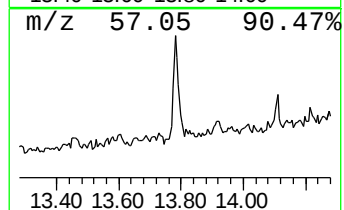
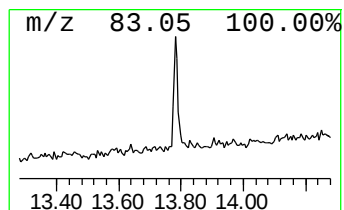
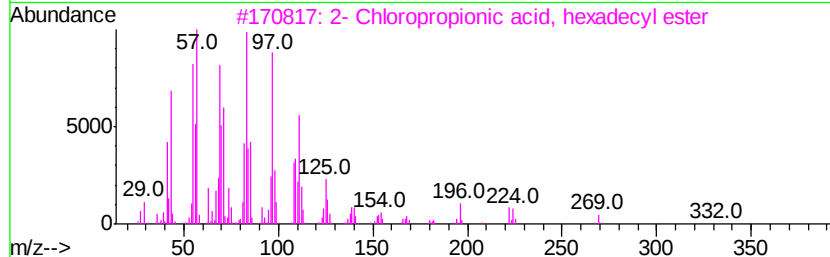
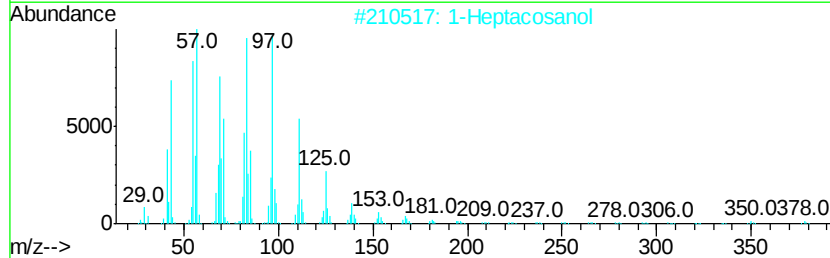
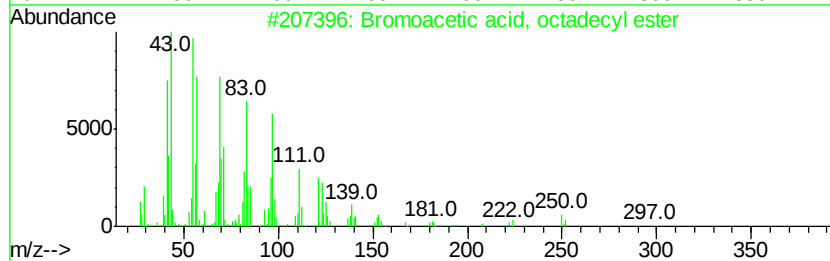
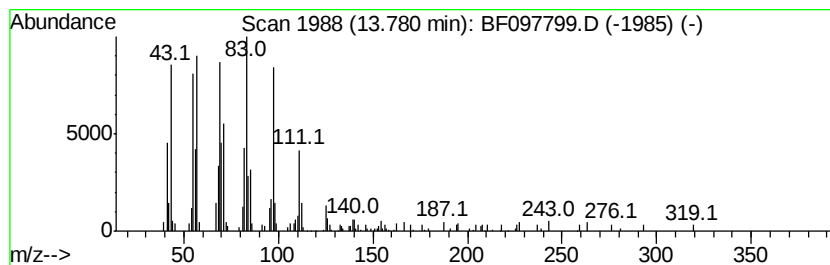
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Peak Number 4 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	3.08 ng	124130	Chrysene-d12	13.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4		Behenic alcohol	326	C22H46O	000661-19-8	90
5		1-Heneicosanol	312	C21H44O	015594-90-8	87



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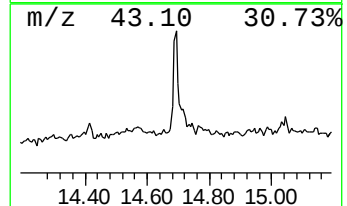
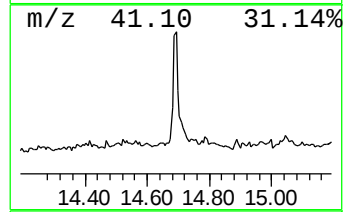
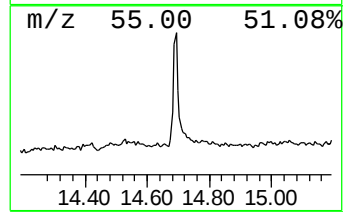
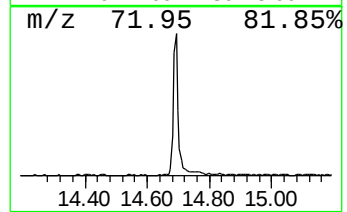
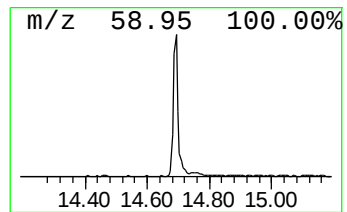
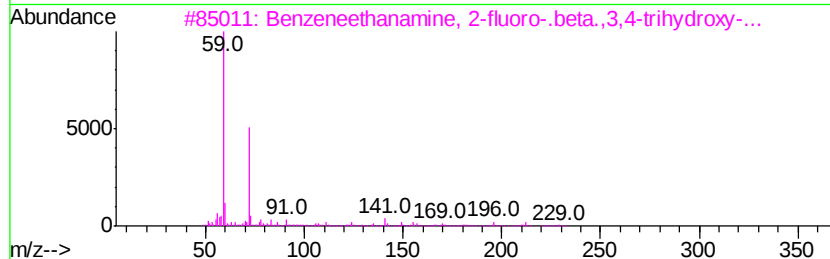
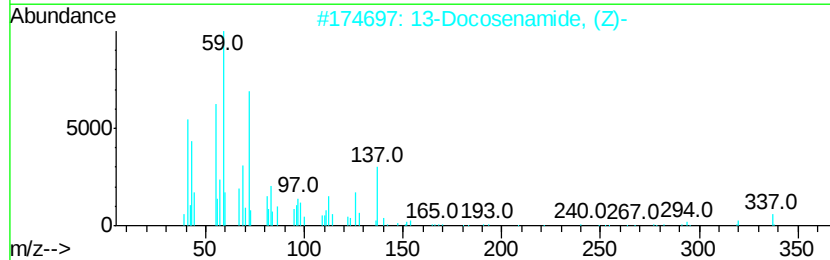
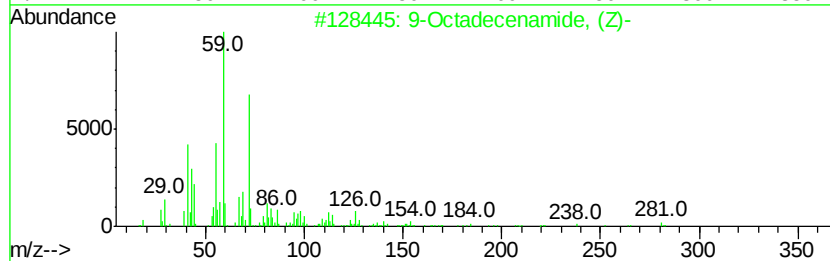
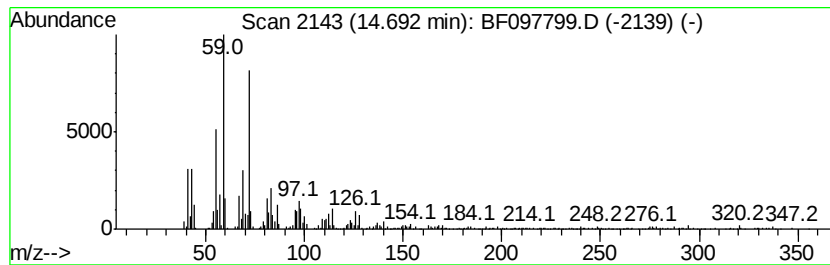
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	17.60 ng	483195	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50
4		3-Pentadecanone	226	C15H30O	018787-66-1	35
5		4-Cyclohexylbutyramide	169	C10H19NO	004441-62-7	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	12.2	ng	525209	1	6.77	860590	20.0
unknown6.55	6.55	84.8	ng	3648310	1	6.77	860590	20.0
Bromoacetic acid,...	13.78	3.1	ng	124130	5	13.93	805508	20.0
9-Octadecenamide,...	14.69	17.6	ng	483195	6	15.36	549020	20.0