

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
 Data File : BF108836.D
 Acq On : 6 Sep 2018 21:09
 Operator : JU/SJ
 Sample : J4803-09
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q2-G7

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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	4.931	437	441	451	rVB	133844	173314	4.30%	0.445%
2	5.348	507	512	515	rBV	3523230	3475954	86.25%	8.927%
3	6.366	680	685	688	rBV	3947570	3591652	89.12%	9.224%
4	6.501	704	708	712	rBV	3903544	3691578	91.60%	9.481%
5	6.566	716	719	722	rBV	57035	45965	1.14%	0.118%
6	6.736	742	748	751	rBV	1808349	1470149	36.48%	3.776%
7	6.766	751	753	757	rVB	124791	101958	2.53%	0.262%
8	6.807	757	760	763	rBV	58606	59390	1.47%	0.153%
9	6.889	768	774	778	rBV	3160907	2944665	73.07%	7.563%
10	7.025	792	797	800	rVB4	48341	77919	1.93%	0.200%
11	7.289	834	842	846	rBV	2376498	2386207	59.21%	6.128%
12	7.389	855	859	864	rVB4	57272	91627	2.27%	0.235%
13	7.536	881	884	885	rBV2	51102	48657	1.21%	0.125%
14	7.666	904	906	910	rVB3	45750	53282	1.32%	0.137%
15	8.013	961	965	969	rBV	1950586	1787107	44.34%	4.590%
16	9.089	1144	1148	1152	rBV	4605008	4030108	100.00%	10.350%
17	9.483	1211	1215	1218	rBV	1378215	1046470	25.97%	2.688%
18	9.766	1259	1263	1267	rBV	2192429	1838172	45.61%	4.721%
19	10.548	1391	1396	1399	rBV	2161439	2030424	50.38%	5.215%
20	11.242	1510	1514	1517	rBV	1831265	1591175	39.48%	4.087%
21	11.777	1600	1605	1615	rBV3	169231	239484	5.94%	0.615%
22	12.442	1715	1718	1724	rBV	50701	50811	1.26%	0.130%
23	12.495	1724	1727	1733	rBV3	39504	47247	1.17%	0.121%
24	12.824	1778	1783	1786	rBV	3402413	3103641	77.01%	7.971%
25	13.736	1935	1938	1947	rBV	164376	202778	5.03%	0.521%
26	13.865	1956	1960	1963	rBV	1910051	1709370	42.41%	4.390%
27	14.054	1989	1992	1995	rBV2	50273	53213	1.32%	0.137%
28	14.359	2041	2044	2047	rBV	58727	47959	1.19%	0.123%
29	14.624	2086	2089	2092	rBV2	184034	198103	4.92%	0.509%
30	14.654	2092	2094	2103	rVV	107742	124026	3.08%	0.319%
31	14.724	2103	2106	2110	rVB	283216	258914	6.42%	0.665%
32	14.971	2145	2148	2153	rVB	118619	126819	3.15%	0.326%
33	15.271	2194	2199	2204	rVV	1544549	1772226	43.97%	4.551%
34	15.330	2206	2209	2213	rVB	111309	131707	3.27%	0.338%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.736	2274	2278	2284	rVB2	98888	140068	3.48%	0.360%
36	16.112	2340	2342	2349	rVB8	43014	76413	1.90%	0.196%
37	16.206	2355	2358	2367	rVB2	68324	118649	2.94%	0.305%

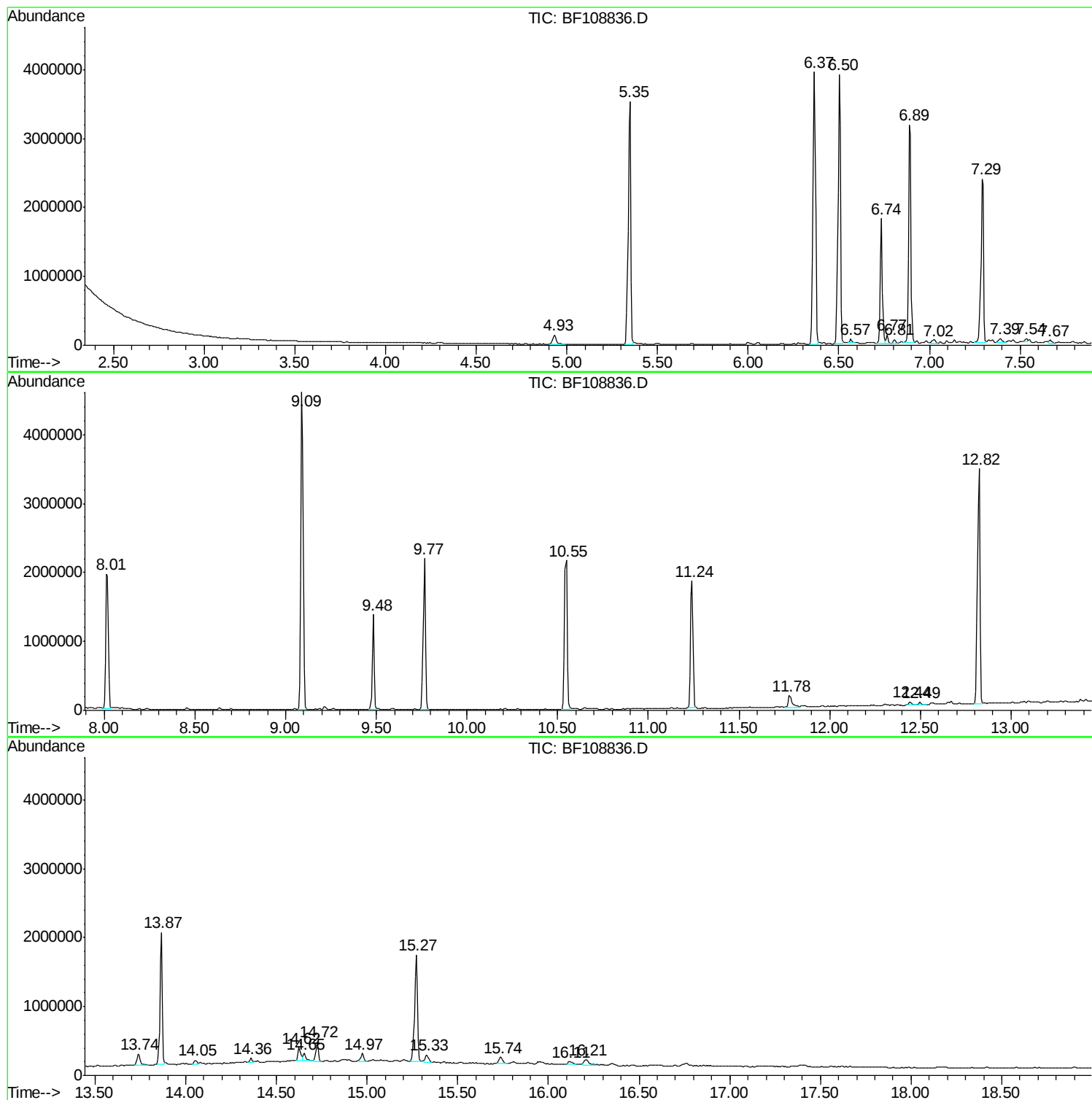
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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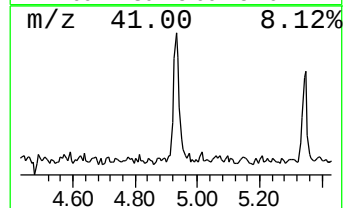
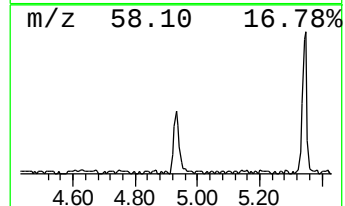
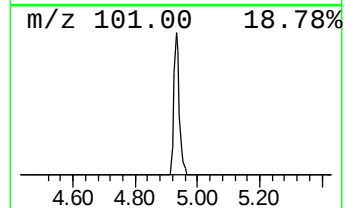
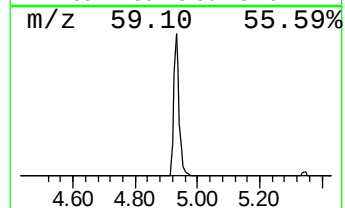
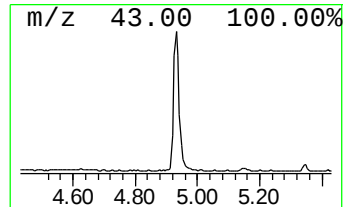
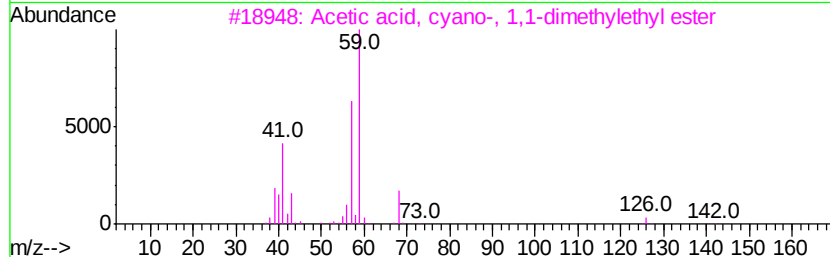
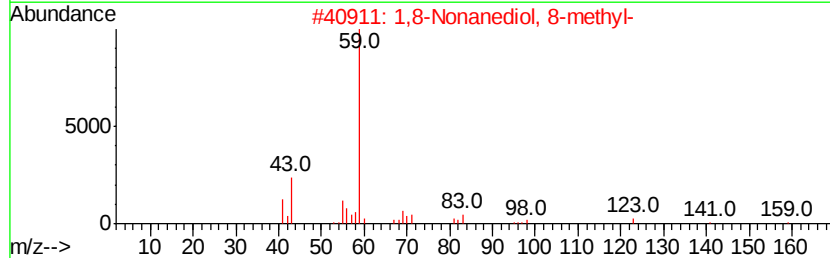
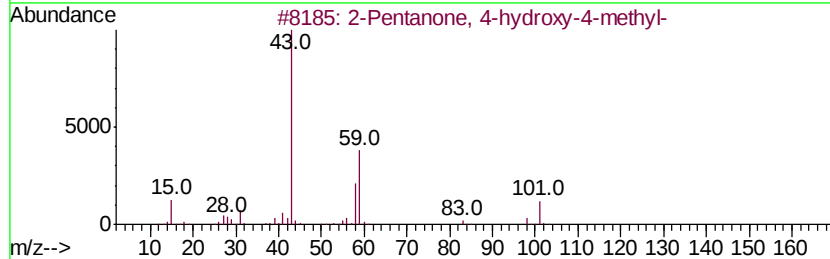
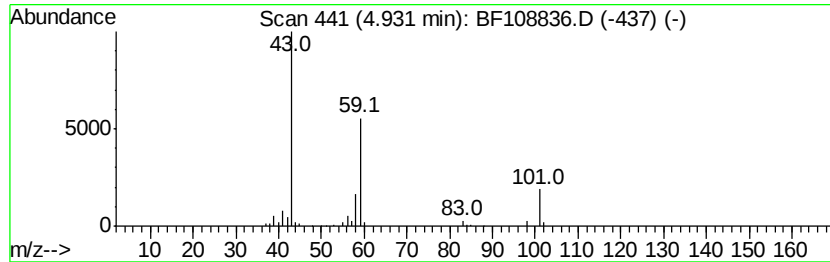
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.36 ng	173314	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25		
4	3-Hexanol	102	C6H14O	000623-37-0	23		
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	17		



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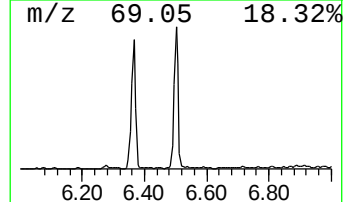
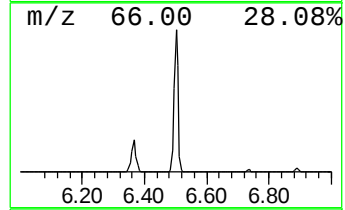
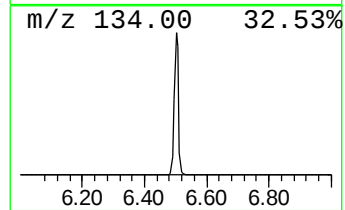
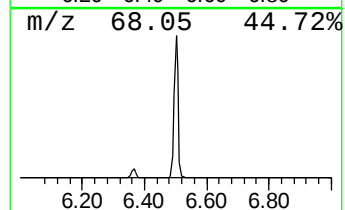
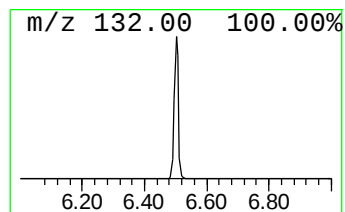
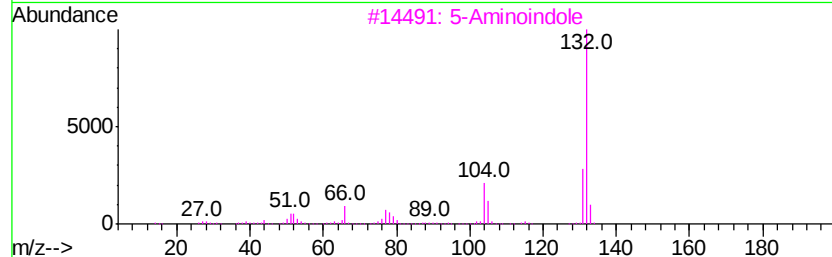
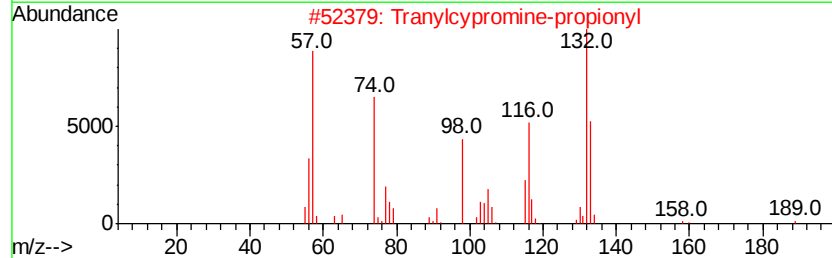
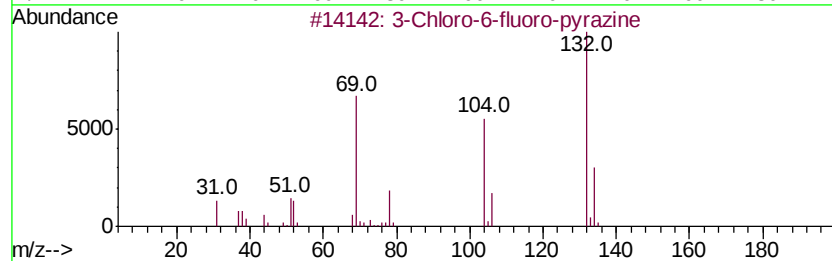
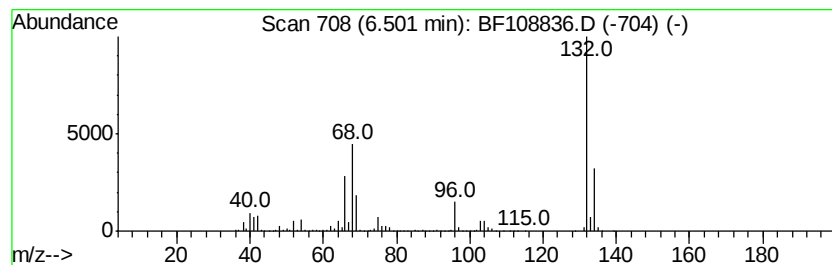
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	50.22 ng	3691580	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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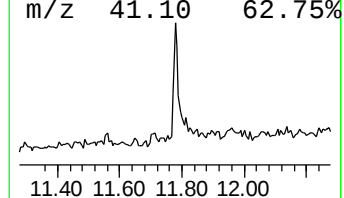
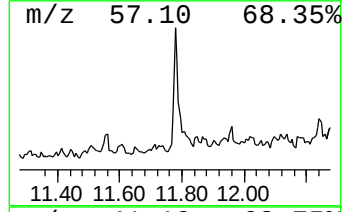
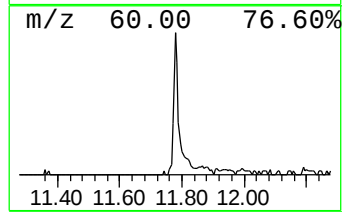
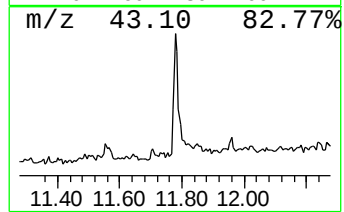
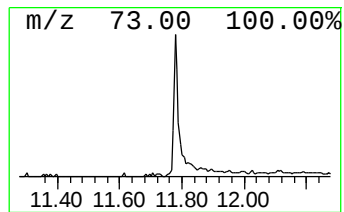
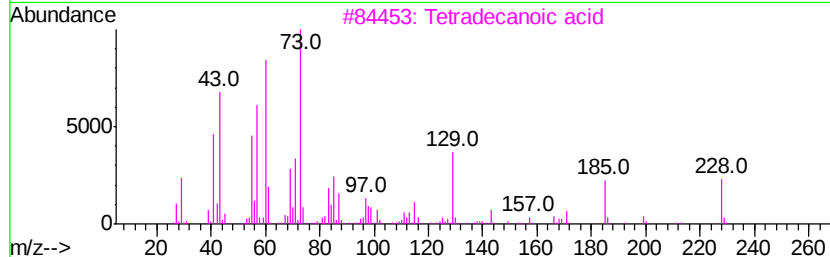
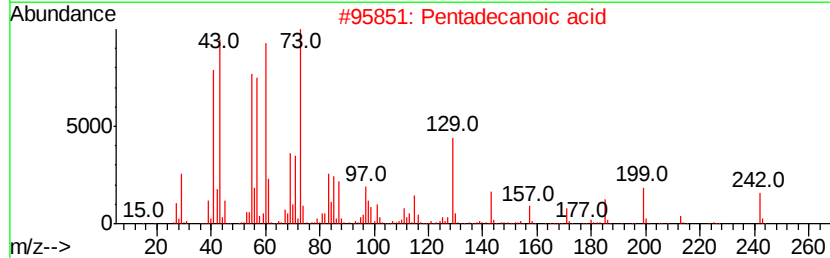
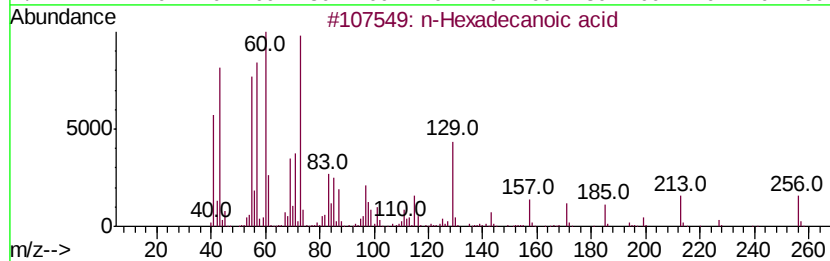
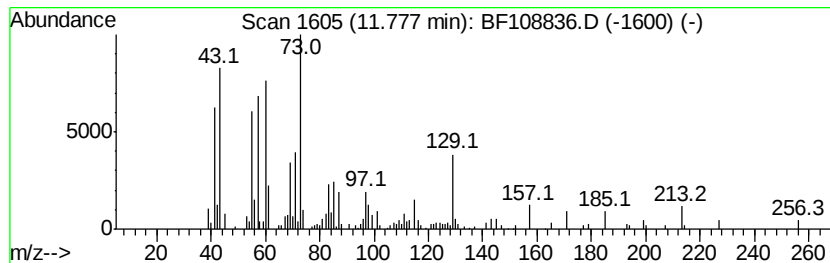
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	3.01 ng	239484	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	11



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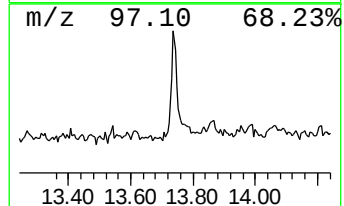
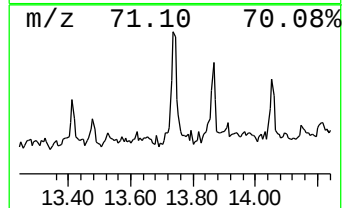
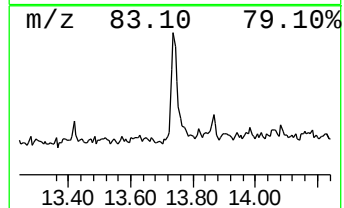
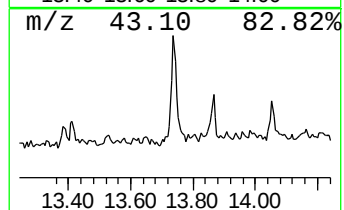
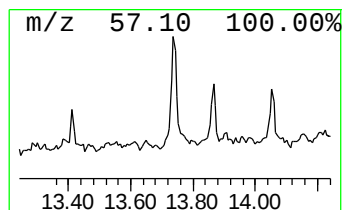
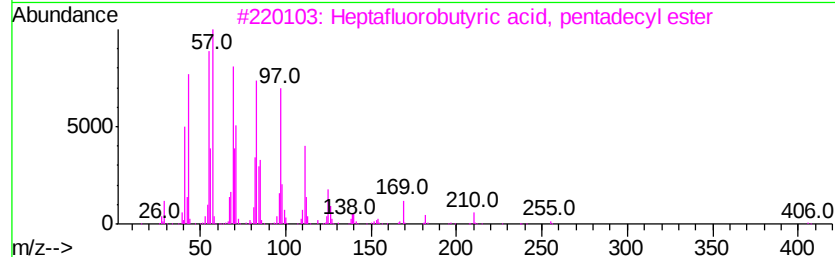
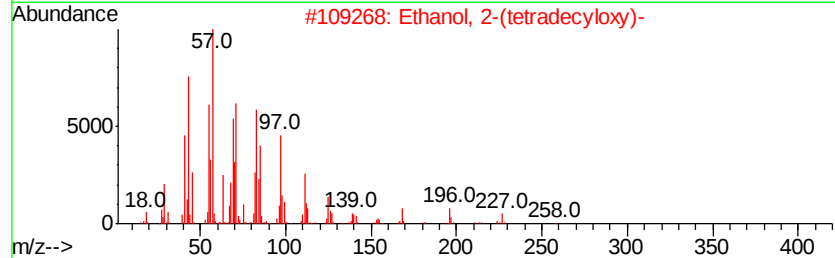
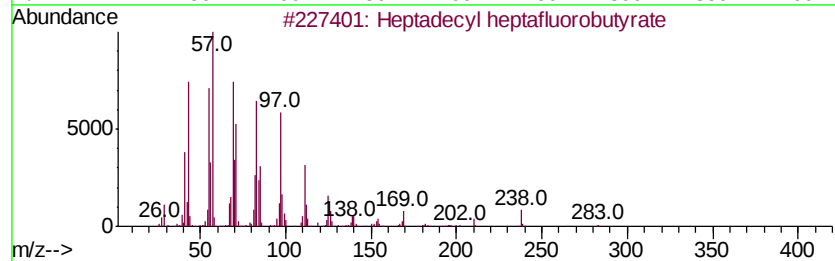
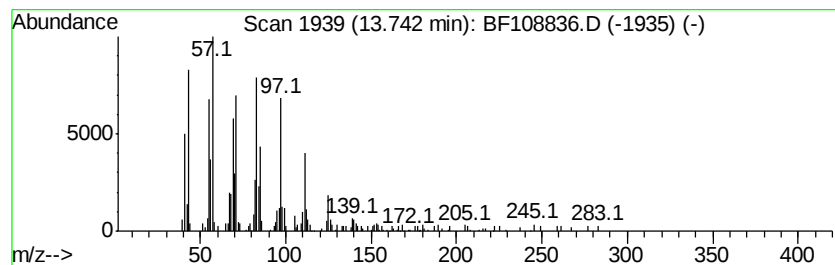
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.37 ng	202778	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5		1-Docosene	308	C22H44	001599-67-3	87



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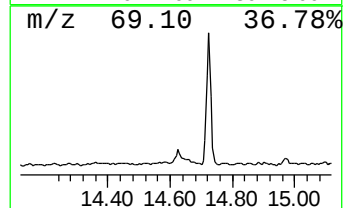
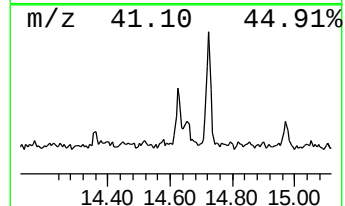
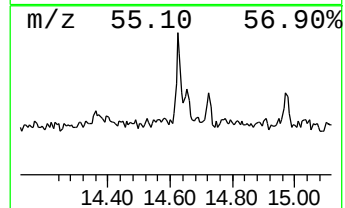
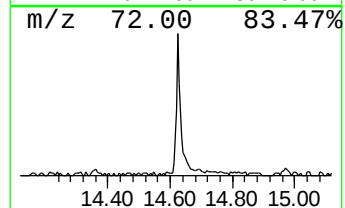
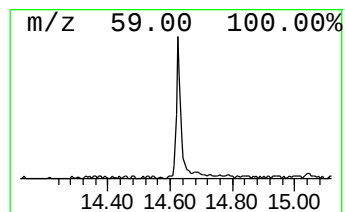
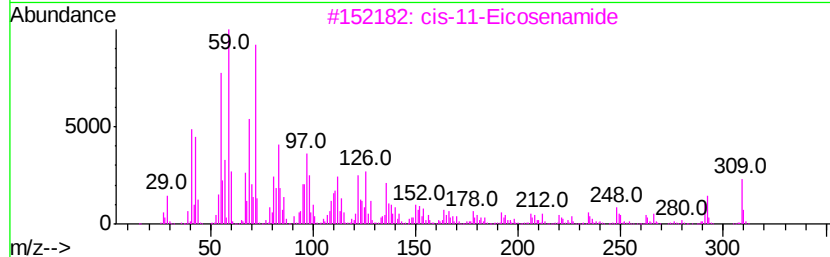
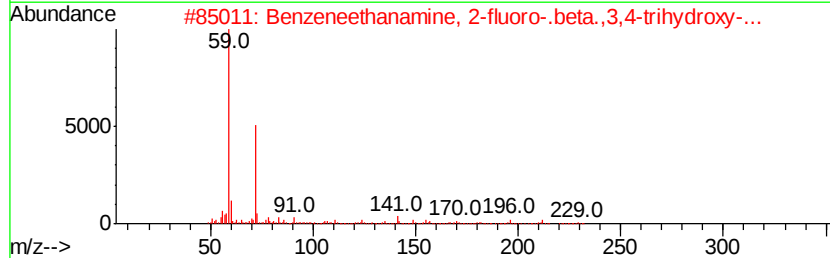
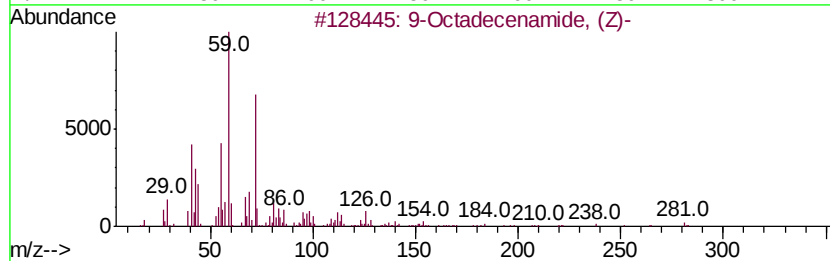
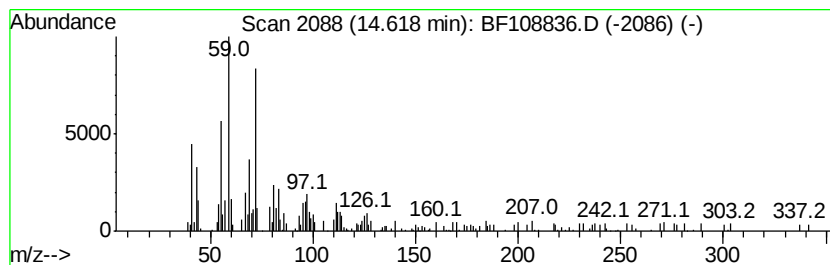
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TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.24 ng	198103	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
3		cis-11-Eicosenamide	309	C20H39NO	010436-08-5	49
4		Dodecanamide	199	C12H25NO	001120-16-7	43
5		Octadecanamide	283	C18H37NO	000124-26-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108836.D
Acq On : 6 Sep 2018 21:09
Operator : JU/SJ
Sample : J4803-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-G7

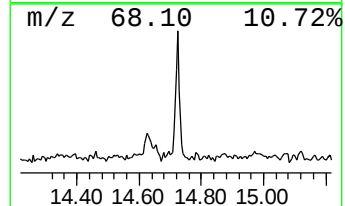
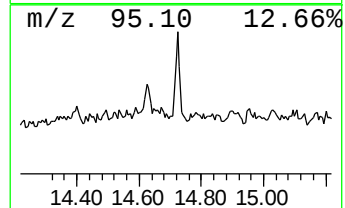
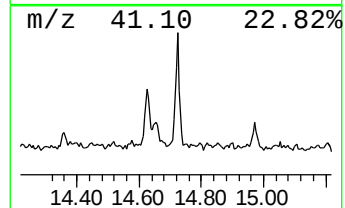
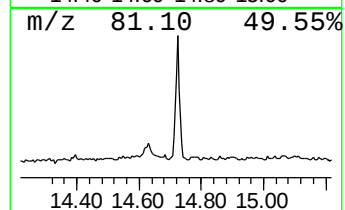
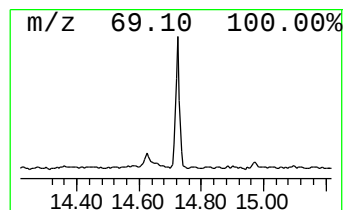
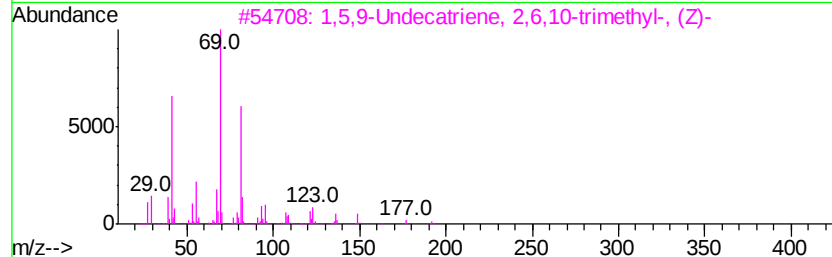
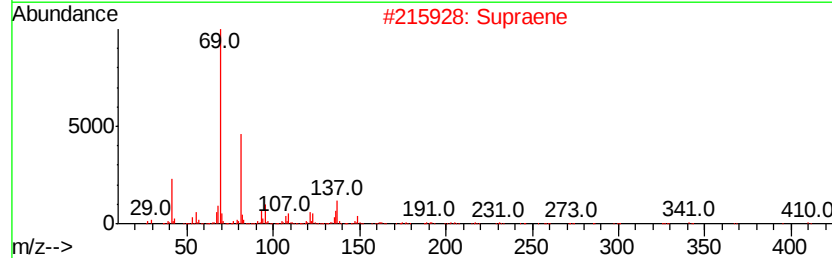
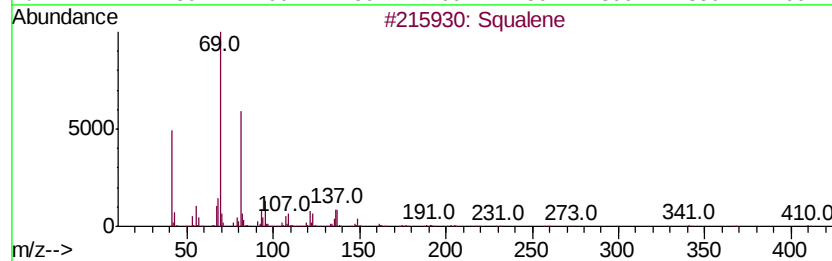
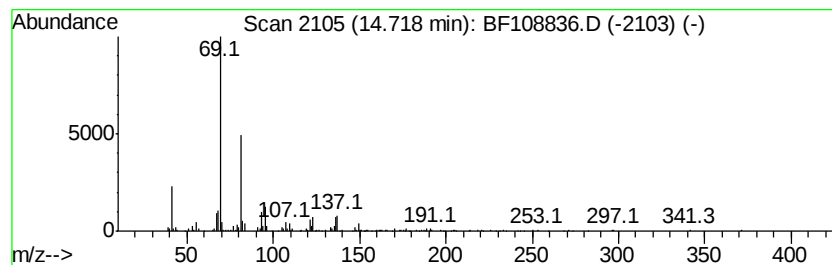
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.92 ng	258914	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	78
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
Data File : BF108836.D
Acq On : 6 Sep 2018 21:09
Operator : JU/SJ
Sample : J4803-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-G7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	4.93	2.4	ng	173314	1	6.74	1470150	20.0
unknown6.50	6.50	50.2	ng	3691580	1	6.74	1470150	20.0
n-Hexadecanoic acid	11.78	3.0	ng	239484	4	11.24	1591180	20.0
Heptadecyl hepta...	13.74	2.4	ng	202778	5	13.87	1709370	20.0
9-Octadecenamide,...	14.62	2.2	ng	198103	6	15.27	1772230	20.0
Squalene	14.72	2.9	ng	258914	6	15.27	1772230	20.0