

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091118\
 Data File : BF108944.D
 Acq On : 11 Sep 2018 19:17
 Operator : JU/SJ
 Sample : J4838-08
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-1B-C-090718-1

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	83765	105802	3.89%	0.368%
2	5.348	507	512	515	rBV	2563820	2471191	90.91%	8.601%
3	6.366	681	685	688	rBV	2557365	2613848	96.16%	9.098%
4	6.507	704	709	712	rBV	2756177	2639367	97.10%	9.187%
5	6.572	717	720	733	rVB	46453	56217	2.07%	0.196%
6	6.737	744	748	751	rBV	1333701	1026785	37.78%	3.574%
7	6.895	771	775	778	rBV	2390508	2034873	74.86%	7.083%
8	7.295	838	843	846	rBV	1921996	1665057	61.26%	5.796%
9	8.019	962	966	969	rBV	1600688	1299262	47.80%	4.522%
10	9.095	1145	1149	1152	rBV	3133053	2718140	100.00%	9.461%
11	9.219	1167	1170	1177	rVB	85891	79142	2.91%	0.275%
12	9.484	1212	1215	1225	rVB	971252	779555	28.68%	2.713%
13	9.766	1259	1263	1267	rBV2	1601177	1383579	50.90%	4.816%
14	10.548	1392	1396	1403	rBV	1728344	1546629	56.90%	5.383%
15	11.242	1510	1514	1517	rBV	1472198	1262385	46.44%	4.394%
16	11.266	1517	1518	1522	rVB	128656	75225	2.77%	0.262%
17	11.783	1602	1606	1610	rBV2	139227	151653	5.58%	0.528%
18	11.854	1615	1618	1620	rBV	34135	31333	1.15%	0.109%
19	12.448	1716	1719	1723	rVB	240297	196168	7.22%	0.683%
20	12.677	1752	1758	1761	rBV	197526	211223	7.77%	0.735%
21	12.824	1779	1783	1786	rBV	2414406	1992162	73.29%	6.934%
22	13.072	1821	1825	1828	rBV	40187	35823	1.32%	0.125%
23	13.748	1936	1940	1950	rBV5	79307	160215	5.89%	0.558%
24	13.871	1956	1961	1963	rBV	1214129	1261232	46.40%	4.390%
25	13.895	1963	1965	1968	rVB	117395	89793	3.30%	0.313%
26	13.971	1974	1978	1982	rBV5	19849	36042	1.33%	0.125%
27	14.254	2022	2026	2029	rBV2	32197	34485	1.27%	0.120%
28	14.360	2037	2044	2046	rBV5	46940	74489	2.74%	0.259%
29	14.654	2091	2094	2099	rVB	61224	61085	2.25%	0.213%
30	14.724	2103	2106	2109	rVB3	41417	42671	1.57%	0.149%
31	14.877	2128	2132	2135	rBV	128763	190780	7.02%	0.664%
32	14.977	2145	2149	2153	rVB2	121080	131265	4.83%	0.457%
33	15.160	2177	2180	2186	rVB	80022	89801	3.30%	0.313%
34	15.218	2186	2190	2195	rVB	110355	129114	4.75%	0.449%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.277	2195	2200	2204	rBV	1065328	1251958	46.06%	4.358%
36	15.330	2206	2209	2213	rVB	93151	116585	4.29%	0.406%
37	15.742	2274	2279	2284	rBV	105825	155533	5.72%	0.541%
38	16.212	2354	2359	2368	rVB	83131	147636	5.43%	0.514%
39	16.630	2425	2430	2435	rVB2	45368	79753	2.93%	0.278%
40	16.765	2448	2453	2461	rVB3	47704	93968	3.46%	0.327%
41	17.042	2495	2500	2505	rVB2	32987	59903	2.20%	0.209%
42	17.407	2557	2562	2569	rVB5	68828	148291	5.46%	0.516%

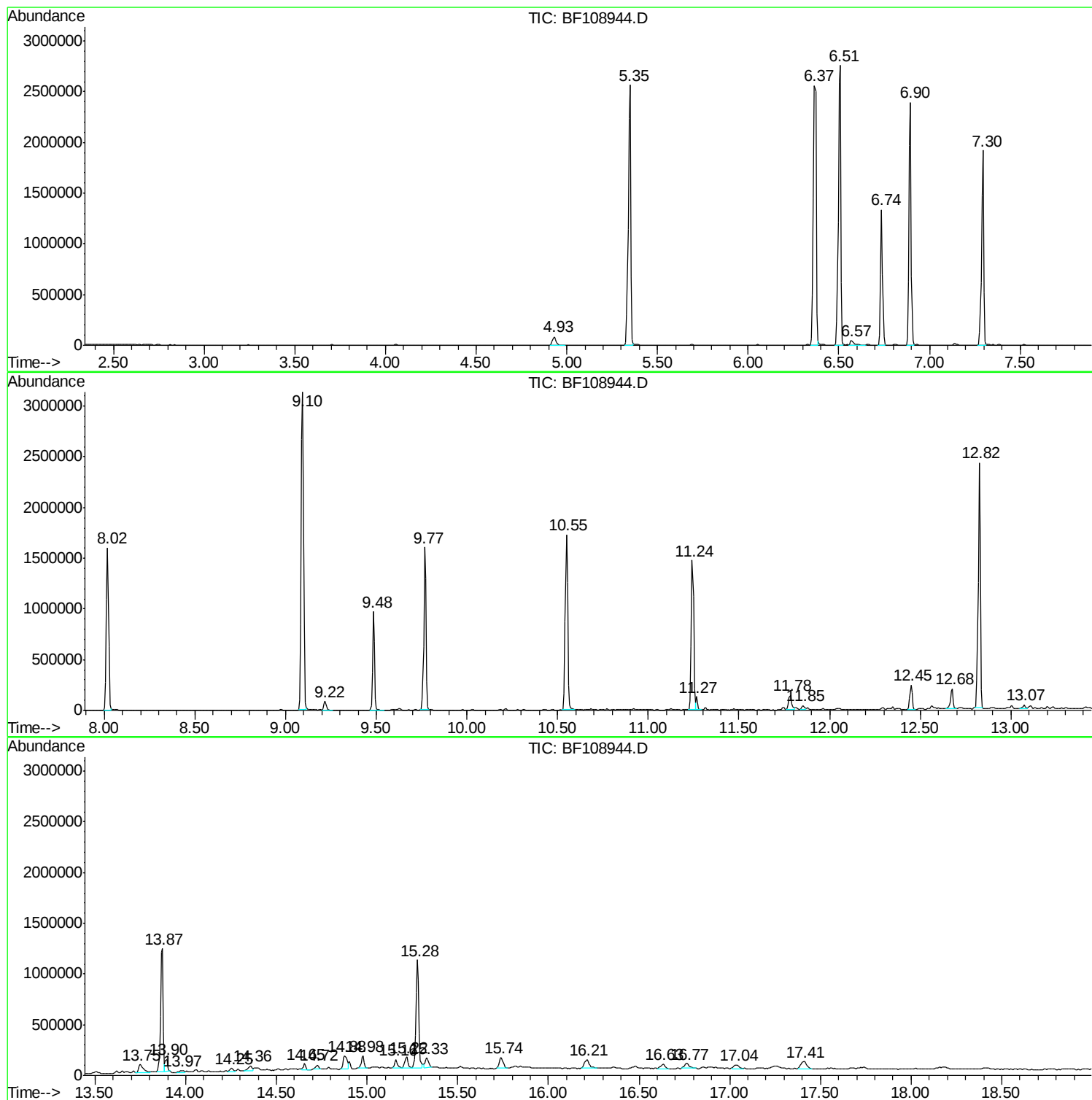
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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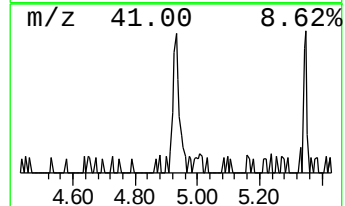
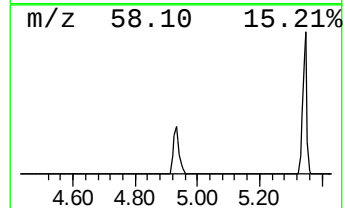
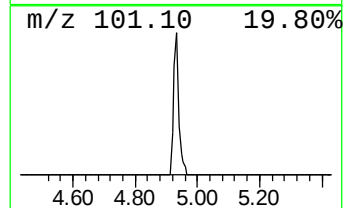
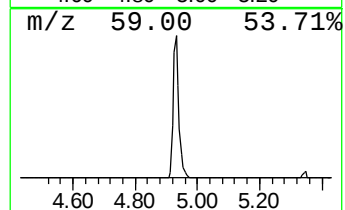
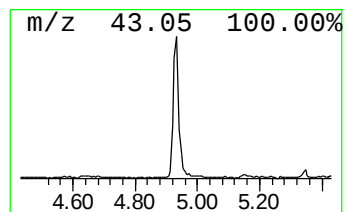
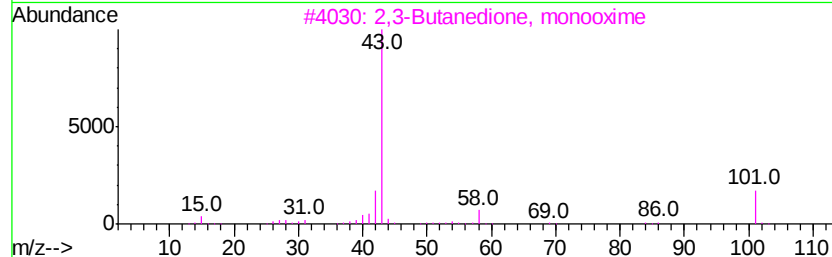
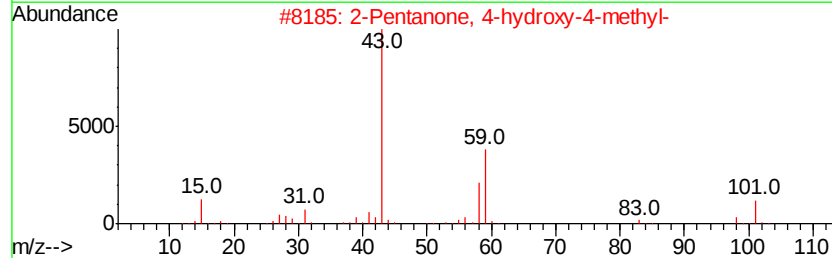
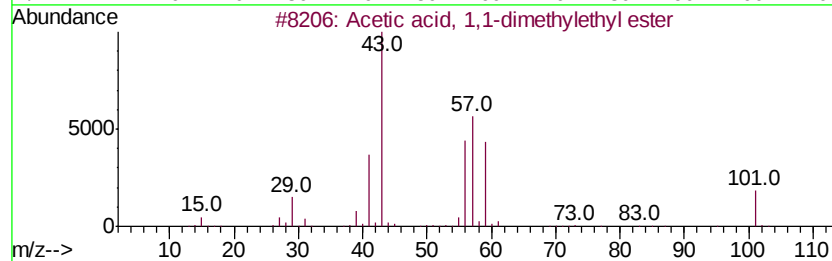
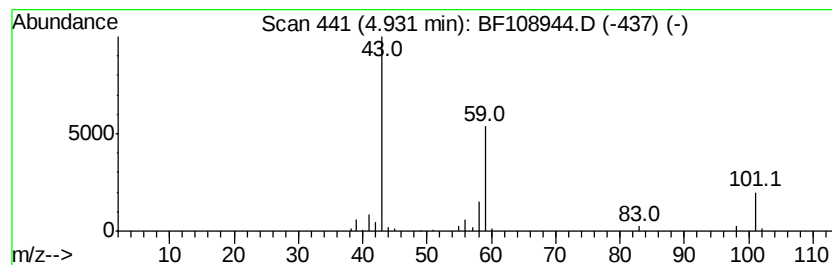
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.06 ng	105802	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



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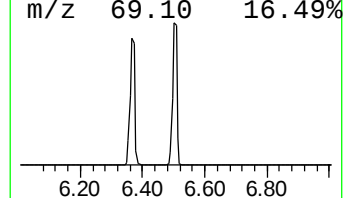
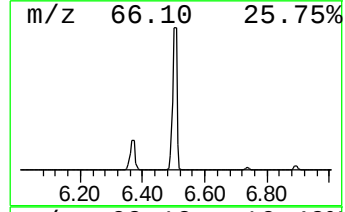
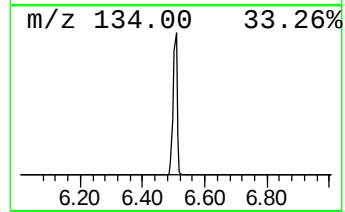
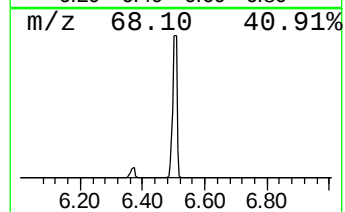
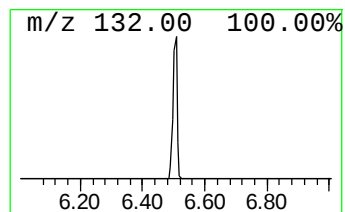
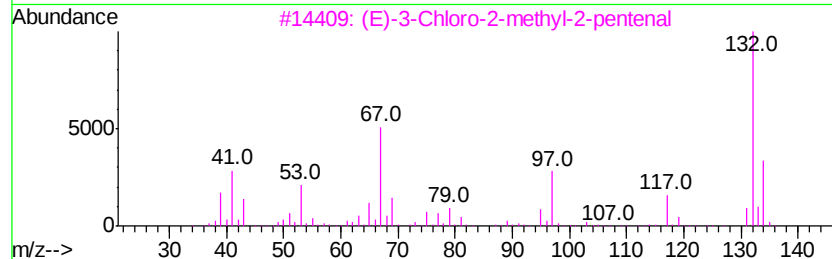
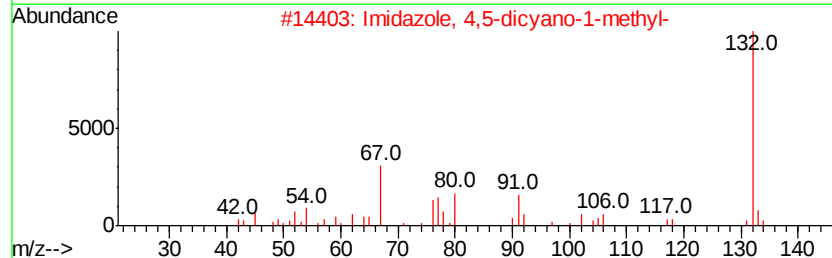
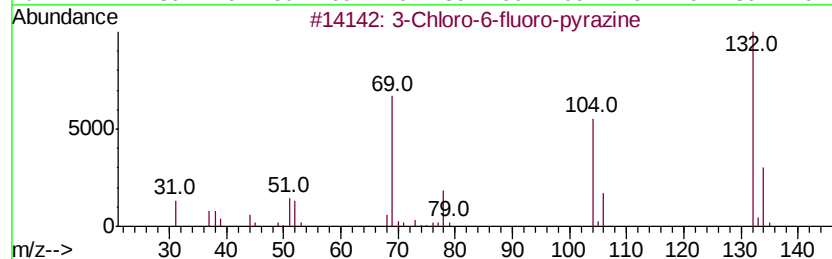
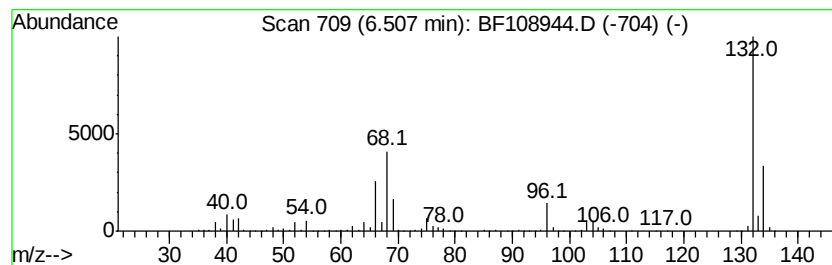
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Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	51.41 ng	2639370	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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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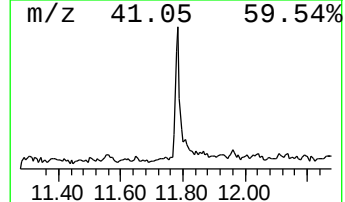
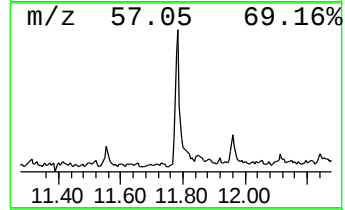
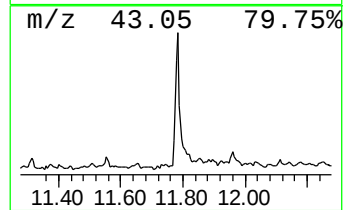
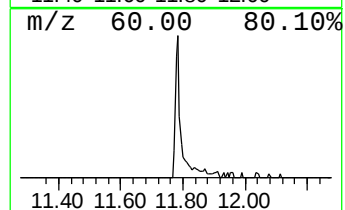
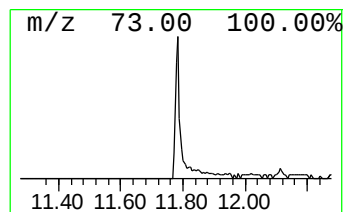
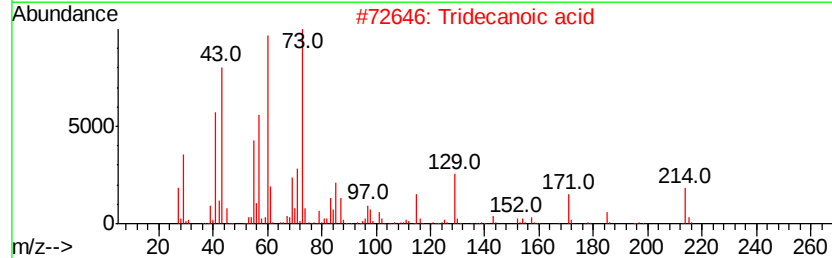
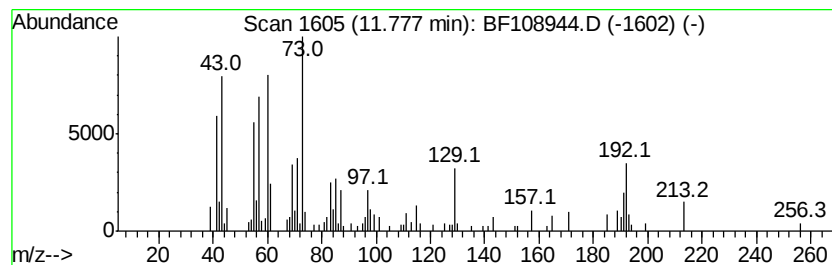
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.40 ng	151653	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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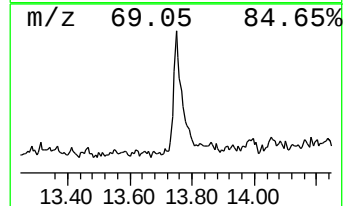
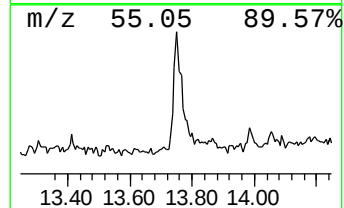
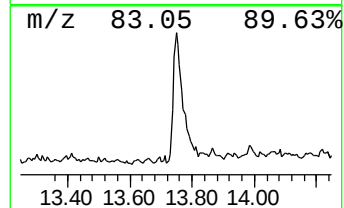
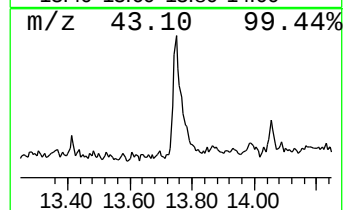
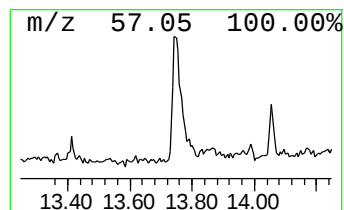
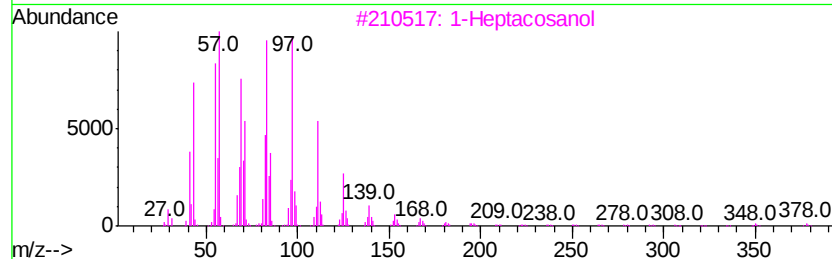
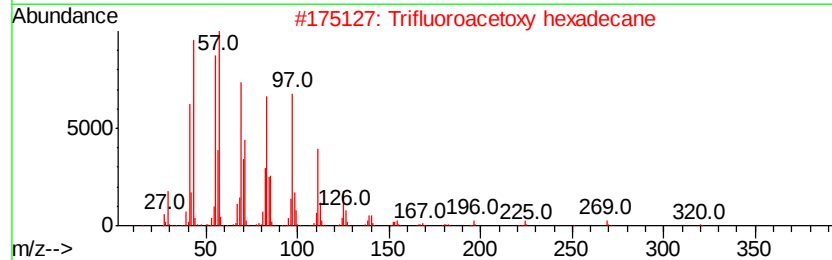
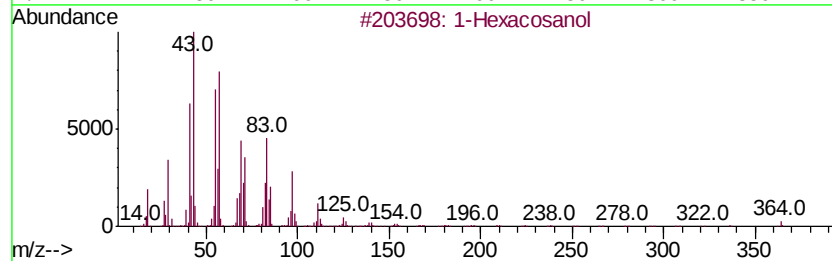
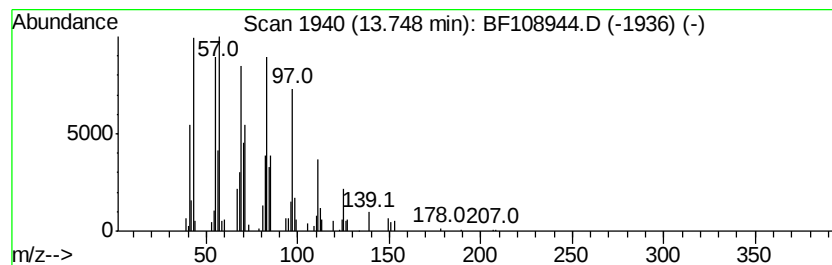
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Peak Number 5 1-Hexacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.54 ng	160215	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexacosanol	382	C26H54O	000506-52-5	91
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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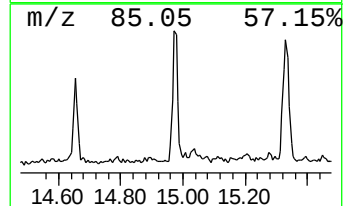
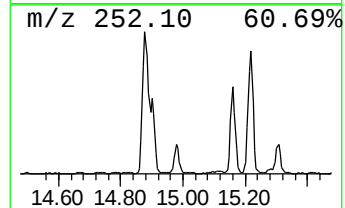
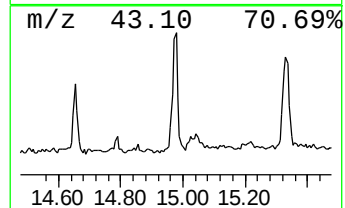
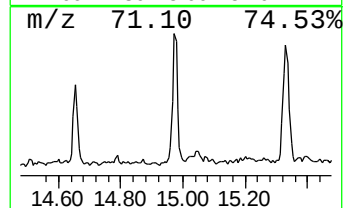
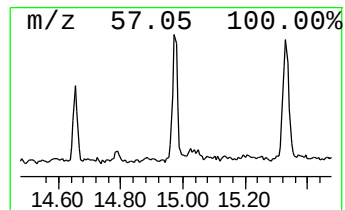
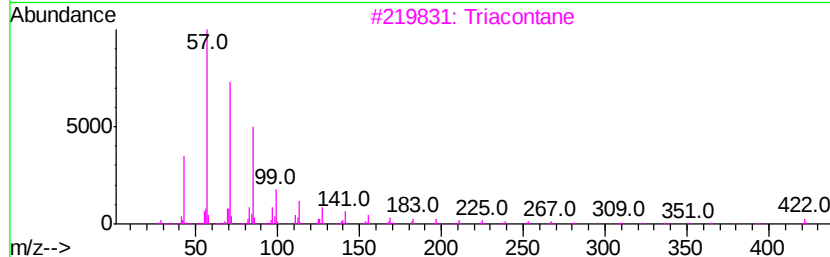
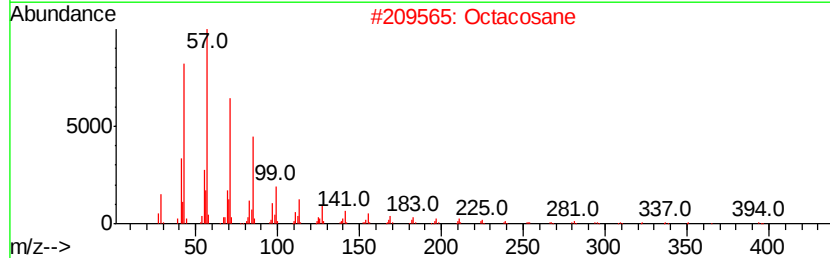
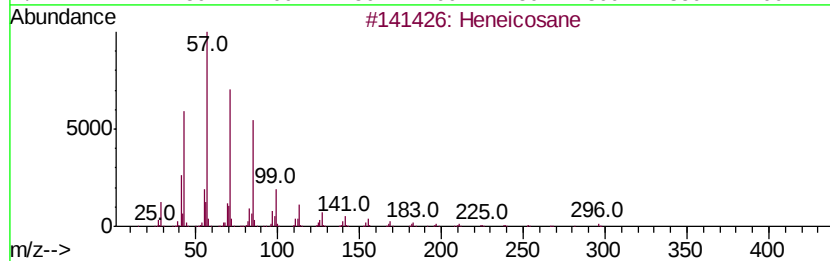
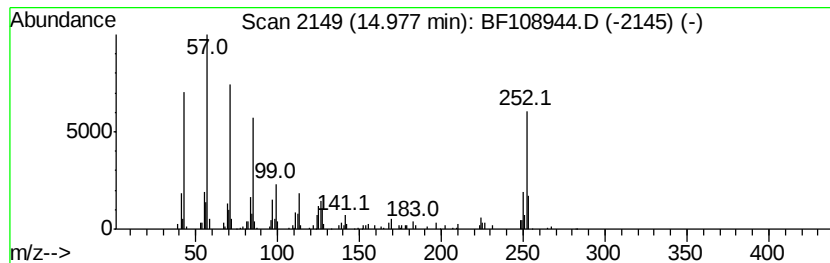
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.10 ng	131265	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	53
2		Octacosane	394	C28H58	000630-02-4	53
3		Triacontane	422	C30H62	000638-68-6	53
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	53
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108944.D
Acq On : 11 Sep 2018 19:17
Operator : JU/SJ
Sample : J4838-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-1B-C-090718-1

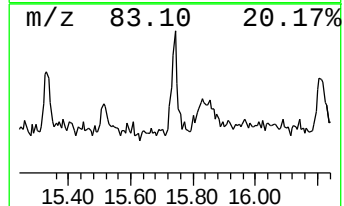
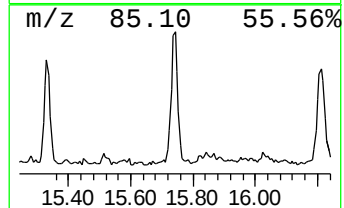
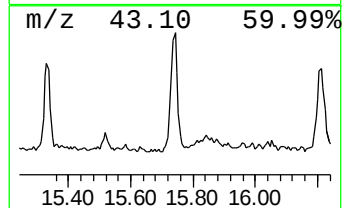
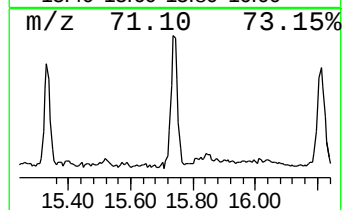
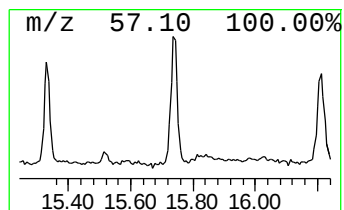
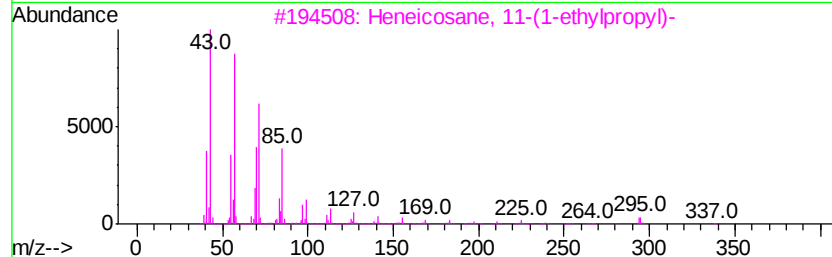
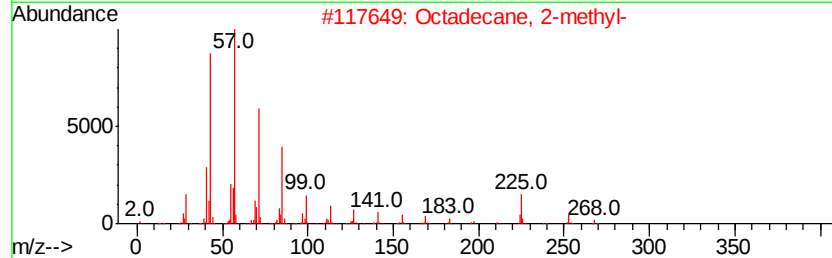
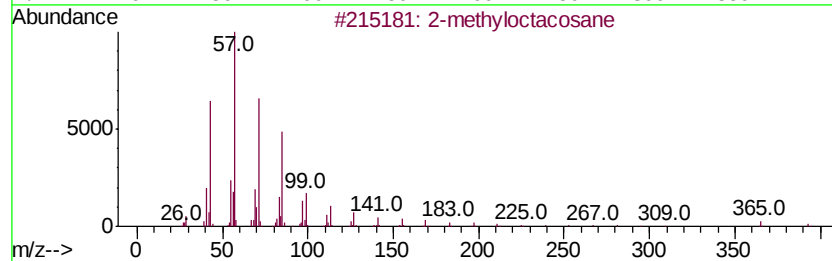
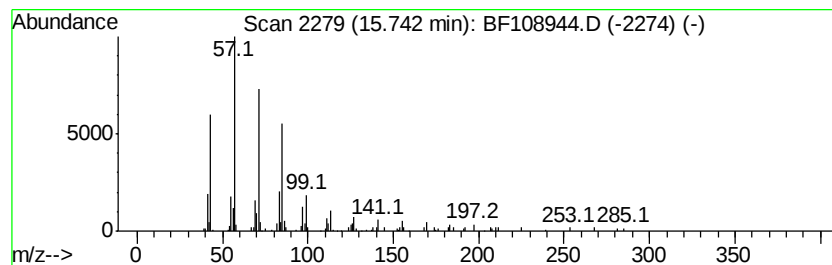
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.48 ng	155533	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108944.D
Acq On : 11 Sep 2018 19:17
Operator : JU/SJ
Sample : J4838-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-1B-C-090718-1

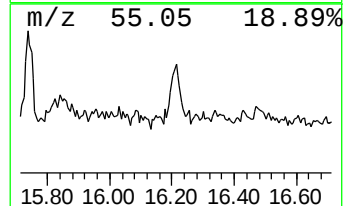
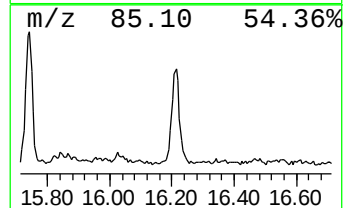
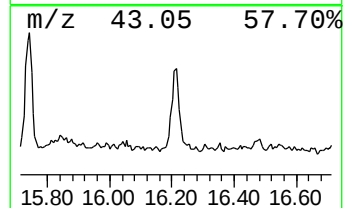
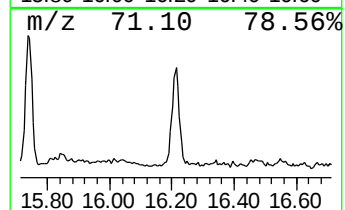
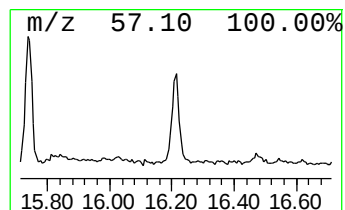
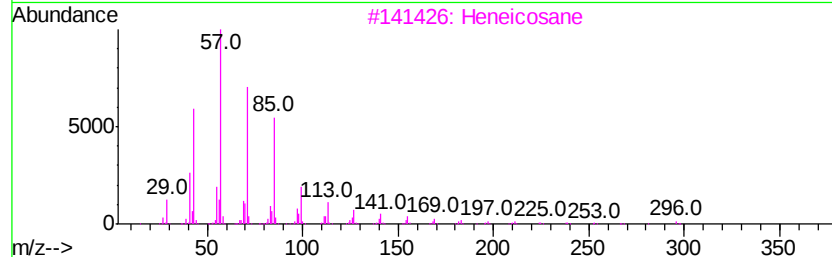
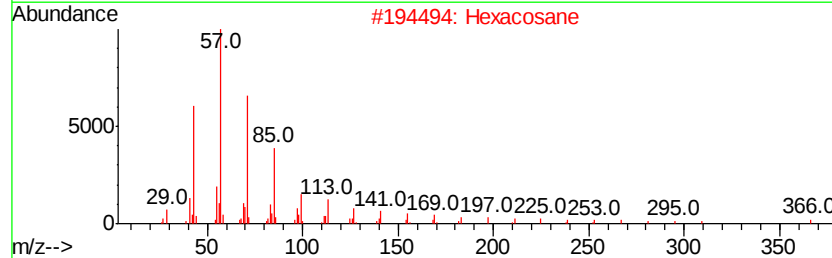
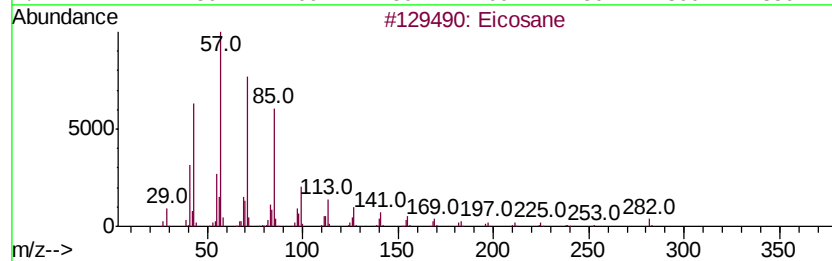
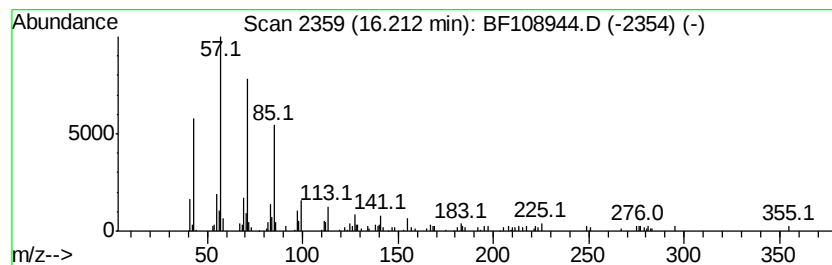
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.36 ng	147636	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	93
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108944.D
Acq On : 11 Sep 2018 19:17
Operator : JU/SJ
Sample : J4838-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-1B-C-090718-1

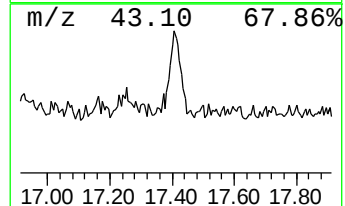
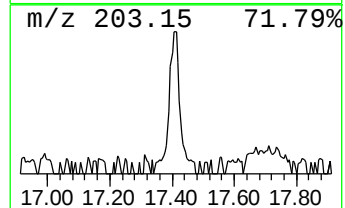
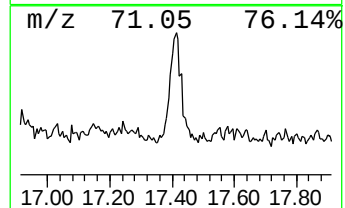
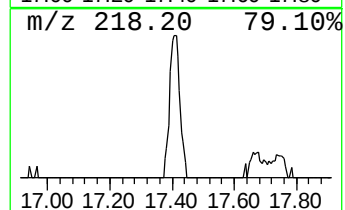
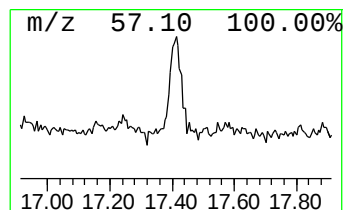
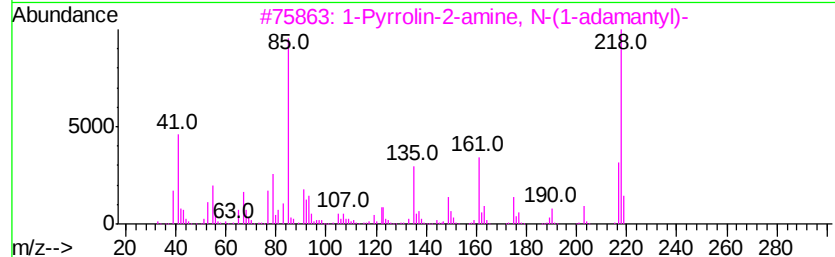
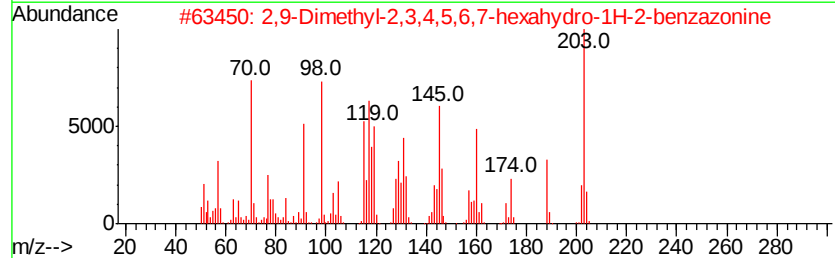
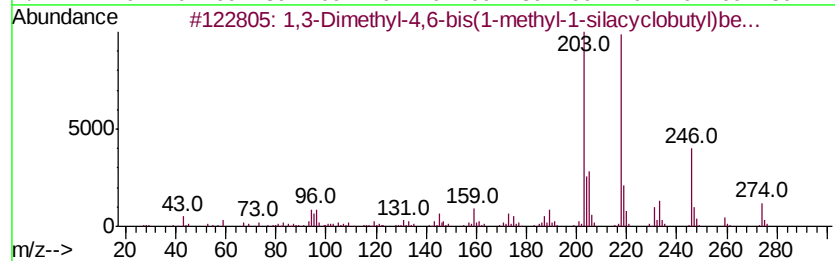
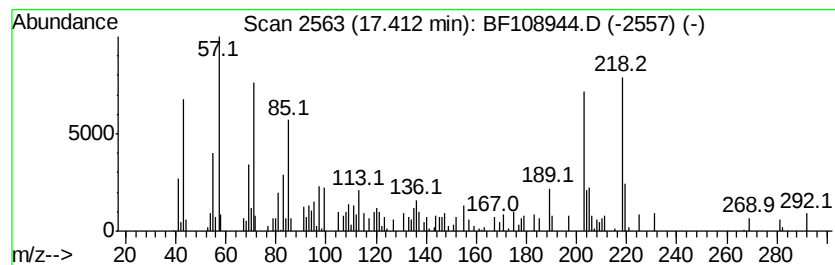
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.41 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.41	2.37 ng	148291	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dimethyl-4,6-bis(1-methyl-1-...	274	C16H26Si2	1000293-75-9	38
2		2,9-Dimethyl-2,3,4,5,6,7-hexahyd...	203	C14H21N	077581-11-4	25
3		1-Pyrrolin-2-amine, N-(1-adamant...	218	C14H22N2	300695-00-5	22
4		Hentriacontane	437	C31H64	000630-04-6	18
5		Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091118\
Data File : BF108944.D
Acq On : 11 Sep 2018 19:17
Operator : JU/SJ
Sample : J4838-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-1B-C-090718-1

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
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unknown6.51	6.51	51.4 ng		2639370	1	6.74	1026790	20.0
n-Hexadecanoic acid	11.78	2.4 ng		151653	4	11.24	1262390	20.0
1-Hexacosanol	13.75	2.5 ng		160215	5	13.87	1261230	20.0
Heneicosane	14.98	2.1 ng		131265	6	15.28	1251960	20.0
2-methyloctacosane	15.74	2.5 ng		155533	6	15.28	1251960	20.0
Eicosane	16.21	2.4 ng		147636	6	15.28	1251960	20.0
unknown17.41	17.41	2.4 ng		148291	6	15.28	1251960	20.0