

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
 Data File : BF108248.D
 Acq On : 17 Aug 2018 17:31
 Operator : JU/SJ
 Sample : J4500-09
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	4.178	308	313	319	rBV	71406	89132	2.24%	0.261%
2	5.254	491	496	508	rVB	682922	790346	19.83%	2.315%
3	5.643	557	562	565	rBV	3451886	3184959	79.89%	9.331%
4	6.637	726	731	734	rBV	3584163	3562540	89.36%	10.437%
5	6.784	752	756	760	rBV	3631496	3456135	86.69%	10.125%
6	7.013	792	795	799	rBV	1184531	1017519	25.52%	2.981%
7	7.172	818	822	825	rBV	3214498	2669144	66.95%	7.820%
8	7.578	886	891	894	rBV	2549640	2246212	56.34%	6.581%
9	8.301	1010	1014	1017	rBV	1403458	1280736	32.13%	3.752%
10	9.372	1192	1196	1199	rBV	4742078	3986564	100.00%	11.679%
11	9.760	1259	1262	1267	rBV	322055	256645	6.44%	0.752%
12	10.060	1309	1313	1317	rBV2	1643949	1423866	35.72%	4.171%
13	10.854	1443	1448	1461	rBV	2260637	2131524	53.47%	6.245%
14	11.554	1563	1567	1571	rBV	1458224	1291629	32.40%	3.784%
15	13.142	1833	1837	1840	rBV	3947368	3336275	83.69%	9.774%
16	13.695	1927	1931	1933	rBV2	47768	47350	1.19%	0.139%
17	14.024	1983	1987	1988	rBV	54132	47560	1.19%	0.139%
18	14.048	1988	1991	2003	rVB3	96219	201092	5.04%	0.589%
19	14.207	2014	2018	2022	rBV	1326327	1261312	31.64%	3.695%
20	14.342	2038	2041	2043	rBV	77494	71476	1.79%	0.209%
21	14.648	2090	2093	2098	rBV	81603	79147	1.99%	0.232%
22	14.977	2145	2149	2153	rVB	92179	97097	2.44%	0.284%
23	15.060	2160	2163	2167	rBV	135001	138783	3.48%	0.407%
24	15.342	2207	2211	2215	rVB2	89186	111855	2.81%	0.328%
25	15.771	2278	2284	2292	rVB	792286	1119396	28.08%	3.279%
26	16.236	2358	2363	2369	rBV	73803	119917	3.01%	0.351%
27	16.789	2453	2457	2469	rVB3	53464	115298	2.89%	0.338%

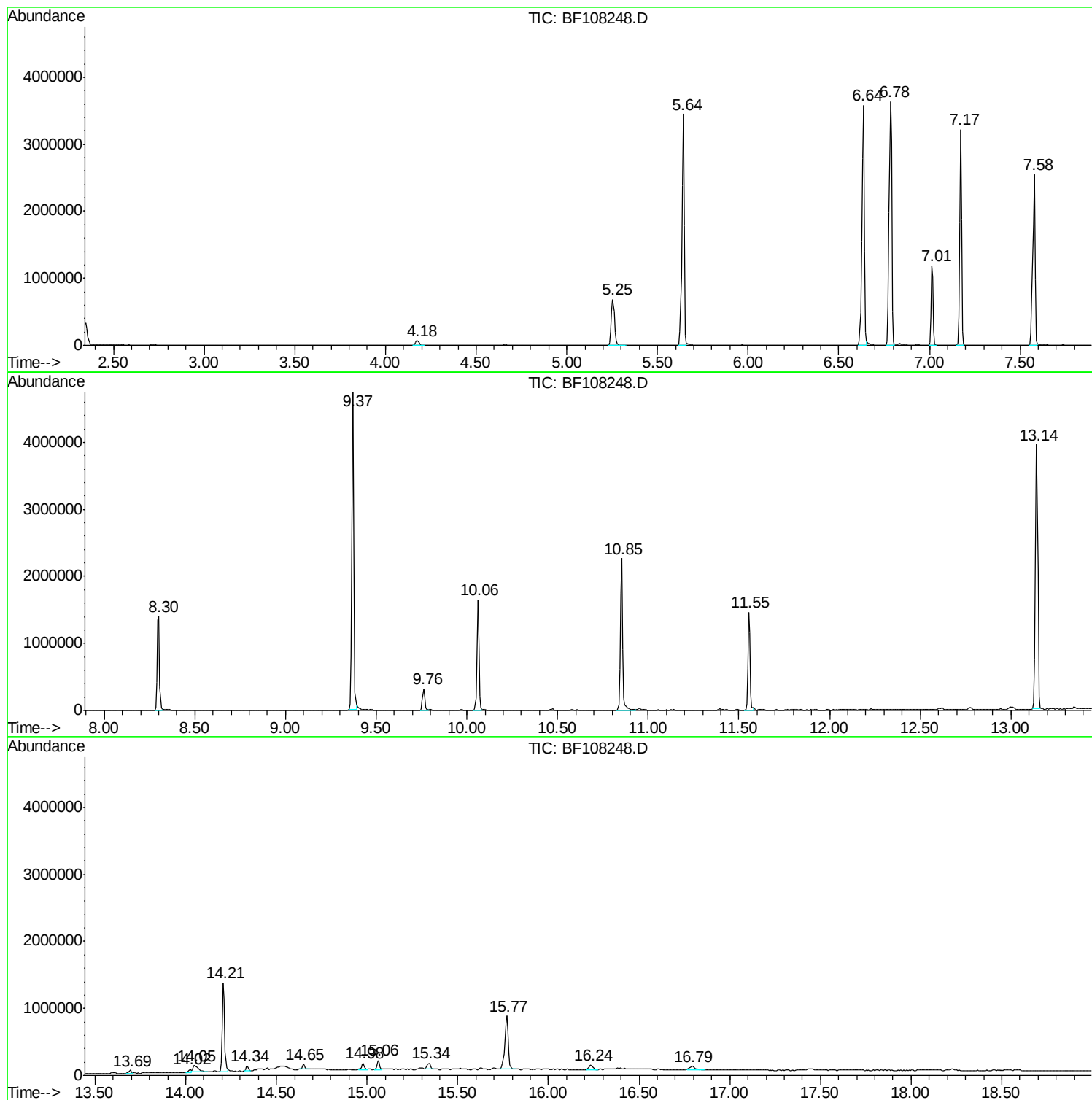
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampled :
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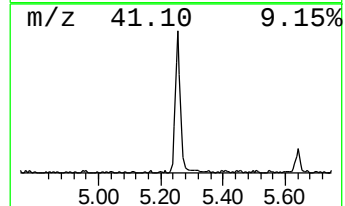
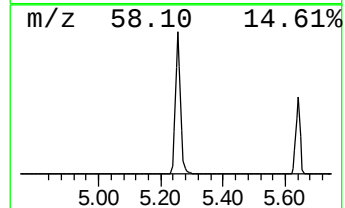
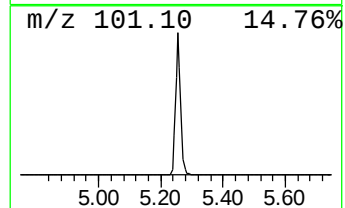
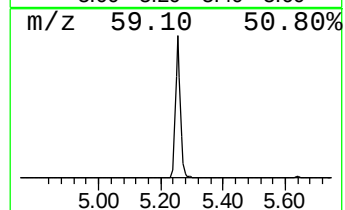
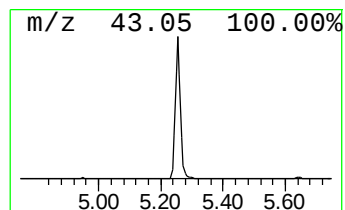
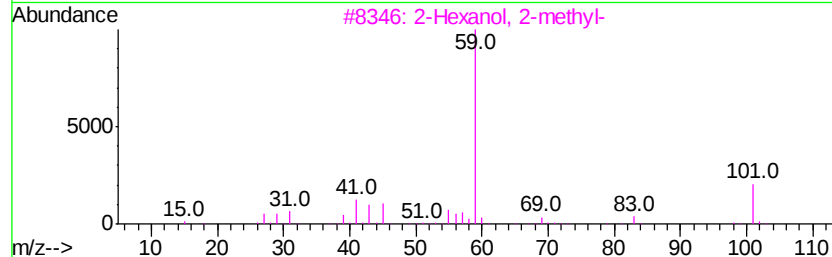
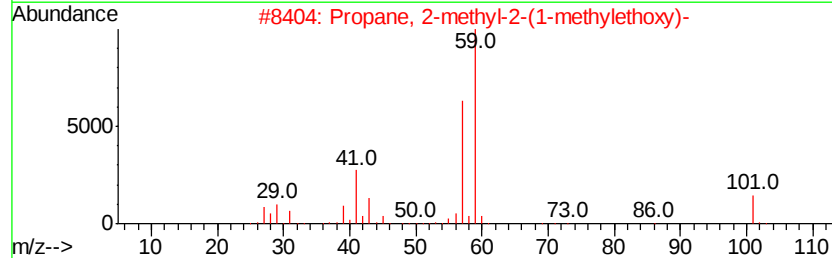
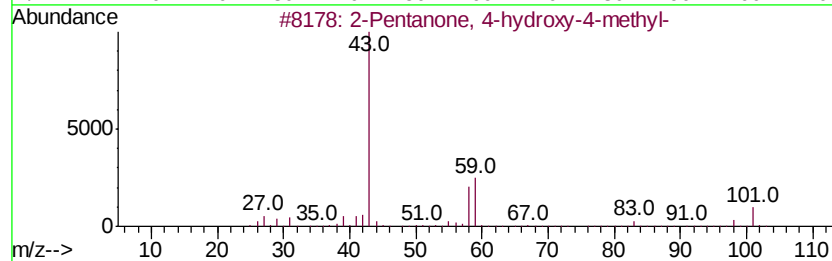
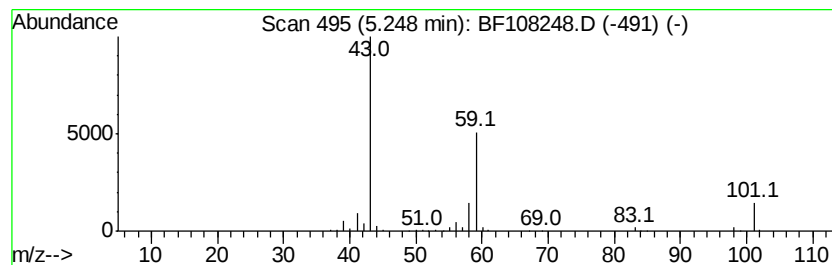
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.25	15.53 ng	790346	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32



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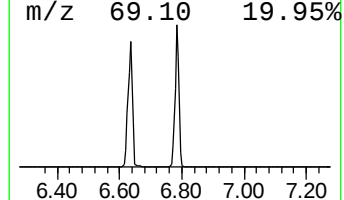
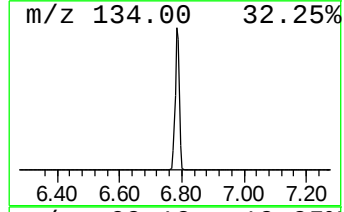
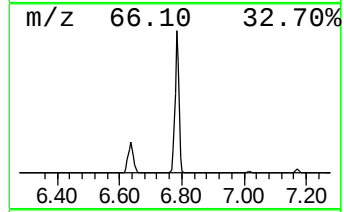
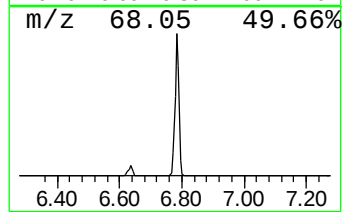
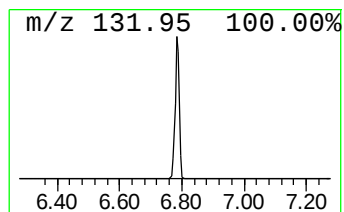
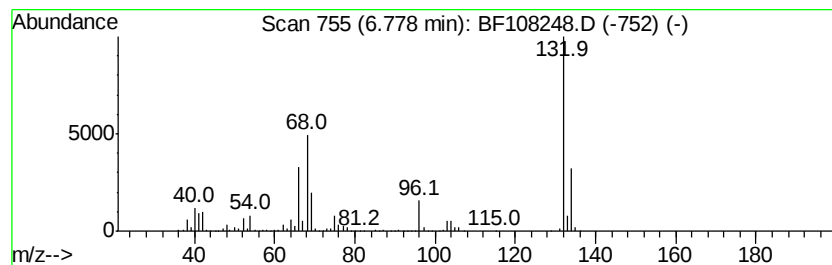
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	67.93 ng	3456140	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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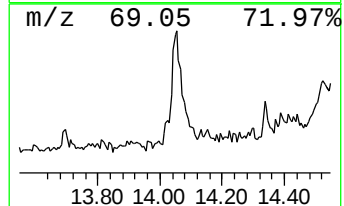
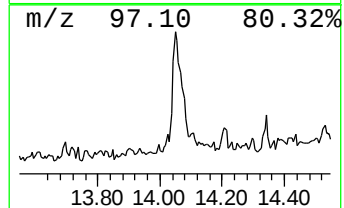
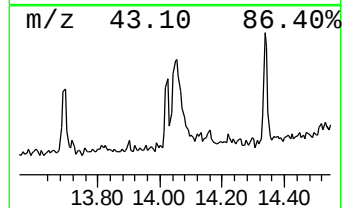
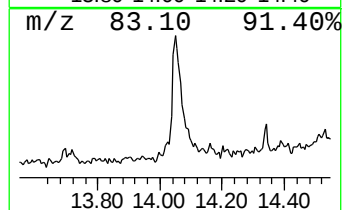
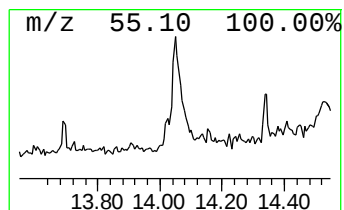
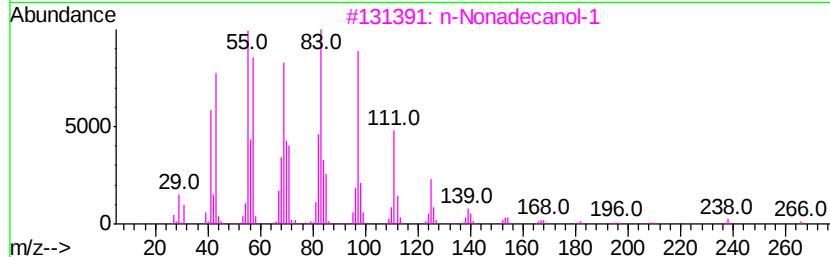
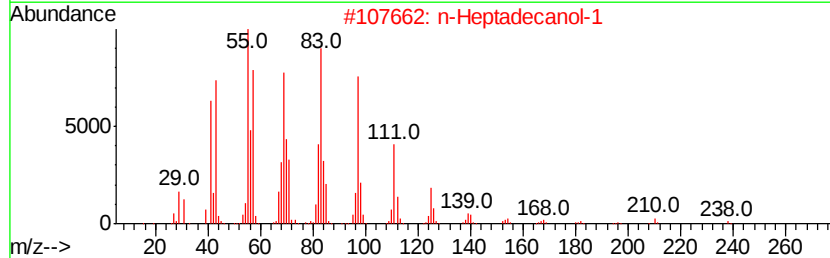
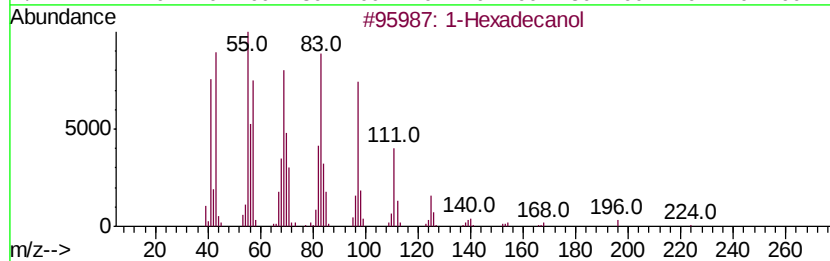
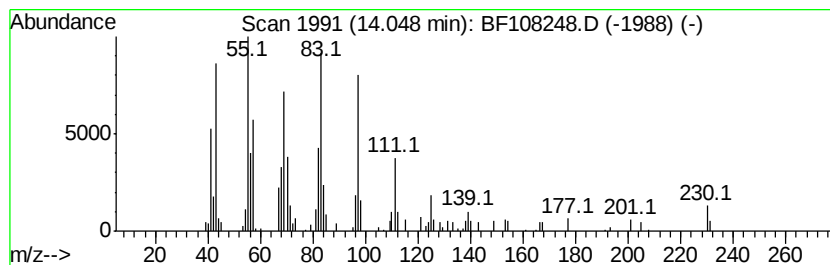
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Peak Number 4 1-Hexadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.05	3.19 ng	201092	Chrysene-d12	14.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	91
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	90



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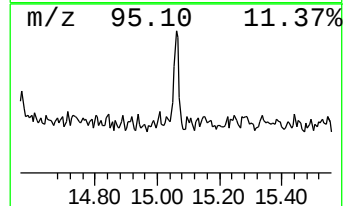
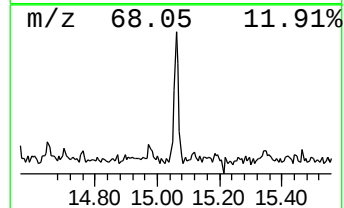
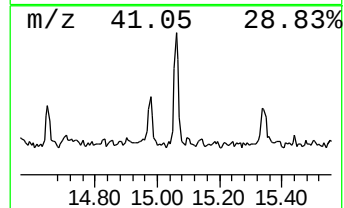
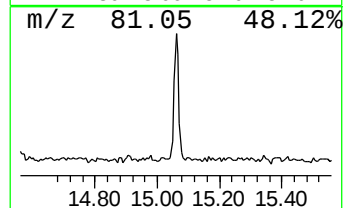
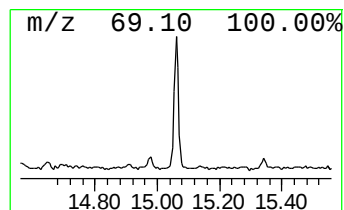
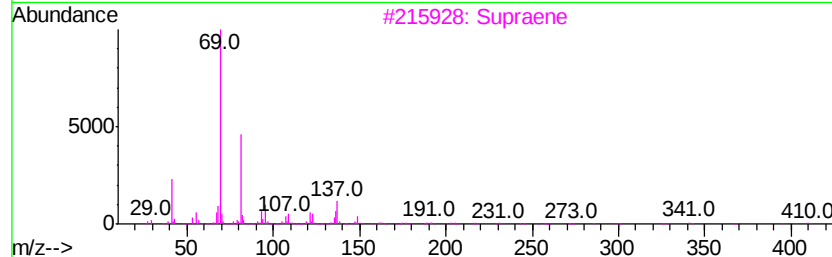
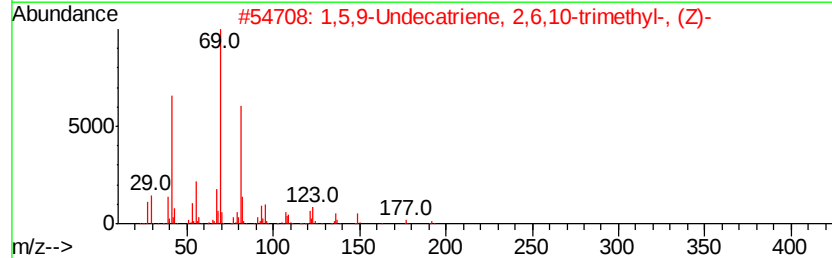
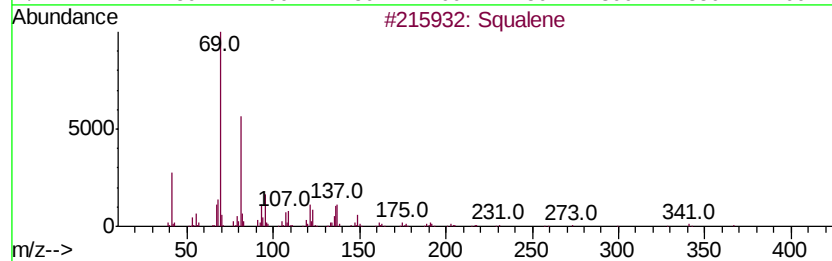
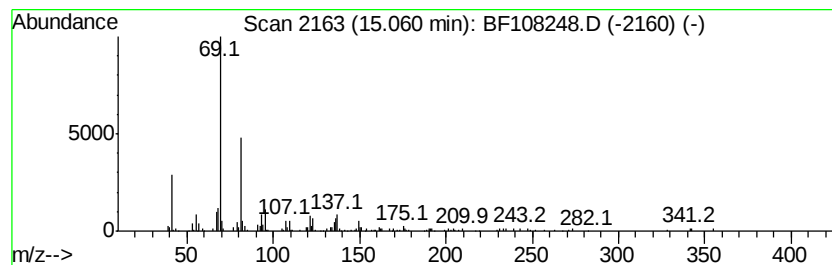
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	2.48 ng	138783	Perylene-d12	15.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	83
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
3		Supraene	410	C30H50	007683-64-9	74
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



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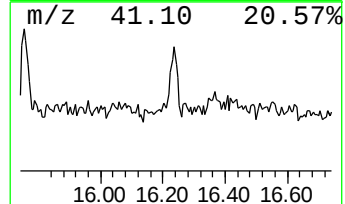
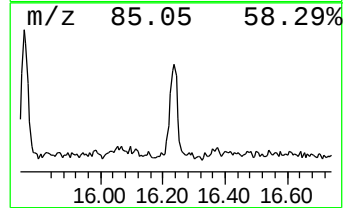
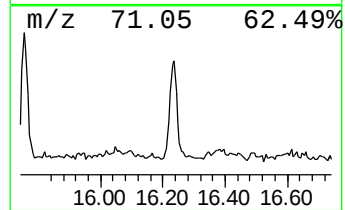
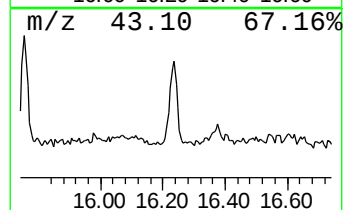
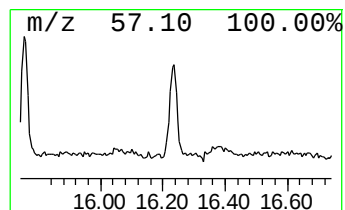
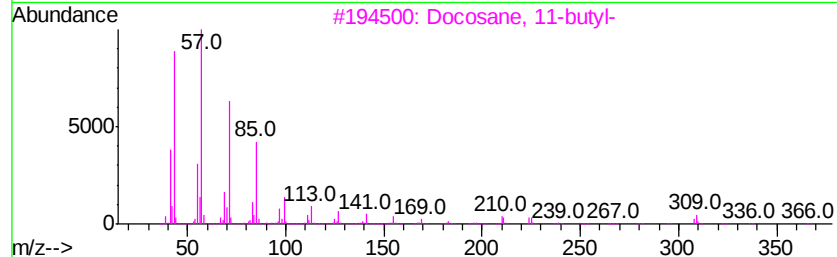
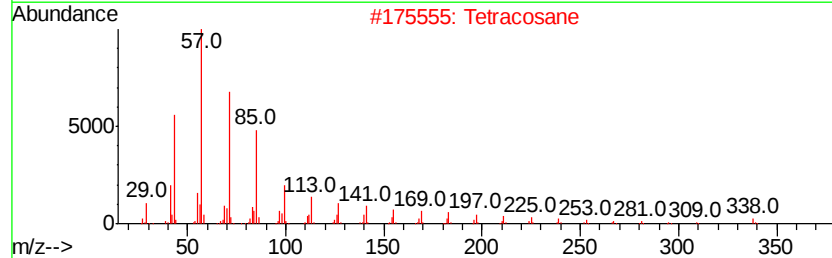
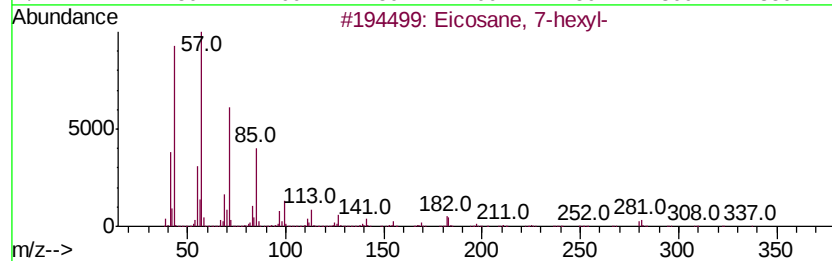
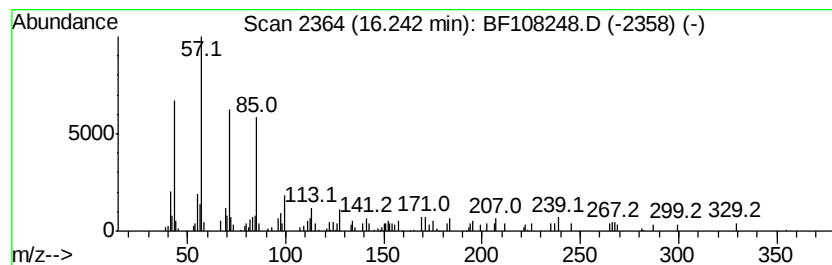
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 6 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	2.14 ng	119917	Perylene-d12	15.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
2		Tetracosane	338	C24H50	000646-31-1	87
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	87
4		Heptacosane	380	C27H56	000593-49-7	83
5		Docosane	310	C22H46	000629-97-0	83



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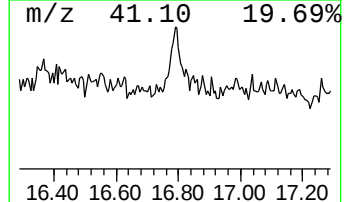
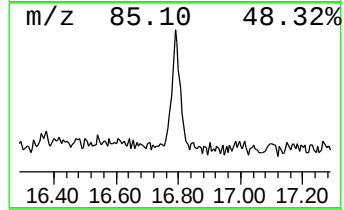
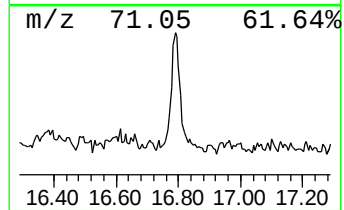
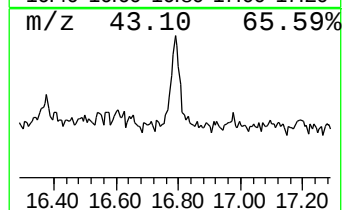
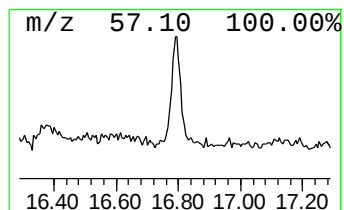
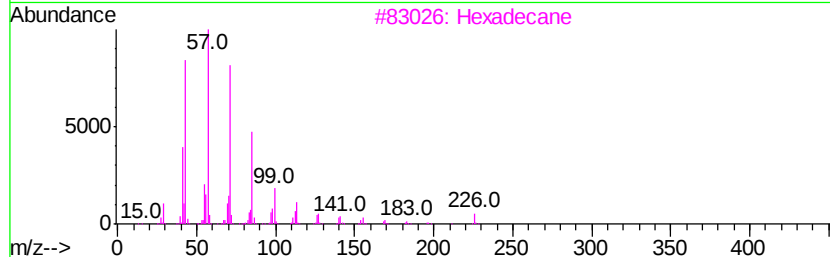
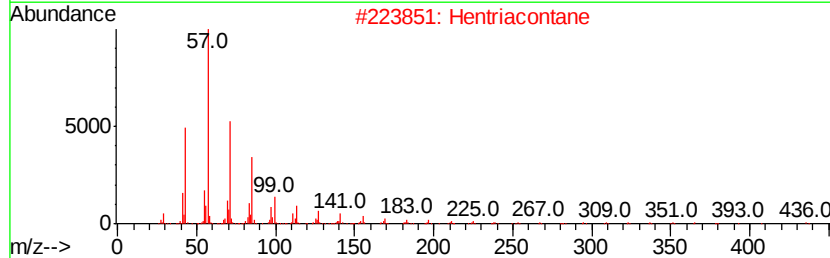
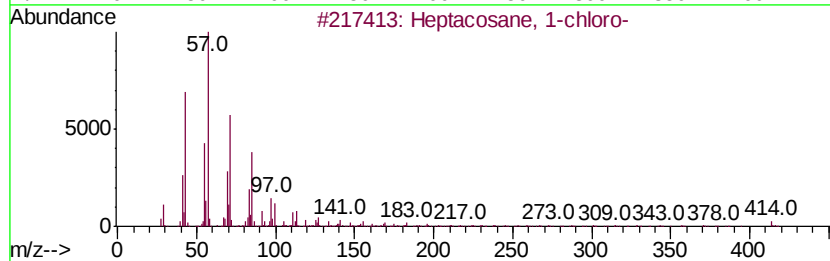
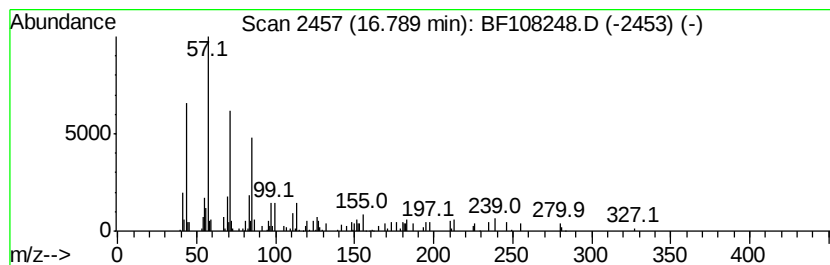
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane, 1-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.79	2.06 ng	115298	Perylene-d12	15.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
2		Hentriacontane	437	C31H64	000630-04-6	80
3		Hexadecane	226	C16H34	000544-76-3	76
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	59
5		Octacosane	394	C28H58	000630-02-4	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
Data File : BF108248.D
Acq On : 17 Aug 2018 17:31
Operator : JU/SJ
Sample : J4500-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.25	15.5	ng	790346	1	7.01	1017520	20.0
unknown6.78	6.78	67.9	ng	3456140	1	7.01	1017520	20.0
1-Hexadecanol	14.05	3.2	ng	201092	5	14.21	1261310	20.0
Squalene	15.06	2.5	ng	138783	6	15.77	1119400	20.0
Eicosane, 7-hexyl-	16.24	2.1	ng	119917	6	15.77	1119400	20.0
Heptacosane, 1-ch...	16.79	2.1	ng	115298	6	15.77	1119400	20.0