

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
 Data File : BF108828.D
 Acq On : 6 Sep 2018 17:31
 Operator : JU/SJ
 Sample : J4803-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q2-E5

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	447	rVB	118958	141838	3.12%	0.317%
2	5.342	507	511	515	rBV	3420178	3328451	73.24%	7.433%
3	6.366	680	685	688	rBV	3870827	3503225	77.08%	7.823%
4	6.501	704	708	712	rBV	3820467	3536726	77.82%	7.898%
5	6.566	717	719	728	rVB	78737	76260	1.68%	0.170%
6	6.736	744	748	751	rBV	2022173	1573529	34.62%	3.514%
7	6.889	770	774	778	rBV	2984465	2766112	60.86%	6.177%
8	7.289	838	842	845	rBV	2398645	2237312	49.23%	4.996%
9	8.019	962	966	969	rBV	2368462	2002393	44.06%	4.471%
10	9.095	1144	1149	1152	rBV	4424273	4036364	88.81%	9.013%
11	9.483	1211	1215	1218	rBV	1424427	1081132	23.79%	2.414%
12	9.766	1259	1263	1267	rBV2	2566302	2153185	47.38%	4.808%
13	10.548	1392	1396	1399	rBV	2406609	2090933	46.01%	4.669%
14	11.242	1510	1514	1517	rBV	2368993	1962778	43.19%	4.383%
15	11.266	1517	1518	1521	rVV	161020	77288	1.70%	0.173%
16	11.313	1521	1526	1530	rVB2	46380	46263	1.02%	0.103%
17	11.783	1601	1606	1615	rBV2	503348	607484	13.37%	1.357%
18	12.448	1715	1719	1723	rBV	282112	249119	5.48%	0.556%
19	12.565	1736	1739	1749	rBV2	182232	259606	5.71%	0.580%
20	12.671	1752	1757	1763	rVV	252412	254108	5.59%	0.567%
21	12.824	1779	1783	1786	rBV	3408657	2914068	64.12%	6.507%
22	13.107	1828	1831	1838	rBV5	32097	45988	1.01%	0.103%
23	13.736	1935	1938	1944	rBV2	466081	506215	11.14%	1.130%
24	13.871	1956	1961	1964	rBV2	4404704	4544719	100.00%	10.148%
25	14.054	1990	1992	1995	rBV	54651	53785	1.18%	0.120%
26	14.359	2042	2044	2053	rVB2	126815	192371	4.23%	0.430%
27	14.654	2091	2094	2100	rVB	204340	232781	5.12%	0.520%
28	14.724	2104	2106	2111	rVB	116979	128606	2.83%	0.287%
29	14.871	2128	2131	2134	rBV	117281	163891	3.61%	0.366%
30	14.977	2145	2149	2153	rBV	326318	368023	8.10%	0.822%
31	15.212	2186	2189	2193	rVB	132438	163128	3.59%	0.364%
32	15.277	2195	2200	2204	rVV	1538484	1934043	42.56%	4.319%
33	15.330	2206	2209	2214	rVB	399091	515613	11.35%	1.151%
34	15.742	2274	2279	2284	rBV	323633	500991	11.02%	1.119%

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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 >
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35	16.212	2355	2359	2373	rVB2	241431	533857	11.75%	1.192%
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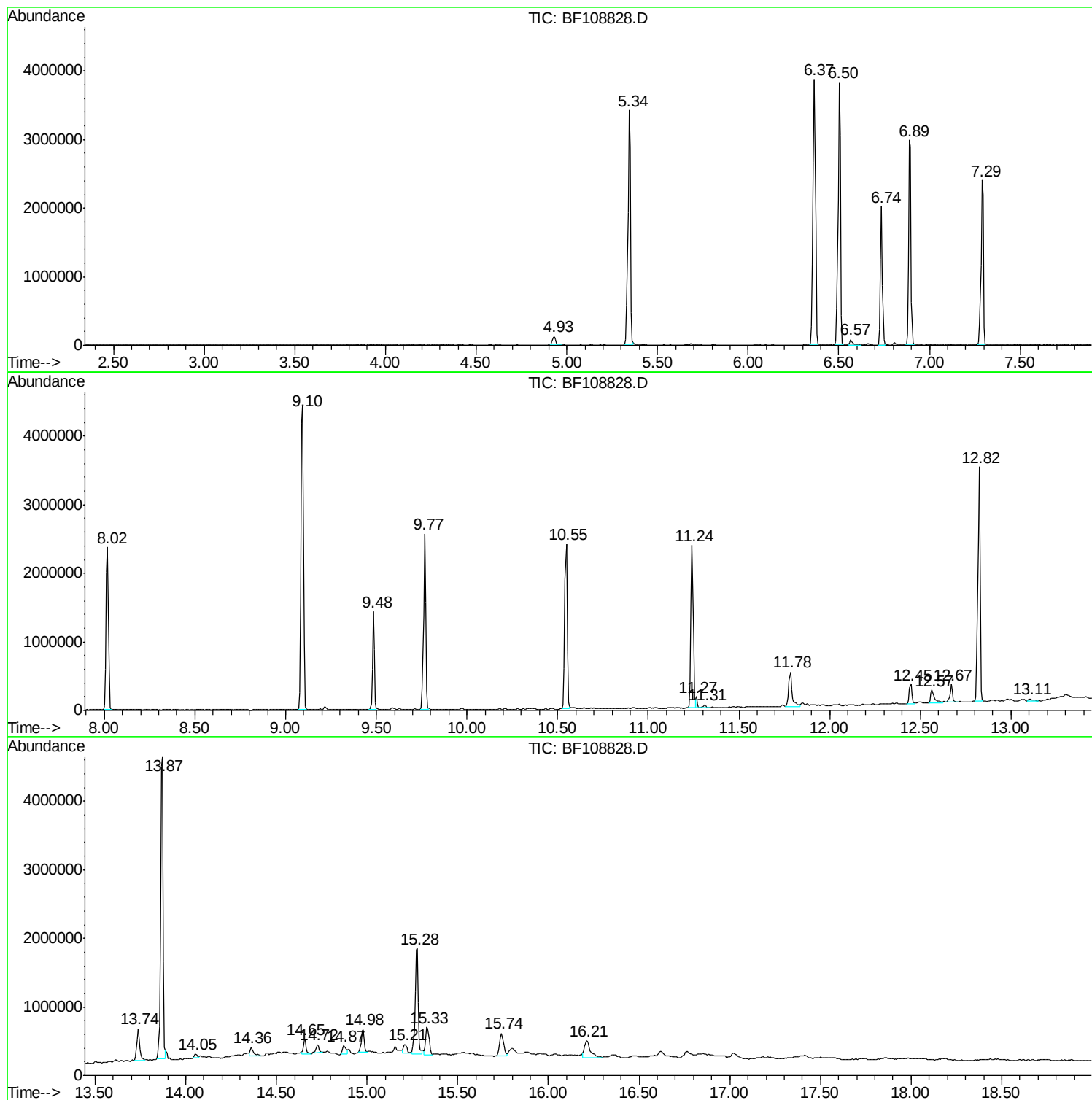
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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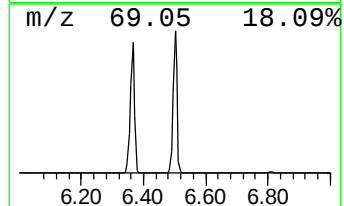
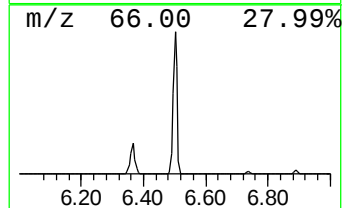
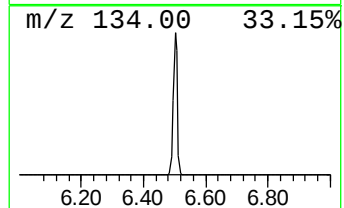
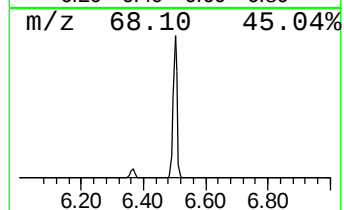
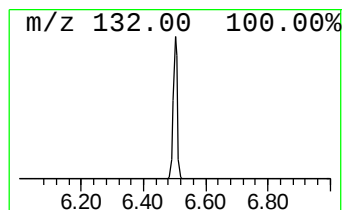
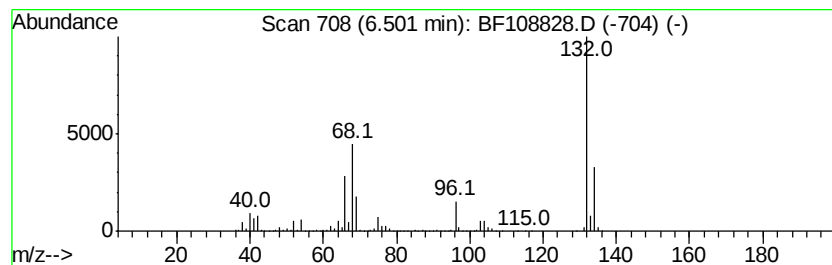
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	44.95 ng	3536730	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	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	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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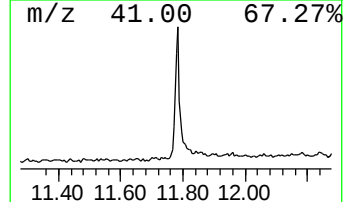
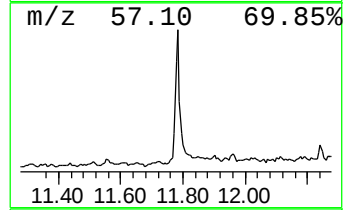
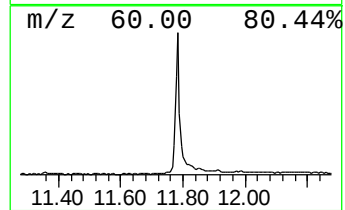
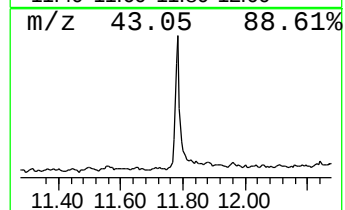
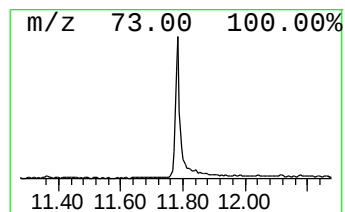
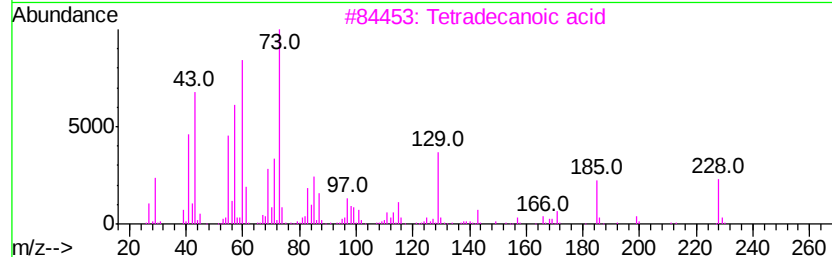
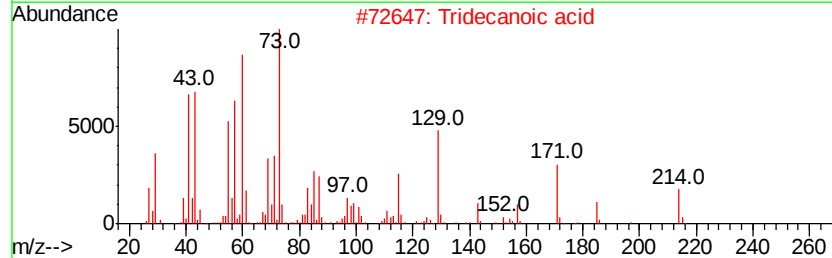
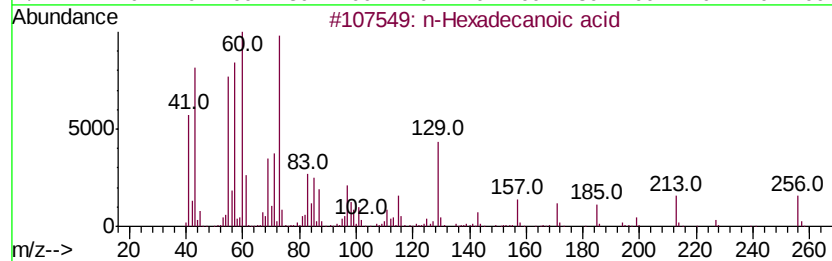
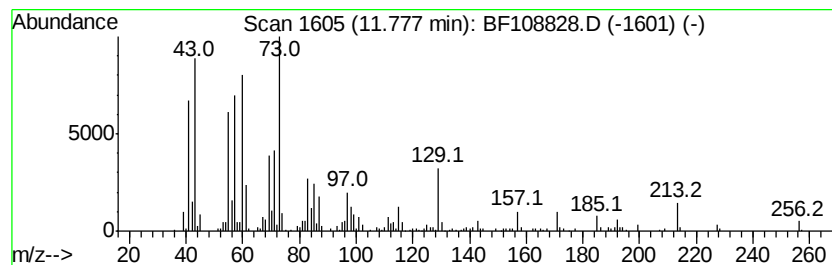
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	6.19 ng	607484	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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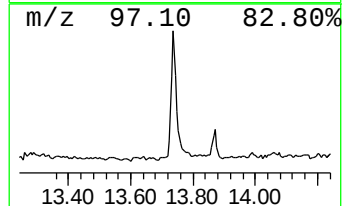
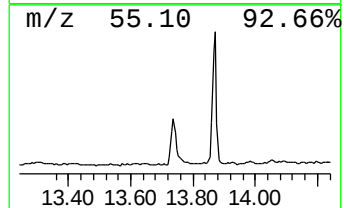
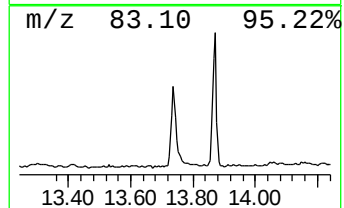
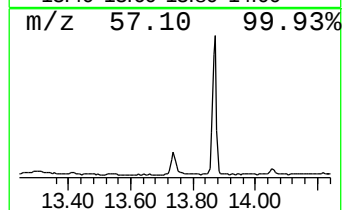
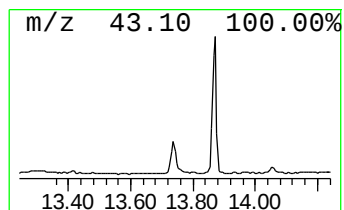
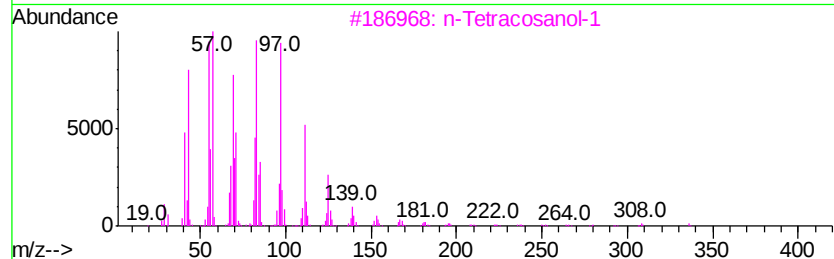
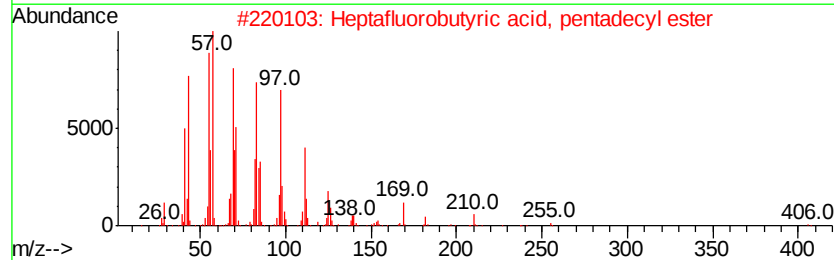
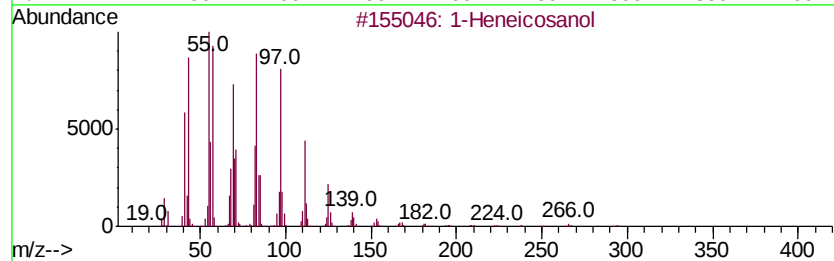
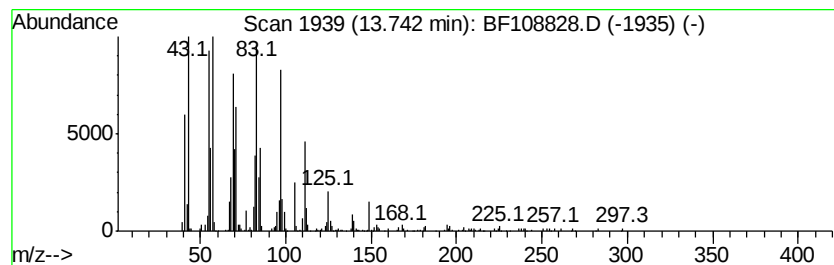
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.23 ng	506215	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	94
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	91
4	1-Nonadecene		266	C19H38	018435-45-5	91
5	Behenic alcohol		326	C22H46O	000661-19-8	91



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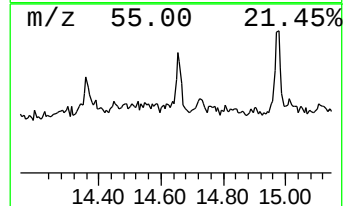
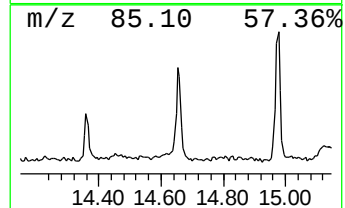
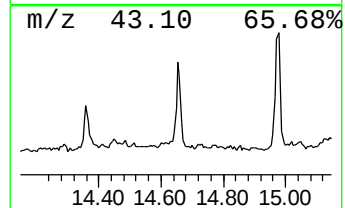
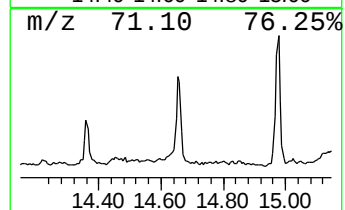
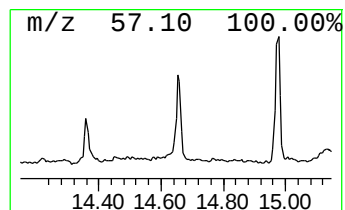
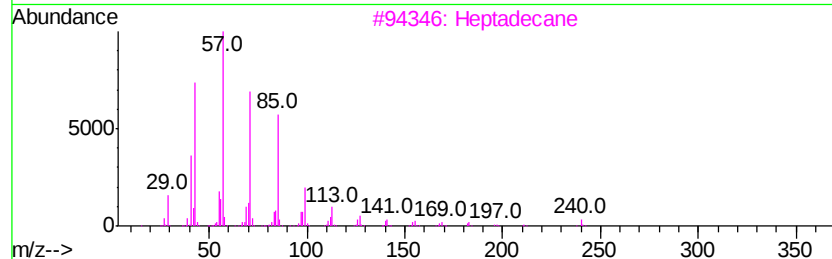
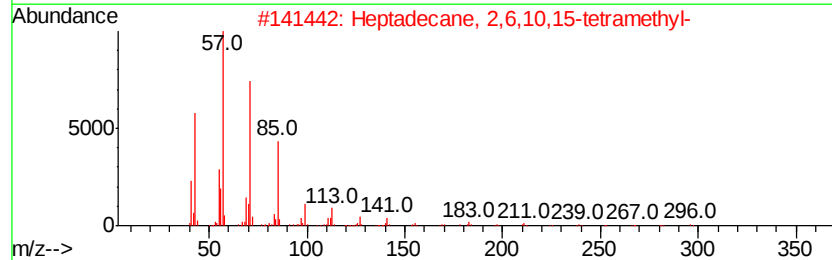
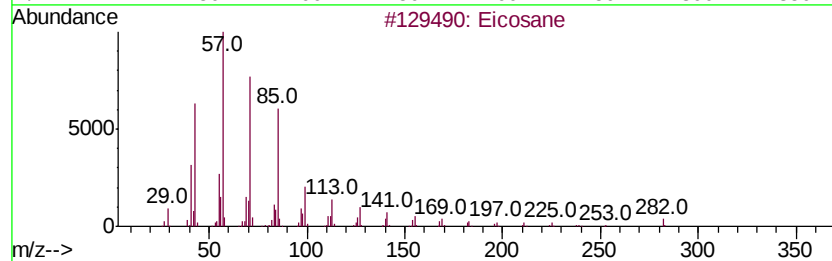
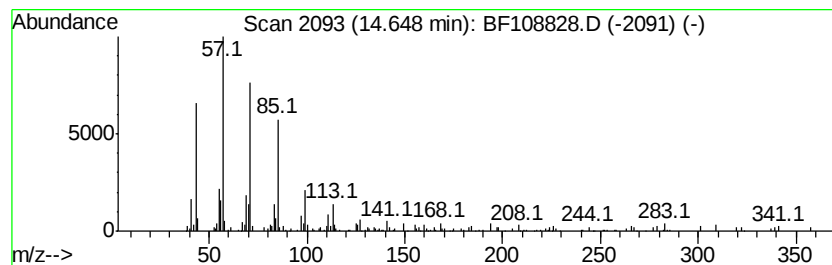
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.41 ng	232781	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	93
3	Heptadecane		240	C17H36	000629-78-7	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Heneicosane		296	C21H44	000629-94-7	90



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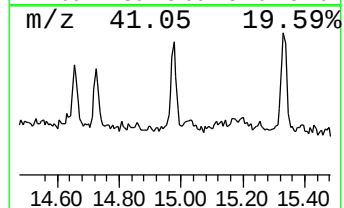
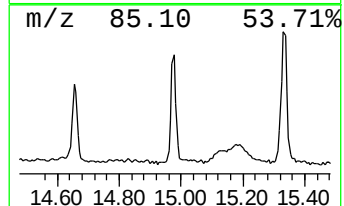
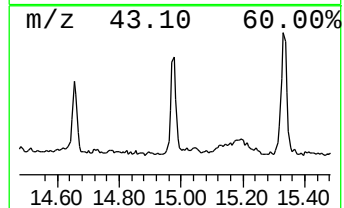
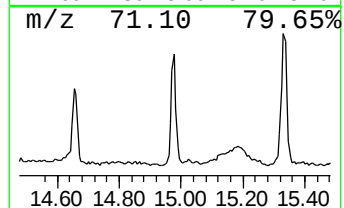
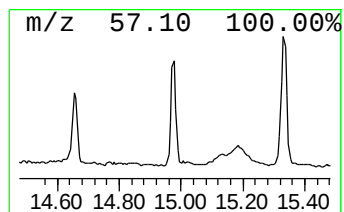
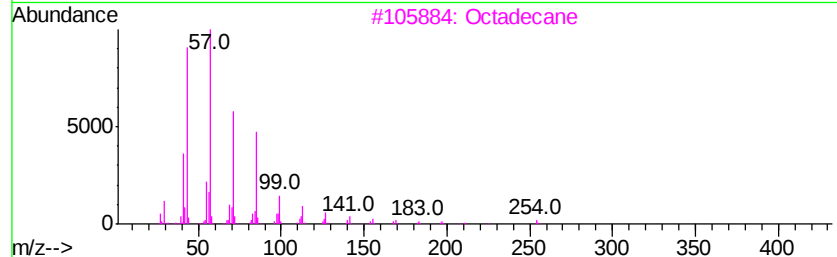
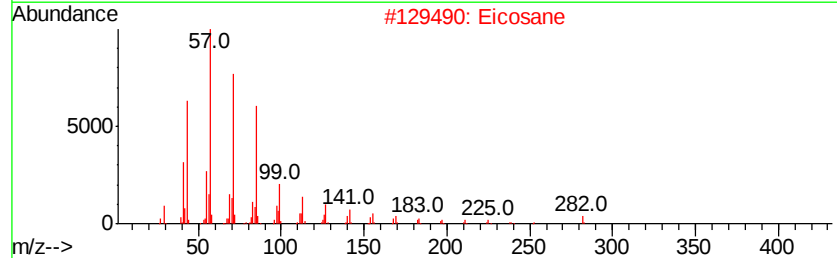
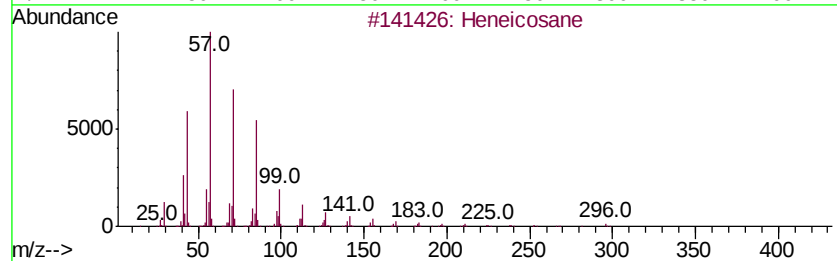
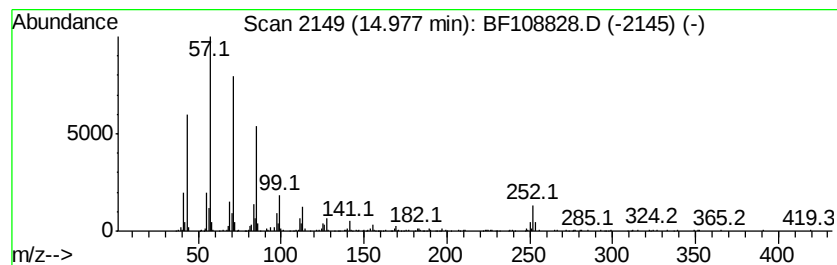
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.81 ng	368023	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Eicosane	282	C20H42	000112-95-8	87
3		Octadecane	254	C18H38	000593-45-3	86
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	80



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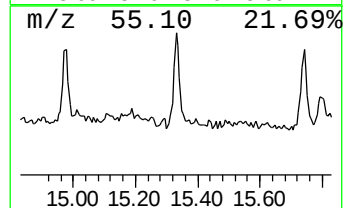
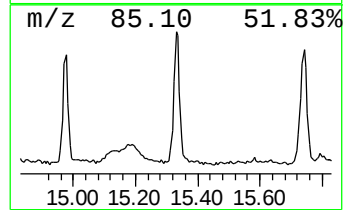
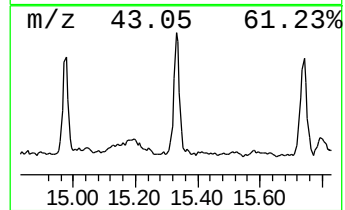
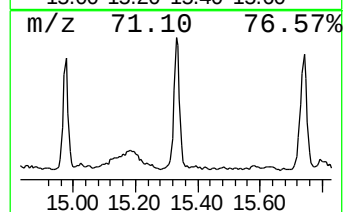
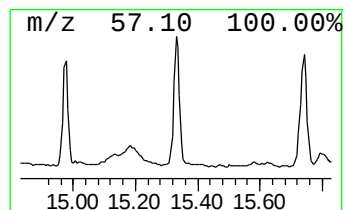
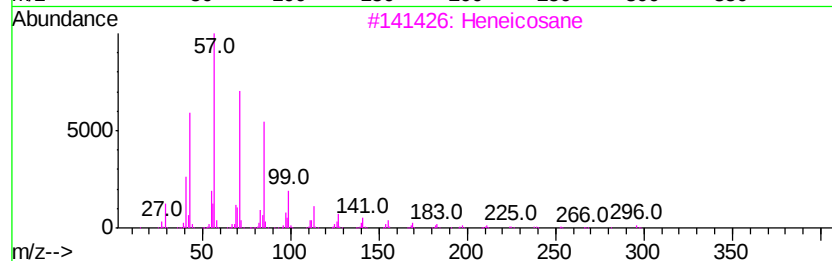
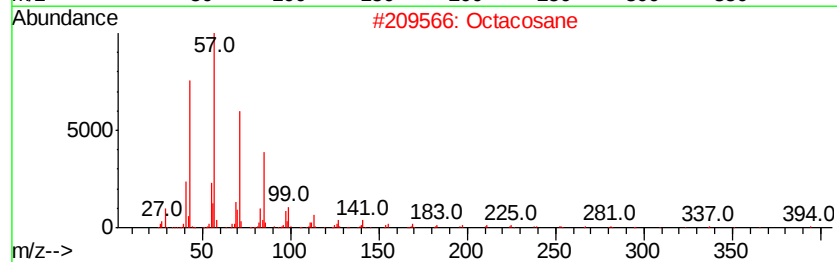
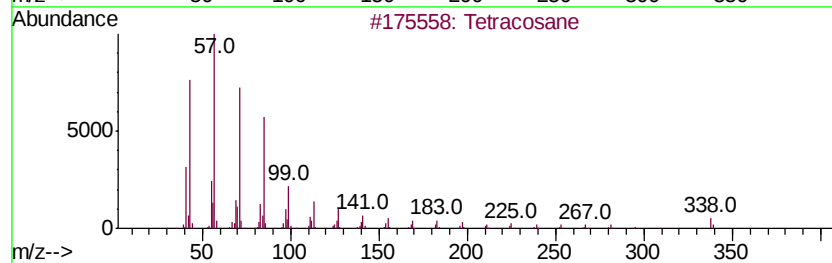
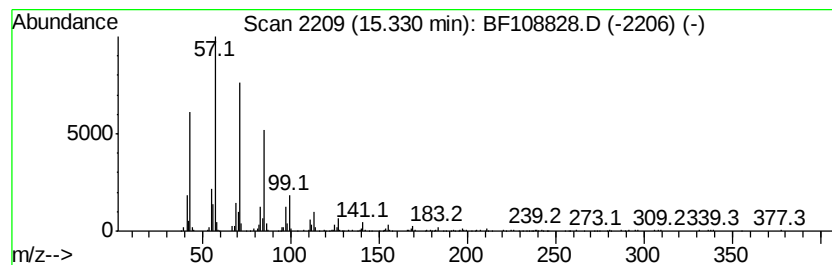
Instrument :
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 ClientSampleId :
 EP1-Q2-E5

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 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.33	5.33 ng	515613	Perylene-d12	15.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108828.D
Acq On : 6 Sep 2018 17:31
Operator : JU/SJ
Sample : J4803-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

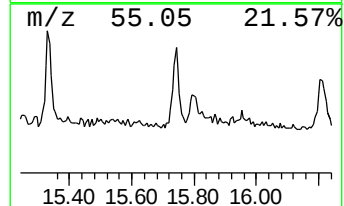
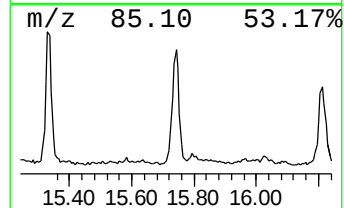
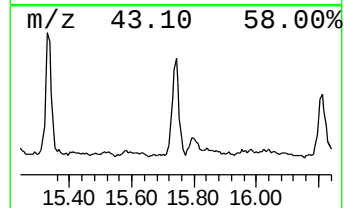
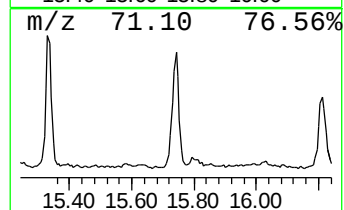
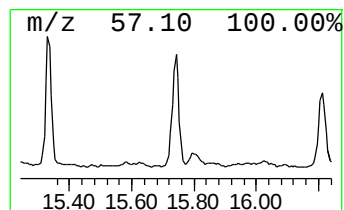
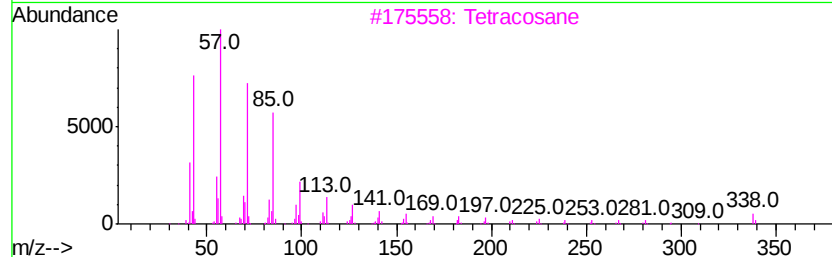
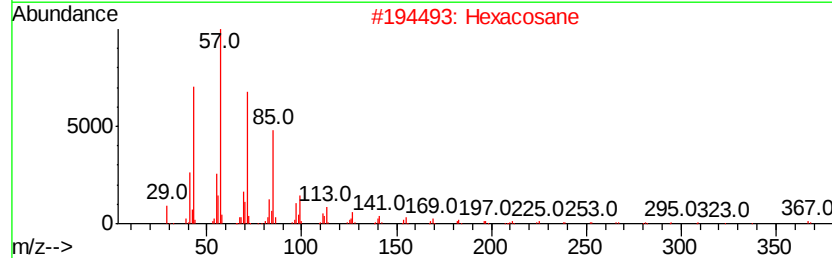
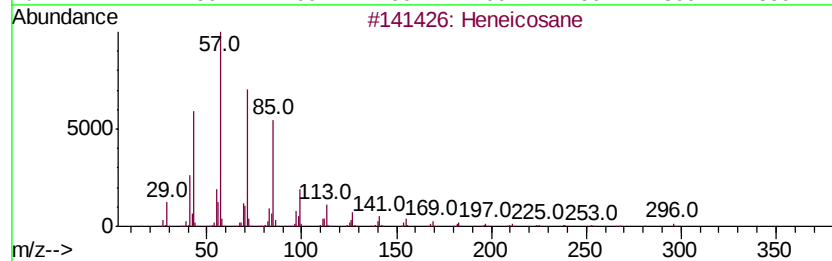
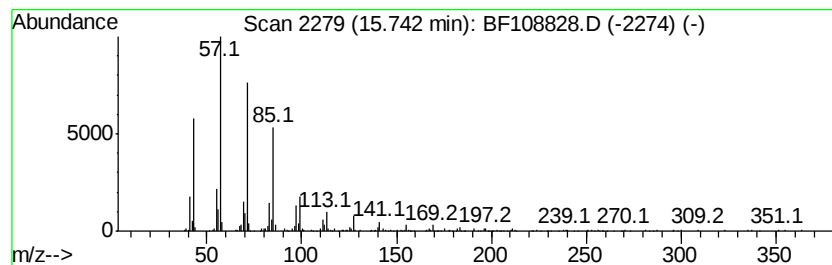
Instrument :
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ClientSampleId :
EP1-Q2-E5

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 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.74	5.18 ng	500991	Perylene-d12	15.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108828.D
Acq On : 6 Sep 2018 17:31
Operator : JU/SJ
Sample : J4803-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-E5

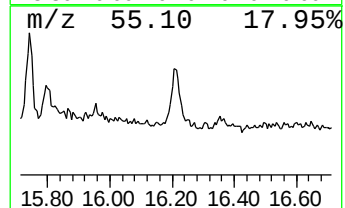
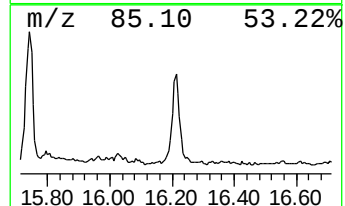
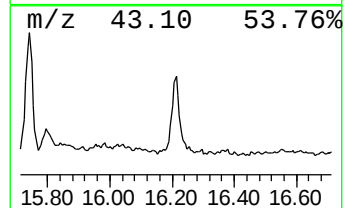
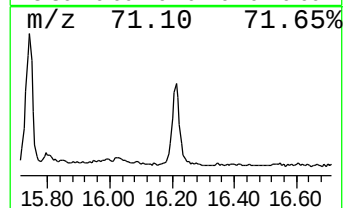
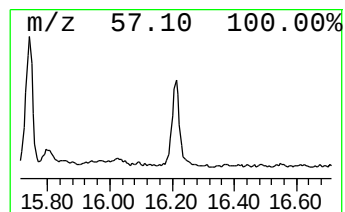
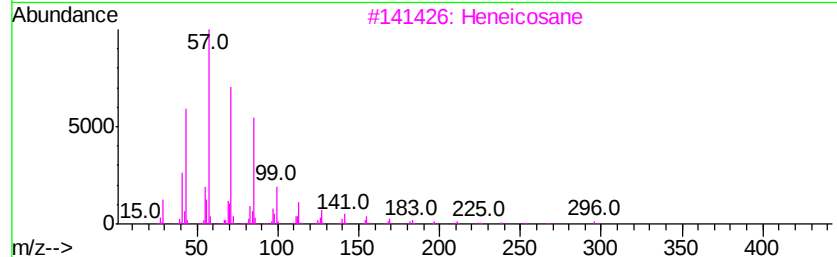
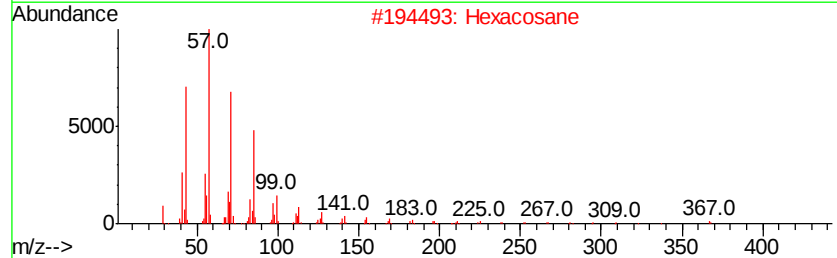
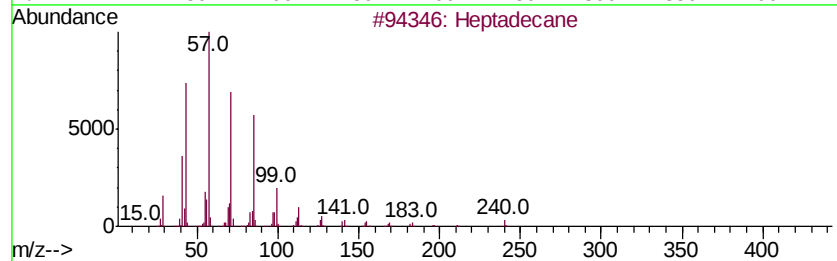
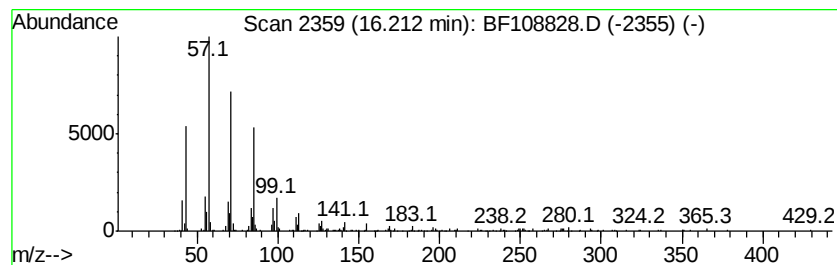
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	5.52 ng	533857	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	95
2		Hexacosane	366	C26H54	000630-01-3	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	87
5		Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
Data File : BF108828.D
Acq On : 6 Sep 2018 17:31
Operator : JU/SJ
Sample : J4803-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-E5

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
unknown6.50	6.50	45.0	ng	3536730	1	6.74	1573530	20.0
n-Hexadecanoic acid	11.78	6.2	ng	607484	4	11.24	1962780	20.0
1-Heneicosanol	13.74	2.2	ng	506215	5	13.87	4544720	20.0
Eicosane	14.65	2.4	ng	232781	6	15.28	1934040	20.0
Octadecane	14.98	3.8	ng	368023	6	15.28	1934040	20.0
Tetracosane	15.33	5.3	ng	515613	6	15.28	1934040	20.0
Hexacosane	15.74	5.2	ng	500991	6	15.28	1934040	20.0
Heptadecane	16.21	5.5	ng	533857	6	15.28	1934040	20.0