

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
 Data File : BF112946.D
 Acq On : 8 Mar 2019 16:05
 Operator : JU/SJ
 Sample : K1787-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-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-BF022719.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	5.340	548	553	556	rBV	3594789	3396318	70.27%	8.721%
2	6.363	722	727	734	rBV	3362027	3698615	76.52%	9.497%
3	6.498	745	750	753	rBV	3971280	3657790	75.67%	9.393%
4	6.728	785	789	793	rBV	1244934	992555	20.53%	2.549%
5	6.886	812	816	819	rBV	3368146	2848489	58.93%	7.314%
6	7.286	879	884	887	rBV	2362912	2242807	46.40%	5.759%
7	8.010	1003	1007	1014	rBV	1291096	1233560	25.52%	3.168%
8	9.086	1186	1190	1204	rBV	4606819	4333738	89.66%	11.128%
9	9.480	1253	1257	1269	rVB	266339	259582	5.37%	0.667%
10	9.757	1300	1304	1313	rBV	1465469	1469365	30.40%	3.773%
11	10.545	1433	1438	1450	rBV	2836716	2976322	61.58%	7.643%
12	11.233	1552	1555	1570	rVB	1512988	1650627	34.15%	4.239%
13	11.774	1644	1647	1651	rBV	230712	263158	5.44%	0.676%
14	11.810	1651	1653	1657	rVB2	113453	118835	2.46%	0.305%
15	12.363	1745	1747	1750	rVB	96931	77760	1.61%	0.200%
16	12.557	1777	1780	1788	rBV	124239	185691	3.84%	0.477%
17	12.816	1820	1824	1828	rBV	4528399	4833563	100.00%	12.412%
18	12.868	1830	1833	1842	rVB	77107	84609	1.75%	0.217%
19	13.339	1910	1913	1917	rVB	52461	49316	1.02%	0.127%
20	13.727	1972	1979	1985	rBV2	153401	270486	5.60%	0.695%
21	13.774	1985	1987	1994	rVV	49241	58174	1.20%	0.149%
22	13.863	1997	2002	2016	rVB	1571301	1814139	37.53%	4.658%
23	14.345	2081	2084	2091	rBV2	85016	104589	2.16%	0.269%
24	14.639	2131	2134	2138	rVB	122906	109079	2.26%	0.280%
25	14.710	2142	2146	2150	rVB	195173	180029	3.72%	0.462%
26	14.957	2184	2188	2195	rBV	129264	149852	3.10%	0.385%
27	15.262	2235	2240	2245	rBV	1054270	1388052	28.72%	3.564%
28	15.309	2245	2248	2253	rVB	120638	166430	3.44%	0.427%
29	15.709	2312	2316	2322	rBV	94995	142112	2.94%	0.365%
30	16.180	2391	2396	2403	rBV	67225	119101	2.46%	0.306%
31	16.727	2484	2489	2496	rVB2	34381	68604	1.42%	0.176%

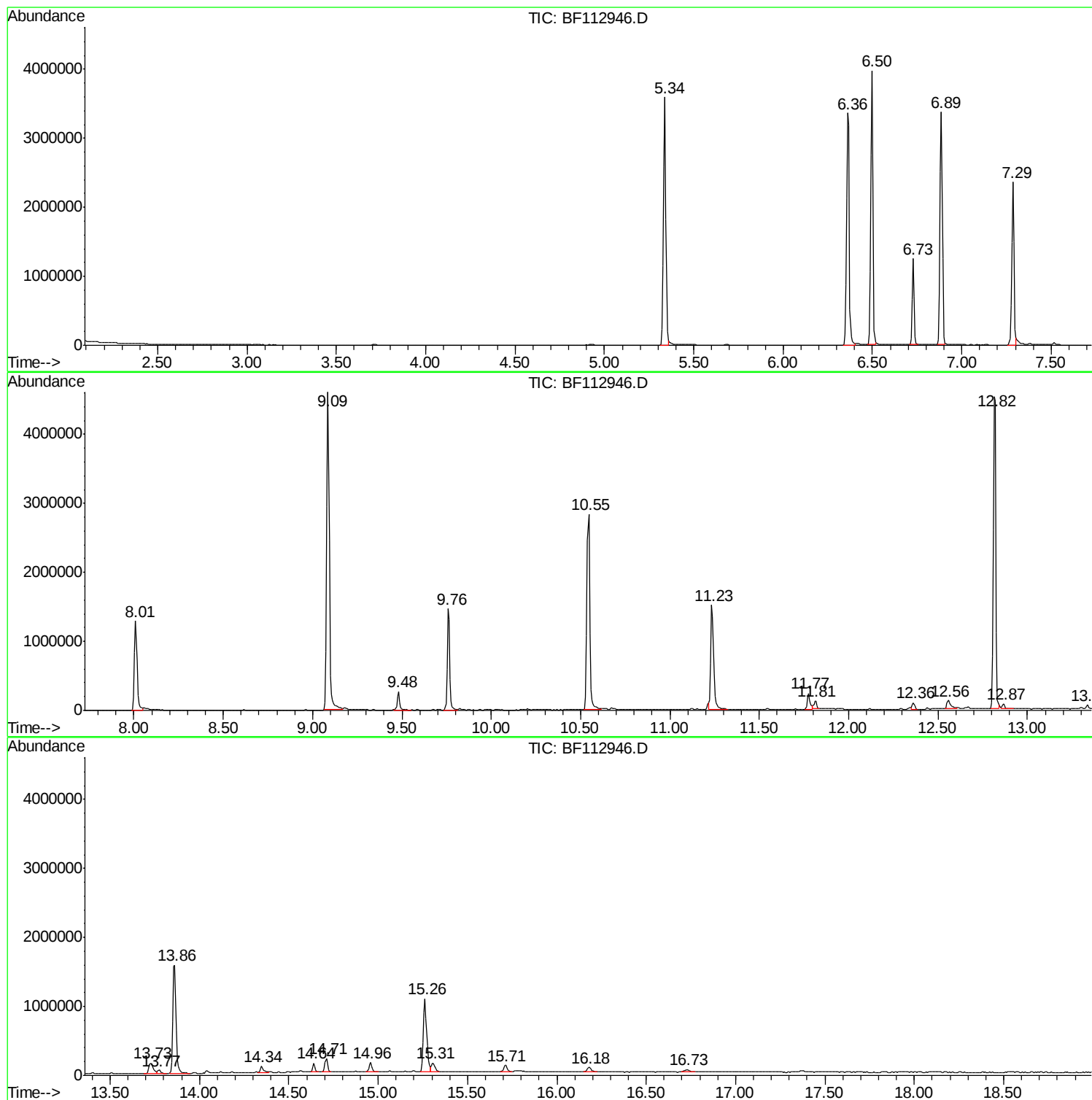
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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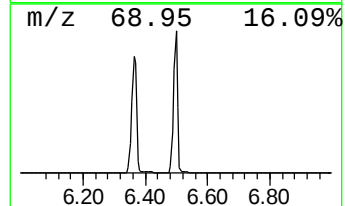
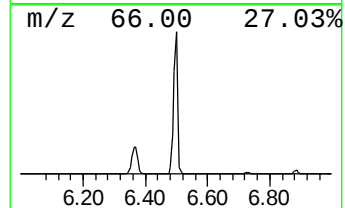
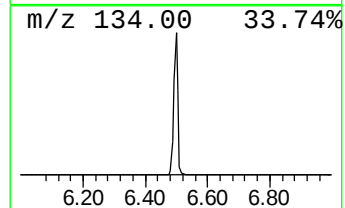
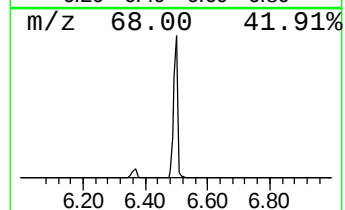
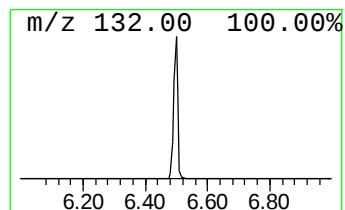
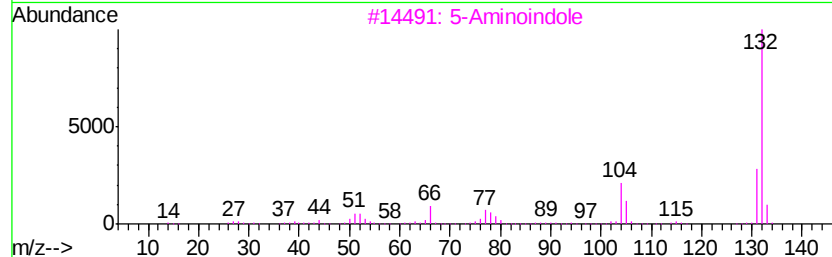
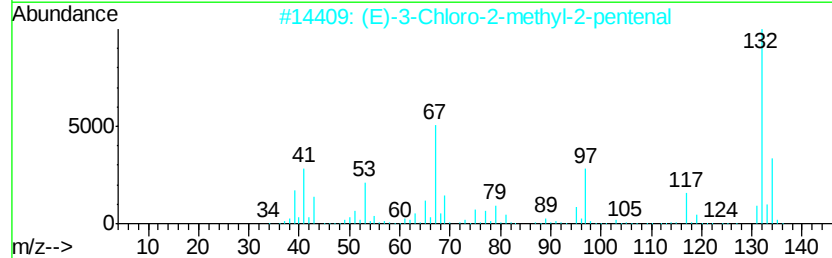
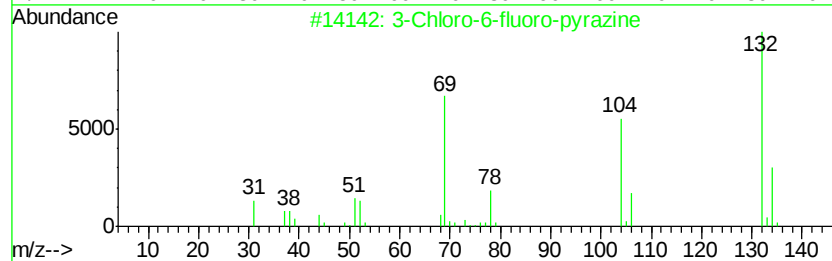
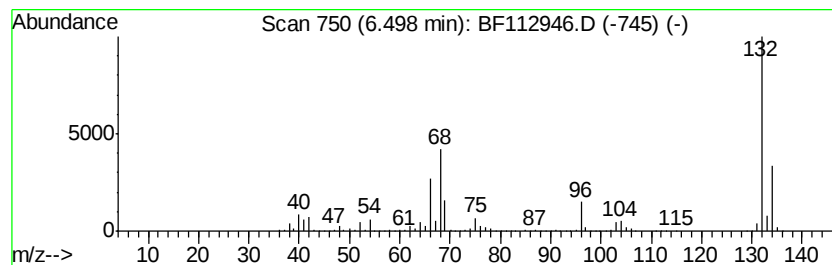
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	73.70 ng	3657790	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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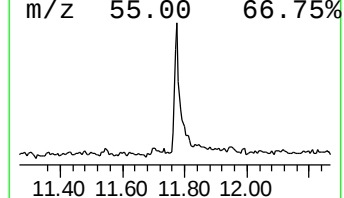
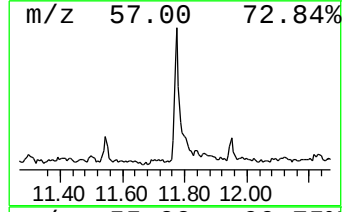
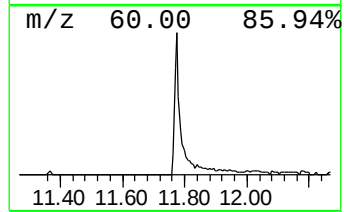
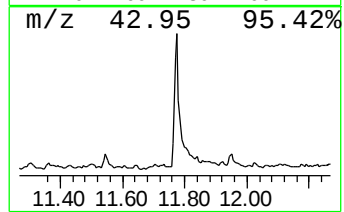
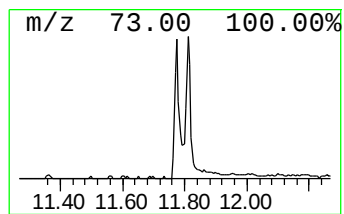
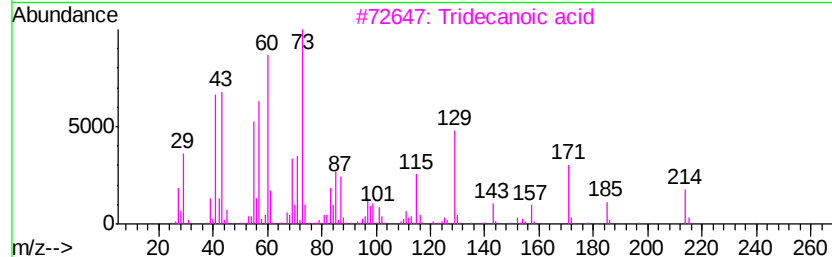
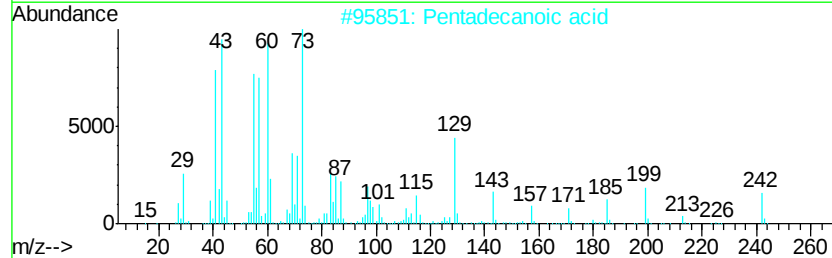
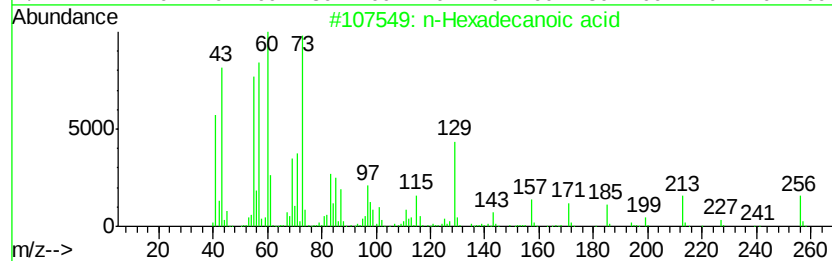
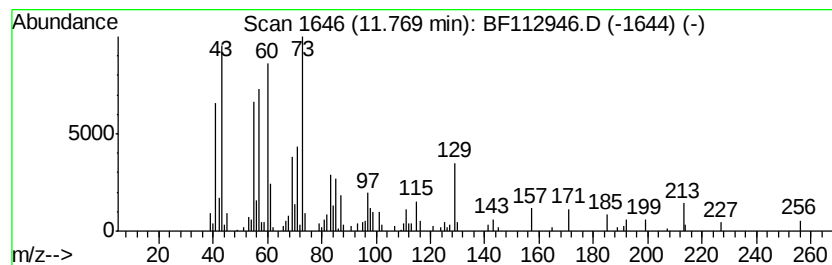
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.19 ng	263158	Phenanthrene-d10	11.23

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	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	92
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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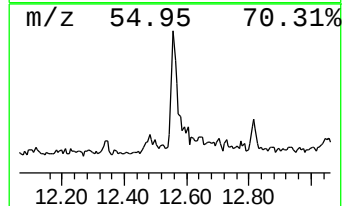
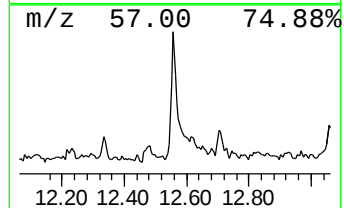
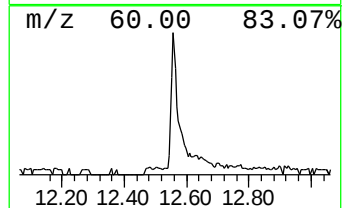
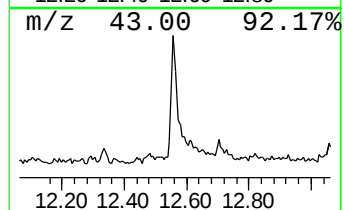
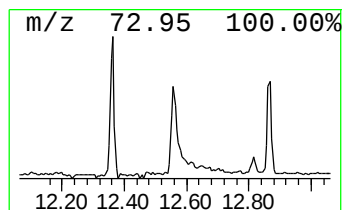
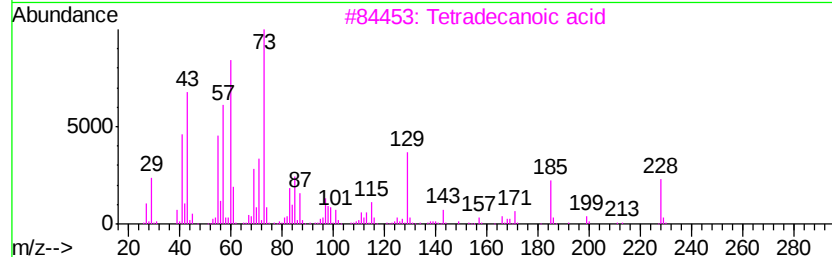
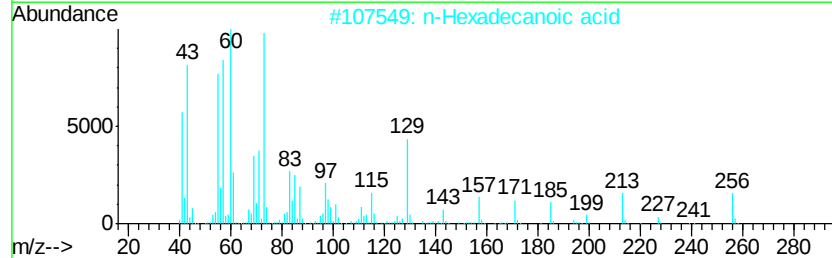
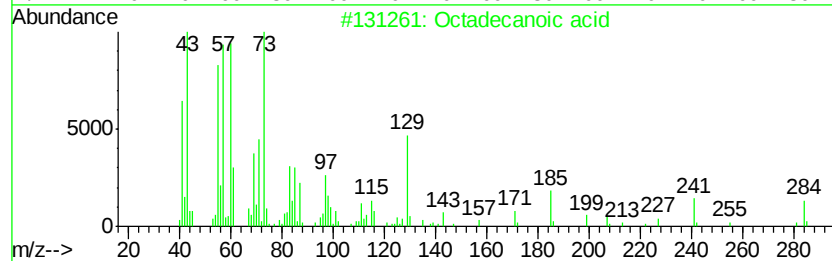
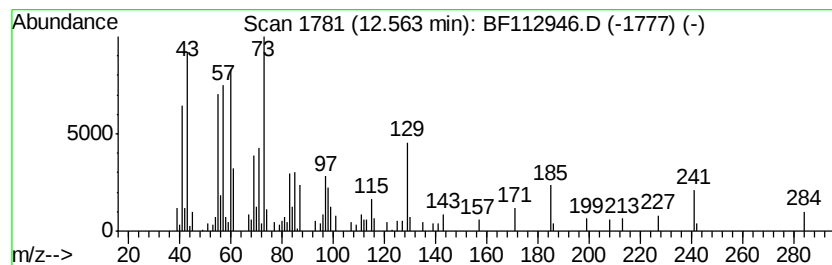
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.05 ng	185691	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5		Undecanoic acid	186	C11H22O2	000112-37-8	60



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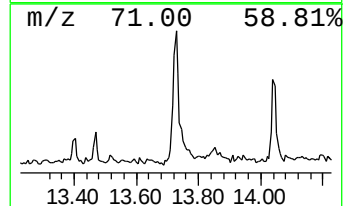
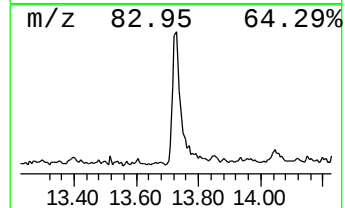
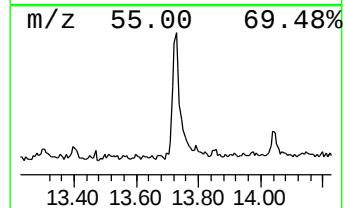
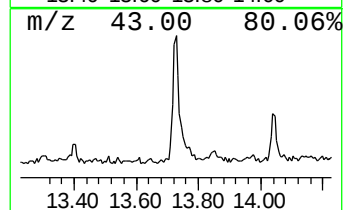
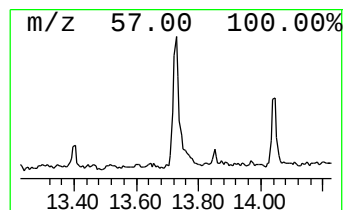
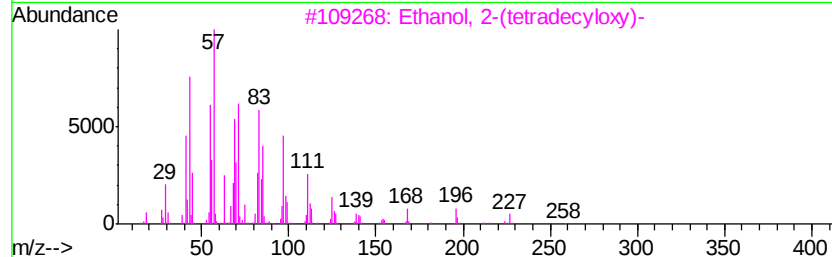
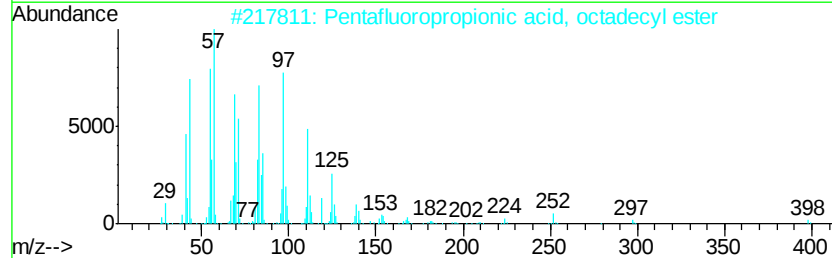
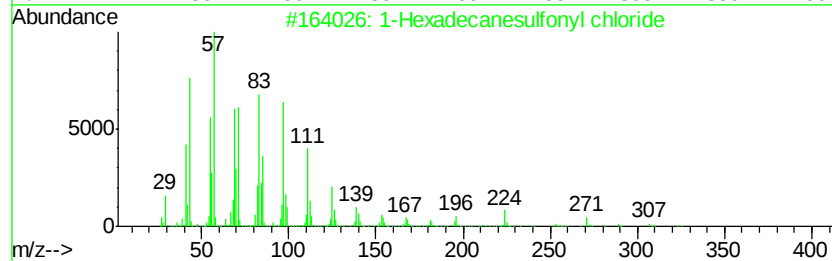
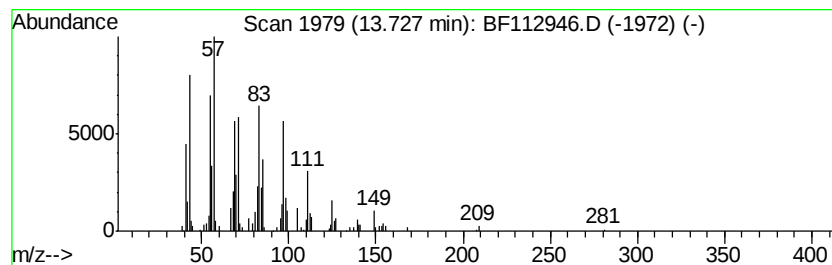
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Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.98 ng	270486	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90



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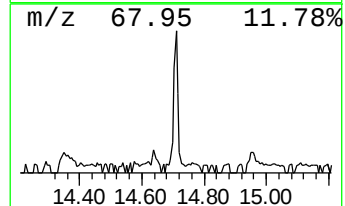
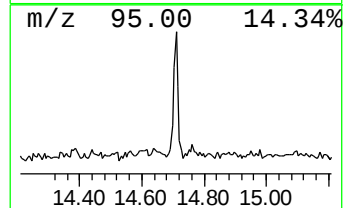
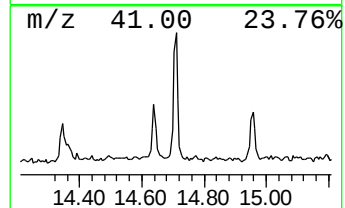
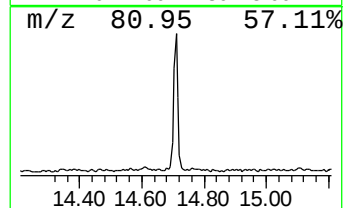
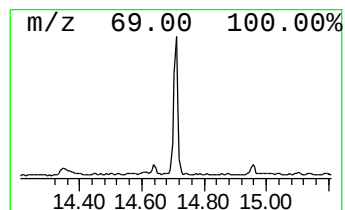
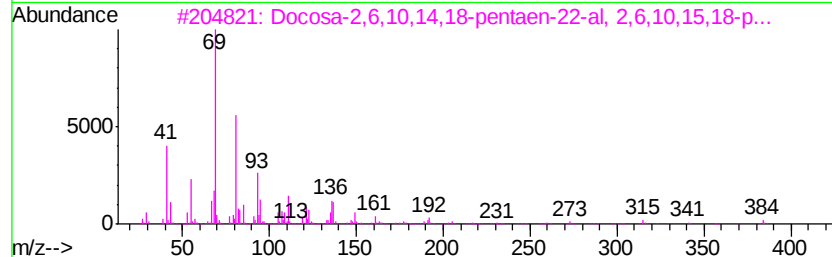
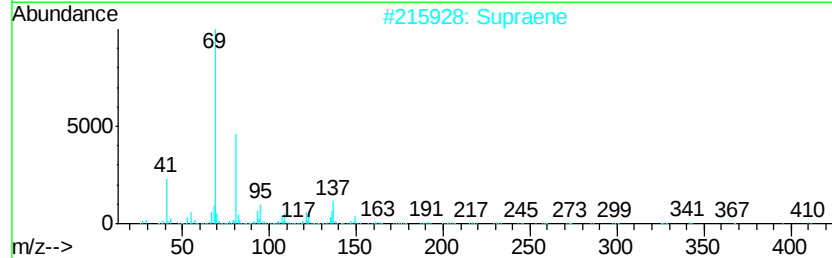
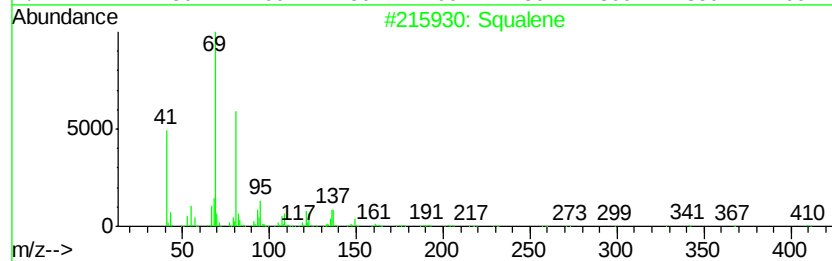
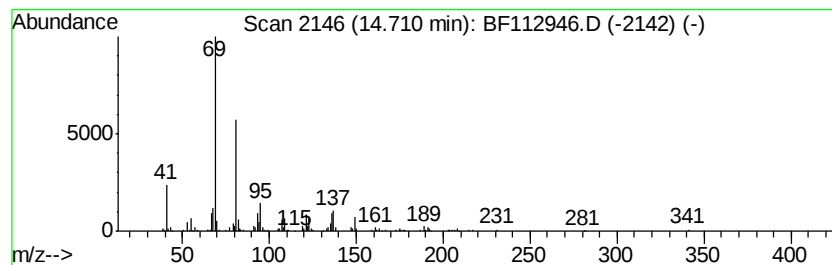
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.59 ng	180029	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	83
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		trans-Farnesol	222	C15H26O	000106-28-5	64



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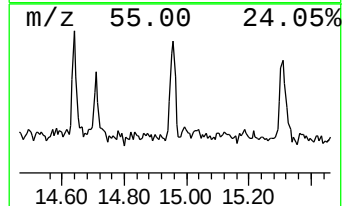
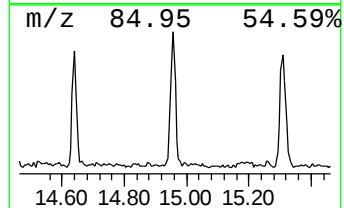
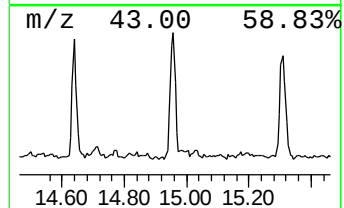
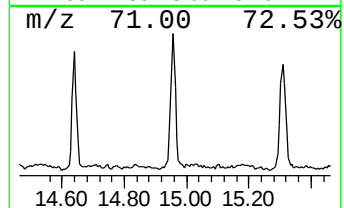
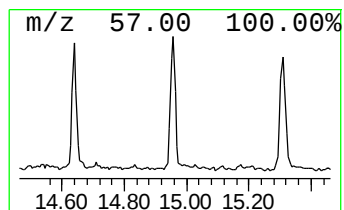
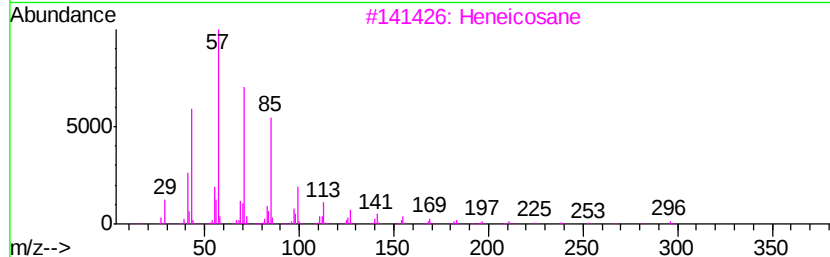
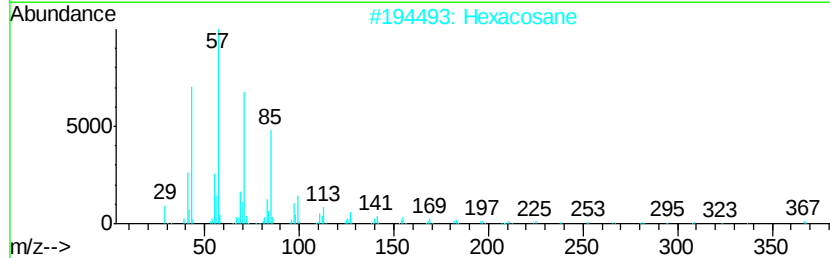
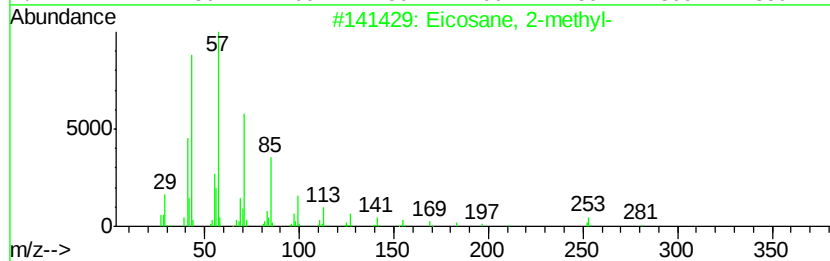
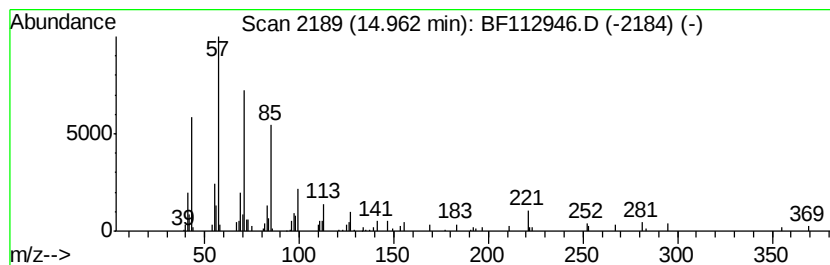
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.16 ng	149852	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 2-methyl-			296	C21H44	001560-84-5	91
2	Hexacosane			366	C26H54	000630-01-3	90
3	Heneicosane			296	C21H44	000629-94-7	90
4	Hentriacontane			437	C31H64	000630-04-6	90
5	Pentacosane			352	C25H52	000629-99-2	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112946.D
Acq On : 8 Mar 2019 16:05
Operator : JU/SJ
Sample : K1787-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

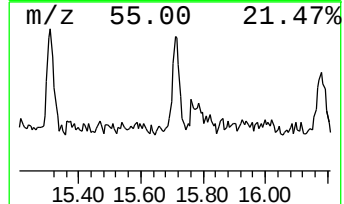
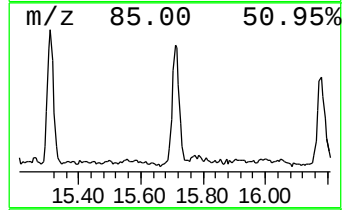
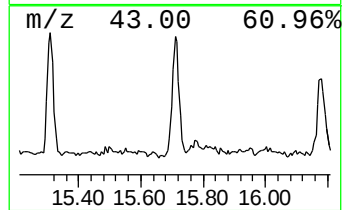
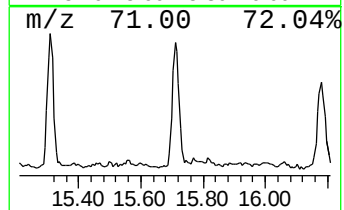
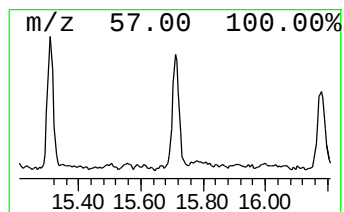
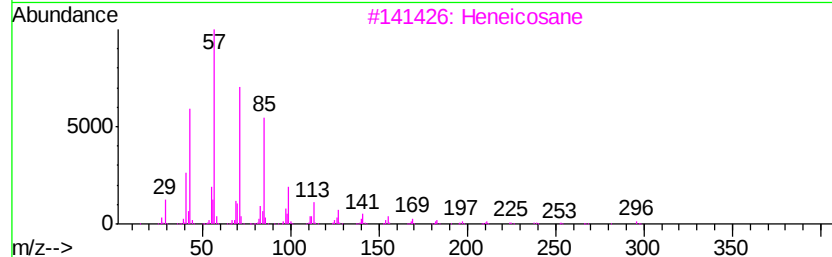
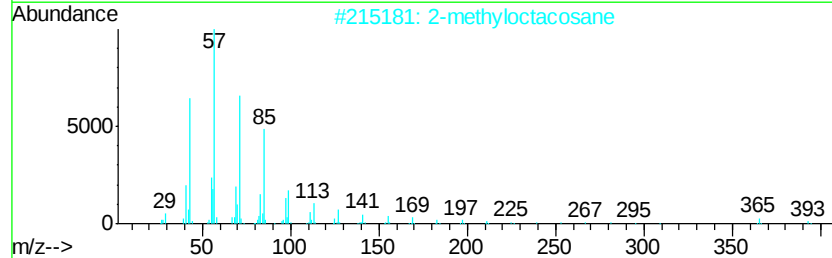
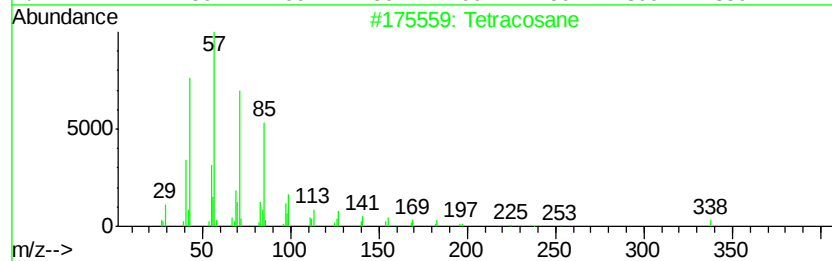
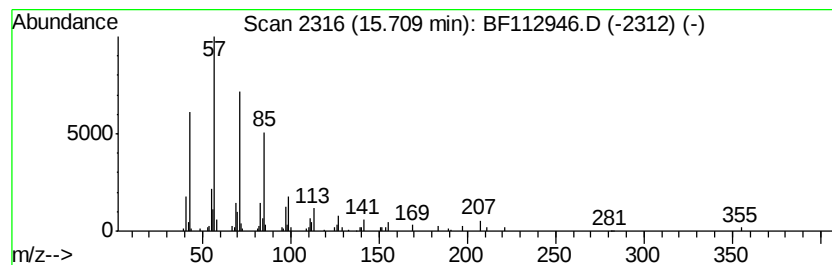
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.05 ng	142112	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112946.D
Acq On : 8 Mar 2019 16:05
Operator : JU/SJ
Sample : K1787-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	73.7	ng	3657790	1	6.73	992555	20.0
n-Hexadecanoic acid	11.77	3.2	ng	263158	4	11.23	1650630	20.0
Octadecanoic acid	12.56	2.0	ng	185691	5	13.86	1814140	20.0
1-Hexadecanesulfo...	13.73	3.0	ng	270486	5	13.86	1814140	20.0
Squalene	14.71	2.6	ng	180029	6	15.26	1388050	20.0
Eicosane, 2-methyl-	14.96	2.2	ng	149852	6	15.26	1388050	20.0
Tetracosane	15.71	2.0	ng	142112	6	15.26	1388050	20.0