

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
 Data File : BF112991.D
 Acq On : 12 Mar 2019 8:29
 Operator : JU/SJ
 Sample : K1817-10
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-027-SW069-030719

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	567	rBV	3077262	3002866	83.83%	8.350%
2	6.369	723	728	746	rVB	3213659	3301447	92.16%	9.180%
3	6.498	746	750	754	rBV	3390967	3118596	87.06%	8.672%
4	6.728	786	789	793	rBV	1104632	917069	25.60%	2.550%
5	6.886	812	816	819	rBV	2943433	2379497	66.43%	6.617%
6	7.286	880	884	897	rBV	1925760	1965901	54.88%	5.467%
7	8.010	1003	1007	1014	rBV	1175908	1133889	31.65%	3.153%
8	9.086	1186	1190	1202	rBV	3762537	3512464	98.06%	9.767%
9	9.480	1254	1257	1265	rBV	303062	285032	7.96%	0.793%
10	9.763	1301	1305	1317	rBV	1509523	1441471	40.24%	4.008%
11	10.545	1434	1438	1452	rBV	2683537	2656921	74.17%	7.388%
12	11.239	1552	1556	1559	rBV	1688621	1532311	42.78%	4.261%
13	11.263	1559	1560	1564	rVV	252863	165353	4.62%	0.460%
14	11.316	1566	1569	1573	rVB	46972	48052	1.34%	0.134%
15	11.780	1644	1648	1657	rBV2	467749	584968	16.33%	1.627%
16	12.445	1757	1761	1766	rBV	238771	223614	6.24%	0.622%
17	12.557	1777	1780	1793	rBV2	147391	222391	6.21%	0.618%
18	12.668	1793	1799	1803	rVV2	177122	235115	6.56%	0.654%
19	12.821	1820	1825	1828	rBV	3860776	3582118	100.00%	9.961%
20	13.063	1864	1866	1869	rVB2	46605	39725	1.11%	0.110%
21	13.104	1869	1873	1878	rBV2	32147	37044	1.03%	0.103%
22	13.304	1899	1907	1912	rBV6	61387	67390	1.88%	0.187%
23	13.404	1918	1924	1926	rBV2	50447	62531	1.75%	0.174%
24	13.504	1937	1941	1946	rVB	30603	40124	1.12%	0.112%
25	13.727	1973	1979	1993	rBV2	370542	553064	15.44%	1.538%
26	13.862	1995	2002	2005	rBV	1503966	1573091	43.92%	4.374%
27	14.045	2029	2033	2037	rBV	146134	141510	3.95%	0.394%
28	14.351	2081	2085	2098	rVB2	246939	429421	11.99%	1.194%
29	14.639	2131	2134	2138	rBV	254237	251392	7.02%	0.699%
30	14.874	2170	2174	2177	rBV	71549	110449	3.08%	0.307%
31	14.957	2184	2188	2191	rBV	266054	302997	8.46%	0.843%
32	14.986	2191	2193	2202	rVB2	86794	153128	4.27%	0.426%
33	15.209	2228	2231	2236	rBV	43809	53860	1.50%	0.150%
34	15.268	2236	2241	2245	rBV	839229	1052240	29.37%	2.926%

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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	15.309	2245	2248	2256	rVB	232179	303980	8.49%	0.845%
36	15.715	2312	2317	2322	rVB	158588	224628	6.27%	0.625%
37	15.774	2324	2327	2335	rVV7	30847	73094	2.04%	0.203%
38	16.180	2392	2396	2401	rBV3	72767	123024	3.43%	0.342%
39	16.733	2485	2490	2495	rVB2	32973	59921	1.67%	0.167%

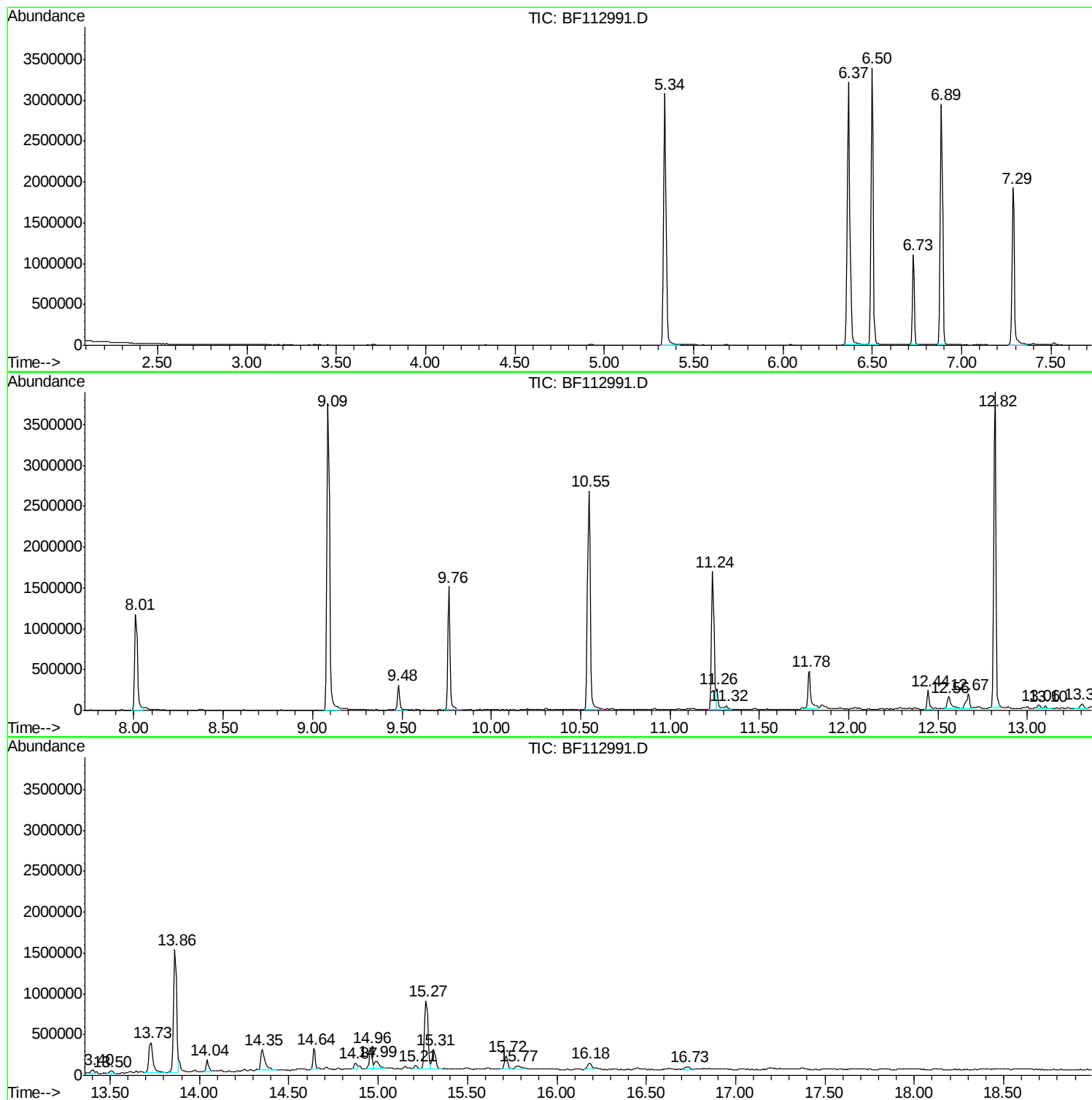
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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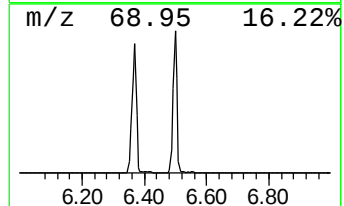
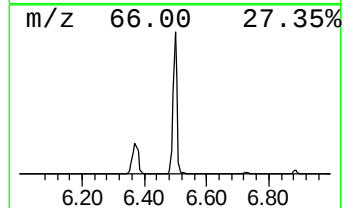
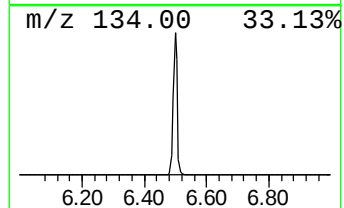
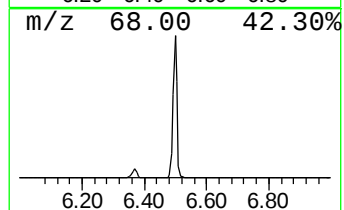
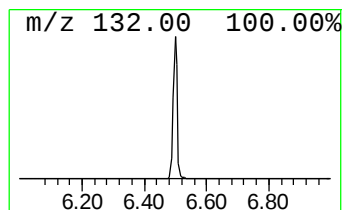
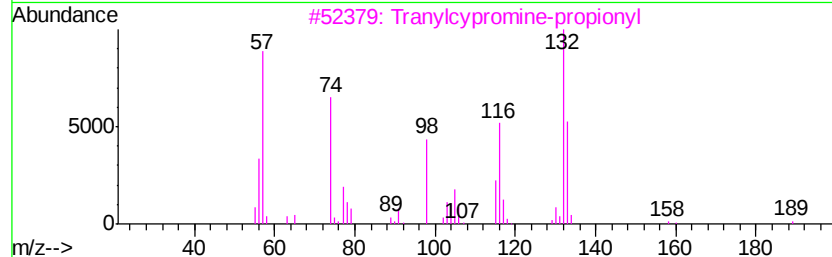
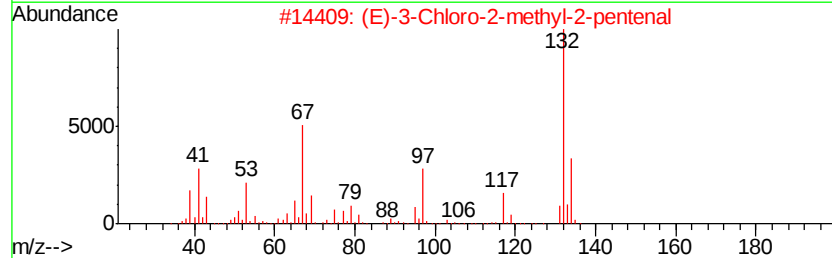
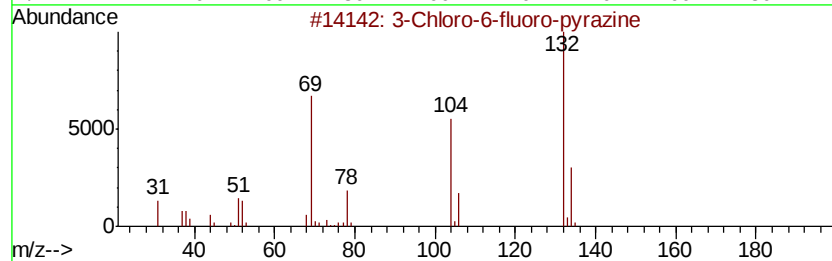
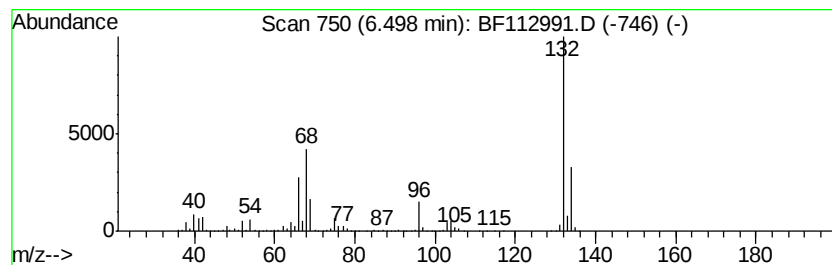
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	68.01 ng	3118600	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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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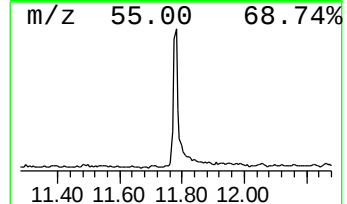
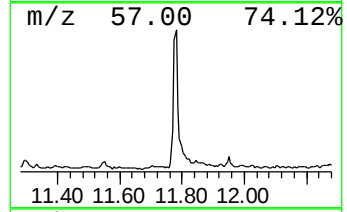
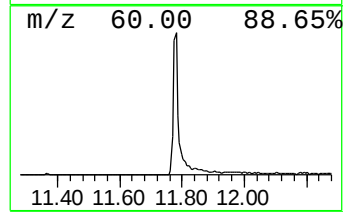
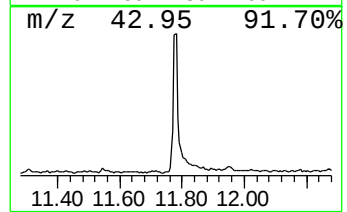
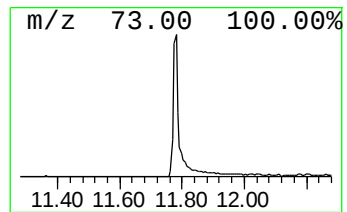
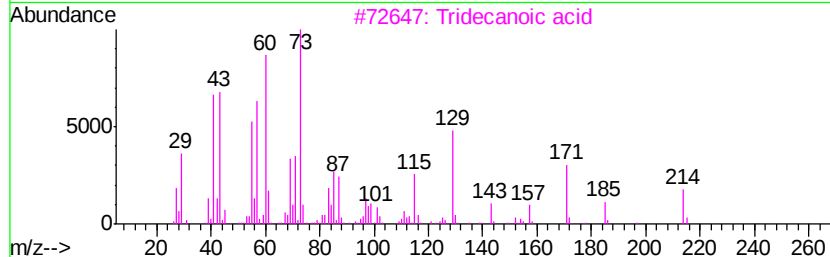
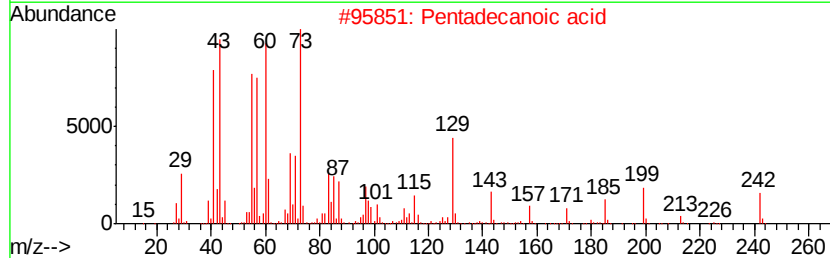
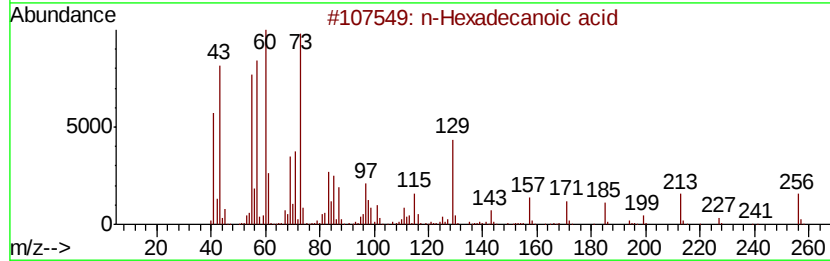
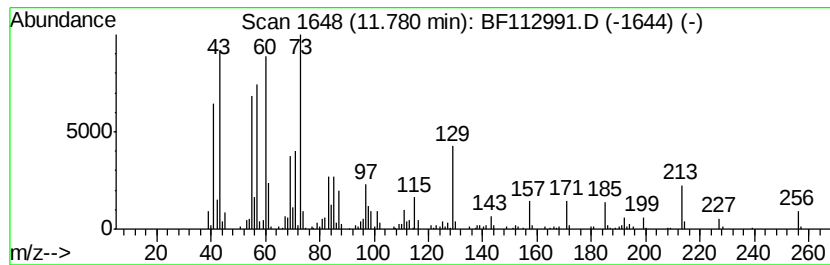
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.78	7.64 ng	584968	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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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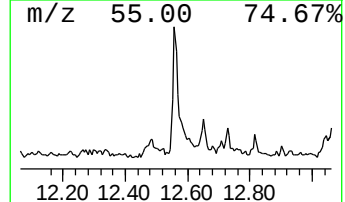
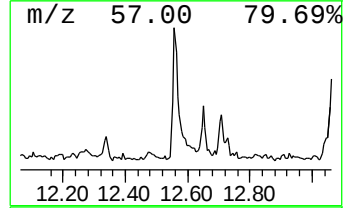
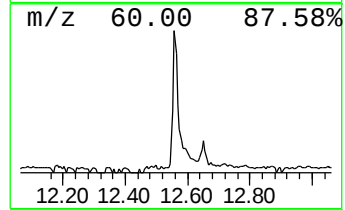
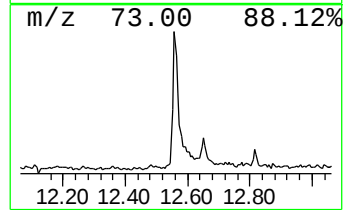
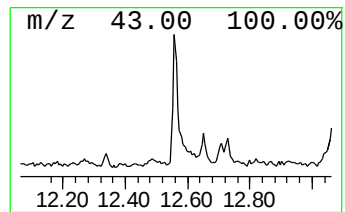
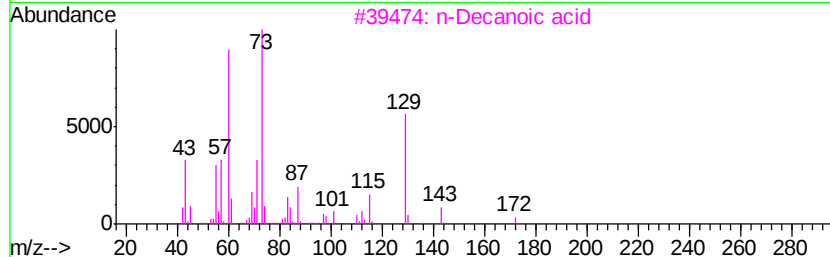
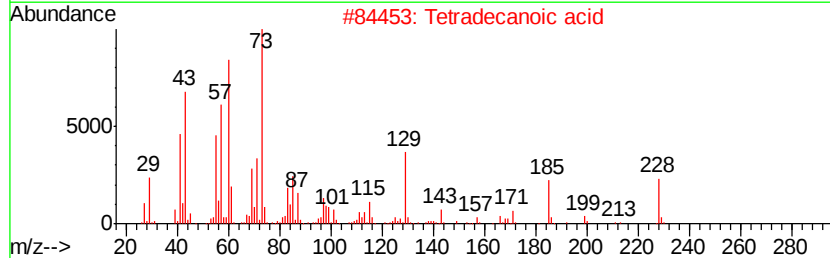
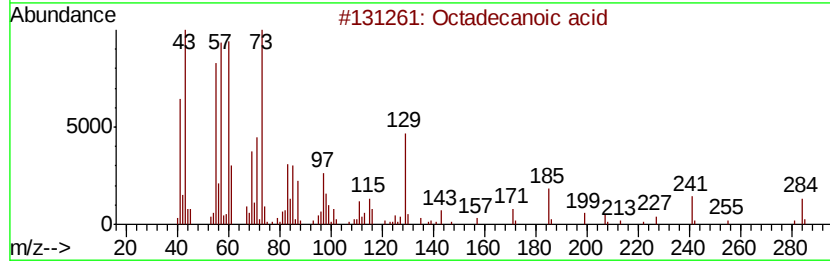
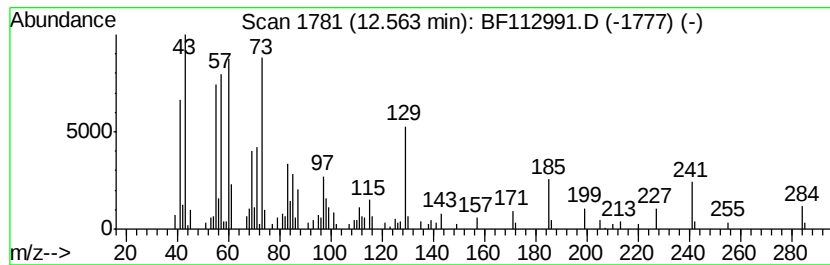
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.56	2.83 ng	222391	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	68
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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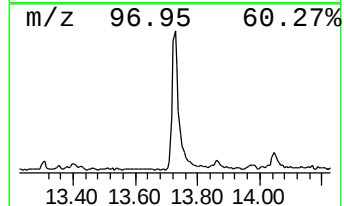
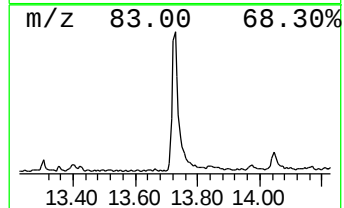
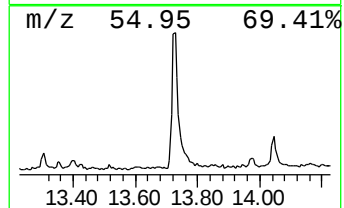
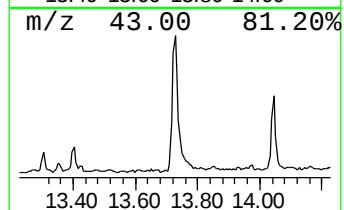
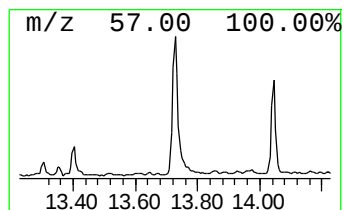
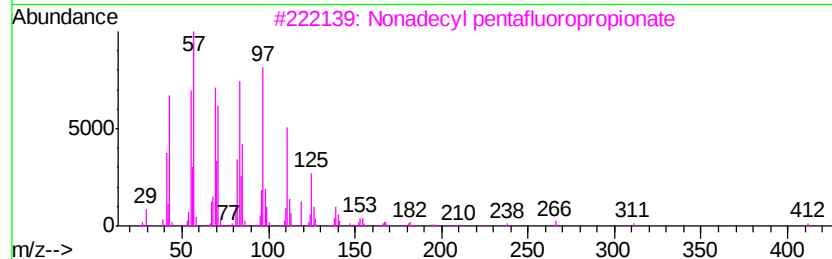
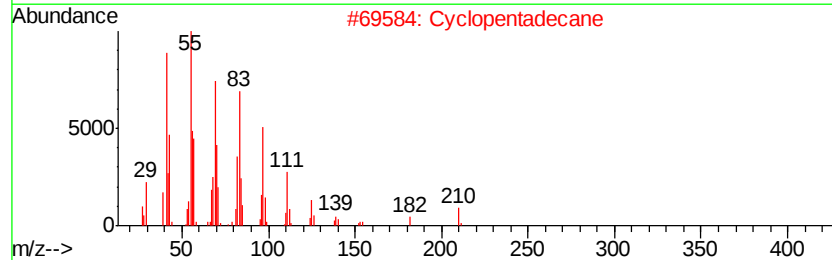
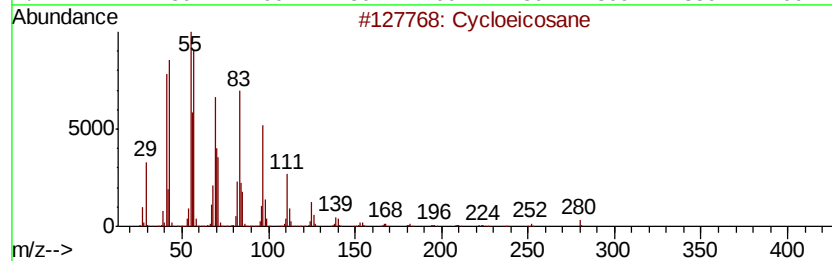
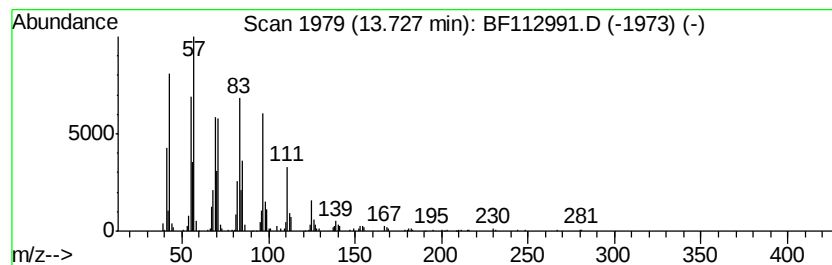
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.03 ng	553064	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloeicosane	280	C20H40	000296-56-0	98
2		Cyclopentadecane	210	C15H30	000295-48-7	93
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91



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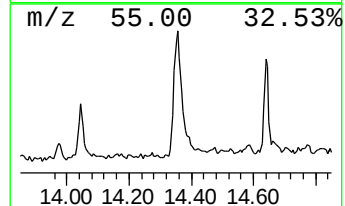
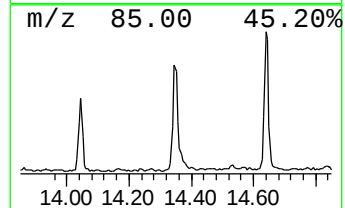
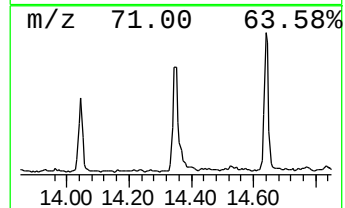
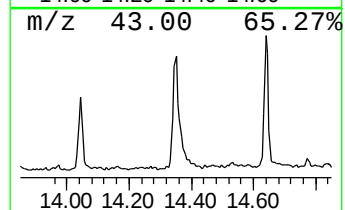
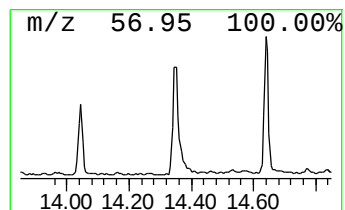
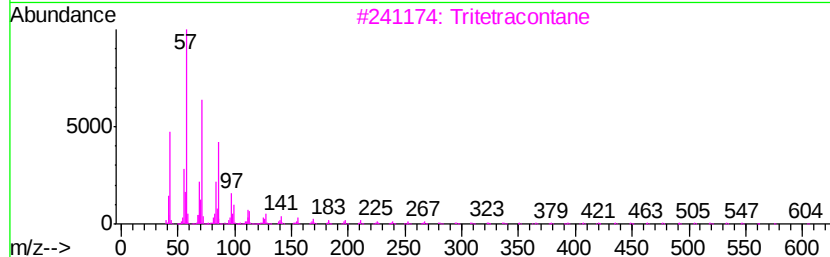
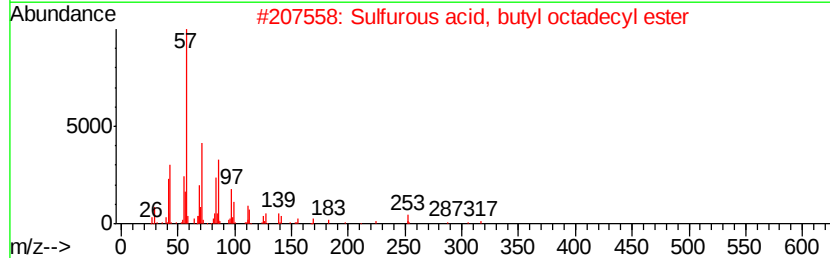
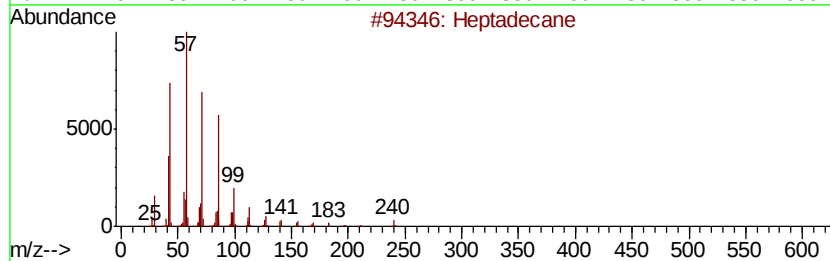
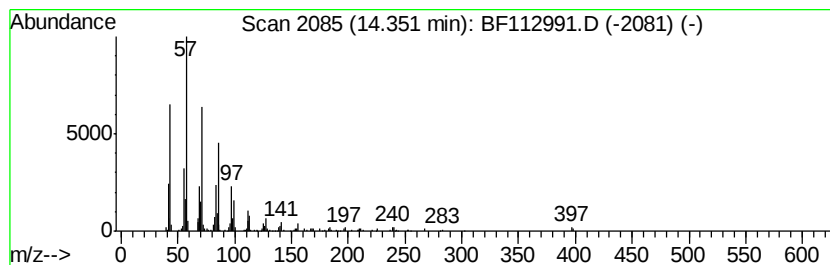
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	5.46 ng	429421	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	96
2		Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	91
3		Tritetracontane	605	C43H88	007098-21-7	87
4		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	87
5		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112991.D
Acq On : 12 Mar 2019 8:29
Operator : JU/SJ
Sample : K1817-10
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PST-027-SW069-030719

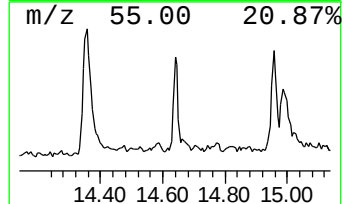
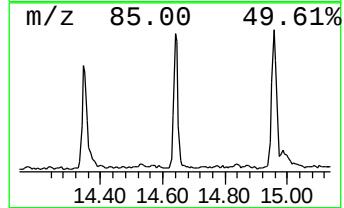
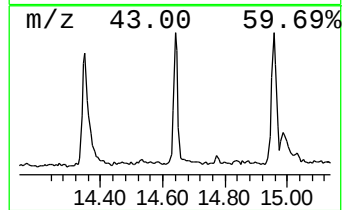
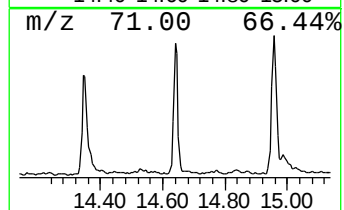
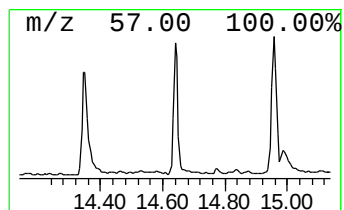
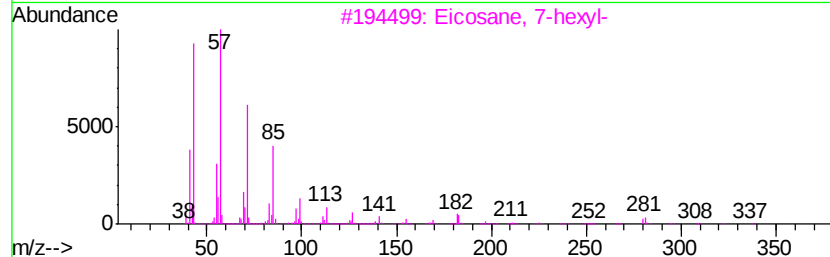
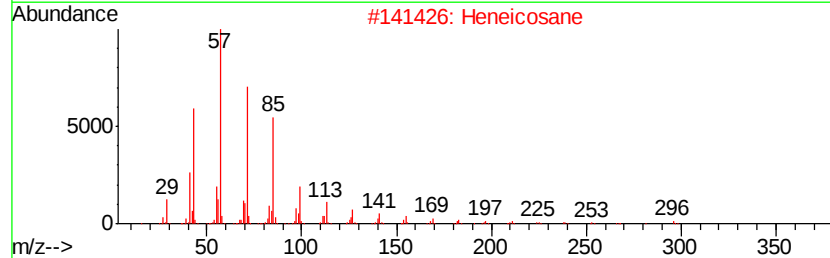
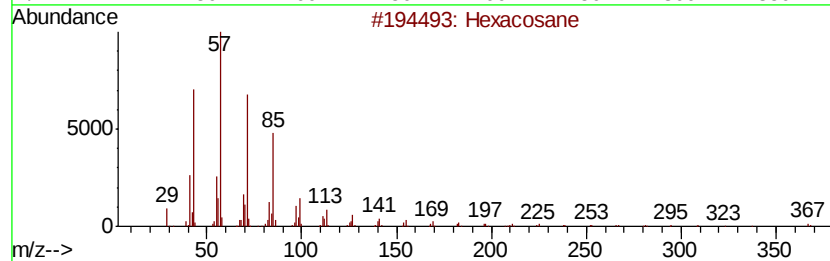
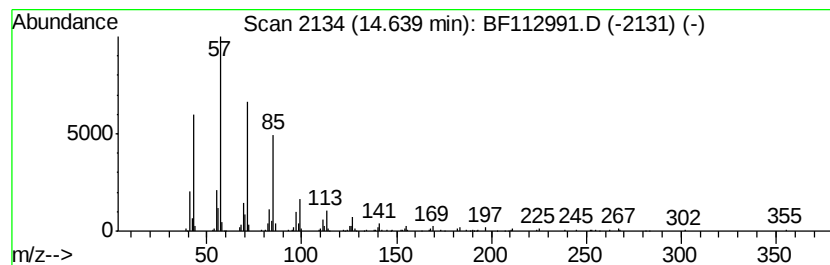
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.78 ng	251392	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4		Nonadecane	268	C19H40	000629-92-5	87
5		Tetratetracontane	619	C44H90	007098-22-8	87



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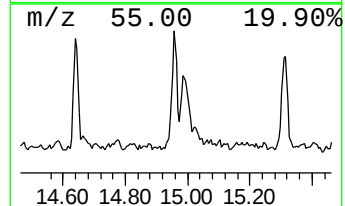
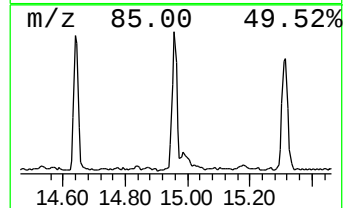
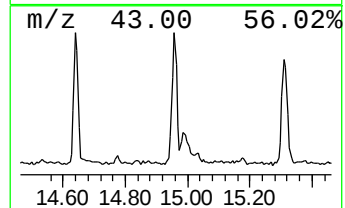
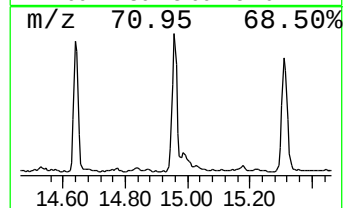
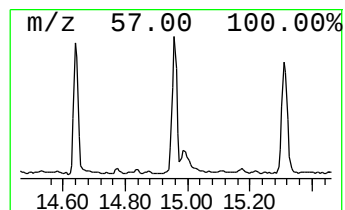
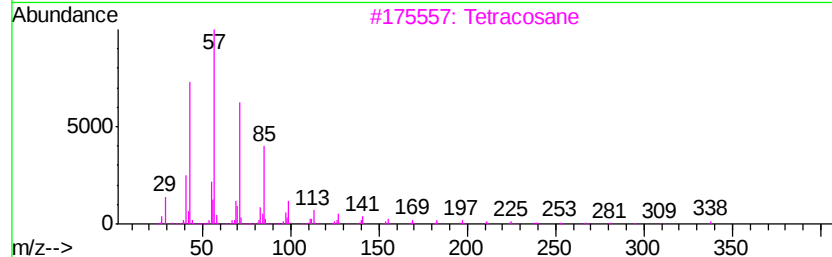
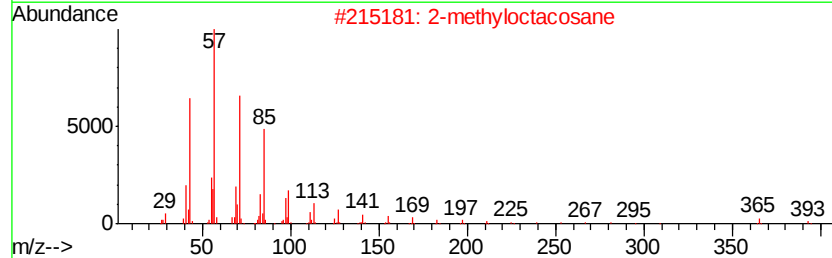
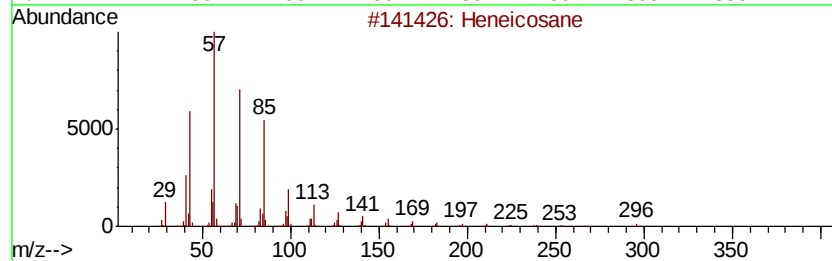
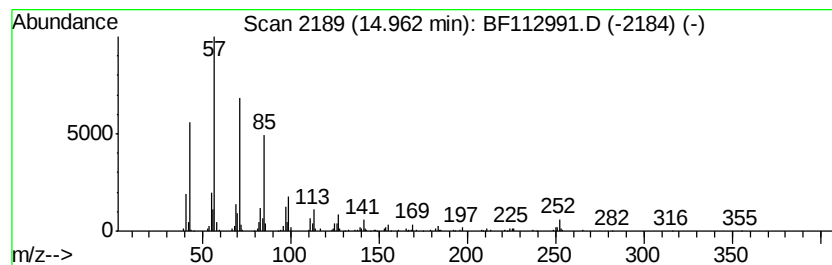
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.96	5.76 ng	302997	Perylene-d12	15.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Eicosane	282	C20H42	000112-95-8	90



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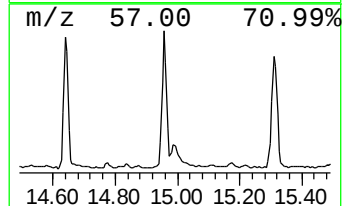
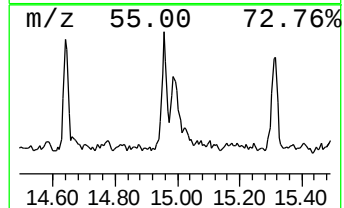
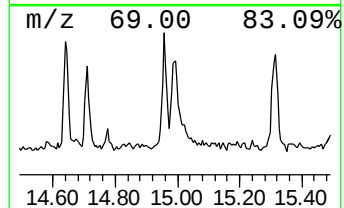
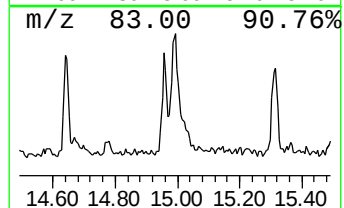
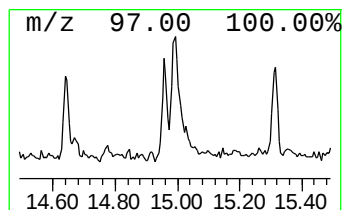
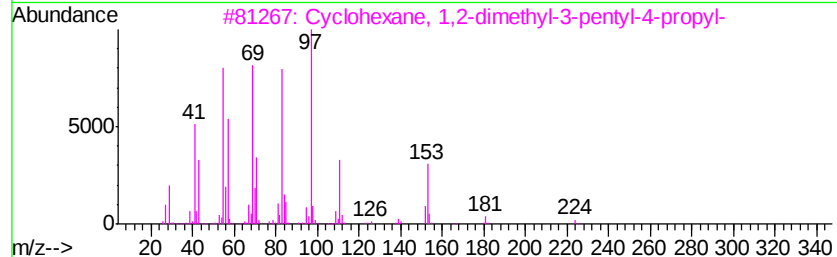
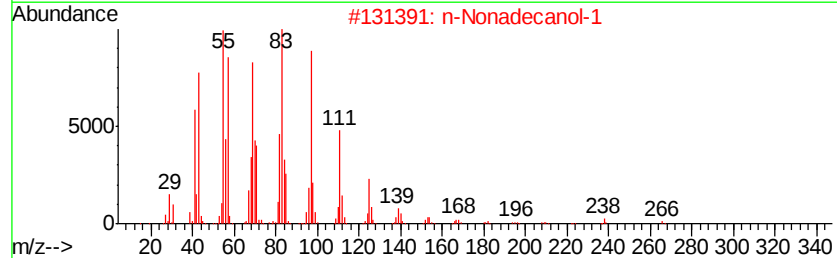
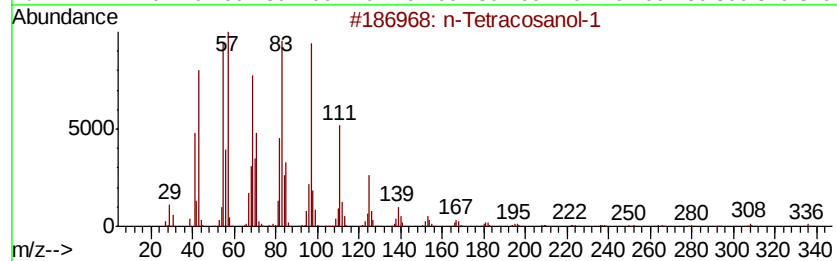
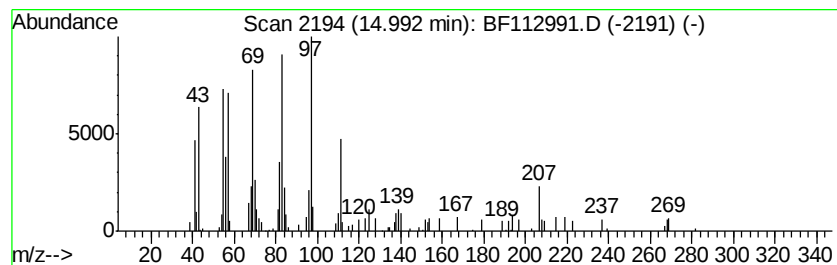
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.91 ng	153128	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	83
3		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	59
4		Silane, [(11-bromoundecyl)oxyl]tr...	322	C14H31BrOSi	026305-83-9	52
5		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112991.D
Acq On : 12 Mar 2019 8:29
Operator : JU/SJ
Sample : K1817-10
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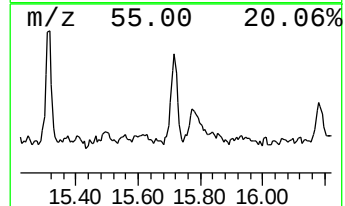
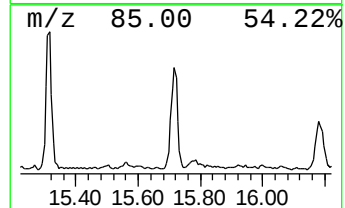
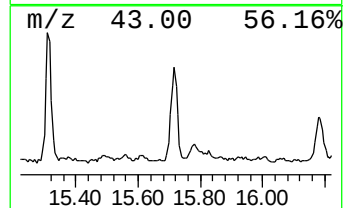
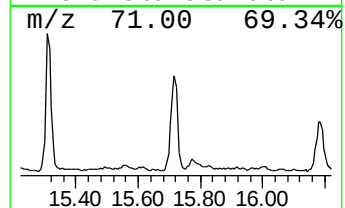
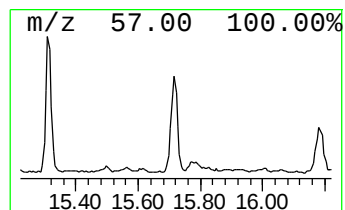
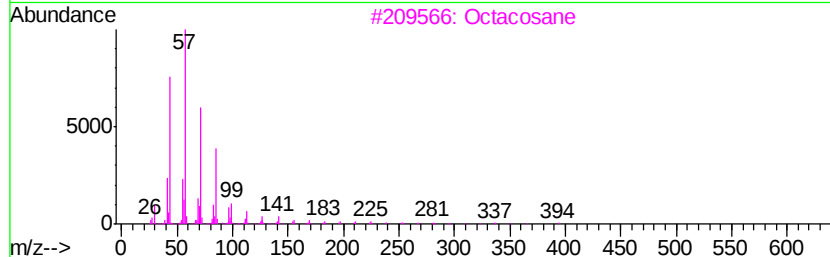
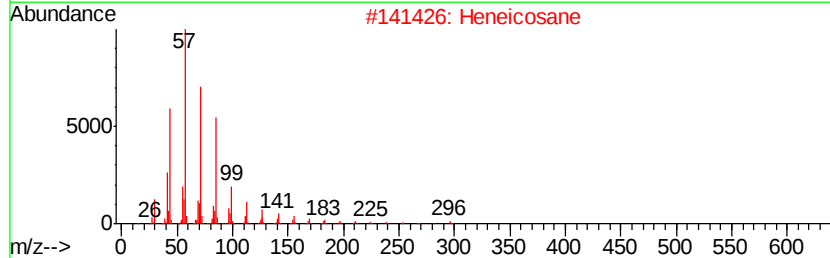
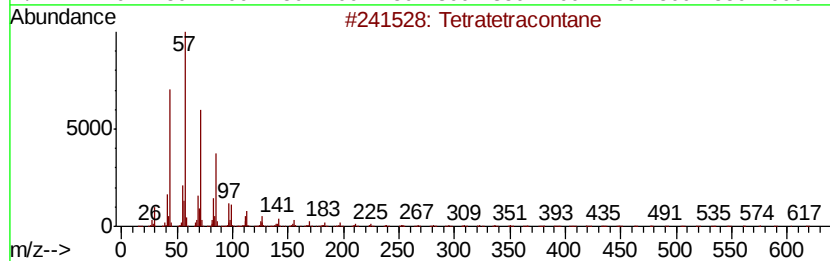
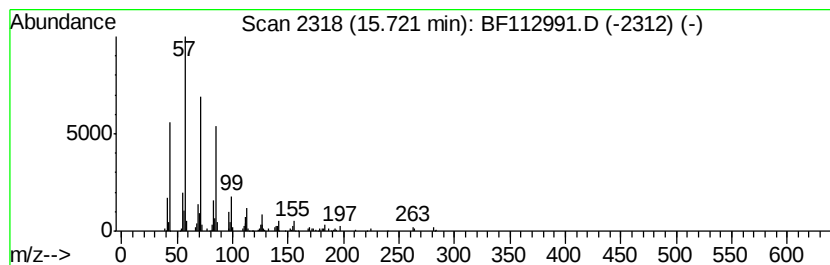
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.27 ng	224628	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112991.D
Acq On : 12 Mar 2019 8:29
Operator : JU/SJ
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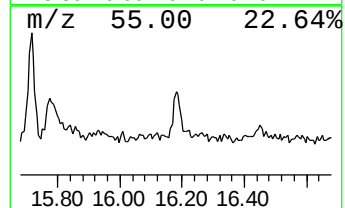
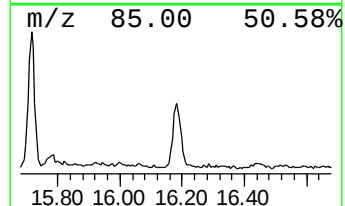
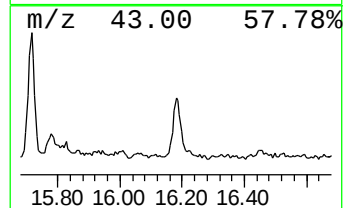
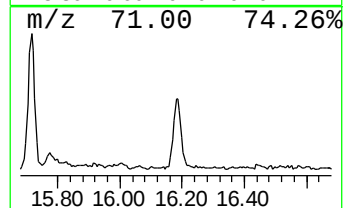
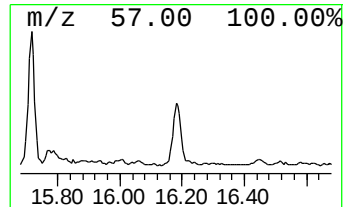
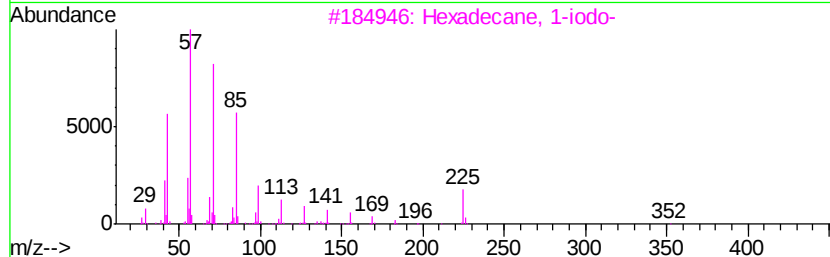
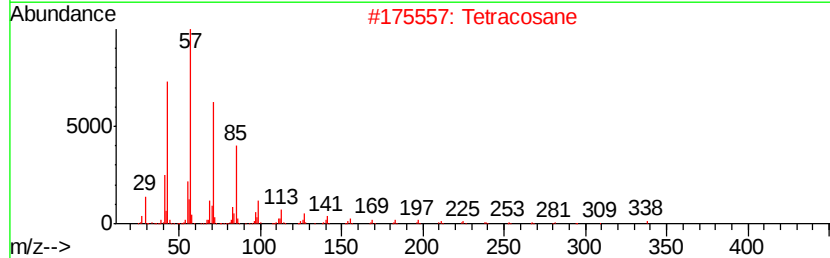
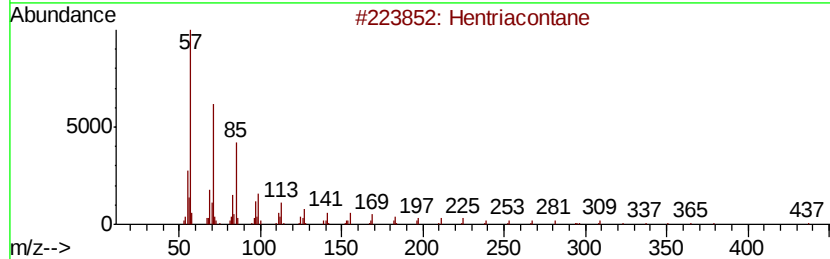
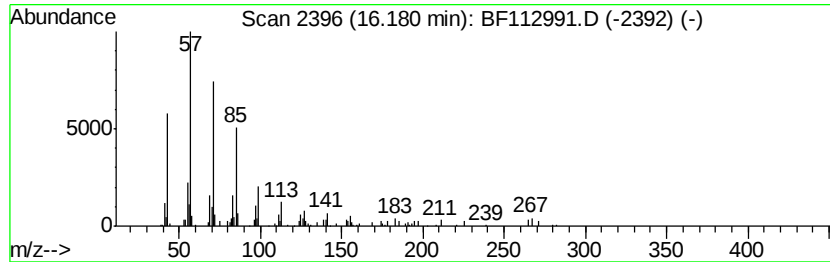
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Hentriacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.34 ng	123024	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Tetracosane	338	C24H50	000646-31-1	90
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
4		triacontane	422	C30H62	000638-68-6	87
5		Pentacosane	352	C25H52	000629-99-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
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 Acq On : 12 Mar 2019 8:29
 Operator : JU/SJ
 Sample : K1817-10
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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 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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n-Hexadecanoic acid	11.78	7.6	ng	584968	4	11.24	1532310	20.0
Octadecanoic acid	12.56	2.8	ng	222391	5	13.86	1573090	20.0
Cycloeicosane	13.73	7.0	ng	553064	5	13.86	1573090	20.0
Heptadecane	14.35	5.5	ng	429421	5	13.86	1573090	20.0
Hexacosane	14.64	4.8	ng	251392	6	15.27	1052240	20.0
Heneicosane	14.96	5.8	ng	302997	6	15.27	1052240	20.0
n-Tetracosanol-1	14.99	2.9	ng	153128	6	15.27	1052240	20.0
Tetratetracontane	15.72	4.3	ng	224628	6	15.27	1052240	20.0
Hentriacontane	16.18	2.3	ng	123024	6	15.27	1052240	20.0