

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
 Data File : BF112775.D
 Acq On : 28 Feb 2019 21:44
 Operator : JU/SJ
 Sample : K1645-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SR-10

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	5.357	550	556	559	rBV	3403585	3510346	95.34%	9.011%
2	6.375	724	729	732	rBV	3600726	3585649	97.38%	9.204%
3	6.510	748	752	756	rBV	3874022	3682069	100.00%	9.452%
4	6.745	788	792	795	rBV	1215146	1090837	29.63%	2.800%
5	6.898	814	818	822	rBV	3249220	2900692	78.78%	7.446%
6	7.298	881	886	894	rBV	2296783	2358161	64.04%	6.053%
7	7.534	922	926	935	rVB2	33655	42560	1.16%	0.109%
8	8.022	1005	1009	1025	rVB	1521675	1369859	37.20%	3.516%
9	9.098	1188	1192	1195	rBV	4060787	3476848	94.43%	8.925%
10	9.486	1255	1258	1262	rBV	190567	168975	4.59%	0.434%
11	9.663	1286	1288	1295	rVB3	32932	59700	1.62%	0.153%
12	9.769	1302	1306	1311	rBV	1299444	1293850	35.14%	3.321%
13	10.551	1435	1439	1451	rVB	2053775	1913543	51.97%	4.912%
14	10.922	1499	1502	1505	rBV	46889	43843	1.19%	0.113%
15	11.245	1554	1557	1560	rBV	1112418	1080434	29.34%	2.773%
16	11.269	1560	1561	1565	rVB	205825	137948	3.75%	0.354%
17	11.322	1565	1570	1573	rBV2	71501	86184	2.34%	0.221%
18	11.786	1645	1649	1658	rBV2	779823	799995	21.73%	2.054%
19	11.857	1658	1661	1664	rBV	49245	47265	1.28%	0.121%
20	12.298	1732	1736	1739	rBV	66631	69935	1.90%	0.180%
21	12.451	1759	1762	1767	rBV	347754	336214	9.13%	0.863%
22	12.569	1778	1782	1792	rBV2	422768	454820	12.35%	1.168%
23	12.680	1796	1801	1803	rVV	345152	350527	9.52%	0.900%
24	12.710	1803	1806	1816	rVB	280642	378953	10.29%	0.973%
25	12.827	1823	1826	1830	rVB	2726148	2463263	66.90%	6.323%
26	13.074	1866	1868	1871	rVB2	56263	47539	1.29%	0.122%
27	13.110	1871	1874	1877	rBV	43695	43000	1.17%	0.110%
28	13.416	1924	1926	1931	rVB2	45700	44736	1.21%	0.115%
29	13.510	1940	1942	1948	rBV	36744	49246	1.34%	0.126%
30	13.621	1957	1961	1964	rBV2	44138	64579	1.75%	0.166%
31	13.733	1974	1980	1985	rBV2	552038	635619	17.26%	1.632%
32	13.874	1999	2004	2006	rBV2	1249628	1357333	36.86%	3.484%
33	13.898	2006	2008	2010	rVB	178098	134516	3.65%	0.345%
34	14.057	2032	2035	2038	rBV	164947	153371	4.17%	0.394%

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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	14.363	2084	2087	2092	rBV	403092	393146	10.68%	1.009%
36	14.663	2134	2138	2143	rBV	364130	409084	11.11%	1.050%
37	14.880	2172	2175	2186	rVB	209867	400643	10.88%	1.028%
38	14.980	2188	2192	2199	rVB	477694	575979	15.64%	1.479%
39	15.162	2220	2223	2227	rVB	143392	152107	4.13%	0.390%
40	15.221	2230	2233	2237	rVB	177398	193008	5.24%	0.495%
41	15.286	2239	2244	2247	rVV	984082	1180140	32.05%	3.029%
42	15.339	2249	2253	2258	rVB	369765	456649	12.40%	1.172%
43	15.745	2318	2322	2326	rBV	306959	433108	11.76%	1.112%
44	15.786	2326	2329	2340	rVB4	141482	241982	6.57%	0.621%
45	16.215	2399	2402	2413	rVB2	164280	287819	7.82%	0.739%

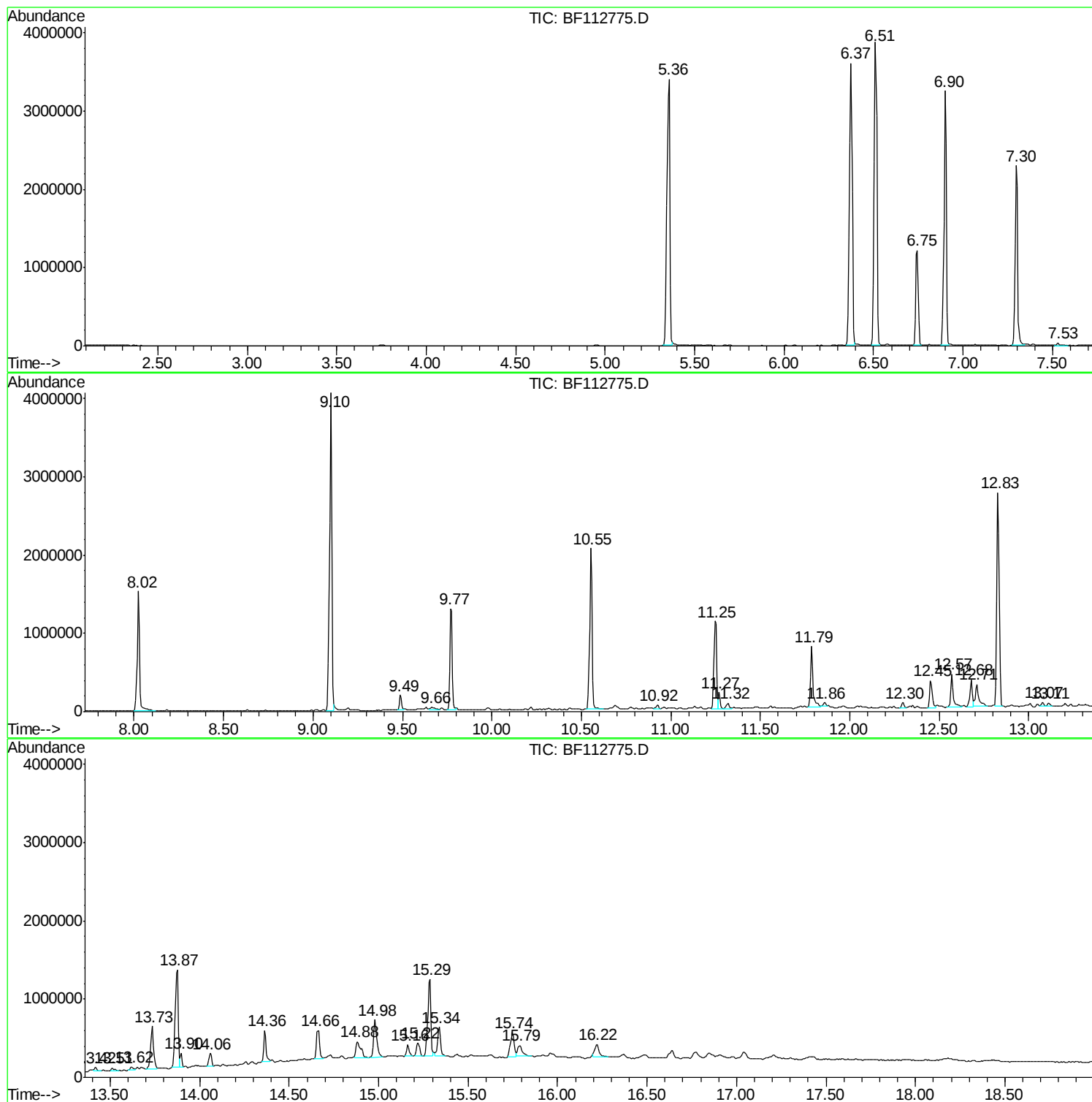
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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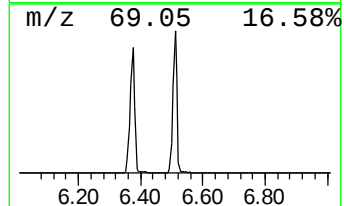
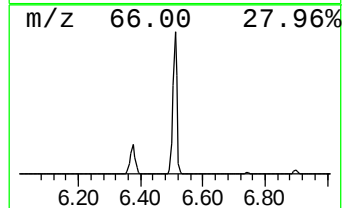
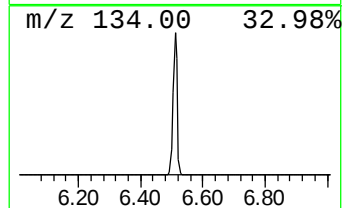
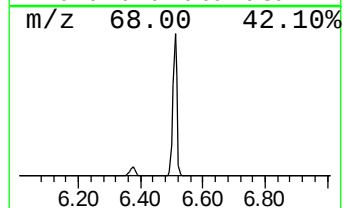
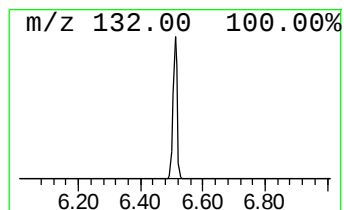
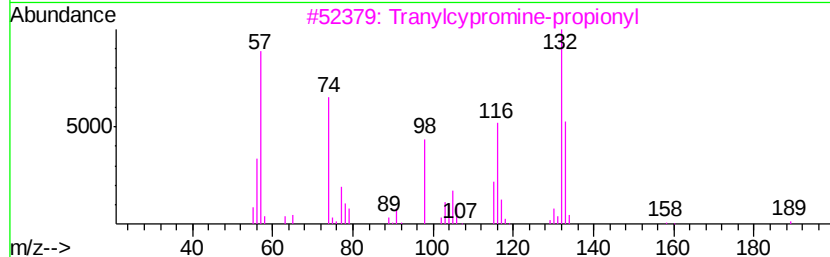
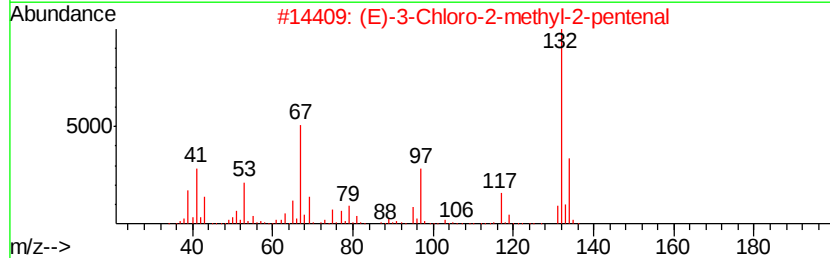
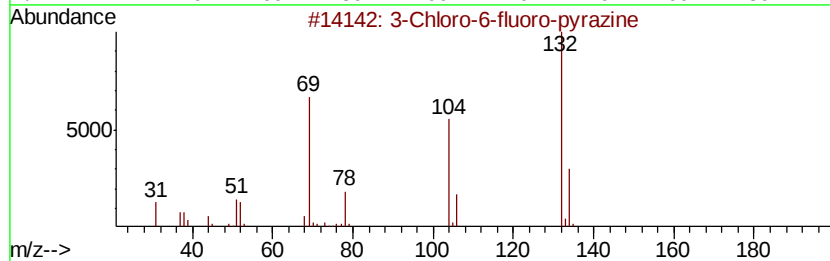
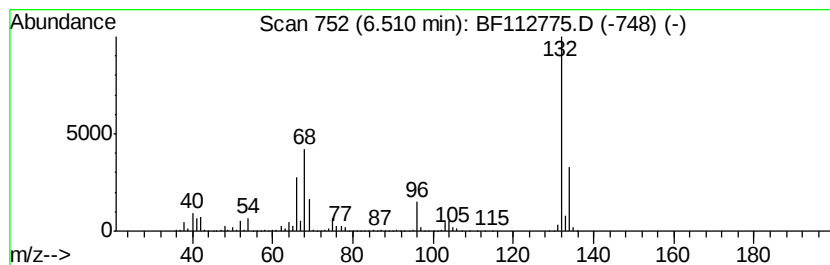
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	67.51 ng	3682070	1,4-Dichlorobenzene-d4	6.75

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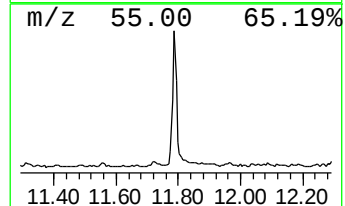
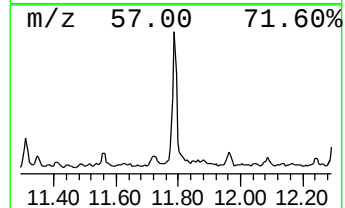
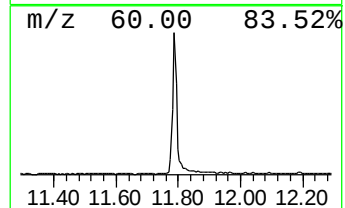
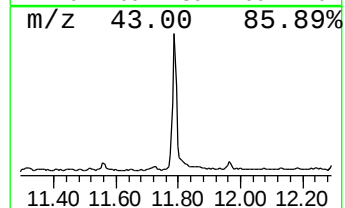
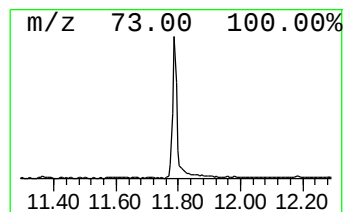
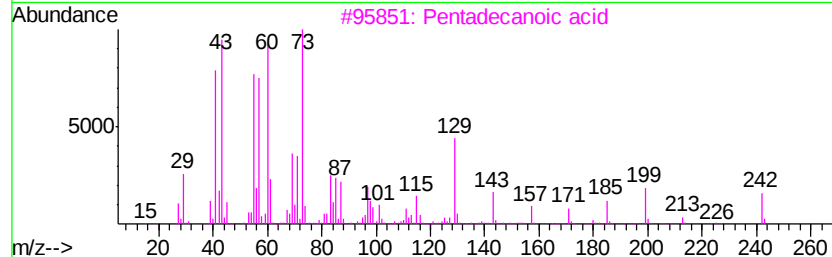
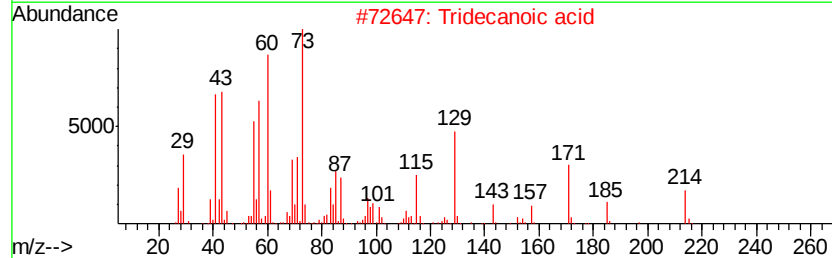
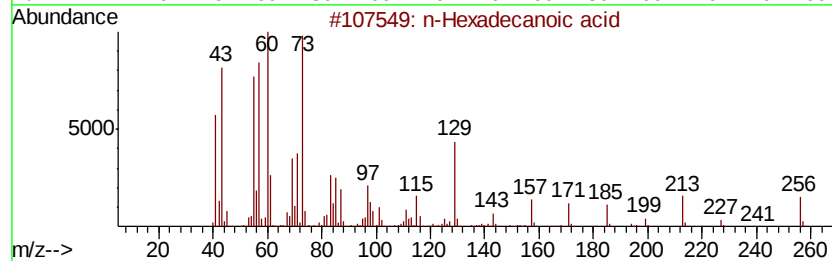
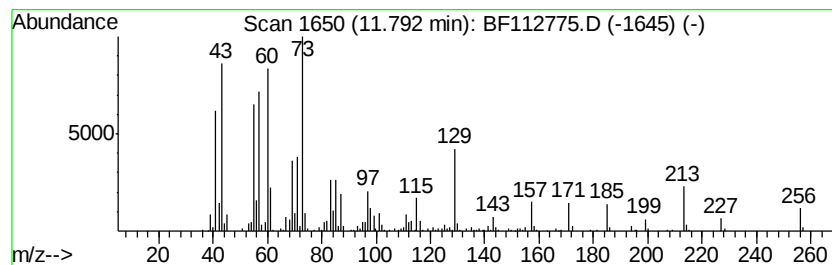
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	14.81 ng	799995	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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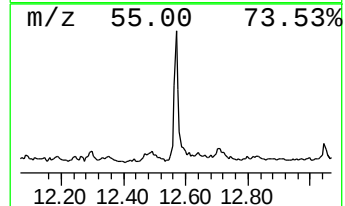
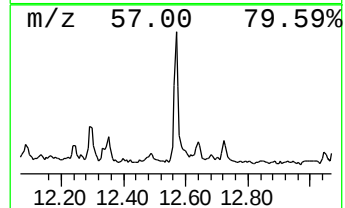
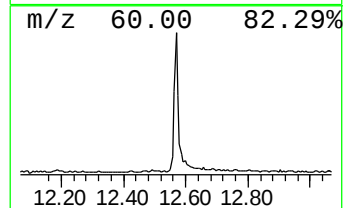
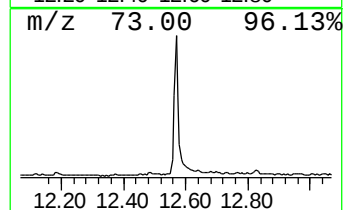
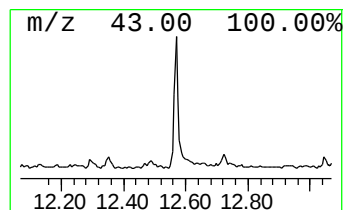
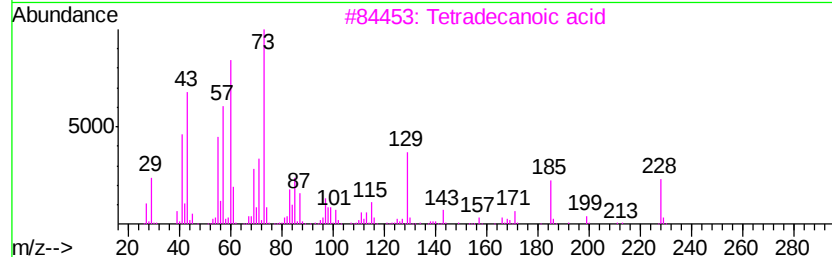
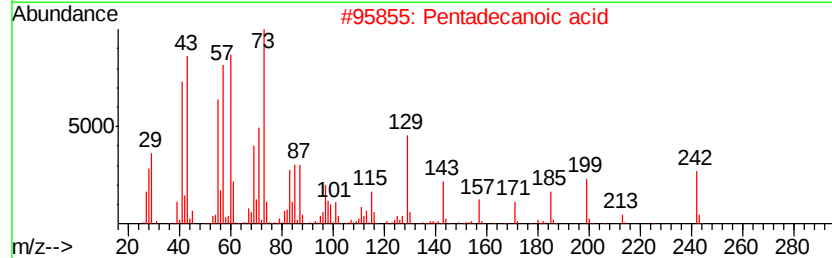
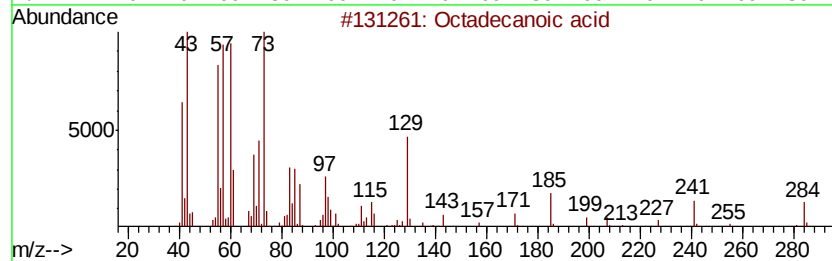
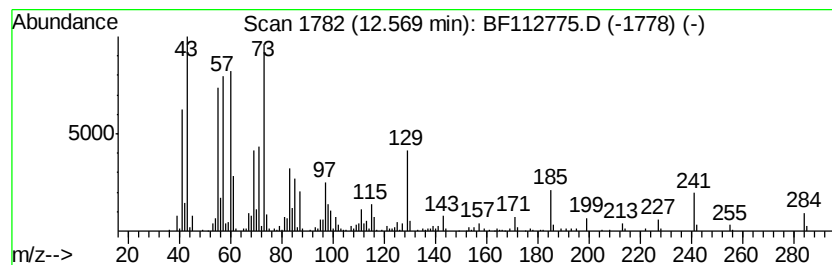
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	6.70 ng	454820	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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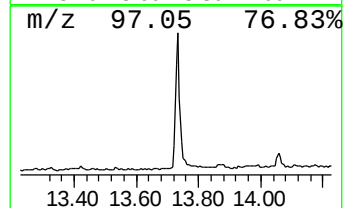
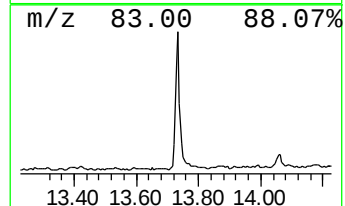
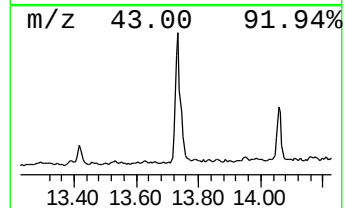
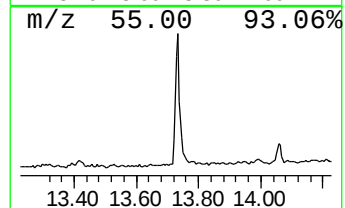
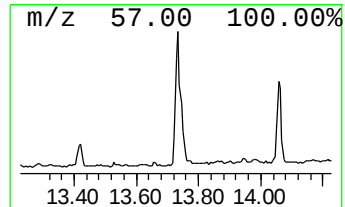
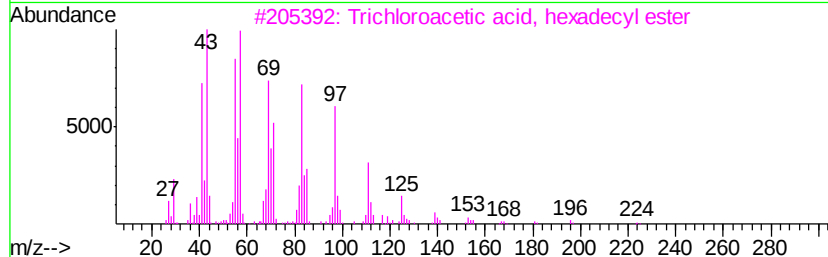
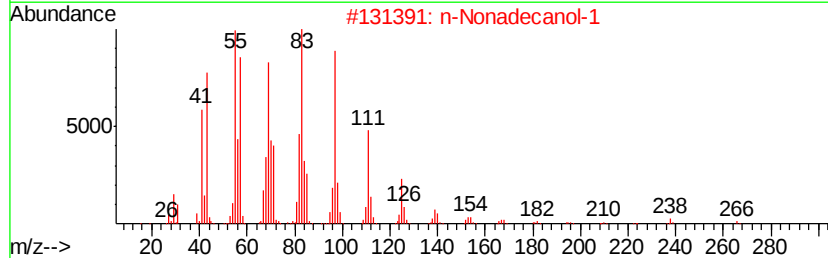
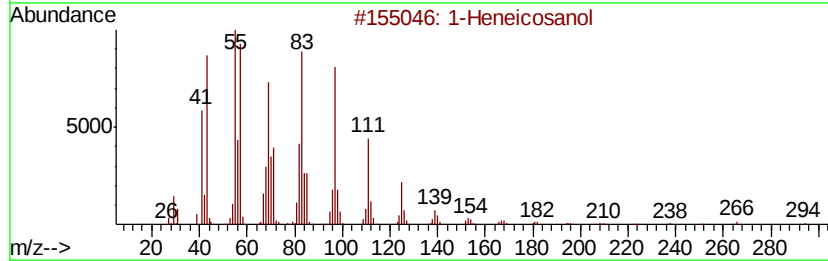
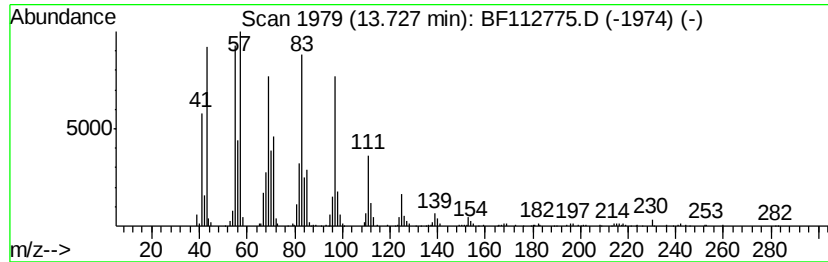
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	9.37 ng	635619	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94



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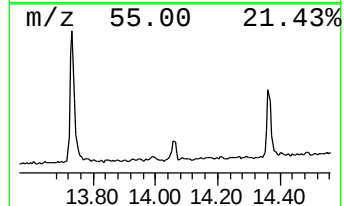
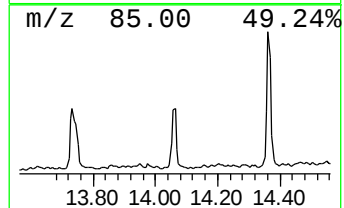
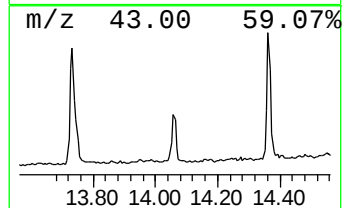
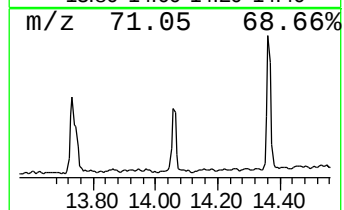
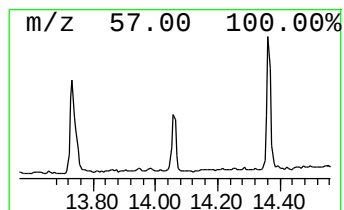
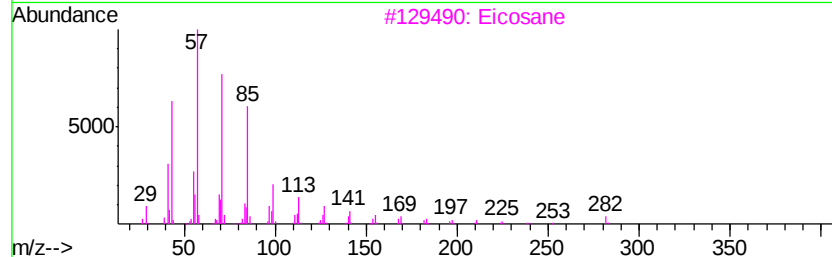
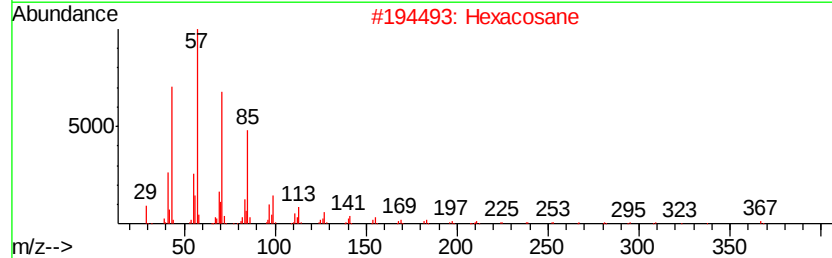
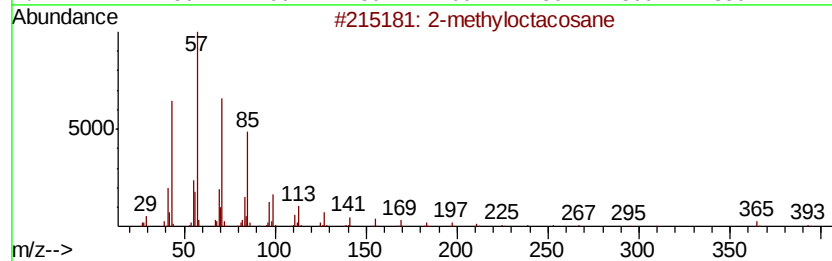
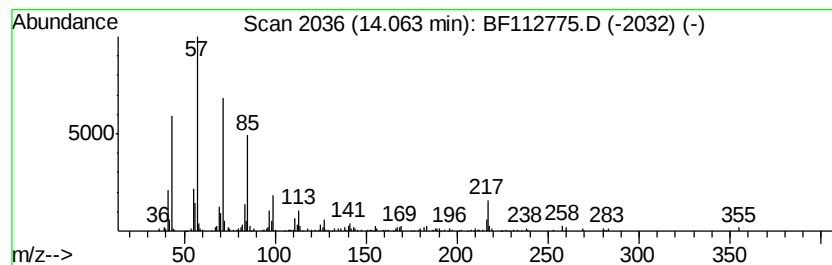
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-methyloctacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.06	2.26 ng	153371	Chrysene-d12		13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	81
2	Hexacosane		366	C26H54	000630-01-3	81
3	Eicosane		282	C20H42	000112-95-8	81
4	Tetratetracontane		619	C44H90	007098-22-8	81
5	Octacosane		394	C28H58	000630-02-4	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112775.D
Acq On : 28 Feb 2019 21:44
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Sample : K1645-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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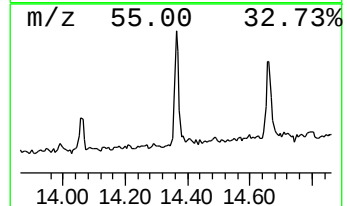
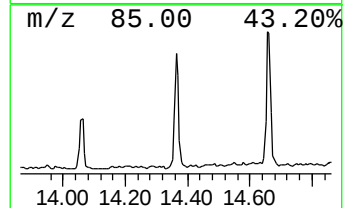
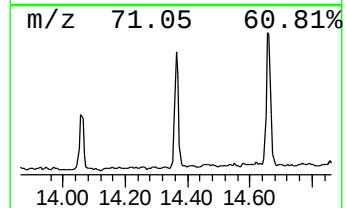
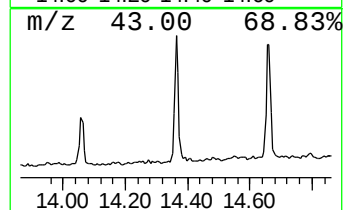
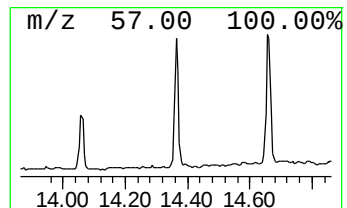
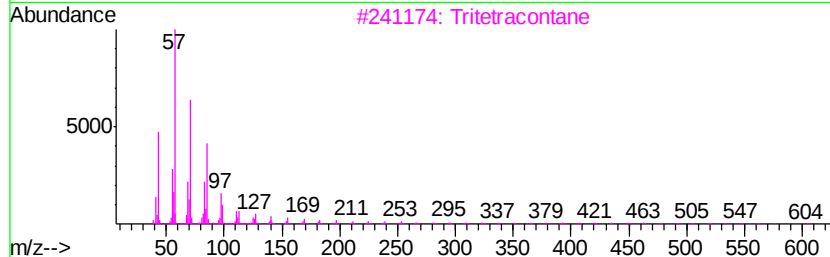
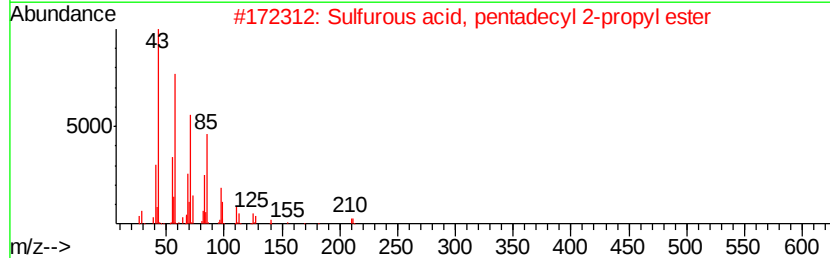
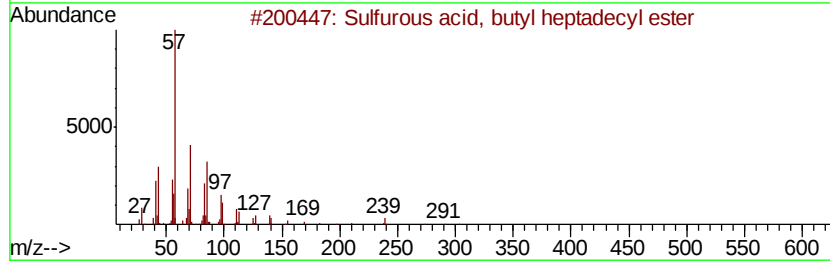
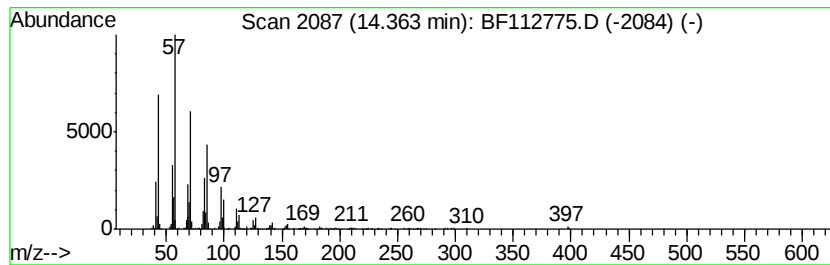
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl hepta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	5.79 ng	393146	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
3		Tritetracontane	605	C43H88	007098-21-7	83
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	70
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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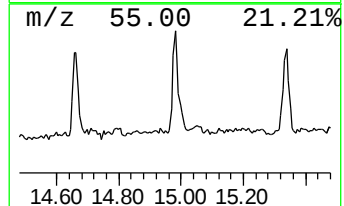
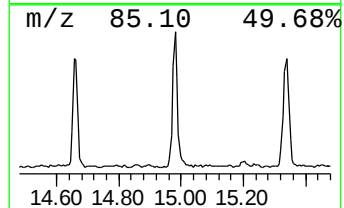
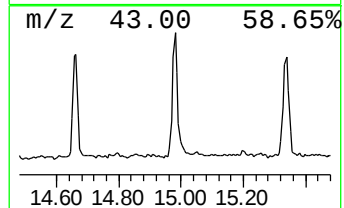
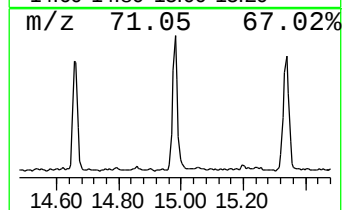
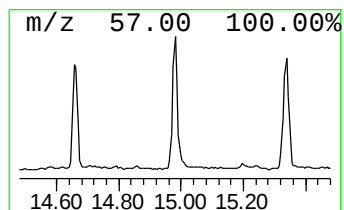
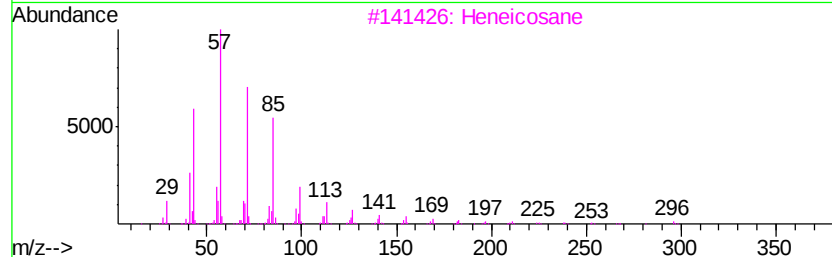
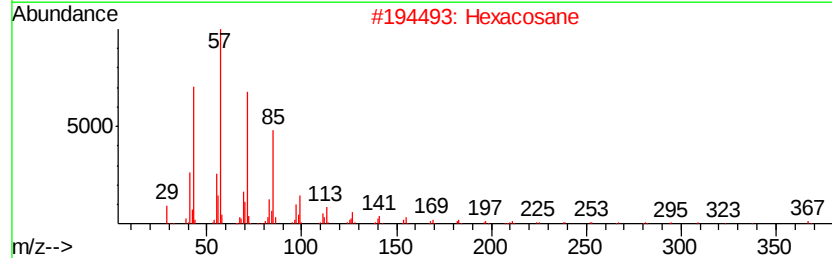
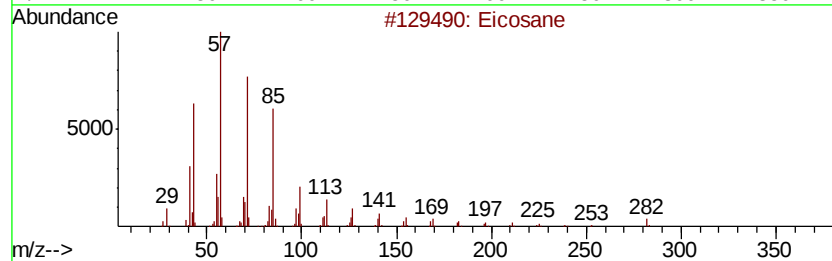
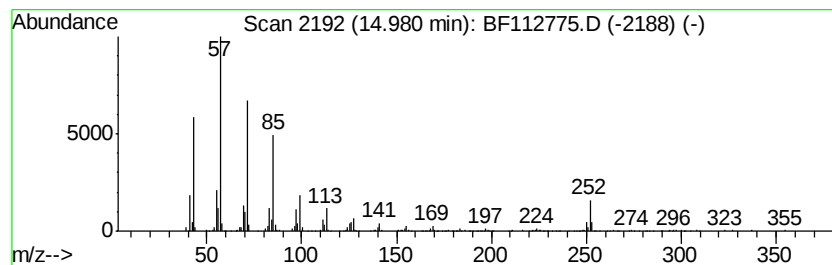
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	9.76 ng	575979	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	93
2	Hexacosane	366 C26H54	000630-01-3	87
3	Heneicosane	296 C21H44	000629-94-7	87
4	Eicosane, 7-hexyl-	366 C26H54	055333-99-8	80
5	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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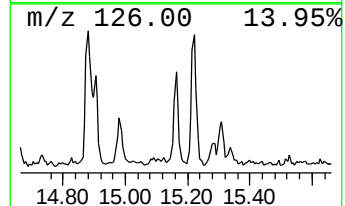
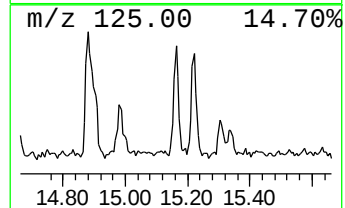
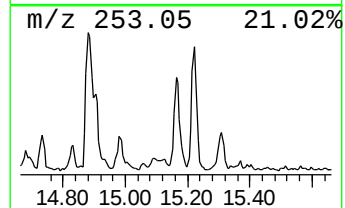
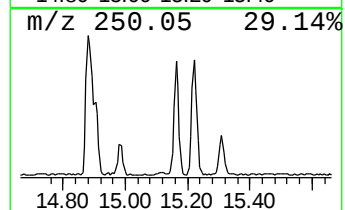
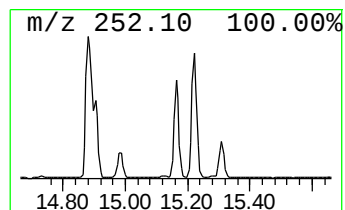
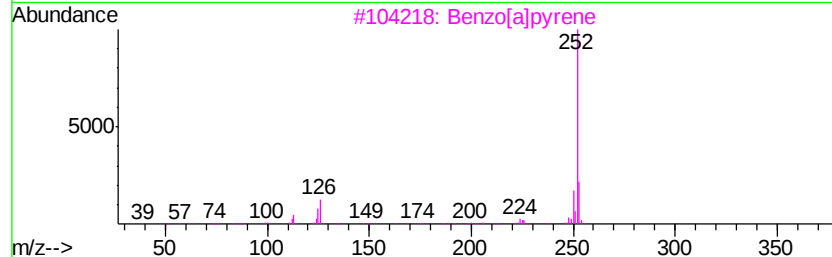
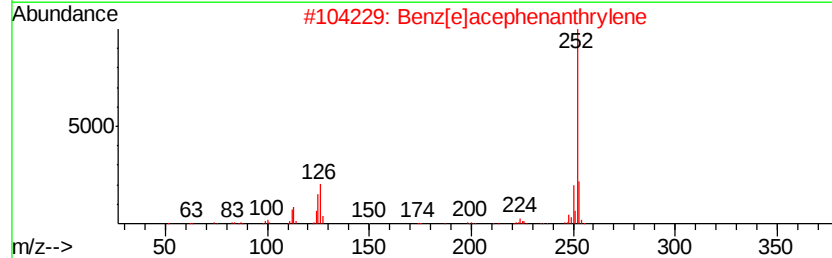
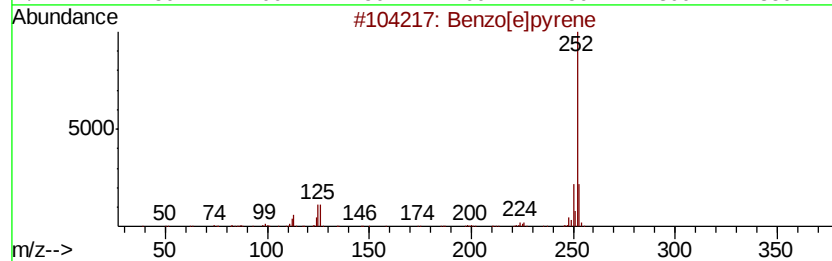
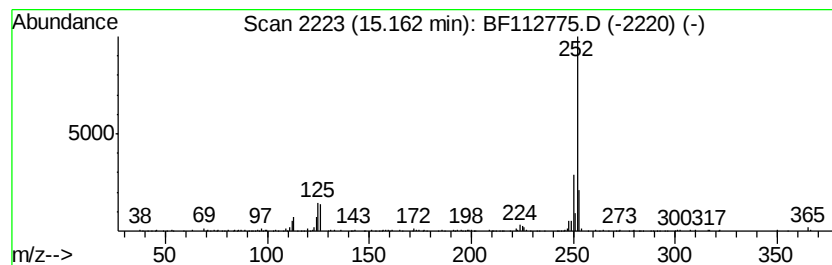
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzo[e]pyrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.58 ng	152107	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	96
3		Benzo[a]pyrene	252	C20H12	000050-32-8	93
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5		Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112775.D
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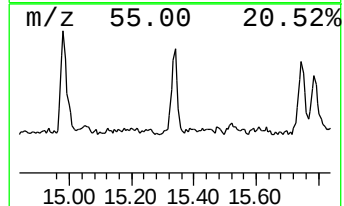
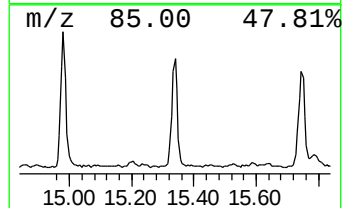
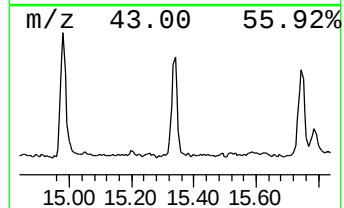
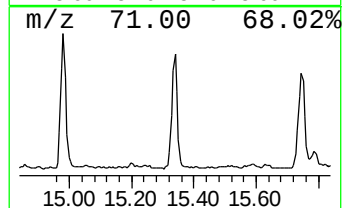
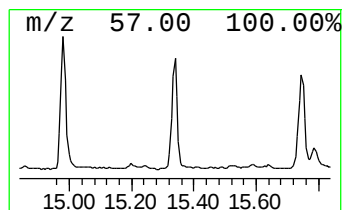
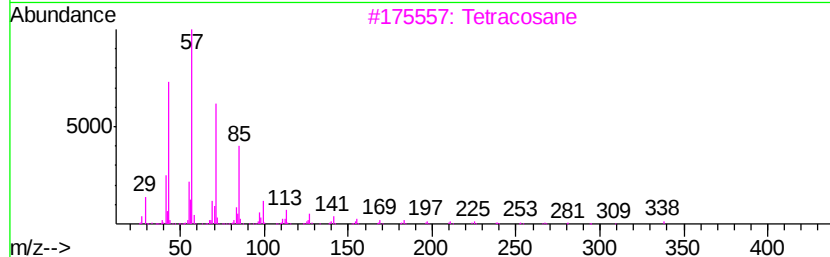
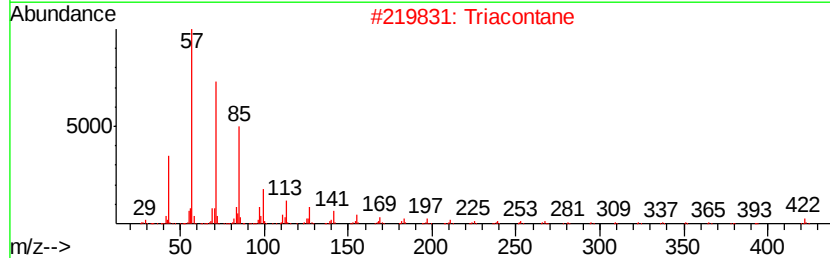
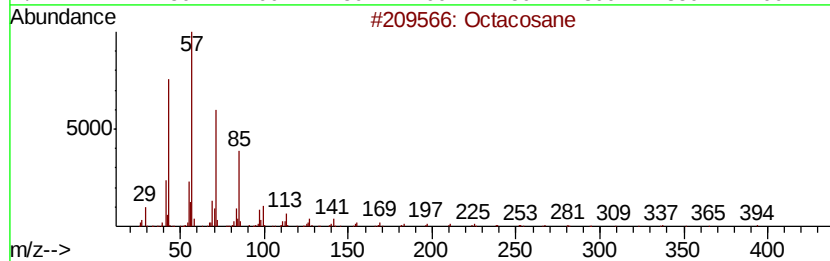
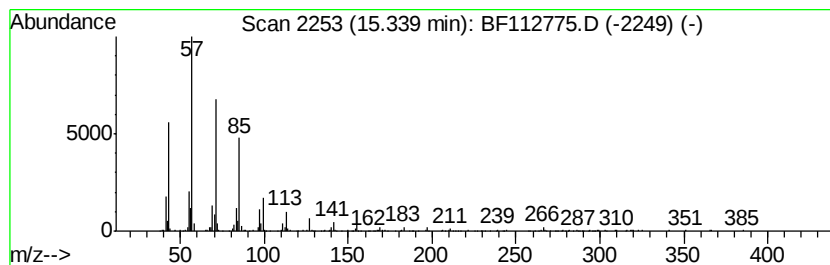
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	7.74 ng	456649	Perylene-d12	15.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Triacontane	422	C30H62	000638-68-6	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
5			Hexacosane	366	C26H54	000630-01-3	90



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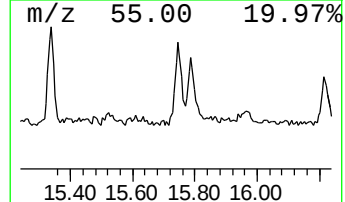
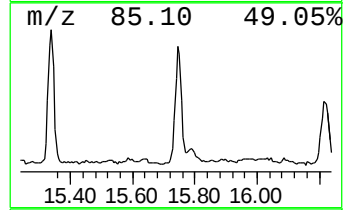
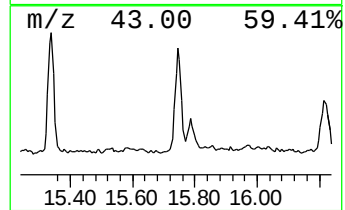
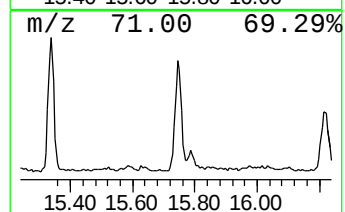
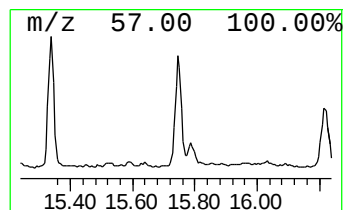
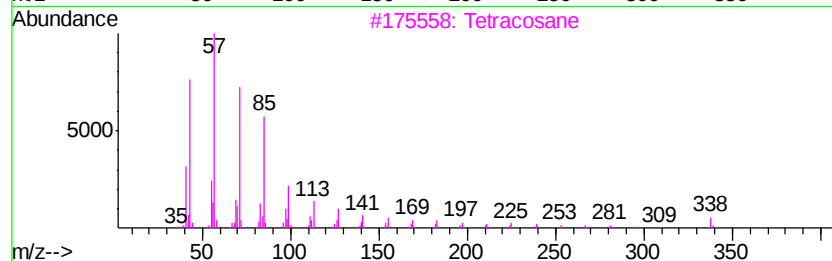
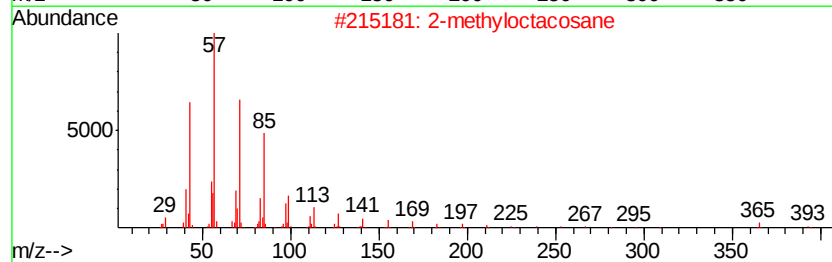
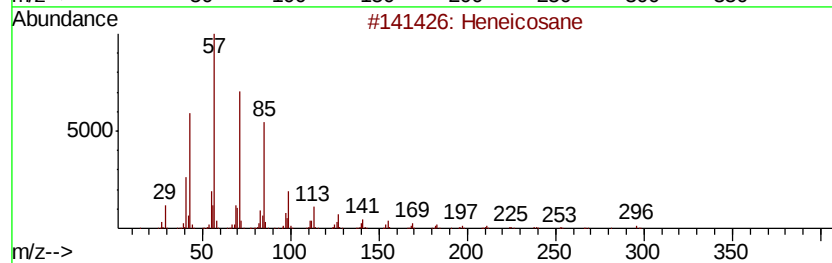
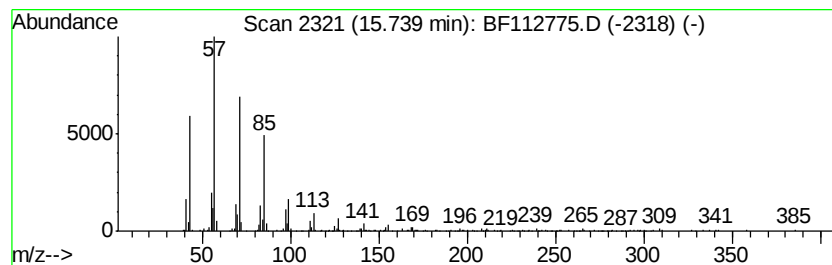
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	7.34 ng	433108	Perylene-d12	15.29

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	triacontane		422	C30H62	000638-68-6	90
5	Tetratetracontane		619	C44H90	007098-22-8	83



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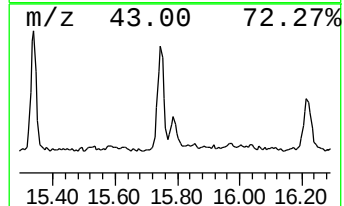
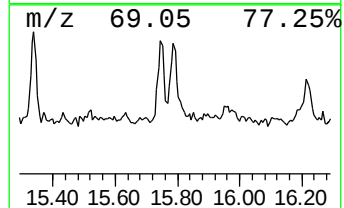
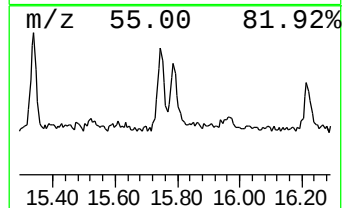
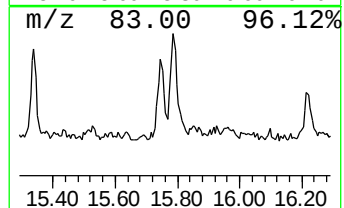
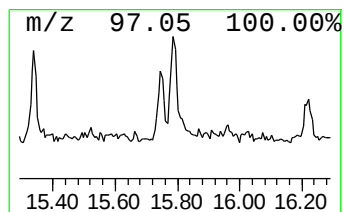
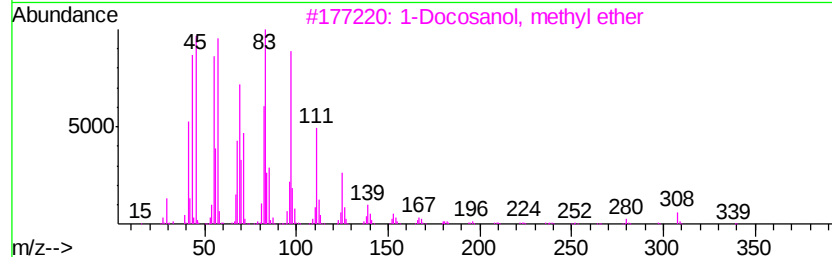
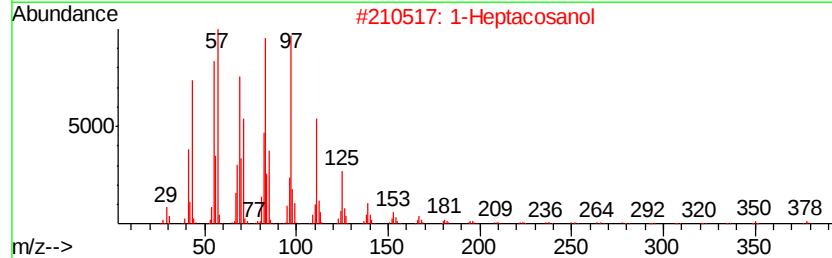
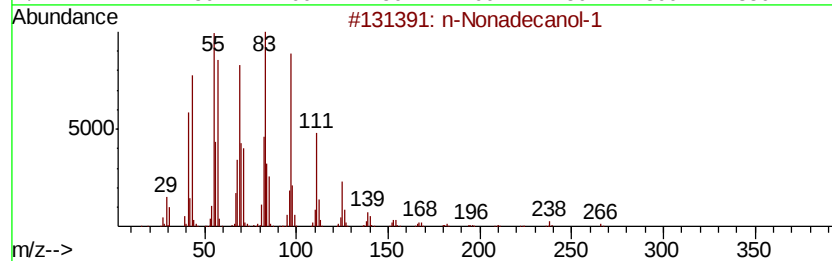
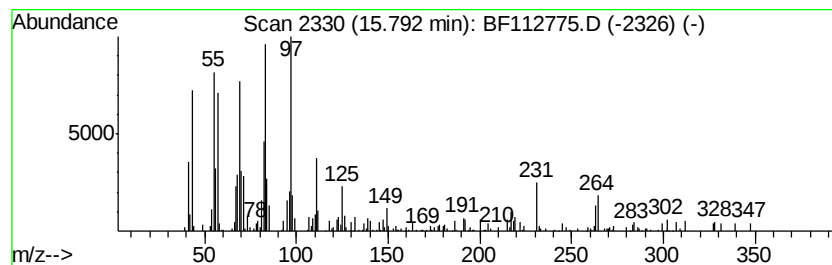
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 n-Nonadecanol-1 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.79	4.10 ng	241982	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	72
3	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	58
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	58
5	Cyclopentadecane	210	C15H30	000295-48-7	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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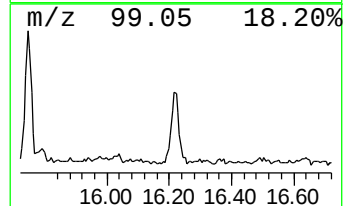
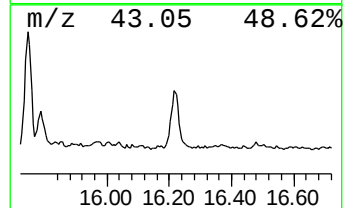
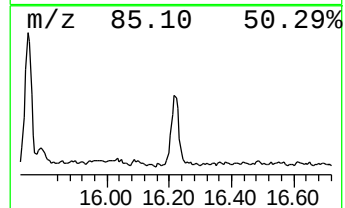
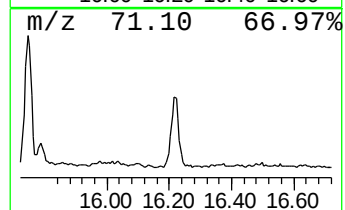
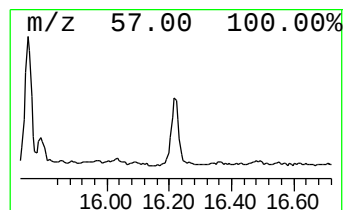
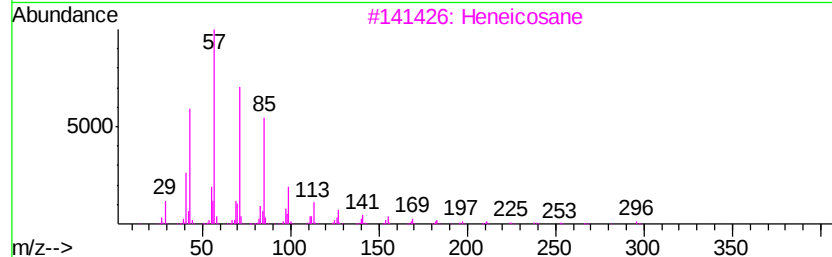
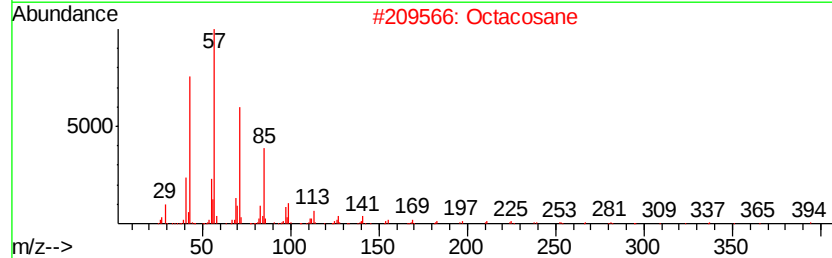
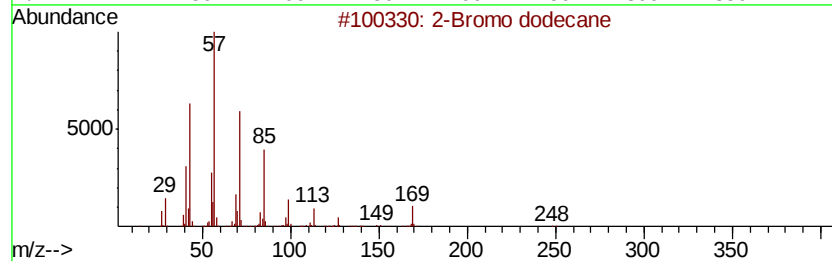
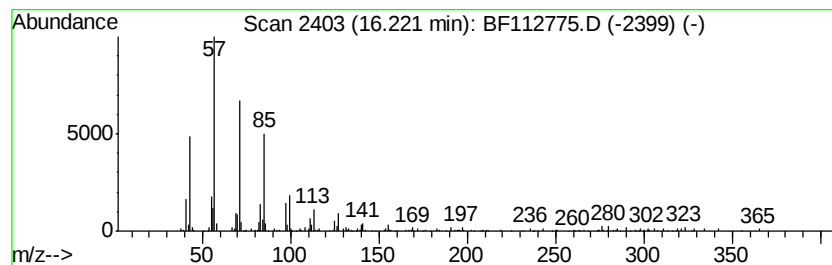
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2-Bromo dodecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	4.88 ng	287819	Perylene-d12	15.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo dodecane	248	C12H25Br	013187-99-0	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Tricosane	324	C23H48	000638-67-5	90
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
Data File : BF112775.D
Acq On : 28 Feb 2019 21:44
Operator : JU/SJ
Sample : K1645-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SR-10

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
unknown6.51	6.51	67.5	ng	3682070	1	6.75	1090840	20.0
n-Hexadecanoic acid	11.79	14.8	ng	799995	4	11.25	1080430	20.0
Octadecanoic acid	12.57	6.7	ng	454820	5	13.87	1357330	20.0
1-Heneicosanol	13.73	9.4	ng	635619	5	13.87	1357330	20.0
2-methyloctacosane	14.06	2.3	ng	153371	5	13.87	1357330	20.0
Sulfurous acid, b...	14.36	5.8	ng	393146	5	13.87	1357330	20.0
Eicosane	14.98	9.8	ng	575979	6	15.29	1180140	20.0
Benzo[e]pyrene	15.16	2.6	ng	152107	6	15.29	1180140	20.0
Octacosane	15.34	7.7	ng	456649	6	15.29	1180140	20.0
Heneicosane	15.74	7.3	ng	433108	6	15.29	1180140	20.0
n-Nonadecanol-1	15.79	4.1	ng	241982	6	15.29	1180140	20.0
2-Bromo dodecane	16.22	4.9	ng	287819	6	15.29	1180140	20.0