

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
 Data File : BF112873.D
 Acq On : 6 Mar 2019 1:03
 Operator : JU/SJ
 Sample : K1705-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EXT-028-SW004-022719

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	5.351	550	555	558	rBV	2951124	3055066	89.95%	7.895%
2	6.022	666	669	672	rBV	49056	39972	1.18%	0.103%
3	6.375	724	729	732	rBV	3211459	3319866	97.75%	8.580%
4	6.445	739	741	747	rVB	87232	78838	2.32%	0.204%
5	6.510	747	752	755	rBV	3703561	3360470	98.95%	8.685%
6	6.739	787	791	795	rBV	1183939	935124	27.53%	2.417%
7	6.898	814	818	821	rBV	2877999	2507162	73.82%	6.479%
8	7.298	881	886	889	rBV	2221353	2035453	59.93%	5.260%
9	7.733	956	960	970	rBV2	36364	60725	1.79%	0.157%
10	8.022	1005	1009	1015	rBV	1191830	1123104	33.07%	2.902%
11	8.416	1072	1076	1082	rBV	47934	80001	2.36%	0.207%
12	9.098	1188	1192	1202	rBV	3724887	3396276	100.00%	8.777%
13	9.439	1246	1250	1253	rBV	116315	105097	3.09%	0.272%
14	9.486	1255	1258	1265	rVV	207212	205788	6.06%	0.532%
15	9.769	1302	1306	1315	rBV2	1320587	1241364	36.55%	3.208%
16	10.557	1435	1440	1455	rBV	2293240	2339661	68.89%	6.046%
17	11.251	1554	1558	1560	rBV	1191393	1160305	34.16%	2.999%
18	11.268	1560	1561	1566	rVB	172042	144281	4.25%	0.373%
19	11.792	1645	1650	1659	rBV2	827554	987270	29.07%	2.551%
20	12.063	1694	1696	1703	rVB	46293	59351	1.75%	0.153%
21	12.304	1733	1737	1739	rBV2	41925	47396	1.40%	0.122%
22	12.380	1747	1750	1755	rVB2	26006	36428	1.07%	0.094%
23	12.457	1759	1763	1767	rBV	434344	427064	12.57%	1.104%
24	12.492	1767	1769	1777	rVB7	38120	72060	2.12%	0.186%
25	12.568	1779	1782	1796	rVV	384943	599796	17.66%	1.550%
26	12.680	1796	1801	1805	rVB	354067	395921	11.66%	1.023%
27	12.804	1819	1822	1823	rBV	37613	37256	1.10%	0.096%
28	12.833	1823	1827	1830	rVV	3185928	3062099	90.16%	7.914%
29	13.010	1851	1857	1859	rBV2	55489	84965	2.50%	0.220%
30	13.074	1866	1868	1872	rVB	42257	39427	1.16%	0.102%
31	13.115	1872	1875	1877	rBV	47714	47809	1.41%	0.124%
32	13.321	1902	1910	1912	rBV4	75155	135474	3.99%	0.350%
33	13.351	1912	1915	1920	rVV4	64895	77813	2.29%	0.201%
34	13.515	1940	1943	1949	rBV	61256	83700	2.46%	0.216%

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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	13.592	1953	1956	1959	rVV4	87486	99250	2.92%	0.256%
36	13.621	1959	1961	1965	rVV2	47107	65585	1.93%	0.169%
37	13.680	1968	1971	1974	rVV2	70431	81507	2.40%	0.211%
38	13.733	1977	1980	1988	rVB2	632932	718947	21.17%	1.858%
39	13.874	1998	2004	2007	rBV2	2481101	2770445	81.57%	7.160%
40	13.898	2007	2008	2011	rVB	232816	174963	5.15%	0.452%
41	14.057	2032	2035	2039	rBV2	162022	156443	4.61%	0.404%
42	14.362	2084	2087	2093	rBV2	304355	395075	11.63%	1.021%
43	14.656	2134	2137	2145	rVB	281851	278990	8.21%	0.721%
44	14.792	2158	2160	2163	rVB2	104529	86278	2.54%	0.223%
45	14.886	2173	2176	2184	rVB	199417	342348	10.08%	0.885%
46	14.980	2188	2192	2194	rBV	264261	313168	9.22%	0.809%
47	15.168	2221	2224	2230	rBV	105609	118613	3.49%	0.307%
48	15.227	2231	2234	2239	rVV	109336	130274	3.84%	0.337%
49	15.286	2240	2244	2249	rVV	688927	849656	25.02%	2.196%
50	15.333	2249	2252	2257	rVB	219800	280746	8.27%	0.726%
51	15.745	2318	2322	2326	rBV	185315	257323	7.58%	0.665%
52	15.792	2327	2330	2337	rVV3	115533	192482	5.67%	0.497%

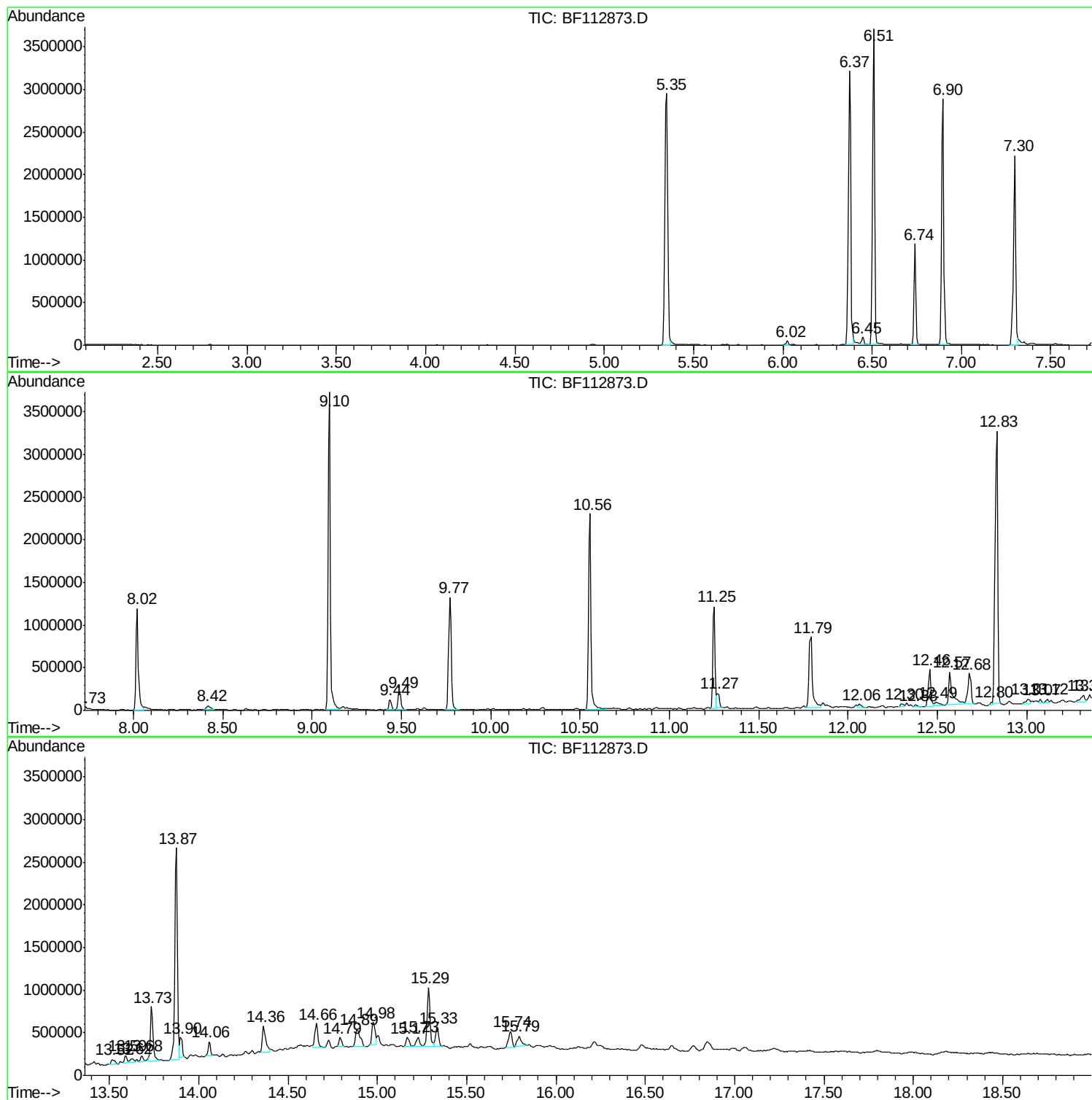
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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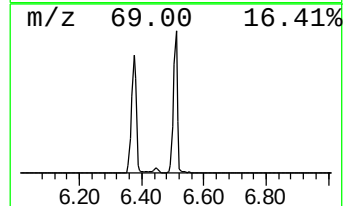
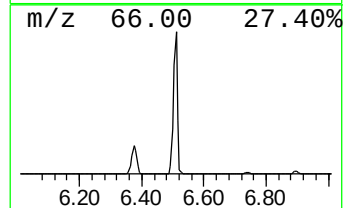
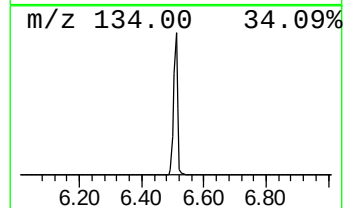
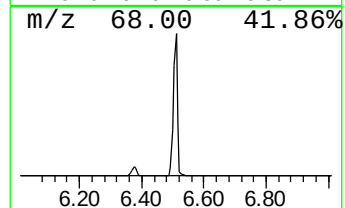
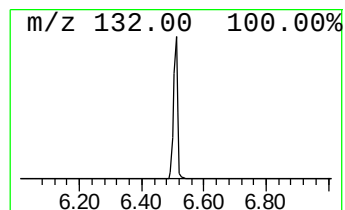
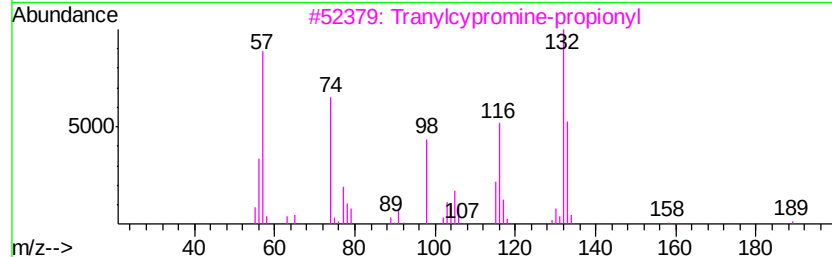
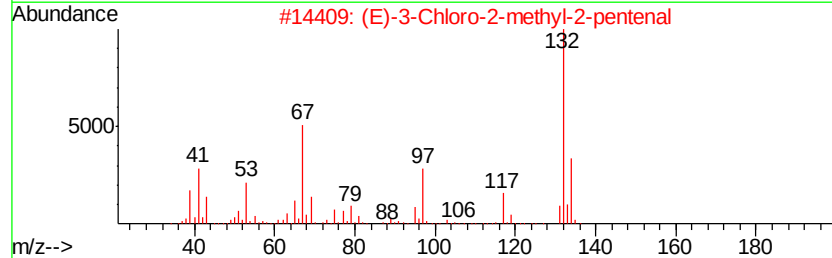
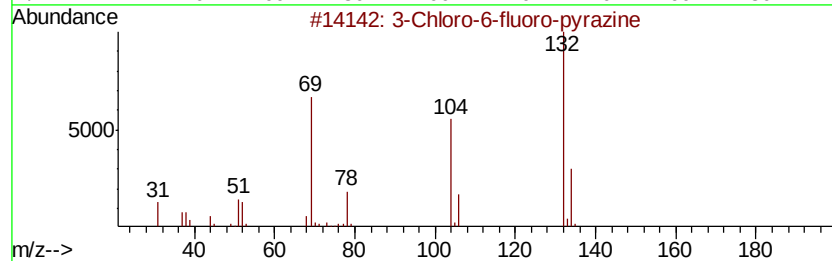
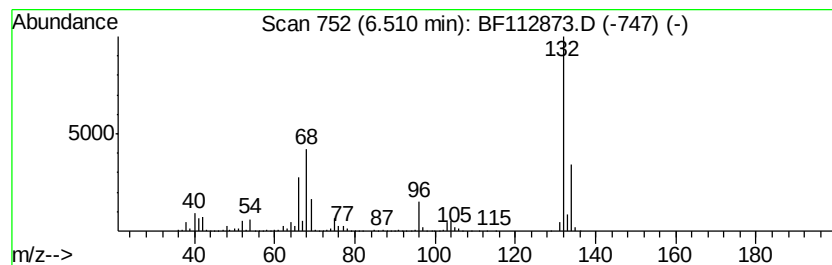
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	71.87 ng	3360470	1,4-Dichlorobenzene-d4	6.74

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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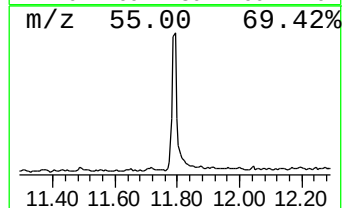
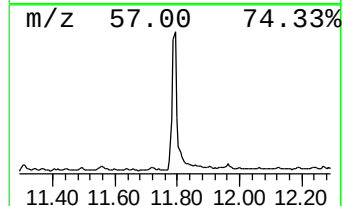
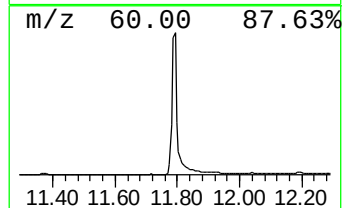
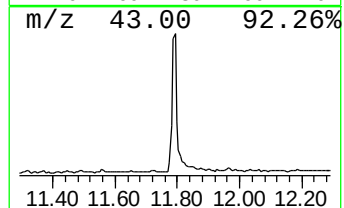
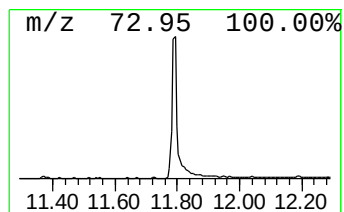
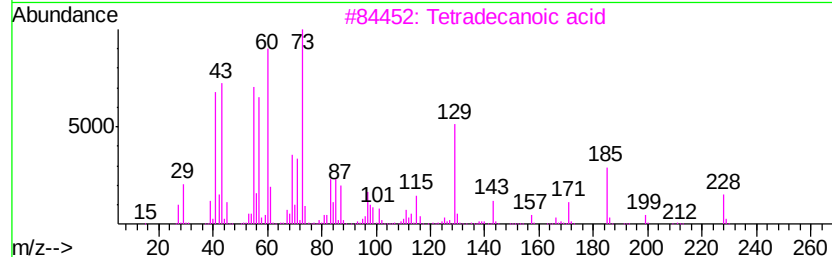
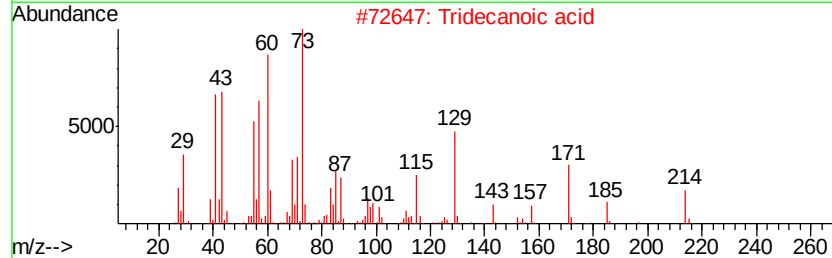
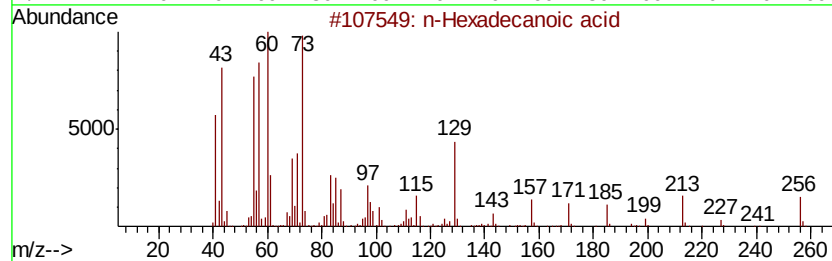
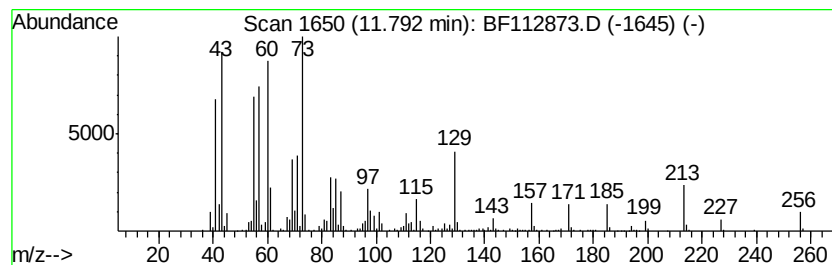
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.79	17.02 ng	987270	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	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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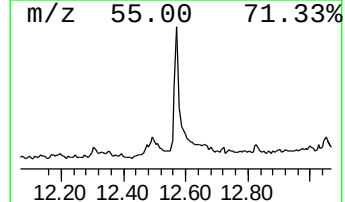
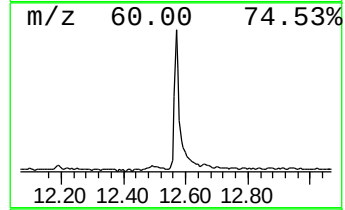
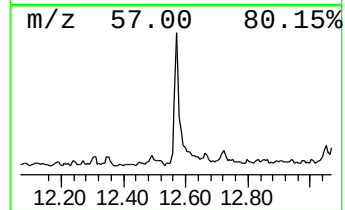
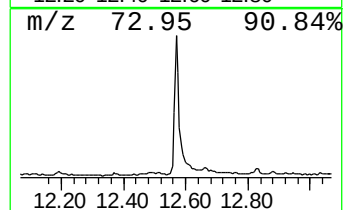
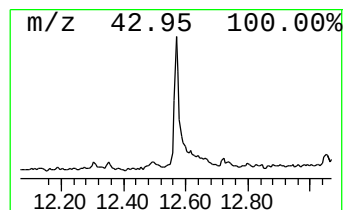
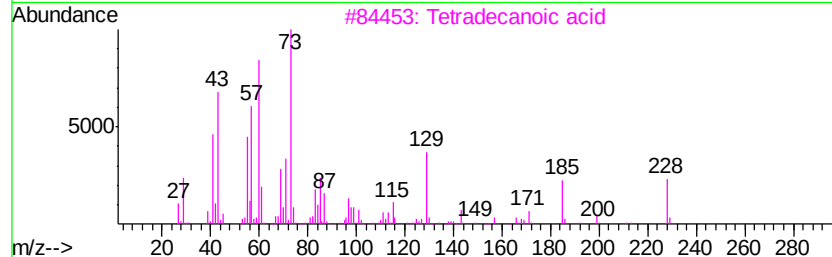
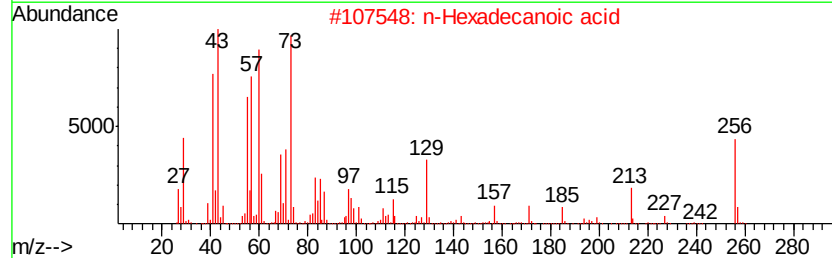
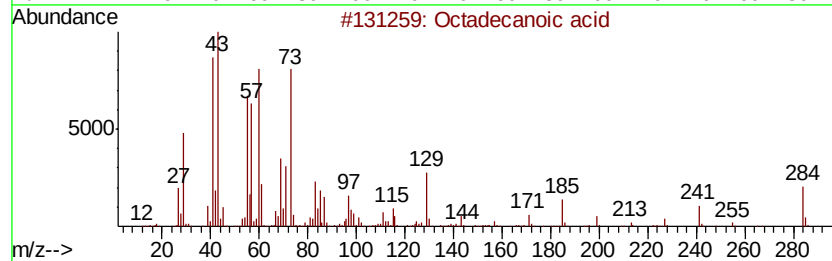
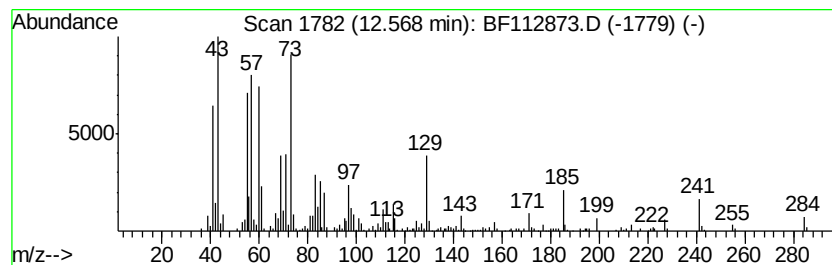
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.57	4.33 ng	599796	Chrysene-d12	13.87	
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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83



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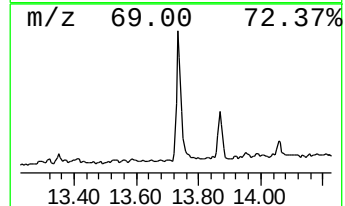
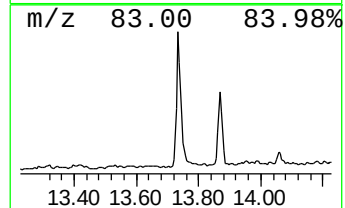
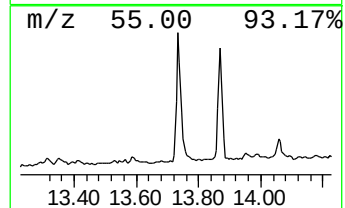
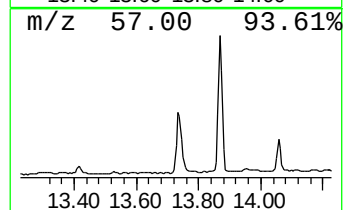
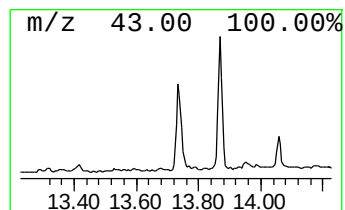
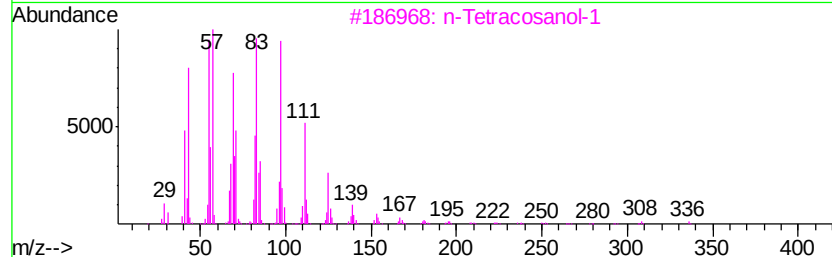
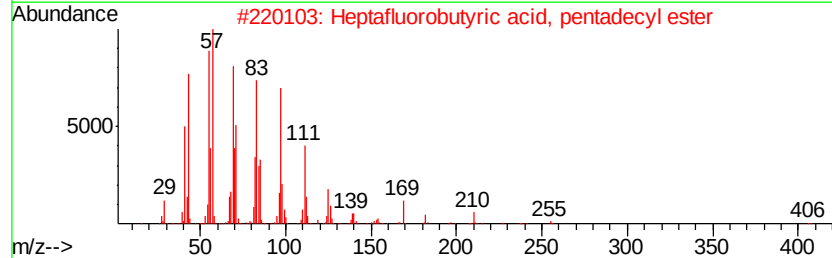
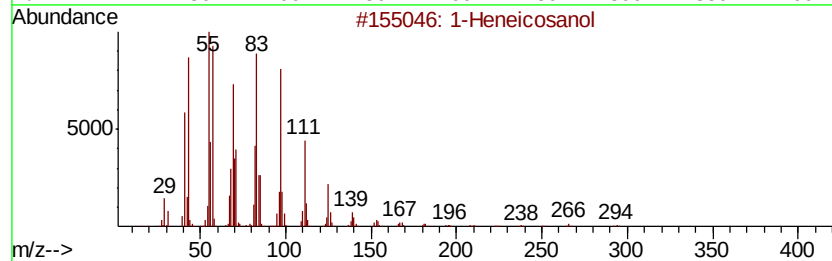
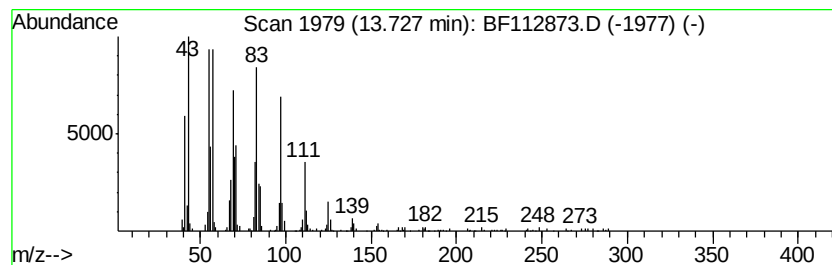
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	5.19 ng	718947	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	94
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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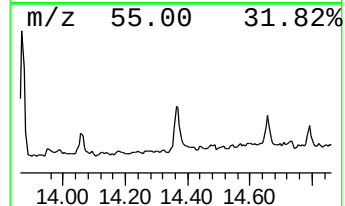
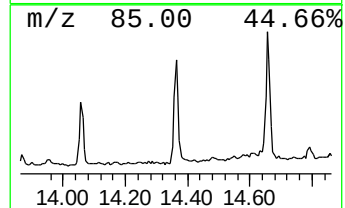
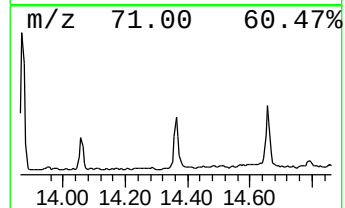
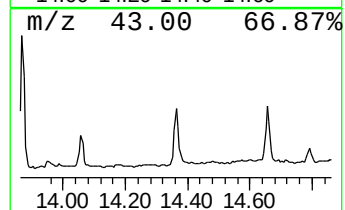
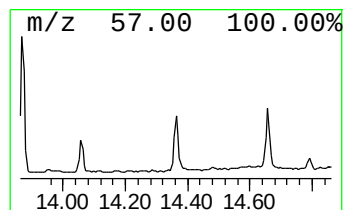
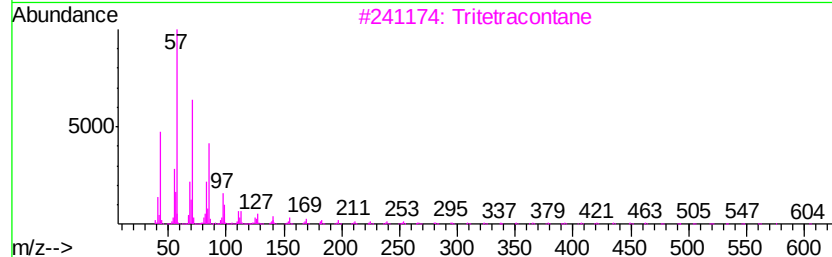
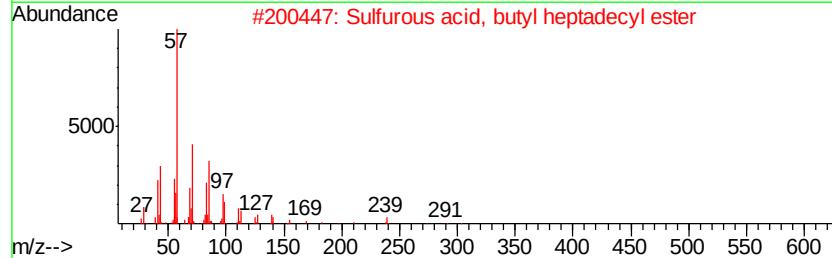
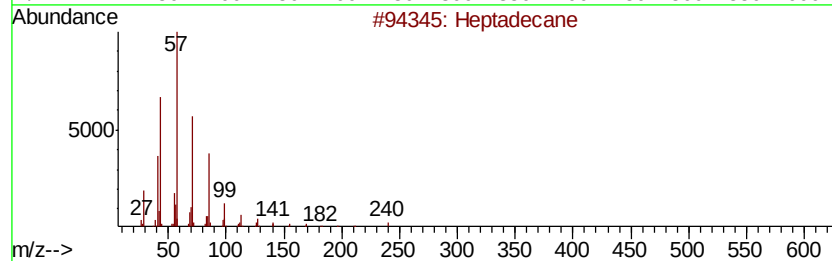
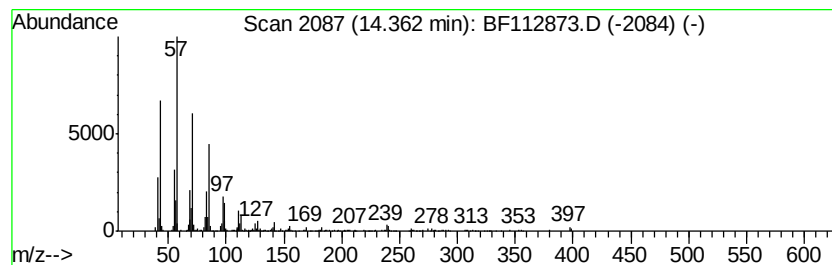
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.85 ng	395075	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	96
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
3		Tritetracontane	605	C43H88	007098-21-7	91
4		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
5		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112873.D
Acq On : 6 Mar 2019 1:03
Operator : JU/SJ
Sample : K1705-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

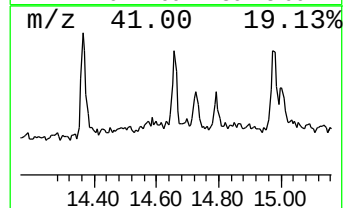
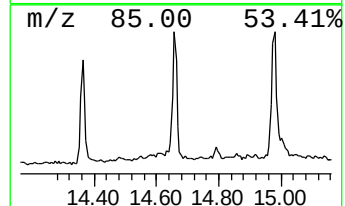
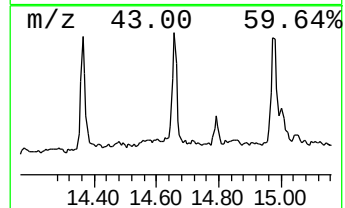
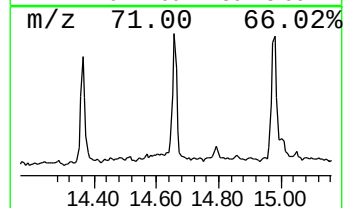
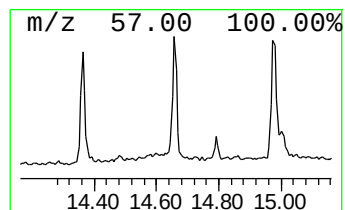
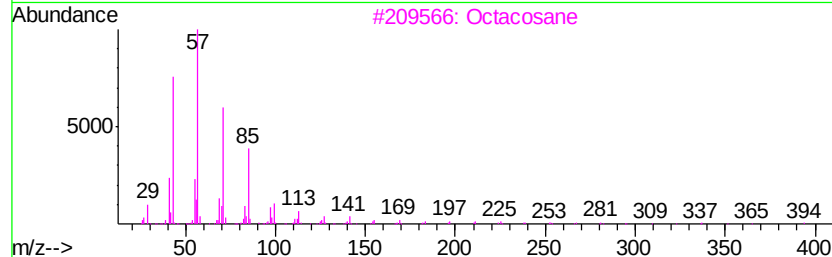
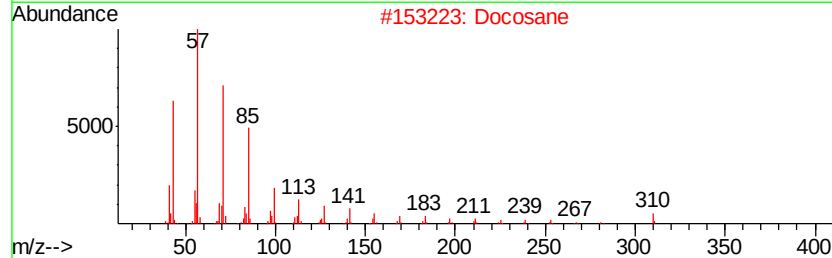
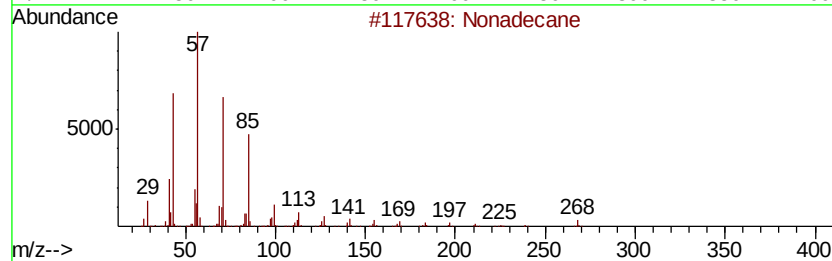
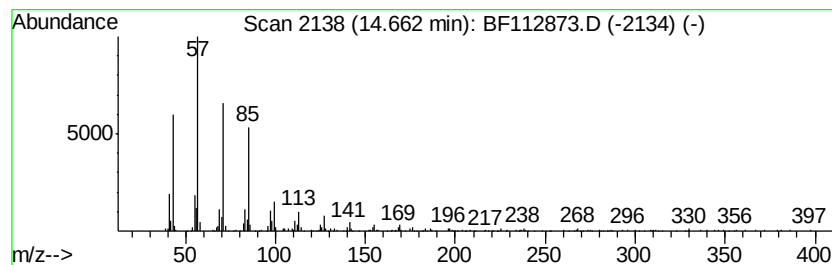
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.66	6.57 ng	278990	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Docosane	310	C22H46	000629-97-0	93
3	Octacosane	394	C28H58	000630-02-4	87
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
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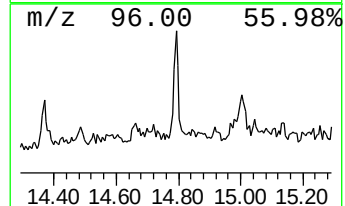
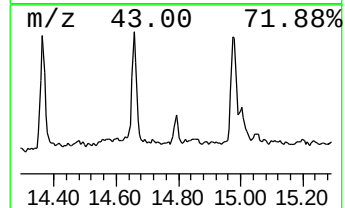
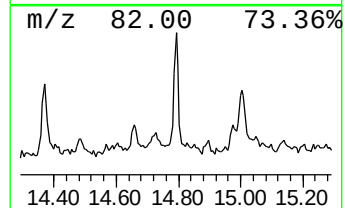
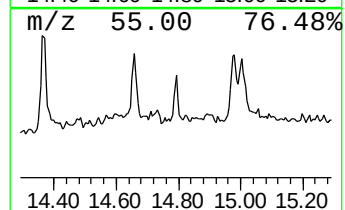
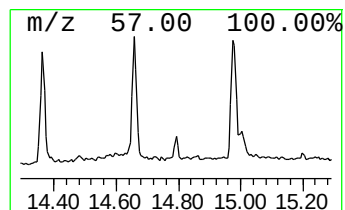
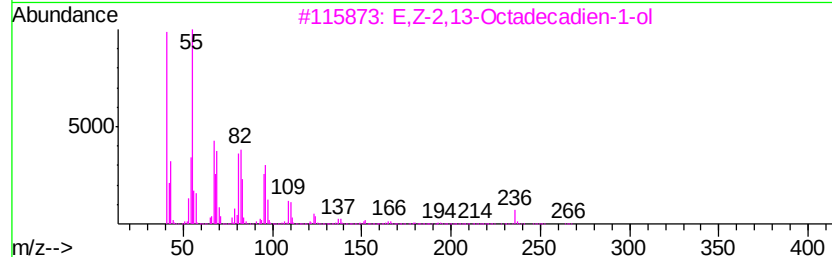
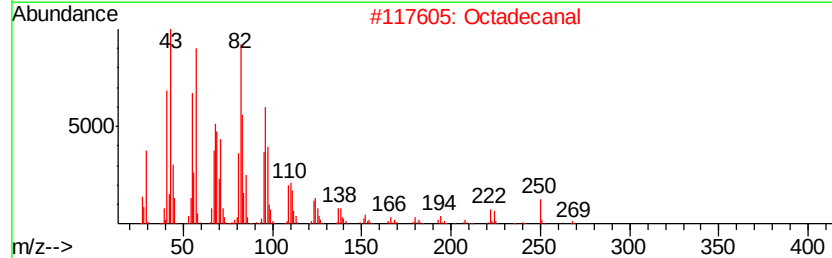
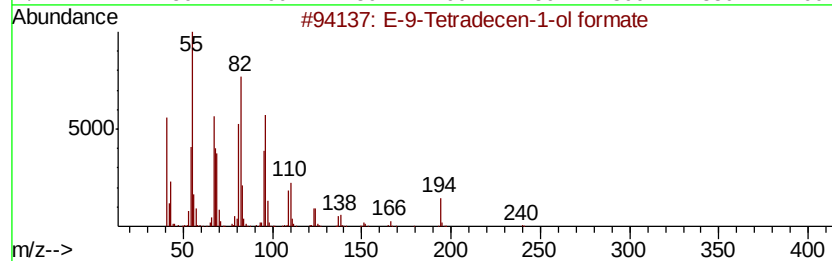
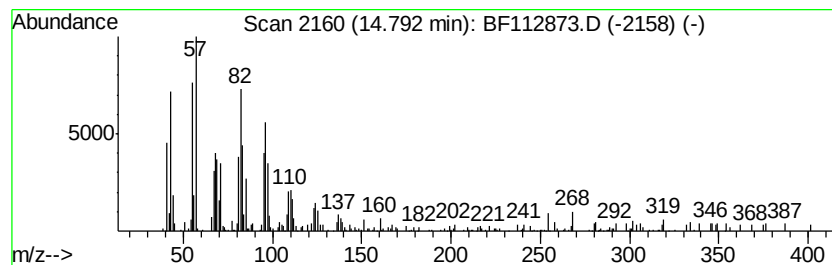
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 E-9-Tetradecen-1-ol formate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.79	2.03 ng	86278	Perylene-d12		15.29	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-9-Tetradecen-1-ol formate	240	C15H28O2	1000130-78-2	90	
2	Octadecanal	268	C18H36O	000638-66-4	81	
3	E,Z-2,13-Octadecadien-1-ol	266	C18H34O	1000131-10-0	81	
4	Pentadecanal-	226	C15H30O	002765-11-9	81	
5	Tetradecanal	212	C14H28O	000124-25-4	81	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112873.D
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Operator : JU/SJ
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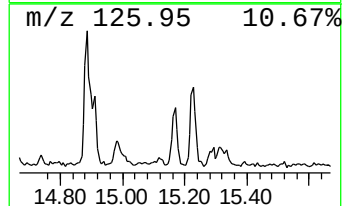
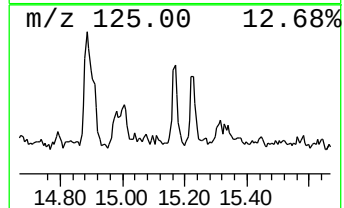
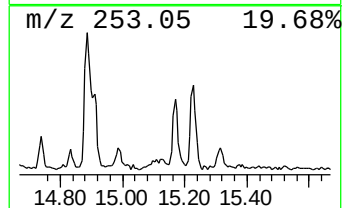
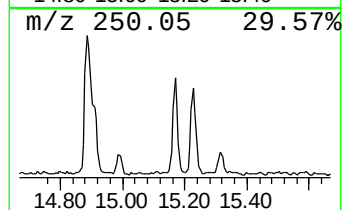
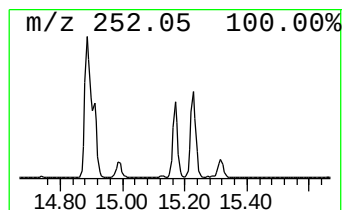
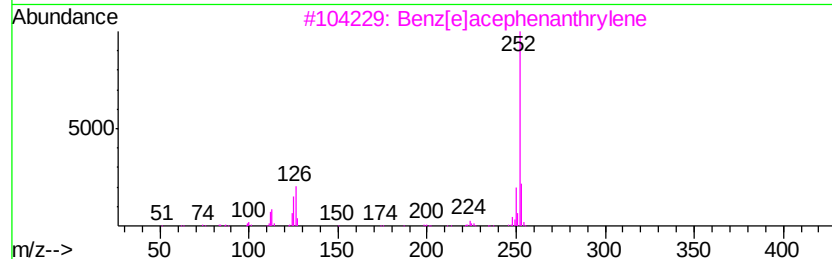
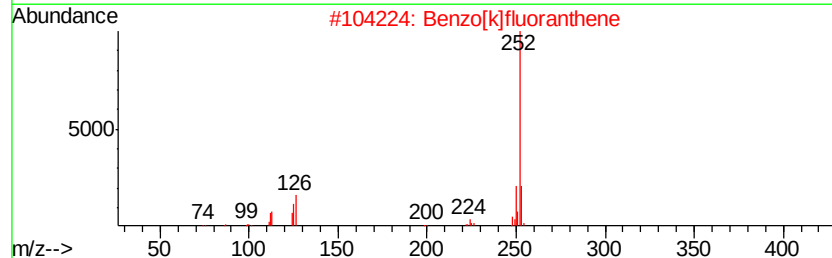
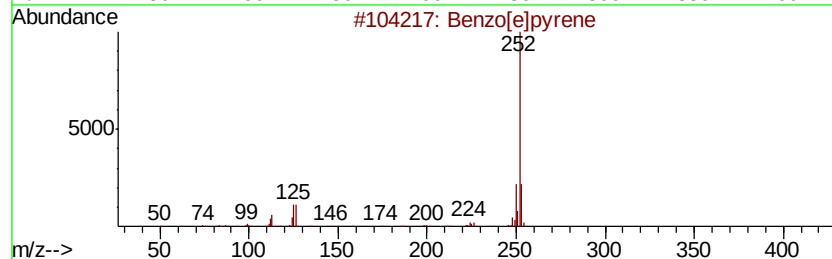
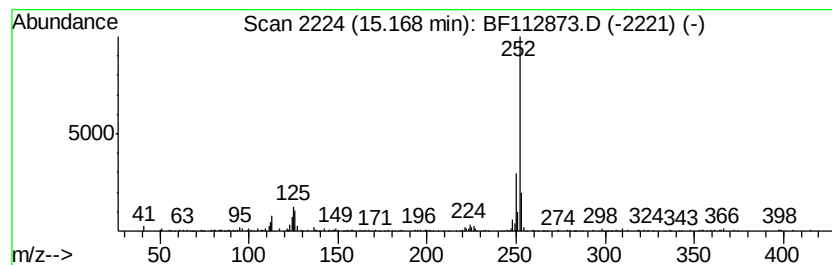
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.79 ng	118613	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[k]fluoranthene	252	C20H12	000207-08-9	97
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	95
4		Benzo[a]pyrene	252	C20H12	000050-32-8	91
5		Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
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Acq On : 6 Mar 2019 1:03
Operator : JU/SJ
Sample : K1705-03
Misc :
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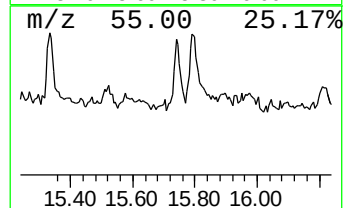
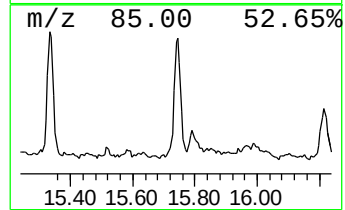
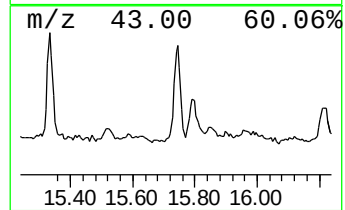
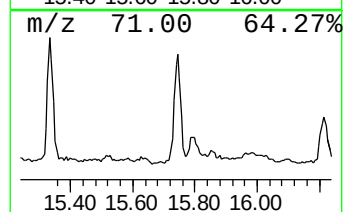
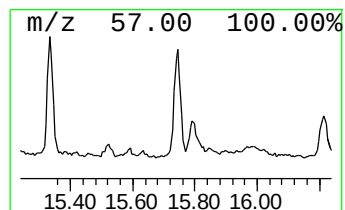
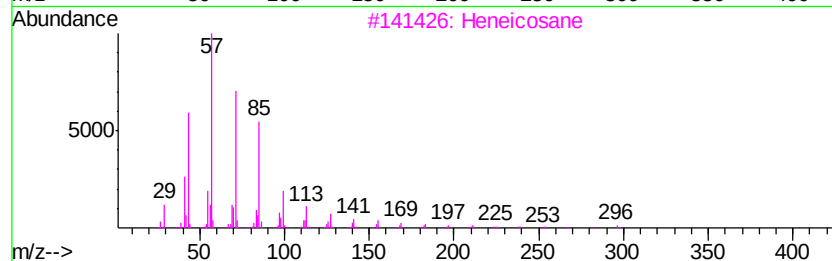
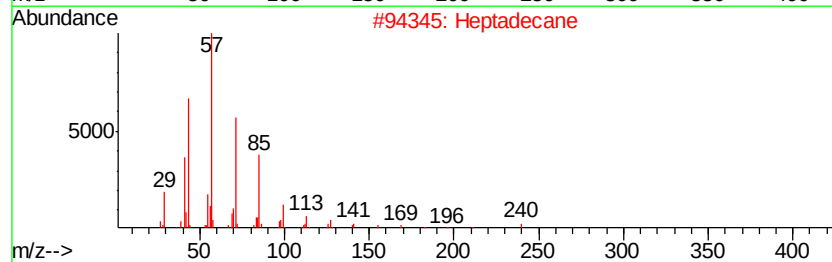
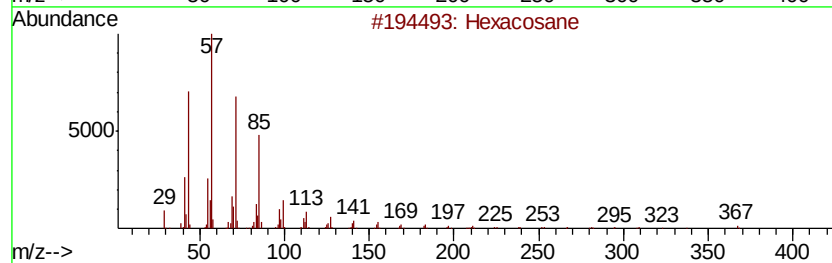
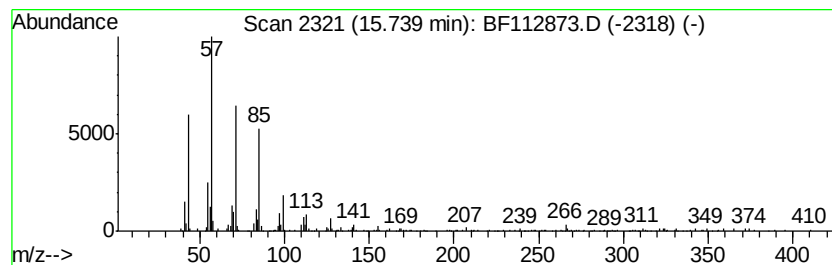
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.74	6.06 ng	257323	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
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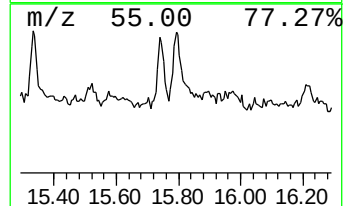
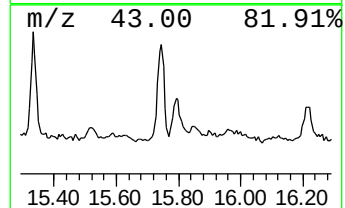
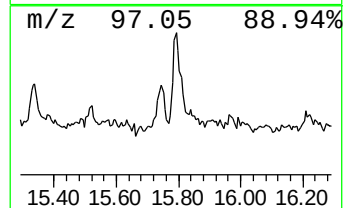
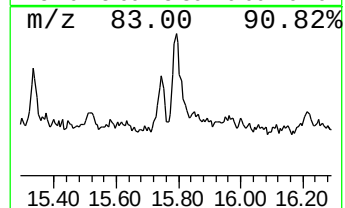
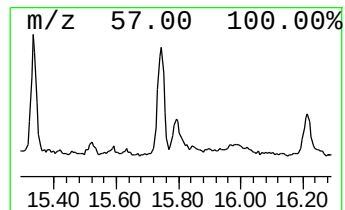
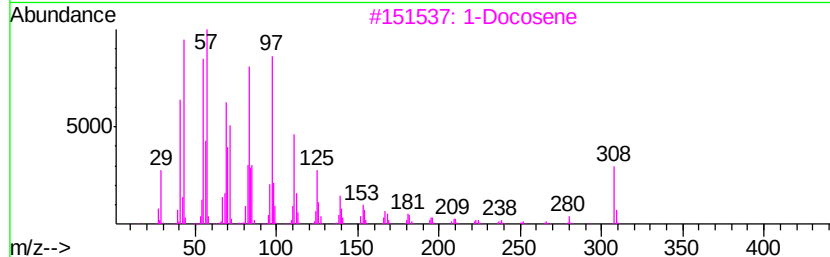
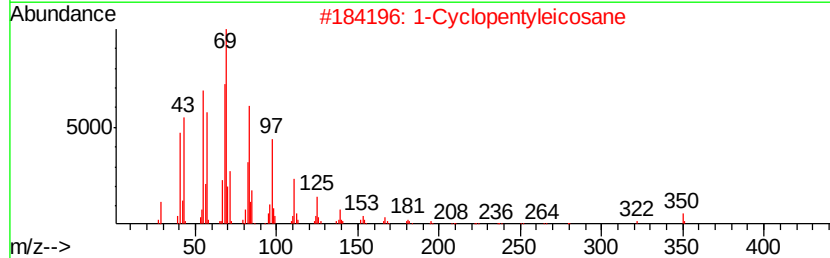
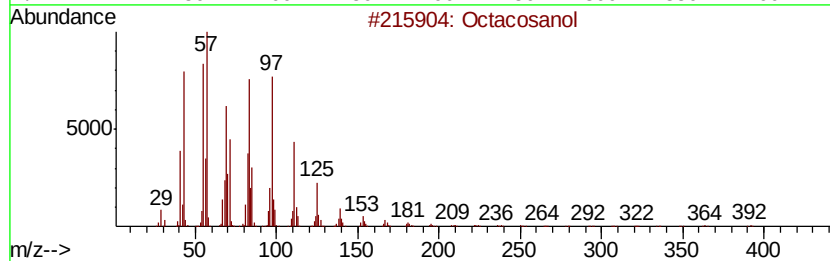
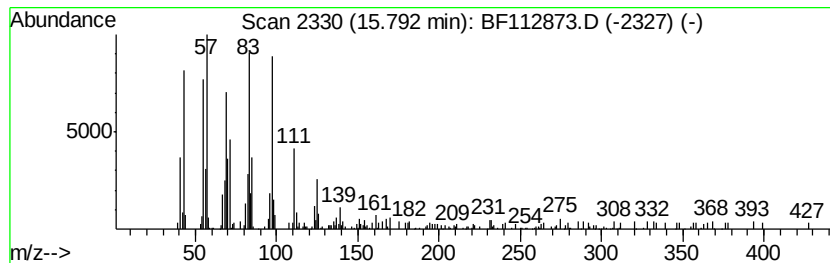
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.79	4.53 ng	192482	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	1-Cyclopentyleicosane	350	C25H50	1000357-25-6	91
3	1-Docosene	308	C22H44	001599-67-3	83
4	Cyclooctacosane	392	C28H56	000297-24-5	74
5	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
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 Acq On : 6 Mar 2019 1:03
 Operator : JU/SJ
 Sample : K1705-03
 Misc :
 ALS Vial : 18 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	11.79	17.0	ng	987270	4	11.25	1160310	20.0
Octadecanoic acid	12.57	4.3	ng	599796	5	13.87	2770450	20.0
1-Heneicosanol	13.73	5.2	ng	718947	5	13.87	2770450	20.0
Heptadecane	14.36	2.9	ng	395075	5	13.87	2770450	20.0
Nonadecane	14.66	6.6	ng	278990	6	15.29	849656	20.0
E-9-Tetradecen-1-...	14.79	2.0	ng	86278	6	15.29	849656	20.0
Benzo[e]pyrene	15.17	2.8	ng	118613	6	15.29	849656	20.0
Hexacosane	15.74	6.1	ng	257323	6	15.29	849656	20.0
Octacosanol	15.79	4.5	ng	192482	6	15.29	849656	20.0