

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
 Data File : BF100696.D
 Acq On : 18 Nov 2017 1:31
 Operator : SJ/JU
 Sample : I6423-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B8(0-10)COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	5.110	511	514	526	rVB	310067	437841	17.33%	1.733%
2	5.504	576	581	584	rBV	2160312	2227751	88.17%	8.818%
3	6.510	746	752	756	rBV	2104598	2307249	91.32%	9.133%
4	6.651	771	776	779	rBV	2343313	2290002	90.64%	9.064%
5	6.881	811	815	819	rBV	811410	636529	25.19%	2.520%
6	7.040	837	842	845	rBV	2082670	1834401	72.61%	7.261%
7	7.445	905	911	914	rBV	1491676	1450395	57.41%	5.741%
8	8.163	1029	1033	1036	rBV	1012048	832054	32.93%	3.293%
9	8.716	1123	1127	1130	rBV	137458	114681	4.54%	0.454%
10	9.239	1210	1216	1219	rBV	2695458	2526546	100.00%	10.001%
11	9.628	1278	1282	1285	rBV	250490	202055	8.00%	0.800%
12	9.916	1327	1331	1335	rBV2	1002700	836704	33.12%	3.312%
13	10.628	1448	1452	1457	rBV	348908	280540	11.10%	1.110%
14	10.704	1461	1465	1469	rBV	1355775	1233214	48.81%	4.881%
15	11.404	1580	1584	1586	rBV	785133	701810	27.78%	2.778%
16	11.428	1586	1588	1591	rVV	307869	239245	9.47%	0.947%
17	11.475	1593	1596	1599	rVB	90813	74031	2.93%	0.293%
18	11.627	1616	1622	1626	rBV2	27819	30439	1.20%	0.120%
19	11.904	1664	1669	1670	rBV	43398	46085	1.82%	0.182%
20	11.922	1670	1672	1676	rVB2	91174	116199	4.60%	0.460%
21	12.016	1684	1688	1690	rBV	64576	65612	2.60%	0.260%
22	12.451	1758	1762	1765	rBV	28196	27230	1.08%	0.108%
23	12.533	1774	1776	1781	rVB	27984	29037	1.15%	0.115%
24	12.616	1786	1790	1793	rVB	489196	423495	16.76%	1.676%
25	12.845	1823	1829	1832	rBV	389327	418510	16.56%	1.657%
26	12.986	1849	1853	1856	rBV	1864971	1582758	62.65%	6.265%
27	13.063	1861	1866	1869	rBV3	31871	52871	2.09%	0.209%
28	13.169	1881	1884	1888	rVB	47443	48588	1.92%	0.192%
29	13.274	1898	1902	1904	rBV2	46679	48616	1.92%	0.192%
30	13.545	1944	1948	1950	rBV4	21492	29292	1.16%	0.116%
31	13.674	1967	1970	1974	rVB	61294	55274	2.19%	0.219%
32	13.786	1984	1989	1992	rBV2	52444	74711	2.96%	0.296%
33	13.869	2000	2003	2014	rVB2	263900	322409	12.76%	1.276%
34	14.039	2024	2032	2035	rBV2	819049	1027008	40.65%	4.065%

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35	14.063	2035	2036	2043	rVB	259735	196250	7.77%	0.777%
36	14.145	2047	2050	2054	rBV	34129	33408	1.32%	0.132%
37	14.192	2054	2058	2061	rBV4	22953	40357	1.60%	0.160%
38	14.263	2066	2070	2073	rBV2	26477	40229	1.59%	0.159%
39	14.421	2093	2097	2100	rVB	52675	55925	2.21%	0.221%
40	14.457	2100	2103	2107	rVB	35169	28832	1.14%	0.114%
41	14.504	2107	2111	2116	rBV5	42798	88130	3.49%	0.349%
42	14.616	2129	2130	2135	rVB4	24639	26848	1.06%	0.106%
43	15.080	2204	2209	2217	rBV	238781	469358	18.58%	1.858%
44	15.145	2217	2220	2223	rVV4	38051	50414	2.00%	0.200%
45	15.186	2225	2227	2231	rVB	46132	45831	1.81%	0.181%
46	15.386	2257	2261	2267	rVB	137752	181392	7.18%	0.718%
47	15.451	2267	2272	2278	rBV	179295	235601	9.33%	0.933%
48	15.515	2278	2283	2287	rBV	524200	679509	26.89%	2.690%
49	15.739	2316	2321	2325	rVB7	23604	37312	1.48%	0.148%
50	15.963	2356	2359	2363	rBV3	29351	37049	1.47%	0.147%
51	16.021	2367	2369	2376	rVB6	26101	48216	1.91%	0.191%
52	16.774	2492	2497	2500	rBV5	16715	33581	1.33%	0.133%
53	16.992	2528	2534	2540	rVB2	68220	124790	4.94%	0.494%
54	17.168	2560	2564	2571	rBV4	19147	37879	1.50%	0.150%
55	17.439	2603	2610	2617	rBV2	48735	112358	4.45%	0.445%
56	17.586	2631	2635	2645	rVB2	15431	37370	1.48%	0.148%

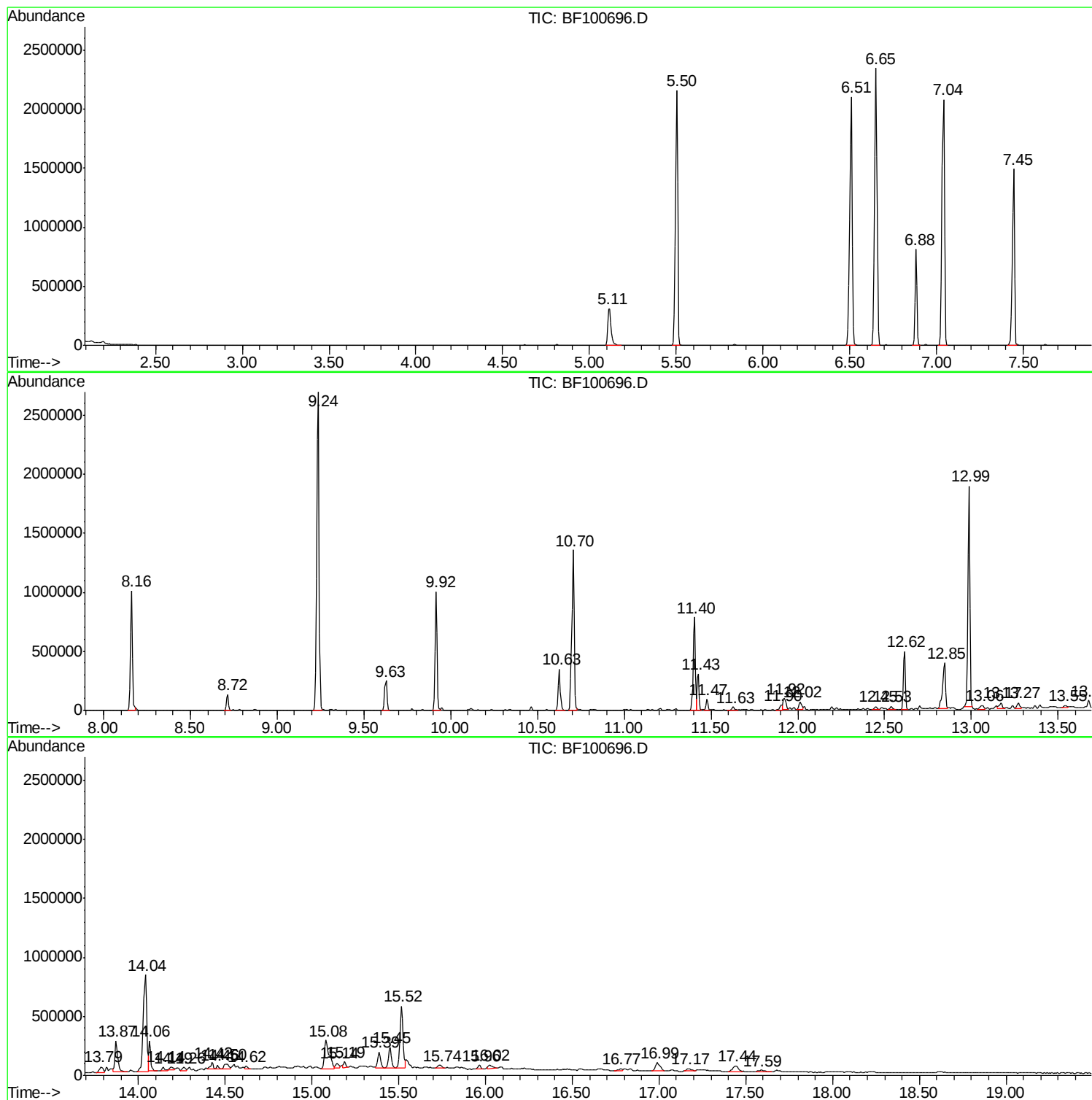
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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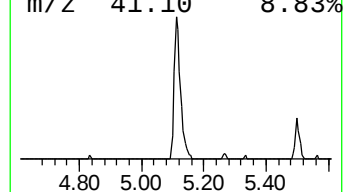
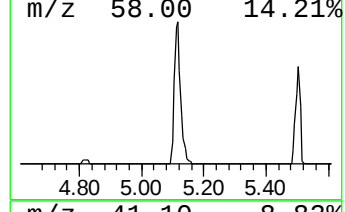
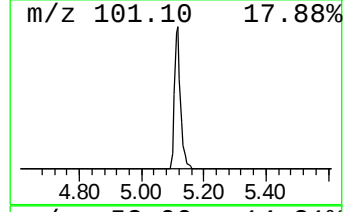
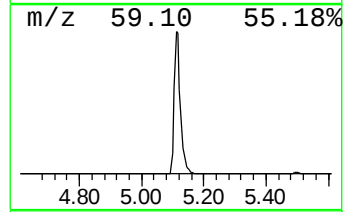
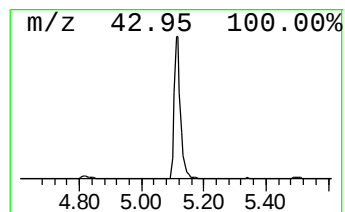
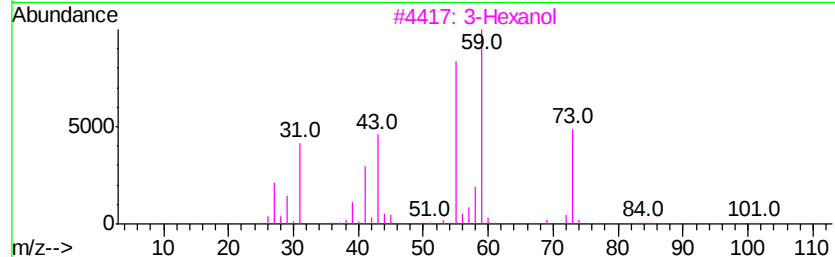
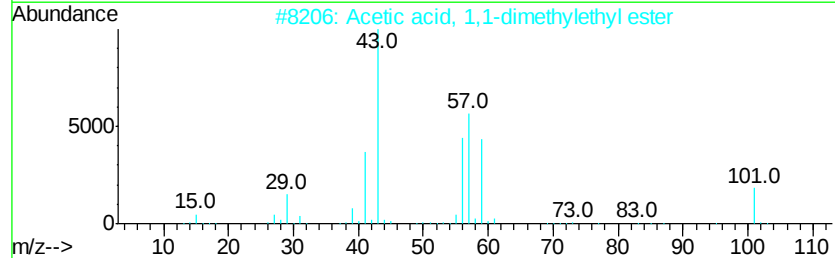
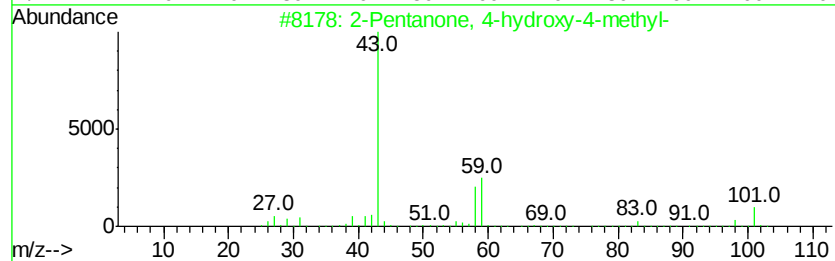
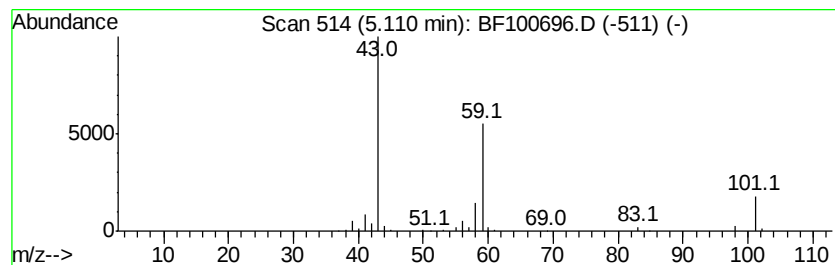
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	13.76 ng	437841	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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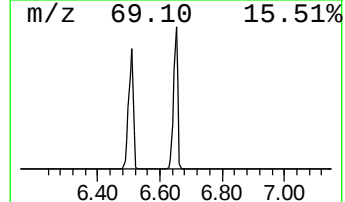
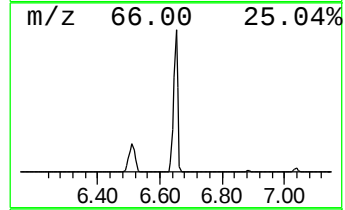
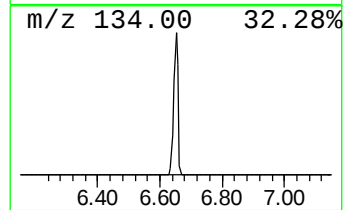
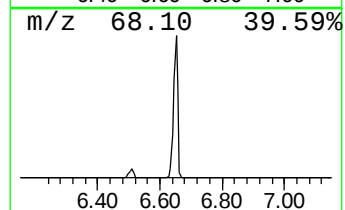
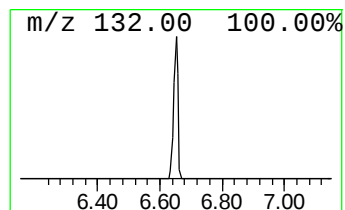
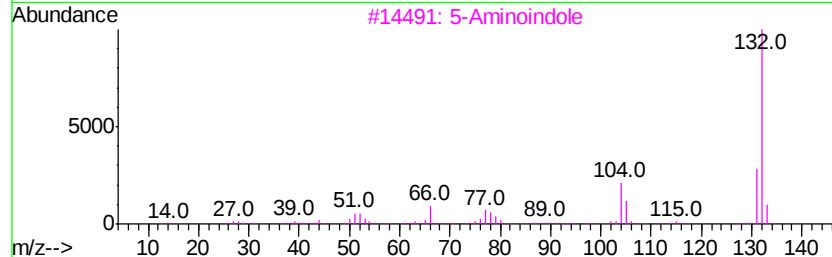
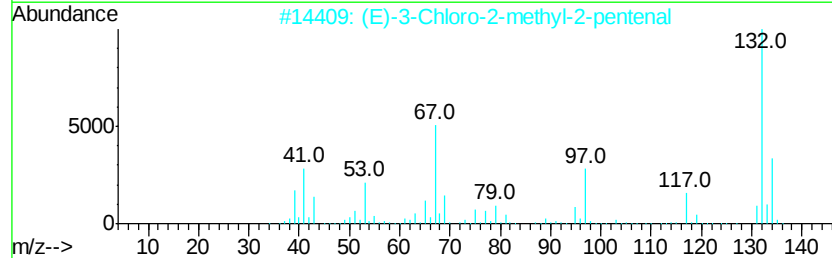
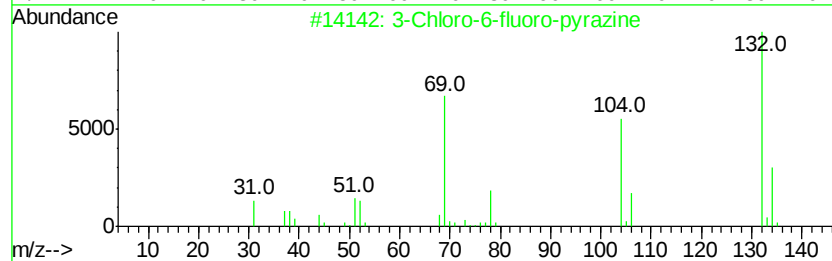
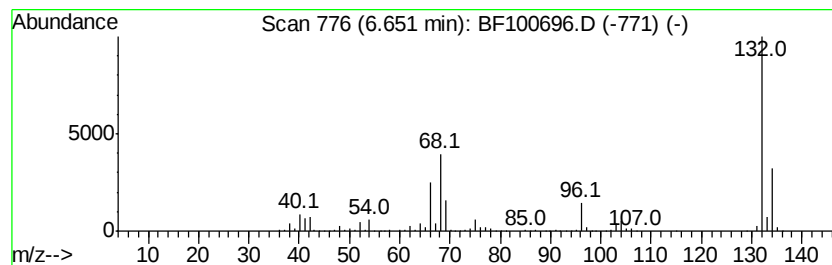
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	71.95 ng	2290000	1,4-Dichlorobenzene-d4	6.88

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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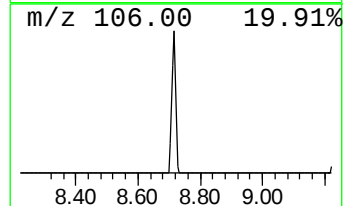
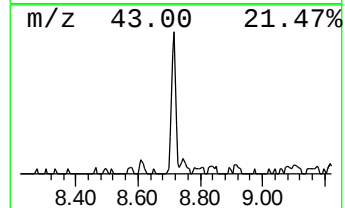
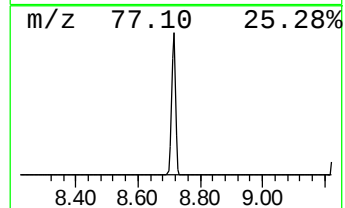
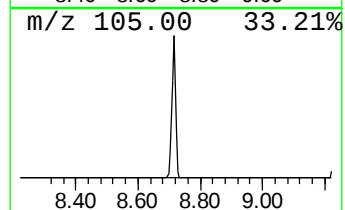
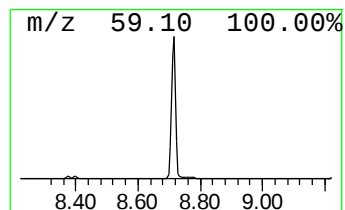
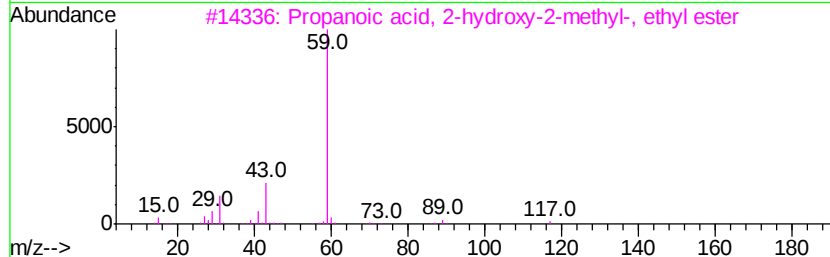
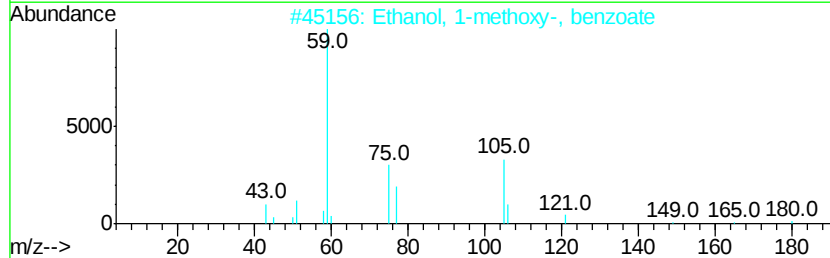
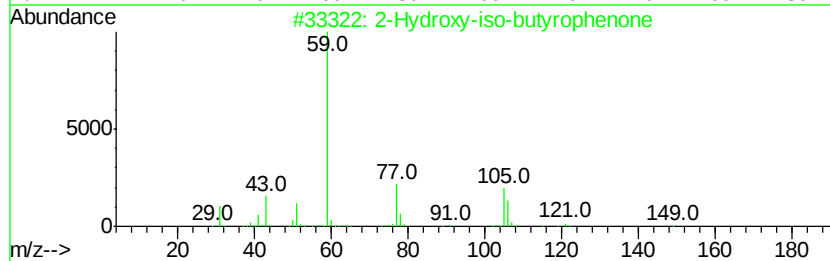
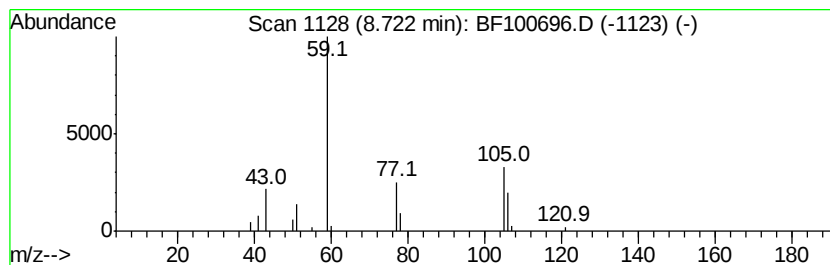
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.76 ng	114681	Napthalene-d8	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	86
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3		Propanoic acid, 2-hydroxy-2-methyl-, ethyl ester	132	C6H12O3	000080-55-7	9
4		Guanidine	59	CH5N3	000113-00-8	7
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5



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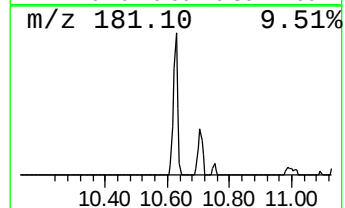
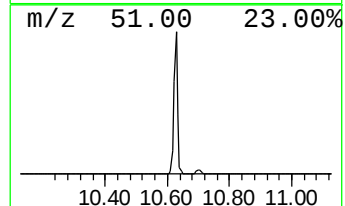
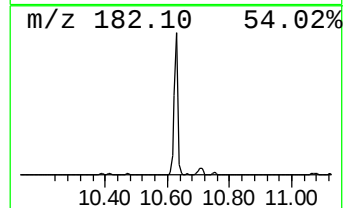
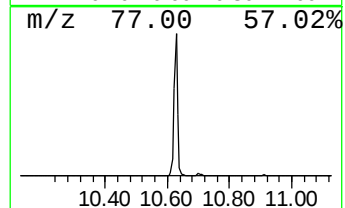
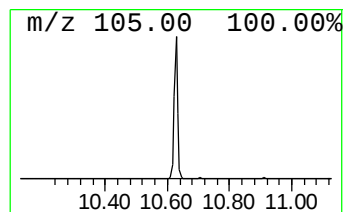
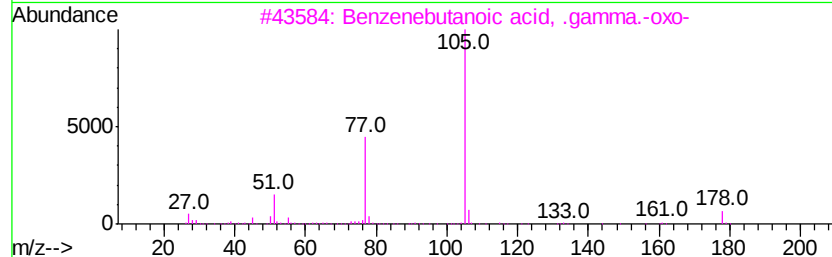
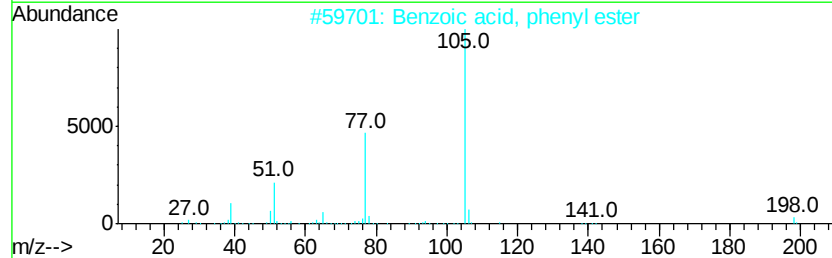
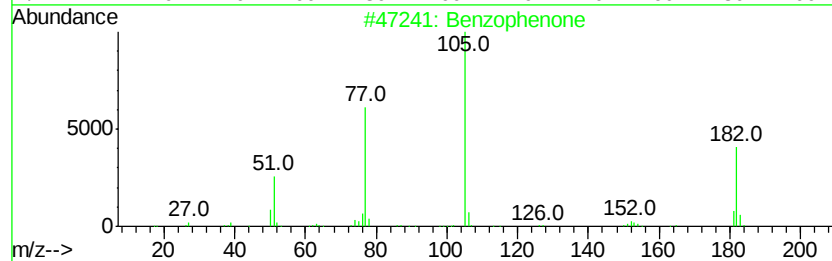
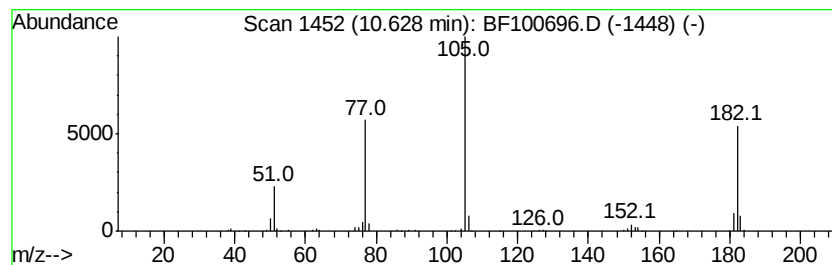
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	6.71 ng	280540	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		Benzoic acid, phenyl ester	198 C13H10O2	000093-99-2 47
3		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
4		1,2-Propanedione, 1-phenyl-	148 C9H8O2	000579-07-7 47
5		Vinyl benzoate	148 C9H8O2	000769-78-8 47



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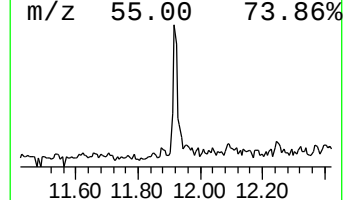
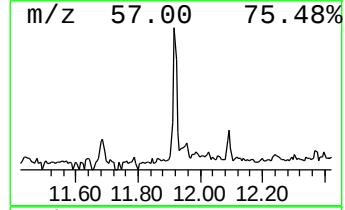
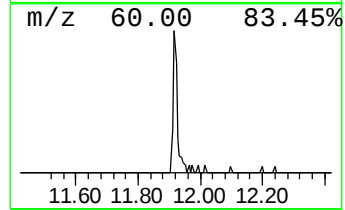
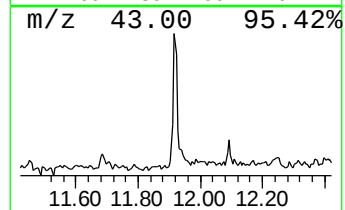
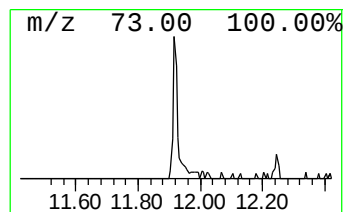
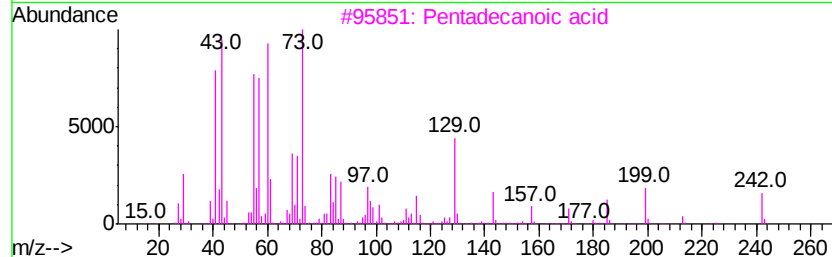
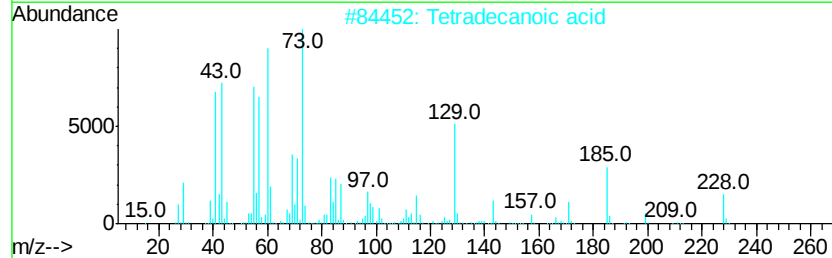
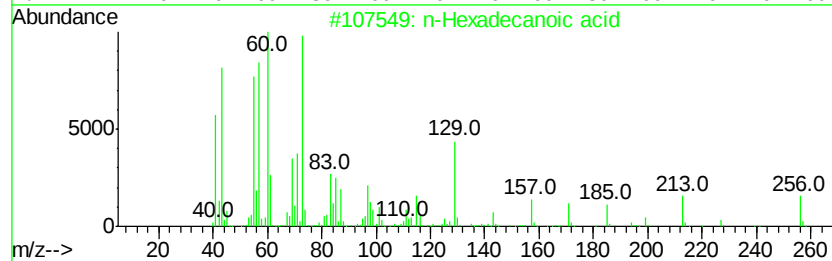
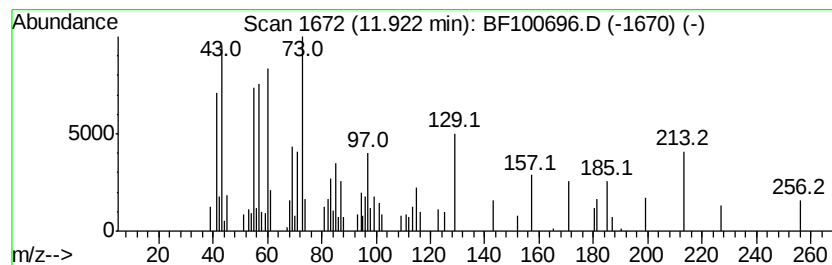
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.31 ng	116199	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	Dodecanoic acid	200	C12H24O2	000143-07-7	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111717\
Data File : BF100696.D
Acq On : 18 Nov 2017 1:31
Operator : SJ/JU
Sample : I6423-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B8(0-10)COMP

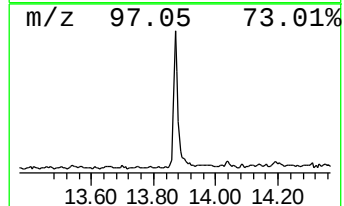
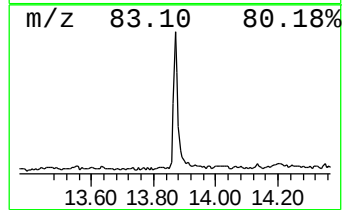
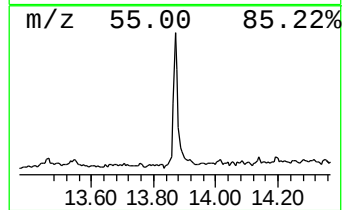
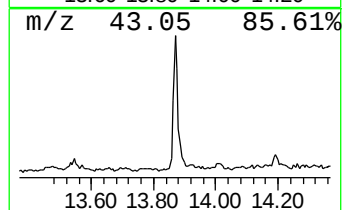
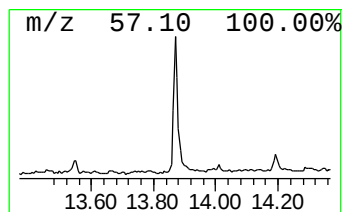
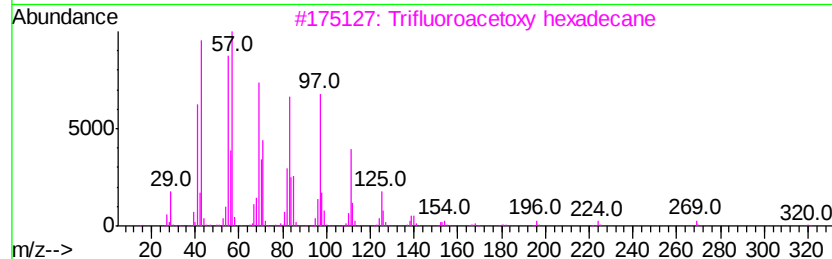
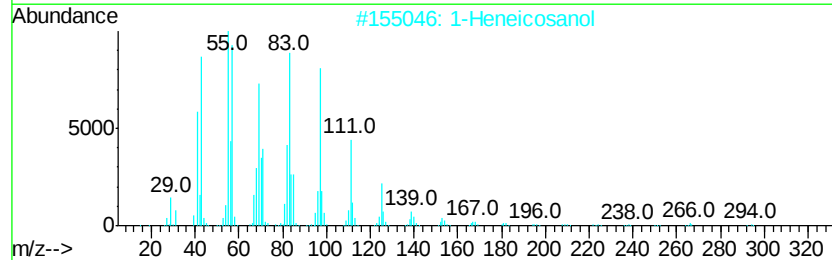
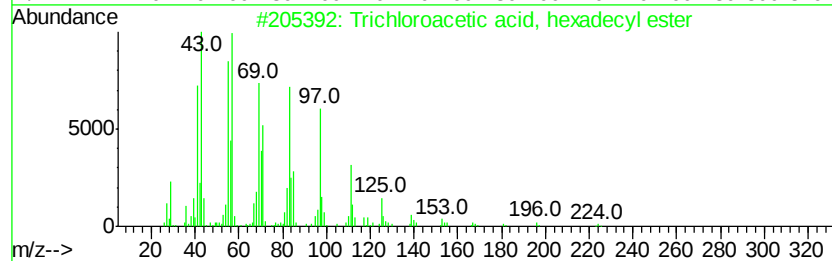
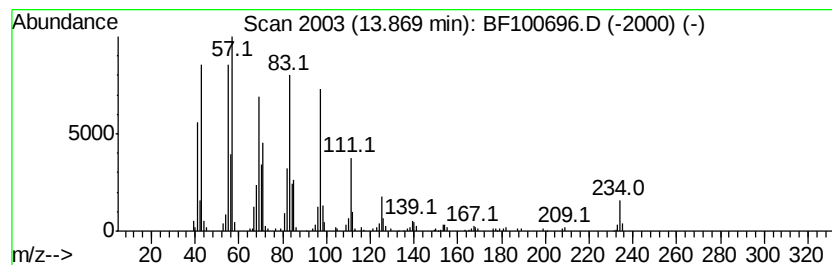
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.28 ng	322409	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5		Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
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Acq On : 18 Nov 2017 1:31
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Sample : I6423-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B8(0-10)COMP

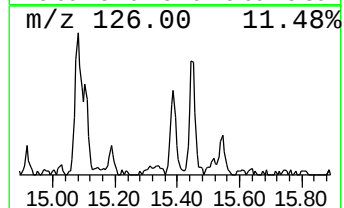
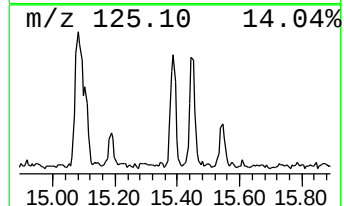
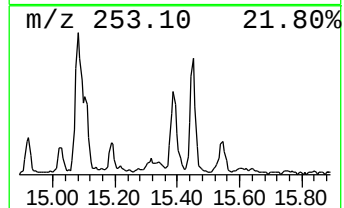
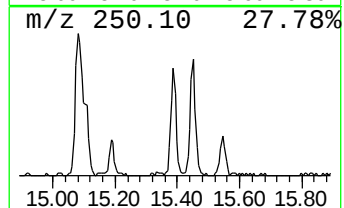
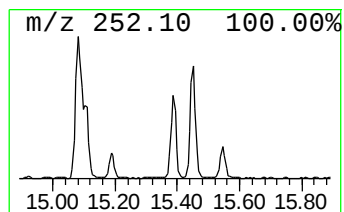
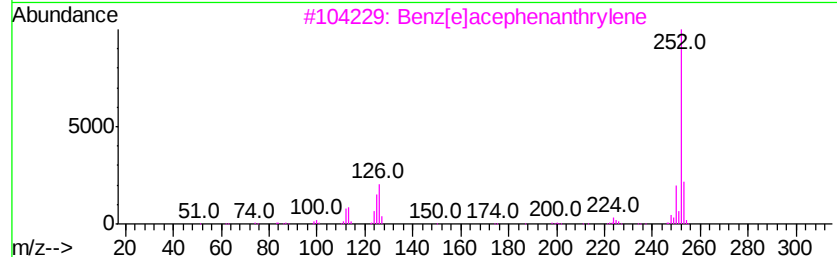
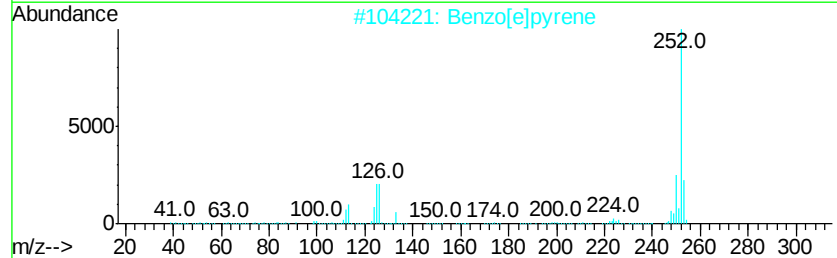
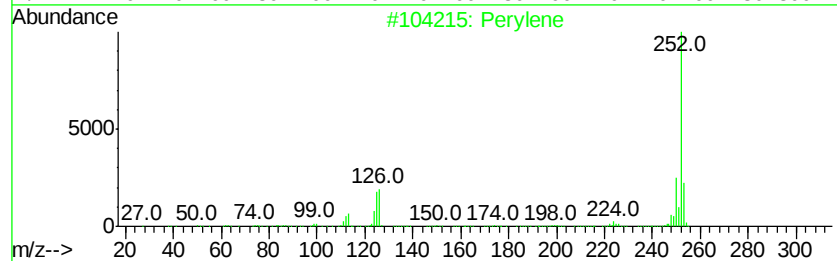
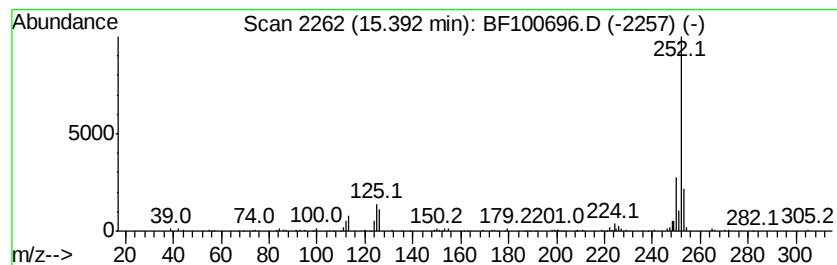
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	5.34 ng	181392	Perylene-d12	15.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Perylene	252	C20H12	000198-55-0	98
2		Benzo[el]pyrene	252	C20H12	000192-97-2	96
3		Benzo[el]acephenanthrylene	252	C20H12	000205-99-2	93
4		Benzo[al]pyrene	252	C20H12	000050-32-8	91
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111717\
Data File : BF100696.D
Acq On : 18 Nov 2017 1:31
Operator : SJ/JU
Sample : I6423-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B8(0-10)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
2-Pentanone, 4-hy...	5.11	13.8	ng	437841	1	6.88	636529	20.0
unknown6.65	6.65	72.0	ng	2290000	1	6.88	636529	20.0
2-Hydroxy-iso-but...	8.72	2.8	ng	114681	2	8.16	832054	20.0
Benzophenone	10.63	6.7	ng	280540	3	9.92	836704	20.0
n-Hexadecanoic acid	11.92	3.3	ng	116199	4	11.40	701810	20.0
Trichloroacetic a...	13.87	6.3	ng	322409	5	14.04	1027010	20.0
Perylene	15.39	5.3	ng	181392	6	15.52	679509	20.0