

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102117\
 Data File : BF099725.D
 Acq On : 21 Oct 2017 14:03
 Operator : SJ/JU
 Sample : I6017-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	5.034	498	501	518	rBV	196496	266959	15.66%	1.400%
2	5.440	566	570	593	rBV	1688558	1642896	96.35%	8.618%
3	6.457	739	743	761	rBV	1646458	1690721	99.15%	8.869%
4	6.587	761	765	768	rBV	1984222	1705187	100.00%	8.945%
5	6.810	800	803	811	rBV	597683	536347	31.45%	2.813%
6	6.969	826	830	846	rBV	1454397	1262027	74.01%	6.620%
7	7.381	896	900	903	rBV	1129883	1012573	59.38%	5.311%
8	8.092	1017	1021	1033	rVB	882239	741211	43.47%	3.888%
9	8.651	1113	1116	1119	rBV	108598	85799	5.03%	0.450%
10	9.169	1199	1204	1207	rBV	1935436	1687021	98.93%	8.849%
11	9.563	1268	1271	1276	rVB	89738	67466	3.96%	0.354%
12	9.710	1293	1296	1303	rBV	23539	21378	1.25%	0.112%
13	9.845	1315	1319	1323	rBV2	858110	791518	46.42%	4.152%
14	10.239	1382	1386	1388	rBV	17903	22419	1.31%	0.118%
15	10.563	1437	1441	1444	rBV	413745	360530	21.14%	1.891%
16	10.639	1450	1454	1465	rBV	1121516	1034641	60.68%	5.427%
17	11.333	1569	1572	1575	rBV	784004	750537	44.01%	3.937%
18	11.357	1575	1576	1581	rVB	223607	180582	10.59%	0.947%
19	11.416	1581	1586	1588	rBV	38401	33558	1.97%	0.176%
20	11.575	1609	1613	1617	rBV2	19729	24180	1.42%	0.127%
21	11.851	1654	1660	1661	rBV2	80119	98512	5.78%	0.517%
22	11.869	1661	1663	1668	rVB2	63789	60901	3.57%	0.319%
23	11.951	1673	1677	1679	rVV2	62072	65820	3.86%	0.345%
24	11.975	1679	1681	1686	rVB	26865	24159	1.42%	0.127%
25	12.133	1705	1708	1711	rBV	23815	21793	1.28%	0.114%
26	12.175	1711	1715	1718	rVB	29648	28380	1.66%	0.149%
27	12.386	1748	1751	1754	rBV	27562	25034	1.47%	0.131%
28	12.486	1763	1768	1771	rBV2	22279	25827	1.51%	0.135%
29	12.551	1775	1779	1783	rBV	483675	401716	23.56%	2.107%
30	12.633	1790	1793	1801	rVB3	45202	60327	3.54%	0.316%
31	12.763	1812	1815	1816	rBV	62149	61558	3.61%	0.323%
32	12.780	1816	1818	1824	rVV	383857	329399	19.32%	1.728%
33	12.833	1824	1827	1830	rVB	21160	21169	1.24%	0.111%
34	12.916	1836	1841	1844	rBV	1483673	1286886	75.47%	6.750%

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Filtering: 5
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 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	12.945	1844	1846	1851	rVB	18840	21923	1.29%	0.115%
36	13.004	1851	1856	1860	rBV3	26225	43389	2.54%	0.228%
37	13.086	1867	1870	1871	rBV2	22520	23282	1.37%	0.122%
38	13.110	1871	1874	1878	rVB	53303	52308	3.07%	0.274%
39	13.174	1882	1885	1888	rBV	32583	27856	1.63%	0.146%
40	13.216	1888	1892	1895	rBV2	36493	38932	2.28%	0.204%
41	13.339	1910	1913	1916	rBV2	25019	22504	1.32%	0.118%
42	13.627	1959	1962	1965	rVB	31483	29515	1.73%	0.155%
43	13.733	1974	1980	1982	rBV	44800	62052	3.64%	0.325%
44	13.751	1982	1983	1986	rVV	39292	30955	1.82%	0.162%
45	13.798	1986	1991	1995	rVV3	86580	130859	7.67%	0.686%
46	13.833	1995	1997	2002	rVB2	39149	51202	3.00%	0.269%
47	13.939	2012	2015	2017	rBV	27605	30079	1.76%	0.158%
48	13.980	2017	2022	2025	rVV2	620404	714603	41.91%	3.748%
49	14.004	2025	2026	2030	rVB	162209	116854	6.85%	0.613%
50	14.404	2091	2094	2095	rBV	21689	21914	1.29%	0.115%
51	15.015	2194	2198	2201	rBV	161019	222998	13.08%	1.170%
52	15.127	2215	2217	2221	rVB	35434	34455	2.02%	0.181%
53	15.315	2246	2249	2253	rBV	89576	113926	6.68%	0.598%
54	15.380	2257	2260	2265	rVV	126355	144782	8.49%	0.759%
55	15.439	2266	2270	2274	rVV	399577	486370	28.52%	2.551%
56	16.909	2516	2520	2530	rVB	72646	155995	9.15%	0.818%
57	17.362	2593	2597	2602	rVB	35576	58176	3.41%	0.305%

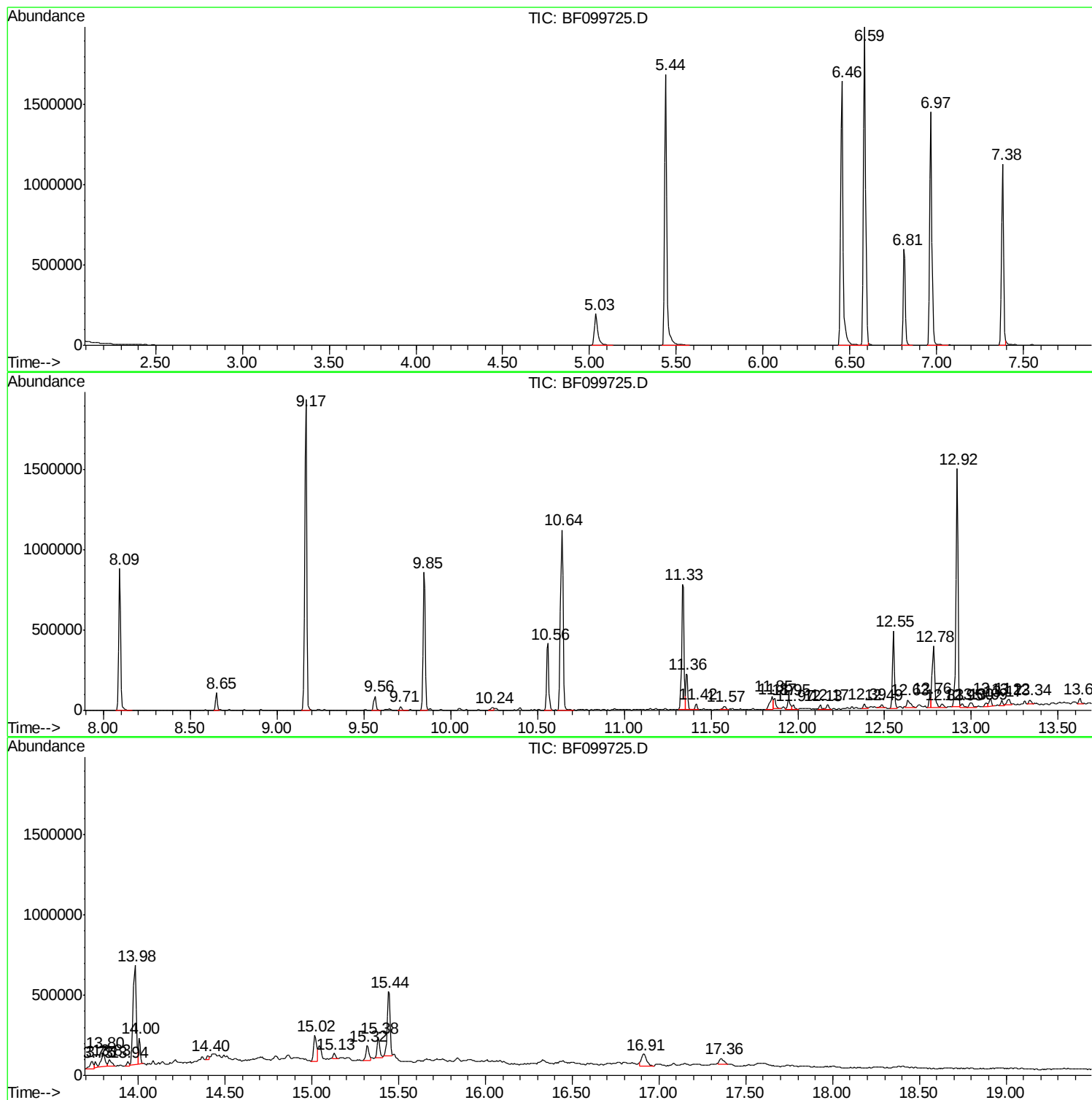
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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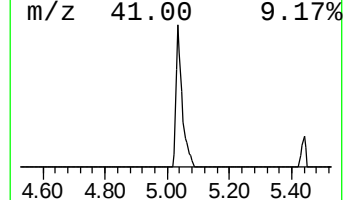
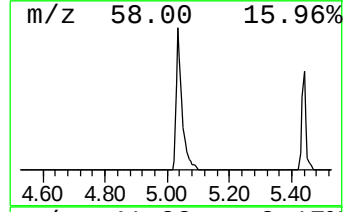
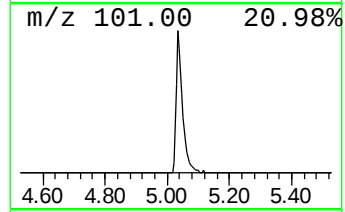
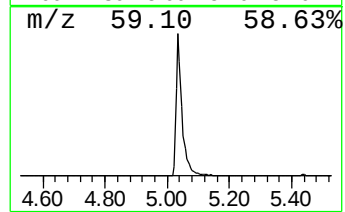
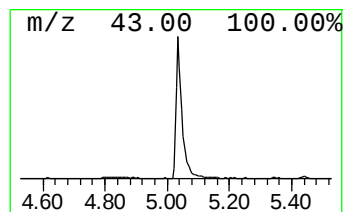
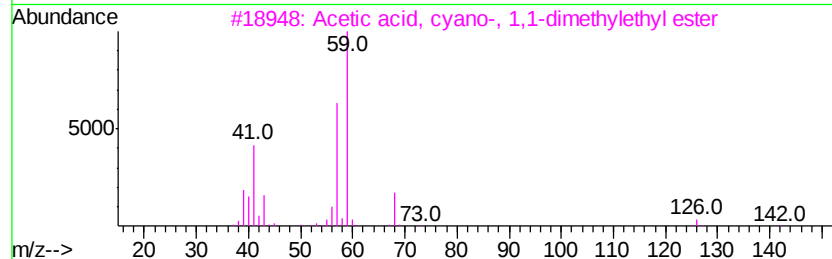
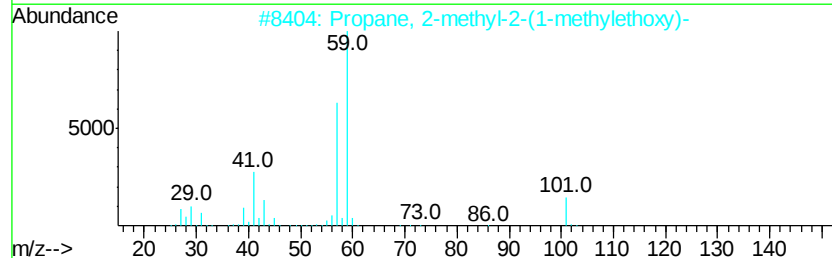
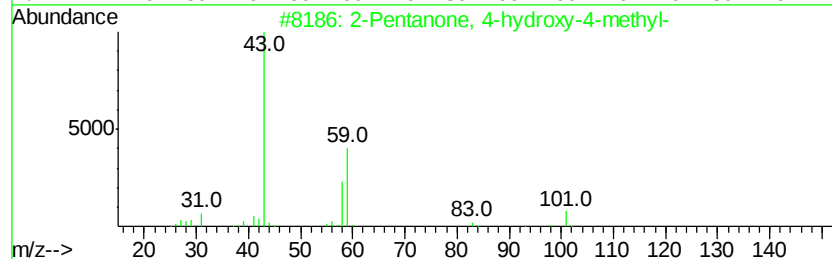
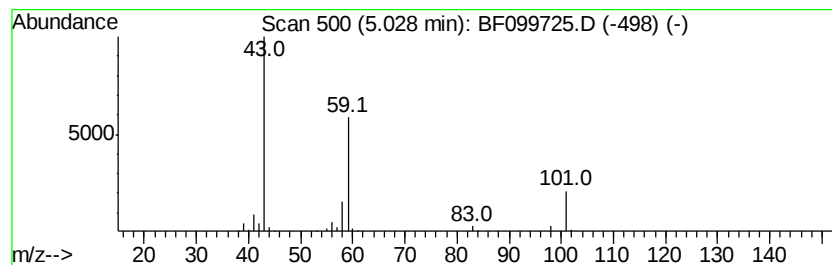
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.03	9.95 ng	266959	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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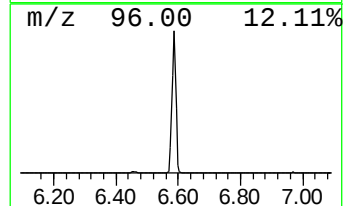
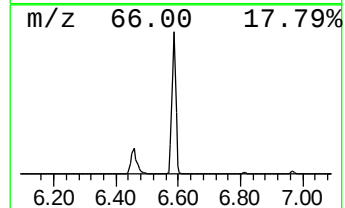
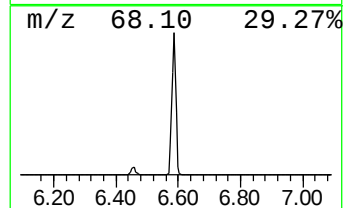
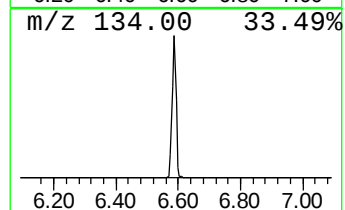
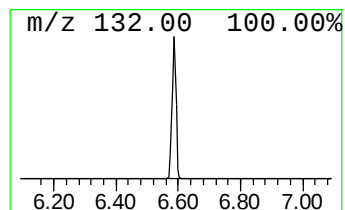
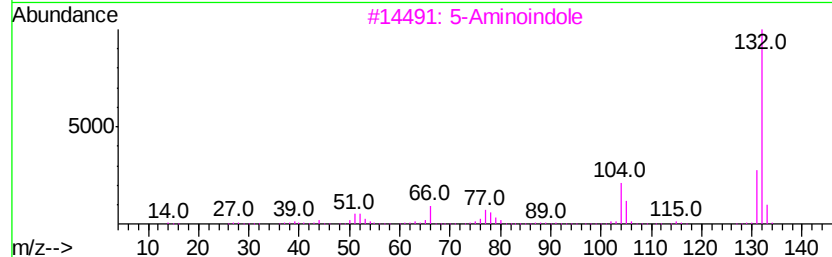
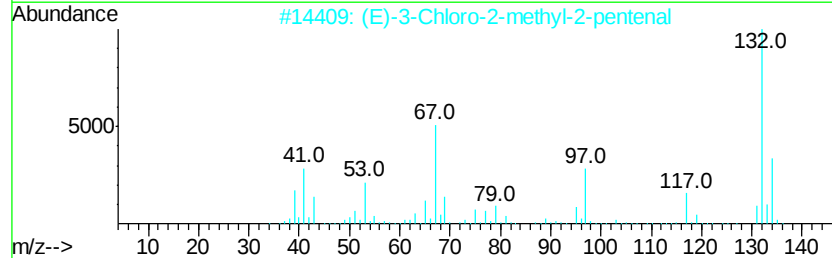
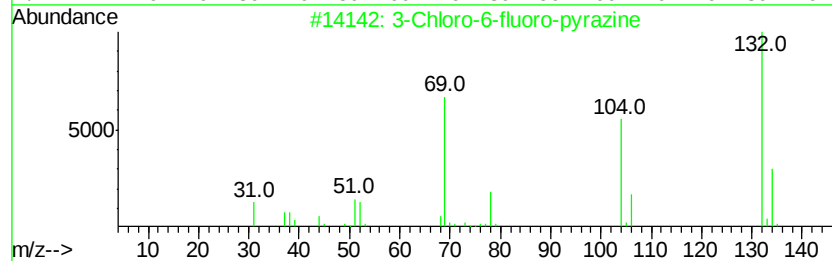
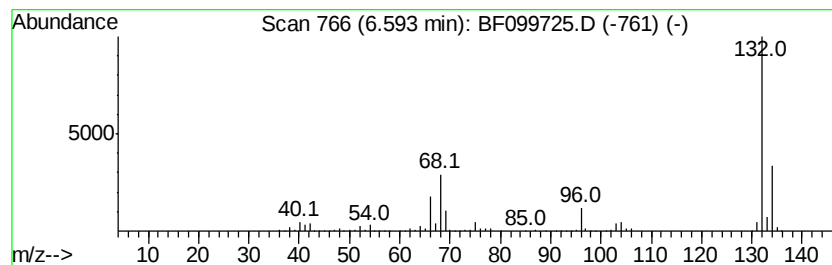
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	63.59 ng	1705190	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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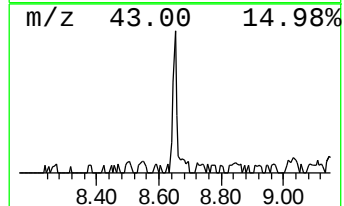
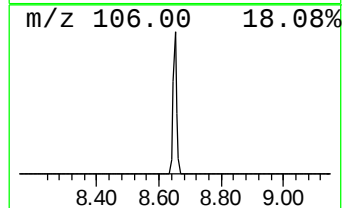
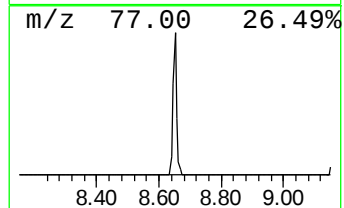
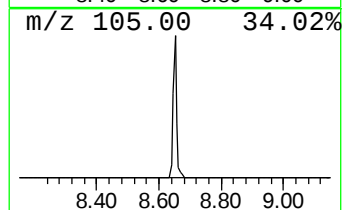
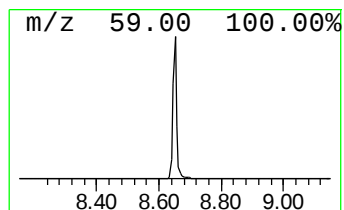
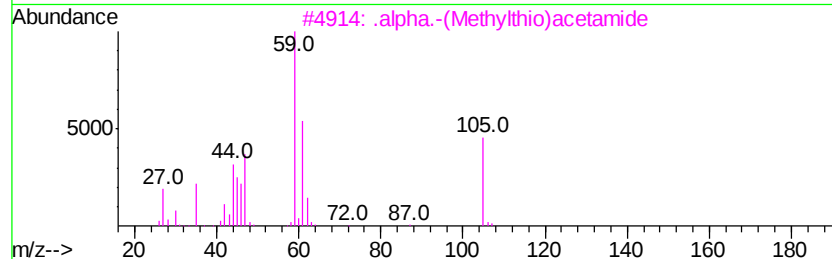
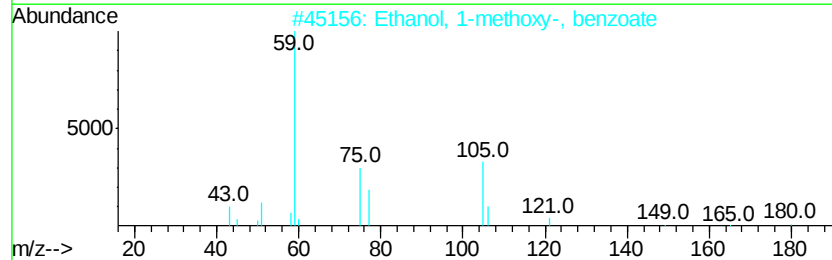
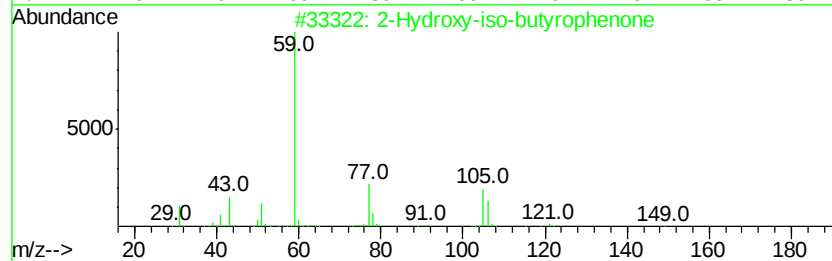
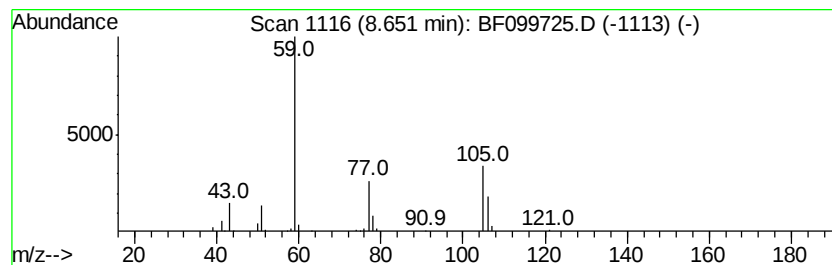
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	2.32 ng	85799	Napthalene-d8	8.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	78	
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64	
3	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7	
4	Guanidine	59	CH5N3	000113-00-8	7	
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5	



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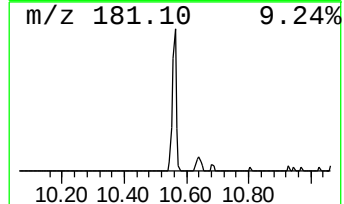
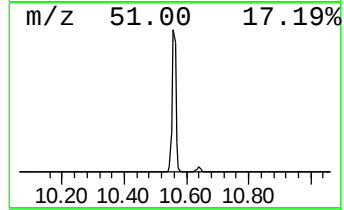
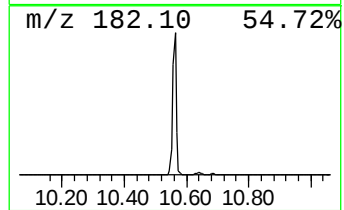
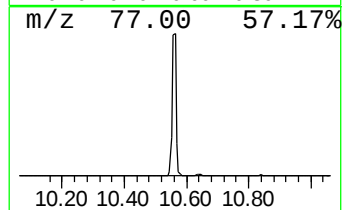
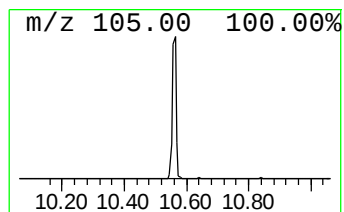
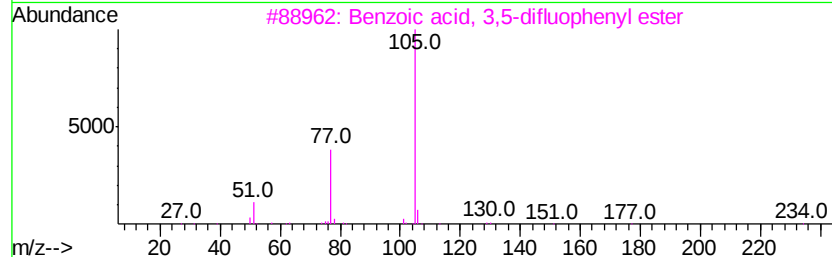
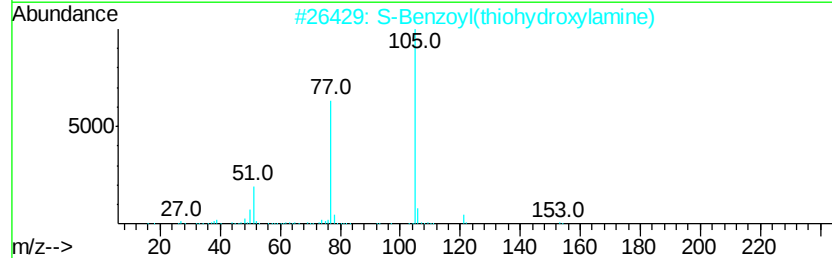
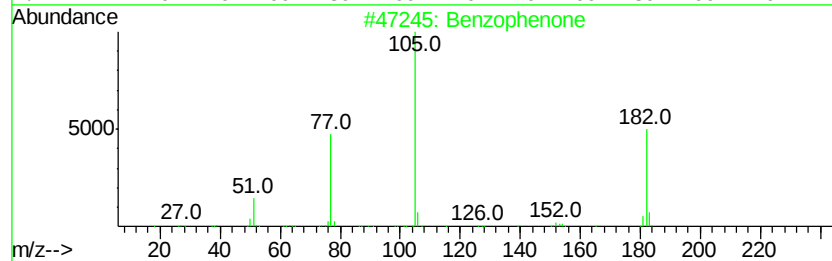
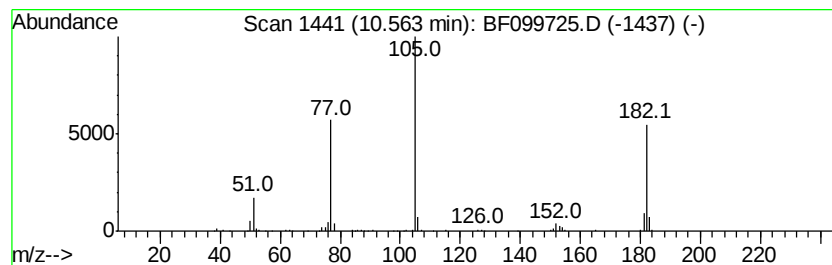
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.56	9.11 ng	360530	Acenaphthene-d10		9.85	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	43
3		Benzoic acid, 3,5-difluophenvl e...	234	C13H8F2O2	1000357-79-5	43
4		Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	43
5		.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	43



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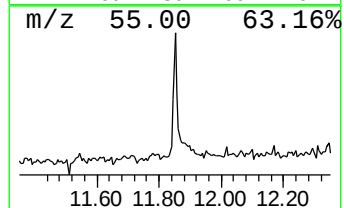
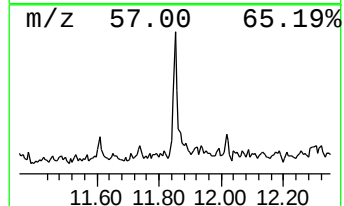
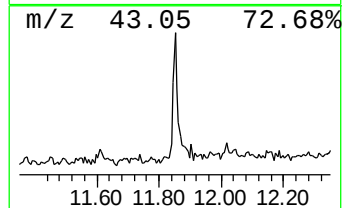
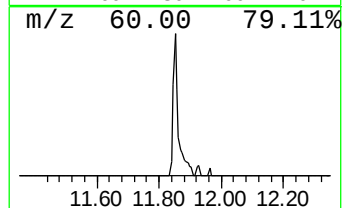
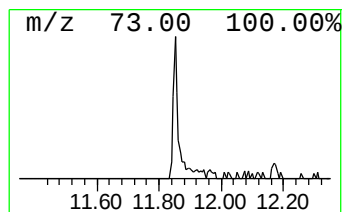
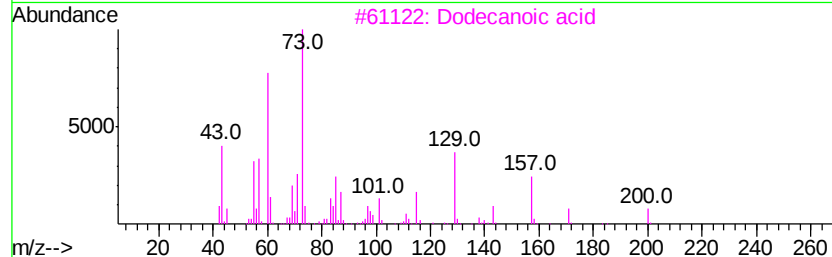
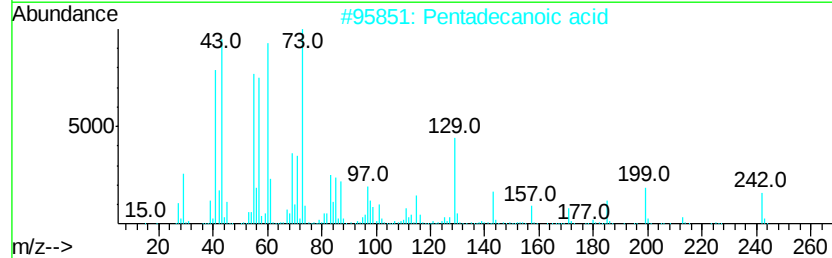
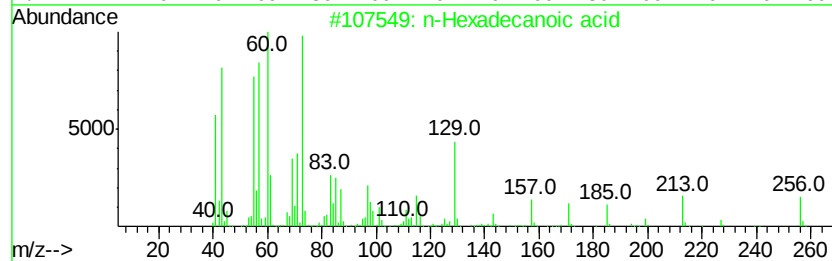
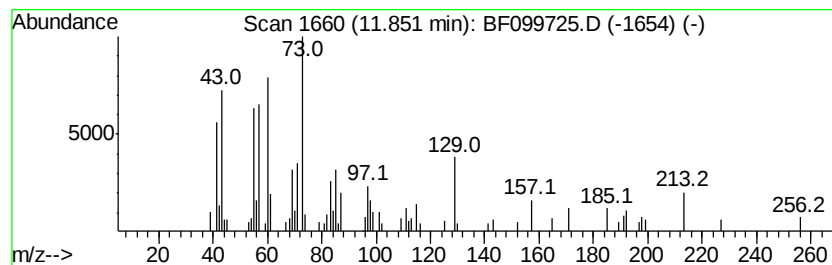
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.85	2.63 ng	98512	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		Dodecanoic acid	200	C12H24O2	000143-07-7	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102117\
Data File : BF099725.D
Acq On : 21 Oct 2017 14:03
Operator : SJ/JU
Sample : I6017-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

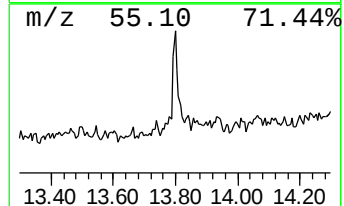
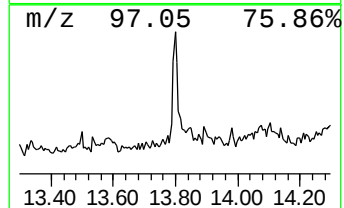
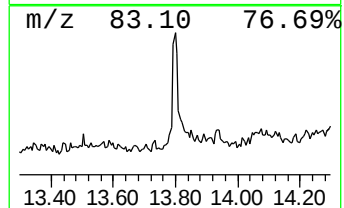
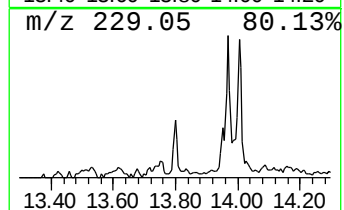
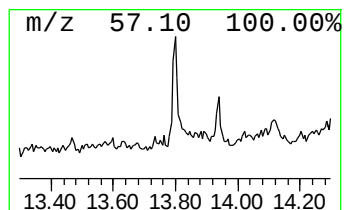
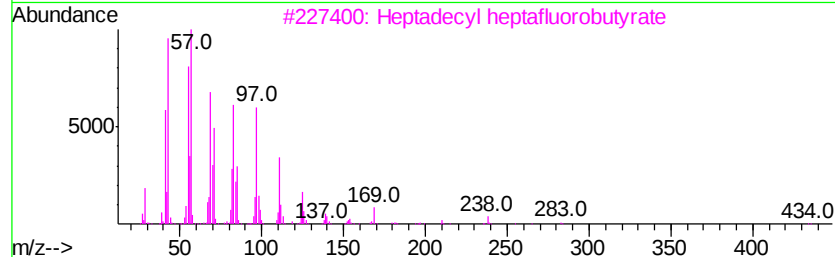
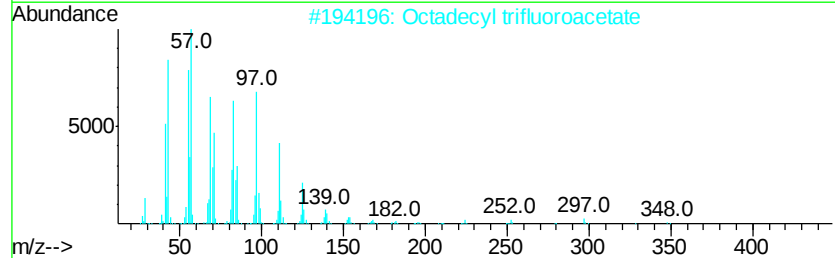
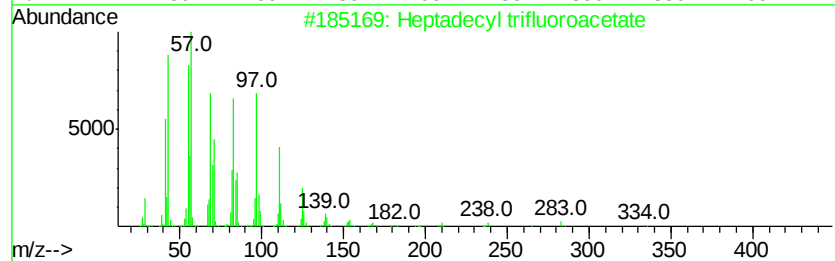
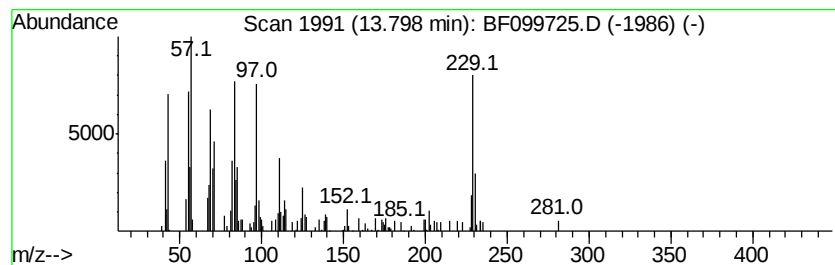
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.66 ng	130859	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92
3		Heptadecyl heptafluorobutrate	452	C21H35F7O2	959085-66-6	86
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	86
5		Octacosanol	410	C28H58O	000557-61-9	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102117\
Data File : BF099725.D
Acq On : 21 Oct 2017 14:03
Operator : SJ/JU
Sample : I6017-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

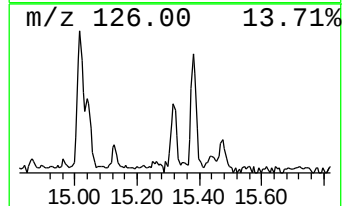
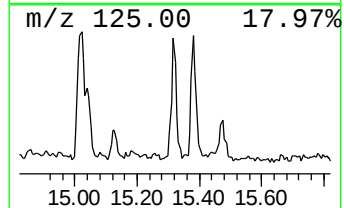
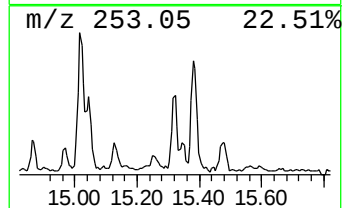
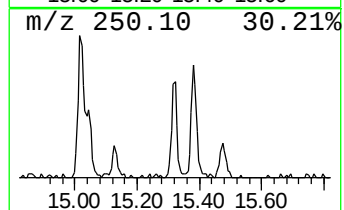
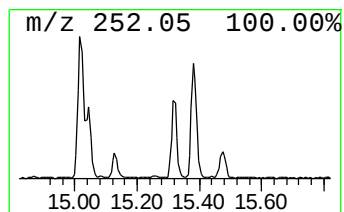
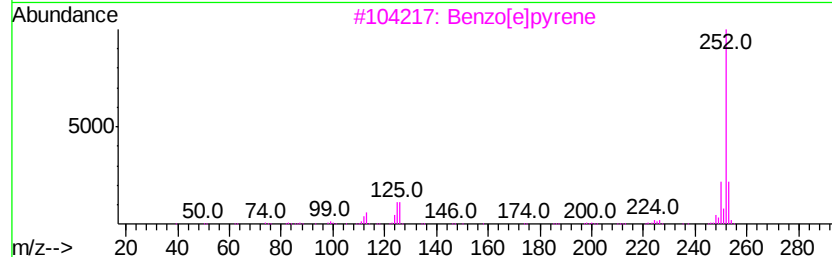
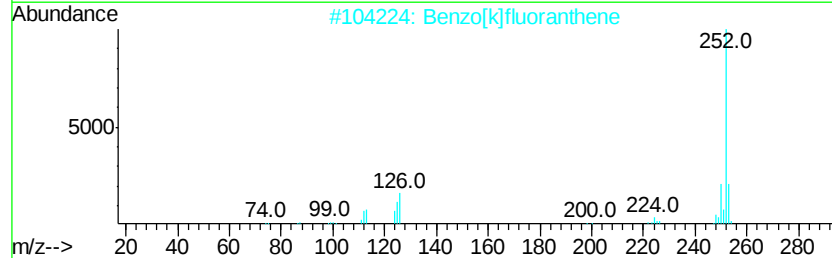
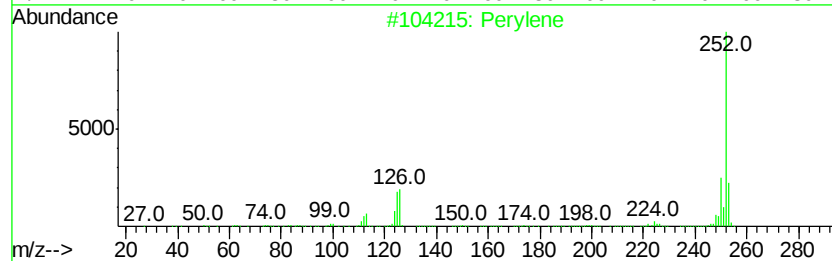
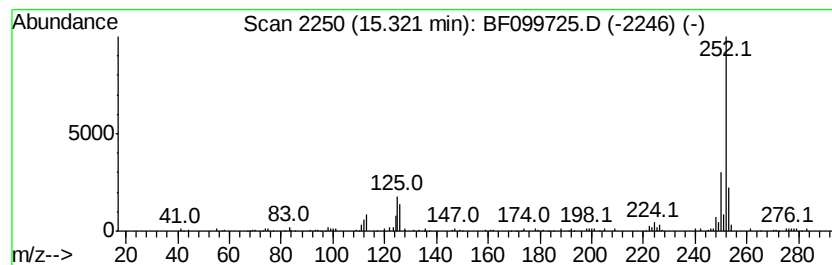
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	4.68 ng	113926	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Perylene	252	C20H12	000198-55-0	98
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3		Benzo[e]pyrene	252	C20H12	000192-97-2	96
4		Benzo[i]fluoranthene	252	C20H12	000205-82-3	93
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102117\
Data File : BF099725.D
Acq On : 21 Oct 2017 14:03
Operator : SJ/JU
Sample : I6017-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.03	9.9 ng		266959	1	6.81	536347	20.0
unknown6.59	6.59	63.6 ng		1705190	1	6.81	536347	20.0
2-Hydroxy-iso-but...	8.65	2.3 ng		85799	2	8.09	741211	20.0
Benzophenone	10.56	9.1 ng		360530	3	9.85	791518	20.0
n-Hexadecanoic acid	11.85	2.6 ng		98512	4	11.33	750537	20.0
Heptadecyl triflu...	13.80	3.7 ng		130859	5	13.98	714603	20.0
Perylene	15.32	4.7 ng		113926	6	15.44	486370	20.0