

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
 Data File : BF101348.D
 Acq On : 12 Dec 2017 23:35
 Operator : SJ/JU
 Sample : I6814-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHMHC-WC1

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-BF113017.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	5.040	499	502	518	rBB	42505	57036	6.22%	0.563%
2	5.446	567	571	584	rBV	842325	845488	92.24%	8.340%
3	6.463	739	744	758	rBV	901533	907180	98.97%	8.949%
4	6.592	762	766	770	rVV	1045648	916617	100.00%	9.042%
5	6.645	772	775	781	rVB3	12591	16746	1.83%	0.165%
6	6.822	802	805	812	rBB	291580	228732	24.95%	2.256%
7	6.975	828	831	835	rBV	738413	680584	74.25%	6.714%
8	7.387	897	901	915	rBV	552937	530986	57.93%	5.238%
9	8.104	1020	1023	1026	rBV	345246	288032	31.42%	2.841%
10	9.181	1202	1206	1209	rBV	1071772	911119	99.40%	8.988%
11	9.575	1270	1273	1280	rVB2	66855	69571	7.59%	0.686%
12	9.722	1295	1298	1303	rBV	48392	40738	4.44%	0.402%
13	9.781	1306	1308	1311	rVB	22731	15809	1.72%	0.156%
14	9.863	1318	1322	1325	rBV	346752	290268	31.67%	2.863%
15	9.892	1325	1327	1330	rVB	16187	13691	1.49%	0.135%
16	10.280	1390	1393	1396	rVB	26489	20603	2.25%	0.203%
17	10.410	1413	1415	1420	rVB	13663	13517	1.47%	0.133%
18	10.657	1453	1457	1466	rVB	591363	510668	55.71%	5.038%
19	10.757	1471	1474	1475	rBV	22959	24668	2.69%	0.243%
20	10.828	1483	1486	1488	rBV	29114	25070	2.74%	0.247%
21	10.857	1488	1491	1495	rVV2	26921	37423	4.08%	0.369%
22	10.892	1495	1497	1500	rVV	28447	27427	2.99%	0.271%
23	10.963	1504	1509	1513	rVV3	12790	27189	2.97%	0.268%
24	11.004	1513	1516	1520	rVB2	20065	24106	2.63%	0.238%
25	11.045	1520	1523	1525	rBV	29027	26659	2.91%	0.263%
26	11.086	1525	1530	1532	rVB3	13656	15728	1.72%	0.155%
27	11.163	1538	1543	1547	rBV2	9902	12534	1.37%	0.124%
28	11.204	1547	1550	1552	rBV	22698	19340	2.11%	0.191%
29	11.351	1572	1575	1578	rBV	309324	285440	31.14%	2.816%
30	11.380	1578	1580	1584	rVV	112540	93672	10.22%	0.924%
31	11.427	1586	1588	1591	rBV	35435	30780	3.36%	0.304%
32	11.586	1611	1615	1619	rBV3	10556	15846	1.73%	0.156%
33	11.627	1619	1622	1627	rVB2	18612	22378	2.44%	0.221%
34	11.857	1656	1661	1664	rBV	19523	29564	3.23%	0.292%

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 Integrator: RTE
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 Sampling : 1
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Filtering: 5
 Min Area: 3 % of largest Peak
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.886	1664	1666	1669	rVB	26867	21841	2.38%	0.215%
36	11.933	1669	1674	1677	rBV2	15398	17455	1.90%	0.172%
37	11.969	1677	1680	1683	rVV	34243	38827	4.24%	0.383%
38	11.992	1683	1684	1687	rVB	16257	10326	1.13%	0.102%
39	12.039	1689	1692	1695	rBV2	17599	15677	1.71%	0.155%
40	12.151	1708	1711	1714	rVB	23186	18335	2.00%	0.181%
41	12.404	1752	1754	1756	rBV	21479	17292	1.89%	0.171%
42	12.504	1767	1771	1773	rBV3	19484	23539	2.57%	0.232%
43	12.574	1779	1783	1786	rBV	184353	171722	18.73%	1.694%
44	12.669	1796	1799	1801	rBV	19742	16759	1.83%	0.165%
45	12.722	1804	1808	1810	rVV5	12337	15097	1.65%	0.149%
46	12.751	1810	1813	1815	rVB3	11667	11724	1.28%	0.116%
47	12.804	1815	1822	1827	rBV	223564	242890	26.50%	2.396%
48	12.851	1828	1830	1834	rVB2	15831	15544	1.70%	0.153%
49	12.939	1841	1845	1848	rVV	820282	680428	74.23%	6.712%
50	12.963	1848	1849	1854	rVB2	13854	11967	1.31%	0.118%
51	13.021	1854	1859	1864	rBV3	24787	45834	5.00%	0.452%
52	13.127	1871	1877	1880	rBV2	31414	51344	5.60%	0.506%
53	13.198	1886	1889	1892	rBV	21223	17024	1.86%	0.168%
54	13.233	1892	1895	1899	rBV2	29577	37220	4.06%	0.367%
55	13.327	1908	1911	1914	rVB2	26795	25047	2.73%	0.247%
56	13.357	1914	1916	1922	rVB2	24288	26316	2.87%	0.260%
57	13.498	1936	1940	1944	rBV6	19810	30224	3.30%	0.298%
58	13.616	1958	1960	1963	rBV4	8654	11163	1.22%	0.110%
59	13.645	1963	1965	1968	rVB2	25529	22188	2.42%	0.219%
60	13.704	1973	1975	1978	rBV3	8897	10983	1.20%	0.108%
61	13.757	1981	1984	1986	rBB	12869	12258	1.34%	0.121%
62	13.780	1986	1988	1990	rVB	22318	15641	1.71%	0.154%
63	13.827	1993	1996	2000	rVB3	86307	82820	9.04%	0.817%
64	14.004	2021	2026	2029	rBV2	339295	405810	44.27%	4.003%
65	14.033	2029	2031	2033	rVB	90483	72511	7.91%	0.715%
66	14.110	2042	2044	2046	rBV	16675	14069	1.53%	0.139%
67	14.357	2084	2086	2087	rBV2	18353	13641	1.49%	0.135%
68	14.392	2090	2092	2095	rVB	32248	28994	3.16%	0.286%
69	14.427	2096	2098	2100	rBV	18233	14850	1.62%	0.146%
70	15.051	2201	2204	2208	rBV	103742	156060	17.03%	1.539%
71	15.163	2220	2223	2226	rVB	34018	34985	3.82%	0.345%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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72	15.357	2253	2256	2261	rVB	85750	104378	11.39%	1.030%
73	15.421	2263	2267	2271	rBV	95517	113468	12.38%	1.119%
74	15.486	2274	2278	2281	rVB	146602	169306	18.47%	1.670%
75	16.974	2526	2531	2539	rVB2	56676	112694	12.29%	1.112%
76	17.157	2558	2562	2565	rBV5	23772	37803	4.12%	0.373%
77	17.433	2605	2609	2613	rVB	40414	65886	7.19%	0.650%

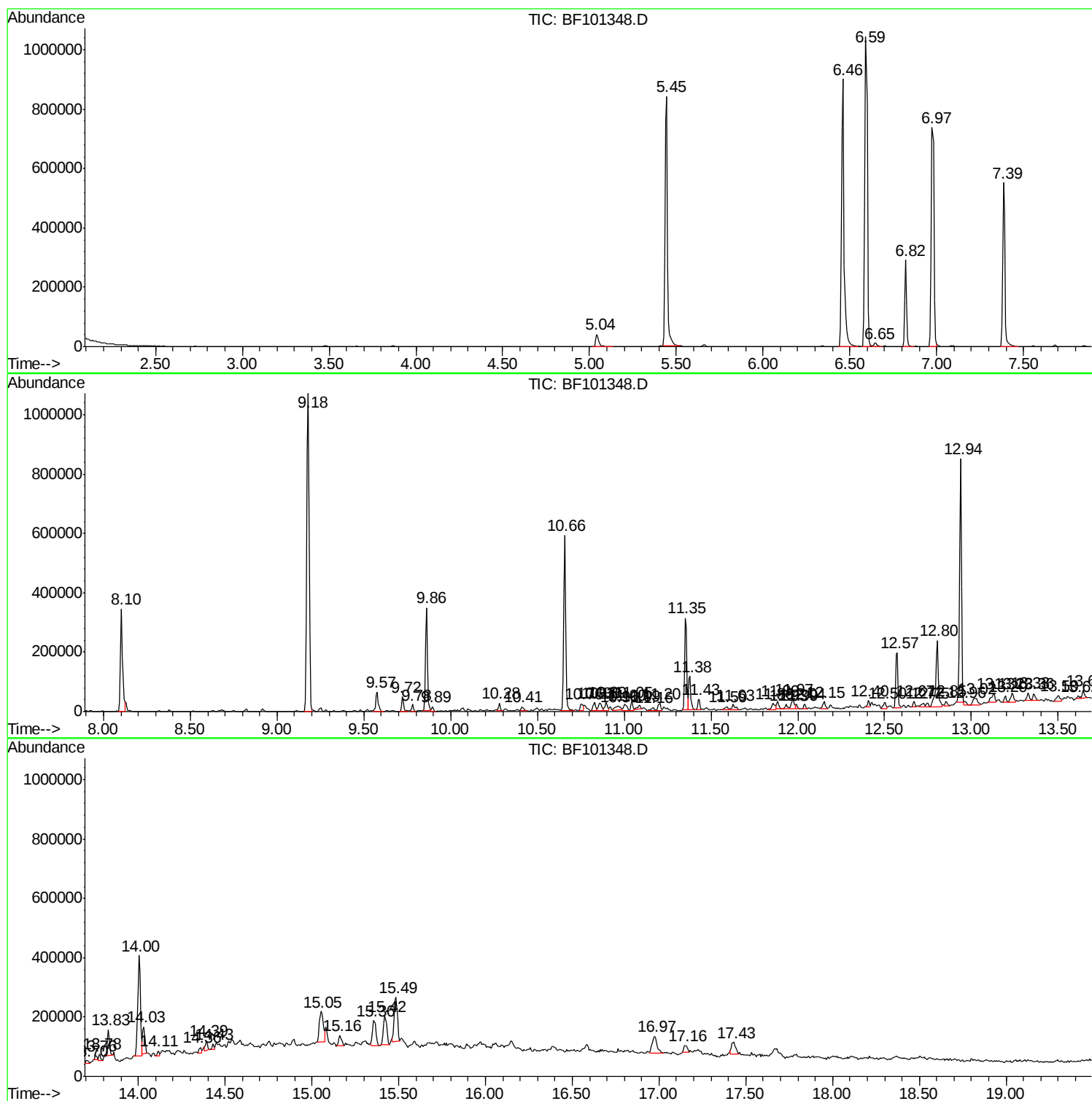
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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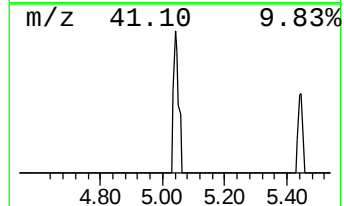
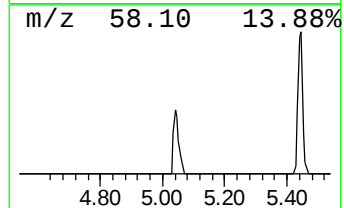
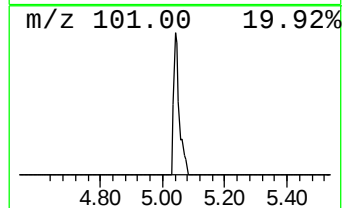
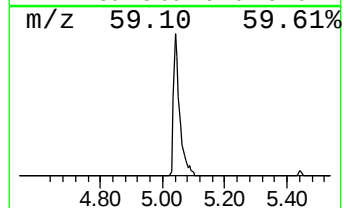
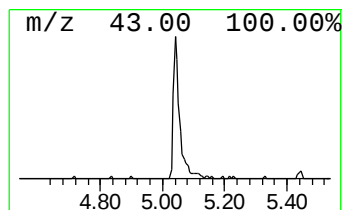
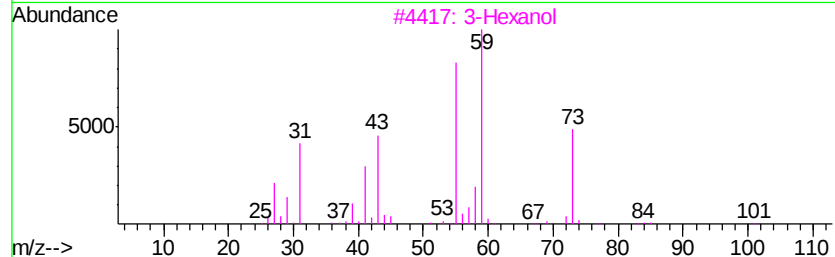
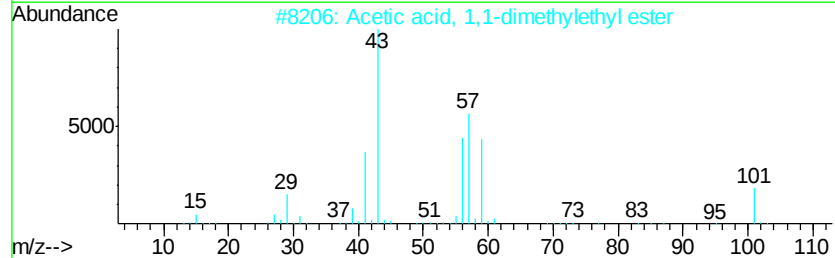
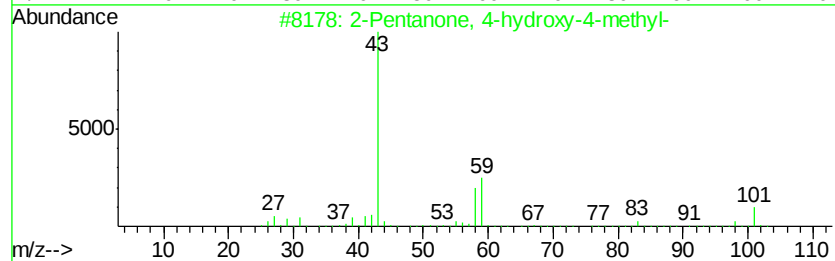
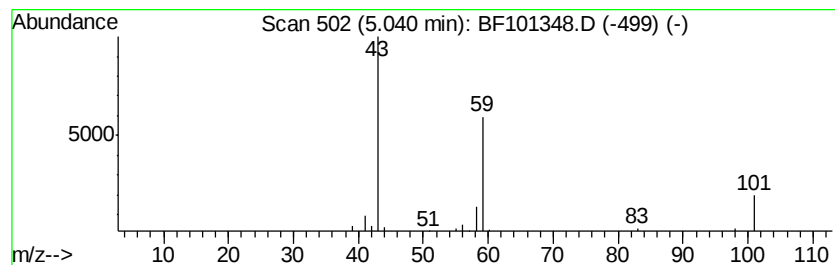
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.99 ng	57036	1,4-Dichlorobenzene-d4	6.82

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
3		3-Hexanol	102	C6H14O	000623-37-0	33
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23



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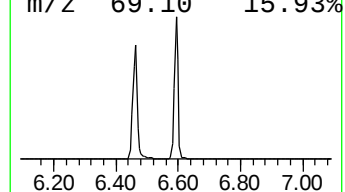
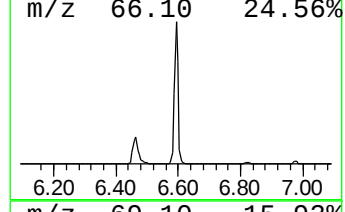
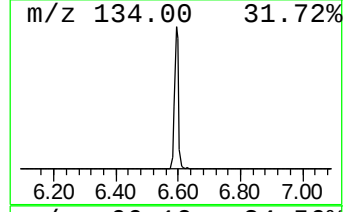
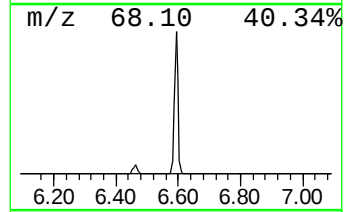
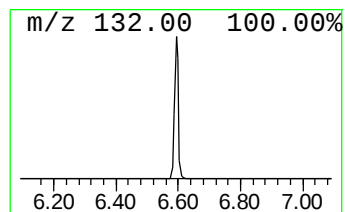
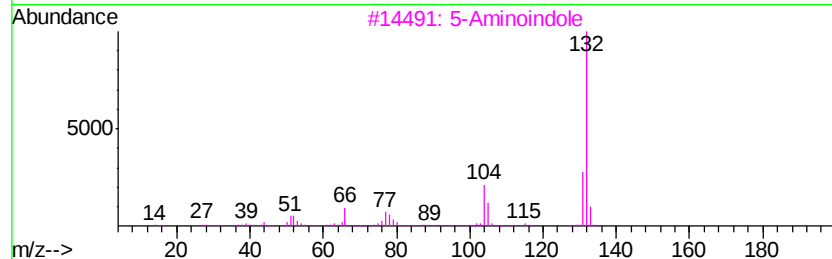
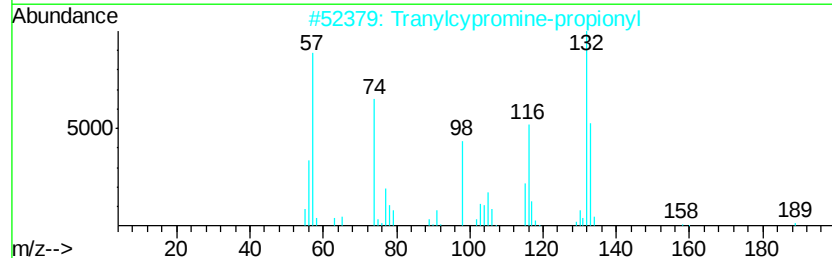
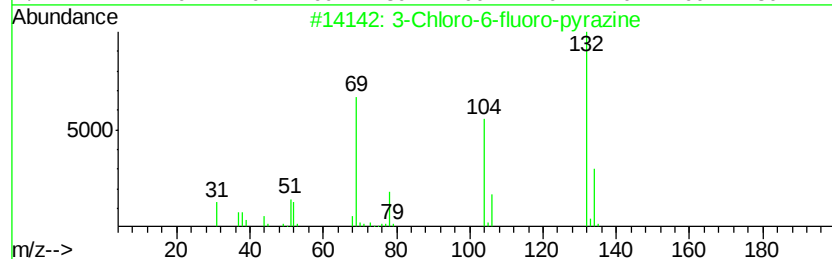
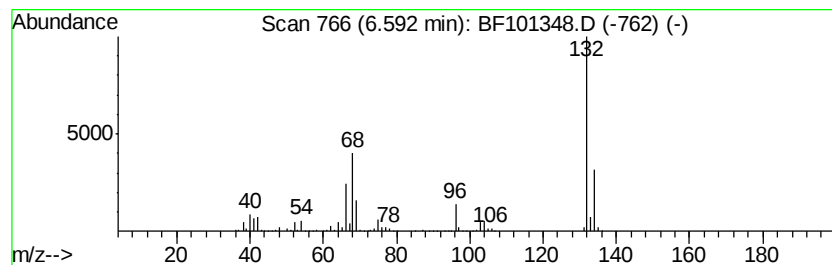
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	80.15 ng	916617	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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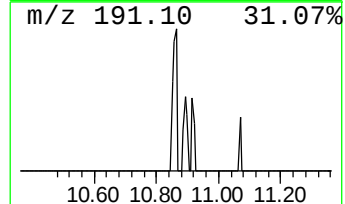
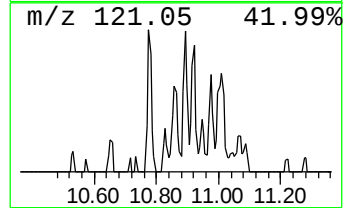
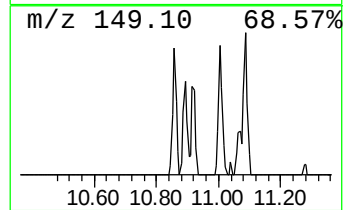
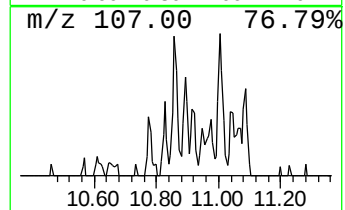
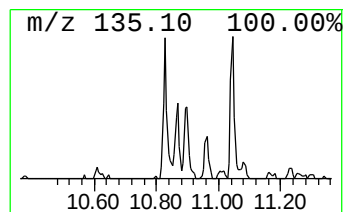
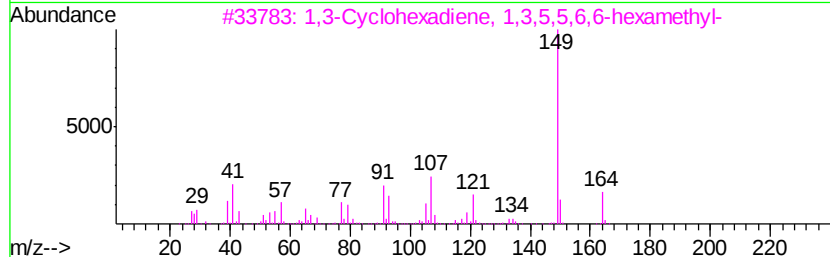
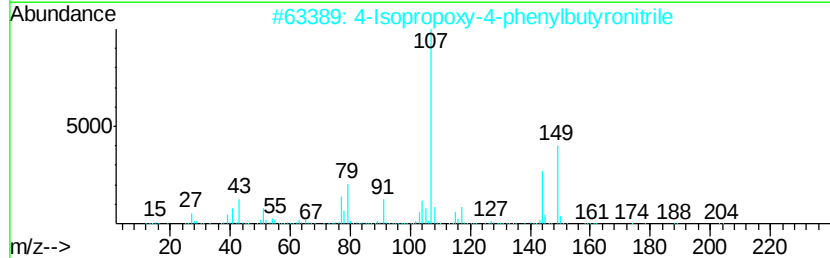
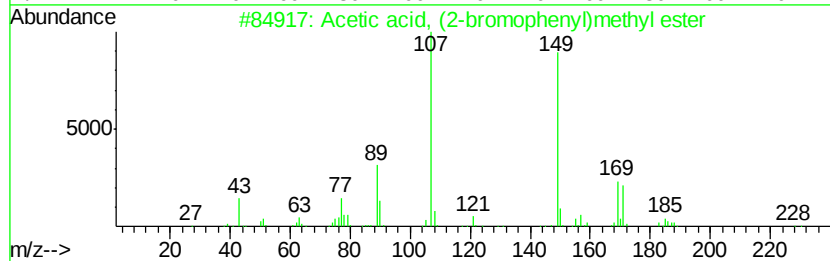
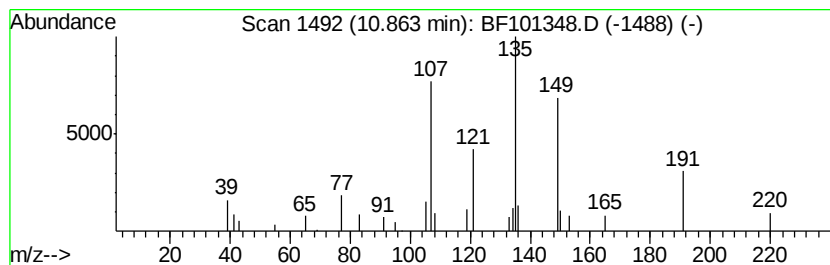
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.86 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.62 ng	37423	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, (2-bromophenyl)meth...	228	C9H9BrO2	1000368-71-4	45
2		4-Isopropoxy-4-phenylbutyronitrile	203	C13H17NO	1000370-35-3	42
3		1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	40
4		1H-Purin-6-amine, N-methyl-	149	C6H7N5	000443-72-1	35
5		Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	27



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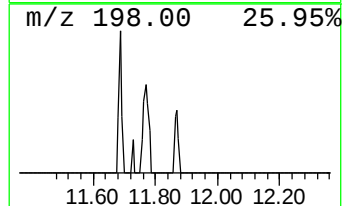
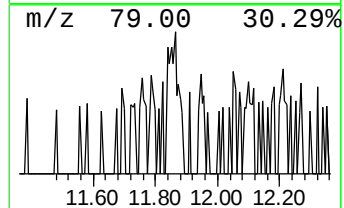
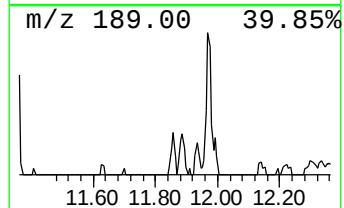
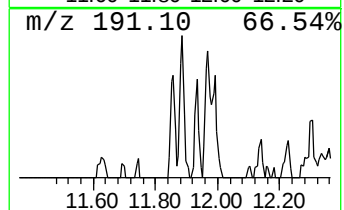
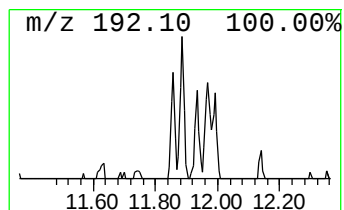
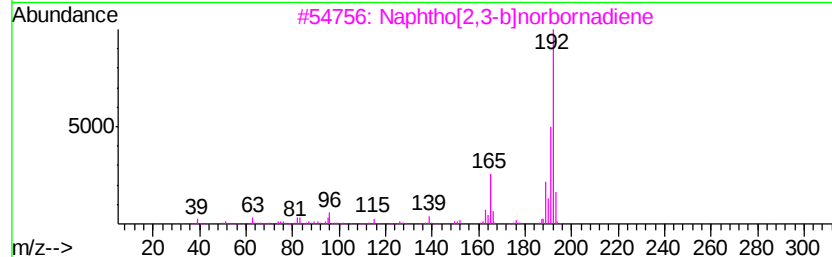
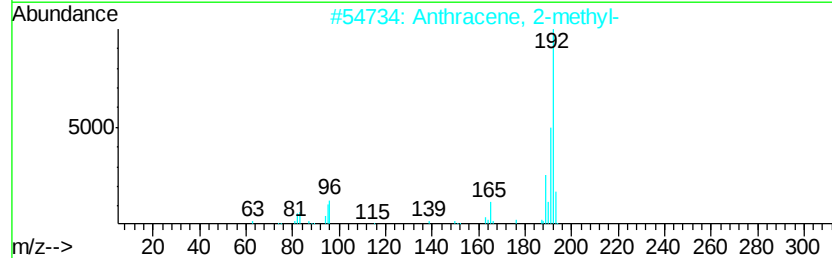
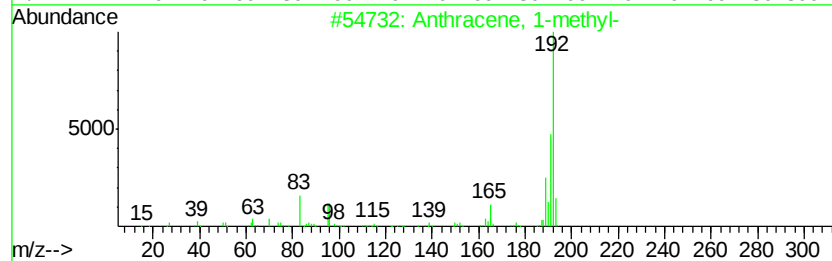
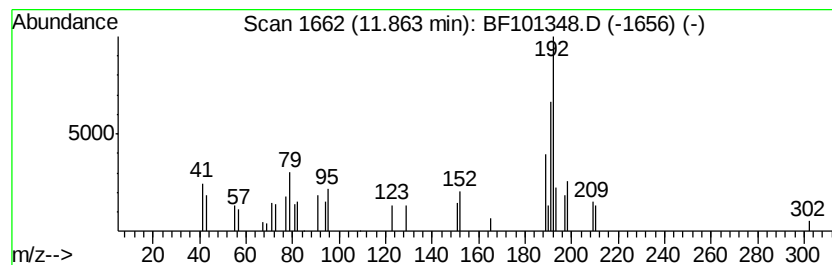
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.86	2.07 ng	29564	Phenanthrene-d10		11.35
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	72
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	64
4	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	59
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101348.D
Acq On : 12 Dec 2017 23:35
Operator : SJ/JU
Sample : I6814-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHMHC-WC1

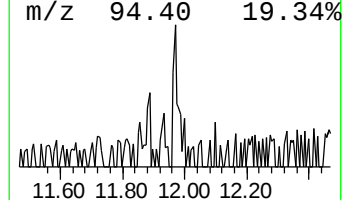
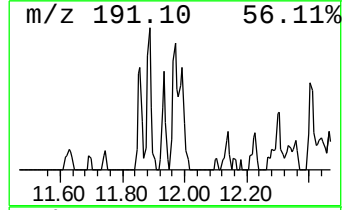
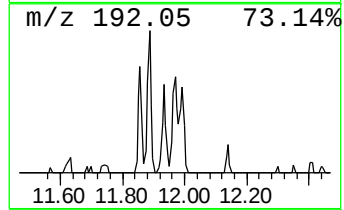
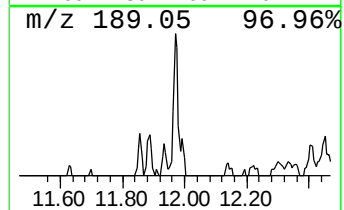
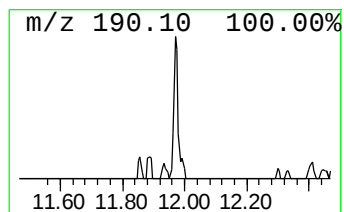
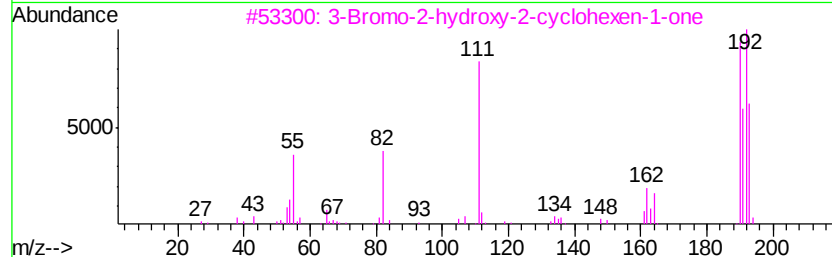
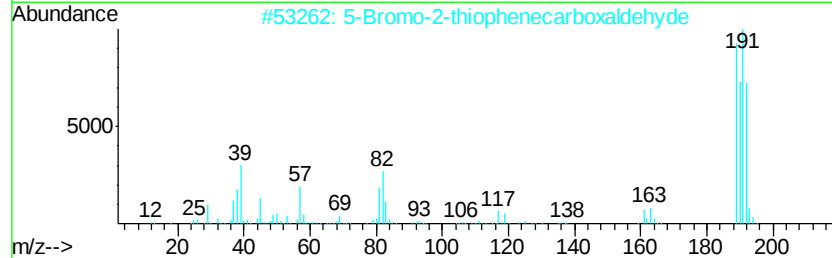
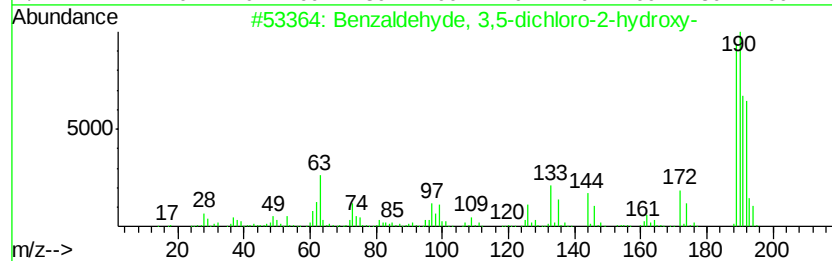
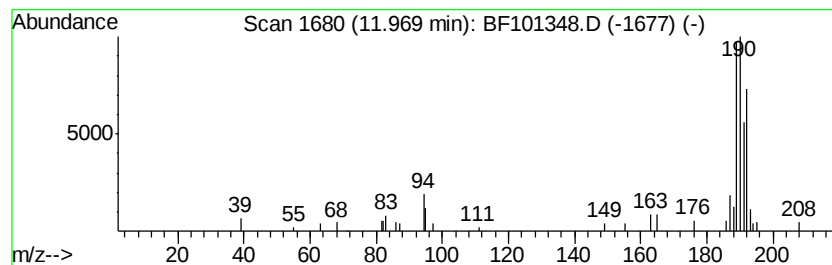
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.72 ng	38827	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2		5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	64
3		3-Bromo-2-hydroxy-2-cyclohexen-1...	190	C6H7BrO2	010324-65-9	47
4		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43
5		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121217\
Data File : BF101348.D
Acq On : 12 Dec 2017 23:35
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Sample : I6814-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

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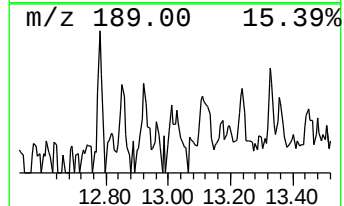
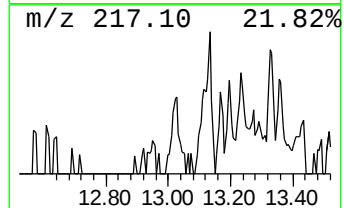
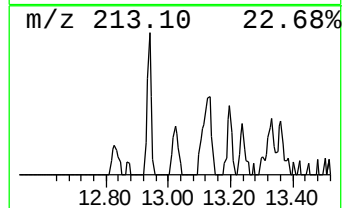
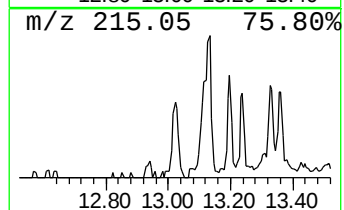
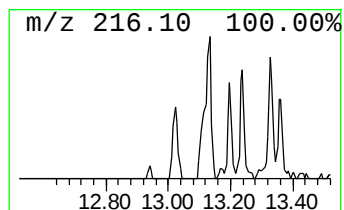
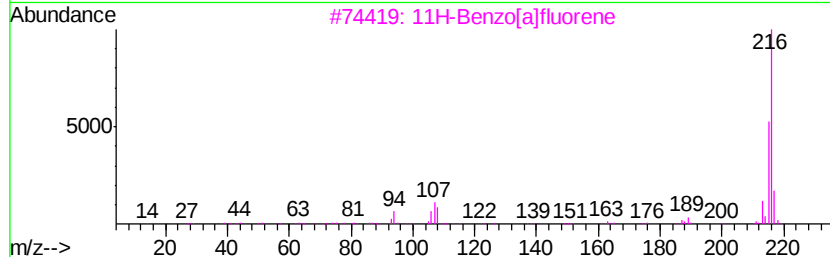
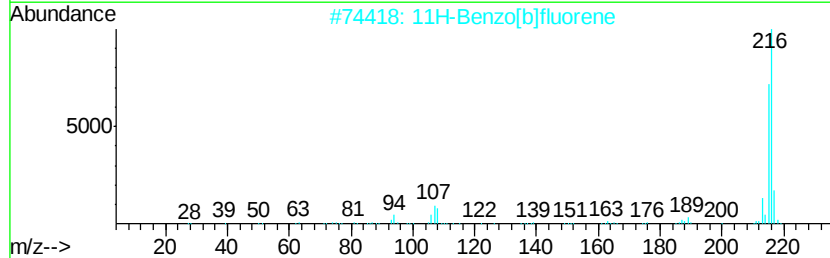
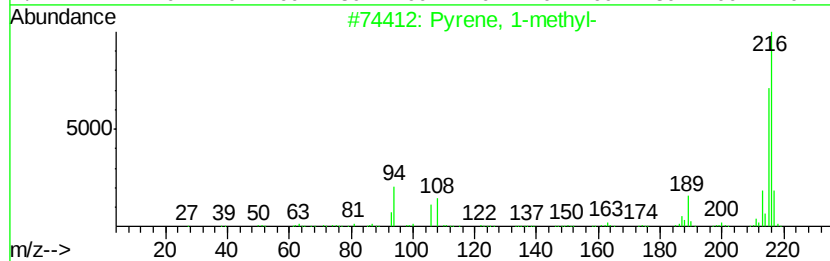
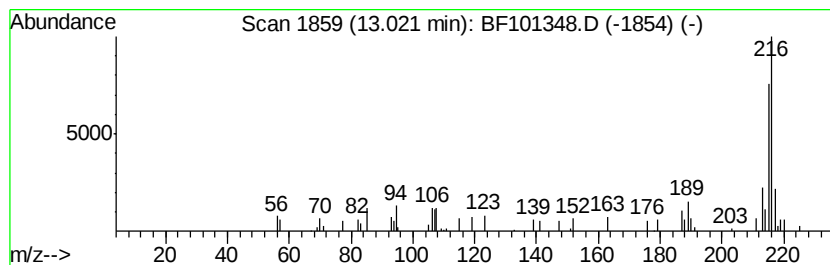
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	2.26 ng	45834	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4		Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
5		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101348.D
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ClientSampleId :
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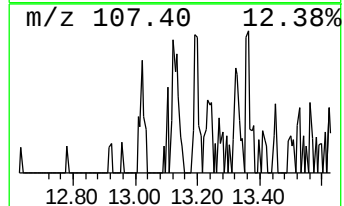
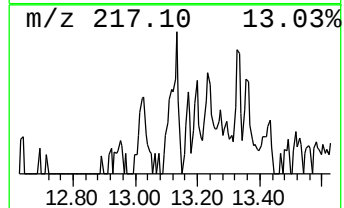
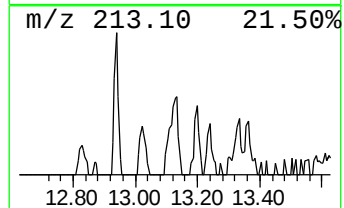
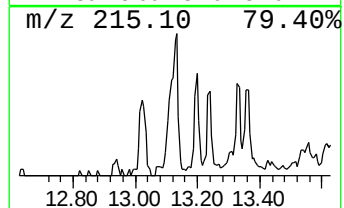
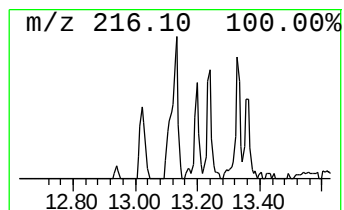
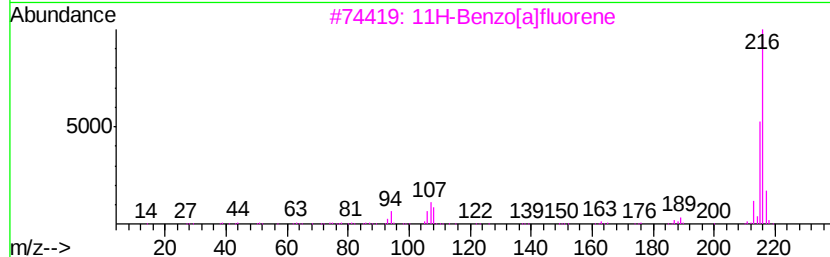
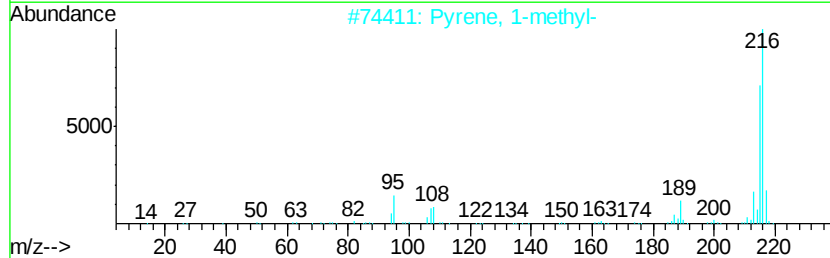
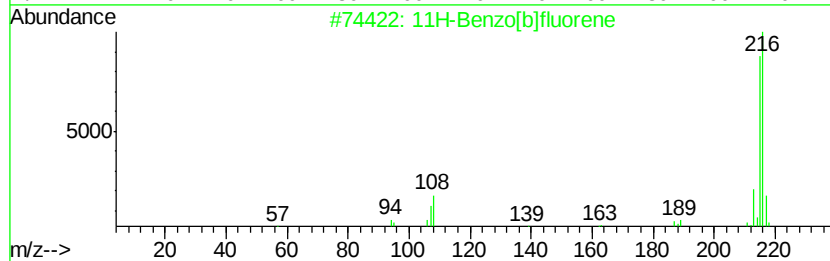
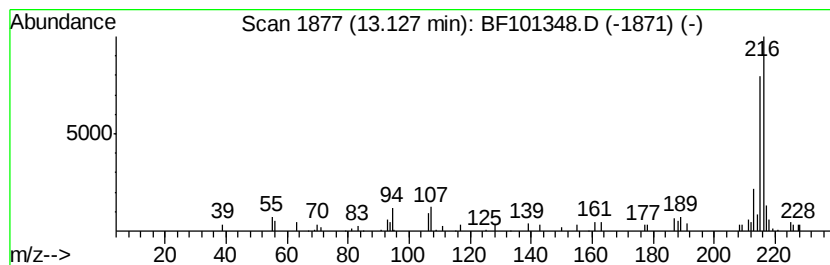
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	2.53 ng	51344	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2		Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	80
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121217\
Data File : BF101348.D
Acq On : 12 Dec 2017 23:35
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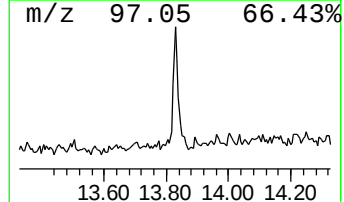
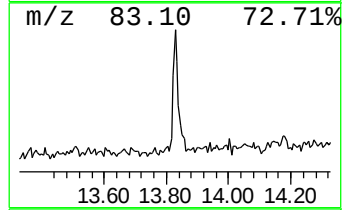
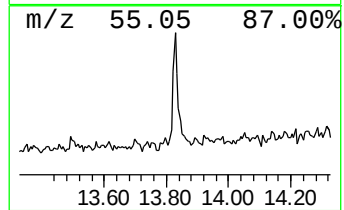
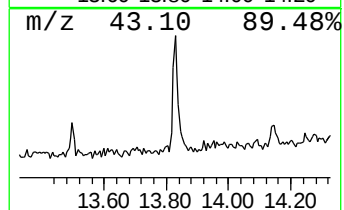
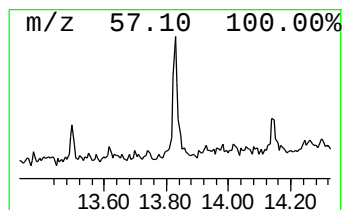
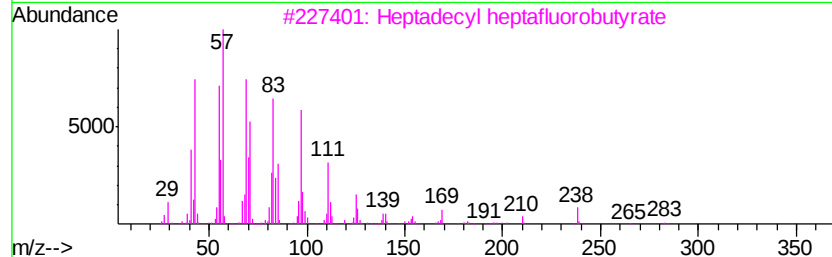
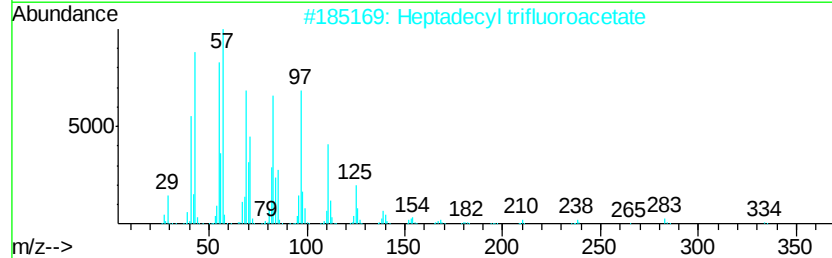
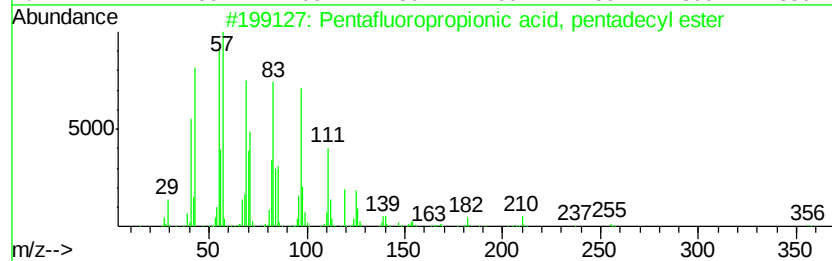
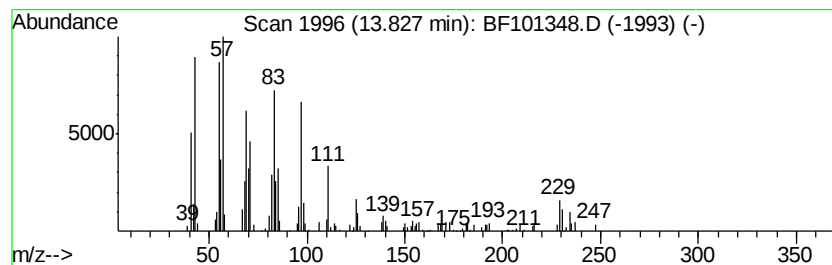
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.08 ng	82820	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	91
4		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	91
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101348.D
Acq On : 12 Dec 2017 23:35
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Misc :
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Instrument :
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ClientSampleId :
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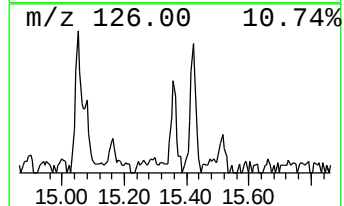
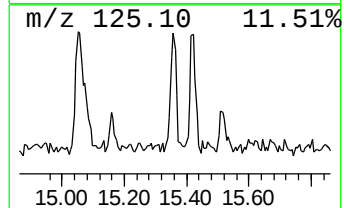
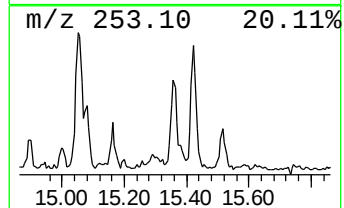
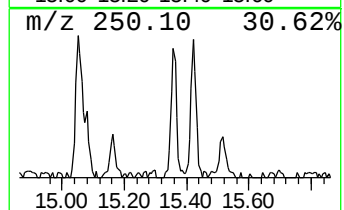
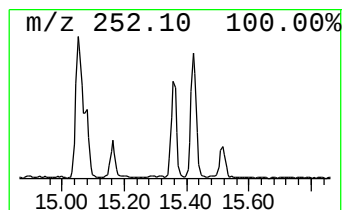
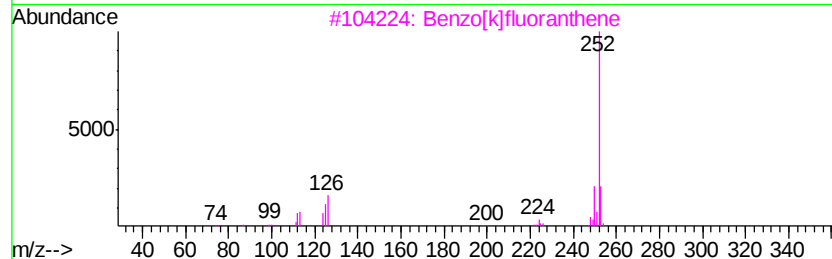
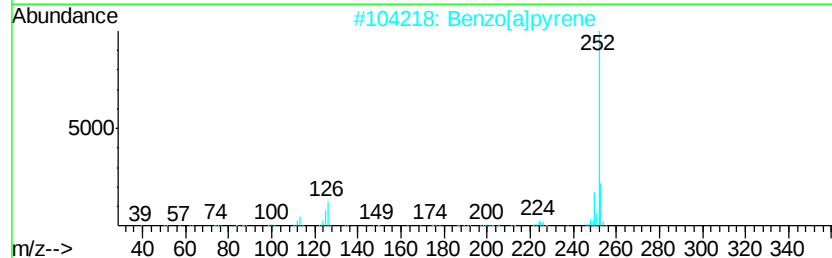
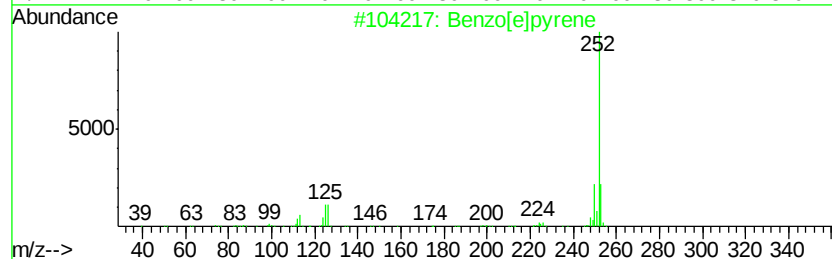
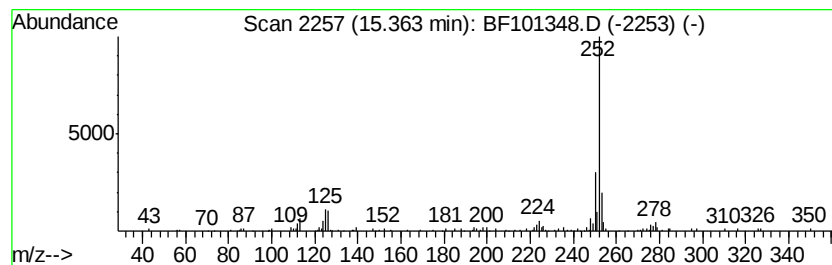
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	12.33 ng	104378	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benzo[a]pyrene	252	C20H12	000050-32-8	95
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	91
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	87



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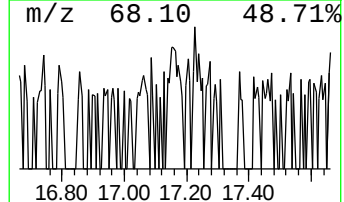
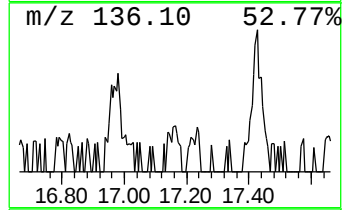
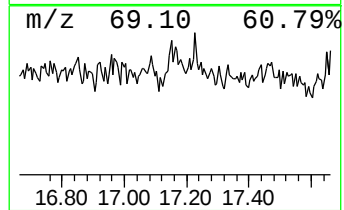
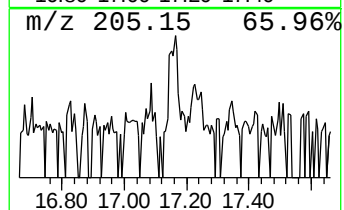
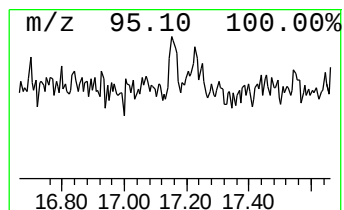
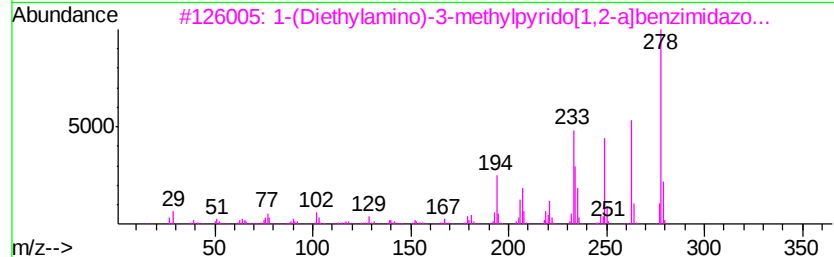
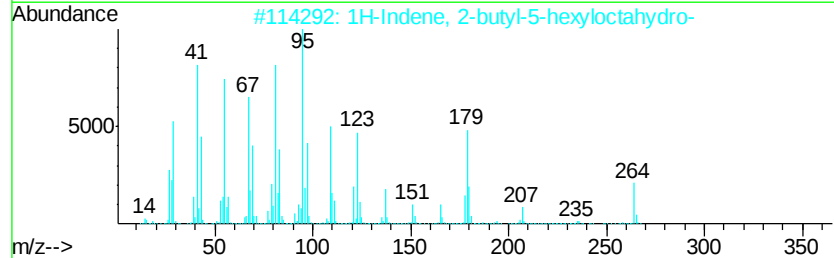
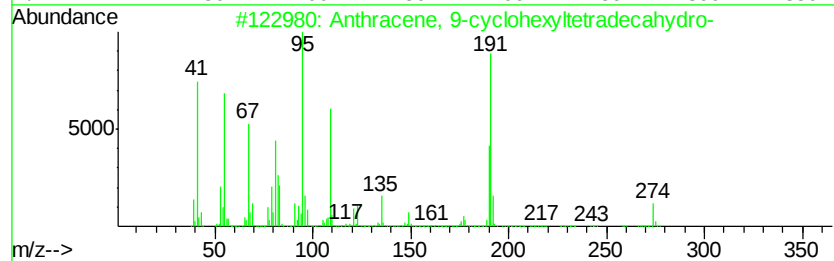
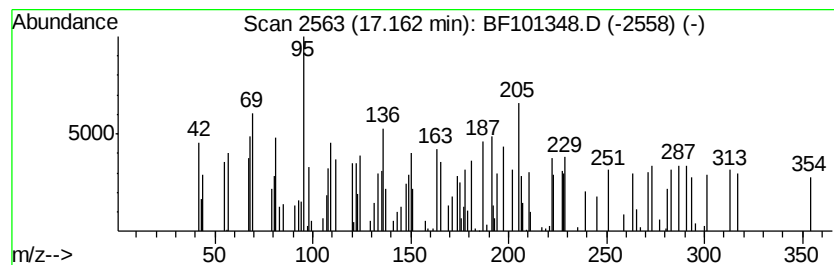
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	4.47 ng	37803	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	14
2		1H-Indene, 2-butyl-5-hexyloctahy...	264	C19H36	055044-33-2	14
3		1-(Diethylamino)-3-methylpyrido[...	278	C17H18N4	1000331-84-4	11
4		Pyrimidine, 5-ethyl-2-(4'-fluoro...	278	C18H15FN2	095495-16-2	10
5		6-[(3-Allylsalicylidene)amino]-1...	278	C16H14N4O	339108-60-0	10



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Sample : I6814-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHMHC-WC1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.04	5.0	ng	57036	1	6.82	228732	20.0
unknown6.59	6.59	80.2	ng	916617	1	6.82	228732	20.0
unknown10.86	10.86	2.6	ng	37423	4	11.35	285440	20.0
Anthracene, 1-met...	11.86	2.1	ng	29564	4	11.35	285440	20.0
Benzaldehyde, 3,5...	11.97	2.7	ng	38827	4	11.35	285440	20.0
Pyrene, 1-methyl-	13.02	2.3	ng	45834	5	14.00	405810	20.0
11H-Benzo[b]fluorene	13.13	2.5	ng	51344	5	14.00	405810	20.0
Pentafluoropropio...	13.83	4.1	ng	82820	5	14.00	405810	20.0
Benzo[e]pyrene	15.36	12.3	ng	104378	6	15.49	169306	20.0
unknown17.16	17.16	4.5	ng	37803	6	15.49	169306	20.0