

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
 Data File : BF106356.D
 Acq On : 12 Jun 2018 20:30
 Operator : JU/SJ
 Sample : J3354-05
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CAS1-SB-102-103-1-27

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-BF061118.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	5.213	485	489	497	rVB	315904	387787	9.39%	1.012%
2	5.601	550	555	558	rBV	3633467	3724713	90.15%	9.718%
3	6.601	719	725	728	rBV	3395032	3689367	89.29%	9.625%
4	6.748	745	750	753	rBV	3497918	3653845	88.43%	9.533%
5	6.972	785	788	792	rVB	1075155	906323	21.94%	2.365%
6	7.131	811	815	818	rBV	3292499	2960561	71.65%	7.724%
7	7.536	879	884	887	rVB	2521845	2344347	56.74%	6.116%
8	7.601	891	895	901	rVB2	63486	68529	1.66%	0.179%
9	8.254	1002	1006	1009	rBV	1267376	1009095	24.42%	2.633%
10	9.330	1184	1189	1192	rBV	4025199	3668900	88.80%	9.572%
11	9.666	1243	1246	1249	rBV2	37220	42713	1.03%	0.111%
12	9.719	1252	1255	1258	rVB	476329	358257	8.67%	0.935%
13	9.930	1284	1291	1294	rBV	84768	82883	2.01%	0.216%
14	10.013	1301	1305	1309	rBV2	1094553	939390	22.74%	2.451%
15	10.248	1343	1345	1350	rBV3	40737	42217	1.02%	0.110%
16	10.430	1373	1376	1379	rVB	111893	94372	2.28%	0.246%
17	10.648	1408	1413	1416	rBV	73205	83445	2.02%	0.218%
18	10.807	1435	1440	1443	rBV	2284501	2166960	52.45%	5.653%
19	10.907	1453	1457	1466	rVB2	324157	360871	8.73%	0.941%
20	11.354	1529	1533	1535	rBV	52216	48331	1.17%	0.126%
21	11.507	1555	1559	1561	rBV	1108219	1009605	24.44%	2.634%
22	11.524	1561	1562	1568	rVV	199608	172097	4.17%	0.449%
23	11.577	1568	1571	1574	rVB	55836	42363	1.03%	0.111%
24	12.007	1641	1644	1646	rBV2	99708	96321	2.33%	0.251%
25	12.036	1646	1649	1652	rVB	93801	86449	2.09%	0.226%
26	12.083	1653	1657	1660	rVV	37633	44683	1.08%	0.117%
27	12.118	1660	1663	1665	rVV2	123592	137345	3.32%	0.358%
28	12.142	1665	1667	1670	rVB	64802	50239	1.22%	0.131%
29	12.301	1691	1694	1696	rBV	70814	55479	1.34%	0.145%
30	12.554	1734	1737	1739	rBV	73611	71757	1.74%	0.187%
31	12.583	1739	1742	1746	rVV4	52419	94691	2.29%	0.247%
32	12.642	1749	1752	1761	rVB5	33390	63401	1.53%	0.165%
33	12.718	1761	1765	1769	rBV	530756	426239	10.32%	1.112%
34	12.895	1792	1795	1798	rVB3	117007	99377	2.41%	0.259%

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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	12.948	1798	1804	1807	rBV	606493	619677	15.00%	1.617%
36	13.001	1810	1813	1817	rBV4	37584	51362	1.24%	0.134%
37	13.089	1824	1828	1832	rVB	3822692	4131704	100.00%	10.779%
38	13.165	1837	1841	1847	rBV5	48891	82191	1.99%	0.214%
39	13.277	1852	1860	1863	rBV	121563	196746	4.76%	0.513%
40	13.342	1868	1871	1874	rVB	80200	64752	1.57%	0.169%
41	13.383	1874	1878	1881	rBV	70817	66301	1.60%	0.173%
42	13.477	1891	1894	1896	rBV	60766	56075	1.36%	0.146%
43	13.507	1896	1899	1902	rVB	58580	52637	1.27%	0.137%
44	13.601	1913	1915	1918	rVB	70162	54412	1.32%	0.142%
45	13.924	1968	1970	1973	rBV	56739	50258	1.22%	0.131%
46	13.971	1973	1978	1981	rBV3	246247	303870	7.35%	0.793%
47	14.154	2004	2009	2011	rBV2	1275159	1404877	34.00%	3.665%
48	14.177	2011	2013	2018	rVB	242312	210855	5.10%	0.550%
49	14.542	2073	2075	2078	rVB	52724	48839	1.18%	0.127%
50	14.612	2084	2087	2090	rBV2	98031	109004	2.64%	0.284%
51	15.018	2153	2156	2158	rBV2	98125	103049	2.49%	0.269%
52	15.230	2189	2192	2195	rBV	110031	161744	3.91%	0.422%
53	15.295	2200	2203	2214	rVB5	127219	318050	7.70%	0.830%
54	15.554	2244	2247	2253	rVB	80531	95025	2.30%	0.248%
55	15.618	2255	2258	2262	rVB	111617	136707	3.31%	0.357%
56	15.689	2265	2270	2281	rBV	663751	928678	22.48%	2.423%

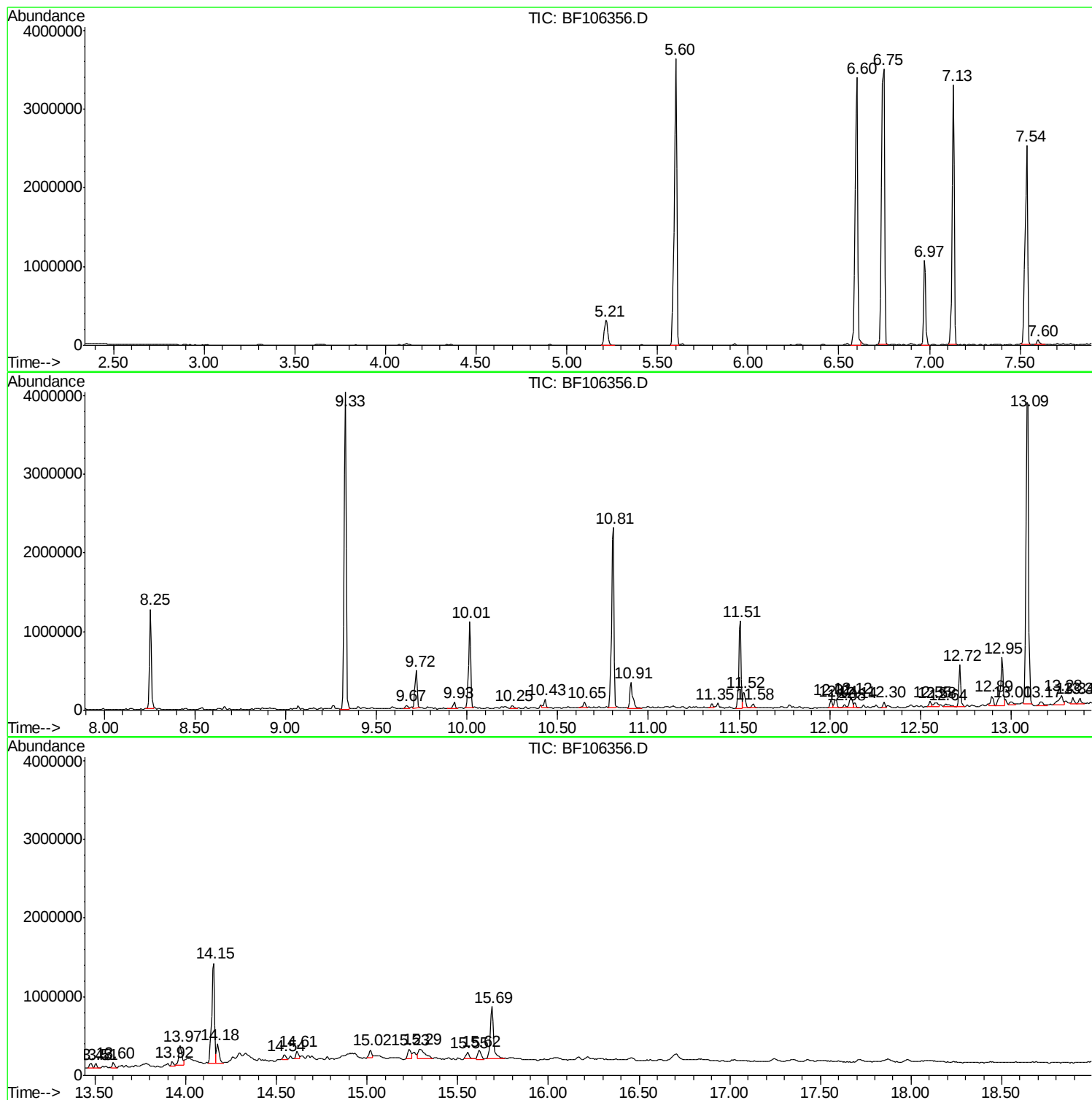
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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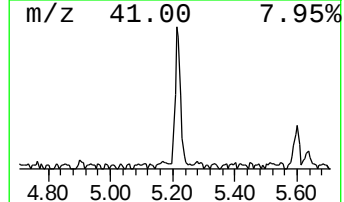
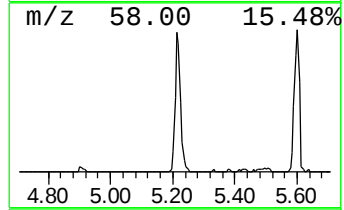
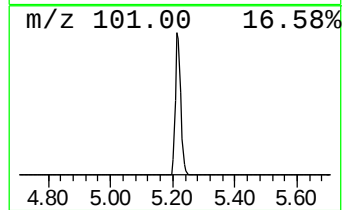
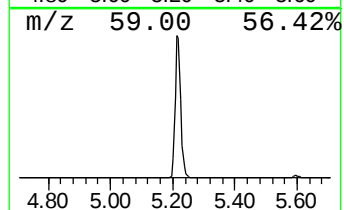
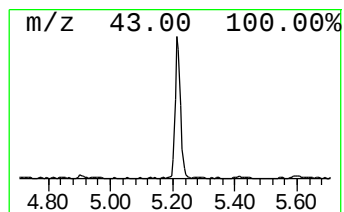
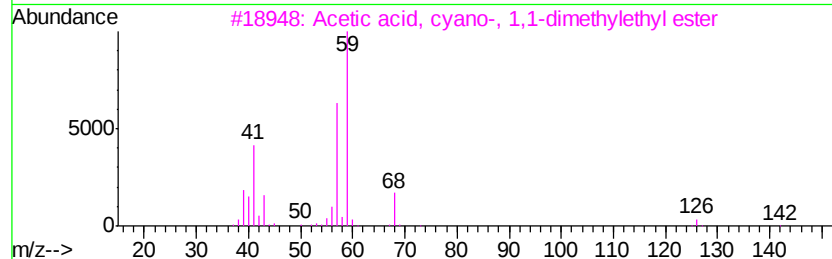
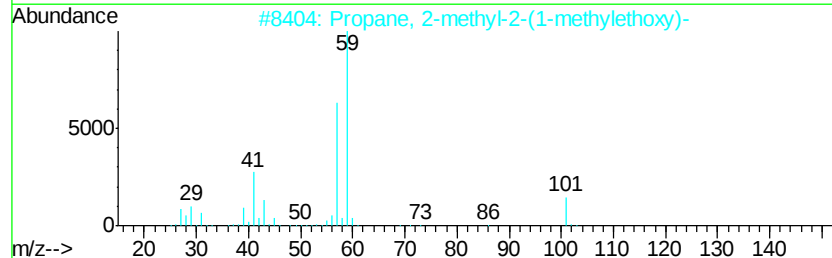
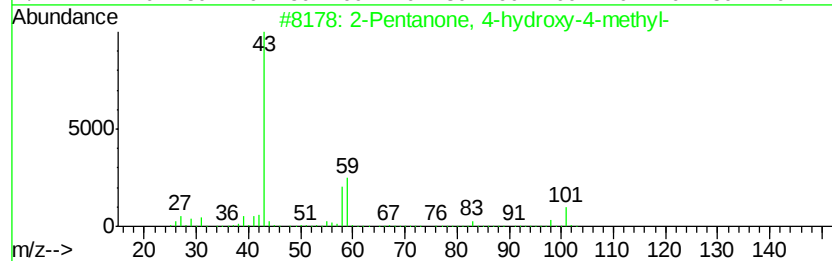
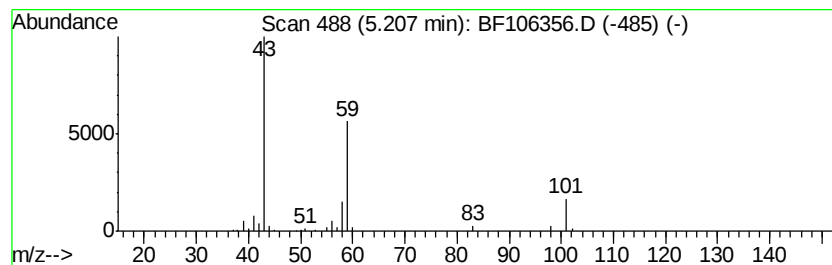
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.21	8.56 ng	387787	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	33
3			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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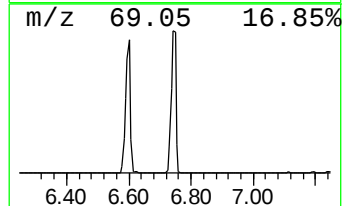
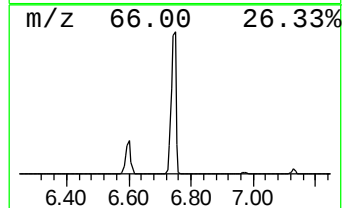
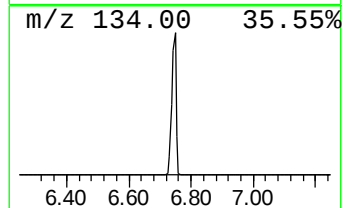
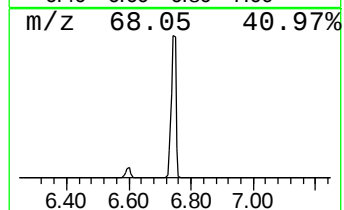
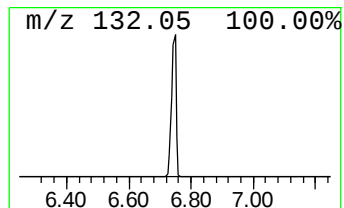
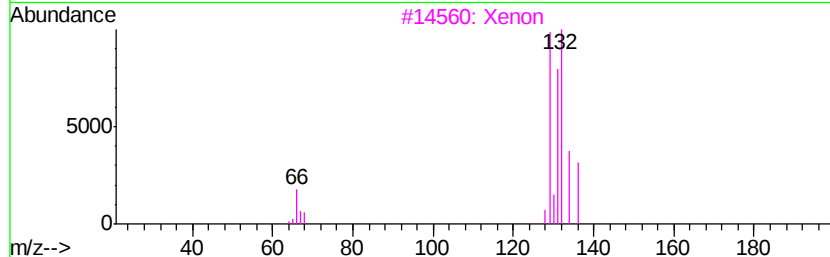
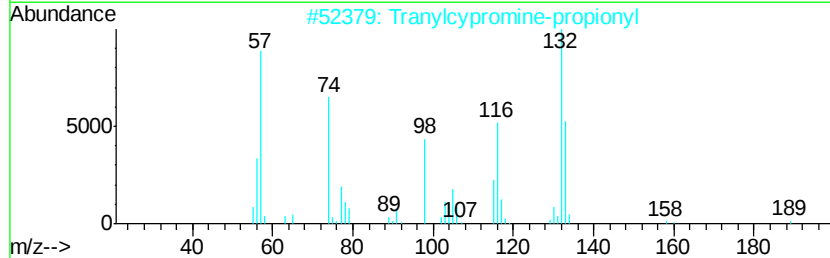
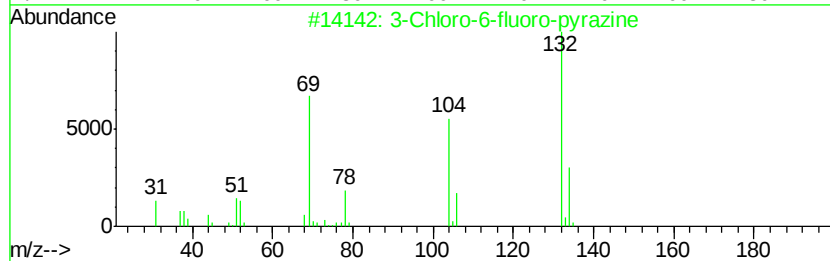
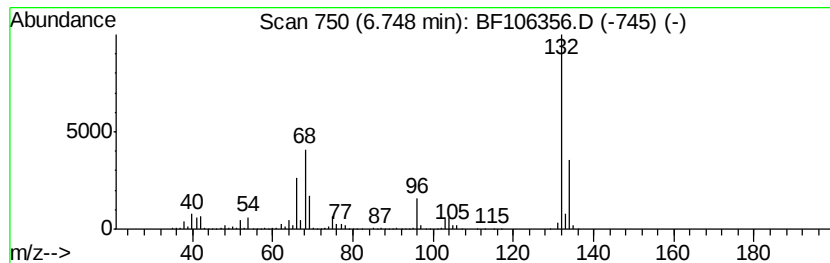
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	80.63 ng	3653850	1,4-Dichlorobenzene-d4	6.97

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		Xenon	132	Xe	007440-63-3	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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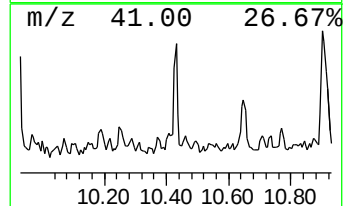
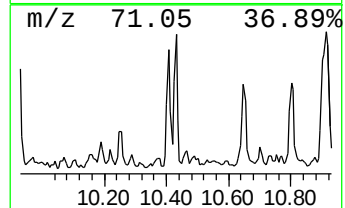
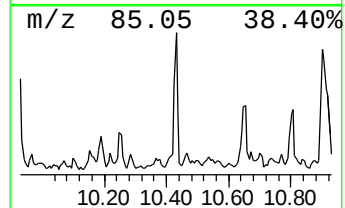
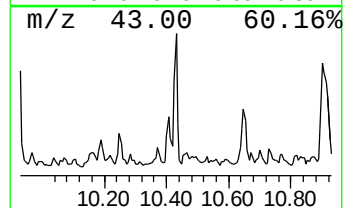
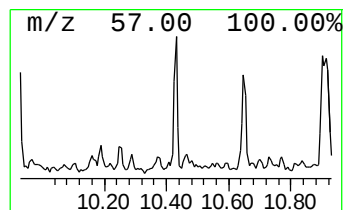
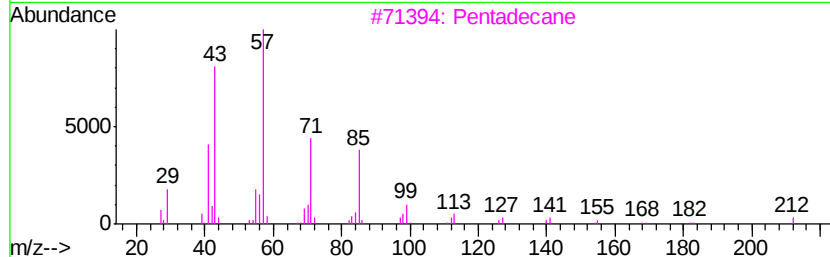
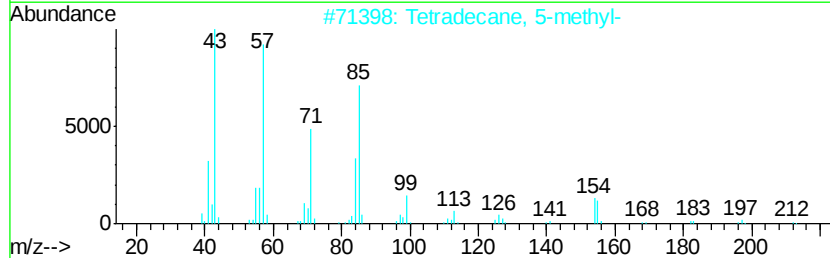
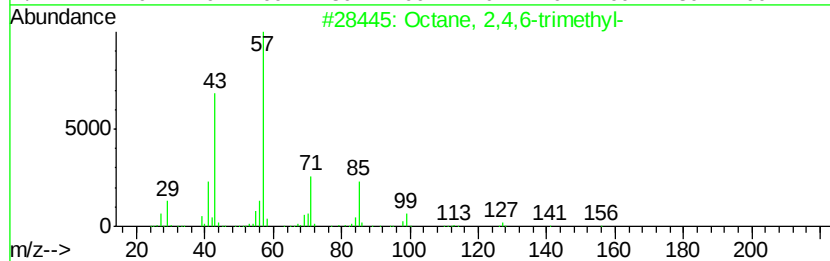
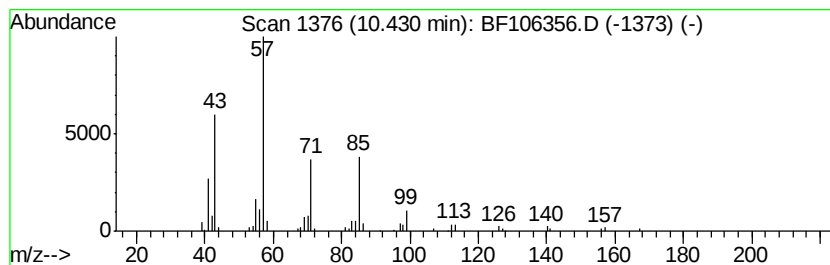
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octane, 2,4,6-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.43	2.01 ng	94372	Acenaphthene-d10		10.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	86
2	Tetradecane, 5-methyl-	212	C15H32	025117-32-2	80
3	Pentadecane	212	C15H32	000629-62-9	78
4	Tetradecane	198	C14H30	000629-59-4	72
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	53



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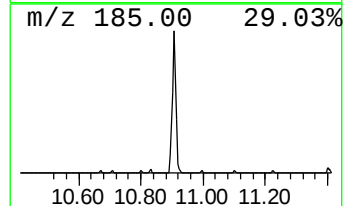
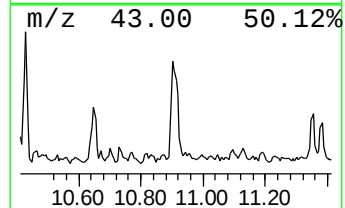
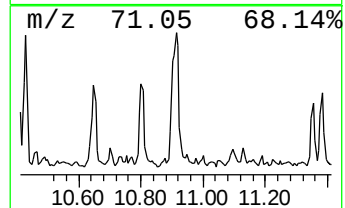
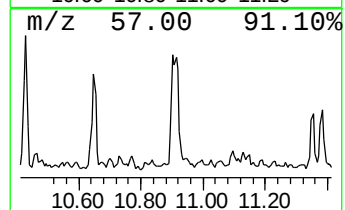
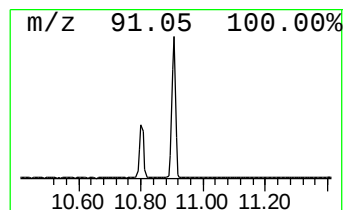
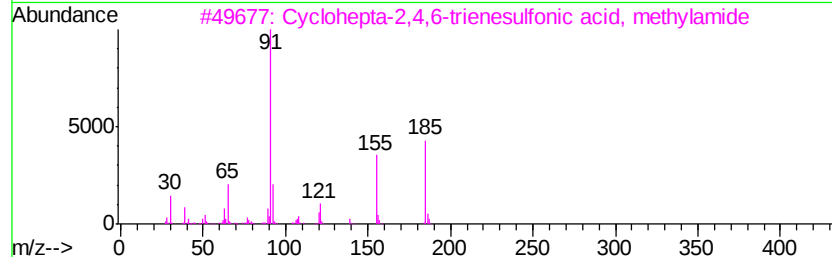
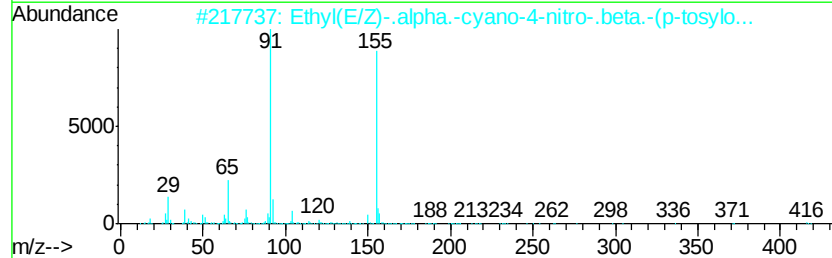
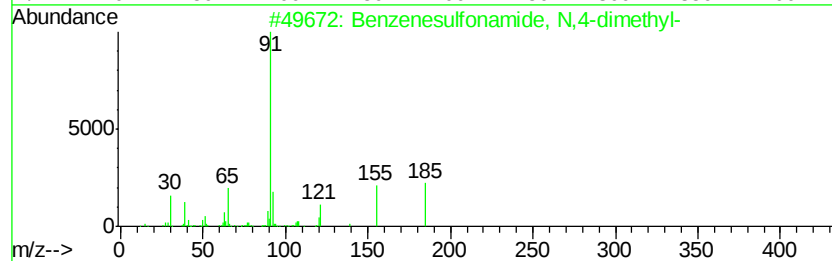
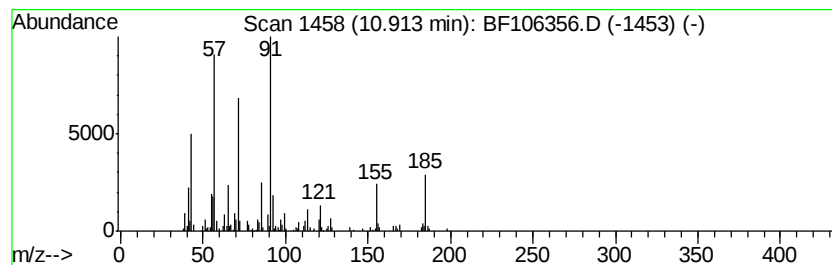
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	7.15 ng	360871	Phenanthrene-d10	11.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	91
2		Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50
3		Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	46
4		Benzeneacetaldehyde	120	C8H8O	000122-78-1	45
5		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	38



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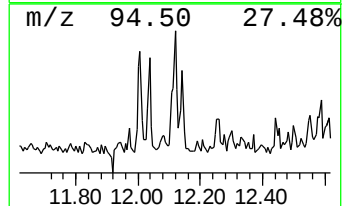
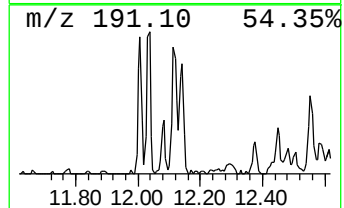
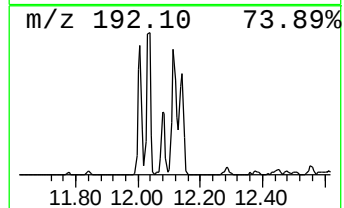
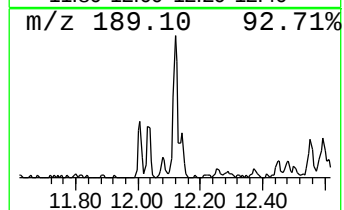
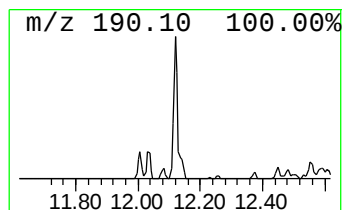
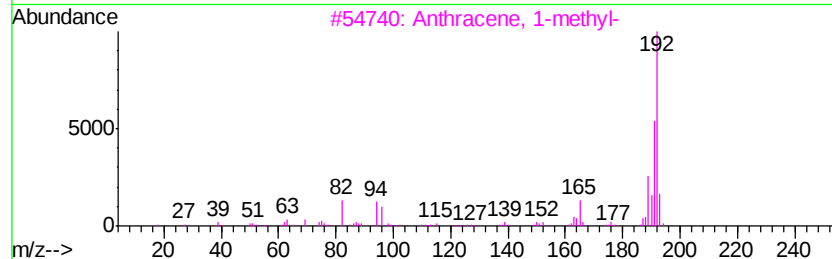
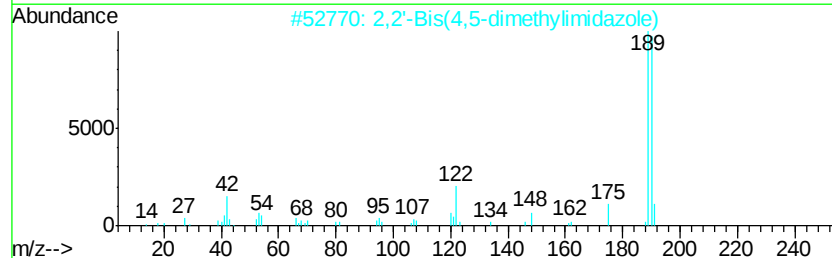
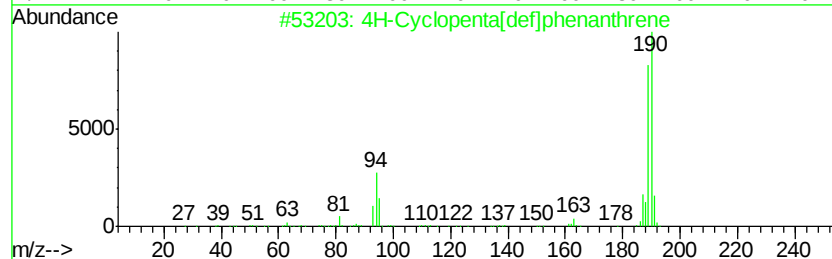
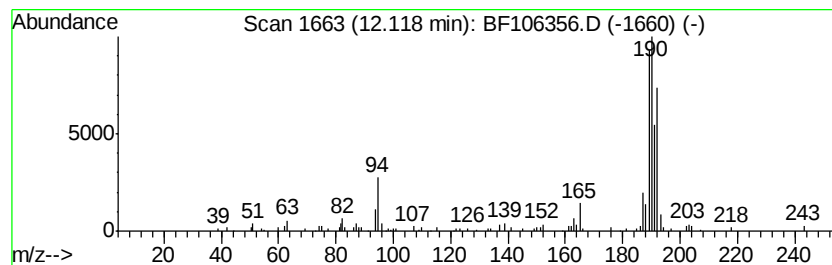
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	2.72 ng	137345	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	30
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106356.D
Acq On : 12 Jun 2018 20:30
Operator : JU/SJ
Sample : J3354-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-102-103-1-27

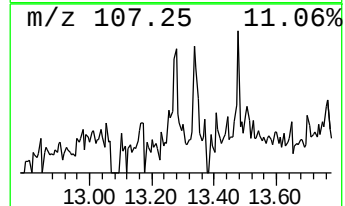
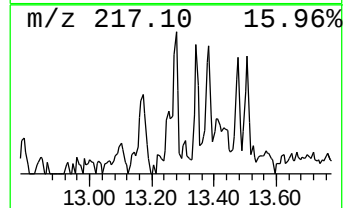
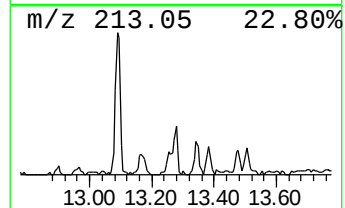
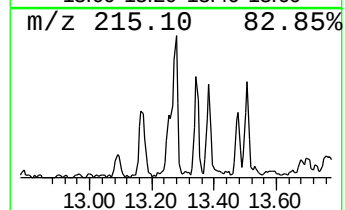
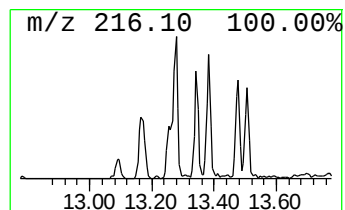
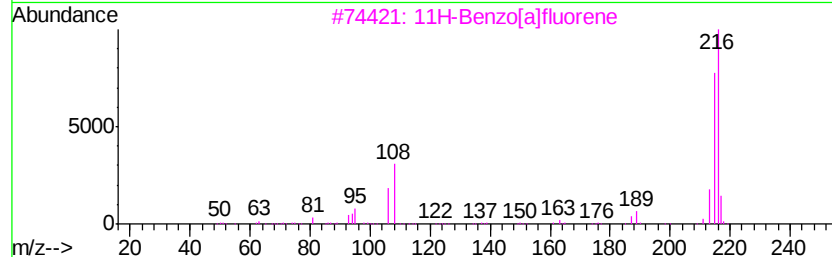
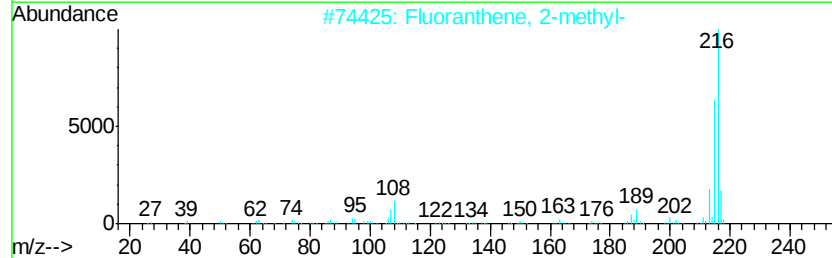
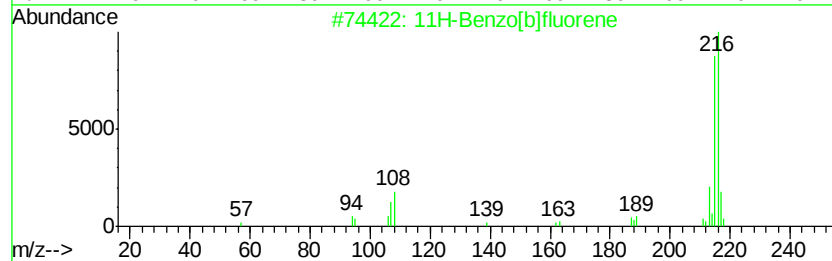
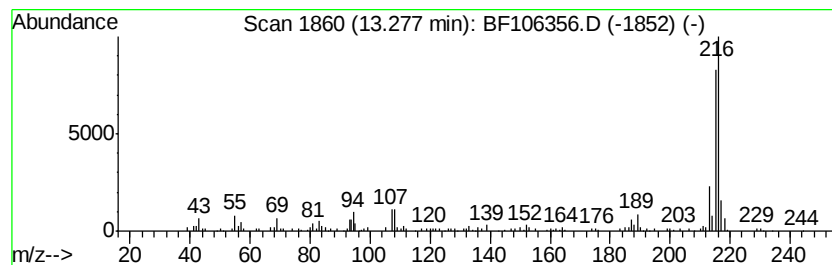
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	2.80 ng	196746	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4		Pyrene, 1-methyl-	216	C17H12	002381-21-7	80
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106356.D
Acq On : 12 Jun 2018 20:30
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Sample : J3354-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

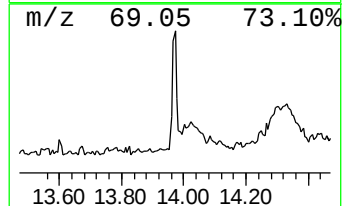
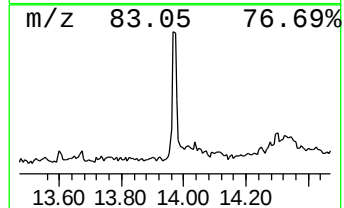
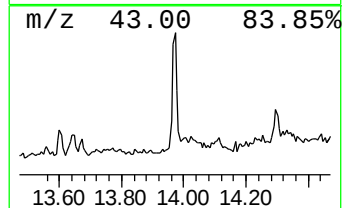
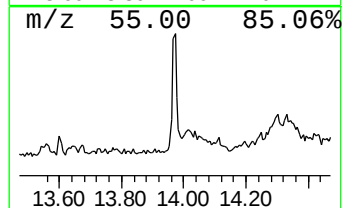
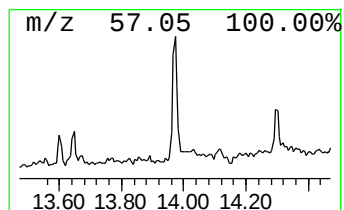
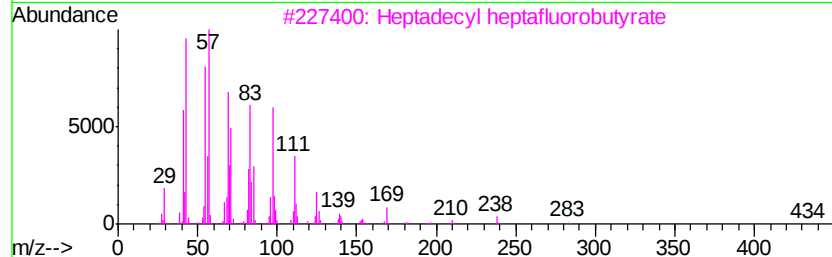
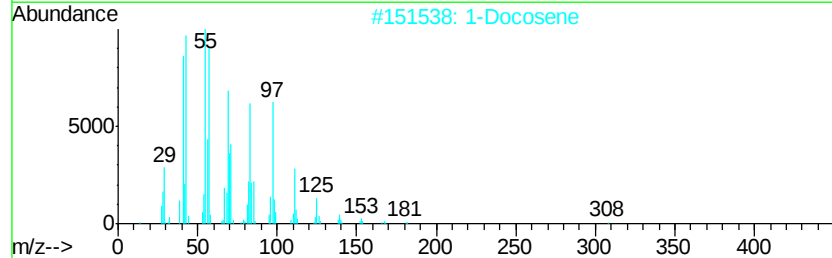
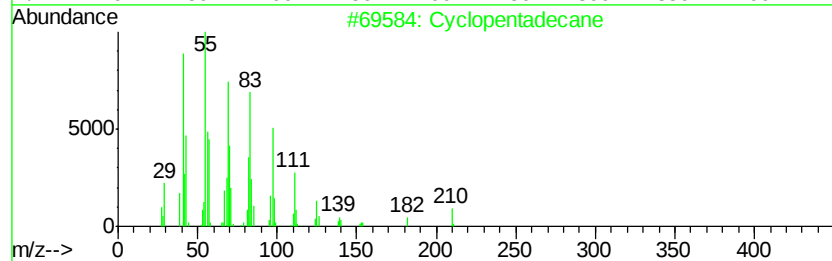
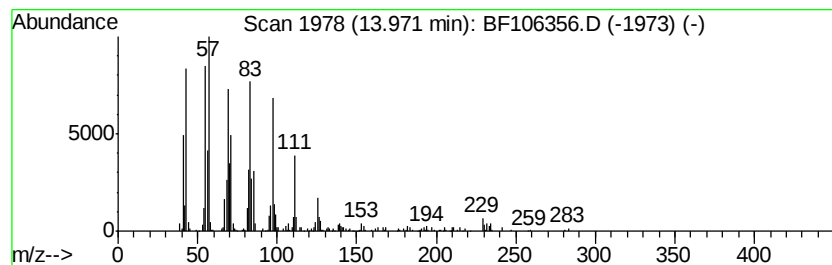
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CAS1-SB-102-103-1-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.97	4.33 ng	303870	Chrysene-d12		14.15	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclopentadecane	210	C15H30	000295-48-7	92
2		1-Docosene	308	C22H44	001599-67-3	91
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
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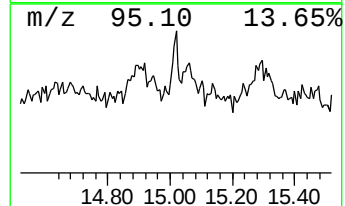
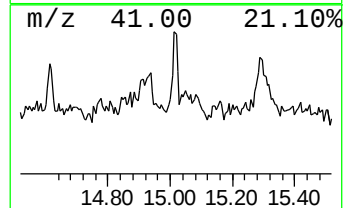
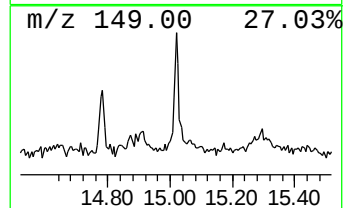
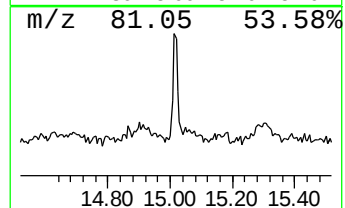
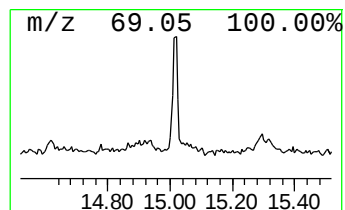
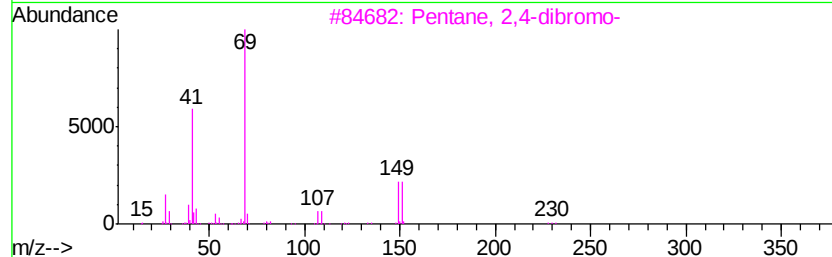
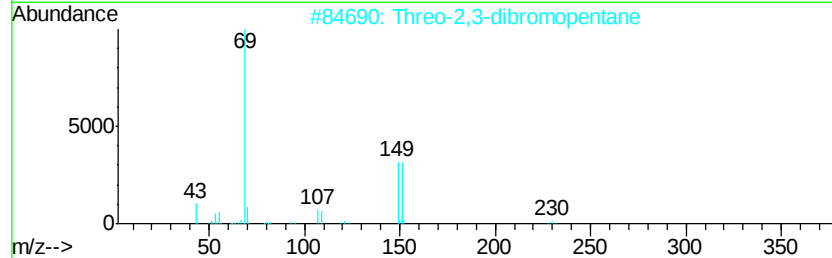
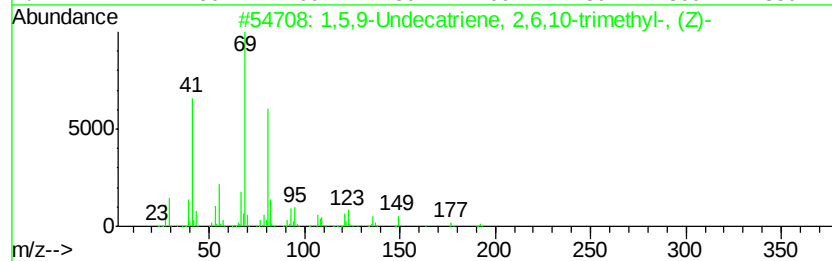
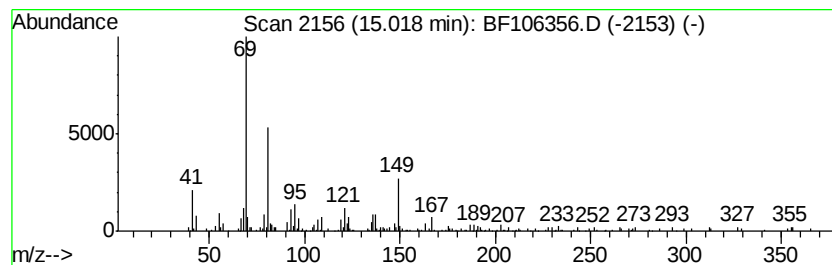
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.02	2.22 ng	103049	Perylene-d12	15.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
2	Threo-2,3-dibromopentane	228	C5H10Br2	1000288-18-6	64
3	Pentane, 2,4-dibromo-	228	C5H10Br2	019398-53-9	64
4	Pentane, 1,4-dibromo-	228	C5H10Br2	000626-87-9	59
5	Supraene	410	C30H50	007683-64-9	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
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Sample : J3354-05
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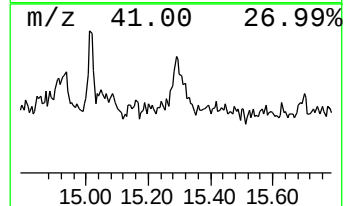
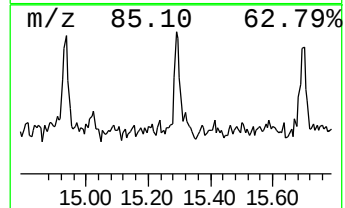
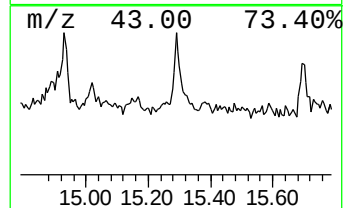
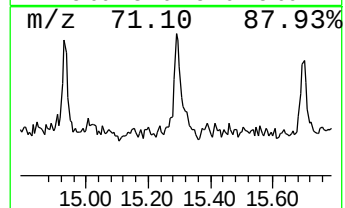
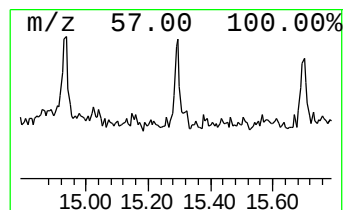
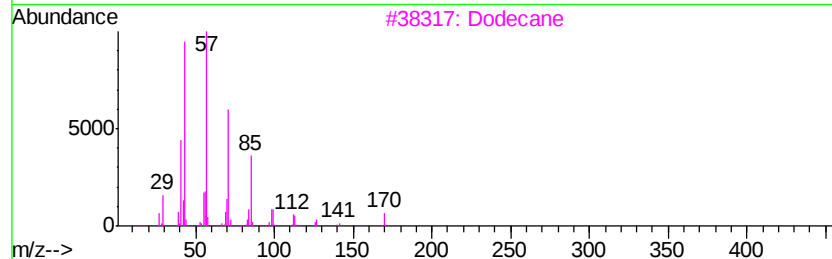
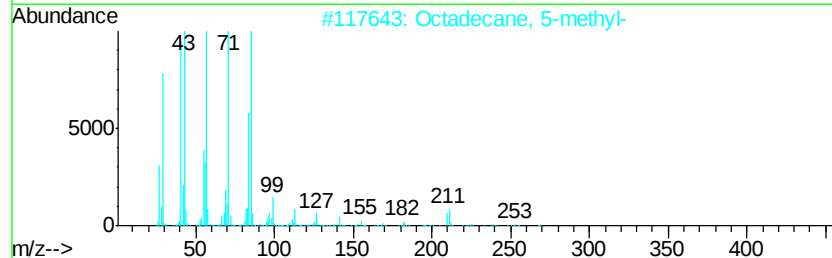
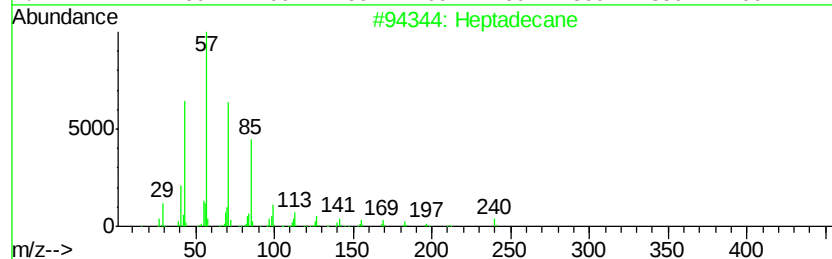
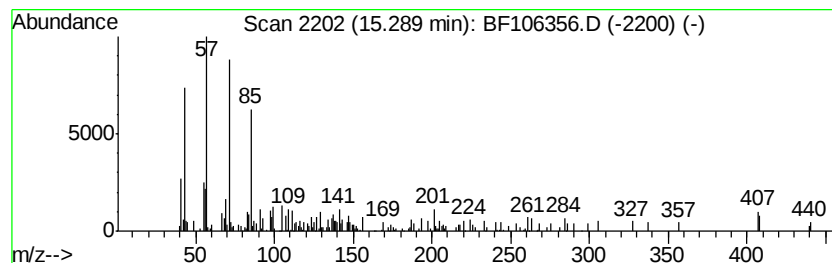
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.29	6.85 ng	318050	Perylene-d12	15.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	58
2	Octadecane, 5-methyl-	268	C19H40	025117-35-5	52
3	Dodecane	170	C12H26	000112-40-3	50
4	Undecane	156	C11H24	001120-21-4	50
5	Tetradecane	198	C14H30	000629-59-4	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
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Operator : JU/SJ
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Misc :
ALS Vial : 21 Sample Multiplier: 1

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CAS1-SB-102-103-1-27

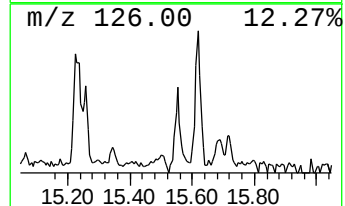
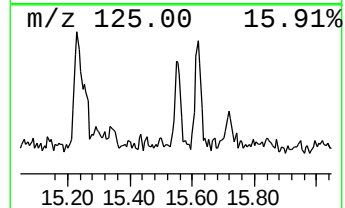
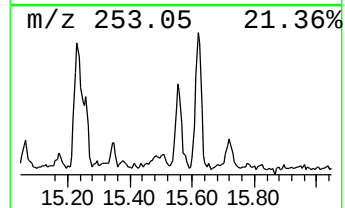
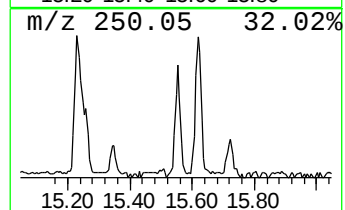
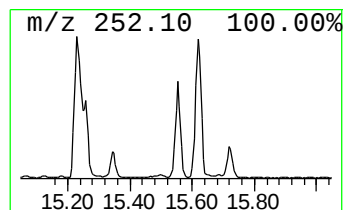
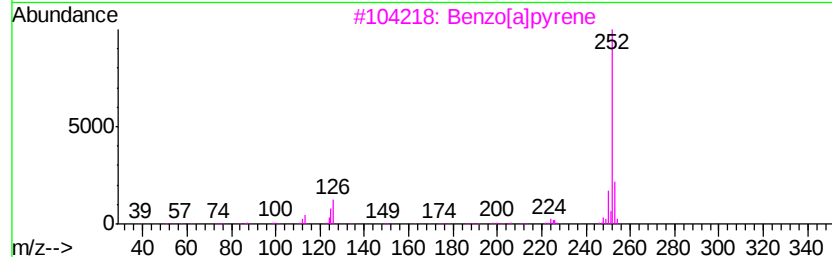
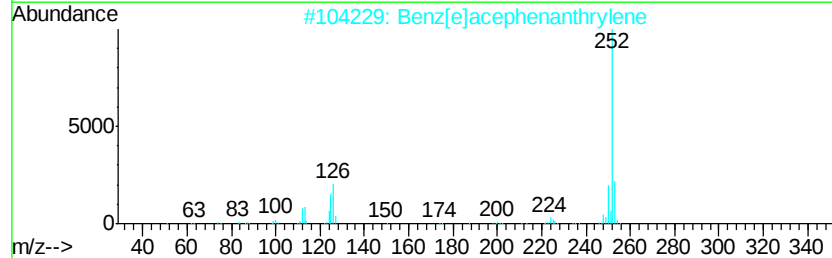
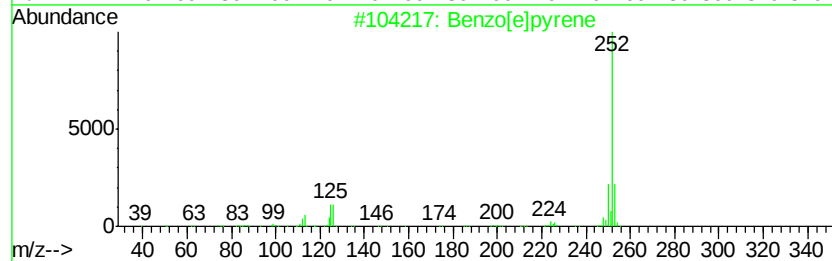
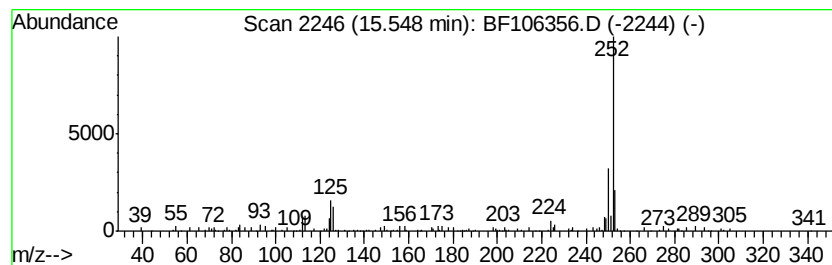
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	2.05 ng	95025	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	96
3		Benzo[a]pyrene	252	C20H12	000050-32-8	96
4		Perylene	252	C20H12	000198-55-0	94
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061218\
Data File : BF106356.D
Acq On : 12 Jun 2018 20:30
Operator : JU/SJ
Sample : J3354-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CAS1-SB-102-103-1-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.21	8.6	ng	387787	1	6.97	906323	20.0
unknown6.75	6.75	80.6	ng	3653850	1	6.97	906323	20.0
Octane, 2,4,6-tri...	10.43	2.0	ng	94372	3	10.01	939390	20.0
Benzenesulfonamid...	10.91	7.2	ng	360871	4	11.51	1009610	20.0
4H-Cyclopenta[def...	12.12	2.7	ng	137345	4	11.51	1009610	20.0
11H-Benzo[b]fluorene	13.28	2.8	ng	196746	5	14.15	1404880	20.0
Cyclopentadecane	13.97	4.3	ng	303870	5	14.15	1404880	20.0
1,5,9-Undecatrien...	15.02	2.2	ng	103049	6	15.69	928678	20.0
Heptadecane	15.29	6.8	ng	318050	6	15.69	928678	20.0
Benzo[e]pyrene	15.55	2.0	ng	95025	6	15.69	928678	20.0