

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122315\
 Data File : BF084044.D
 Acq On : 23 Dec 2015 20:14
 Operator : UM/SJ
 Sample : G4889-01
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LIBERTY-SF-121815

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-BF122215.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	5.001	253	255	264	rBB	248577	375427	20.89%	2.123%
2	5.436	291	293	296	rBV	1073787	1231339	68.50%	6.963%
3	6.476	381	384	386	rBV	1040662	1404254	78.12%	7.941%
4	6.590	392	394	397	rBV	1327897	1340155	74.55%	7.578%
5	6.819	412	414	416	rBV	383770	326864	18.18%	1.848%
6	6.979	425	428	430	rBV	1181079	1216307	67.66%	6.878%
7	7.379	460	463	466	rBV	641651	883098	49.13%	4.994%
8	8.099	524	526	531	rBV2	400150	472768	26.30%	2.673%
9	8.819	586	589	591	rBV	44315	37487	2.09%	0.212%
10	8.910	595	597	600	rVB4	19999	28349	1.58%	0.160%
11	9.185	618	621	623	rBV	1928785	1797590	100.00%	10.165%
12	9.265	625	628	630	rBV2	17700	26283	1.46%	0.149%
13	9.310	630	632	633	rVB	41043	46073	2.56%	0.261%
14	9.448	640	644	647	rBV2	14066	28347	1.58%	0.160%
15	9.516	647	650	652	rVV	28515	39713	2.21%	0.225%
16	9.573	653	655	657	rVV	257613	265714	14.78%	1.503%
17	9.642	657	661	663	rVV3	12589	32076	1.78%	0.181%
18	9.722	666	668	671	rBV2	21882	26580	1.48%	0.150%
19	9.802	673	675	677	rVB	32423	32738	1.82%	0.185%
20	9.859	677	680	682	rBV	548519	516700	28.74%	2.922%
21	9.893	682	683	685	rVB	43676	33854	1.88%	0.191%
22	10.019	691	694	696	rBV3	10541	25453	1.42%	0.144%
23	10.065	696	698	699	rVB	38404	36147	2.01%	0.204%
24	10.179	705	708	711	rBV3	17538	27872	1.55%	0.158%
25	10.271	714	716	717	rBV	19147	24991	1.39%	0.141%
26	10.293	717	718	720	rVB	52750	47196	2.63%	0.267%
27	10.408	726	728	730	rBV	47169	59951	3.34%	0.339%
28	10.442	730	731	734	rVV2	39175	59296	3.30%	0.335%
29	10.522	736	738	740	rVV	26196	39157	2.18%	0.221%
30	10.568	740	742	744	rVB	20010	24663	1.37%	0.139%
31	10.648	746	749	751	rBV	960681	890102	49.52%	5.033%
32	10.773	758	760	764	rVB2	66296	109015	6.06%	0.616%
33	10.842	764	766	770	rBV4	12480	33248	1.85%	0.188%
34	10.956	774	776	777	rBV2	17935	21090	1.17%	0.119%

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35	11.094	785	788	792	rVB6	15406	38728	2.15%	0.219%
36	11.219	795	799	800	rBV2	40112	60466	3.36%	0.342%
37	11.242	800	801	805	rVB2	43130	51070	2.84%	0.289%
38	11.345	808	810	814	rBV2	438313	786116	43.73%	4.445%
39	11.414	814	816	818	rVB	84614	85599	4.76%	0.484%
40	11.459	818	820	821	rBV	18603	18779	1.04%	0.106%
41	11.574	828	830	834	rVB2	31219	39477	2.20%	0.223%
42	11.676	837	839	844	rVB4	9335	18875	1.05%	0.107%
43	11.848	851	854	855	rBV	40248	57237	3.18%	0.324%
44	11.871	855	856	858	rVV	80776	72913	4.06%	0.412%
45	11.916	858	860	862	rVV2	25670	36962	2.06%	0.209%
46	11.951	862	863	868	rVB	77814	132095	7.35%	0.747%
47	12.042	868	871	873	rBV3	14092	31309	1.74%	0.177%
48	12.134	878	879	881	rVV2	31389	34276	1.91%	0.194%
49	12.168	881	882	884	rVB	26392	24918	1.39%	0.141%
50	12.316	894	895	899	rBV3	15809	37683	2.10%	0.213%
51	12.397	899	902	903	rVV3	42776	54390	3.03%	0.308%
52	12.431	903	905	908	rVB2	25699	41190	2.29%	0.233%
53	12.477	908	909	911	rBV	18712	24514	1.36%	0.139%
54	12.557	914	916	918	rBV	358315	347387	19.33%	1.964%
55	12.705	927	929	930	rBV2	13244	19144	1.06%	0.108%
56	12.785	931	936	937	rVV	284901	378746	21.07%	2.142%
57	12.831	937	940	943	rVB3	26591	51684	2.88%	0.292%
58	12.922	946	948	951	rVB	1070674	1300797	72.36%	7.356%
59	13.002	952	955	959	rVB3	22333	52597	2.93%	0.297%
60	13.117	961	965	966	rVB	30870	65044	3.62%	0.368%
61	13.174	968	970	972	rBV2	26594	43842	2.44%	0.248%
62	13.219	972	974	977	rVB3	37252	53732	2.99%	0.304%
63	13.311	980	982	983	rVB	17872	19109	1.06%	0.108%
64	13.345	983	985	986	rBV	17374	24688	1.37%	0.140%
65	13.402	988	990	993	rBV2	23637	24700	1.37%	0.140%
66	13.459	993	995	996	rVB	31168	35022	1.95%	0.198%
67	13.505	997	999	1000	rBV2	21526	26784	1.49%	0.151%
68	13.619	1008	1009	1011	rVB	29532	31692	1.76%	0.179%
69	13.734	1016	1019	1020	rBV	24247	41610	2.31%	0.235%
70	13.825	1025	1027	1031	rVB5	71537	110766	6.16%	0.626%
71	13.974	1037	1040	1046	rVB3	323562	643448	35.80%	3.639%

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72	14.088	1048	1050	1052	rVB2	24651	27250	1.52%	0.154%
73	14.145	1052	1055	1059	rBV2	29286	74970	4.17%	0.424%
74	14.454	1080	1082	1084	rBV3	23021	37189	2.07%	0.210%
75	14.854	1115	1117	1120	rBV4	16397	27994	1.56%	0.158%
76	15.002	1128	1130	1134	rVV	105889	181132	10.08%	1.024%
77	15.105	1138	1139	1145	rBV	20219	27067	1.51%	0.153%
78	15.288	1153	1155	1159	rVB	56360	71191	3.96%	0.403%
79	15.357	1159	1161	1163	rVV	81394	113992	6.34%	0.645%
80	15.414	1163	1166	1172	rVB	200942	340921	18.97%	1.928%
81	16.054	1220	1222	1229	rVB5	25212	62037	3.45%	0.351%
82	16.465	1255	1258	1262	rVB4	16460	36952	2.06%	0.209%
83	16.820	1286	1289	1297	rVB	36014	94327	5.25%	0.533%
84	17.243	1324	1326	1331	rBV	26942	65277	3.63%	0.369%
85	17.494	1345	1348	1354	rVB4	14698	46732	2.60%	0.264%

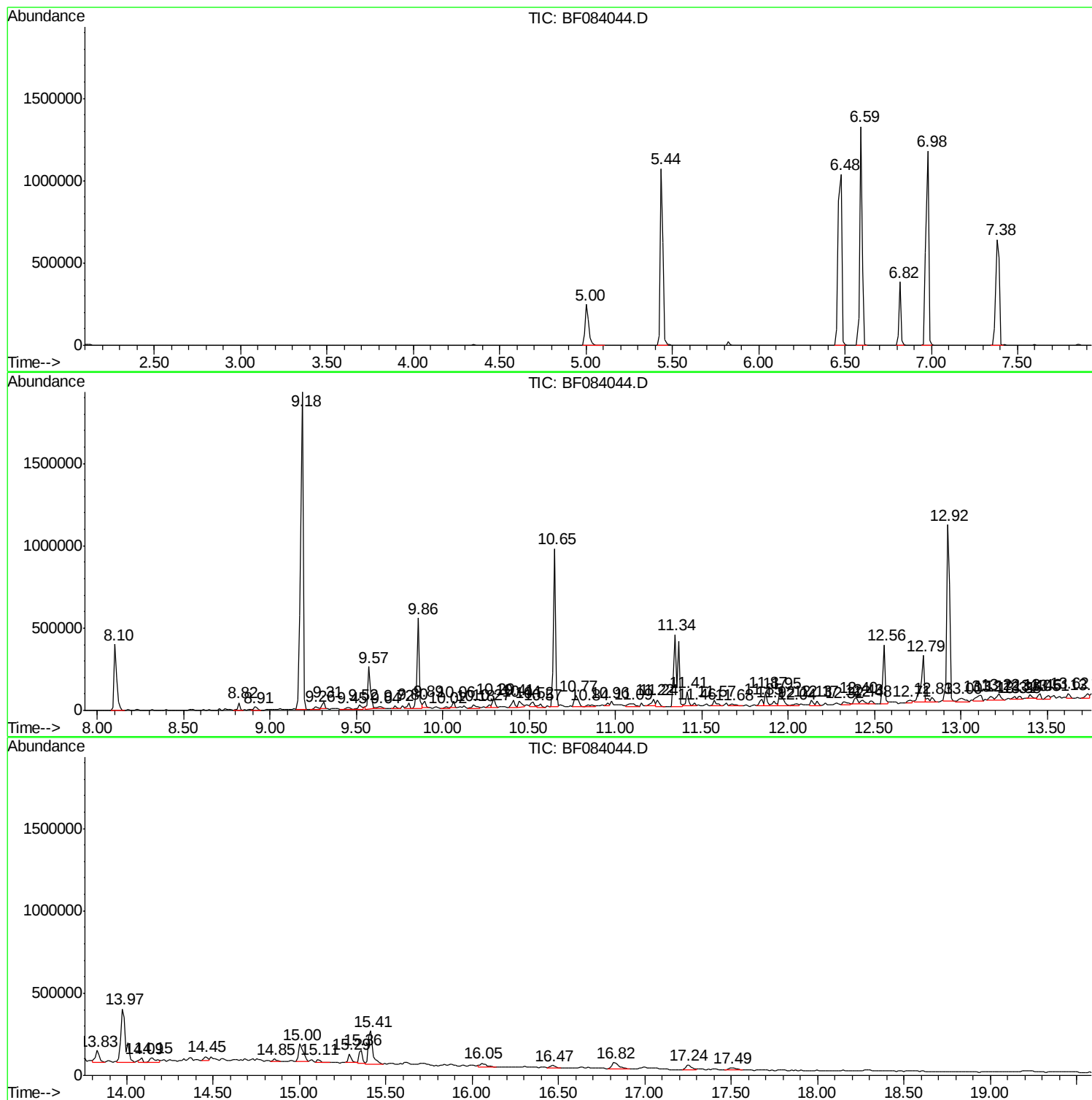
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Acq On : 23 Dec 2015 20:14
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Instrument :
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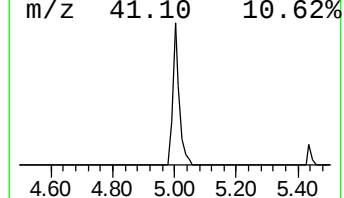
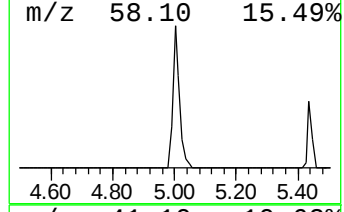
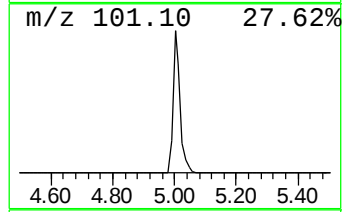
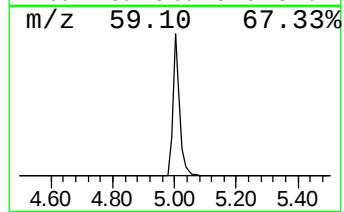
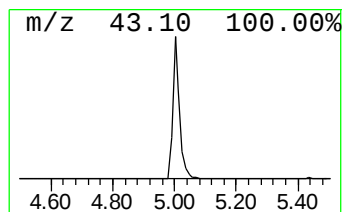
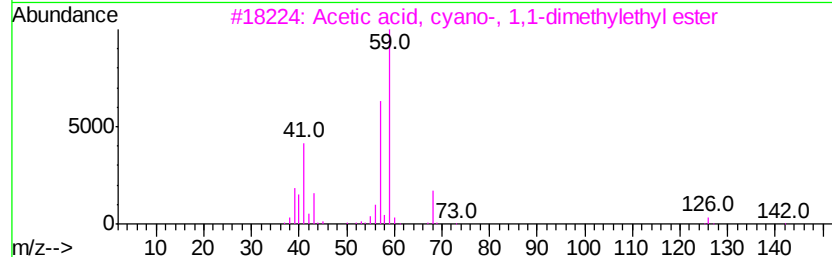
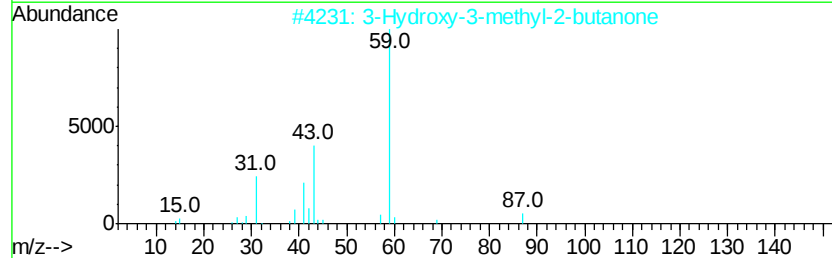
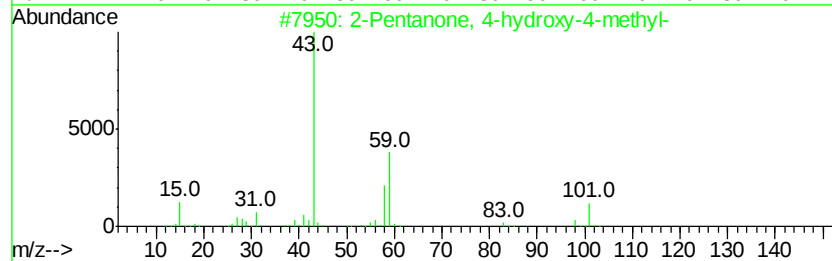
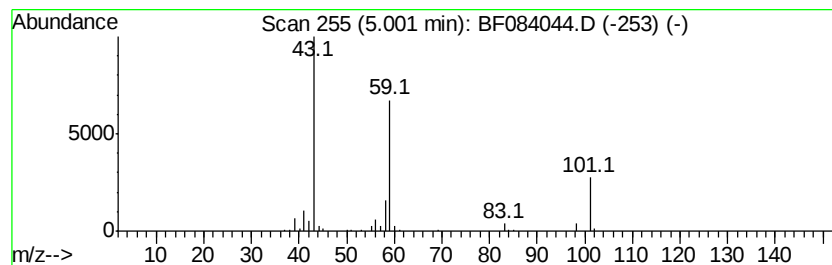
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
5.00	22.97 ng	375427	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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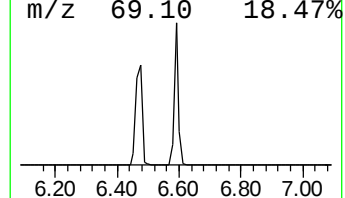
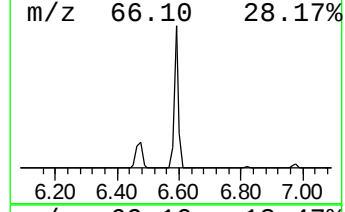
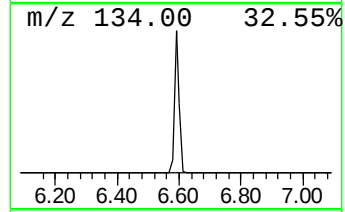
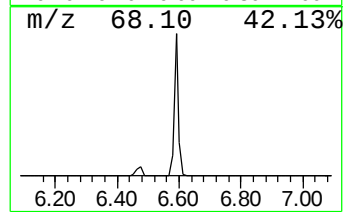
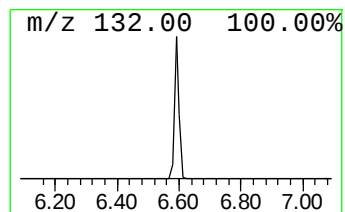
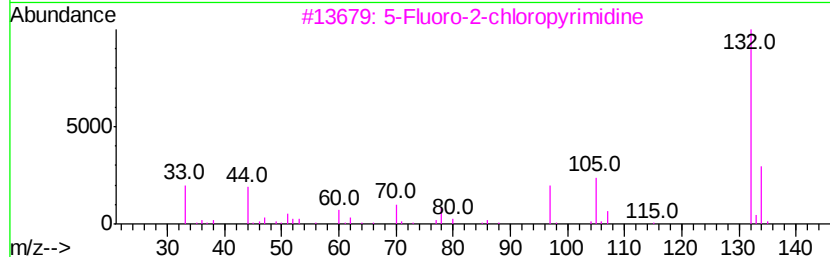
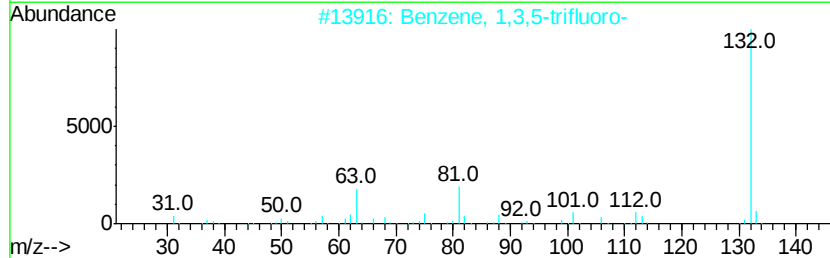
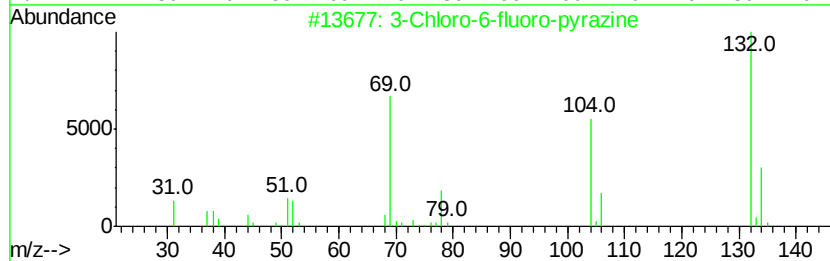
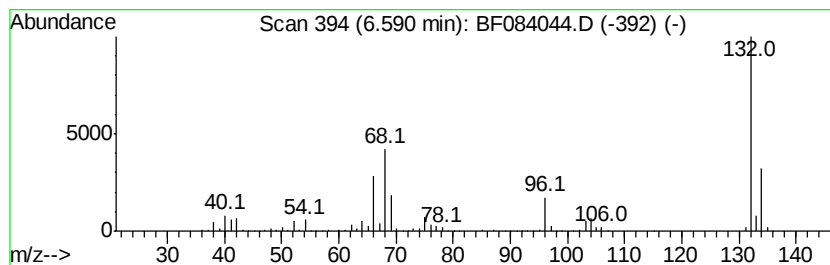
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	82.00 ng	1340160	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		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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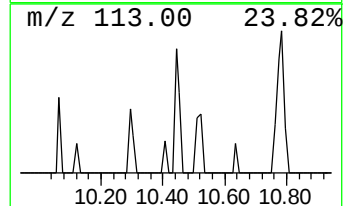
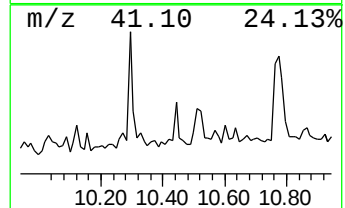
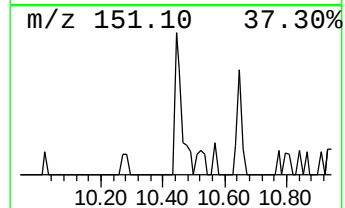
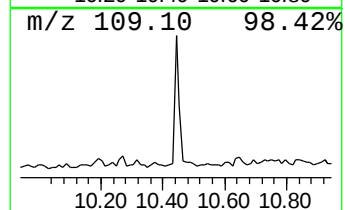
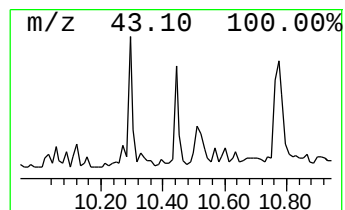
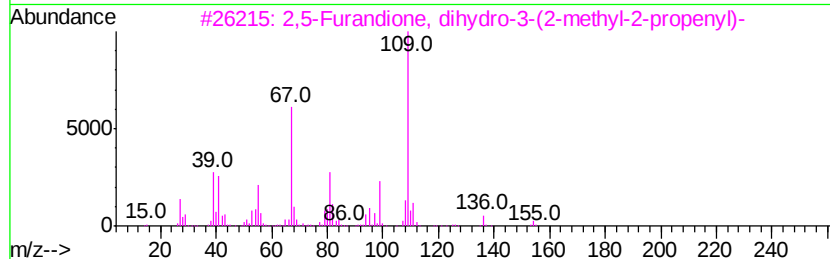
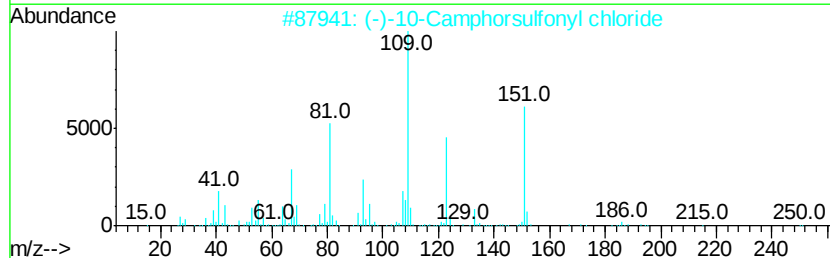
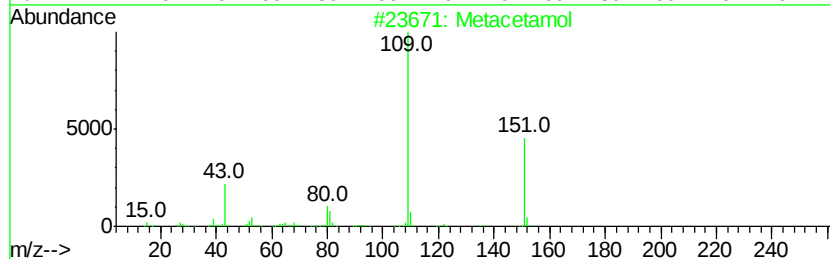
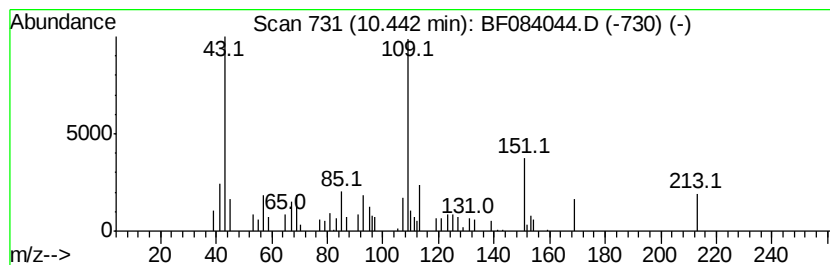
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.44 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.30 ng	59296	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Metacetamol	151	C8H9NO2	000621-42-1	43
2		(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	38
3		2,5-Furandione, dihydro-3-(2-met...	154	C8H10O3	018908-20-8	38
4		Acetaminophen	151	C8H9NO2	000103-90-2	38
5		m-Isopropoxyaniline	151	C9H13NO	041406-00-2	38



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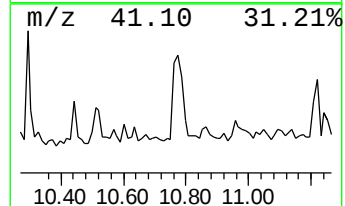
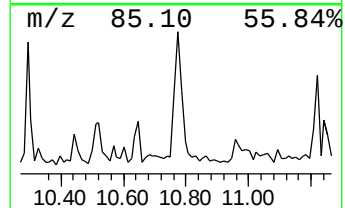
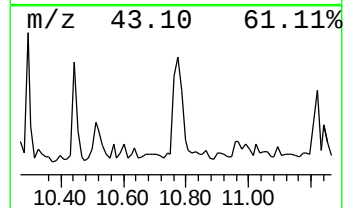
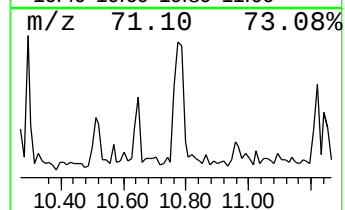
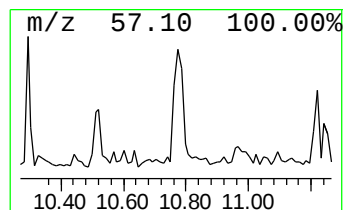
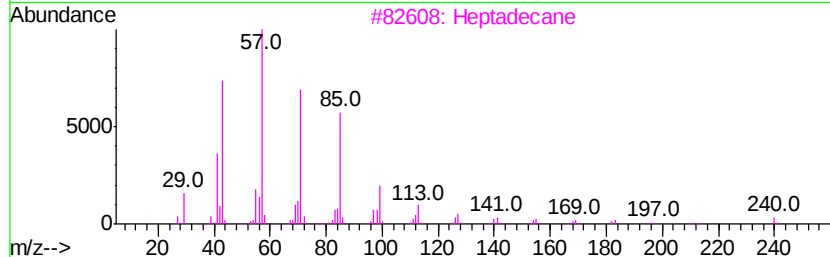
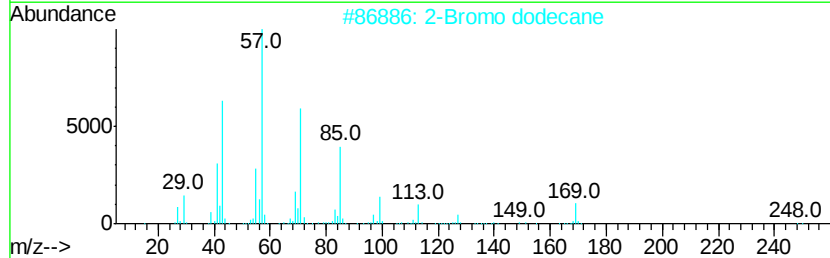
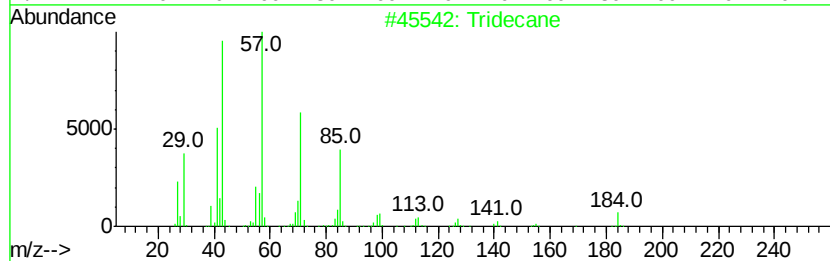
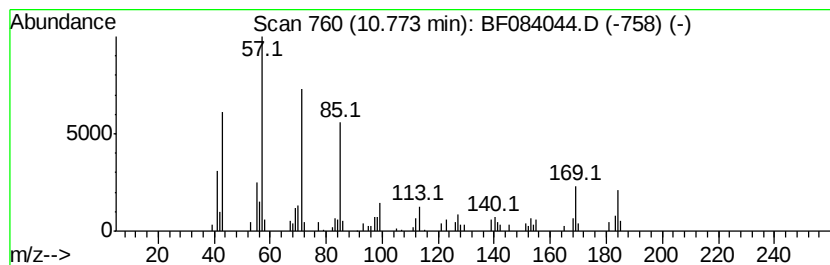
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.77 ng	109015	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	81
2	2-Bromo dodecane		248	C12H25Br	013187-99-0	64
3	Heptadecane		240	C17H36	000629-78-7	64
4	Hexacosane		366	C26H54	000630-01-3	64
5	Eicosane, 10-methyl-		296	C21H44	054833-23-7	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122315\
Data File : BF084044.D
Acq On : 23 Dec 2015 20:14
Operator : UM/SJ
Sample : G4889-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIBERTY-SF-121815

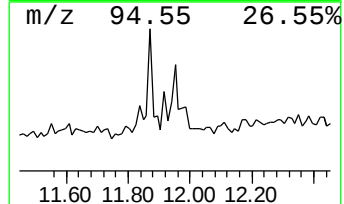
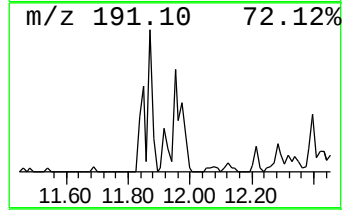
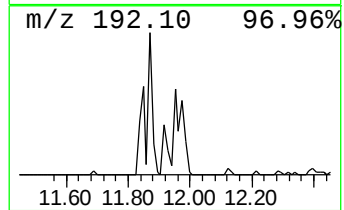
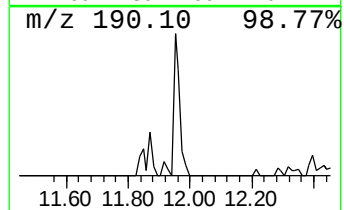
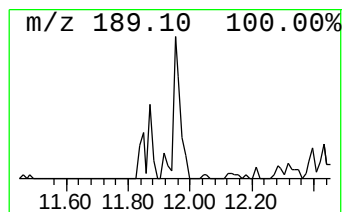
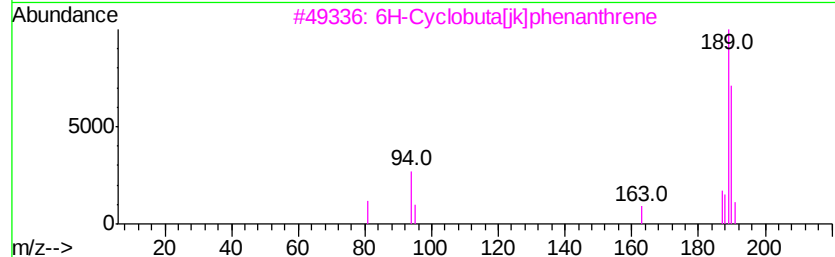
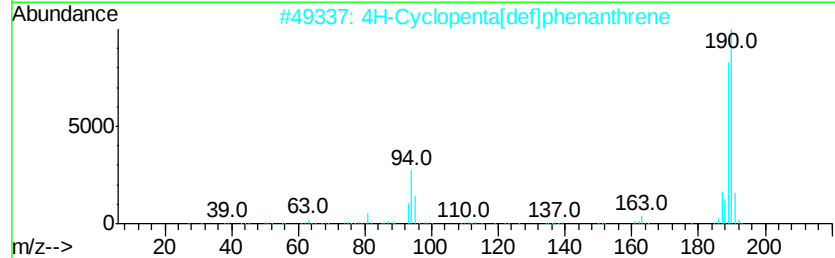
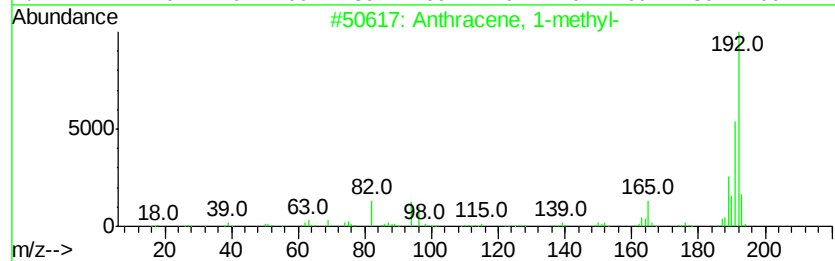
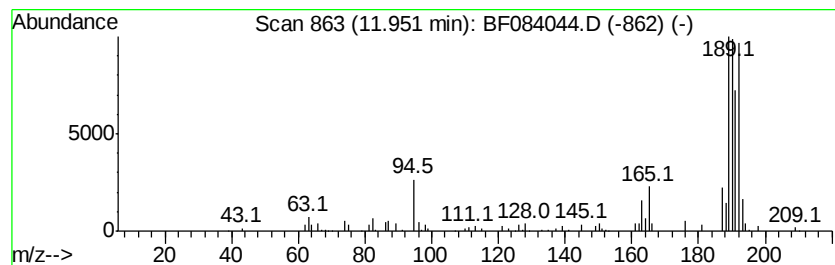
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.36 ng	132095	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	50
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3	6H-Cyclobuta[fik]phenanthrene	190	C15H10	083469-43-6	49
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	41
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	41



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122315\
Data File : BF084044.D
Acq On : 23 Dec 2015 20:14
Operator : UM/SJ
Sample : G4889-01
Misc :
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Instrument :
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ClientSampleId :
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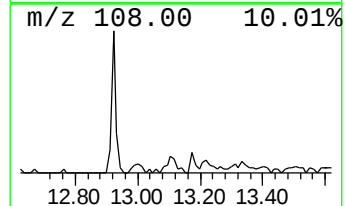
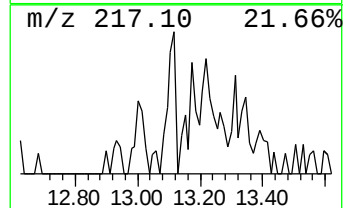
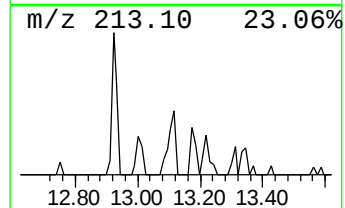
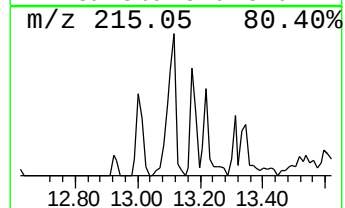
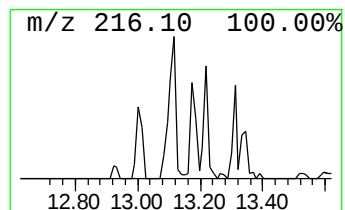
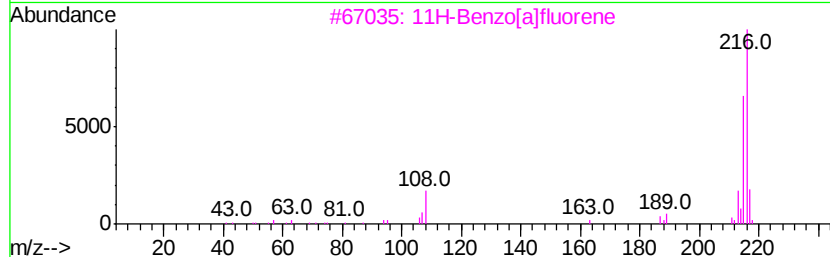
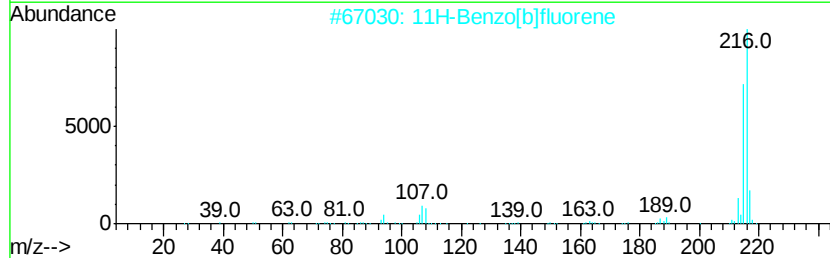
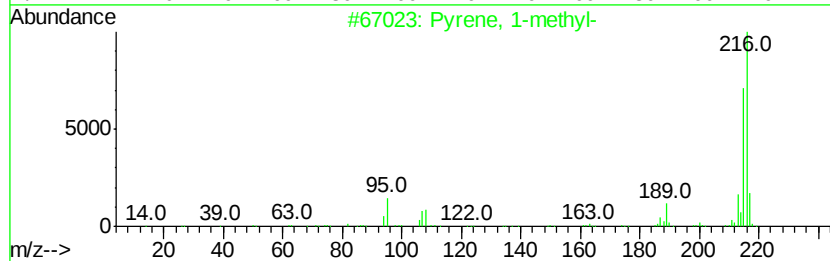
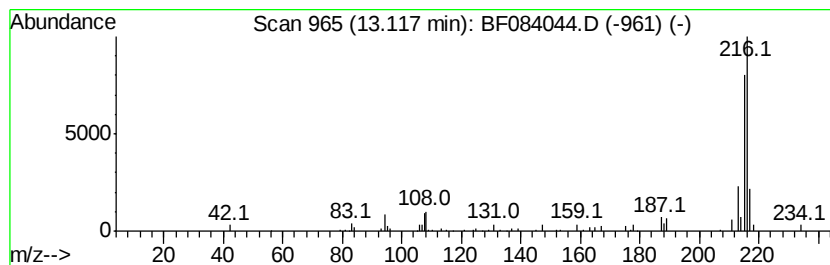
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	2.02 ng	65044	Chrysene-d12	13.99

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	90
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	80
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122315\
Data File : BF084044.D
Acq On : 23 Dec 2015 20:14
Operator : UM/SJ
Sample : G4889-01
Misc :
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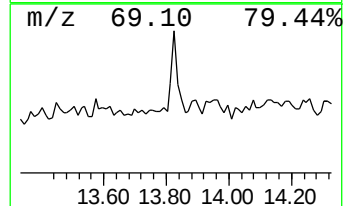
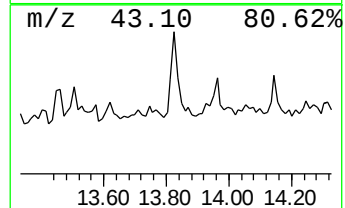
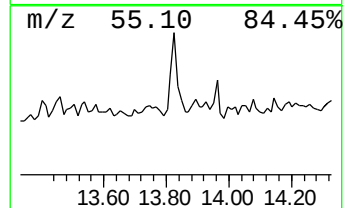
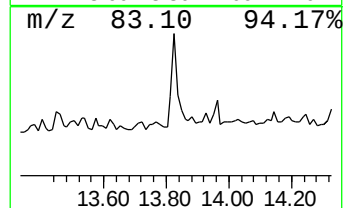
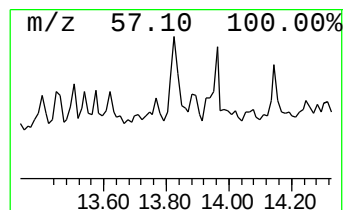
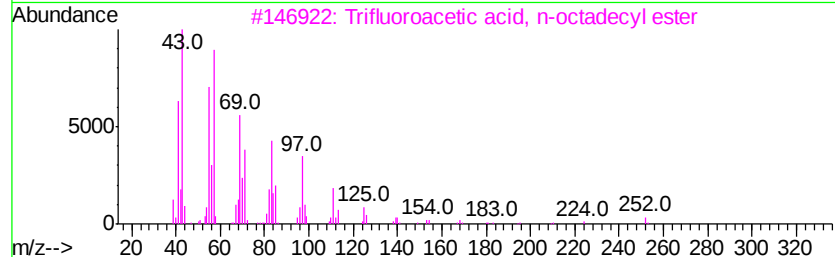
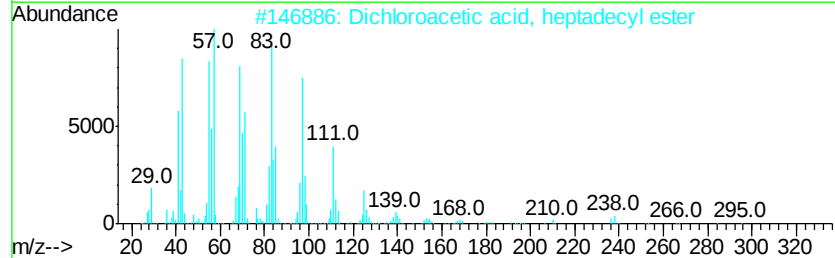
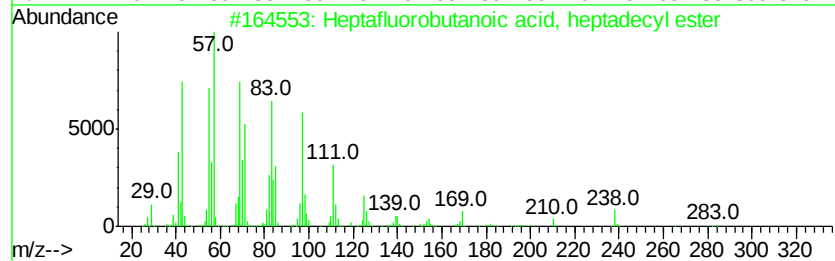
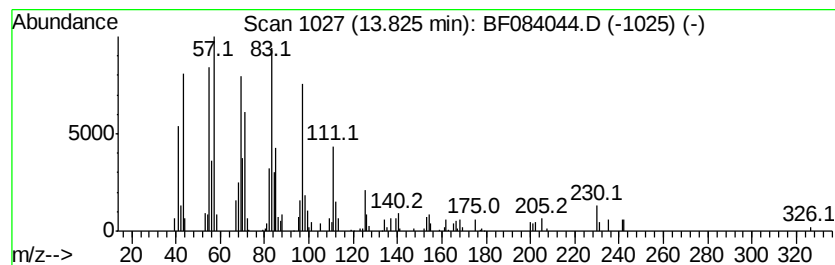
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptafluorobutanoic acid, h... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.44 ng	110766	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3		Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	90



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Operator : UM/SJ
Sample : G4889-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

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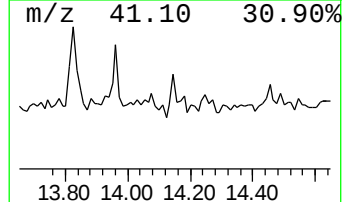
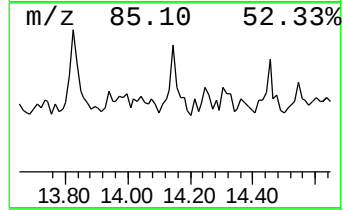
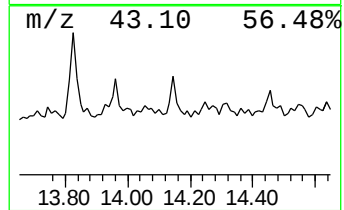
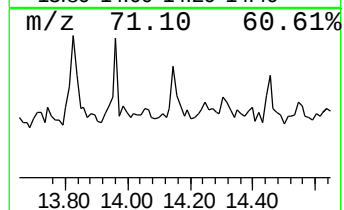
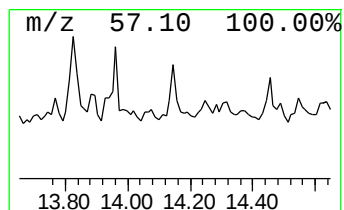
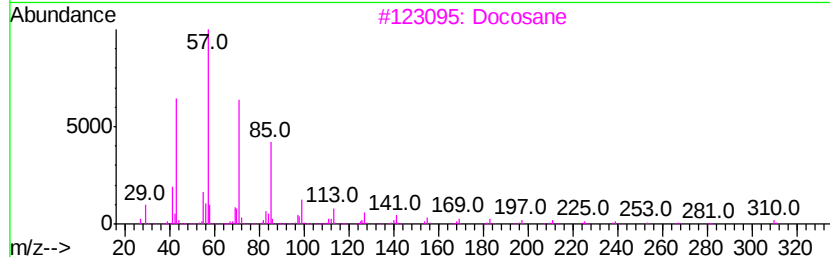
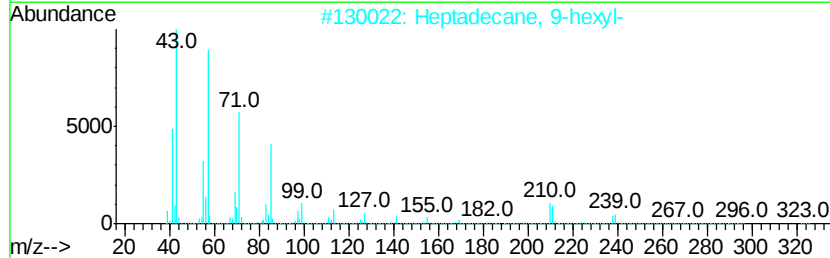
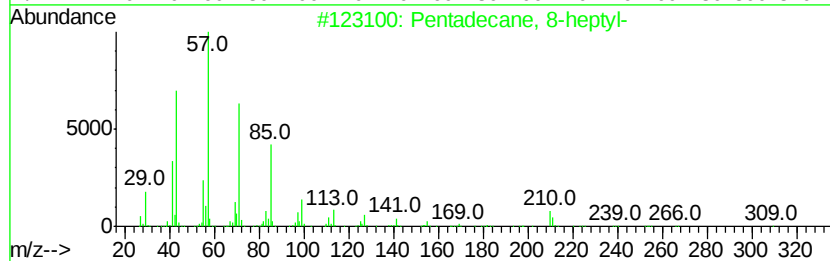
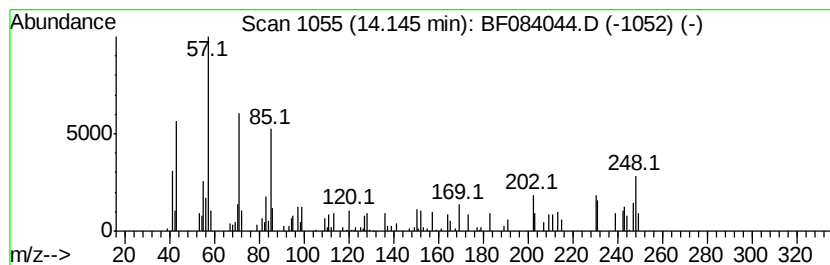
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown14.15 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	2.33 ng	74970	Chrysene-d12	13.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	38
2			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	38
3			Docosane	310	C22H46	000629-97-0	38
4			Octacosane	394	C28H58	000630-02-4	35
5			Dodecane, 2-methyl-	184	C13H28	001560-97-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122315\
Data File : BF084044.D
Acq On : 23 Dec 2015 20:14
Operator : UM/SJ
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Instrument :
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ClientSampleId :
LIBERTY-SF-121815

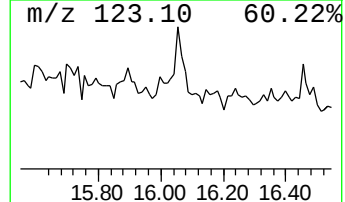
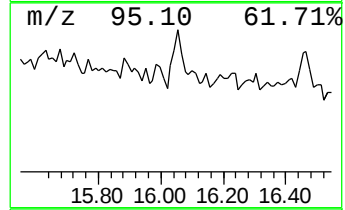
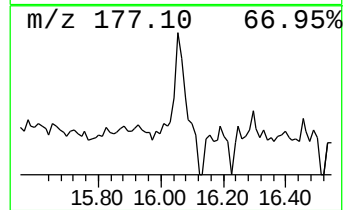
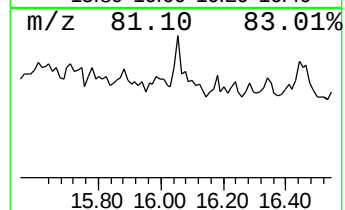
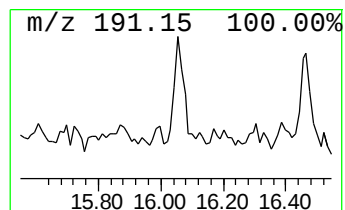
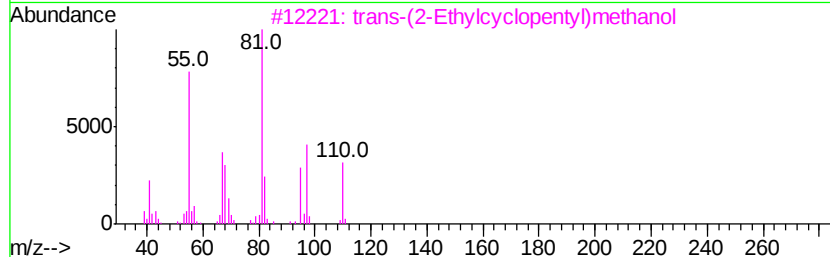
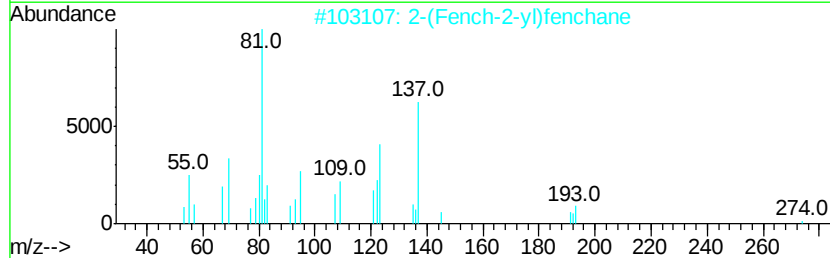
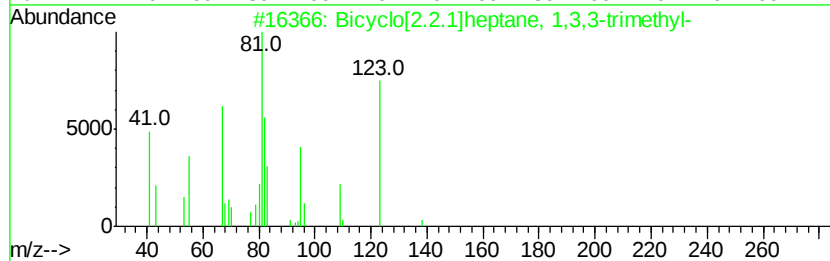
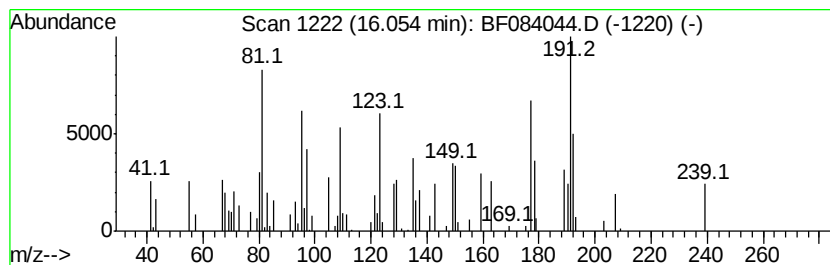
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown16.05 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	3.64 ng	62037	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	22
2		2-(Fench-2-yl)fenchane	274	C20H34	1000105-83-1	14
3		trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	14
4		Cyclopentaneethanol, 2-(hydroxym...	172	C10H20O2	000485-42-7	14
5		2-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122315\
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Acq On : 23 Dec 2015 20:14
Operator : UM/SJ
Sample : G4889-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.59	6.59	82.0	ng	1340160	1	6.82	326864	20.0
unknown10.44	10.44	2.3	ng	59296	3	9.86	516700	20.0
Tridecane	10.77	2.8	ng	109015	4	11.35	786116	20.0
Anthracene, 1-met...	11.95	3.4	ng	132095	4	11.35	786116	20.0
Pyrene, 1-methyl-	13.12	2.0	ng	65044	5	13.99	643448	20.0
Heptafluorobutano...	13.83	3.4	ng	110766	5	13.99	643448	20.0
unknown14.15	14.15	2.3	ng	74970	5	13.99	643448	20.0
unknown16.05	16.05	3.6	ng	62037	6	15.41	340921	20.0