

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
 Data File : BF092564.D
 Acq On : 27 Jan 2017 9:16
 Operator : SJ/MA
 Sample : I1353-02
 Misc :
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-13

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-BF012417.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	4.041	167	171	174	rVB	69040	141329	1.23%	0.121%
2	4.464	203	208	211	rBV3	71660	208463	1.81%	0.178%
3	5.150	266	268	272	rVV	551346	755557	6.55%	0.646%
4	5.241	272	276	278	rVV2	138509	280880	2.43%	0.240%
5	5.276	278	279	282	rVB	205561	250962	2.18%	0.214%
6	5.481	295	297	300	rVB	122369	142947	1.24%	0.122%
7	5.573	302	305	307	rVB	2698756	2540806	22.03%	2.171%
8	5.744	318	320	323	rVB	128358	159062	1.38%	0.136%
9	5.824	323	327	330	rBV5	82135	228239	1.98%	0.195%
10	5.870	330	331	333	rVB	127923	117861	1.02%	0.101%
11	6.007	341	343	345	rVB	159456	168085	1.46%	0.144%
12	6.190	355	359	360	rVV2	63891	133245	1.16%	0.114%
13	6.270	364	366	371	rBV2	99080	196781	1.71%	0.168%
14	6.476	381	384	387	rBV2	123829	190348	1.65%	0.163%
15	6.567	390	392	393	rVV	115769	124536	1.08%	0.106%
16	6.601	393	395	397	rVB	1904178	1852235	16.06%	1.583%
17	6.739	404	407	409	rBV	3913323	3982736	34.53%	3.403%
18	6.773	409	410	411	rVV	211812	215666	1.87%	0.184%
19	6.899	419	421	425	rBV2	176188	256895	2.23%	0.219%
20	6.967	425	427	429	rBV	1247290	1216618	10.55%	1.040%
21	7.036	432	433	438	rVB	176669	138940	1.20%	0.119%
22	7.127	438	441	444	rBV	3726429	4000504	34.68%	3.418%
23	7.219	447	449	450	rVB2	161153	159003	1.38%	0.136%
24	7.310	454	457	460	rBV3	257962	445461	3.86%	0.381%
25	7.379	460	463	464	rBV2	118990	201390	1.75%	0.172%
26	7.424	464	467	469	rVB	261930	488421	4.23%	0.417%
27	7.539	469	477	479	rBV	3027797	5232026	45.36%	4.470%
28	7.584	479	481	483	rVB2	335338	542402	4.70%	0.463%
29	7.619	483	484	486	rBV2	150928	204829	1.78%	0.175%
30	7.664	486	488	489	rBV2	123799	117067	1.01%	0.100%
31	7.699	489	491	494	rVB3	83031	153516	1.33%	0.131%
32	7.744	494	495	497	rVB	197186	251330	2.18%	0.215%
33	7.802	497	500	501	rBV3	185528	330305	2.86%	0.282%
34	7.836	501	503	505	rVB2	124880	173084	1.50%	0.148%

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35	7.927	508	511	514	rBV3	508905	1069668	9.27%	0.914%
36	7.996	514	517	520	rBV4	236999	453950	3.94%	0.388%
37	8.064	520	523	527	rVB3	568632	985654	8.54%	0.842%
38	8.145	527	530	531	rBV2	119197	214946	1.86%	0.184%
39	8.202	531	535	536	rBV2	594107	1077230	9.34%	0.920%
40	8.259	536	540	542	rVB2	1501263	2497402	21.65%	2.134%
41	8.316	544	545	549	rVB4	435856	683501	5.93%	0.584%
42	8.430	549	555	557	rBV3	670282	1470272	12.75%	1.256%
43	8.522	557	563	564	rBV2	1078436	2451625	21.25%	2.095%
44	8.556	564	566	571	rVB4	530582	989835	8.58%	0.846%
45	8.659	571	575	577	rBV4	342480	890126	7.72%	0.761%
46	8.705	577	579	586	rBV3	556300	1888563	16.37%	1.614%
47	8.807	586	588	589	rVB	494856	569706	4.94%	0.487%
48	8.853	589	592	594	rBV3	457016	744033	6.45%	0.636%
49	8.910	594	597	600	rBV4	292533	596744	5.17%	0.510%
50	8.967	600	602	604	rBV2	524337	820656	7.11%	0.701%
51	9.013	604	606	608	rBV	814669	1121095	9.72%	0.958%
52	9.059	608	610	612	rBV	815211	1337276	11.59%	1.143%
53	9.093	612	613	614	rVV	427995	344528	2.99%	0.294%
54	9.127	614	616	618	rVB2	542219	729200	6.32%	0.623%
55	9.162	618	619	621	rBV2	479029	846264	7.34%	0.723%
56	9.219	621	624	625	rVB3	456892	802032	6.95%	0.685%
57	9.310	628	632	633	rBV3	873871	1709379	14.82%	1.461%
58	9.356	633	636	637	rVB	4314289	5470814	47.43%	4.674%
59	9.379	637	638	639	rBV	389707	356494	3.09%	0.305%
60	9.402	639	640	642	rVB2	621853	842188	7.30%	0.720%
61	9.470	642	646	648	rBV5	667564	1768283	15.33%	1.511%
62	9.516	648	650	652	rBV3	835766	949164	8.23%	0.811%
63	9.550	652	653	655	rVB2	362777	328636	2.85%	0.281%
64	9.596	655	657	661	rVB4	600185	1445101	12.53%	1.235%
65	9.676	661	664	665	rBV3	645138	1087105	9.42%	0.929%
66	9.710	665	667	669	rBV3	441991	995459	8.63%	0.851%
67	9.745	669	670	674	rVB	628792	896415	7.77%	0.766%
68	10.030	691	695	696	rBV2	2135062	3068681	26.60%	2.622%
69	10.110	700	702	703	rBV	811693	791150	6.86%	0.676%
70	10.145	703	705	706	rVB	580541	523335	4.54%	0.447%
71	10.202	708	710	712	rBV2	542298	922031	7.99%	0.788%

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72	10.350	721	723	725	rBV2	560233	1170186	10.14%	1.000%
73	10.453	725	732	733	rVV	3562481	11535360	100.00%	9.856%
74	10.488	733	735	737	rVV2	1080284	1877141	16.27%	1.604%
75	10.545	737	740	743	rVB4	1038412	2475504	21.46%	2.115%
76	10.613	743	746	748	rBV2	586267	850915	7.38%	0.727%
77	10.659	748	750	753	rBV3	605713	1331027	11.54%	1.137%
78	10.728	753	756	759	rVB2	1668850	3047963	26.42%	2.604%
79	10.830	763	765	767	rVV2	1327568	1866097	16.18%	1.594%
80	10.922	769	773	777	rVB3	1965462	4388153	38.04%	3.749%
81	11.162	791	794	796	rVB2	1795355	3420203	29.65%	2.922%
82	11.196	796	797	802	rBV3	576089	1163171	10.08%	0.994%
83	11.425	813	817	821	rBV2	2133197	4520151	39.19%	3.862%
84	11.528	824	826	828	rVB	1617638	1603371	13.90%	1.370%
85	11.562	828	829	831	rBV	255232	364036	3.16%	0.311%
86	11.859	853	855	856	rBV	427228	358877	3.11%	0.307%
87	11.962	862	864	865	rVB	246211	244062	2.12%	0.209%
88	12.316	892	895	897	rBV	257739	431114	3.74%	0.368%
89	12.934	947	949	951	rVB	437889	406269	3.52%	0.347%
90	13.116	962	965	968	rVB	3499770	3942144	34.17%	3.368%
91	13.631	1008	1010	1012	rVB	328546	300125	2.60%	0.256%
92	13.676	1012	1014	1024	rVB2	126482	329607	2.86%	0.282%
93	14.168	1054	1057	1059	rVB	1001382	1037493	8.99%	0.886%
94	15.642	1183	1186	1195	rVB	576630	1034943	8.97%	0.884%

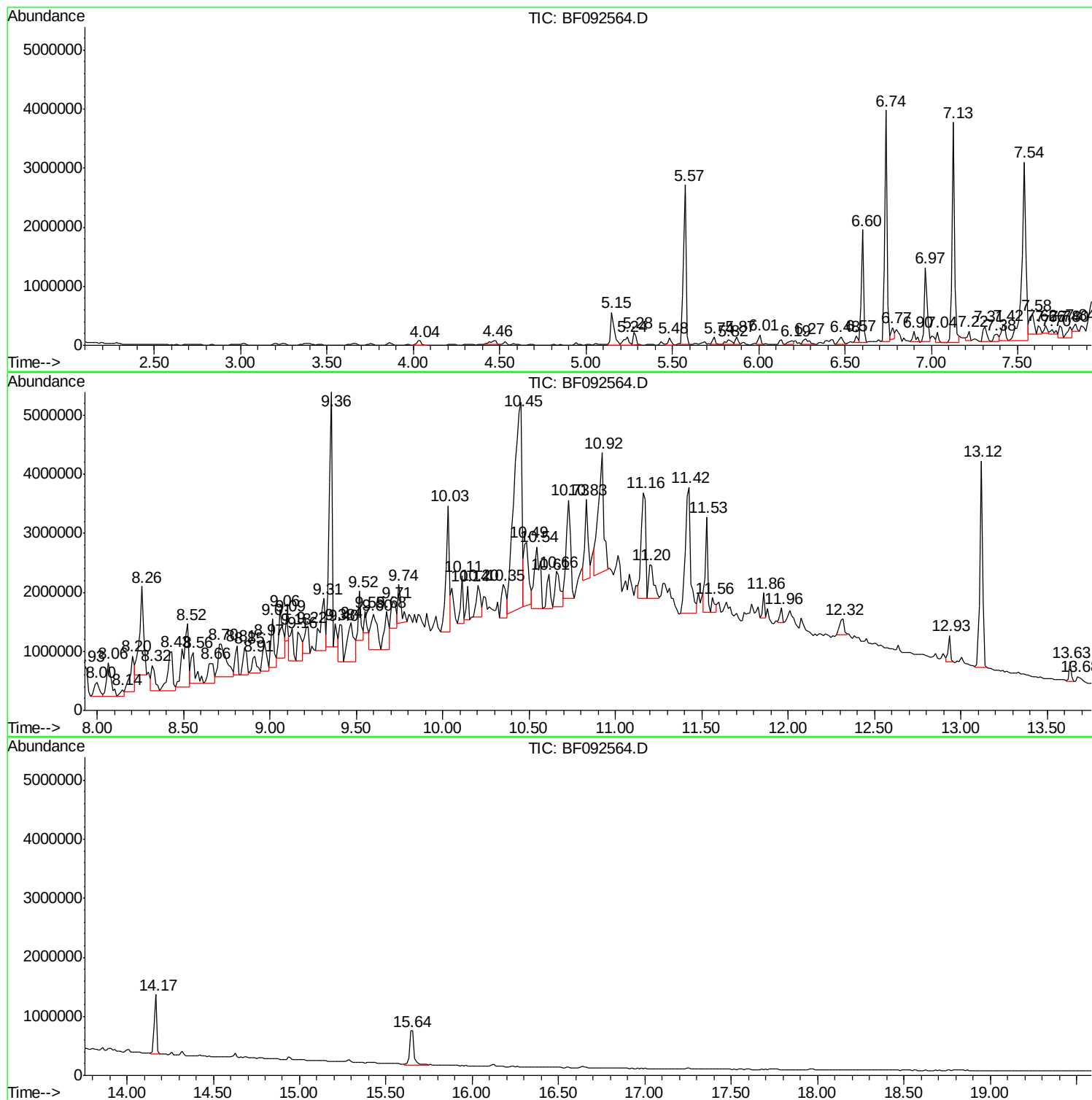
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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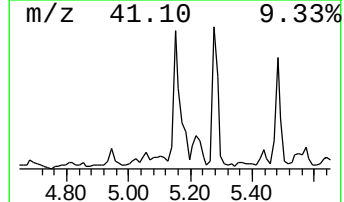
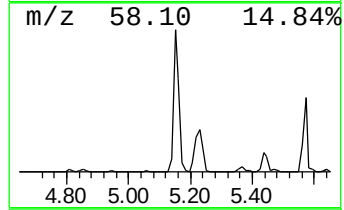
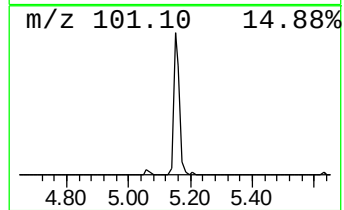
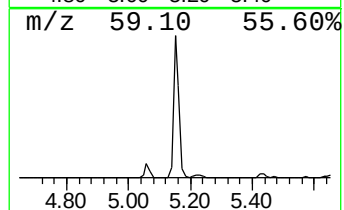
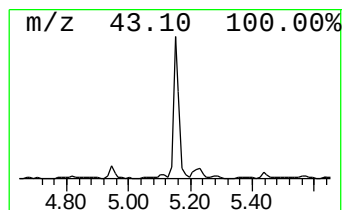
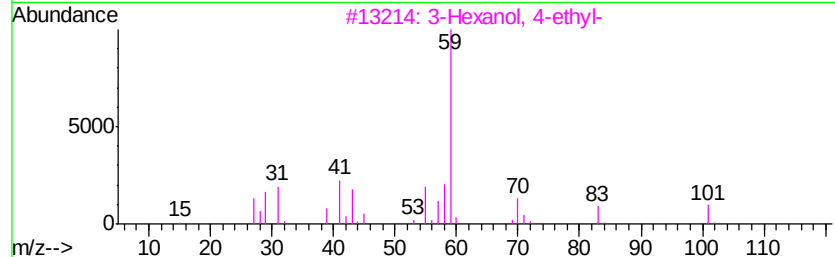
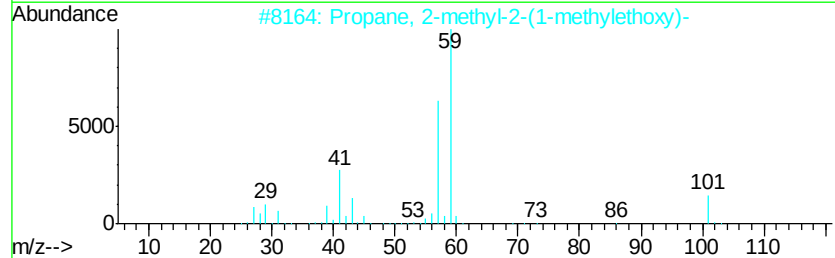
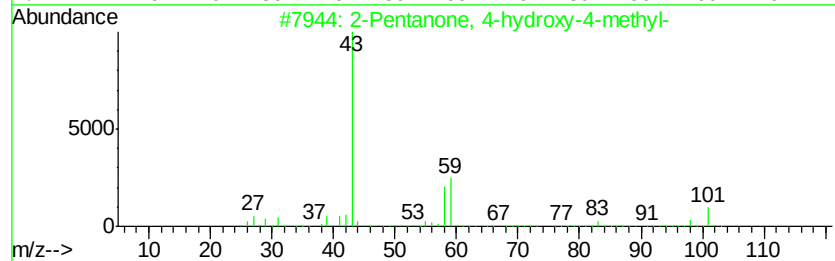
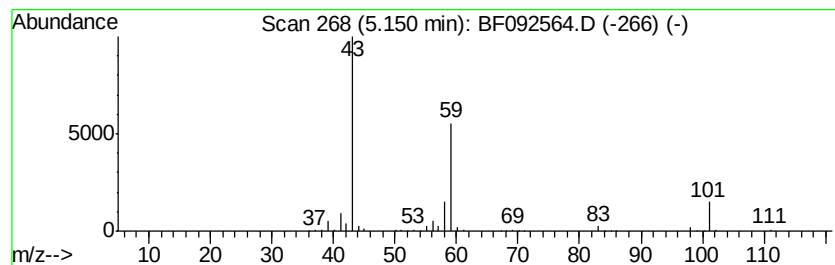
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	12.42 ng	755557	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		3-Octanol	130	C8H18O	000589-98-0	33



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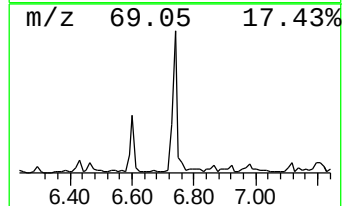
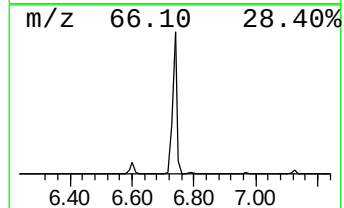
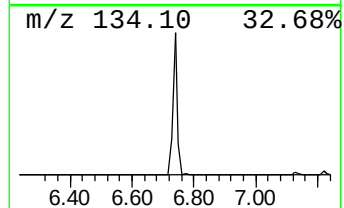
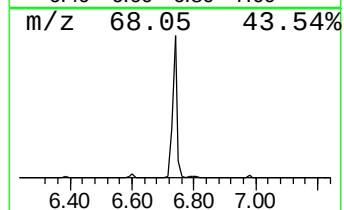
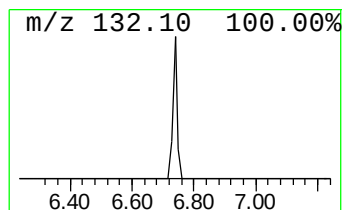
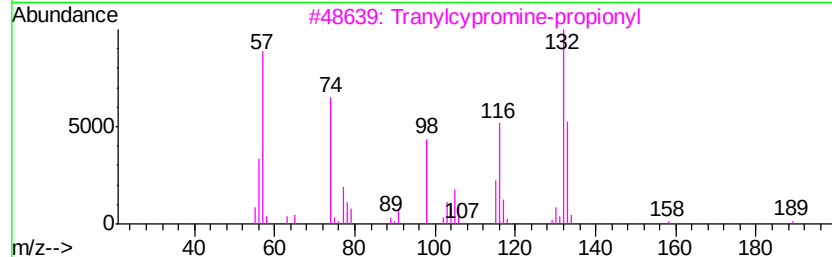
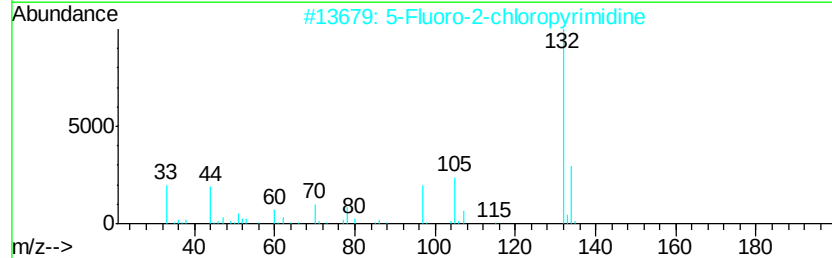
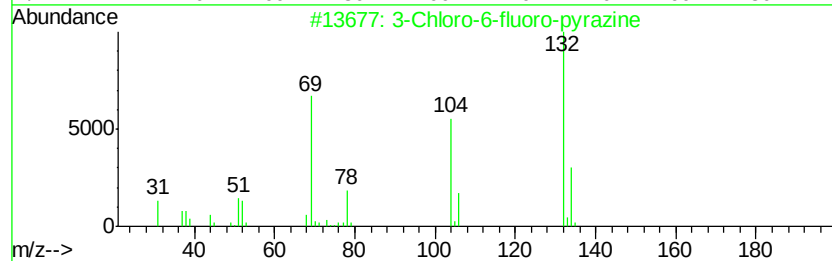
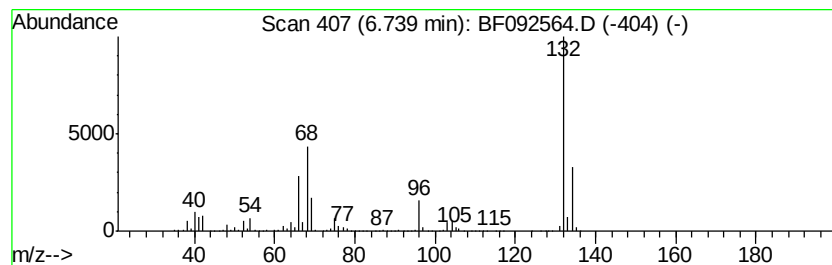
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	65.47 ng	3982740	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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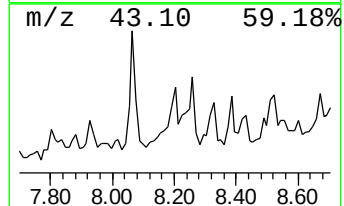
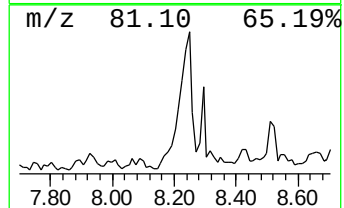
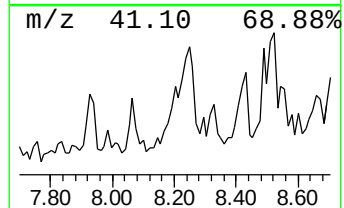
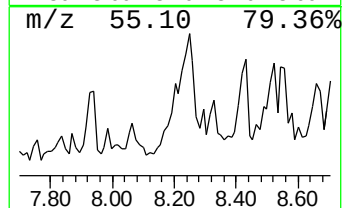
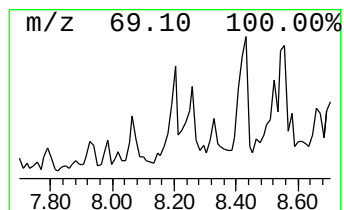
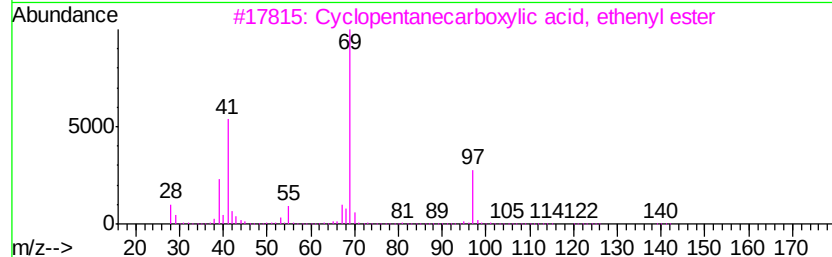
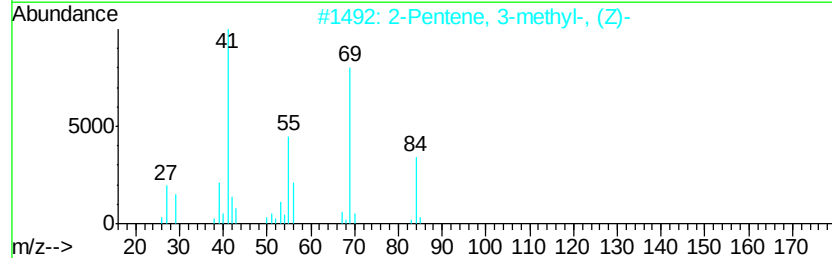
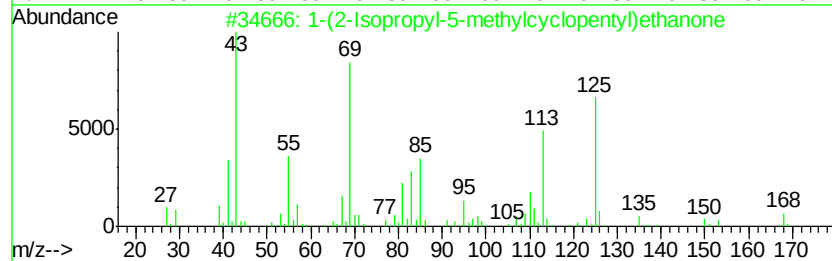
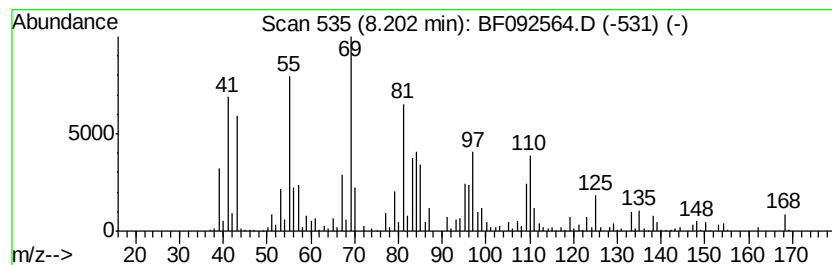
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.20 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.20	8.63 ng	1077230	Naphthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(2-Isopropyl-5-methylcyclopent...	168	C11H20O	1000191-21-0	30
2		2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	30
3		Cyclopentanecarboxylic acid, eth...	140	C8H12O2	016523-06-1	27
4		2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	27
5		3-Penten-2-one	84	C5H8O	000625-33-2	27



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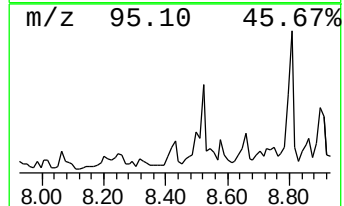
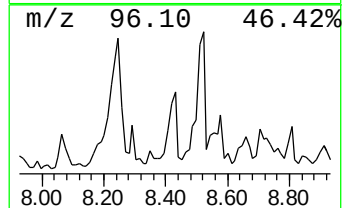
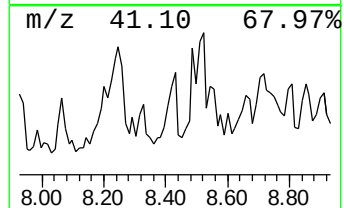
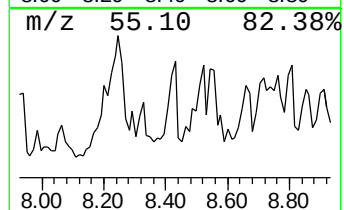
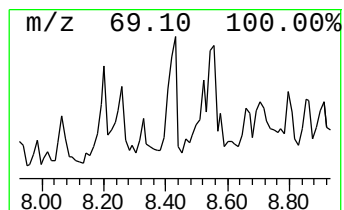
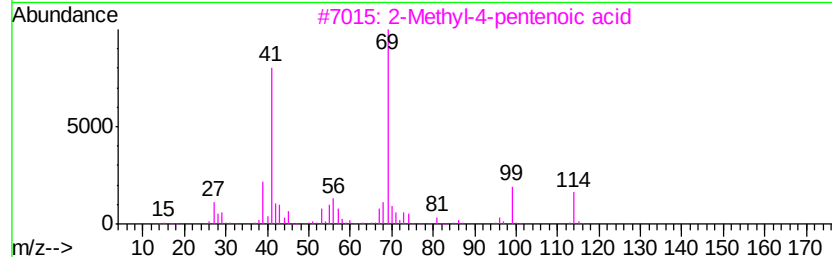
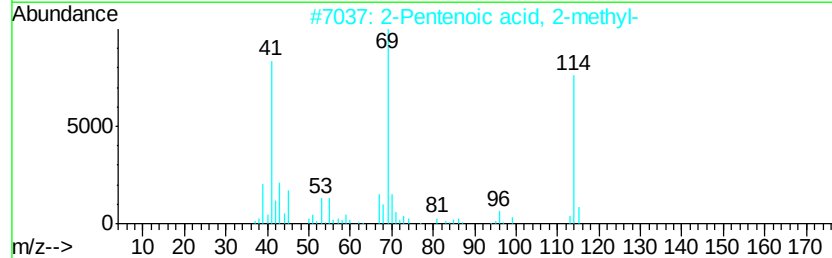
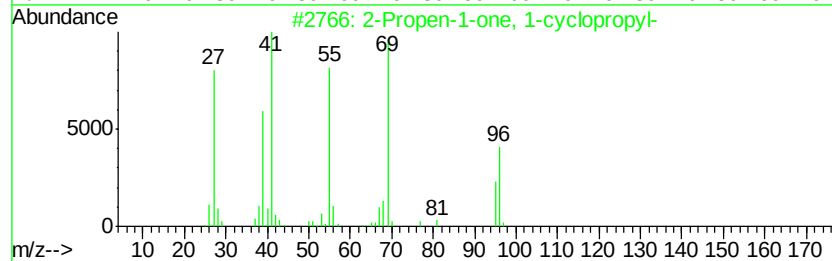
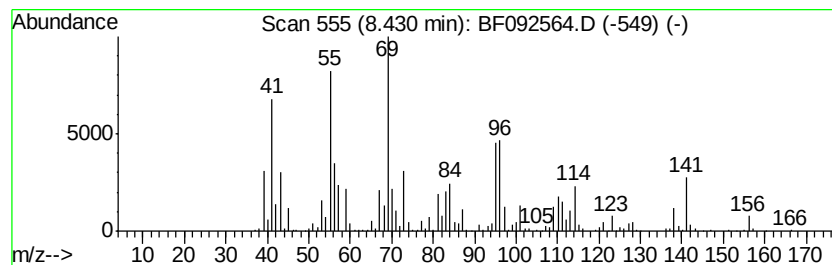
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.43 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.43	11.77 ng	1470270	Naphthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propen-1-one, 1-cyclopropyl-	96	C6H8O	059819-62-4	43
2		2-Pentenoic acid, 2-methyl-	114	C6H10O2	003142-72-1	30
3		2-Methyl-4-pentenoic acid	114	C6H10O2	001575-74-2	27
4		2-Pentenoic acid, 2-methyl-, (E)-	114	C6H10O2	016957-70-3	27
5		2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
Operator : SJ/MA
Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-13

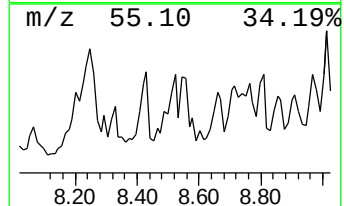
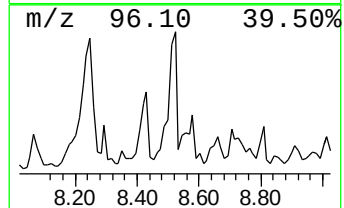
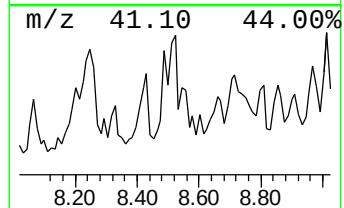
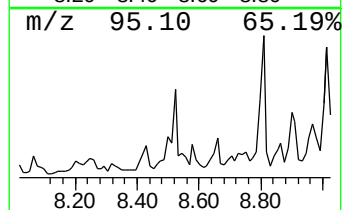
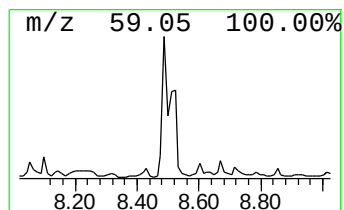
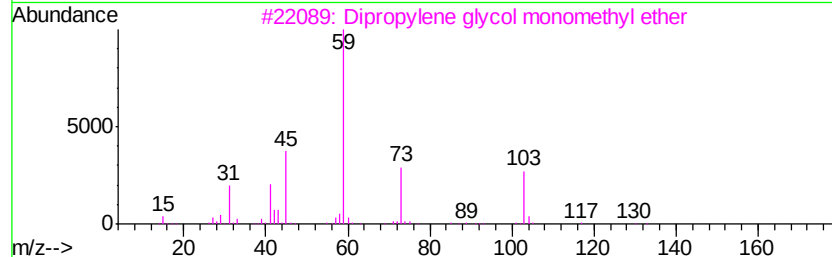
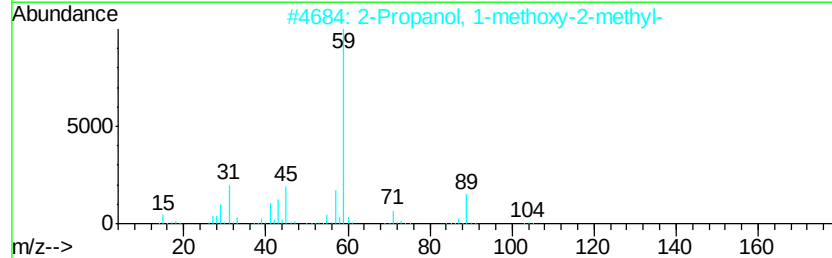
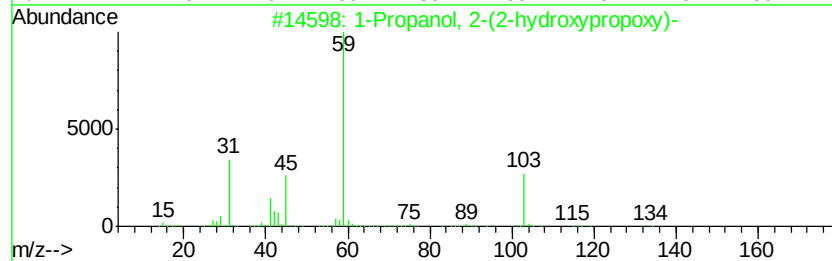
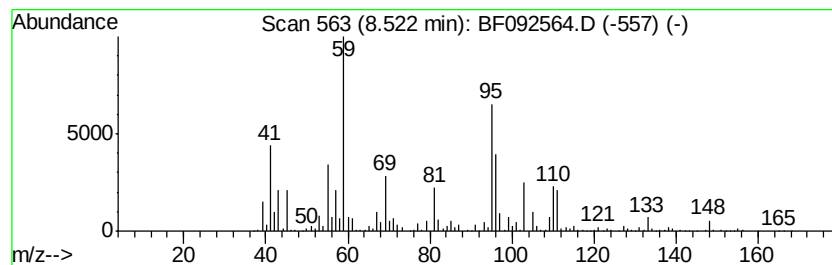
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.52 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	19.63 ng	2451630	Napthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	35
2		2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	27
3		Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	27
4		3-Methyl-oxirane-2-carboxylic ac...	116	C5H8O3	1000194-20-4	27
5		2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
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Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleID :
MW-13

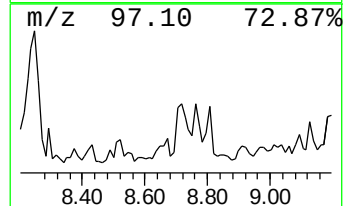
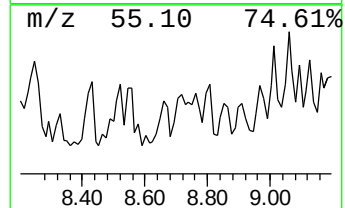
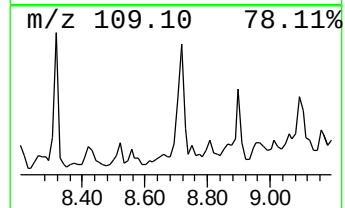
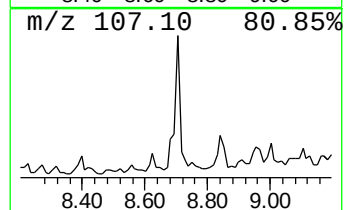
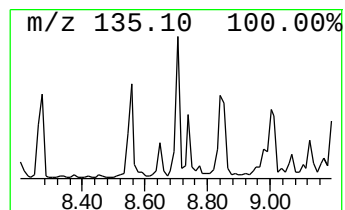
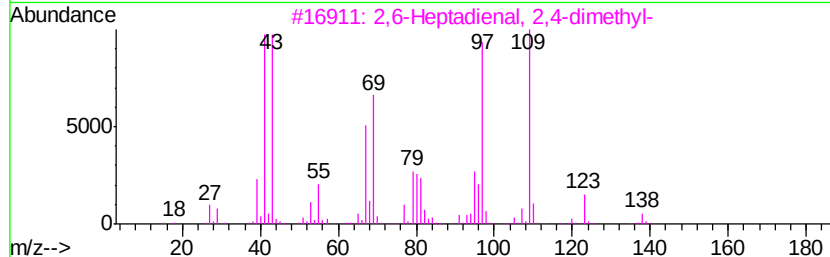
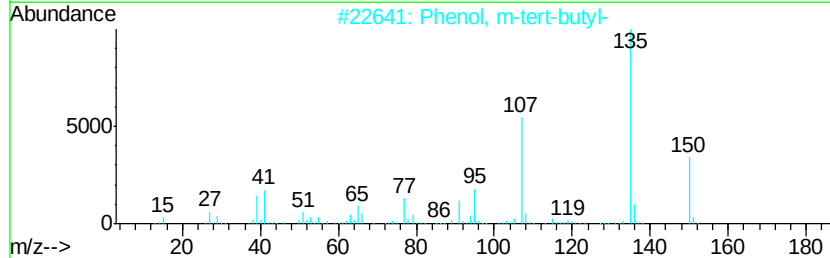
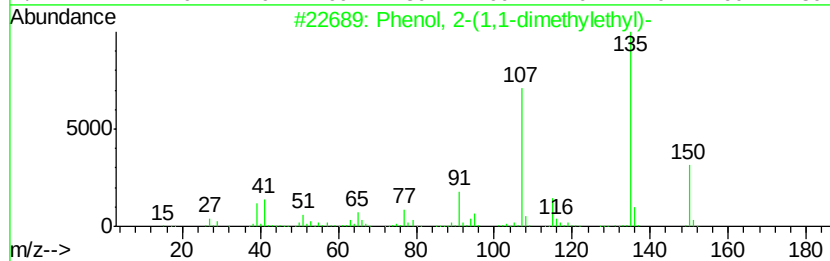
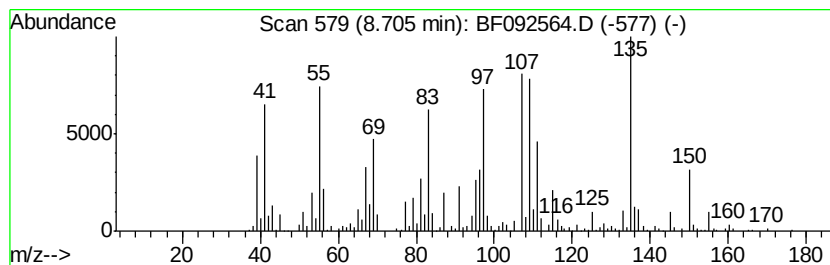
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	15.12 ng	1888560	Napthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	83
2		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	38
3		2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	30
4		1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	25
5		4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
Operator : SJ/MA
Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

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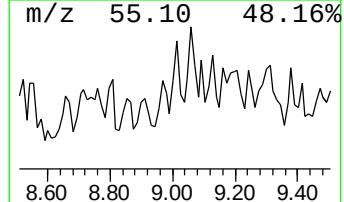
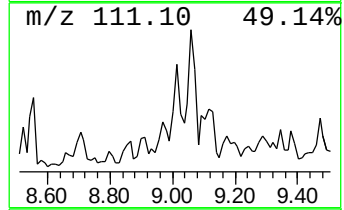
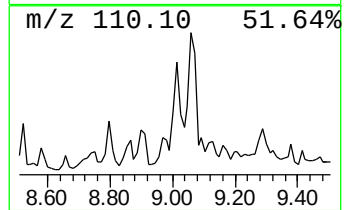
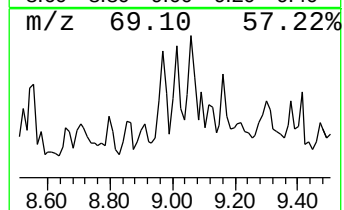
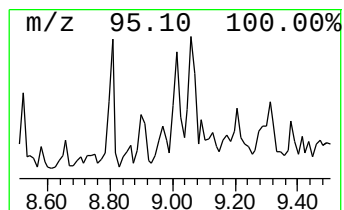
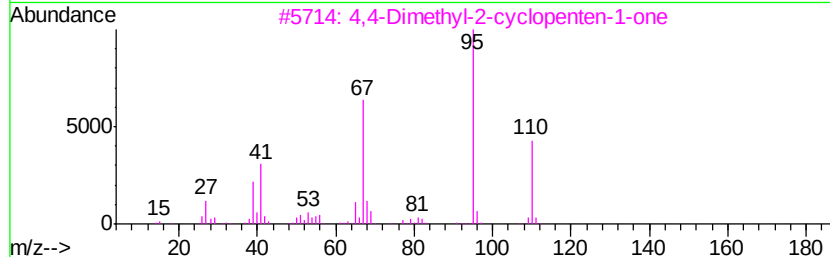
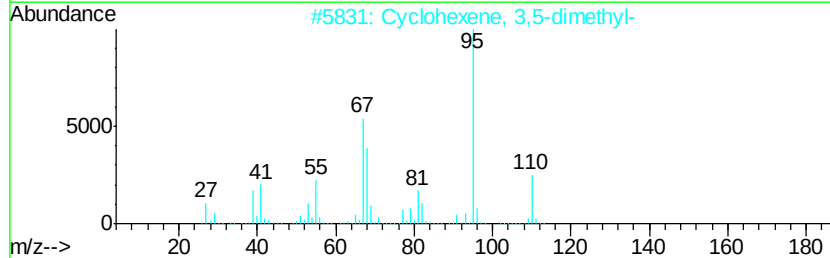
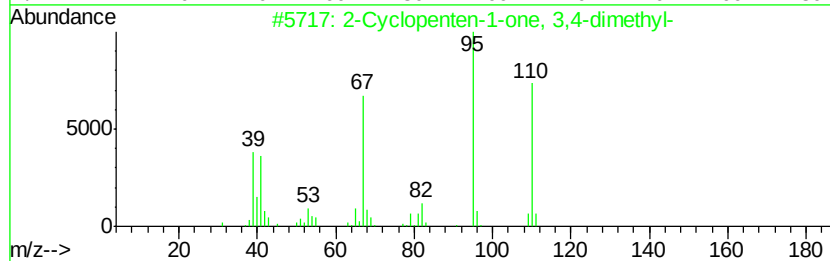
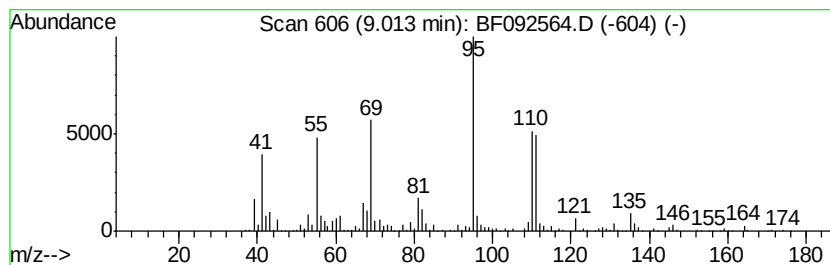
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Cyclopenten-1-one, 3,4-di... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	8.98 ng	1121100	Napthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	52
2		Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	50
3		4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	49
4		Cyclobutene, 1,2,3,4-tetramethyl-	110	C8H14	090346-45-5	47
5		Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
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Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

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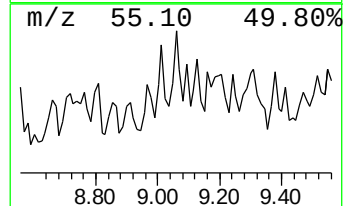
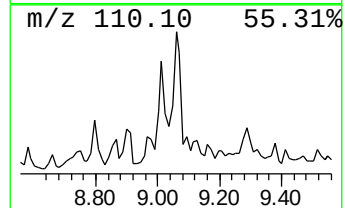
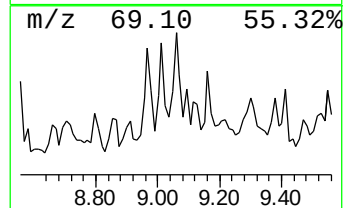
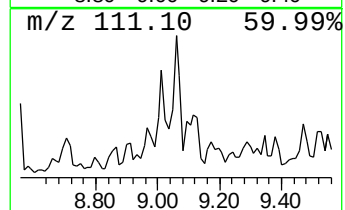
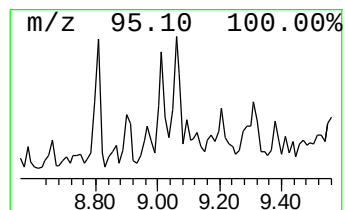
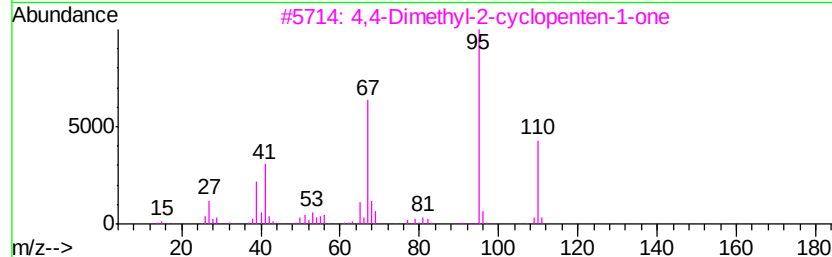
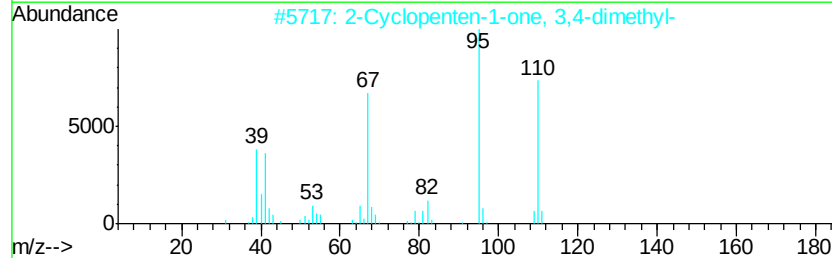
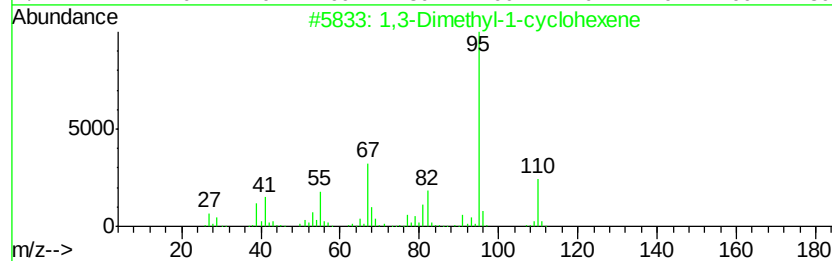
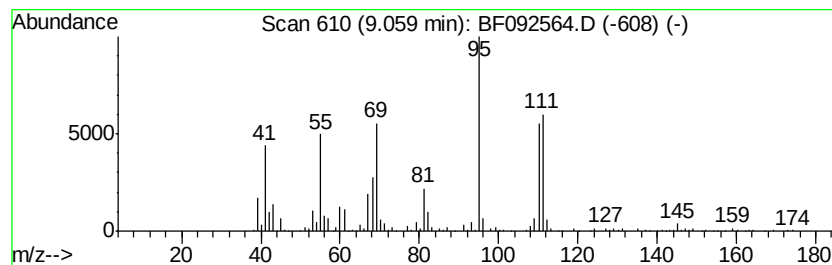
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,3-Dimethyl-1-cyclohexene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	10.71 ng	1337280	Napthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	53
2		2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	49
3		4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	47
4		1,2-Dimethyl-4-heptafluorobutyl...	324	C12H15F7O2	1000216-64-4	38
5		2-Pyrimidinamine	95	C4H5N3	000109-12-6	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
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Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-13

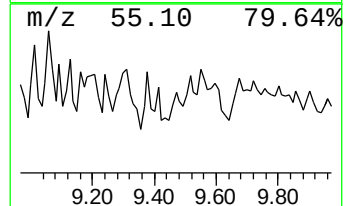
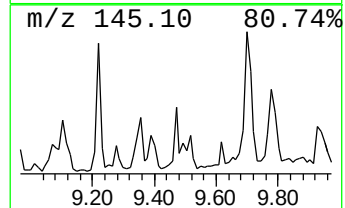
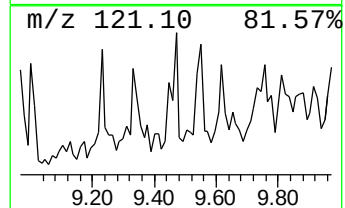
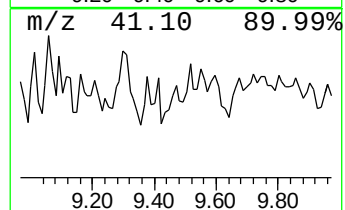
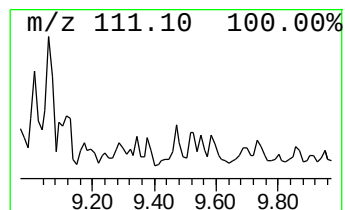
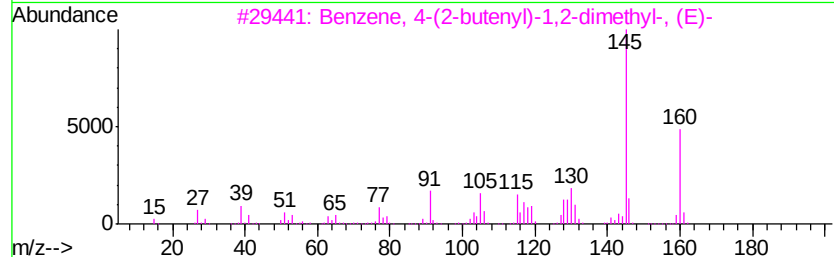
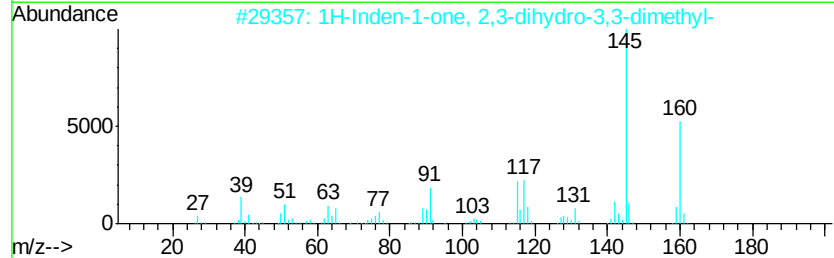
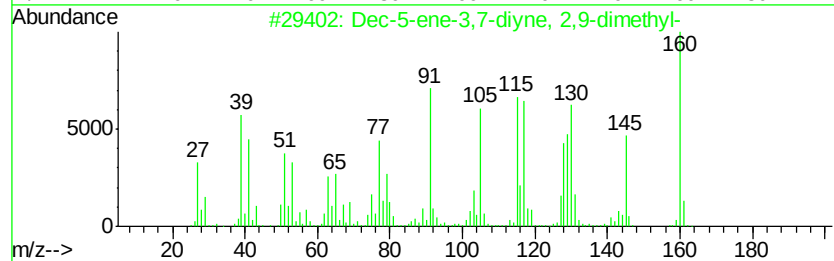
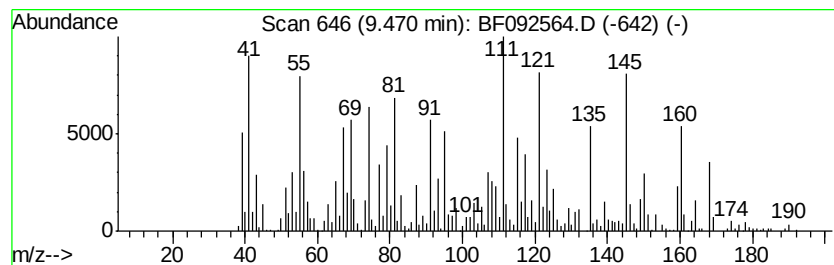
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.47 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.47	11.52 ng	1768280	Acenaphthene-d10	10.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dec-5-ene-3,7-diyne, 2,9-dimethyl-	160	C12H16	1000211-23-3	41
2		1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	30
3		Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	25
4		Hex-3-ene-1,5-diyne, 3,4-diisopr...	160	C12H16	1000211-22-8	25
5		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092564.D
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Misc :
ALS Vial : 51 Sample Multiplier: 1

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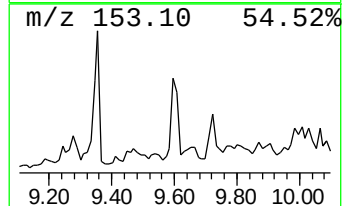
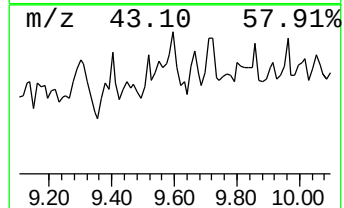
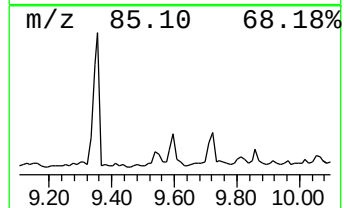
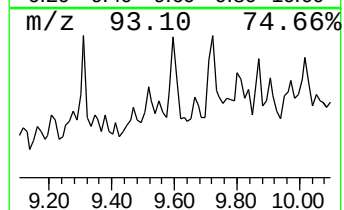
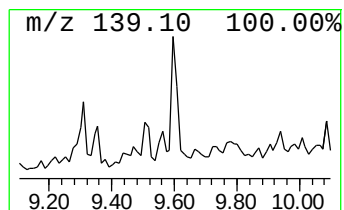
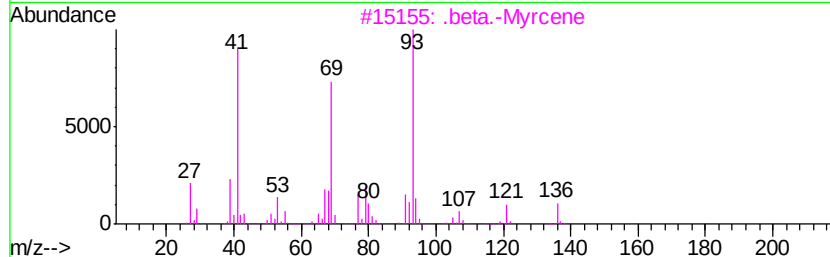
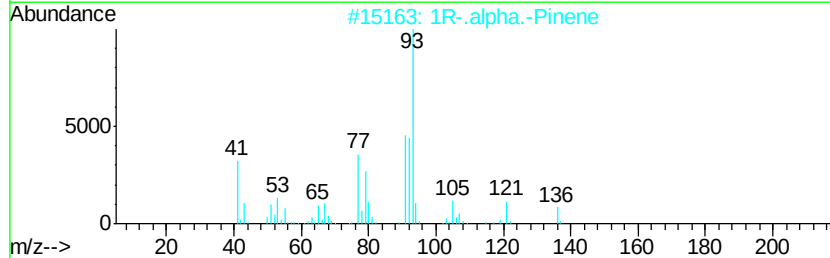
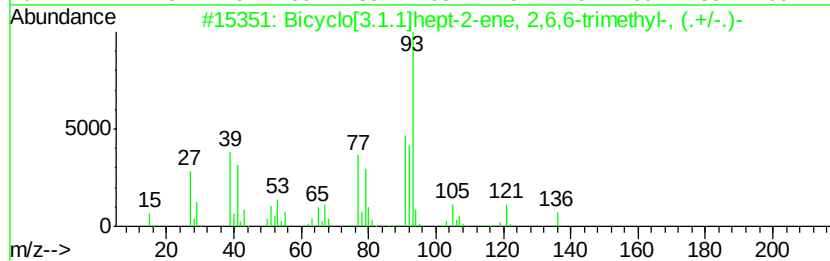
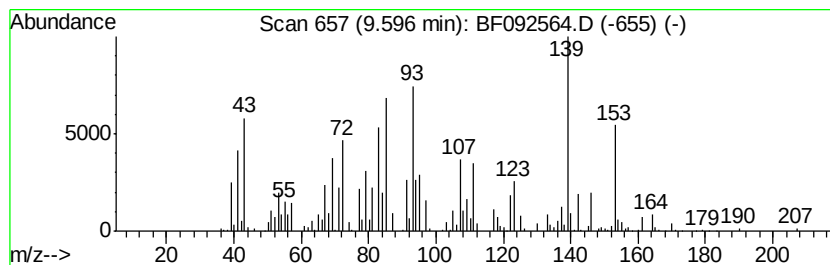
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown9.60 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	9.42 ng	1445100	Acenaphthene-d10	10.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[3.1.1]hept-2-ene, 2,6,6-...	136	C10H16	002437-95-8	11
2		1R-.alpha.-Pinene	136	C10H16	007785-70-8	11
3		.beta.-Myrcene	136	C10H16	000123-35-3	11
4		Pyrindine, 3-(ethylthio)-	139	C7H9NS	026891-59-8	11
5		Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
Operator : SJ/MA
Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

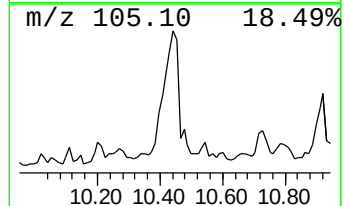
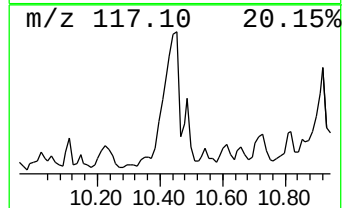
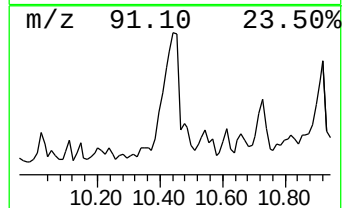
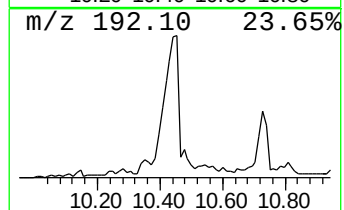
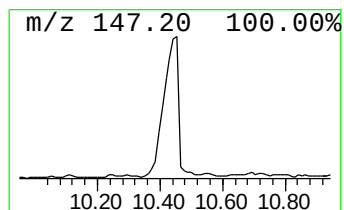
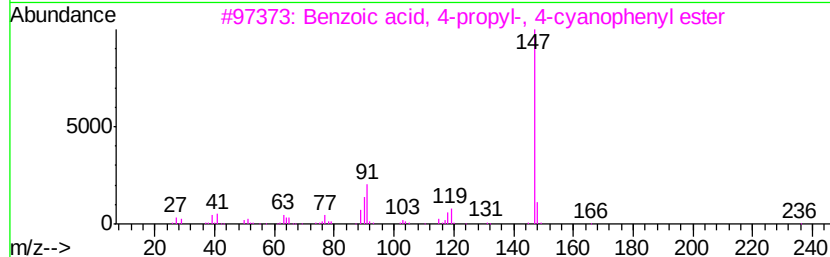
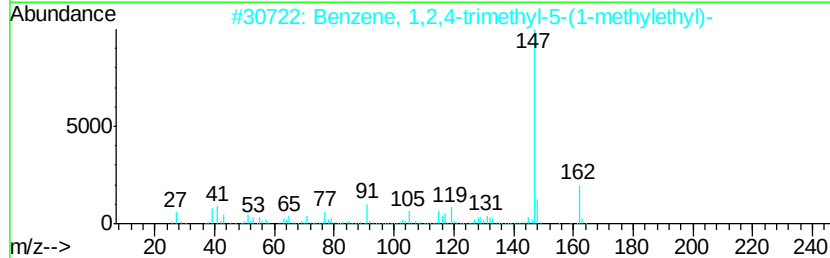
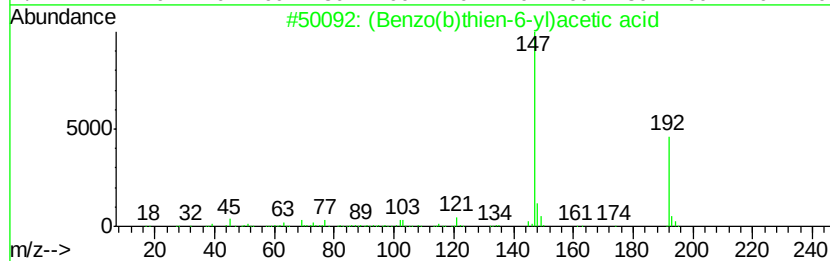
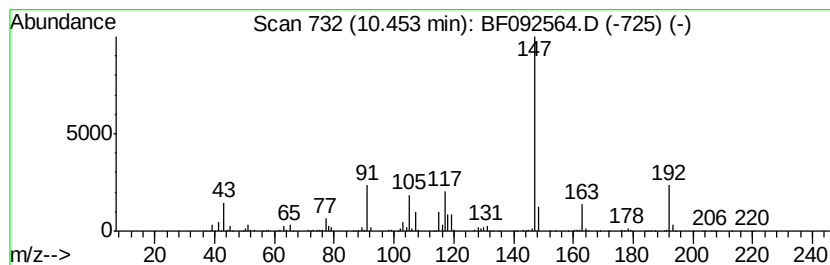
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	75.18 ng	11535400	Acenaphthene-d10	10.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		(Benzo(b)thien-6-yl)acetic acid	192 C10H8O2S	006177-87-3 47
2		Benzene, 1,2,4-trimethyl-5-(1-me...	162 C12H18	010222-95-4 43
3		Benzoic acid, 4-propyl-, 4-cyano...	265 C17H15N02	056131-49-8 43
4		Benzo[b]thiophene, 2-propyl-	176 C11H12S	016587-32-9 43
5		Benzoyl chloride, 4-propyl-	182 C10H11ClO	052710-27-7 43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
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Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
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ClientSampled :
MW-13

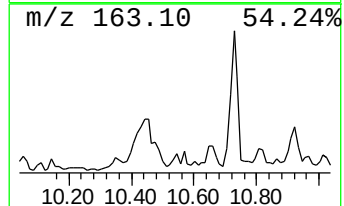
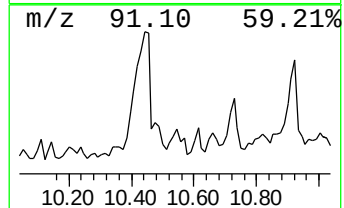
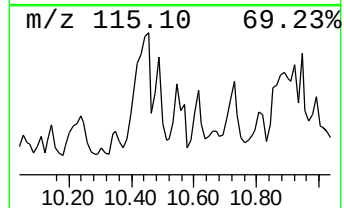
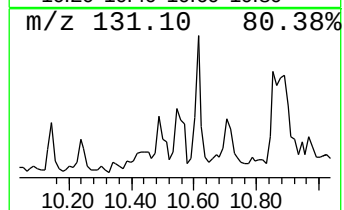
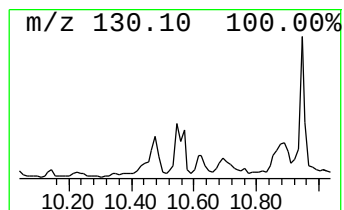
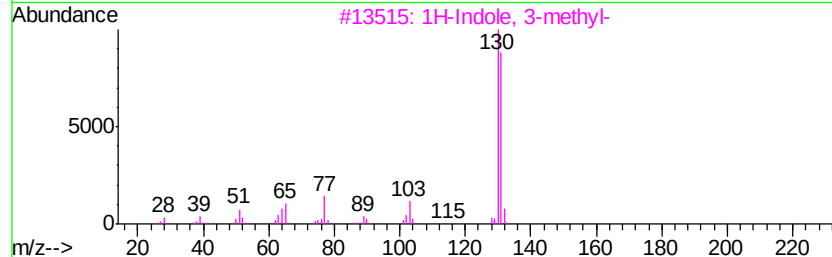
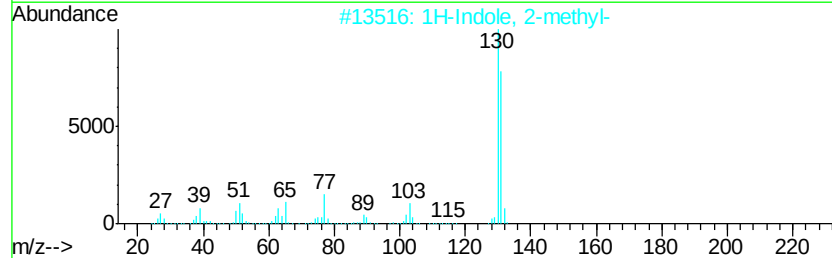
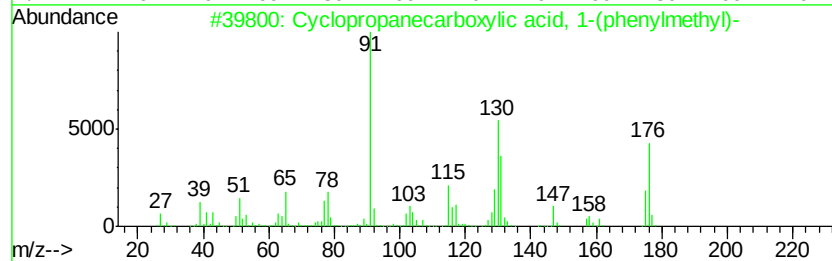
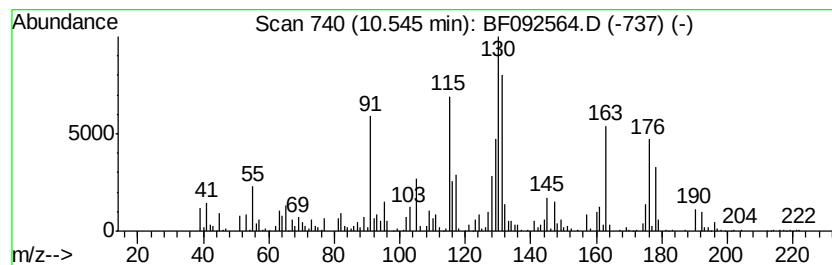
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Cyclopropanecarboxylic acid... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	16.13 ng	2475500	Acenaphthene-d10	10.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanecarboxylic acid, 1-(...	176	C11H12O2	027356-91-8	62
2		1H-Indole, 2-methyl-	131	C9H9N	000095-20-5	41
3		1H-Indole, 3-methyl-	131	C9H9N	000083-34-1	41
4		1H-Indene, 1-methyl-	130	C10H10	000767-59-9	38
5		1H-Indole, 7-methyl-	131	C9H9N	000933-67-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
Operator : SJ/MA
Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

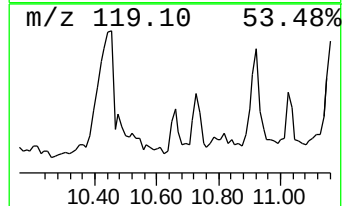
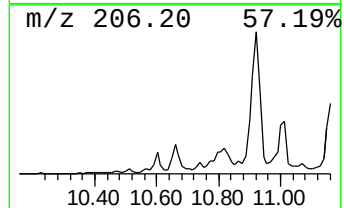
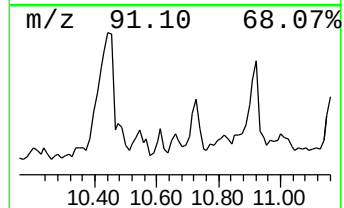
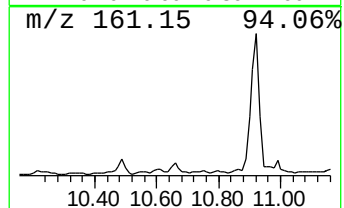
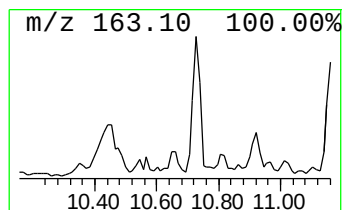
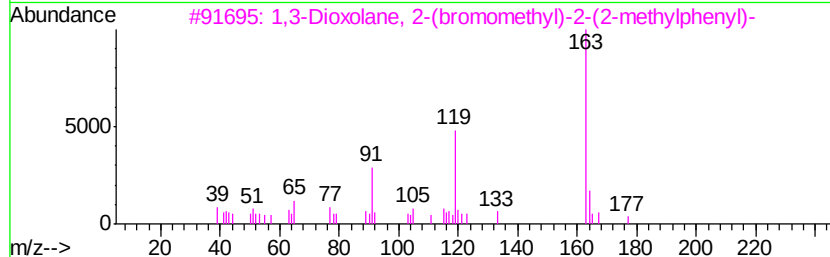
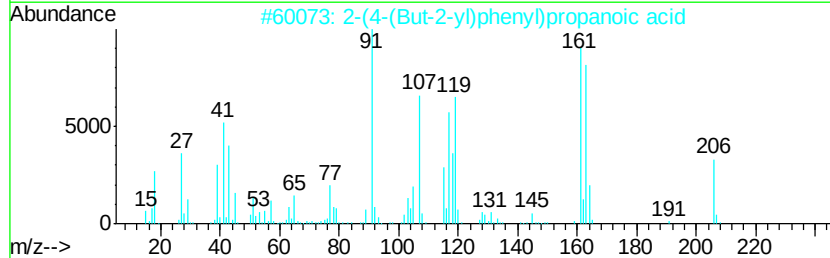
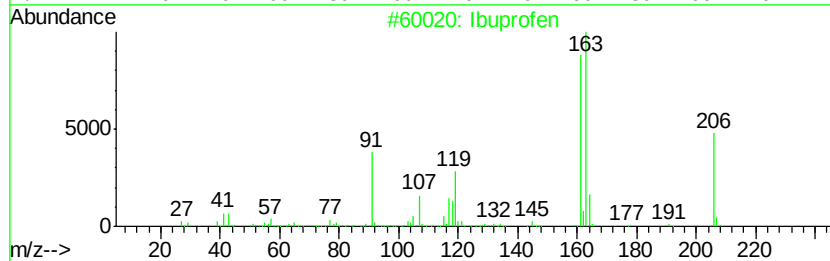
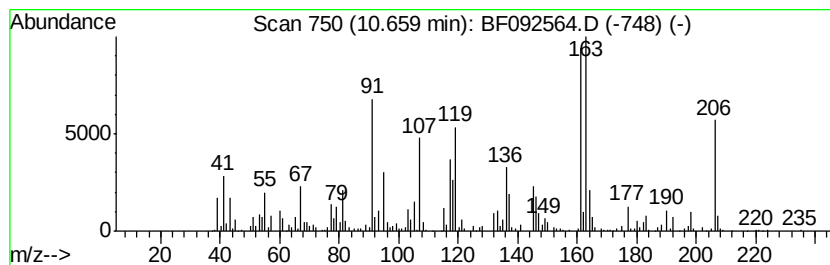
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Ibuprofen Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	8.67 ng	1331030	Acenaphthene-d10	10.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ibuprofen		206 C13H18O2	015687-27-1 90
2	2-(4-(But-2-yl)phenyl)propanoic ...		206 C13H18O2	064451-76-9 90
3	1,3-Dioxolane, 2-(bromomethyl)-2...		256 C11H13BrO2	024169-43-5 22
4	2H-1-Benzopyran-2-one, 7-hydroxy...		206 C11H10O4	003374-03-6 22
5	1,2-Dimethyl-5-nitroadamantane		209 C12H19NO2	006588-68-7 22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
Operator : SJ/MA
Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

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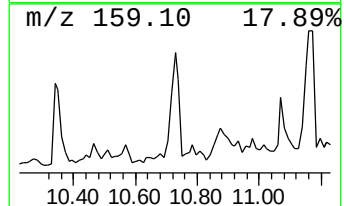
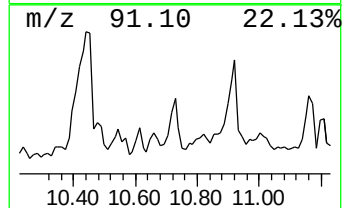
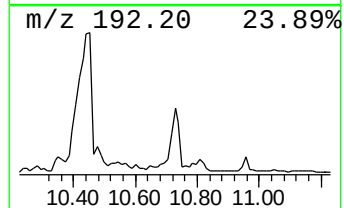
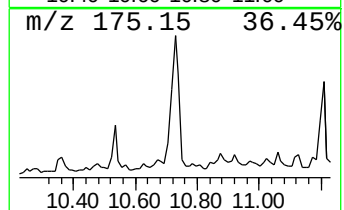
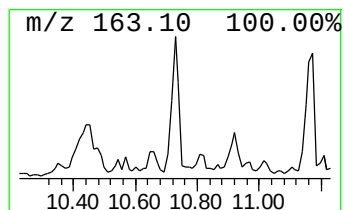
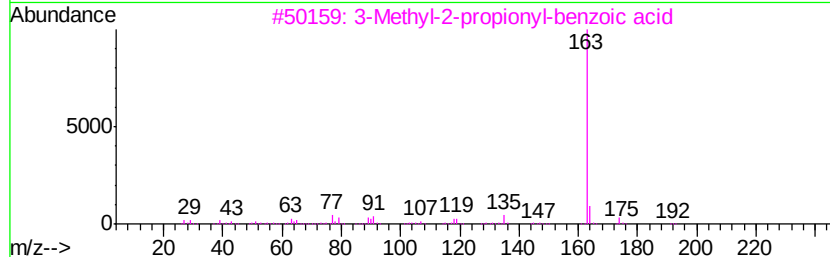
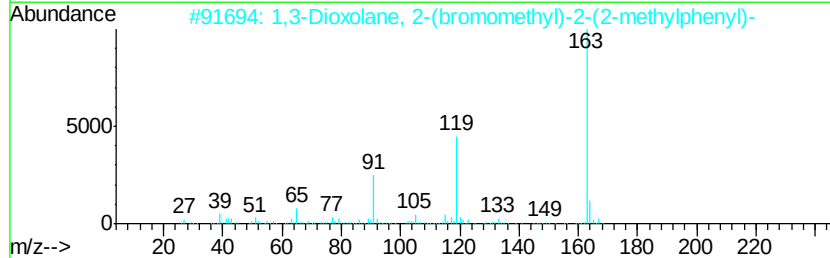
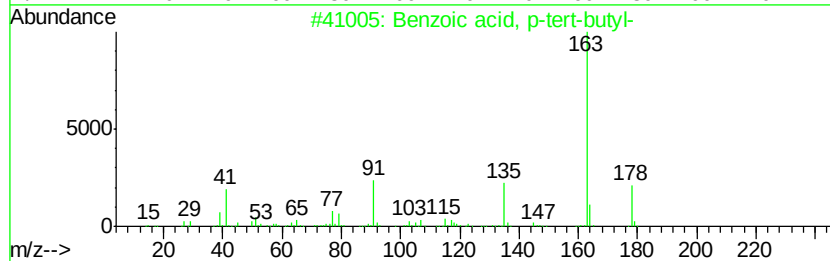
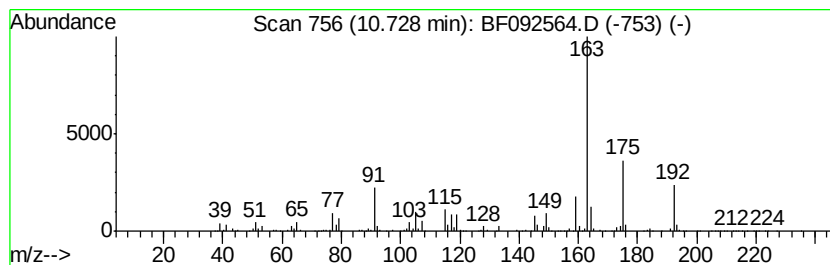
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown10.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	19.87 ng	3047960	Acenaphthene-d10	10.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	43
2		1,3-Dioxolane, 2-(bromomethyl)-2...	256	C11H13BrO2	024169-43-5	38
3		3-Methyl-2-propionyl-benzoic acid	192	C11H12O3	092945-59-0	32
4		1H-Indazole, 5-nitro-	163	C7H5N3O2	005401-94-5	32
5		Propanediamide, 2-ethyl-2-phenyl-	206	C11H14N2O2	007206-76-0	28



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
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Misc :
ALS Vial : 51 Sample Multiplier: 1

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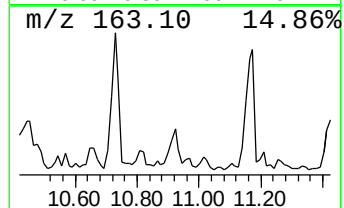
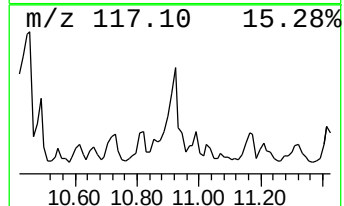
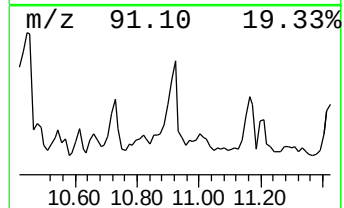
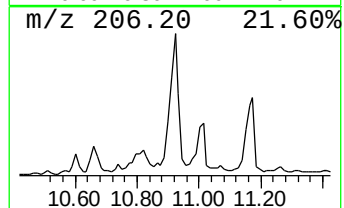
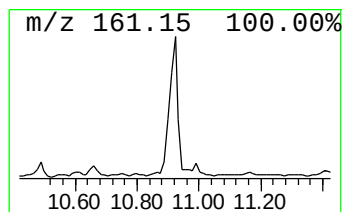
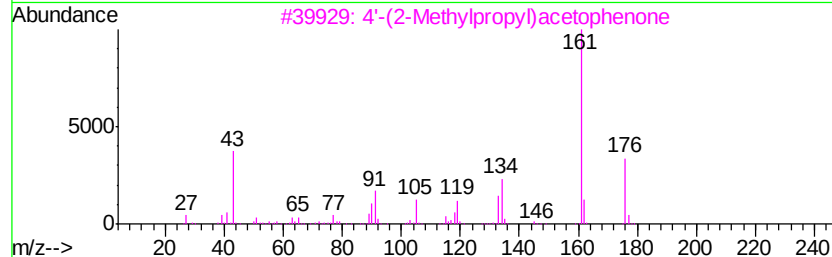
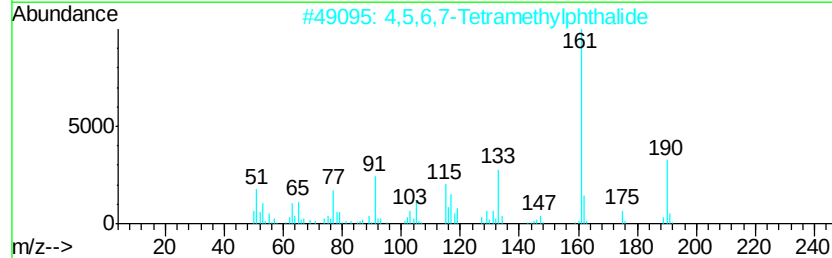
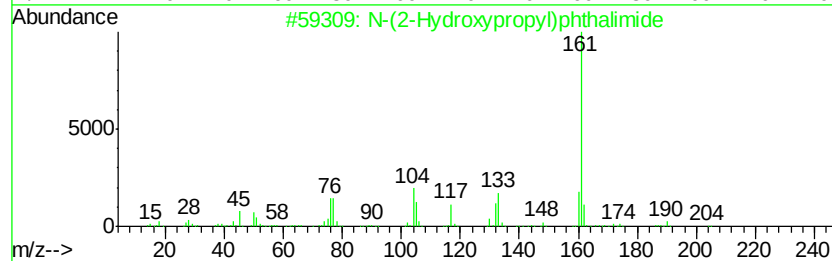
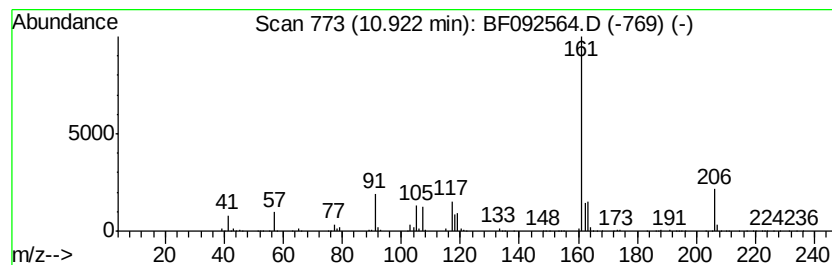
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 N-(2-Hydroxypropyl)phthalimide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.92	54.74 ng	4388150	Phenanthrene-d10	11.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-(2-Hydroxypropyl)phthalimide	205	C11H11NO3	003700-55-8	50
2		4,5,6,7-Tetramethylphthalide	190	C12H14O2	029002-54-8	42
3		4'-(2-Methylpropyl)acetophenone	176	C12H16O	038861-78-8	42
4		4-Methoxy-1-methylindole	161	C10H11NO	007556-35-6	40
5		p-n-Butylacetophenone	176	C12H16O	037920-25-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
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Instrument :
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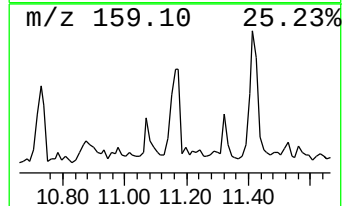
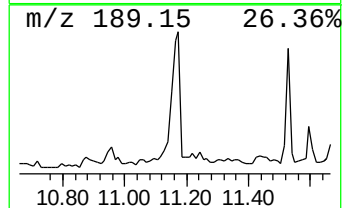
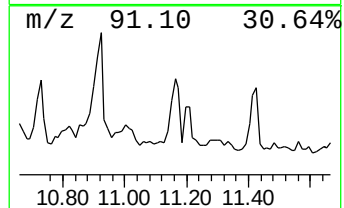
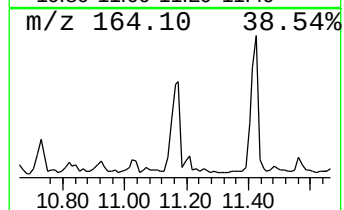
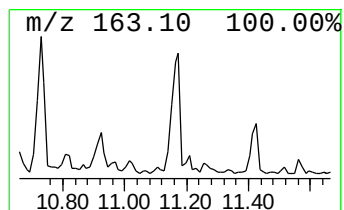
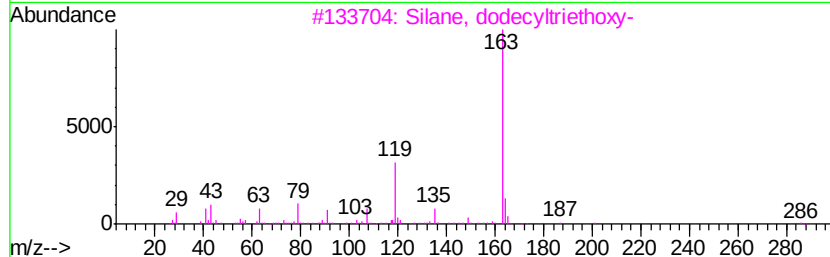
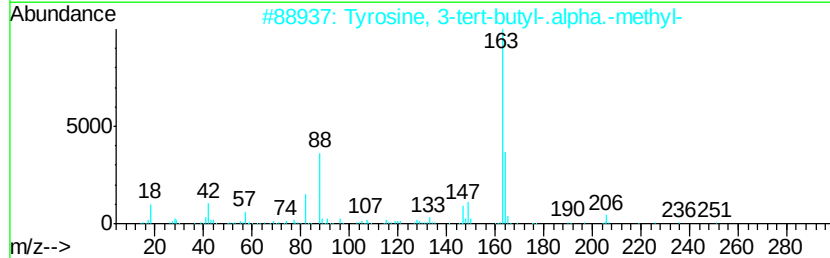
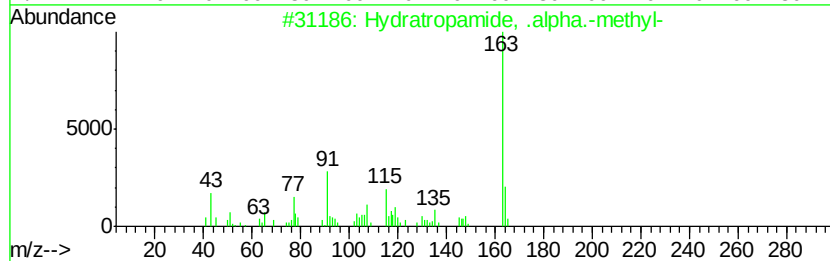
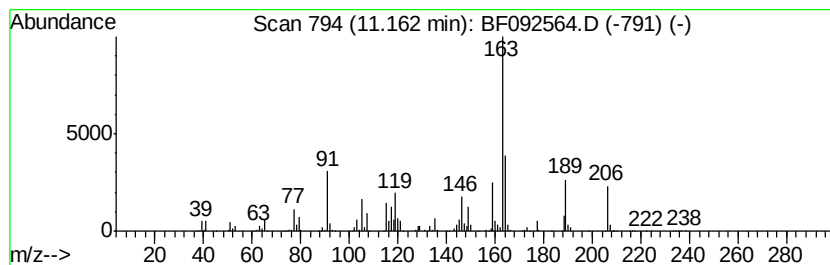
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown11.16 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	42.66 ng	3420200	Phenanthrene-d10	11.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydratropamide, .alpha.-methyl-	163	C10H13NO	000826-54-0	41
2		Tyrosine, 3-tert-butyl-.alpha.-m...	251	C14H21NO3	032919-76-9	37
3		Silane, dodecyltriethoxy-	332	C18H40O3Si	018536-91-9	35
4		p-Amidinobenzamide	163	C8H9N3O	054050-86-1	32
5		Ethanone, 1-[4-(1-hydroxy-1-meth...	178	C11H14O2	054549-72-3	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
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Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-13

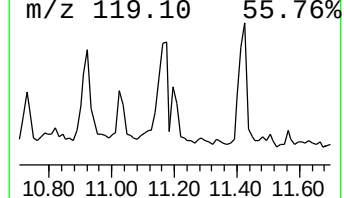
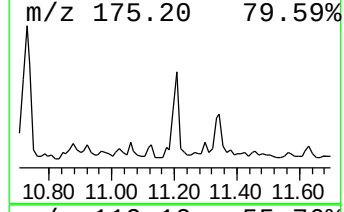
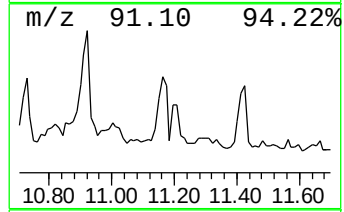
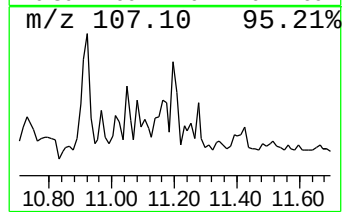
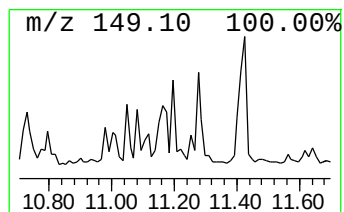
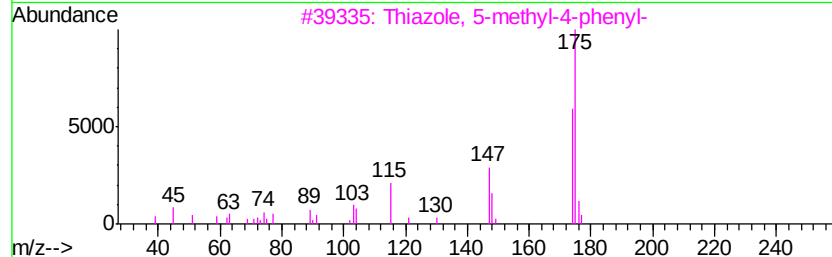
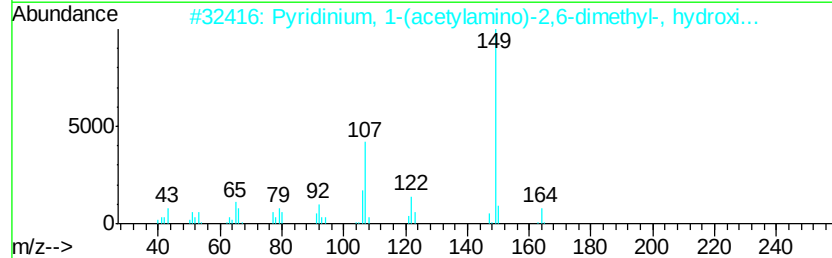
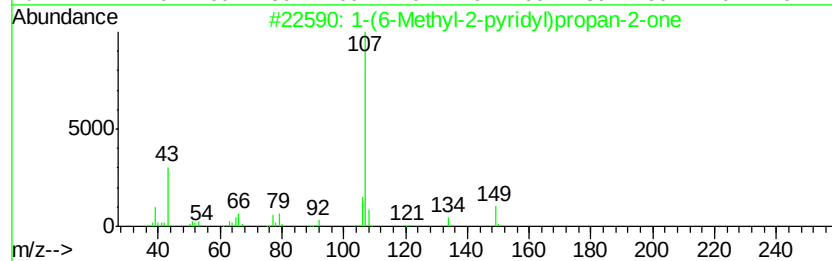
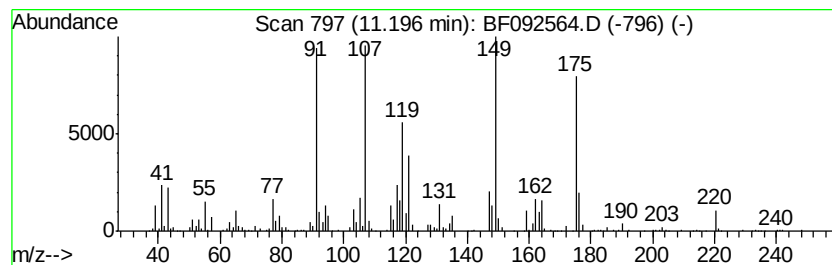
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown11.20 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	14.51 ng	1163170	Phenanthrene-d10	11.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	30
2		Pyridinium, 1-(acetylamino)-2,6-dimethyl-, hydroxi...	164	C9H12N2O	031020-35-6	22
3		Thiazole, 5-methyl-4-phenyl-	175	C10H9NS	001826-18-2	18
4		3-(4-Hydroxyphenyl)propionitrile	147	C9H9NO	017362-17-3	15
5		1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092564.D
Acq On : 27 Jan 2017 9:16
Operator : SJ/MA
Sample : I1353-02
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-13

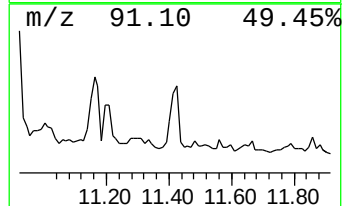
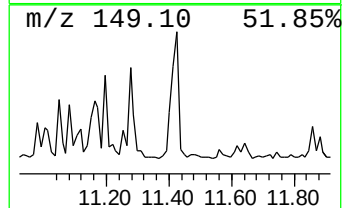
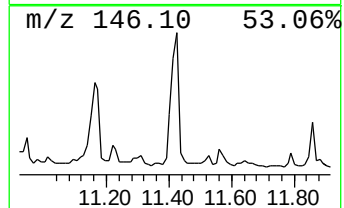
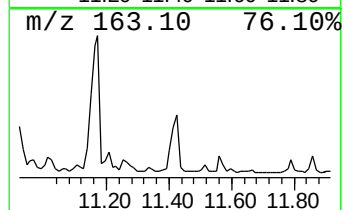
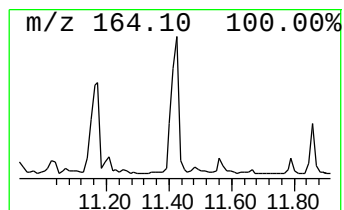
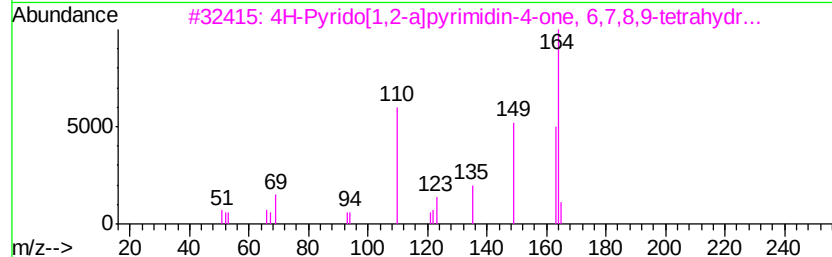
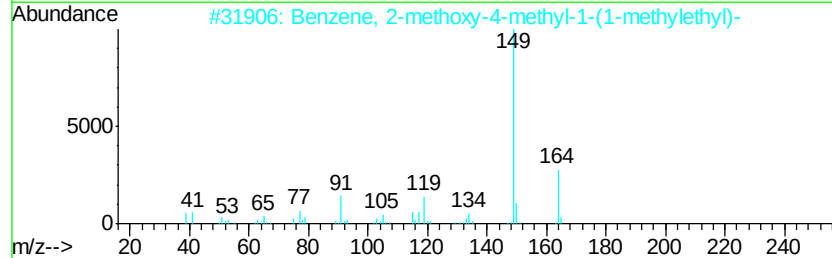
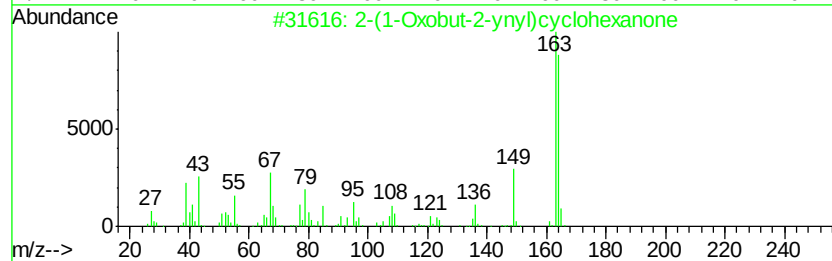
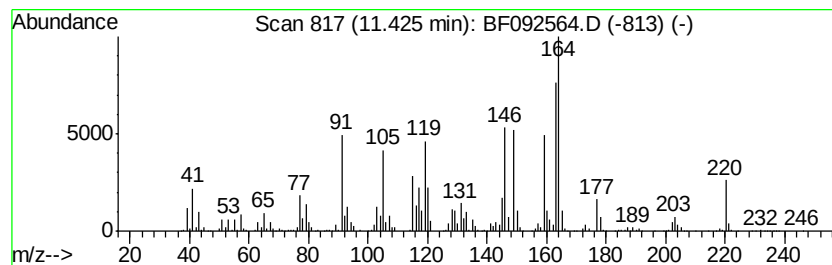
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown11.42 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	56.38 ng	4520150	Phenanthrene-d10	11.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(1-Oxobut-2-ynyl)cyclohexanone	164	C10H12O2	1000191-07-1	35
2		Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-	164	C11H16O	001076-56-8	30
3		4H-Pyrido[1,2-a]pyrimidin-4-one, 6,7,8,9-tetrahydr...	164	C9H12N2O	032092-29-8	27
4		4,6-Dimethyl-2-mercaptopyridine-...	164	C8H8N2S	054585-47-6	25
5		Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
 Data File : BF092564.D
 Acq On : 27 Jan 2017 9:16
 Operator : SJ/MA
 Sample : I1353-02
 Misc :
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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
2-Pentanone, 4-hy...	5.15	12.4	ng	755557	1	6.97	1216620	20.0
unknown6.74	6.74	65.5	ng	3982740	1	6.97	1216620	20.0
unknown8.20	8.20	8.6	ng	1077230	2	8.26	2497400	20.0
unknown8.43	8.43	11.8	ng	1470270	2	8.26	2497400	20.0
unknown8.52	8.52	19.6	ng	2451630	2	8.26	2497400	20.0
Phenol, 2-(1,1-di...	8.70	15.1	ng	1888560	2	8.26	2497400	20.0
2-Cyclopenten-1-o...	9.01	9.0	ng	1121100	2	8.26	2497400	20.0
1,3-Dimethyl-1-cy...	9.06	10.7	ng	1337280	2	8.26	2497400	20.0
unknown9.47	9.47	11.5	ng	1768280	3	10.03	3068680	20.0
unknown9.60	9.60	9.4	ng	1445100	3	10.03	3068680	20.0
unknown10.45	10.45	75.2	ng	11535400	3	10.03	3068680	20.0
Cyclopropanecarbo...	10.54	16.1	ng	2475500	3	10.03	3068680	20.0
Ibuprofen	10.66	8.7	ng	1331030	3	10.03	3068680	20.0
unknown10.73	10.73	19.9	ng	3047960	3	10.03	3068680	20.0
N-(2-Hydroxypropy...	10.92	54.7	ng	4388150	4	11.53	1603370	20.0
unknown11.16	11.16	42.7	ng	3420200	4	11.53	1603370	20.0
unknown11.20	11.20	14.5	ng	1163170	4	11.53	1603370	20.0
unknown11.42	11.42	56.4	ng	4520150	4	11.53	1603370	20.0