

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
 Data File : BF091067.D
 Acq On : 7 Nov 2016 20:23
 Operator : UM/SJ
 Sample : H5543-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-113-0.5-1.0

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-BF110316.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	1.767	5	7	39	rVB	1928661	4432875	79.42%	7.627%
2	4.819	272	274	283	rBV	330783	581769	10.42%	1.001%
3	5.264	311	313	316	rBV	3210067	3642916	65.27%	6.268%
4	6.327	403	406	409	rBV2	3541821	5581684	100.00%	9.603%
5	6.442	414	416	419	rBV	3814899	4175497	74.81%	7.184%
6	6.670	434	436	442	rBV	981524	891802	15.98%	1.534%
7	6.830	447	450	452	rBV	3274739	3081892	55.21%	5.302%
8	7.242	484	486	488	rBV	1456861	1390927	24.92%	2.393%
9	7.345	494	495	503	rVB	44094	73905	1.32%	0.127%
10	7.962	547	549	551	rBV	998739	1047649	18.77%	1.802%
11	8.968	635	637	641	rBV	147862	237575	4.26%	0.409%
12	9.048	641	644	646	rBV	3487462	4642452	83.17%	7.987%
13	9.436	676	678	681	rBV	867381	968799	17.36%	1.667%
14	9.573	688	690	693	rBV	225160	193194	3.46%	0.332%
15	9.711	700	702	704	rBV	1474738	1267933	22.72%	2.181%
16	9.745	704	705	707	rVB	130892	99319	1.78%	0.171%
17	10.156	740	741	743	rVB2	71117	66532	1.19%	0.114%
18	10.259	749	750	753	rVB	78734	72094	1.29%	0.124%
19	10.499	769	771	774	rBV	1345407	1426275	25.55%	2.454%
20	10.625	781	782	786	rVB	95299	154819	2.77%	0.266%
21	10.808	794	798	804	rBV4	36353	136689	2.45%	0.235%
22	10.956	806	811	814	rVV3	45119	89378	1.60%	0.154%
23	11.082	820	822	827	rVB2	69000	148858	2.67%	0.256%
24	11.196	830	832	836	rBV2	1240860	2095140	37.54%	3.605%
25	11.265	836	838	840	rVB	250523	286951	5.14%	0.494%
26	11.436	850	853	856	rBV3	75255	139617	2.50%	0.240%
27	11.699	873	876	877	rBV	131775	156483	2.80%	0.269%
28	11.722	877	878	881	rVV	197052	179933	3.22%	0.310%
29	11.768	881	882	884	rVV	113763	125764	2.25%	0.216%
30	11.802	884	885	890	rVB	273811	419886	7.52%	0.722%
31	11.905	890	894	898	rBV4	32825	100122	1.79%	0.172%
32	11.997	899	902	907	rVB3	81850	185883	3.33%	0.320%
33	12.145	912	915	916	rBV2	40920	66396	1.19%	0.114%
34	12.248	921	924	925	rBV	143076	170339	3.05%	0.293%

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 Start Thrs: 0.2
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 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-BF110316.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.282	925	927	930	rVB2	89441	147236	2.64%	0.253%
36	12.328	930	931	935	rBV2	113943	153082	2.74%	0.263%
37	12.408	935	938	940	rBV	1667536	1695798	30.38%	2.918%
38	12.454	940	942	945	rBV2	42751	61699	1.11%	0.106%
39	12.545	948	950	955	rBV3	57478	152851	2.74%	0.263%
40	12.637	955	958	960	rBV	1266889	1895351	33.96%	3.261%
41	12.682	960	962	965	rVB2	70370	135587	2.43%	0.233%
42	12.751	966	968	969	rBV	91939	108928	1.95%	0.187%
43	12.785	969	971	973	rVV	4129823	3877882	69.48%	6.672%
44	12.854	973	977	979	rVB2	131934	163825	2.94%	0.282%
45	12.957	983	986	988	rVB2	193010	399743	7.16%	0.688%
46	13.025	991	992	994	rBV	152345	136718	2.45%	0.235%
47	13.059	994	995	999	rVB	192225	262019	4.69%	0.451%
48	13.128	999	1001	1002	rBV2	43358	58826	1.05%	0.101%
49	13.151	1002	1003	1005	rVB	124749	115993	2.08%	0.200%
50	13.185	1005	1006	1008	rBV	161225	152206	2.73%	0.262%
51	13.368	1020	1022	1025	rVB2	51060	97692	1.75%	0.168%
52	13.471	1029	1031	1035	rVB	122864	163764	2.93%	0.282%
53	13.574	1038	1040	1041	rBV	167441	200481	3.59%	0.345%
54	13.608	1041	1043	1044	rVV	122234	182725	3.27%	0.314%
55	13.688	1048	1050	1054	rVB3	173346	293417	5.26%	0.505%
56	13.825	1059	1062	1067	rBV	1574466	3196155	57.26%	5.499%
57	13.928	1069	1071	1073	rBV2	142042	204194	3.66%	0.351%
58	14.180	1092	1093	1094	rBV	65897	63194	1.13%	0.109%
59	14.214	1094	1096	1098	rVV	206188	247903	4.44%	0.427%
60	14.305	1102	1104	1106	rBV2	70363	119759	2.15%	0.206%
61	14.545	1121	1125	1128	rBV4	81352	203556	3.65%	0.350%
62	14.831	1147	1150	1155	rBV	908249	1675024	30.01%	2.882%
63	14.923	1156	1158	1161	rVB	153414	215748	3.87%	0.371%
64	15.105	1171	1174	1176	rVB	348180	546731	9.80%	0.941%
65	15.151	1176	1178	1181	rBV	580261	916579	16.42%	1.577%
66	15.208	1181	1183	1185	rBV	631138	982123	17.60%	1.690%
67	16.511	1294	1297	1301	rVB	291849	519422	9.31%	0.894%
68	16.900	1328	1331	1335	rVB	208465	444538	7.96%	0.765%

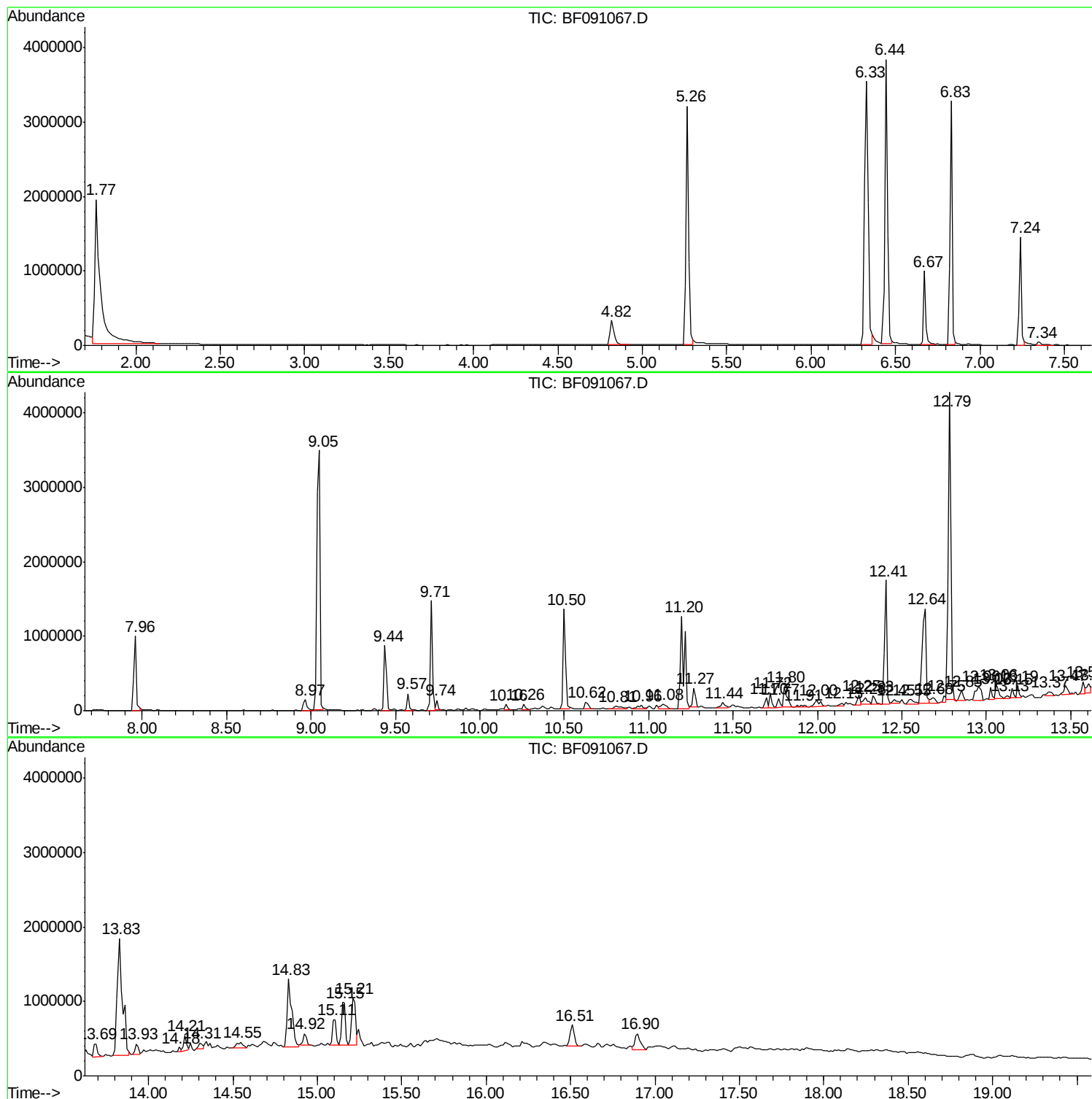
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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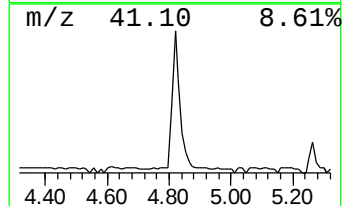
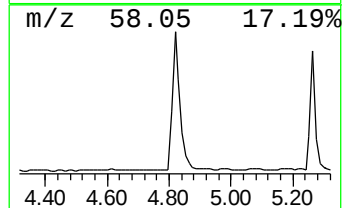
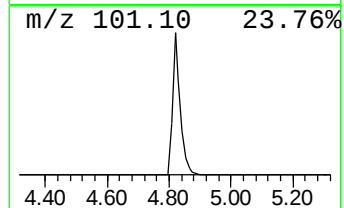
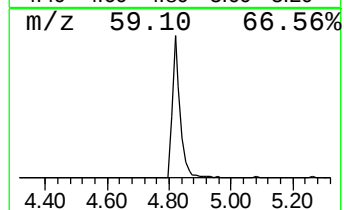
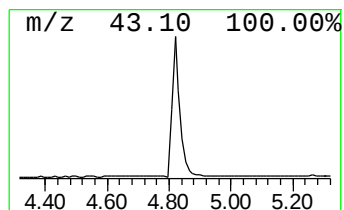
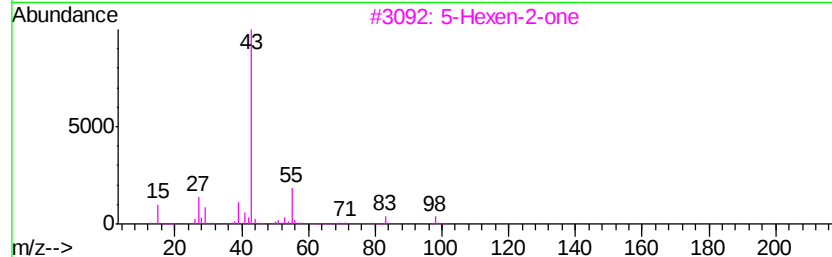
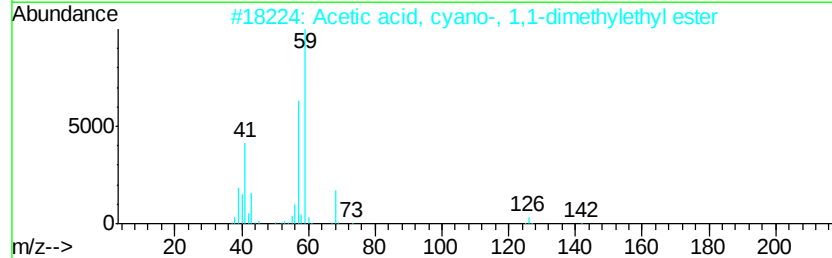
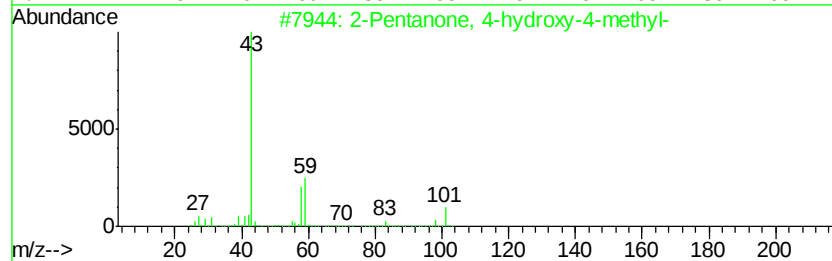
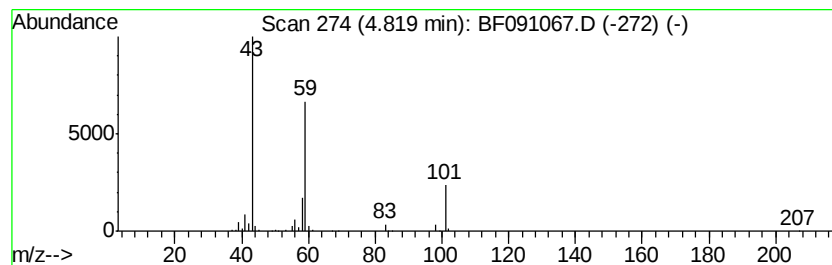
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	13.05 ng	581769	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Guanidine	59	CH5N3	000113-00-8	9



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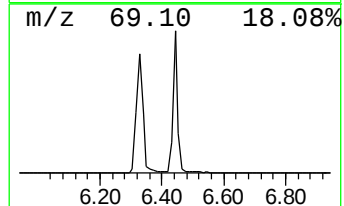
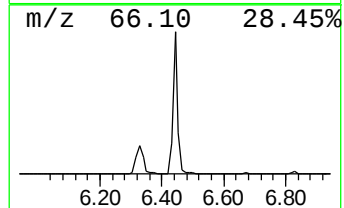
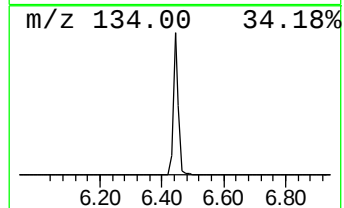
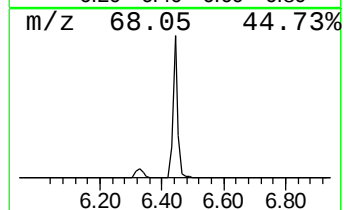
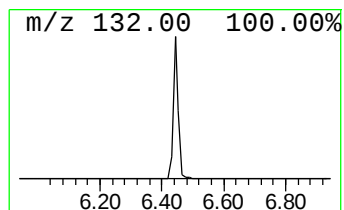
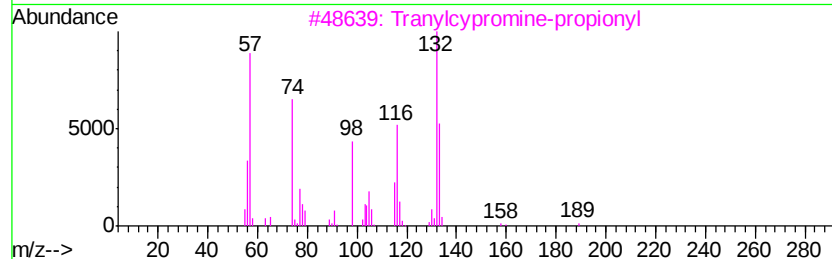
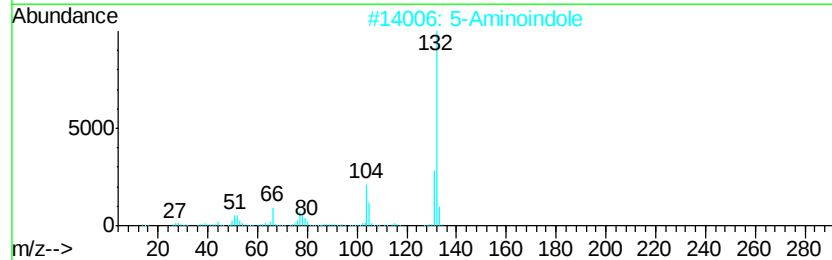
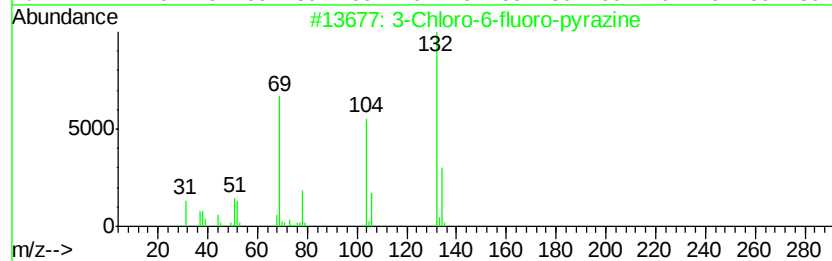
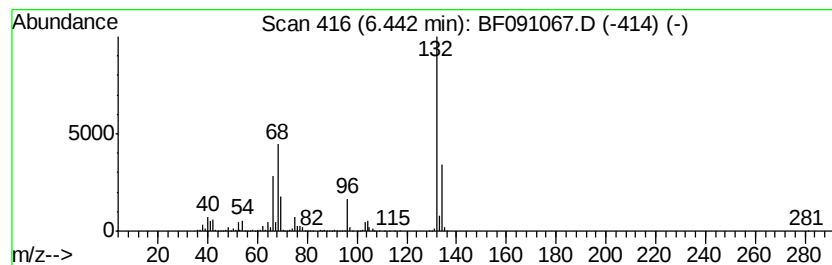
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	93.64 ng	4175500	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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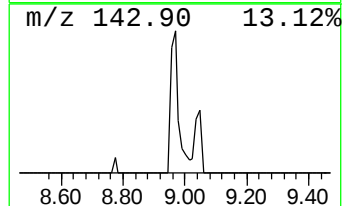
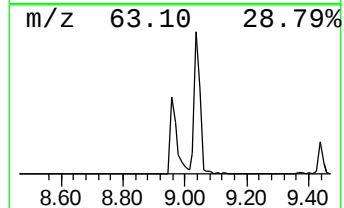
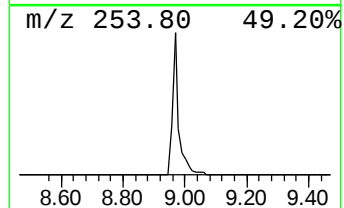
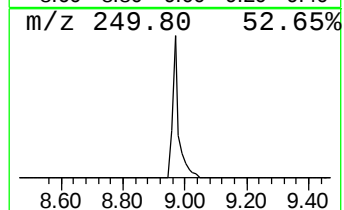
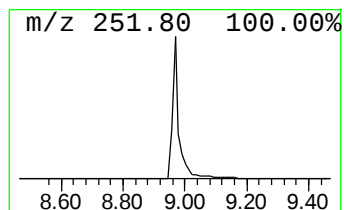
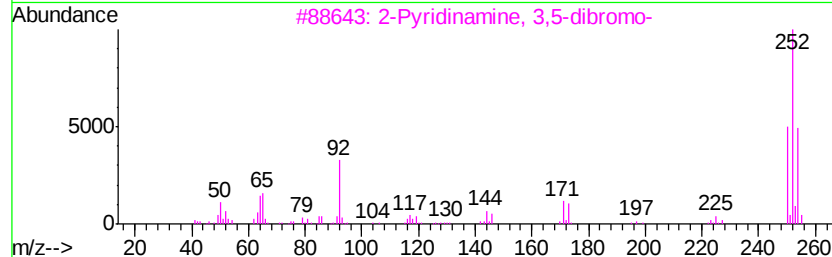
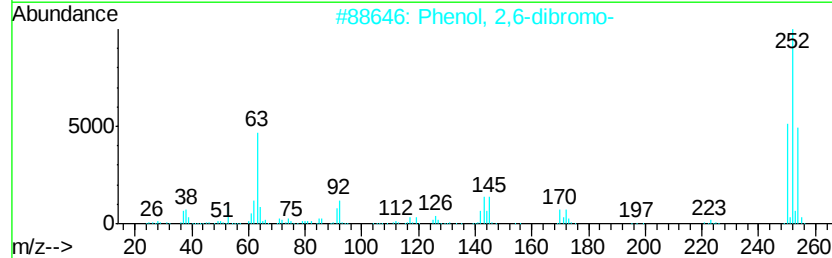
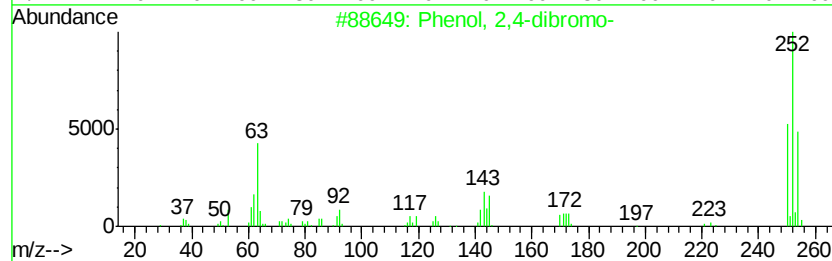
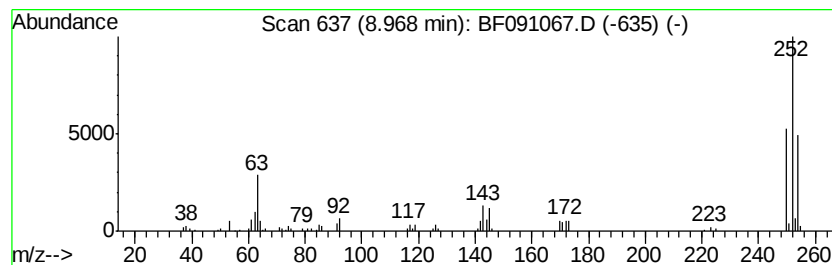
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, 2,4-dibromo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	3.75 ng	237575	Acenaphthene-d10	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	99
2			Phenol, 2,6-dibromo-	250	C6H4Br2O	000608-33-3	97
3			2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	58
4			7-Chloro-6-methoxy-4-methyl-8-ni...	252	C11H9ClN2O3	1000213-13-0	32
5			1-Chloro-11H-indolo[3,2-c]quinoline	252	C15H9ClN2	155249-51-7	23



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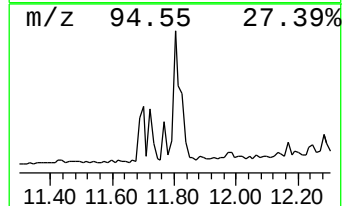
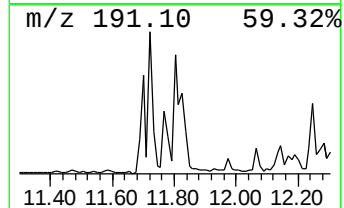
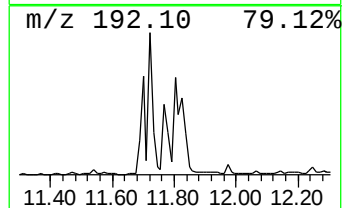
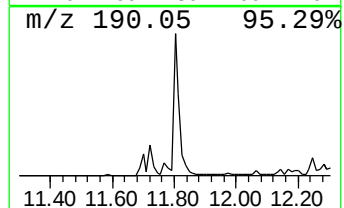
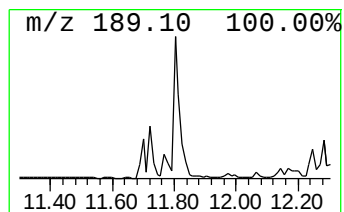
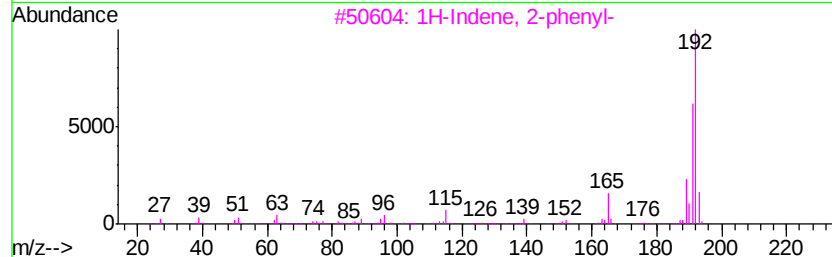
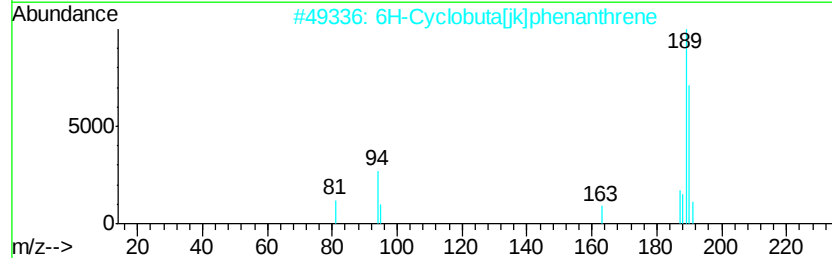
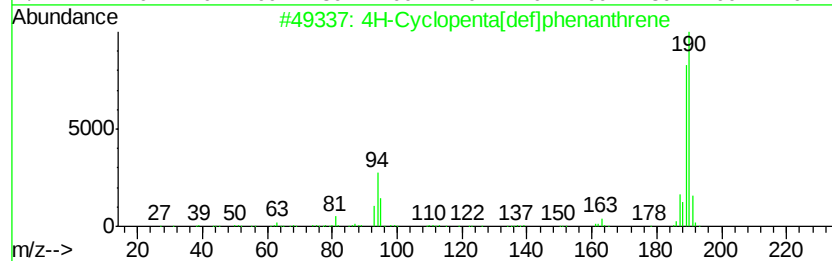
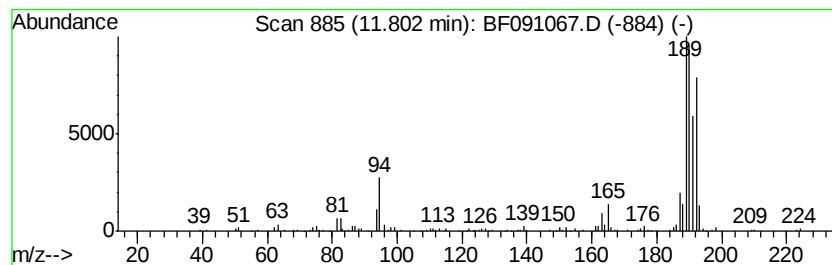
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.80	4.01 ng	419886	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	49
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	42
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
5	Benzene, 1,1'-(1,2-propadienyld...	192	C15H12	014251-57-1	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091067.D
Acq On : 7 Nov 2016 20:23
Operator : UM/SJ
Sample : H5543-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-113-0.5-1.0

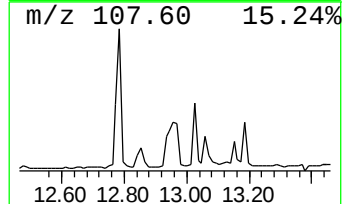
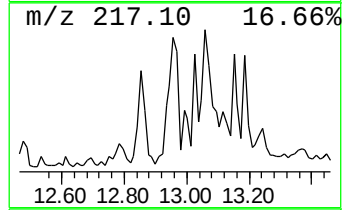
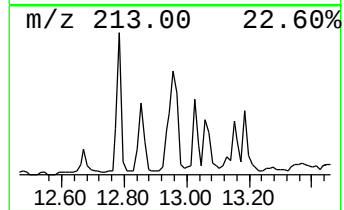
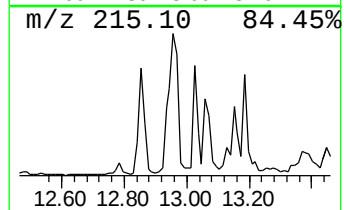
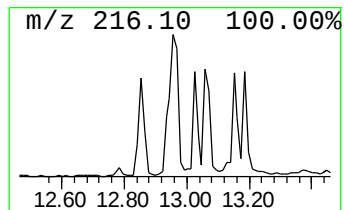
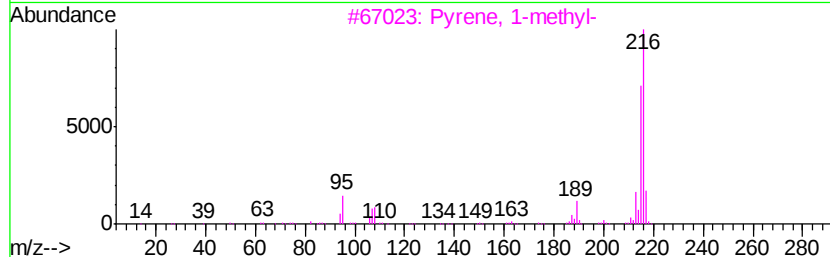
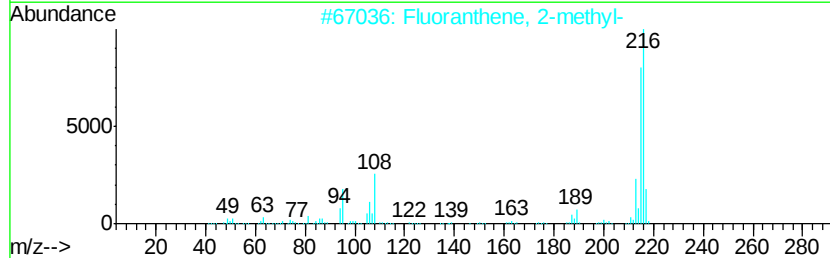
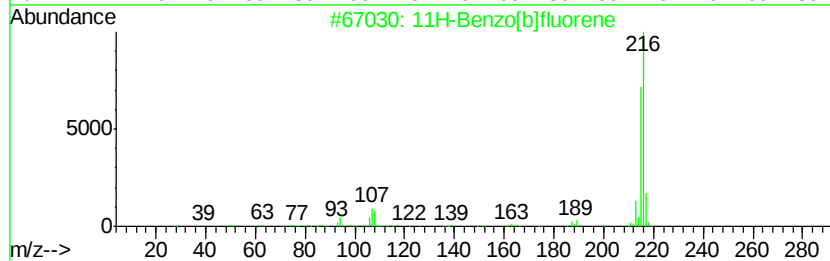
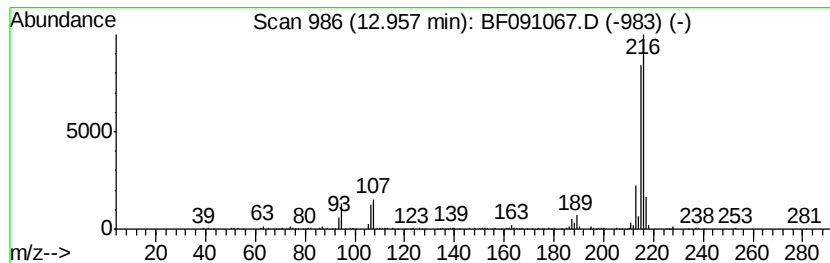
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	2.50 ng	399743	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	95
3		Pvrene, 1-methyl-	216	C17H12	002381-21-7	87
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-113-0.5-1.0

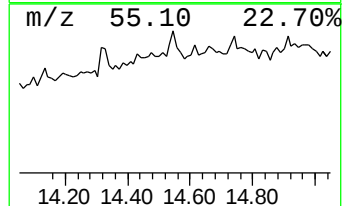
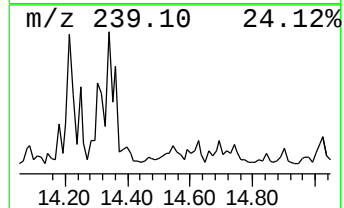
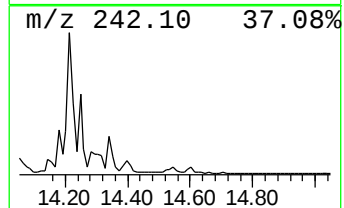
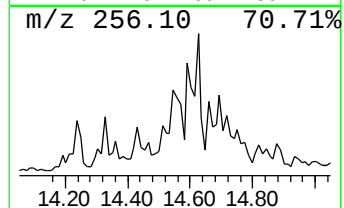
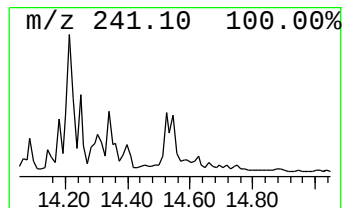
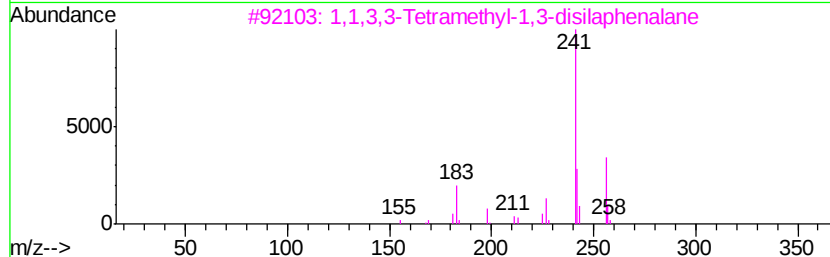
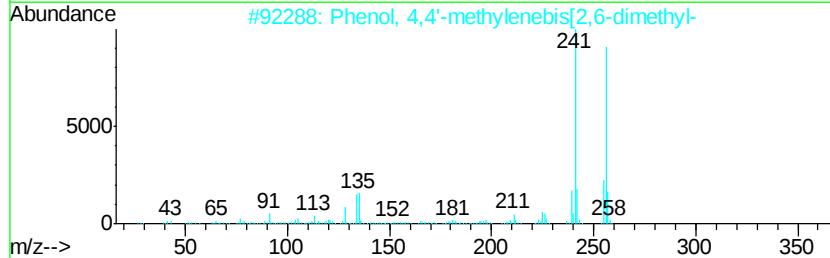
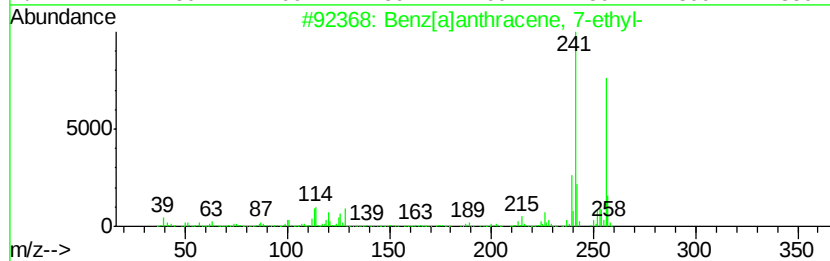
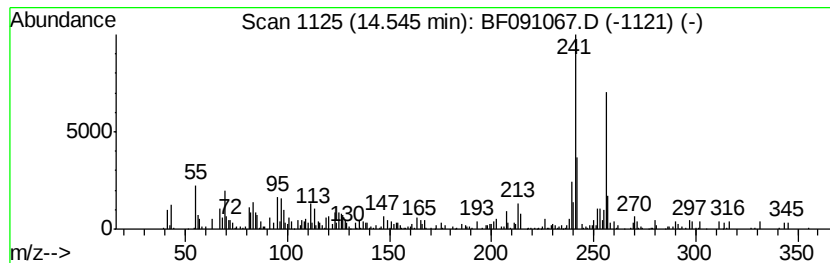
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benz[a]anthracene, 7-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	4.15 ng	203556	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz[a]anthracene, 7-ethyl-	256	C20H16	003697-30-1	74
2		Phenol, 4,4'-methylenebis[2,6-di...	256	C17H20O2	005384-21-4	58
3		1,1,3,3-Tetramethyl-1,3-disilaph...	256	C15H20Si2	032538-51-5	53
4		Phenol, 4,4'-(1-methylethylidene...	256	C17H20O2	000079-97-0	50
5		Benz[a]anthracene, 7,12-dimethyl-	256	C20H16	000057-97-6	46



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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-113-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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...	4.82	13.1	ng	581769	1	6.67	891802	20.0
unknown6.44	6.44	93.6	ng	4175500	1	6.67	891802	20.0
Phenol, 2,4-dibromo-	8.97	3.8	ng	237575	3	9.71	1267930	20.0
4H-Cyclopenta[def...	11.80	4.0	ng	419886	4	11.20	2095140	20.0
11H-Benzo[b]fluorene	12.96	2.5	ng	399743	5	13.83	3196160	20.0
Benz[a]anthracene...	14.55	4.2	ng	203556	6	15.22	982123	20.0