

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100615\
 Data File : BF082092.D
 Acq On : 6 Oct 2015 19:11
 Operator : UM/IZ
 Sample : G3906-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IM-MLA-(1.5-02)

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-BF092815.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	5.063	253	256	268	rVB	643408	1038191	46.21%	4.190%
2	5.486	290	293	295	rBV	1568515	2057340	91.56%	8.304%
3	6.514	380	383	385	rBV	1880032	1976945	87.99%	7.979%
4	6.652	392	395	397	rBV	2043440	2246880	100.00%	9.069%
5	6.880	413	415	419	rBV	553548	485747	21.62%	1.961%
6	7.040	426	429	431	rBV	1644945	1685313	75.01%	6.802%
7	7.452	462	465	467	rBV	1266210	1302541	57.97%	5.257%
8	8.172	525	528	530	rBV	592415	655765	29.19%	2.647%
9	9.246	619	622	624	rBV	2288076	2050189	91.25%	8.275%
10	9.635	655	656	659	rBV	231822	311981	13.89%	1.259%
11	9.920	679	681	683	rBV	658245	725417	32.29%	2.928%
12	9.955	683	684	686	rVB	93827	74811	3.33%	0.302%
13	10.126	697	699	701	rBV2	24650	27209	1.21%	0.110%
14	10.355	715	719	720	rBV	37184	59097	2.63%	0.239%
15	10.469	727	729	732	rBV	64410	63240	2.81%	0.255%
16	10.560	732	737	740	rBV3	21197	45301	2.02%	0.183%
17	10.720	748	751	753	rBV	1136027	1469761	65.41%	5.932%
18	10.823	758	760	765	rVB	79806	101078	4.50%	0.408%
19	11.018	774	777	779	rBV	17669	28125	1.25%	0.114%
20	11.166	786	790	793	rBV5	10226	25670	1.14%	0.104%
21	11.269	797	799	801	rBV	58366	61002	2.71%	0.246%
22	11.303	801	802	805	rVB2	26571	33179	1.48%	0.134%
23	11.418	809	812	816	rBV2	507458	1237982	55.10%	4.997%
24	11.486	816	818	824	rVB	147303	186756	8.31%	0.754%
25	11.646	830	832	835	rBV2	23430	42946	1.91%	0.173%
26	11.692	835	836	839	rVB	23303	33081	1.47%	0.134%
27	11.943	853	858	861	rBV2	77042	157111	6.99%	0.634%
28	12.023	863	865	870	rVB2	97577	130419	5.80%	0.526%
29	12.206	880	881	886	rBV3	17846	30343	1.35%	0.122%
30	12.458	901	903	905	rBV	20523	29806	1.33%	0.120%
31	12.629	915	918	920	rBV	454350	561925	25.01%	2.268%
32	12.858	935	938	940	rBV	370371	562287	25.03%	2.270%
33	12.995	948	950	953	rBV	1379050	1698810	75.61%	6.857%
34	13.064	955	956	959	rVB2	23338	35752	1.59%	0.144%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.178	963	966	968	rBV	61377	98470	4.38%	0.397%
36	13.246	971	972	974	rVV	60257	64228	2.86%	0.259%
37	13.281	974	975	979	rVB2	34921	59909	2.67%	0.242%
38	13.406	985	986	988	rBV	20995	27698	1.23%	0.112%
39	13.567	998	1000	1002	rBV	33562	43069	1.92%	0.174%
40	13.692	1007	1011	1015	rBV5	16939	50432	2.24%	0.204%
41	13.898	1027	1029	1034	rVB2	129132	207393	9.23%	0.837%
42	14.058	1038	1043	1050	rBV2	516678	1114680	49.61%	4.499%
43	14.161	1050	1052	1053	rVB	40965	42061	1.87%	0.170%
44	14.207	1054	1056	1059	rBV4	30547	48297	2.15%	0.195%
45	14.435	1074	1076	1078	rVB2	19771	32173	1.43%	0.130%
46	14.515	1081	1083	1086	rBV3	45026	83051	3.70%	0.335%
47	14.824	1108	1110	1111	rBV	19826	23956	1.07%	0.097%
48	15.087	1130	1133	1137	rBV	150745	337652	15.03%	1.363%
49	15.190	1140	1142	1144	rBV	29784	27909	1.24%	0.113%
50	15.384	1157	1159	1162	rVB	79021	110063	4.90%	0.444%
51	15.441	1162	1164	1167	rVV	133712	182148	8.11%	0.735%
52	15.510	1167	1170	1176	rVB	346166	622843	27.72%	2.514%
53	16.184	1226	1229	1232	rVB2	33580	73179	3.26%	0.295%
54	16.595	1263	1265	1274	rVB5	27989	74819	3.33%	0.302%
55	16.927	1291	1294	1299	rBV2	47334	98385	4.38%	0.397%
56	17.167	1312	1315	1317	rBV3	21237	45050	2.01%	0.182%
57	17.361	1329	1332	1336	rBV	36416	76198	3.39%	0.308%

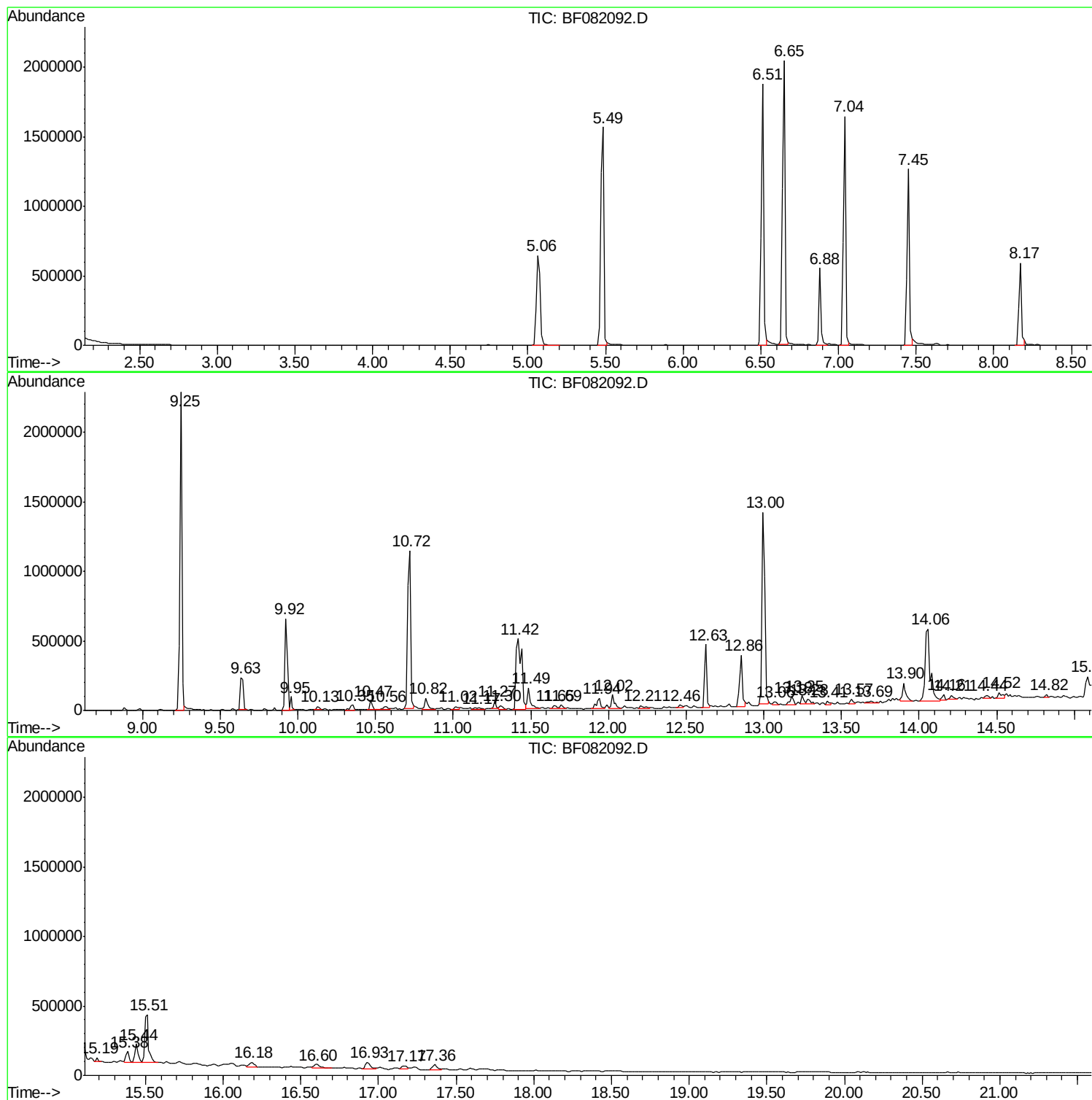
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ClientSampleId :
IM-MLA-(1.5-02)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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Sample : G3906-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
IM-MLA-(1.5-02)

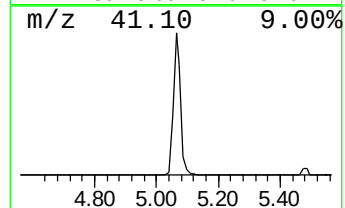
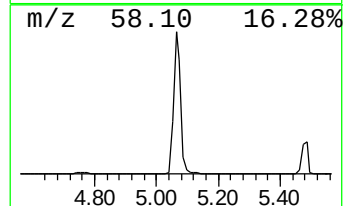
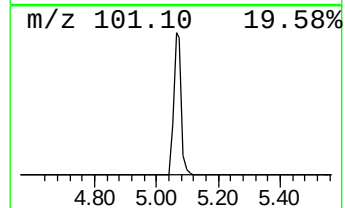
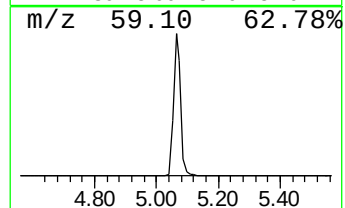
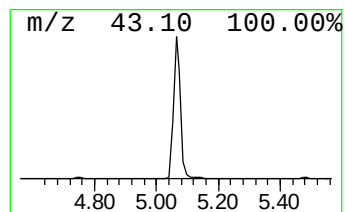
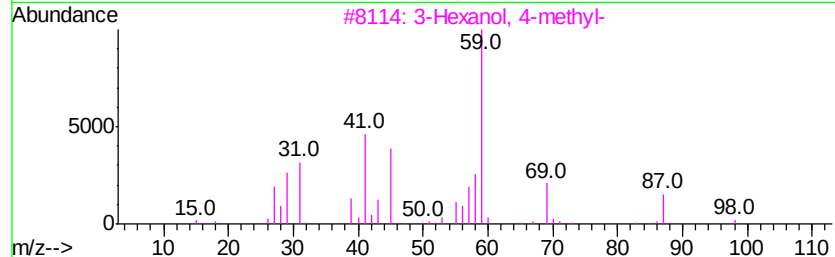
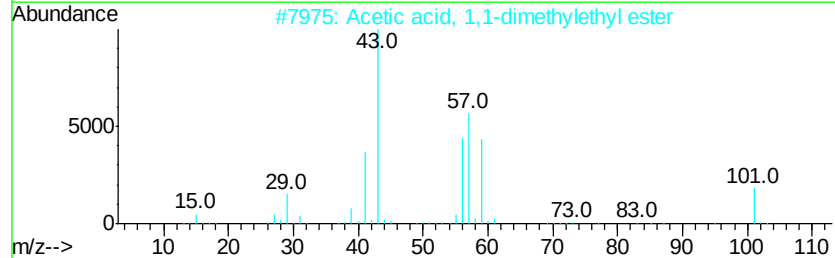
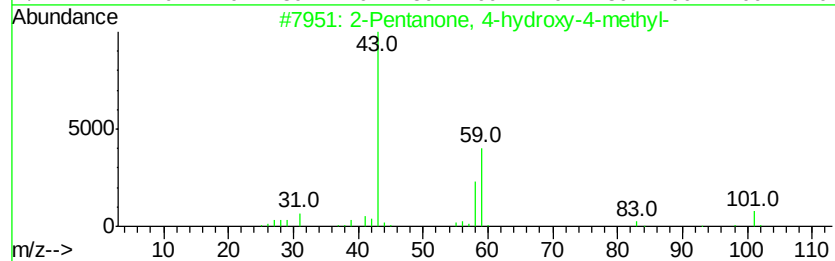
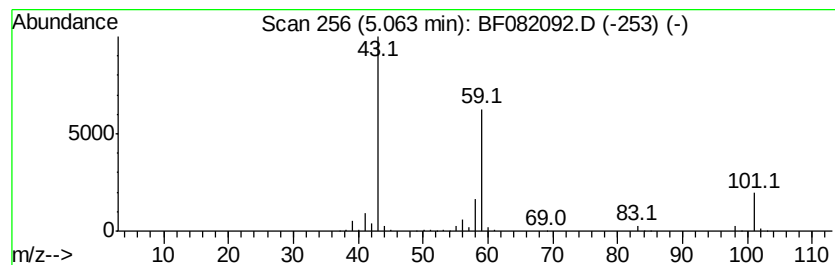
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.06	42.75 ng	1038190	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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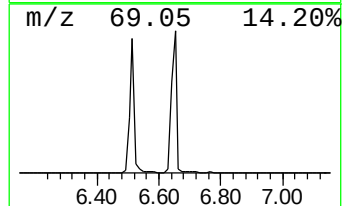
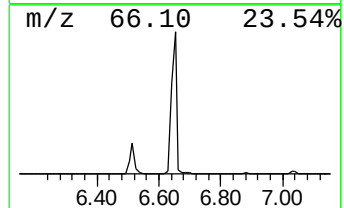
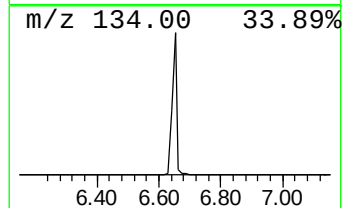
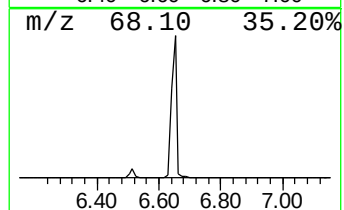
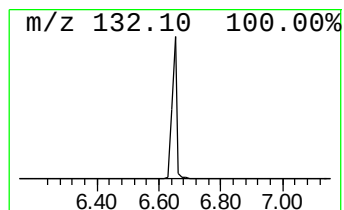
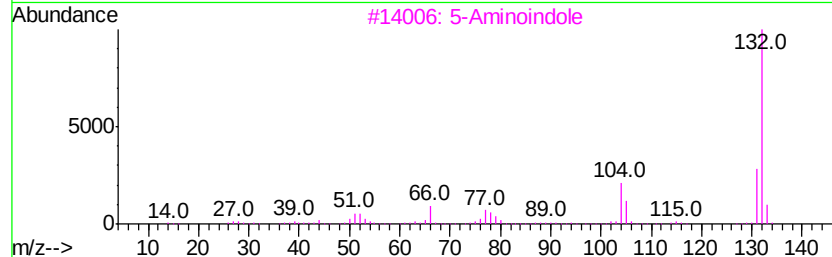
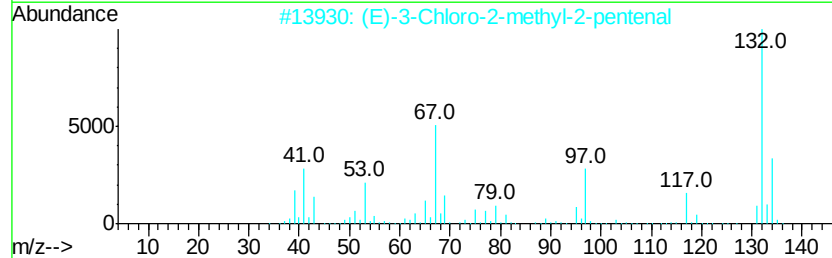
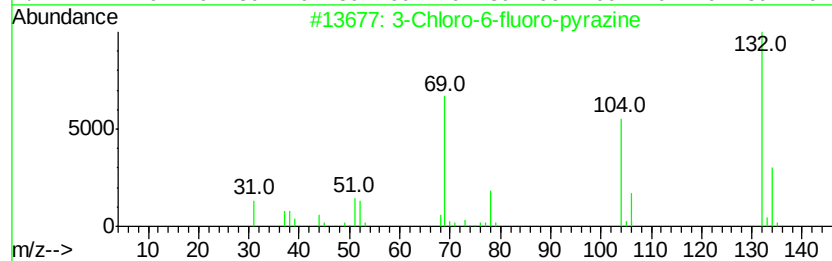
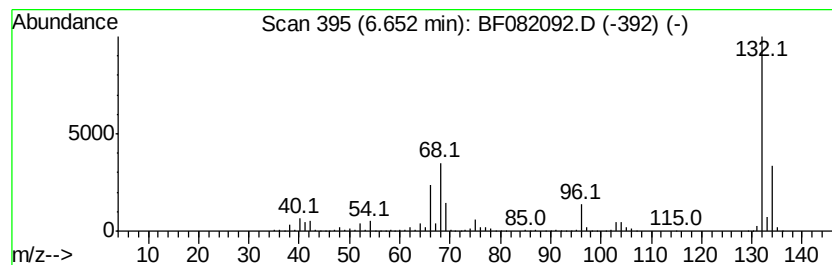
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	92.51 ng	2246880	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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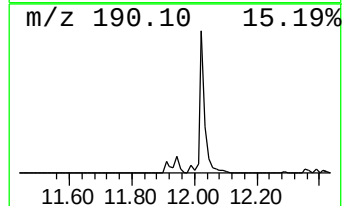
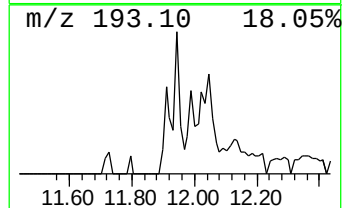
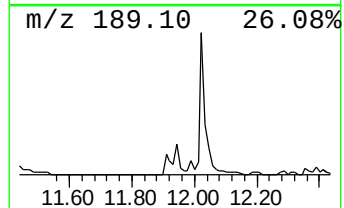
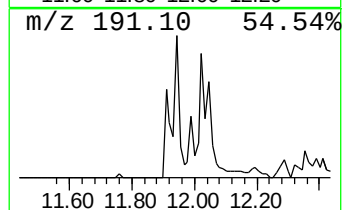
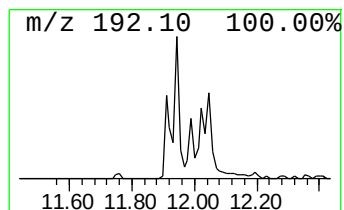
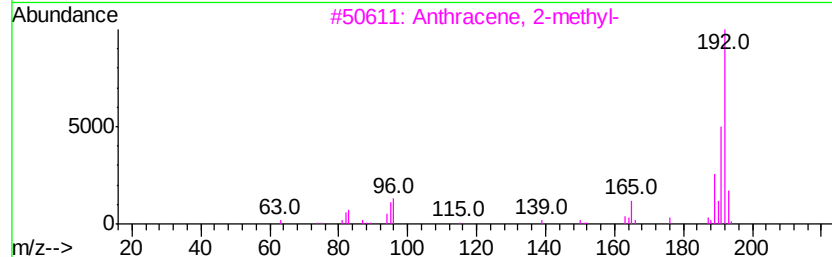
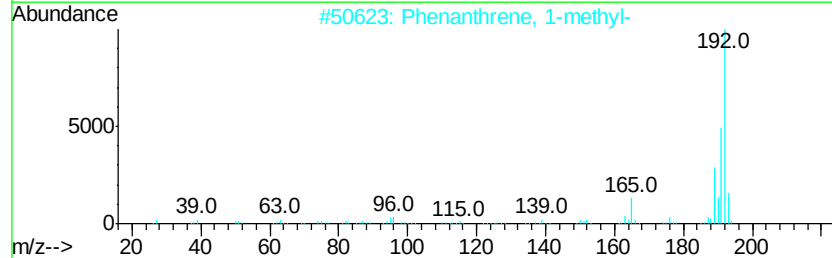
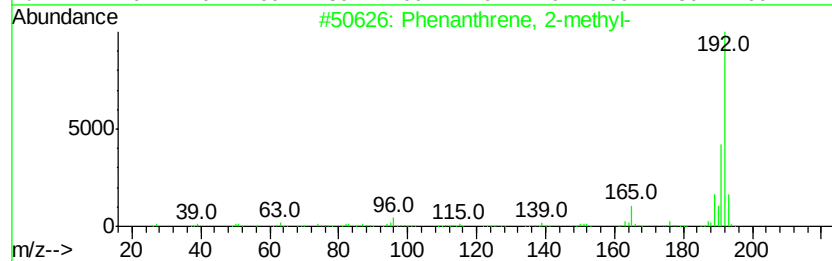
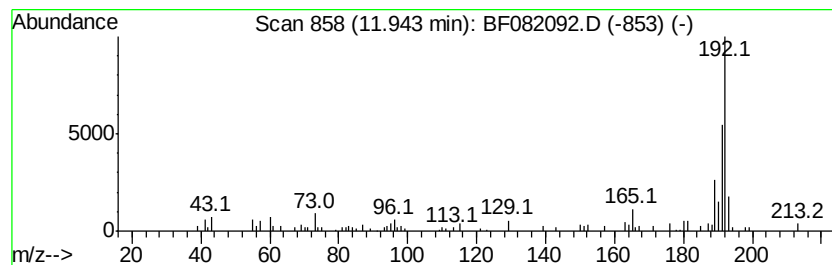
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.54 ng	157111	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	95



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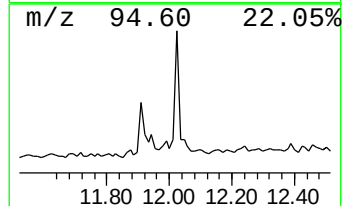
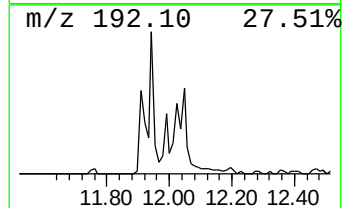
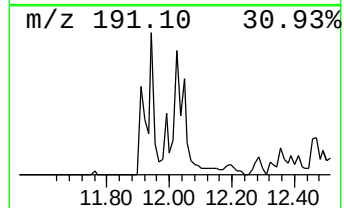
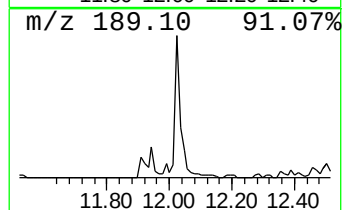
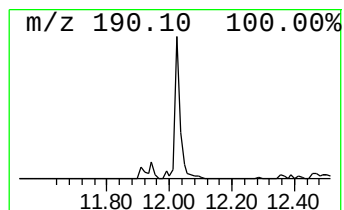
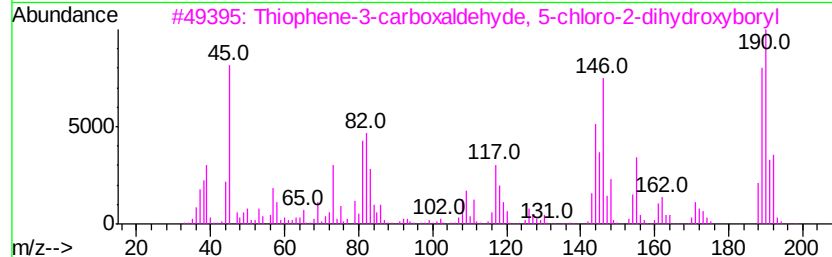
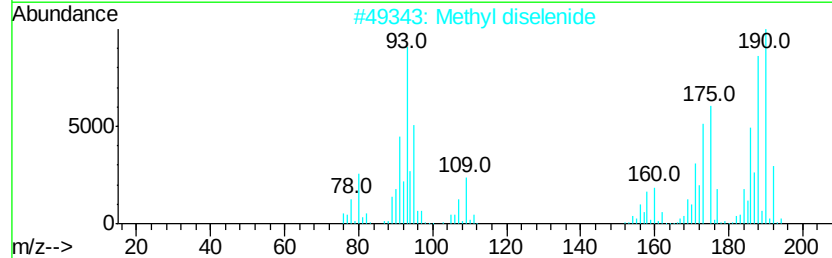
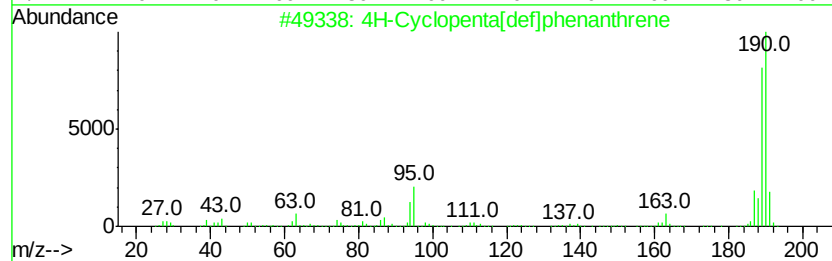
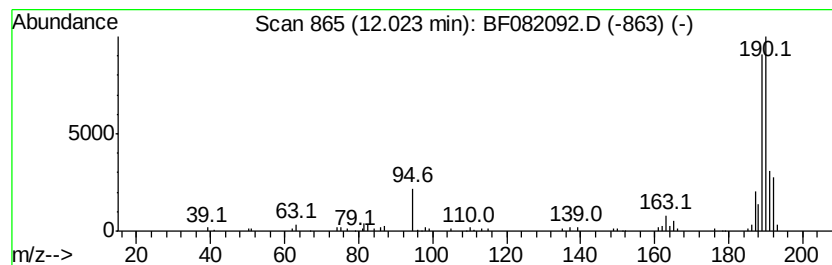
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.02	2.11 ng	130419	Phenanthrene-d10	11.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2		Methyl diselenide	190	C2H6Se2	007101-31-7	55
3		Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
4		6H-Cyclobuta[flk]phenanthrene	190	C15H10	083469-43-6	50
5		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45



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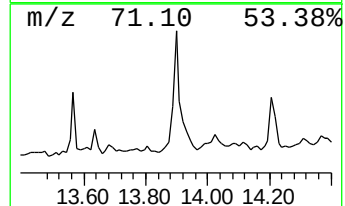
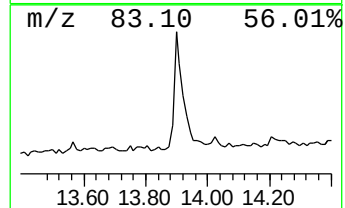
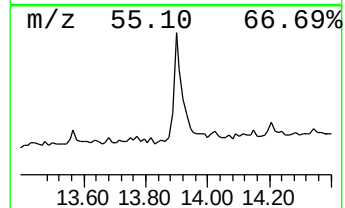
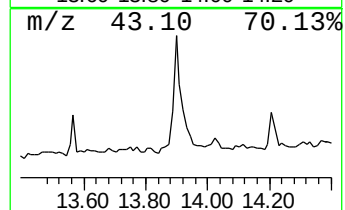
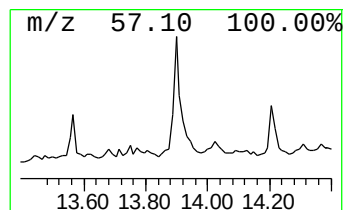
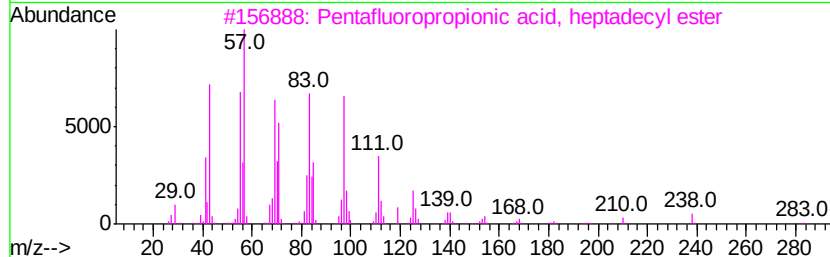
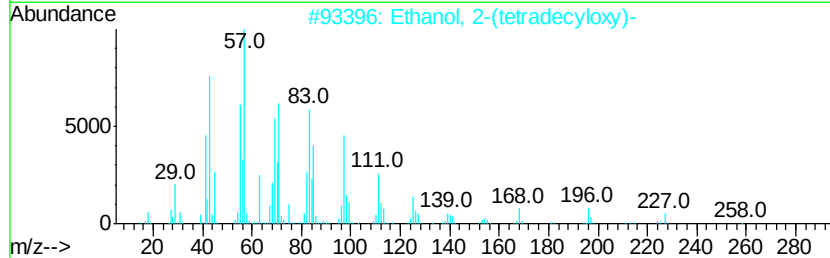
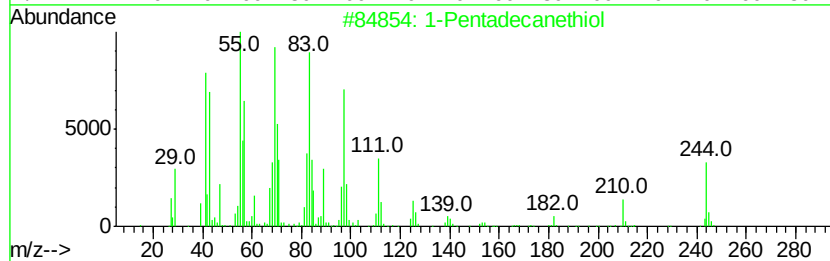
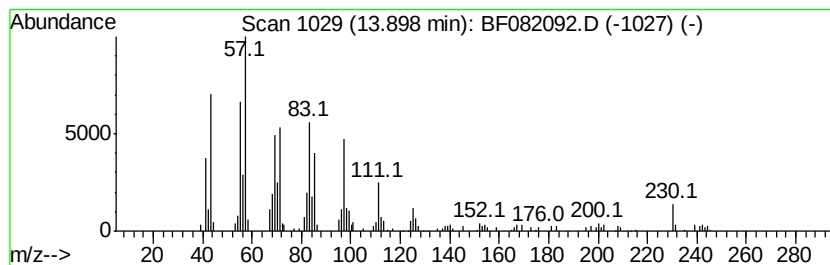
Instrument :
BNA_F
ClientSampleId :
IM-MLA-(1.5-02)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Pentadecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.90	3.72 ng	207393	Chrysene-d12	14.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	90
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	81
4		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	70
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100615\
Data File : BF082092.D
Acq On : 6 Oct 2015 19:11
Operator : UM/IZ
Sample : G3906-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IM-MLA-(1.5-02)

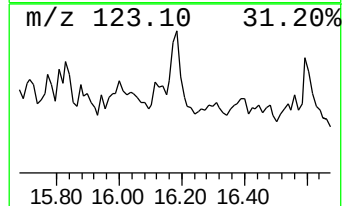
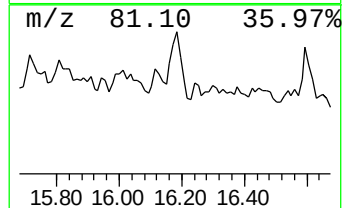
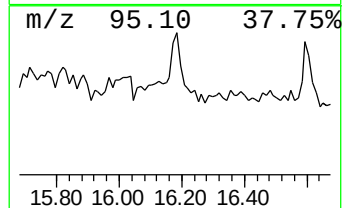
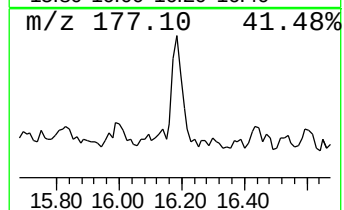
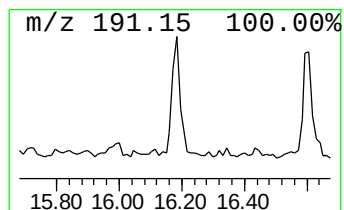
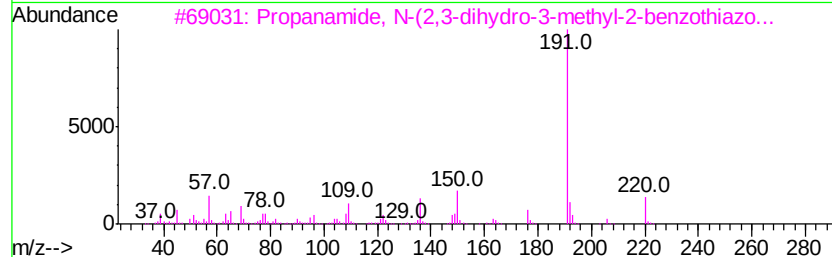
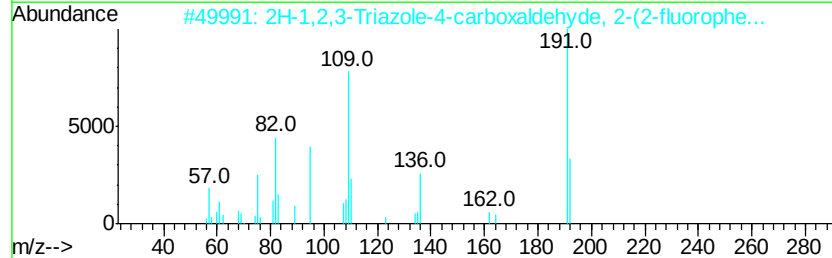
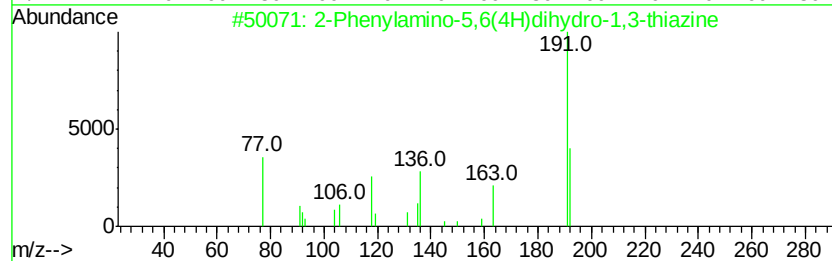
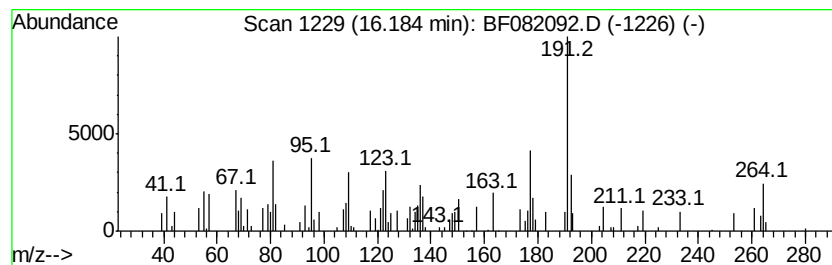
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.18 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.35 ng	73179	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	45
2		2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	35
3		Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	27
4		(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	27
5		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100615\
Data File : BF082092.D
Acq On : 6 Oct 2015 19:11
Operator : UM/IZ
Sample : G3906-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

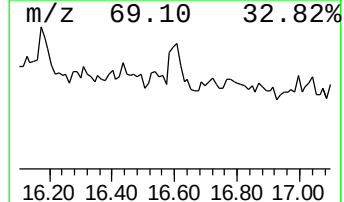
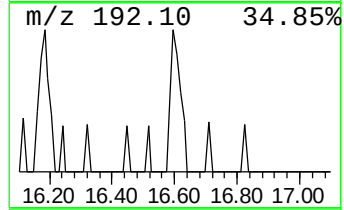
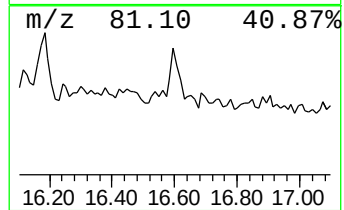
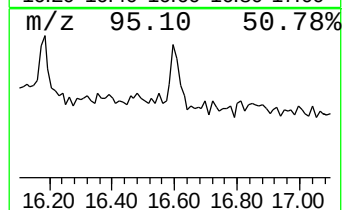
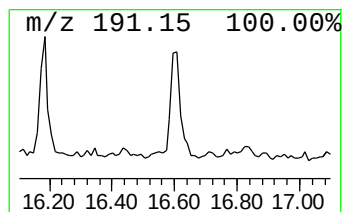
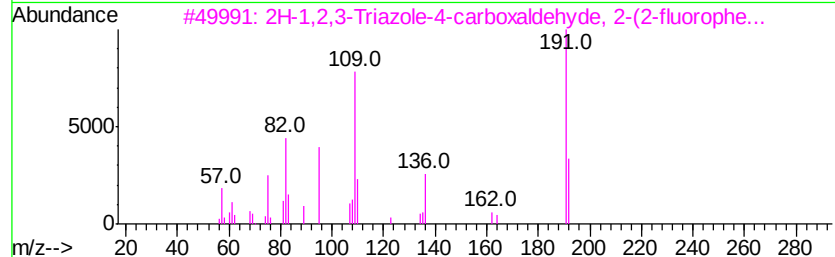
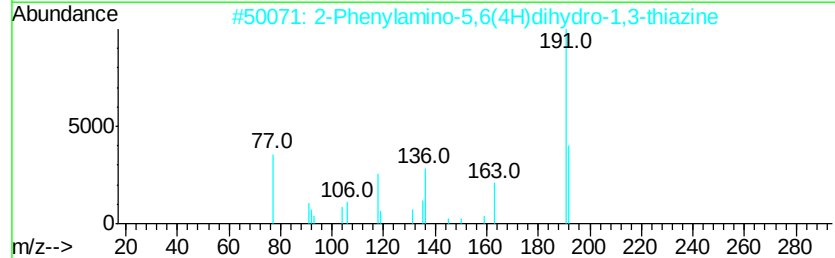
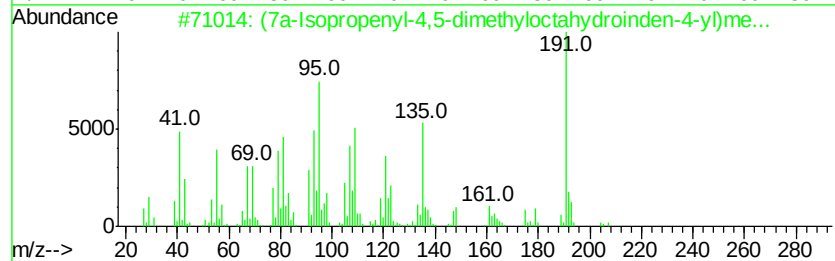
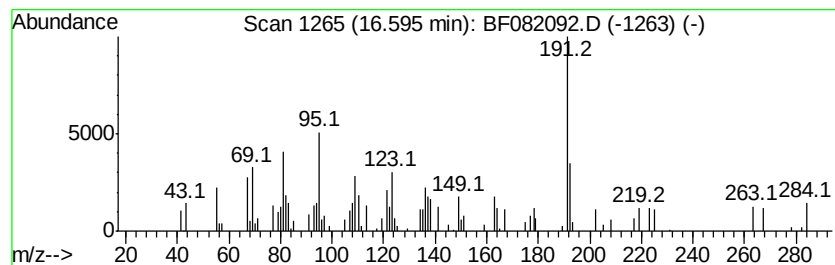
Instrument :
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ClientSampleId :
IM-MLA-(1.5-02)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 (7a-Isopropenyl-4,5-dimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.60	2.40 ng	74819	Perylene-d12	15.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(7a-Isopropenyl-4,5-dimethyl-octa...	222	C15H26O	1000187-02-9	50
2	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	50
3	2H-1,2,3-Triazole-4-carboxaldeh...	191	C9H6FN3O	051306-43-5	47
4	2-Phenyliminoperhydro-1,3-thiazine	192	C10H12N2S	1000138-91-3	43
5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100615\
Data File : BF082092.D
Acq On : 6 Oct 2015 19:11
Operator : UM/IZ
Sample : G3906-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IM-MLA-(1.5-02)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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...	5.06	42.8	ng	1038190	1	6.88	485747	20.0
unknown6.65	6.65	92.5	ng	2246880	1	6.88	485747	20.0
Phenanthrene, 2-m...	11.94	2.5	ng	157111	4	11.42	1237980	20.0
4H-Cyclopenta[def...	12.02	2.1	ng	130419	4	11.42	1237980	20.0
1-Pentadecanethiol	13.90	3.7	ng	207393	5	14.06	1114680	20.0
unknown16.18	16.18	2.4	ng	73179	6	15.51	622843	20.0
(7a-Isopropenyl-4...	16.60	2.4	ng	74819	6	15.51	622843	20.0