

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
 Data File : BG017247.D
 Acq On : 22 May 2015 15:31
 Operator : TP/IZ
 Sample : G2255-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SS043MW009-150512

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_G\METHODS\8270-BG051315.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	2.770	8	14	25	rBV4	56807	137103	1.53%	0.652%
2	2.858	25	29	39	rVB	142608	242536	2.71%	1.153%
3	3.604	150	156	165	rBV	115985	191567	2.14%	0.911%
4	7.012	729	736	742	rBV	705114	1122043	12.54%	5.333%
5	7.071	742	746	752	rVB	77488	112686	1.26%	0.536%
6	7.570	823	831	838	rVB	188746	329673	3.69%	1.567%
7	7.682	843	850	852	rBV	175471	254697	2.85%	1.211%
8	7.723	852	857	864	rVB	735279	1200539	13.42%	5.707%
9	8.046	900	912	919	rVB	5086626	8944624	100.00%	42.517%
10	8.293	949	954	957	rVV2	110956	169981	1.90%	0.808%
11	8.328	957	960	966	rVB	107137	159630	1.78%	0.759%
12	8.622	1004	1010	1016	rBV3	62505	105919	1.18%	0.503%
13	8.793	1030	1039	1044	rBV	199382	345153	3.86%	1.641%
14	8.863	1044	1051	1057	rVB5	36150	92738	1.04%	0.441%
15	8.981	1064	1071	1078	rBV3	99037	215900	2.41%	1.026%
16	9.098	1086	1091	1093	rBV2	217503	358395	4.01%	1.704%
17	9.122	1093	1095	1101	rVB	249423	315808	3.53%	1.501%
18	9.251	1110	1117	1118	rBV2	60573	108530	1.21%	0.516%
19	9.386	1133	1140	1147	rBV6	55761	137282	1.53%	0.653%
20	9.486	1152	1157	1163	rVB2	168411	269215	3.01%	1.280%
21	9.897	1214	1227	1234	rVB2	156229	356769	3.99%	1.696%
22	10.120	1259	1265	1274	rBV3	93794	191277	2.14%	0.909%
23	10.256	1282	1288	1296	rBV	204406	365394	4.09%	1.737%
24	10.473	1319	1325	1331	rBV	238607	409736	4.58%	1.948%
25	11.019	1412	1418	1424	rBV	247843	390955	4.37%	1.858%
26	11.589	1508	1515	1520	rVB2	64291	126400	1.41%	0.601%
27	12.100	1595	1602	1609	rVB2	68637	140135	1.57%	0.666%
28	12.947	1741	1746	1752	rVB3	92724	161441	1.80%	0.767%
29	13.305	1800	1807	1812	rBV4	51935	108859	1.22%	0.517%
30	13.364	1812	1817	1822	rVV	118295	209849	2.35%	0.997%
31	13.657	1861	1867	1872	rBV9	39981	89715	1.00%	0.426%
32	13.793	1886	1890	1900	rVB2	83227	155985	1.74%	0.741%
33	14.333	1977	1982	1990	rVB2	324201	510507	5.71%	2.427%
34	15.825	2233	2236	2244	rVB4	73300	117413	1.31%	0.558%

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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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35	16.037	2268	2272	2277	rBV2	77047	125735	1.41%	0.598%
36	17.083	2444	2450	2456	rBV2	401679	574196	6.42%	2.729%
37	17.994	2600	2605	2610	rBV	280006	390396	4.36%	1.856%
38	19.274	2819	2823	2833	rVB2	227403	319569	3.57%	1.519%
39	19.715	2894	2898	2904	rVB	136756	170330	1.90%	0.810%
40	20.984	3110	3114	3120	rBV2	86607	128335	1.43%	0.610%
41	21.266	3157	3162	3167	rBV	485518	602675	6.74%	2.865%
42	23.516	3538	3545	3553	rBV2	297671	578307	6.47%	2.749%

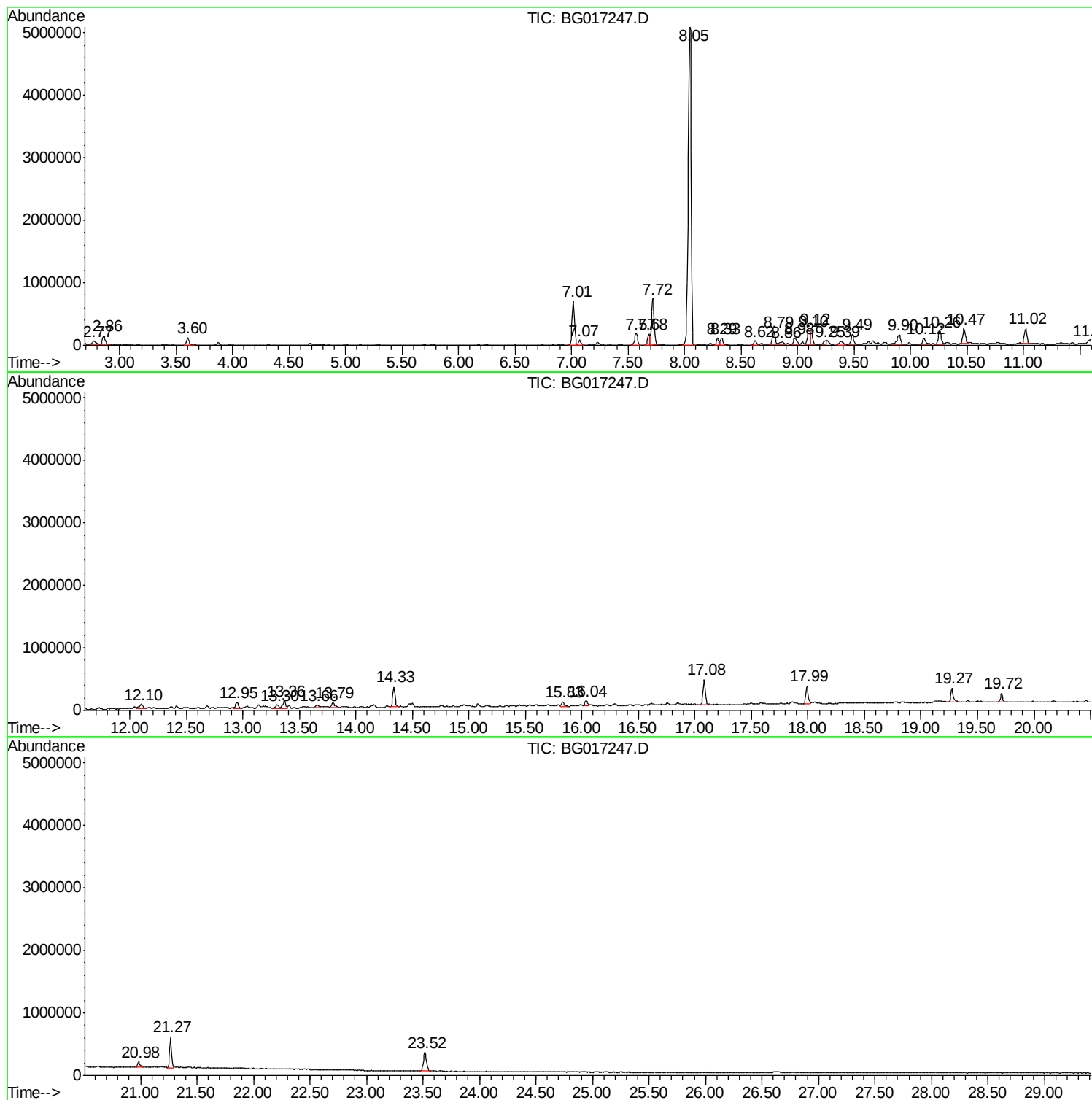
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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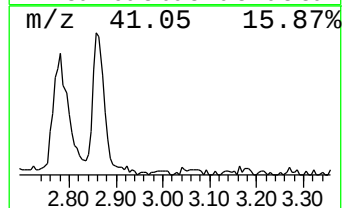
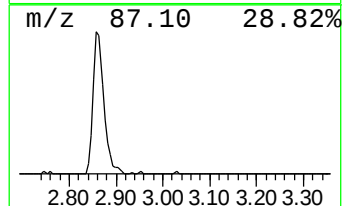
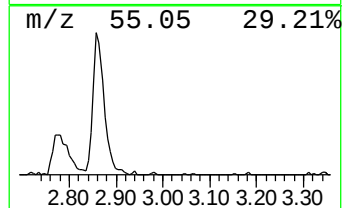
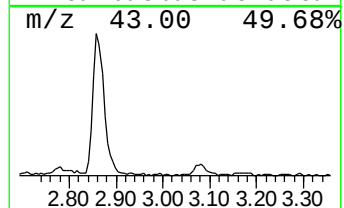
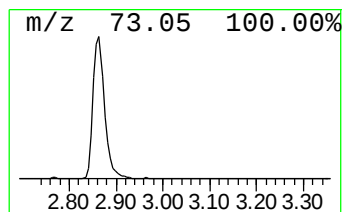
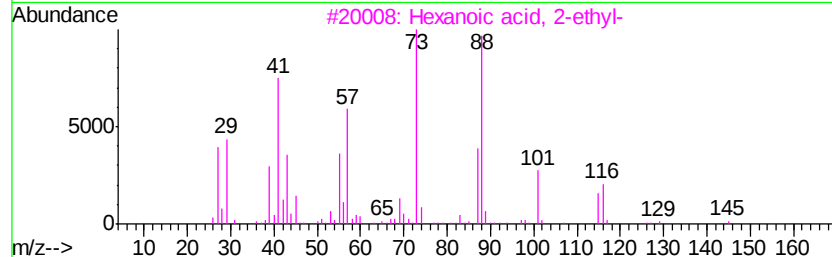
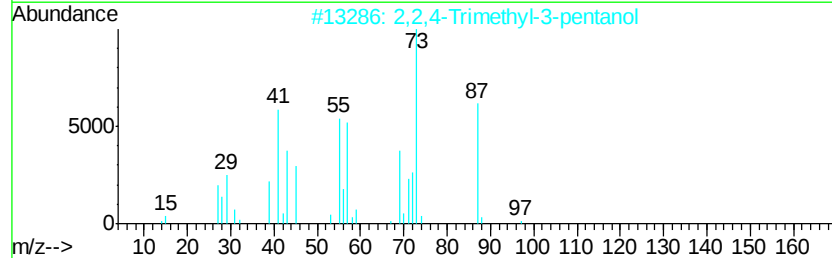
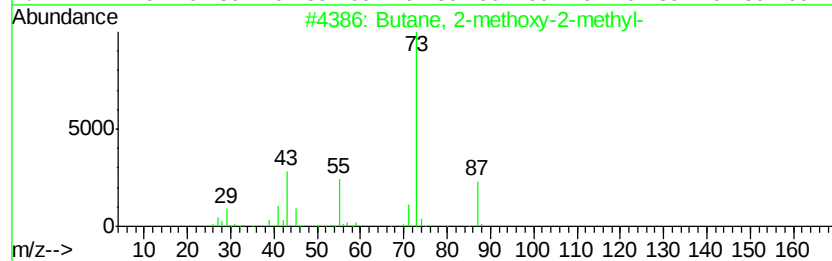
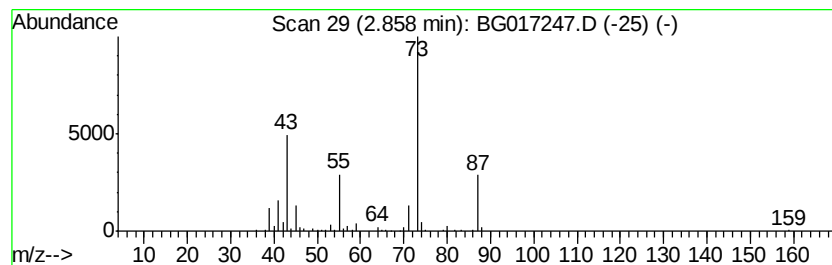
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	19.05 ng	242536	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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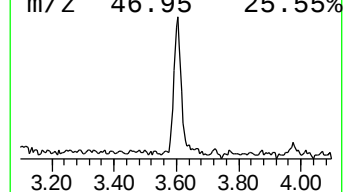
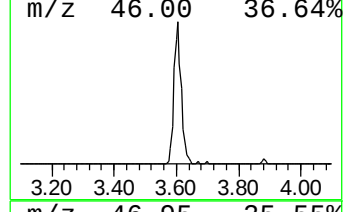
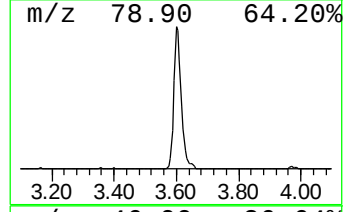
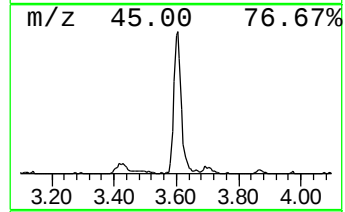
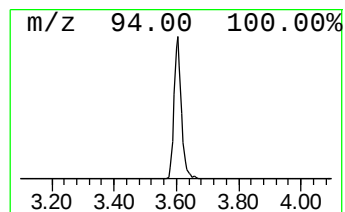
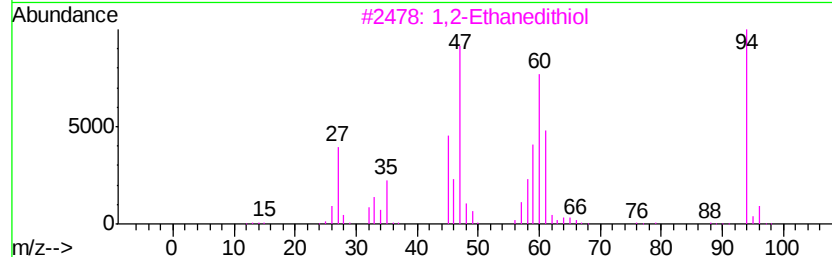
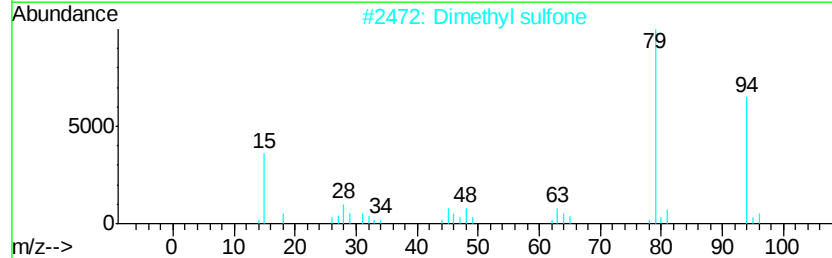
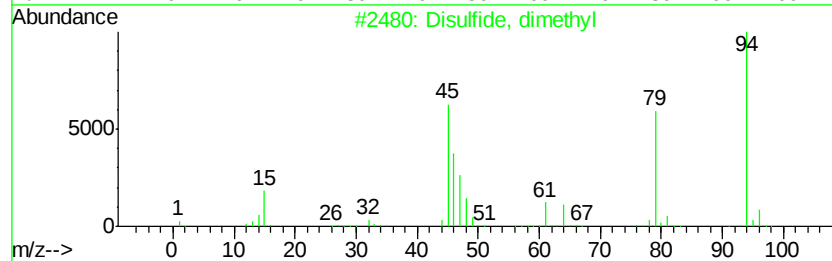
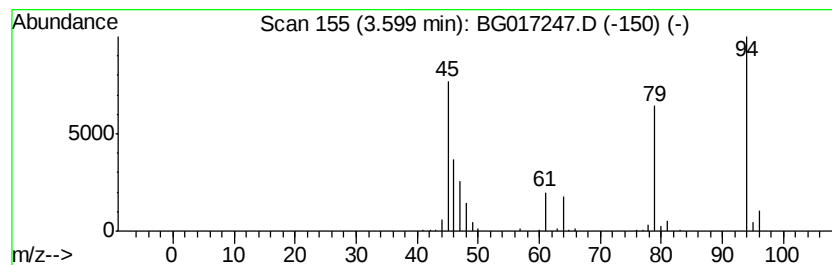
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 Disulfide, dimethyl Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	15.04 ng	191567	1,4-Dichlorobenzene-d4	7.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2		Dimethyl sulfone	94	C2H6O2S	000067-71-0	43
3		1,2-Ethanedithiol	94	C2H6S2	000540-63-6	38
4		S-(2,2,2-Trifluoroethyl) methane...	194	C3H5F3O2S2	069466-44-0	28
5		Ethyl 3-methyl-8-[p-sulfamylbenz...	416	C18H20N6O4S	021271-88-5	12



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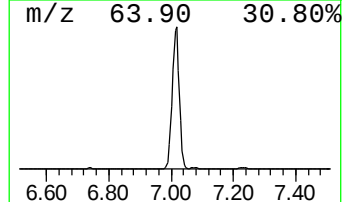
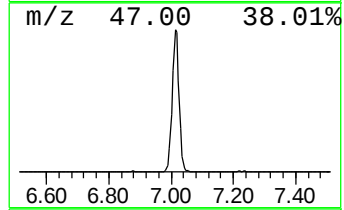
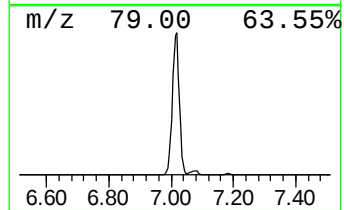
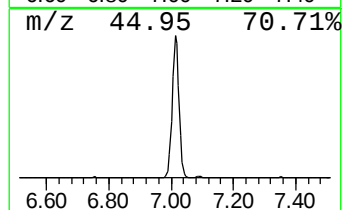
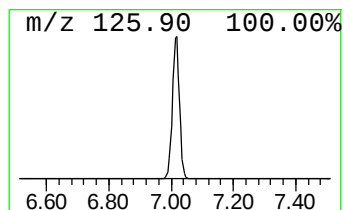
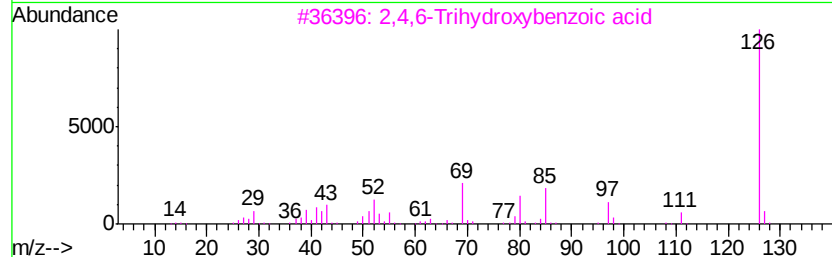
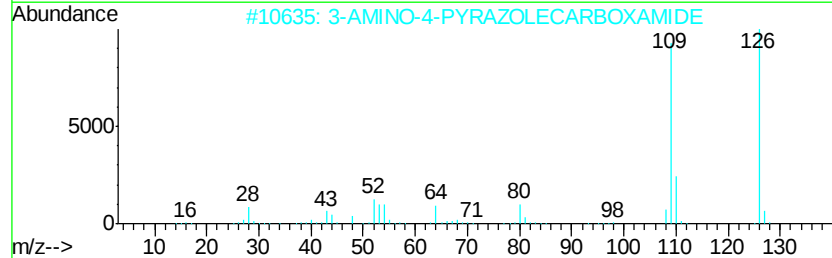
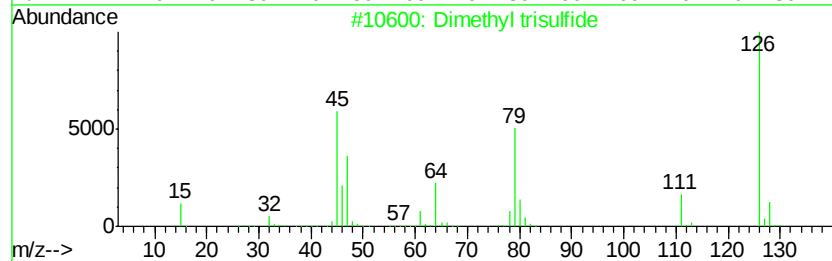
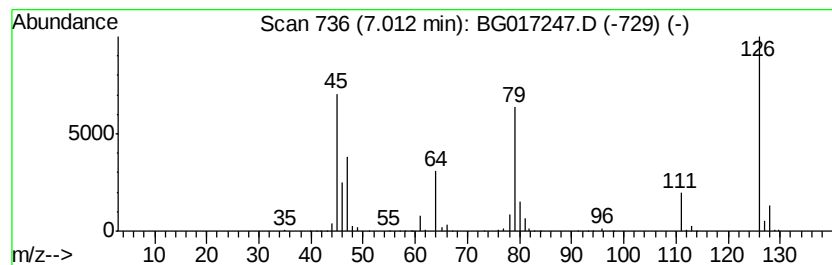
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dimethyl trisulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.01	88.11 ng	1122040	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethyl trisulfide	126	C2H6S3	003658-80-8	97
2		3-AMINO-4-PYRAZOLECARBOXAMIDE	126	C4H6N4O	1000239-42-1	22
3		2,4,6-Trihydroxybenzoic acid	170	C7H6O5	000083-30-7	12
4		3H-Pyrazol-3-one, 1,2-dihydro-1,...	126	C6H10N2O	003201-26-1	9
5		4-Methyl-2-pyrimidinethiol	126	C5H6N2S	035071-17-1	9



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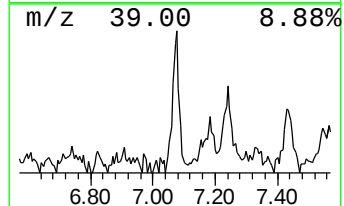
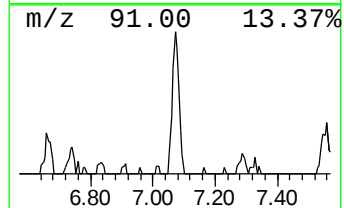
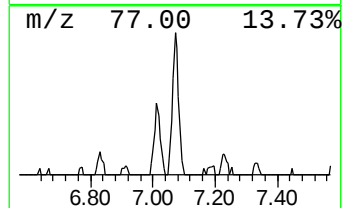
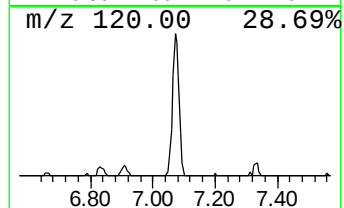
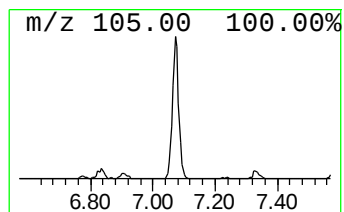
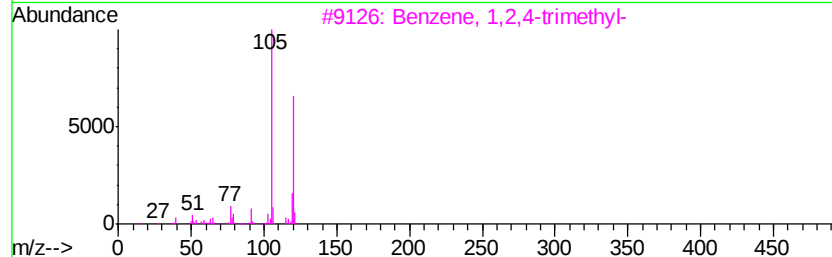
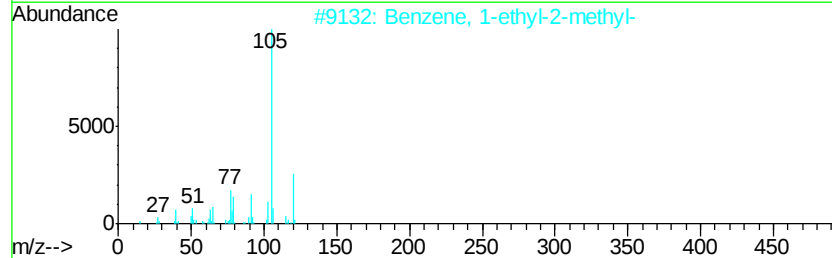
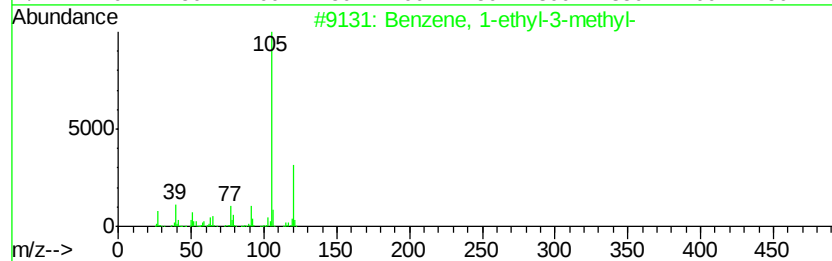
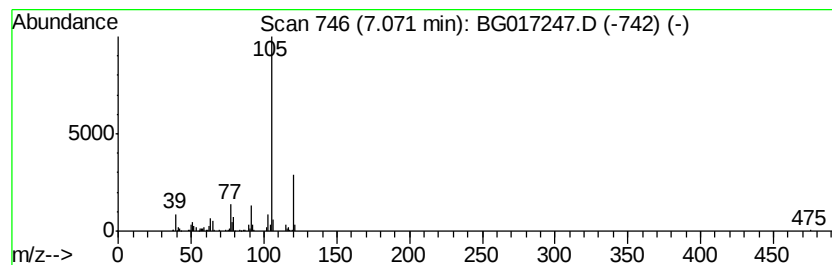
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	8.85 ng	112686	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87
4		Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	87
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87



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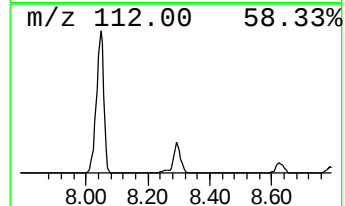
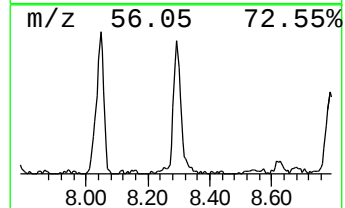
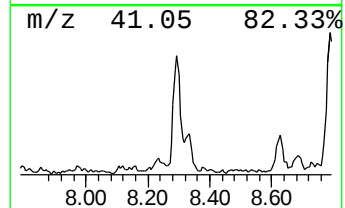
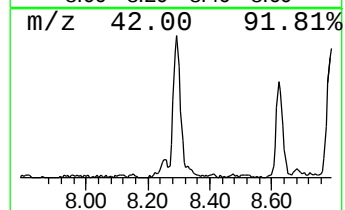
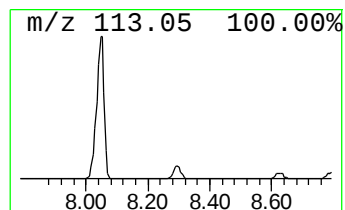
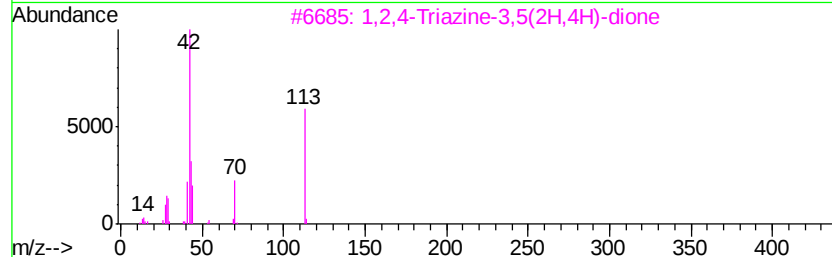
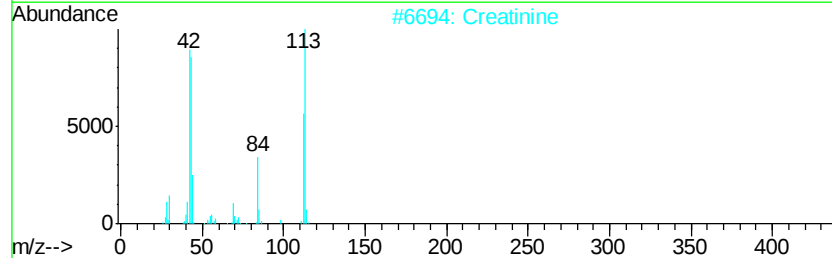
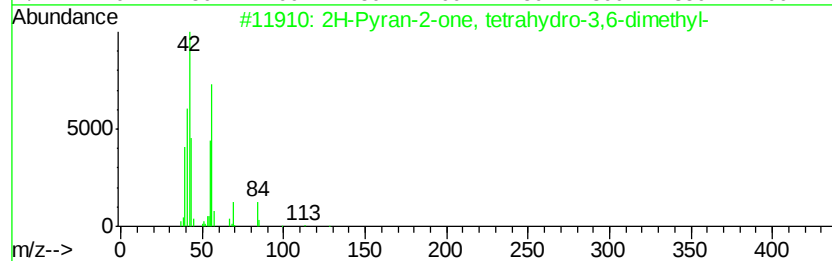
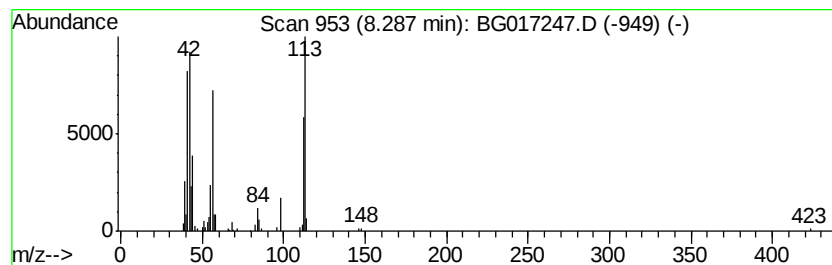
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown8.29 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	13.35 ng	169981	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Pyran-2-one, tetrahydro-3,6-d...	128	C7H12O2	003720-22-7	32
2		Creatinine	113	C4H7N3O	000060-27-5	32
3		1,2,4-Triazine-3,5(2H,4H)-dione	113	C3H3N3O2	000461-89-2	25
4		1,4-Cyclohexanedione	112	C6H8O2	000637-88-7	22
5		Piperidine-2,5-dione	113	C5H7N O2	052065-78-8	22



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

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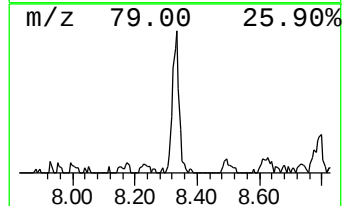
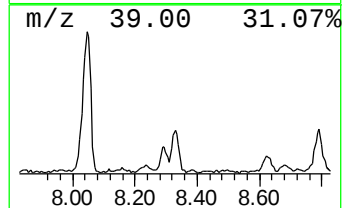
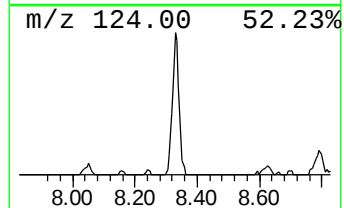
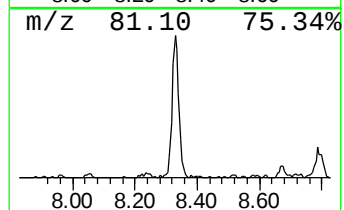
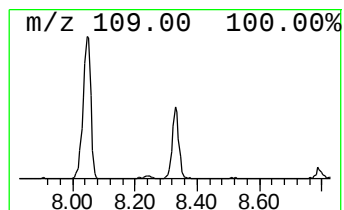
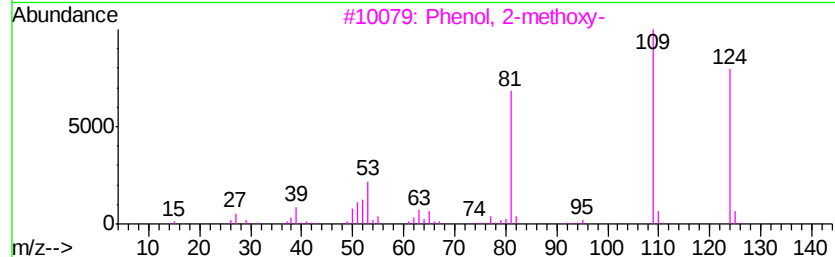
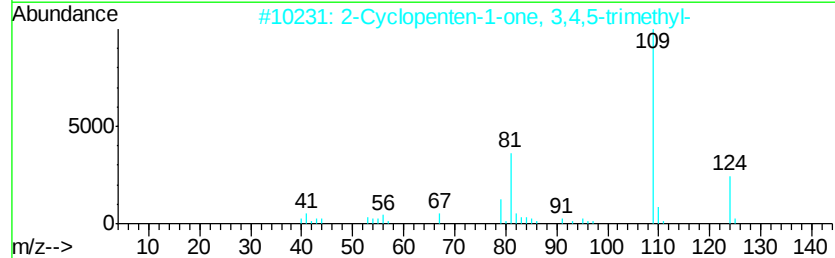
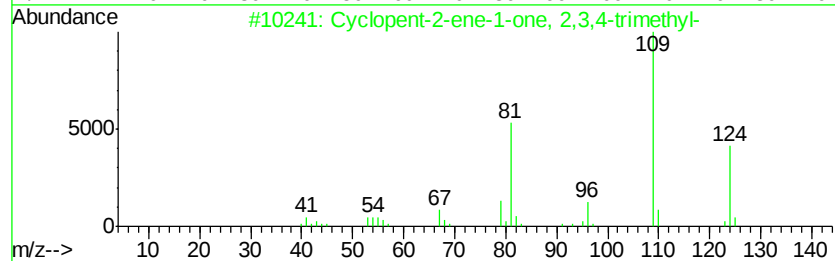
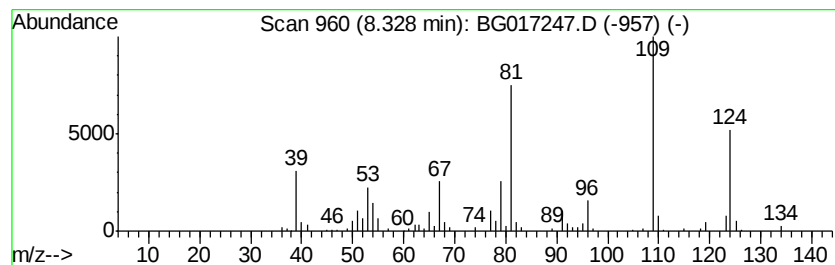
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopent-2-ene-1-one, 2,3,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.33	12.53 ng	159630	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopent-2-ene-1-one, 2,3,4-tri...	124	C8H12O	083321-16-8	87
2		2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	87
3		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	76
4		2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	74
5		Mequinol	124	C7H8O2	000150-76-5	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS043MW009-150512

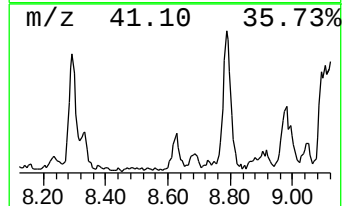
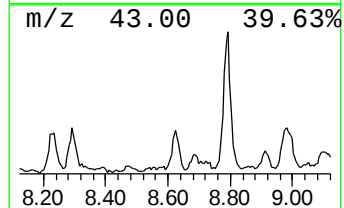
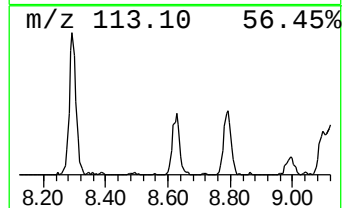
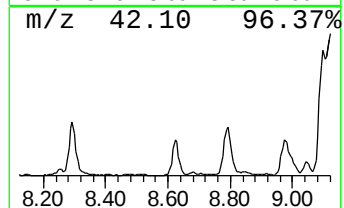
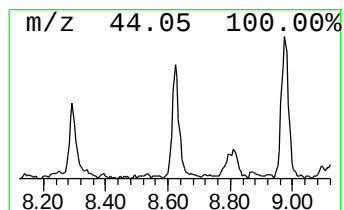
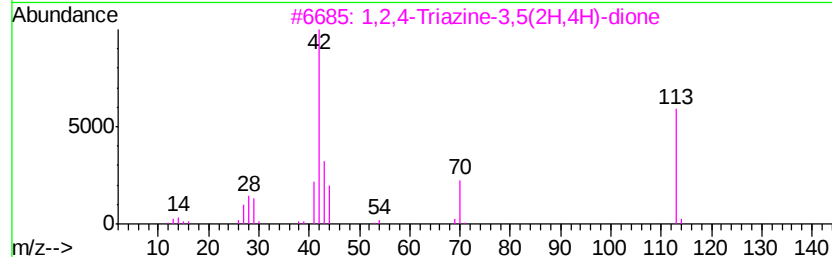
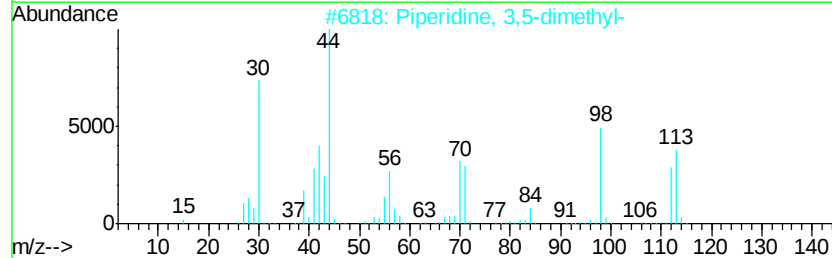
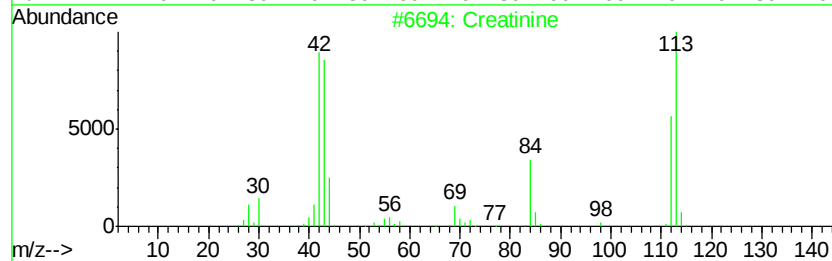
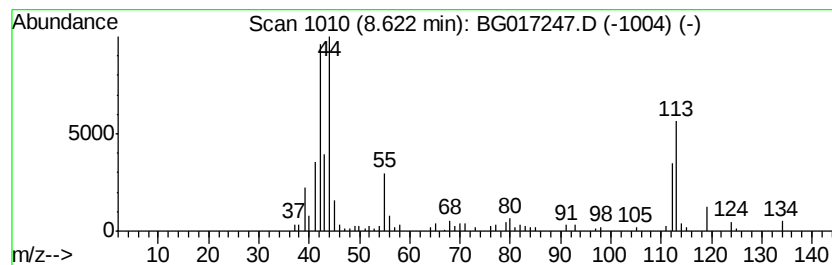
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.62 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	8.32 ng	105919	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Creatinine	113	C4H7N3O	000060-27-5	40
2		Piperidine, 3,5-dimethyl-	113	C7H15N	035794-11-7	38
3		1,2,4-Triazine-3,5(2H,4H)-dione	113	C3H3N3O2	000461-89-2	38
4		1,3-Cyclohexanedione	112	C6H8O2	000504-02-9	27
5		4-Amino-3,5-dimethyl-1,2,4-triazole	112	C4H8N4	003530-15-2	16



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
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Misc :
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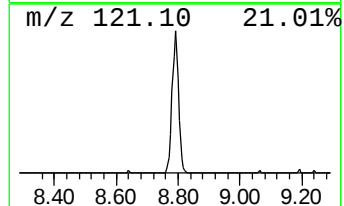
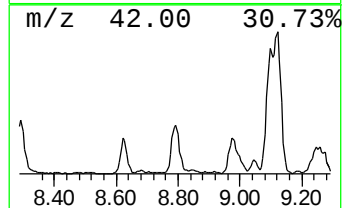
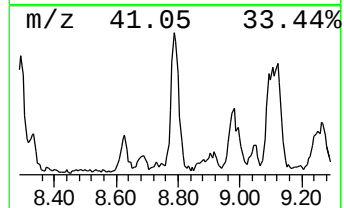
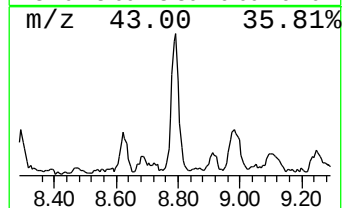
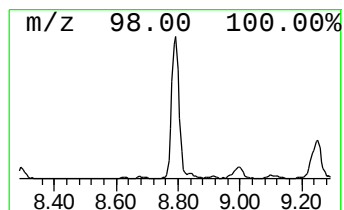
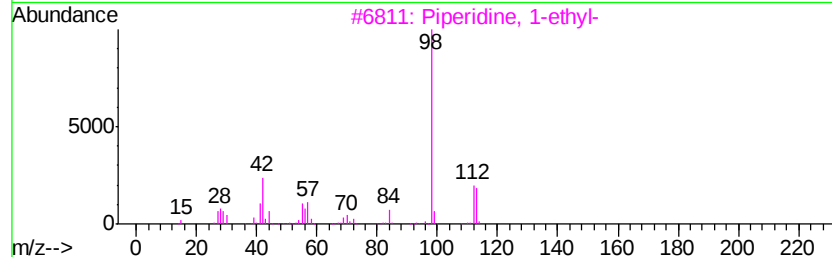
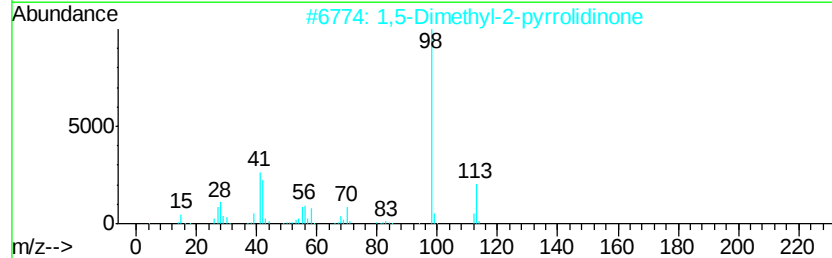
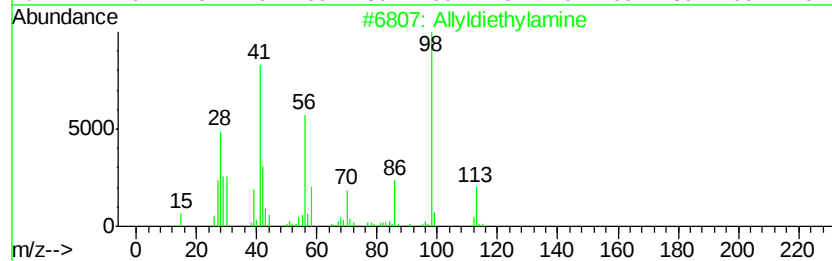
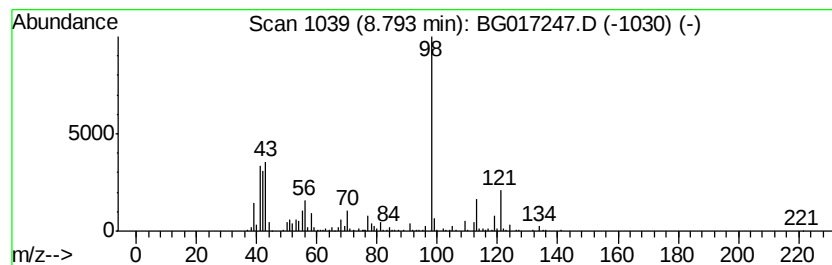
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Allyldiethylamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.79	27.10 ng	345153	1,4-Dichlorobenzene-d4	7.68		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Allyldiethylamine	113	C7H15N	005666-17-1	80
2		1,5-Dimethyl-2-pyrrolidinone	113	C6H11NO	005075-92-3	76
3		Piperidine, 1-ethyl-	113	C7H15N	000766-09-6	72
4		Piperidine, 1-(2-phenylethyl)-	189	C13H19N	000332-14-9	53
5		3H-Pyrazol-3-one, 1,2-dihydro-5-...	98	C4H6N2O	004344-87-0	50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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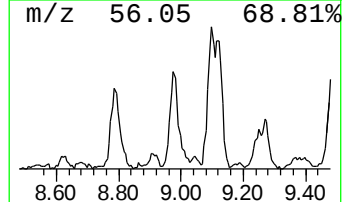
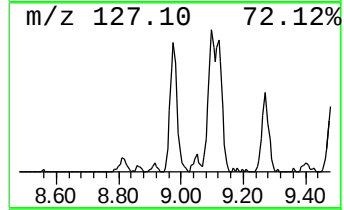
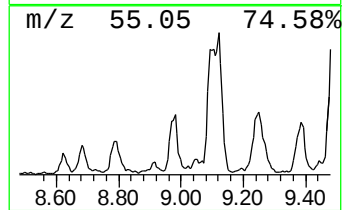
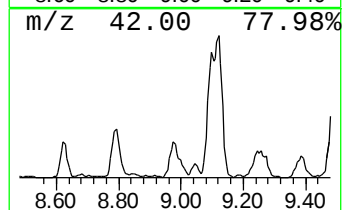
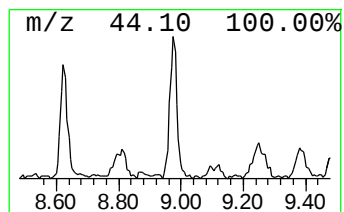
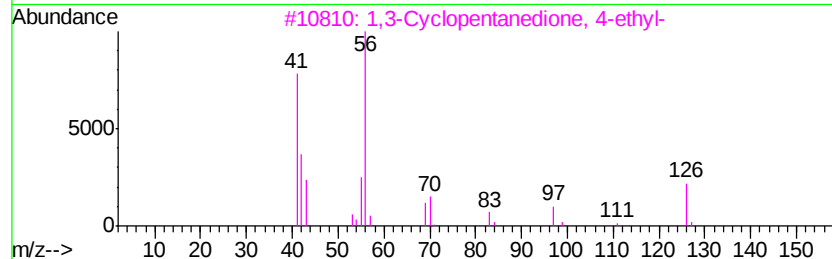
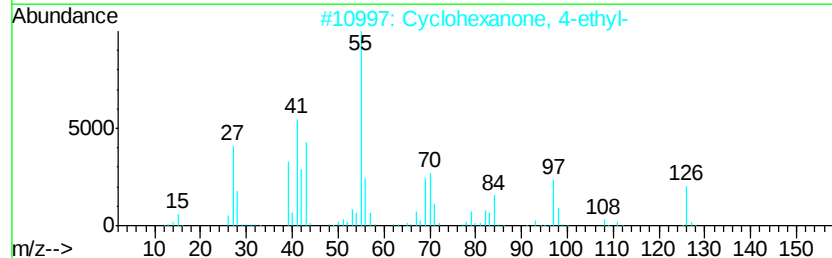
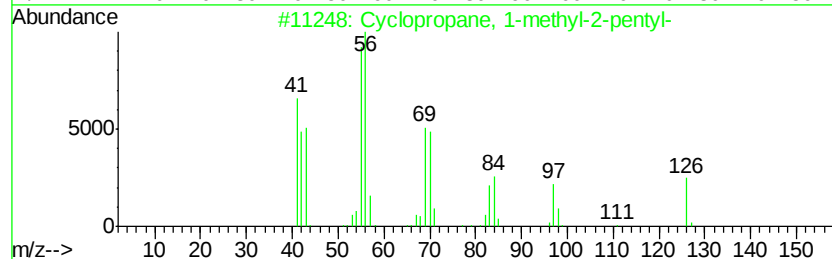
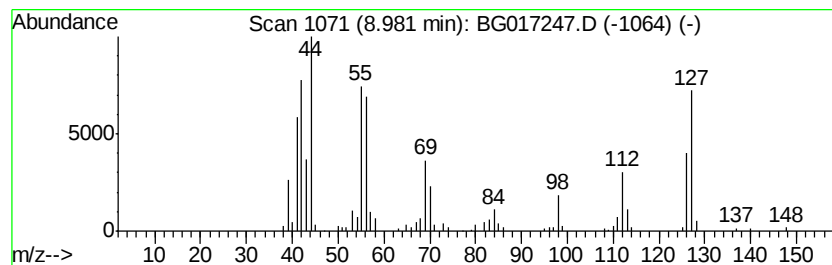
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.98 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	16.95 ng	215900	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, 1-methyl-2-pentyl-	126	C9H18	041977-37-1	49
2		Cyclohexanone, 4-ethyl-	126	C8H14O	005441-51-0	38
3		1,3-Cyclopentanedione, 4-ethyl-	126	C7H10O2	057157-03-6	27
4		4,4-Dimethylazetidin-2-one	99	C5H9NO	004879-95-2	25
5		2-Hexene, (E)-	84	C6H12	004050-45-7	18



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
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Acq On : 22 May 2015 15:31
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Misc :
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Instrument :
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ClientSampleId :
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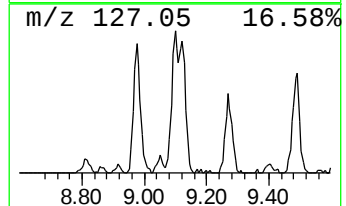
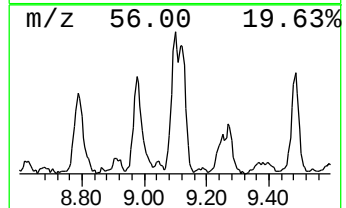
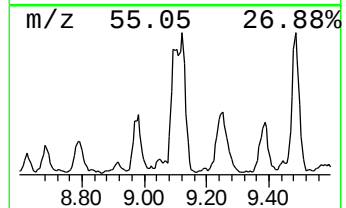
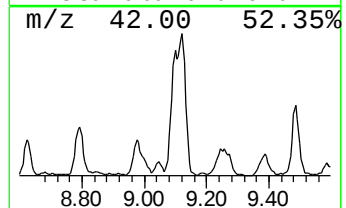
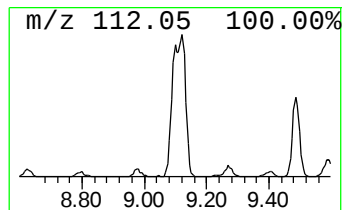
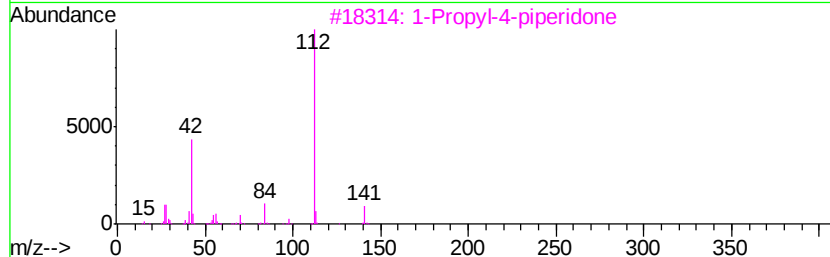
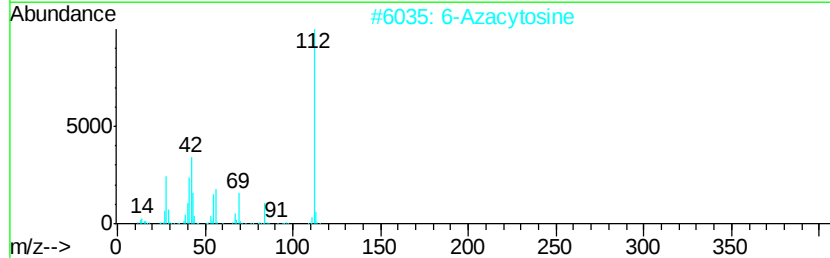
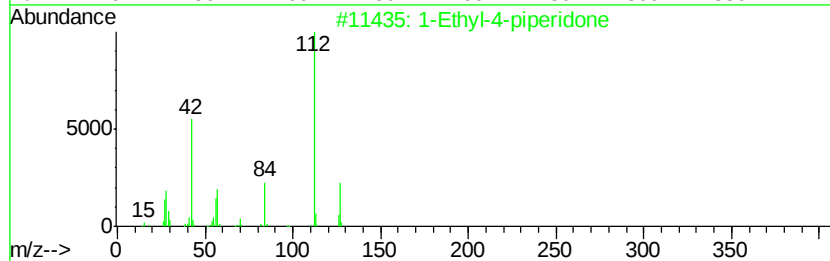
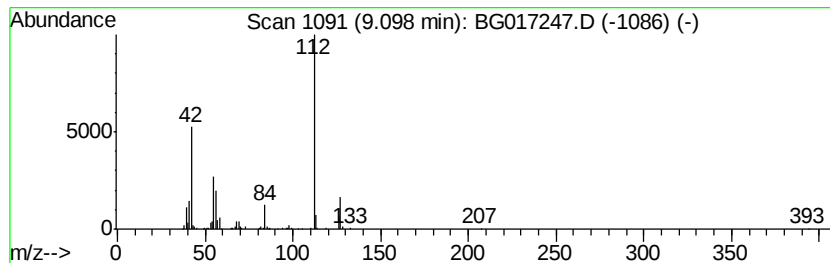
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Ethyl-4-piperidone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.10	17.49 ng	358395	Naphthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-4-piperidone	127	C7H13NO	003612-18-8	80
2		6-Azacytosine	112	C3H4N4O	000931-85-1	72
3		1-Propyl-4-piperidone	141	C8H15NO	023133-37-1	50
4		2-Cyclopenten-1-one, 2-hydroxy-3...	112	C6H8O2	000080-71-7	47
5		2-Pyrrolidinecarboxylic acid, 1,...	171	C8H13NO3	056145-23-4	40



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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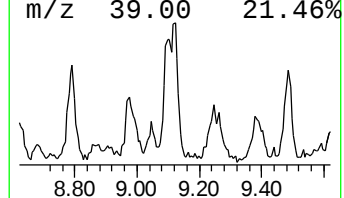
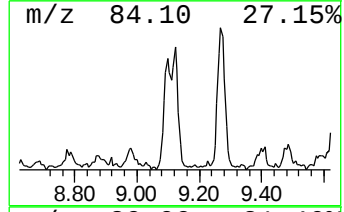
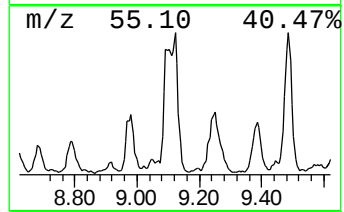
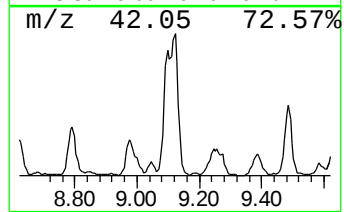
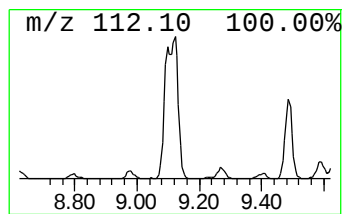
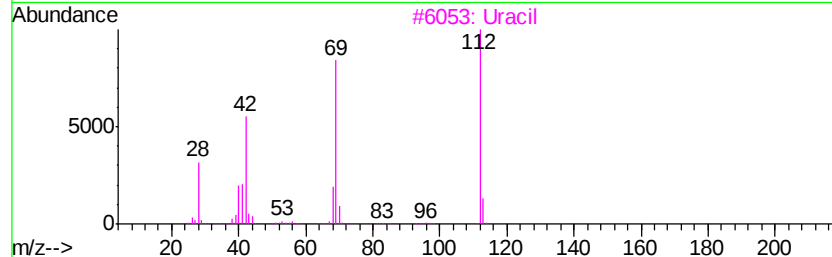
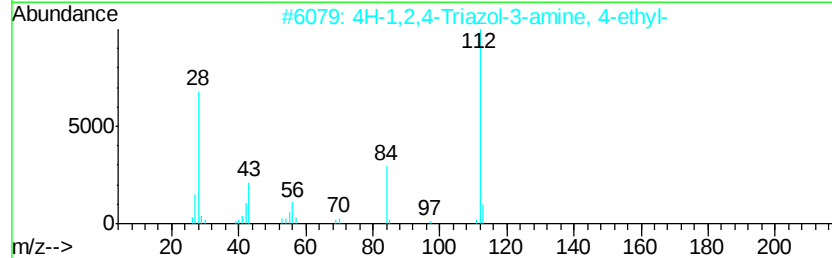
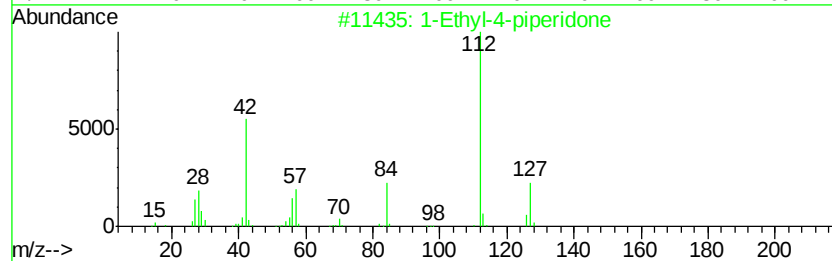
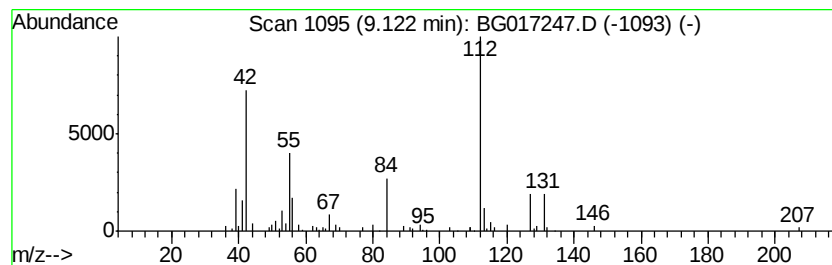
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 4H-1,2,4-Triazol-3-amine, 4... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.12	15.42 ng	315808	Naphthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-4-piperidone	127	C7H13NO	003612-18-8	72
2		4H-1,2,4-Triazol-3-amine, 4-ethyl-	112	C4H8N4	042786-06-1	50
3		Uracil	112	C4H4N2O2	000066-22-8	47
4		2H-Pyran-2,6(3H)-dione	112	C5H4O3	005926-95-4	47
5		6-Azacytosine	112	C3H4N4O	000931-85-1	47



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
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Misc :
ALS Vial : 7 Sample Multiplier: 1

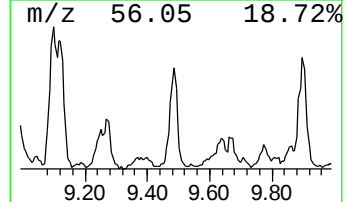
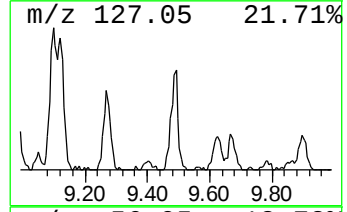
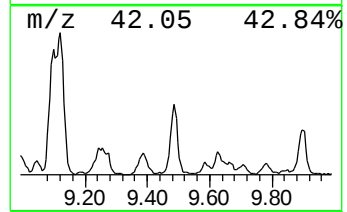
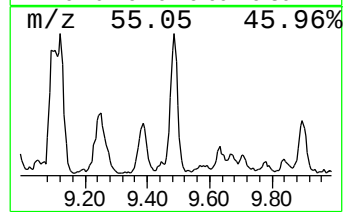
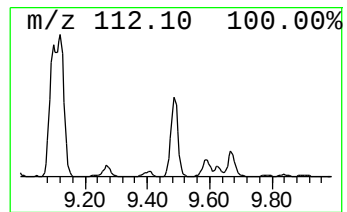
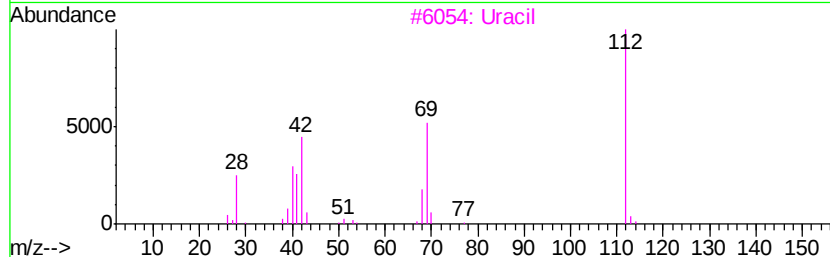
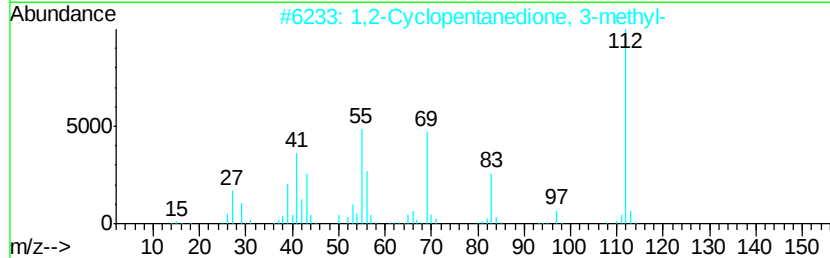
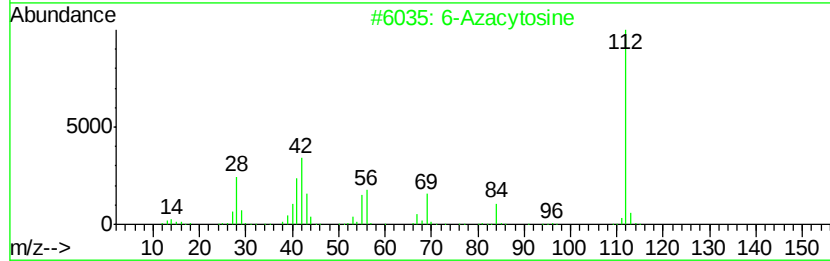
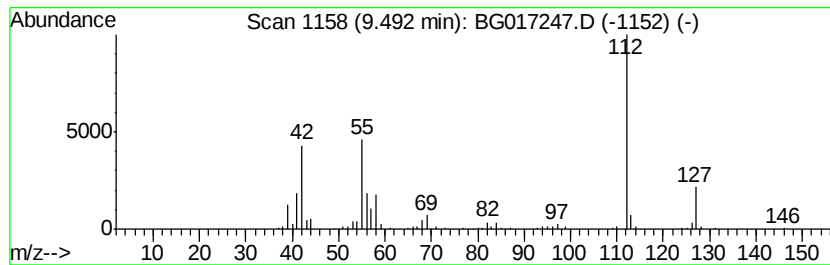
Instrument :
BNA_G
ClientSampleId :
SS043MW009-150512

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 6-Azacytosine Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.49	13.14 ng	269215	Naphthalene-d8	10.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Azacytosine	112	C3H4N4O	000931-85-1	58
2	1,2-Cyclopentanedione, 3-methyl-	112	C6H8O2	000765-70-8	49
3	Uracil	112	C4H4N2O2	000066-22-8	47
4	1-Ethyl-4-piperidone	127	C7H13NO	003612-18-8	42
5	1H-1,3-Diazepine, 4,5,6,7-tetra...	112	C6H12N2	018237-68-8	40



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

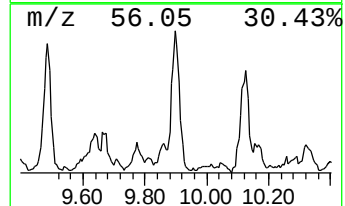
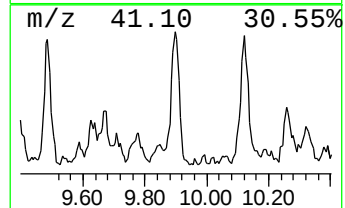
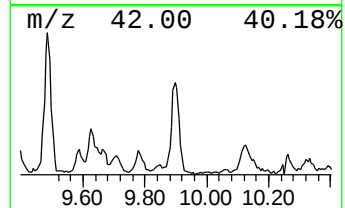
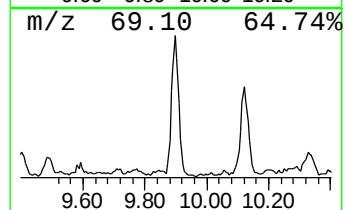
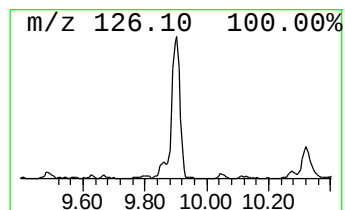
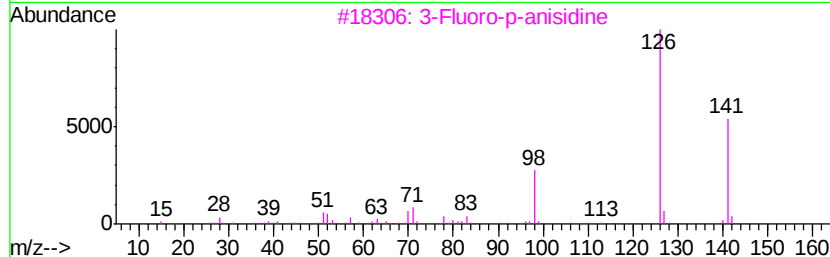
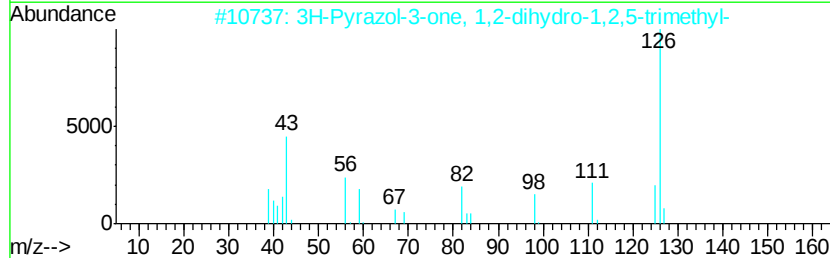
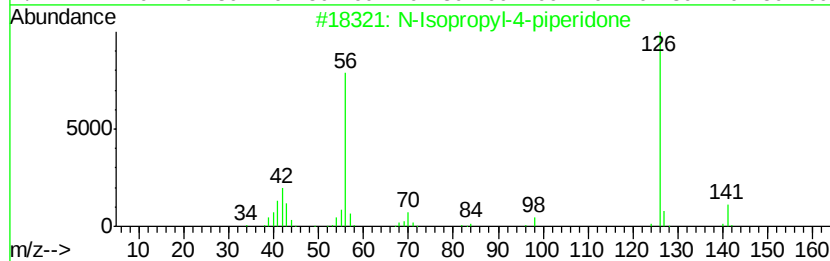
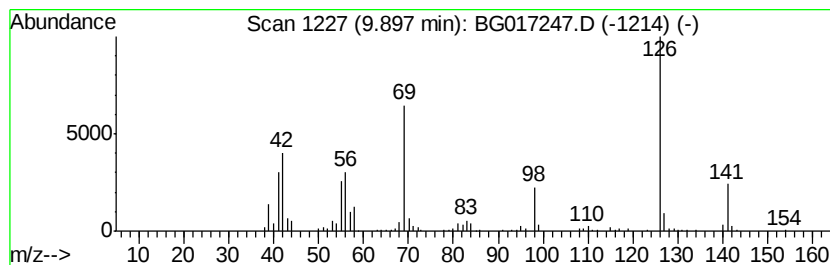
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ClientSampleId :
SS043MW009-150512

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 N-Isopropyl-4-piperidone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.90	17.41 ng	356769	Naphthalene-d8	10.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Isopropyl-4-piperidone	141	C8H15NO	005355-68-0	64
2	3H-Pyrazol-3-one, 1,2-dihydro-1,...	126	C6H10N2O	003201-26-1	50
3	3-Fluoro-p-anisidine	141	C7H8FN0	000366-99-4	47
4	5-Methyl-1,3-cyclohexanedione	126	C7H10O2	004341-24-6	42
5	4,6-Dihydroxy-2-methylpyrimidine	126	C5H6N2O2	040497-30-1	40



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

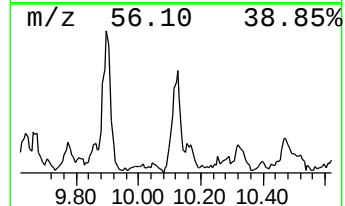
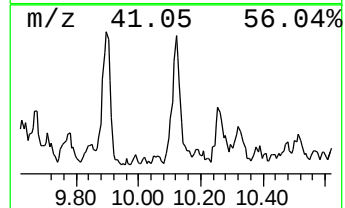
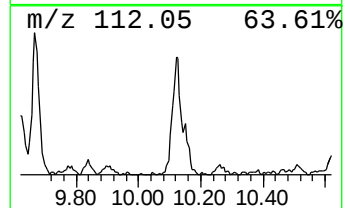
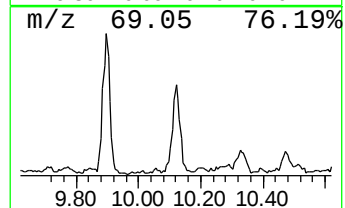
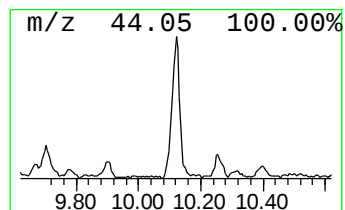
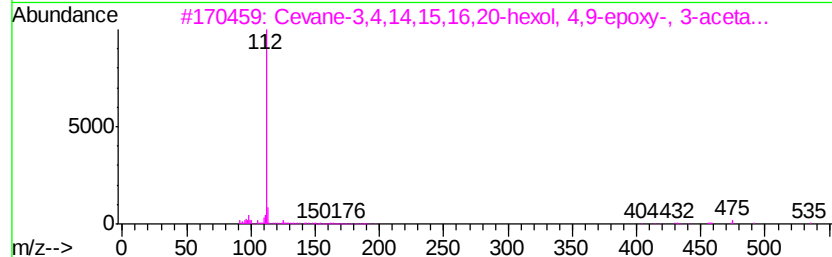
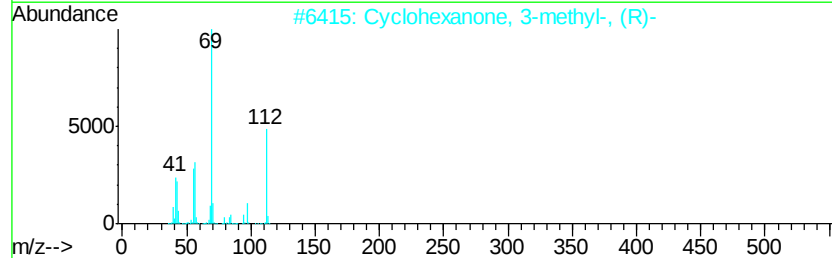
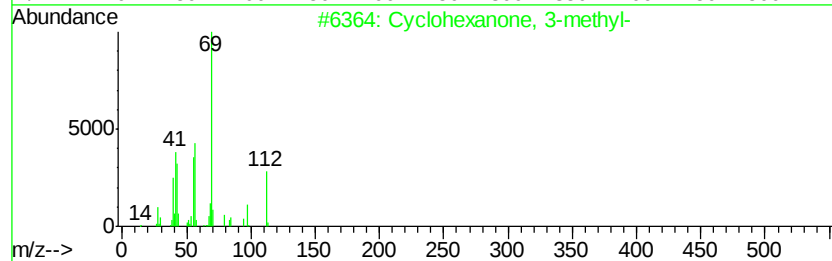
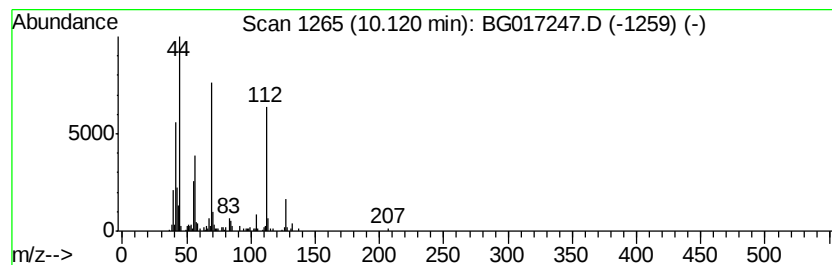
Instrument :
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ClientSampleId :
SS043MW009-150512

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Cyclohexanone, 3-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.12	9.34 ng	191277	Napthalene-d8	10.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexanone, 3-methyl-	112 C7H12O	000591-24-2 52
2		Cyclohexanone, 3-methyl-, (R)-	112 C7H12O	013368-65-5 43
3		Cevane-3,4,14,15,16,20-hexol, 4,...	535 C29H45NO8	002777-79-9 42
4		1H-Imidazole, 2-ethyl-4,5-dihydr...	112 C6H12N2	000931-35-1 42
5		3-Buten-2-amine, N,N-diethyl-	127 C8H17N	037969-64-5 38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS043MW009-150512

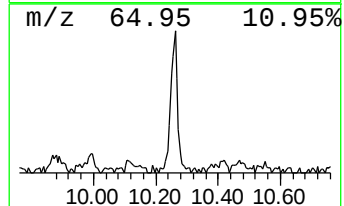
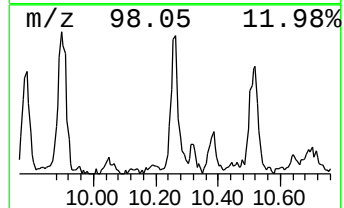
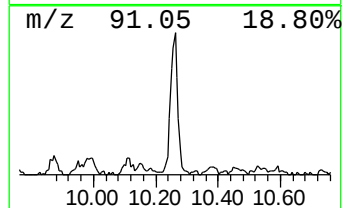
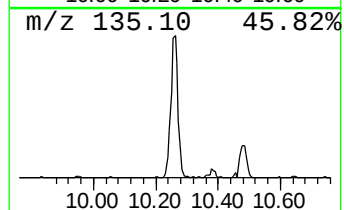
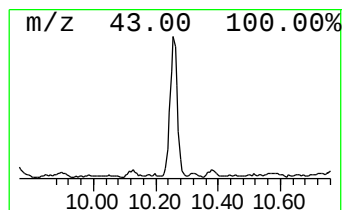
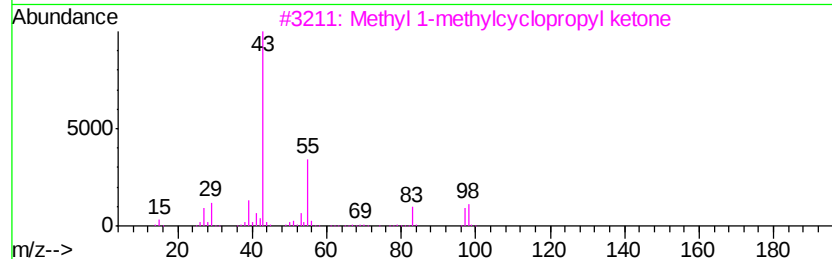
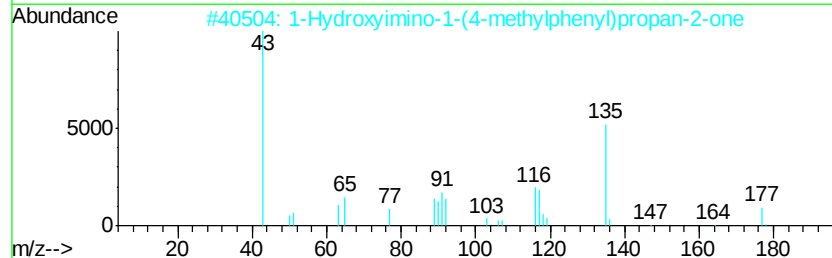
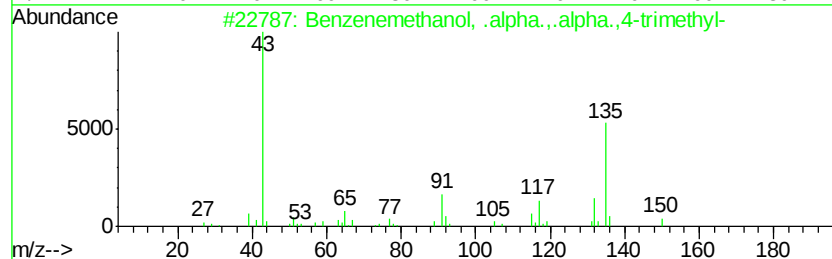
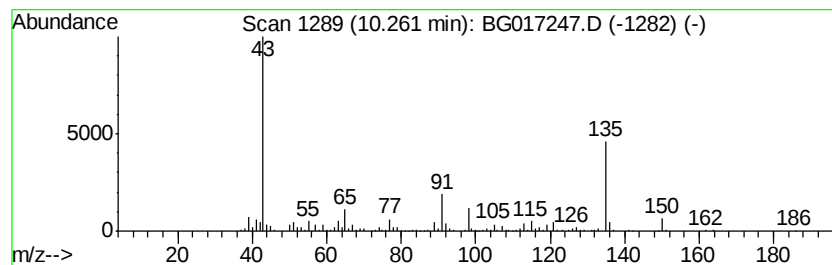
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzenemethanol, .alpha.,.a... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	17.84 ng	365394	Napthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenemethanol, .alpha.,.alpha....	150	C10H14O	001197-01-9	72
2		1-Hydroxyimino-1-(4-methylphenyl)...	177	C10H11NO2	053815-22-8	33
3		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10
4		1,6;2,3-Dianhydro-4-O-acetyl-.be...	186	C8H10O5	1000139-89-3	9
5		Acetic acid, phenyl-, isopentyl ...	206	C13H18O2	000102-19-2	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SS043MW009-150512

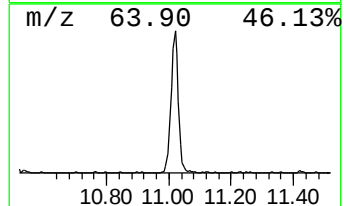
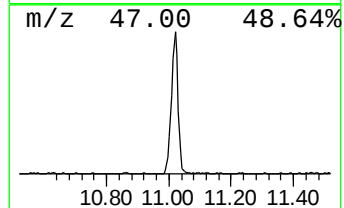
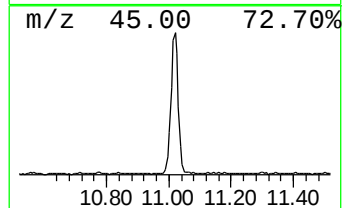
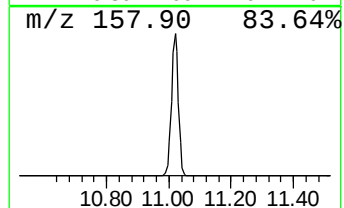
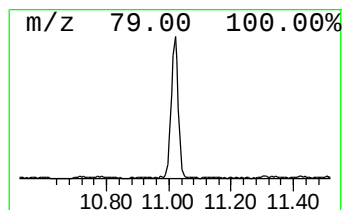
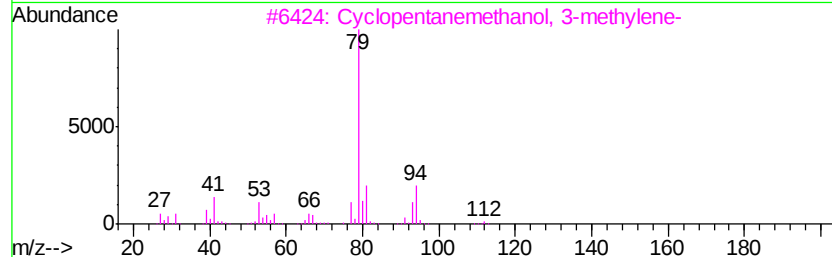
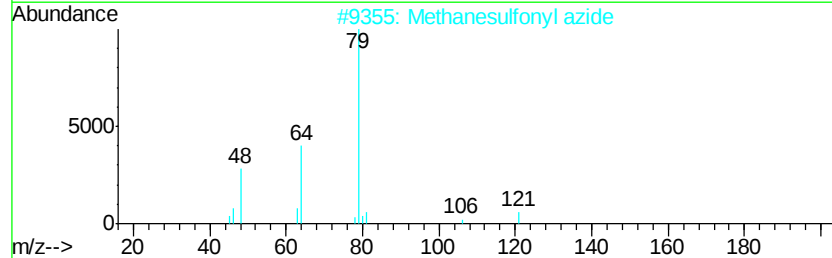
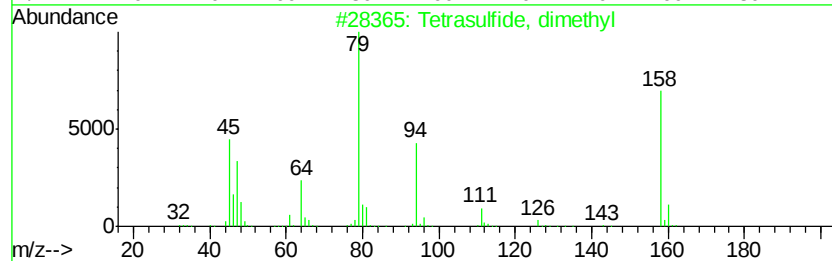
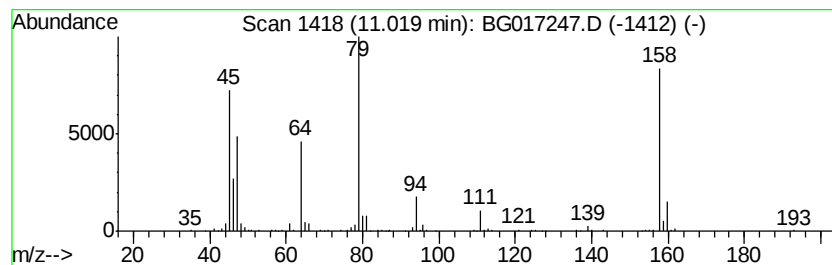
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Tetrasulfide, dimethyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	19.08 ng	390955	Naphthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrasulfide, dimethyl	158	C2H6S4	005756-24-1	83
2		Methanesulfonyl azide	121	CH3N3O2S	001516-70-7	37
3		Cyclopentanemethanol, 3-methylene-	112	C7H12O	074793-20-7	10
4		Butane, 1-(methylsulfinyl)-	120	C5H12OS	002976-98-9	10
5		2-Bromopyrimidine	158	C4H3BrN2	004595-60-2	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

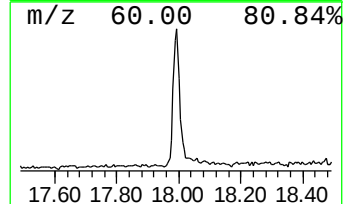
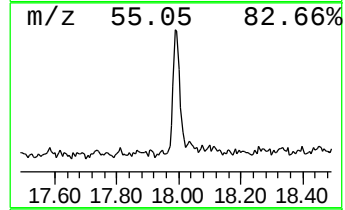
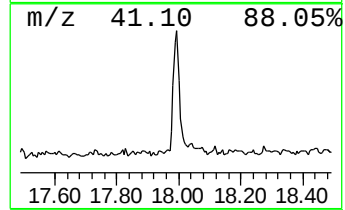
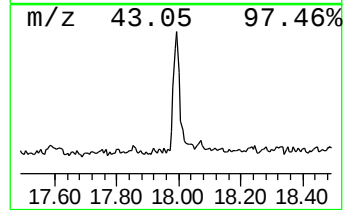
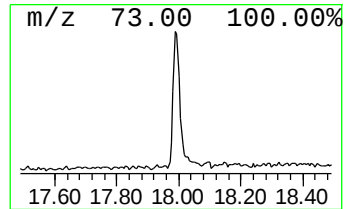
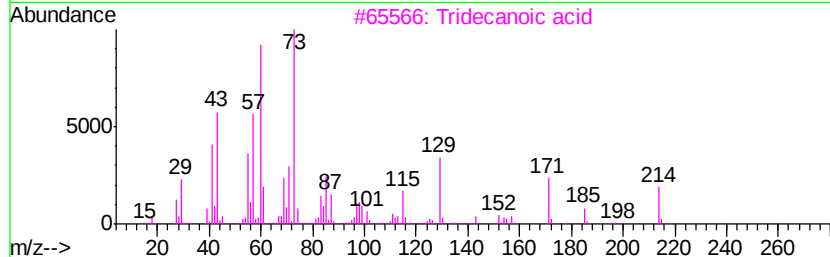
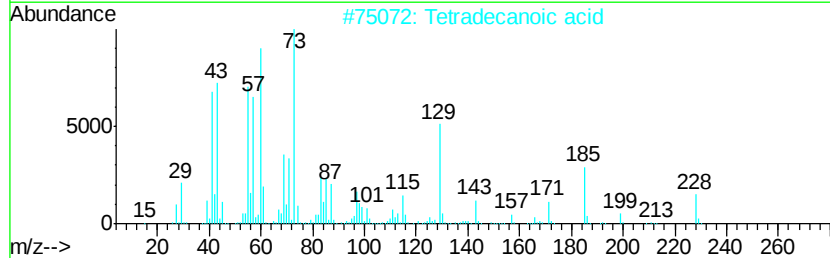
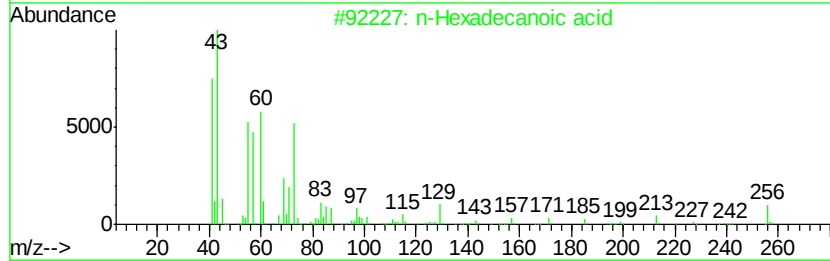
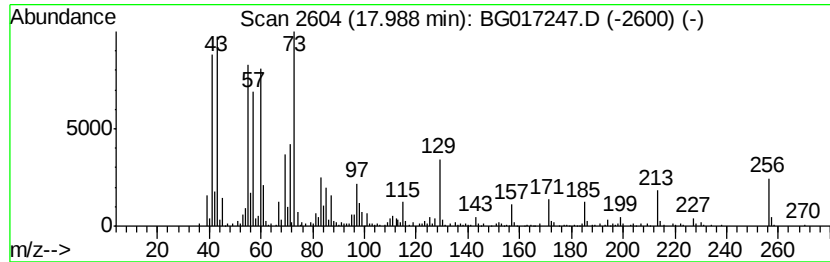
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.99	13.60 ng	390396	Phenanthrene-d10	17.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		Undecanoic acid	186	C11H22O2	000112-37-8	64
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	59



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017247.D
Acq On : 22 May 2015 15:31
Operator : TP/IZ
Sample : G2255-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

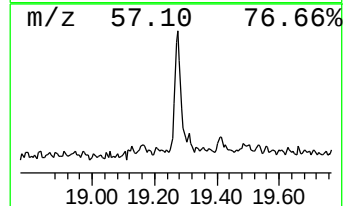
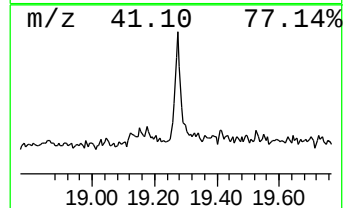
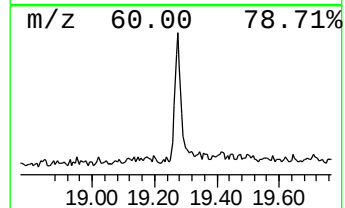
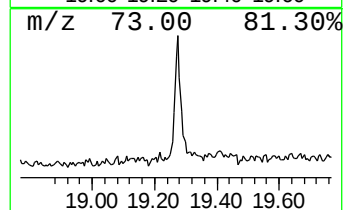
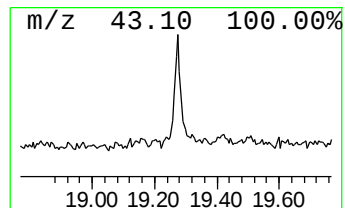
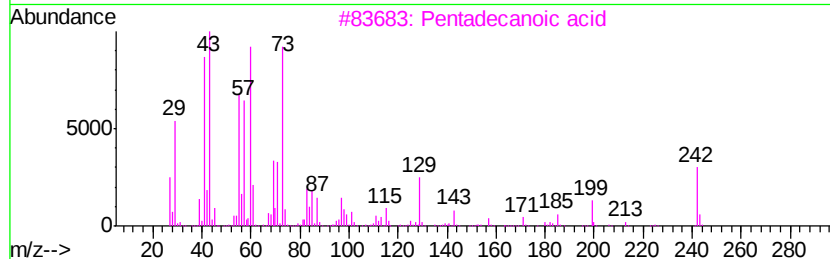
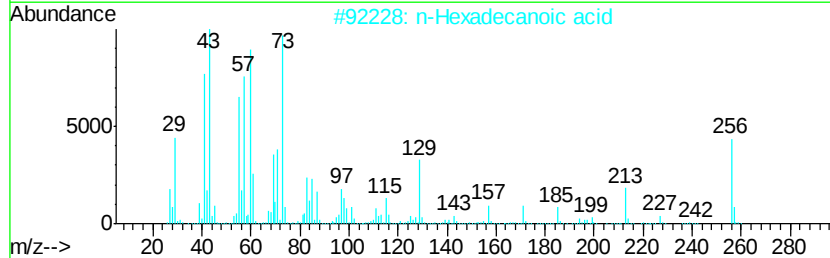
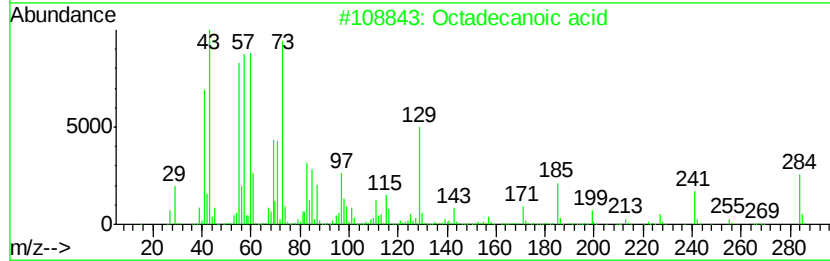
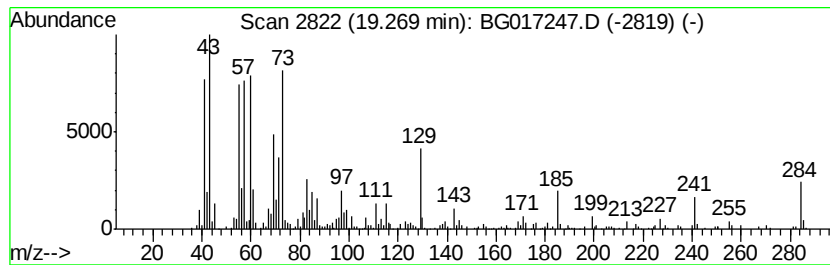
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.27	10.61 ng	319569	Chrysene-d12	21.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
 Data File : BG017247.D
 Acq On : 22 May 2015 15:31
 Operator : TP/IZ
 Sample : G2255-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SS043MW009-150512

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.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
Butane, 2-methoxy...	2.86	19.1	ng	242536	1	7.68	254697	20.0
Disulfide, dimethyl	3.60	15.0	ng	191567	1	7.68	254697	20.0
Dimethyl trisulfide	7.01	88.1	ng	1122040	1	7.68	254697	20.0
Benzene, 1-ethyl-...	7.07	8.8	ng	112686	1	7.68	254697	20.0
unknown8.29	8.29	13.4	ng	169981	1	7.68	254697	20.0
Cyclopent-2-ene-1...	8.33	12.5	ng	159630	1	7.68	254697	20.0
unknown8.62	8.62	8.3	ng	105919	1	7.68	254697	20.0
Allyldiethylamine	8.79	27.1	ng	345153	1	7.68	254697	20.0
unknown8.98	8.98	16.9	ng	215900	1	7.68	254697	20.0
1-Ethyl-4-piperidone	9.10	17.5	ng	358395	2	10.47	409736	20.0
4H-1,2,4-Triazol-...	9.12	15.4	ng	315808	2	10.47	409736	20.0
6-Azacytosine	9.49	13.1	ng	269215	2	10.47	409736	20.0
N-Isopropyl-4-pip...	9.90	17.4	ng	356769	2	10.47	409736	20.0
Cyclohexanone, 3-...	10.12	9.3	ng	191277	2	10.47	409736	20.0
Benzenemethanol, ...	10.26	17.8	ng	365394	2	10.47	409736	20.0
Tetrasulfide, dim...	11.02	19.1	ng	390955	2	10.47	409736	20.0
n-Hexadecanoic acid	17.99	13.6	ng	390396	4	17.08	574196	20.0
Octadecanoic acid	19.27	10.6	ng	319569	5	21.27	602675	20.0