

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

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

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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	2.897	5	10	20	rBV	390928	861715	10.30%	1.418%
2	3.038	29	34	53	rVB	5210414	8369236	100.00%	13.774%
3	3.185	53	59	71	rBV	392264	855070	10.22%	1.407%
4	5.223	400	406	415	rVB	297396	460982	5.51%	0.759%
5	5.699	480	487	497	rBV	2223281	3574932	42.72%	5.884%
6	7.309	752	761	771	rBV	2418028	4347355	51.94%	7.155%
7	7.679	816	824	829	rBV	2290516	4053183	48.43%	6.671%
8	7.721	829	831	842	rVB	405875	606959	7.25%	0.999%
9	8.149	897	904	911	rBV	538700	929164	11.10%	1.529%
10	8.478	951	960	967	rBV	1627611	2851280	34.07%	4.693%
11	9.325	1095	1104	1114	rBV	1484969	2751318	32.87%	4.528%
12	10.981	1377	1386	1393	rBV	769911	1397219	16.69%	2.300%
13	13.414	1791	1800	1811	rBV	3568801	5728526	68.45%	9.428%
14	14.236	1934	1940	1946	rBV	860201	1254655	14.99%	2.065%
15	14.800	2028	2036	2045	rVB2	1207720	2081669	24.87%	3.426%
16	16.287	2283	2289	2299	rBV	3190890	5051076	60.35%	8.313%
17	16.475	2317	2321	2325	rBV2	84520	133248	1.59%	0.219%
18	17.274	2451	2457	2461	rBV3	99275	137394	1.64%	0.226%
19	17.550	2498	2504	2510	rBV	1532931	2373743	28.36%	3.907%
20	18.414	2647	2651	2657	rBV4	140310	232105	2.77%	0.382%
21	19.595	2847	2852	2857	rBV	71192	115651	1.38%	0.190%
22	19.959	2911	2914	2920	rVB3	63882	102501	1.22%	0.169%
23	20.153	2941	2947	2953	rBV	5359487	7175337	85.73%	11.809%
24	21.463	3167	3170	3177	rBV8	79690	162363	1.94%	0.267%
25	21.857	3230	3237	3243	rBV	1554213	2648503	31.65%	4.359%
26	25.229	3802	3811	3825	rVB2	802735	2505024	29.93%	4.123%

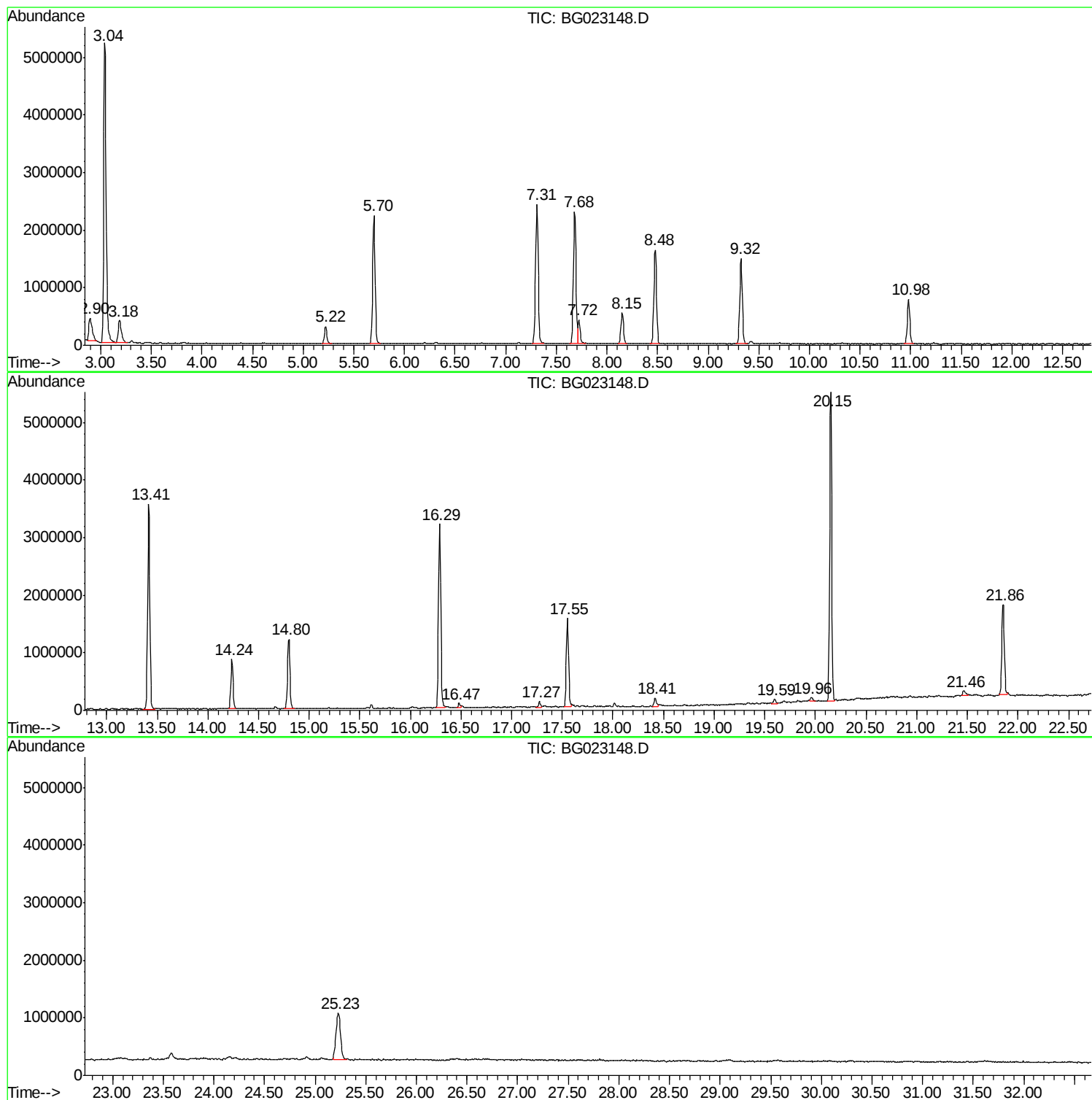
Sum of corrected areas: 60760208

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

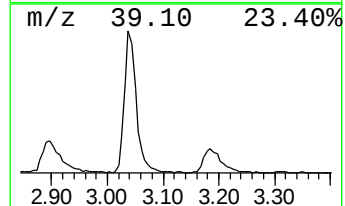
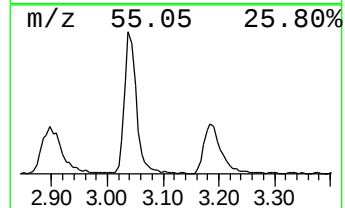
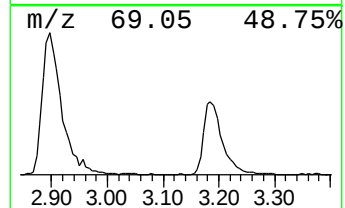
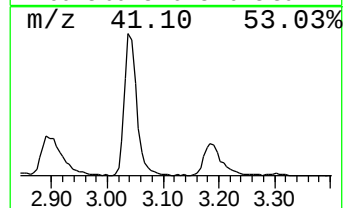
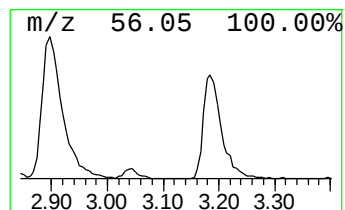
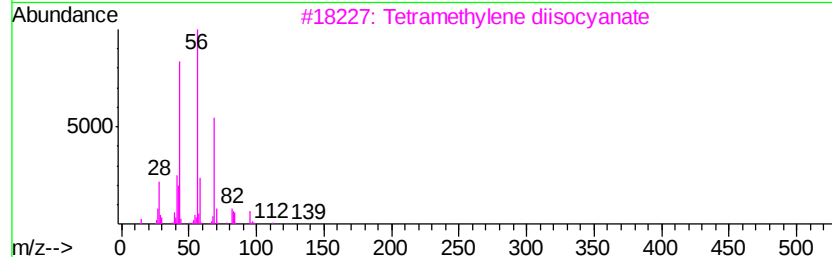
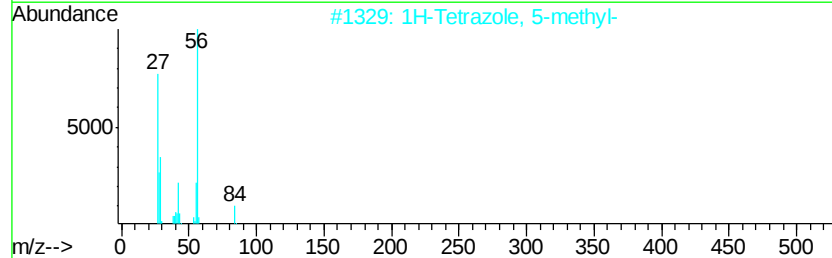
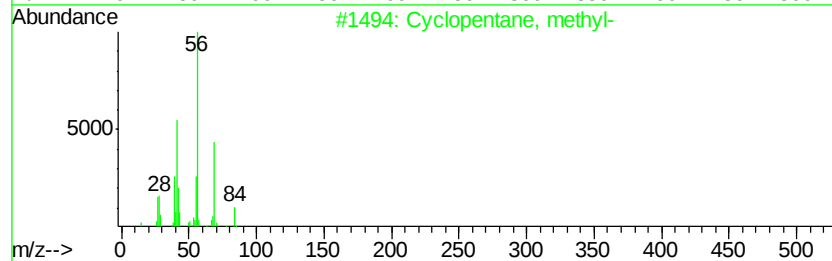
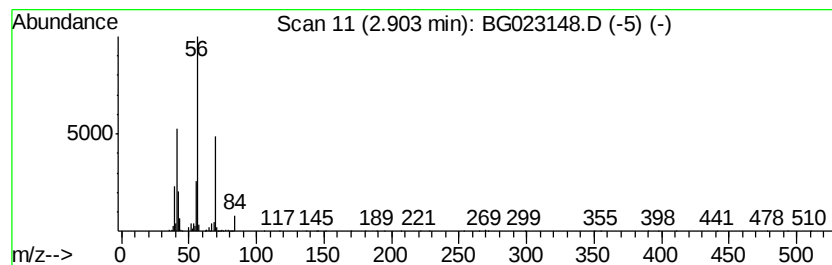
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	18.55 ng	861715	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
3		Tetramethylene diisocyanate	140	C6H8N2O2	004538-37-8	56
4		2-Ethylthiolane, S,S-dioxide	148	C6H12O2S	010178-59-3	40
5		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	40



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

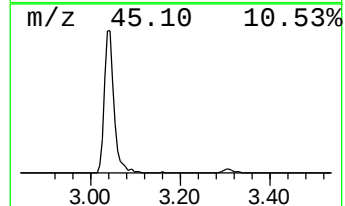
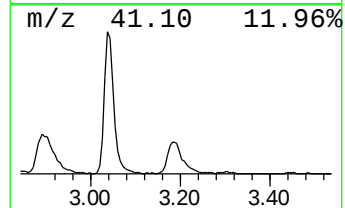
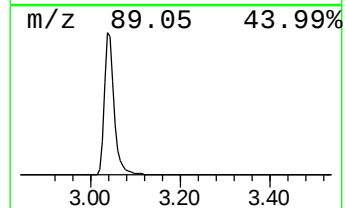
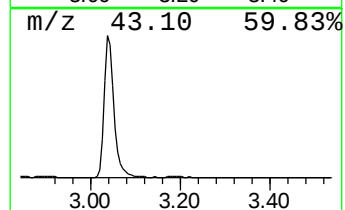
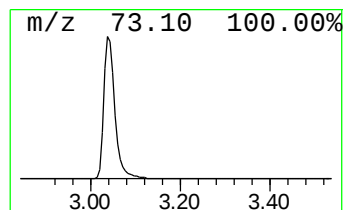
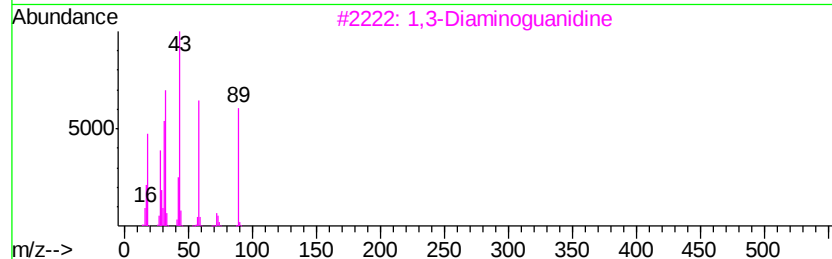
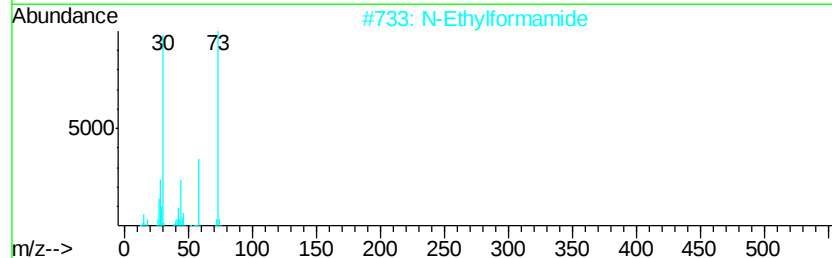
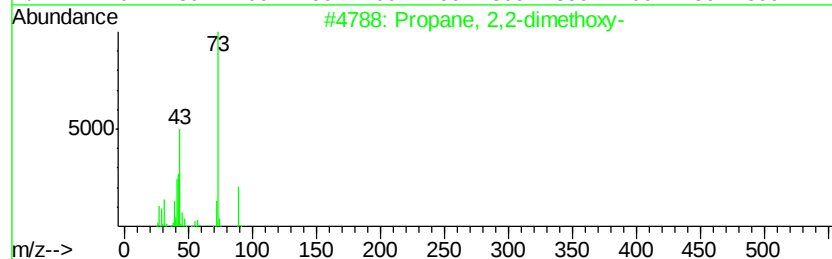
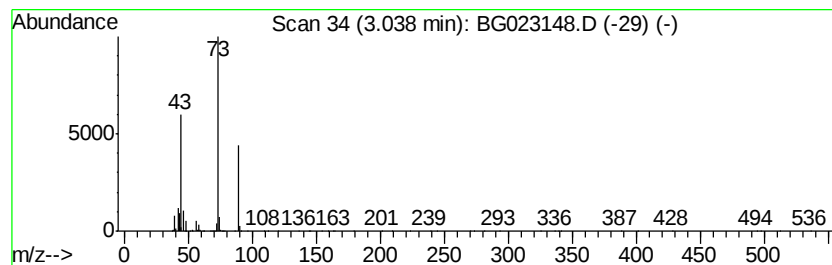
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	180.15 ng	8369240	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

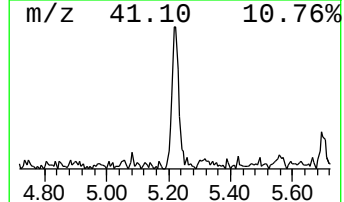
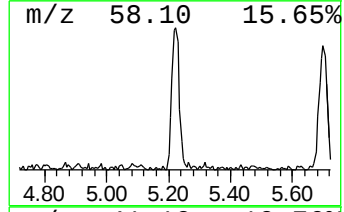
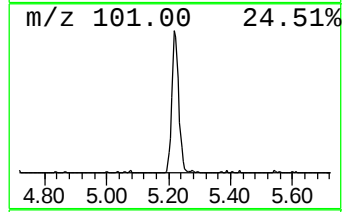
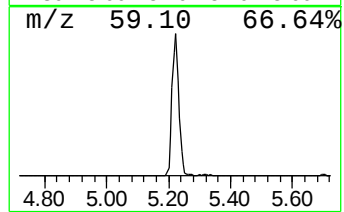
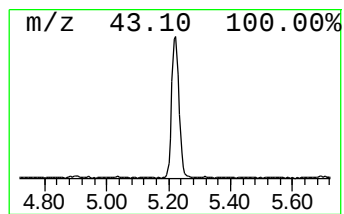
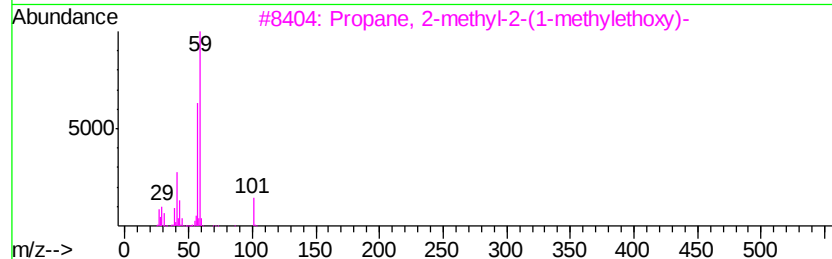
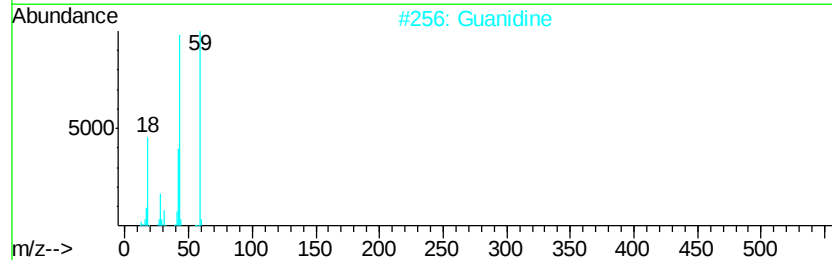
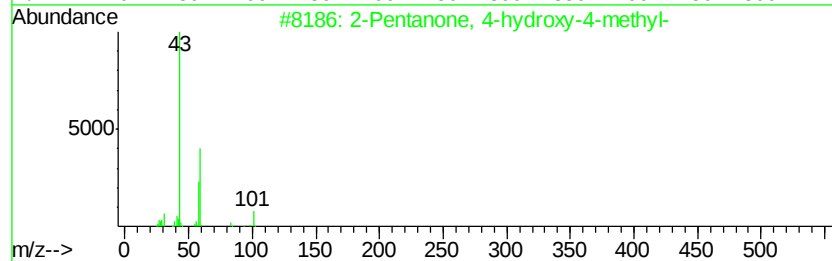
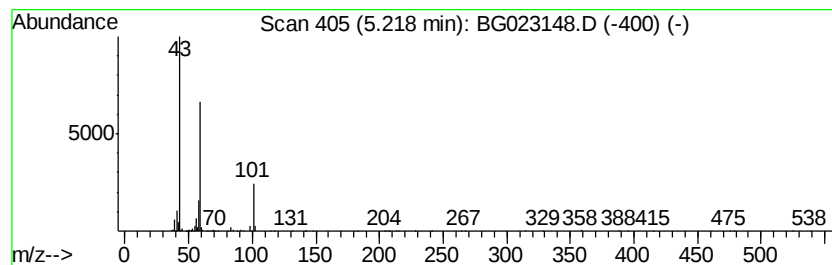
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	9.92 ng	460982	1,4-Dichlorobenzene-d4	8.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	72
2	Guanidine	59	CH5N3		000113-00-8	53
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	45
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5		1000325-80-7	42
5	3-Hexanol	102	C6H14O		000623-37-0	33



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

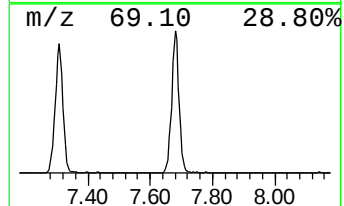
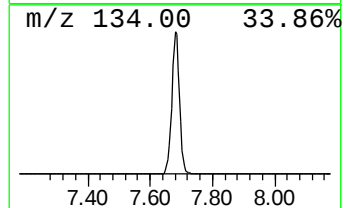
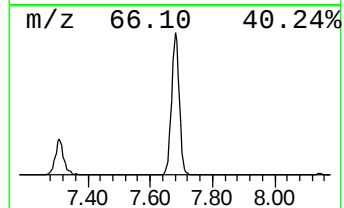
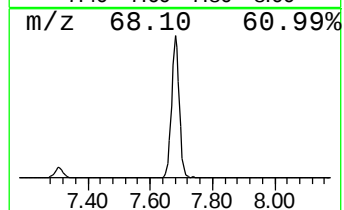
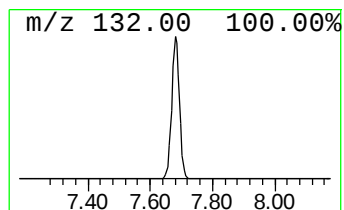
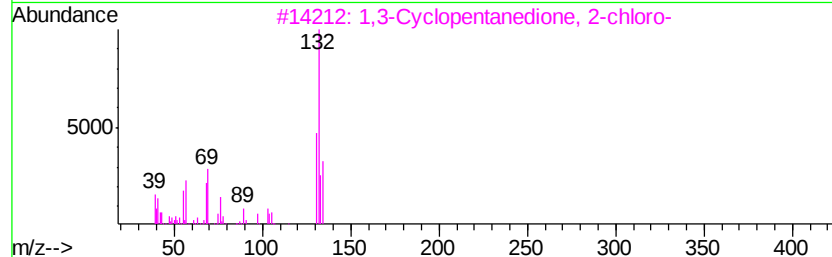
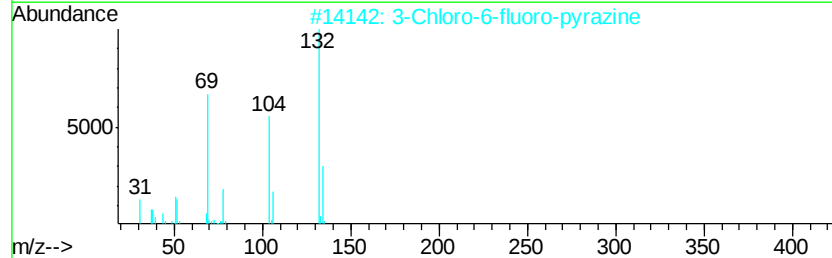
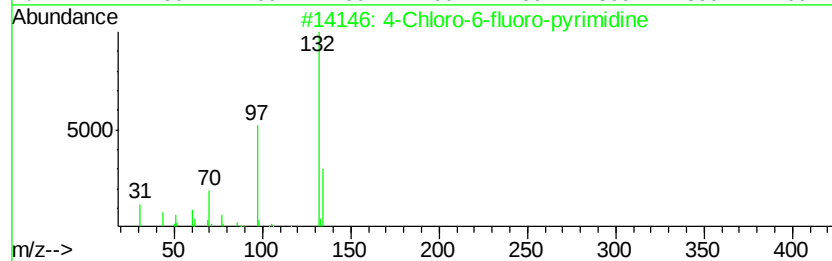
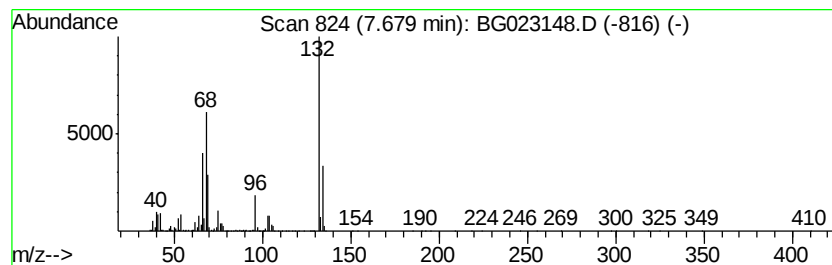
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	87.24 ng	4053180	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

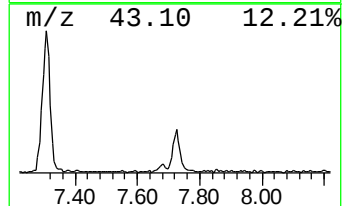
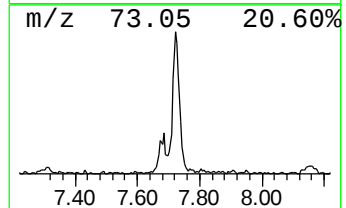
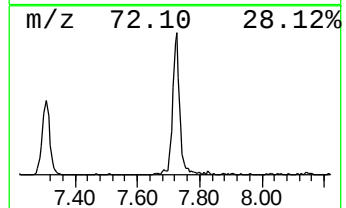
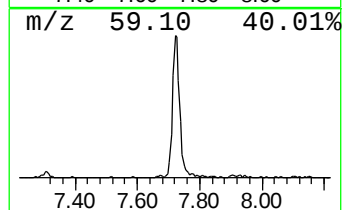
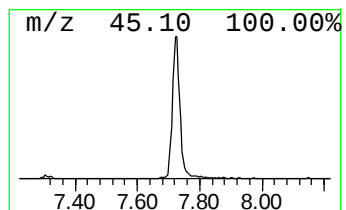
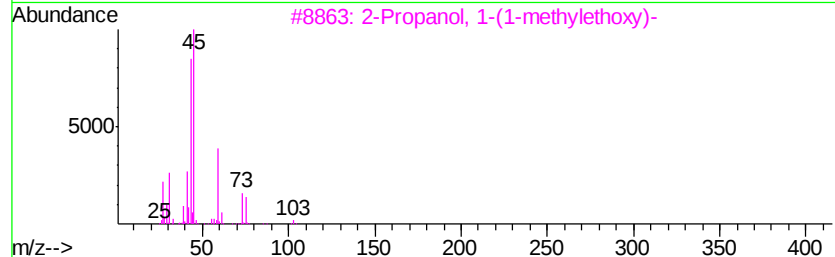
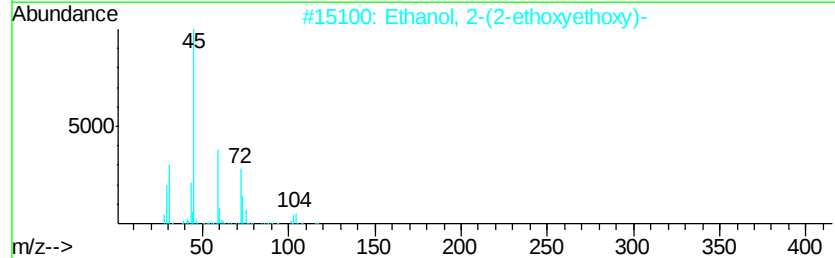
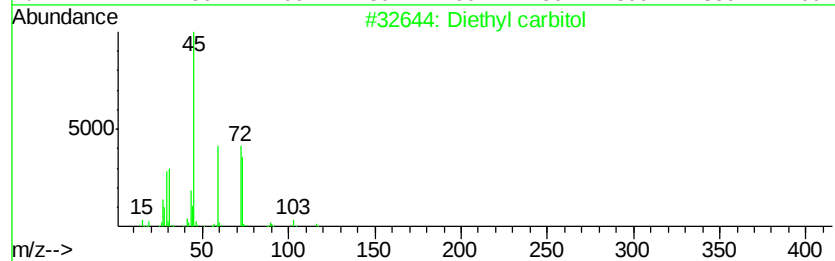
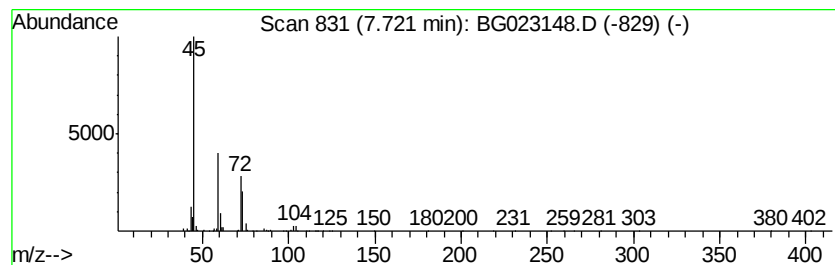
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Diethyl carbitol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	13.06 ng	606959	1,4-Dichlorobenzene-d4	8.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Diethyl carbitol	162	C8H18O3	000112-36-7	78
2		Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	74
3		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	64
4		Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
5		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023148.D
Acq On : 16 Jul 2016 15:41
Operator : UM/SJ
Sample : H4015-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C4.2-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentane, met...	2.90	18.6	ng	861715	1	8.15	929164	20.0
unknown3.04	3.04	180.2	ng	8369240	1	8.15	929164	20.0
2-Pentanone, 4-hy...	5.22	9.9	ng	460982	1	8.15	929164	20.0
unknown7.68	7.68	87.2	ng	4053180	1	8.15	929164	20.0
Diethyl carbitol	7.72	13.1	ng	606959	1	8.15	929164	20.0