

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
 Data File : BG023132.D
 Acq On : 16 Jul 2016 4:56
 Operator : UM/SJ
 Sample : H4045-07
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 H10-B3(12-18)C

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	3.040	29	34	53	rBV	6516725	10177266	100.00%	17.205%
2	5.219	399	405	411	rBV	145550	222911	2.19%	0.377%
3	5.695	479	486	496	rBV	2044990	3348102	32.90%	5.660%
4	7.305	752	760	772	rBV	2367638	4223017	41.49%	7.139%
5	7.681	816	824	834	rBV	2206693	3832528	37.66%	6.479%
6	8.151	897	904	911	rBV	376836	646524	6.35%	1.093%
7	8.474	952	959	968	rVB	1431120	2548712	25.04%	4.309%
8	9.326	1095	1104	1111	rBV	1488879	2728554	26.81%	4.613%
9	10.977	1377	1385	1394	rBV	565167	1036197	10.18%	1.752%
10	13.416	1790	1800	1811	rBV	3527965	5863330	57.61%	9.912%
11	14.238	1933	1940	1948	rBV	643624	942209	9.26%	1.593%
12	14.796	2028	2035	2046	rBV2	1048777	1725623	16.96%	2.917%
13	16.289	2282	2289	2300	rBV	3770536	5971408	58.67%	10.095%
14	16.483	2317	2322	2326	rBV2	77738	112020	1.10%	0.189%
15	17.552	2495	2504	2511	rBV2	1366923	2147556	21.10%	3.631%
16	18.416	2646	2651	2661	rBV2	194380	301415	2.96%	0.510%
17	20.155	2940	2947	2952	rBV	5647910	7982032	78.43%	13.494%
18	21.494	3169	3175	3186	rBV	38593	136283	1.34%	0.230%
19	21.853	3229	3236	3247	rBV2	1413130	2430466	23.88%	4.109%
20	22.282	3305	3309	3314	rVB6	74643	103729	1.02%	0.175%
21	23.580	3523	3530	3537	rVB	200432	370018	3.64%	0.626%
22	25.231	3799	3811	3832	rBV	708642	2303272	22.63%	3.894%

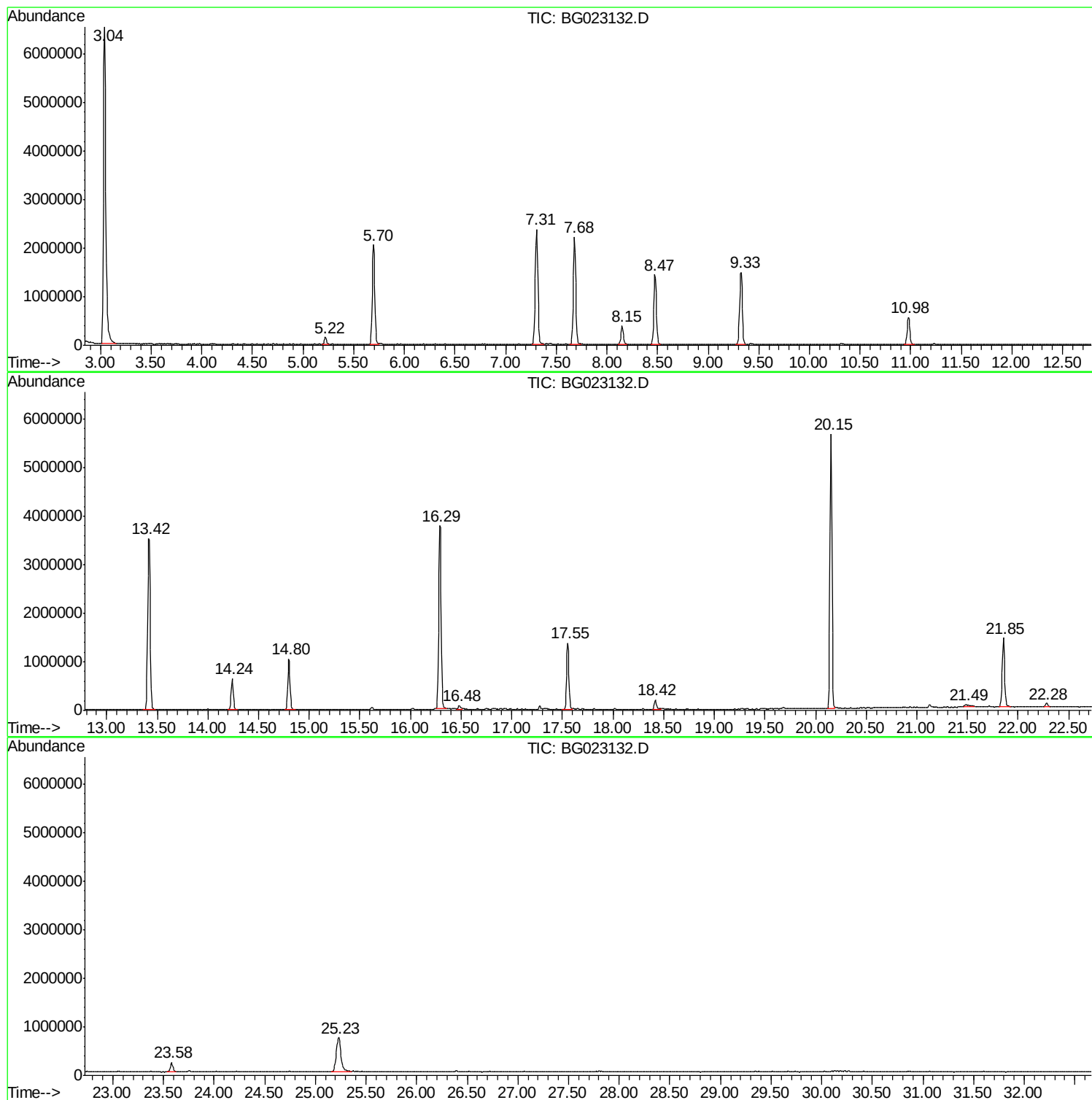
Sum of corrected areas: 59153172

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023132.D
Acq On : 16 Jul 2016 4:56
Operator : UM/SJ
Sample : H4045-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B3(12-18)C

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\BG071516\
Data File : BG023132.D
Acq On : 16 Jul 2016 4:56
Operator : UM/SJ
Sample : H4045-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B3(12-18)C

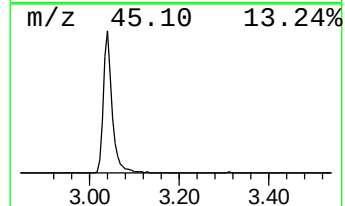
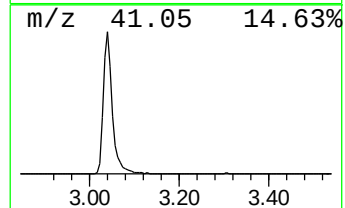
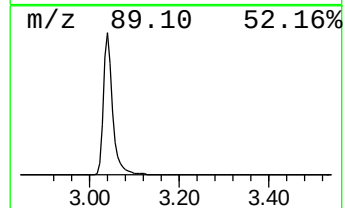
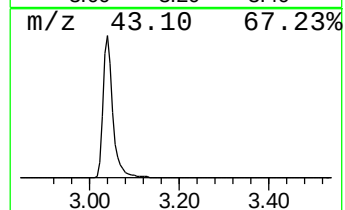
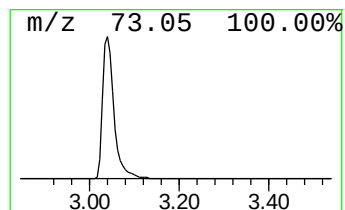
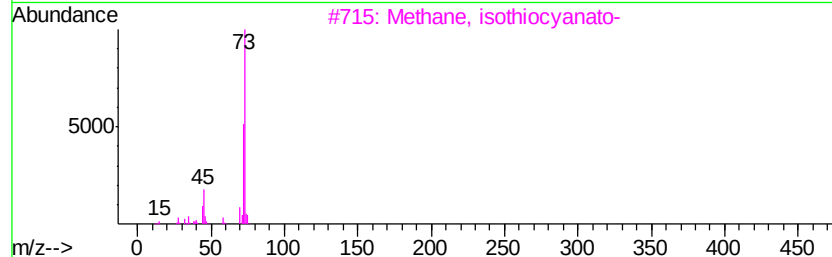
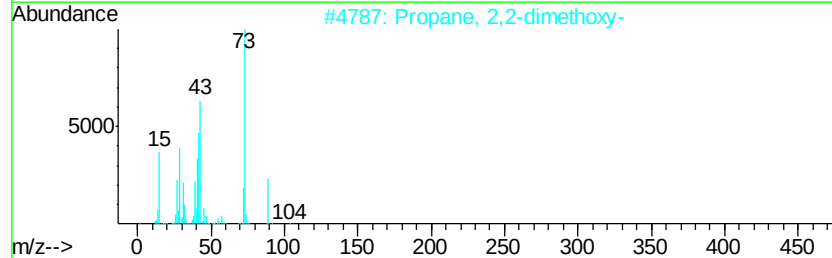
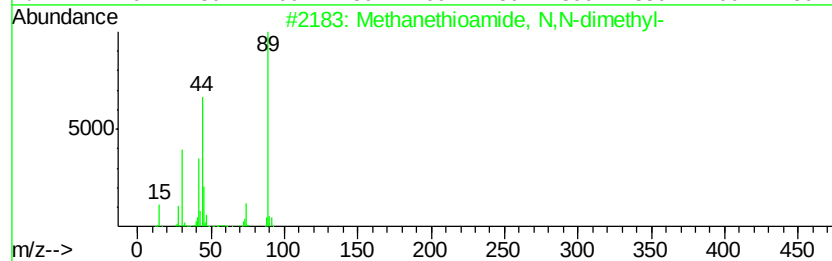
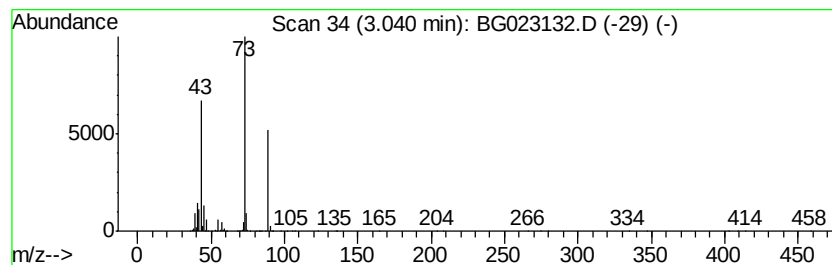
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	314.83 ng	10177300	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
3		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
4		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5		1-Hepten-4-ol	114	C7H14O	003521-91-3	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023132.D
Acq On : 16 Jul 2016 4:56
Operator : UM/SJ
Sample : H4045-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B3(12-18)C

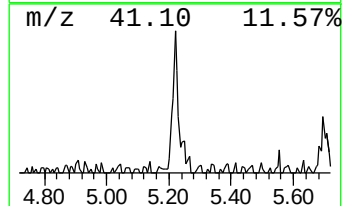
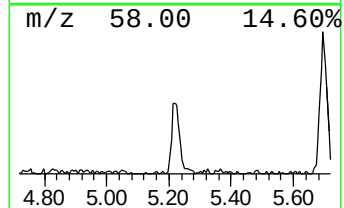
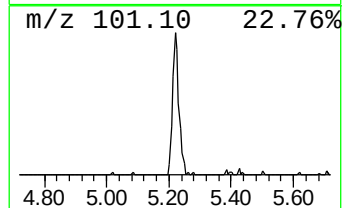
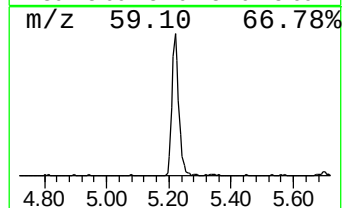
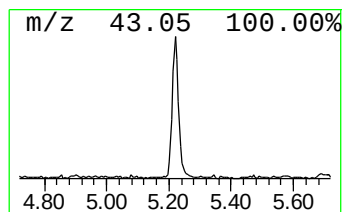
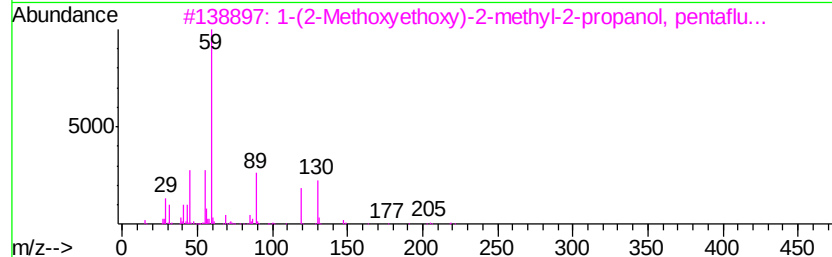
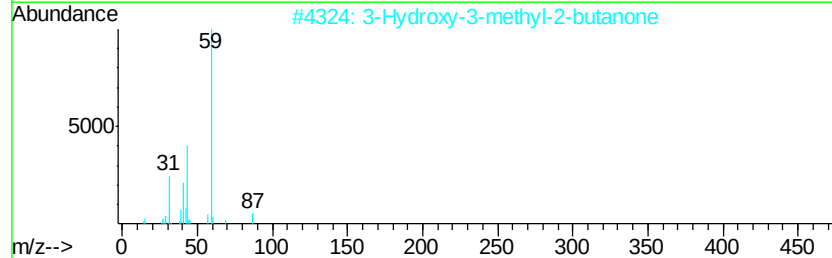
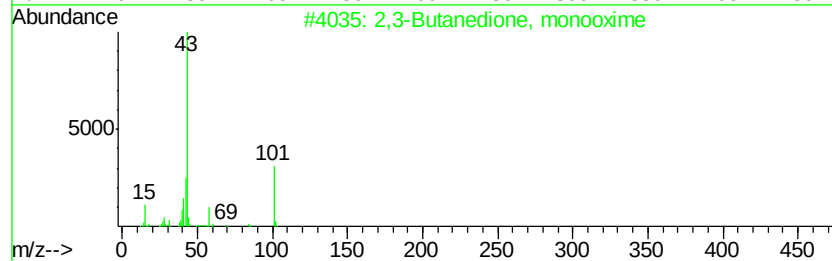
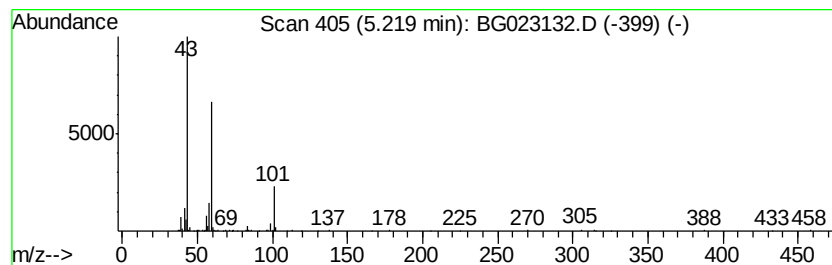
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.22 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	6.90 ng	222911	1,4-Dichlorobenzene-d4	8.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12		
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	294	C10H15F5O4	1000364-25-8	10		
4	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023132.D
Acq On : 16 Jul 2016 4:56
Operator : UM/SJ
Sample : H4045-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B3(12-18)C

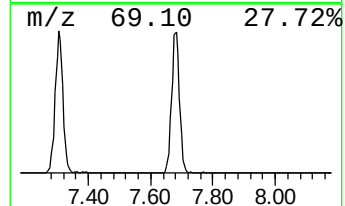
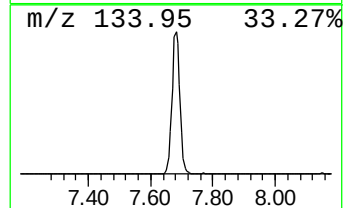
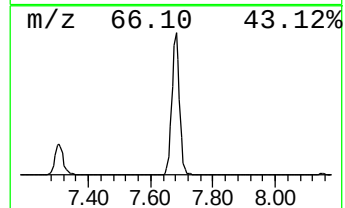
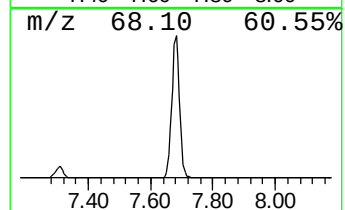
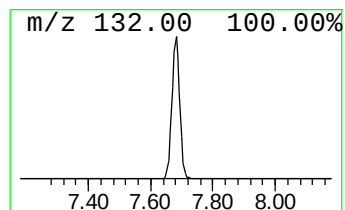
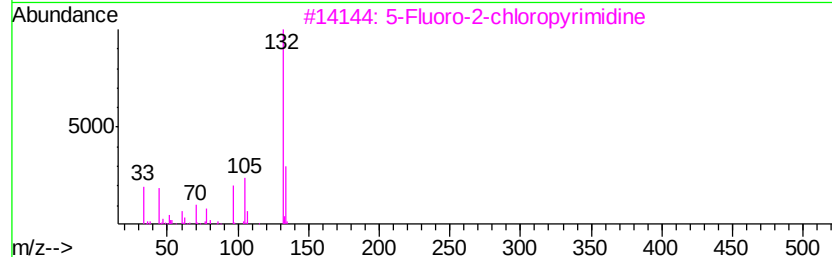
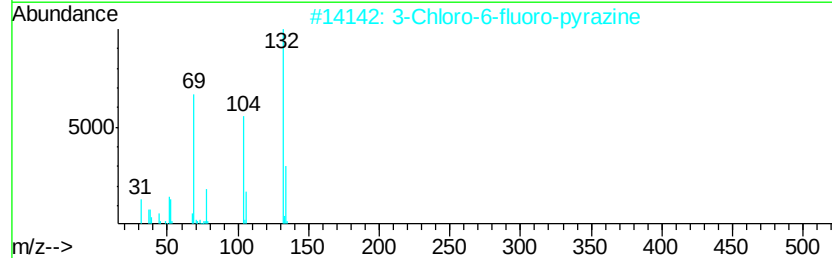
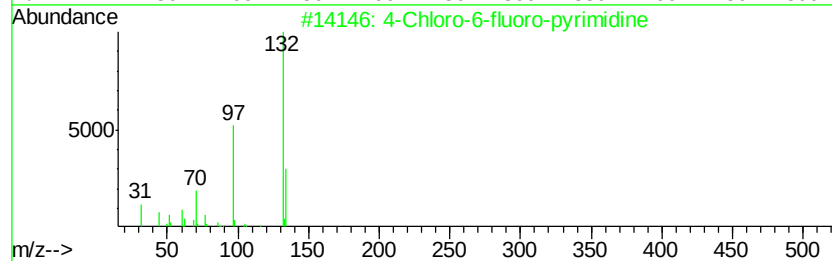
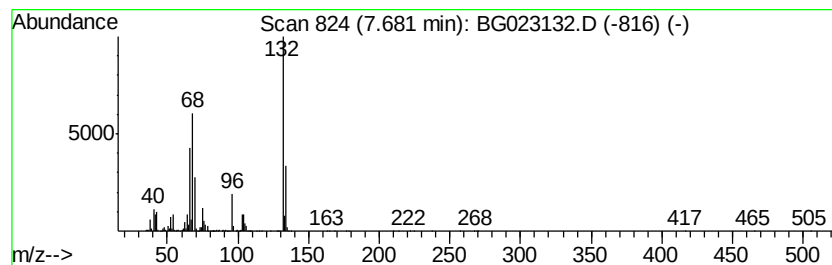
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	118.56 ng	3832530	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
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\BG071516\
Data File : BG023132.D
Acq On : 16 Jul 2016 4:56
Operator : UM/SJ
Sample : H4045-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B3(12-18)C

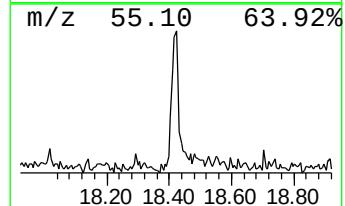
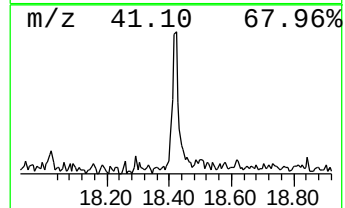
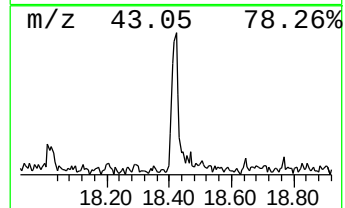
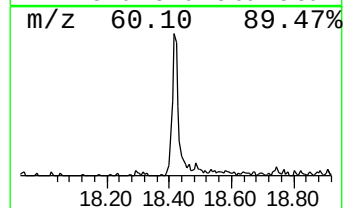
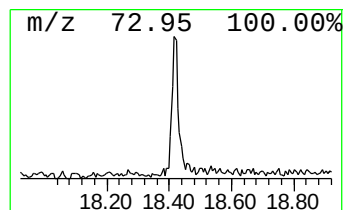
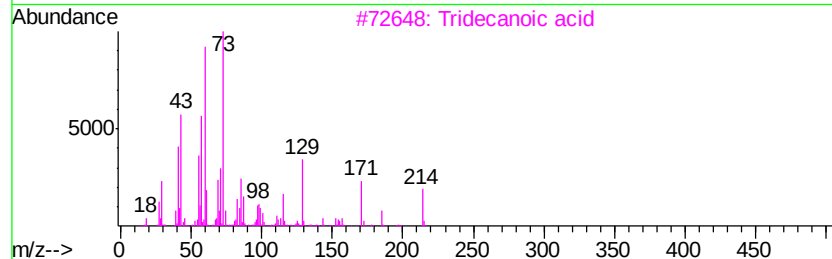
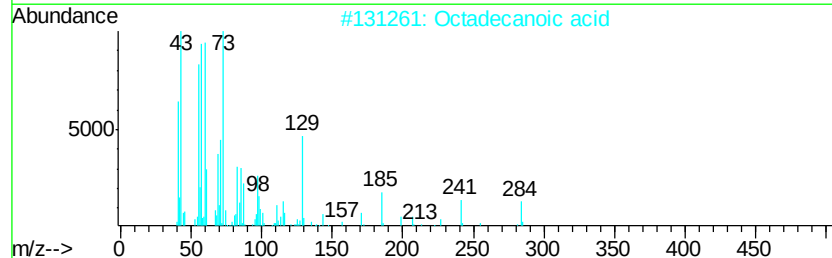
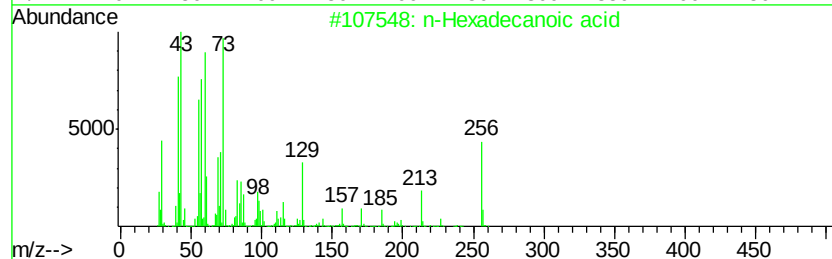
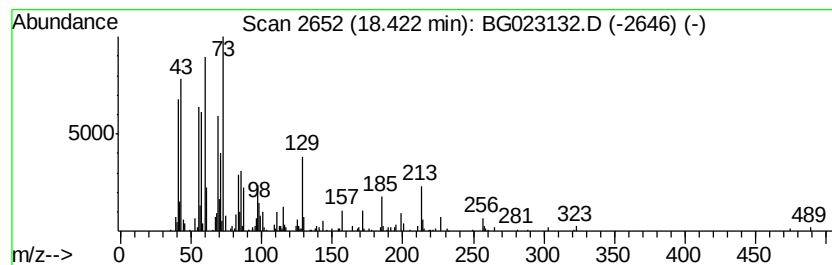
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.81 ng	301415	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Octadecanoic acid	284	C18H36O2	000057-11-4	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Dodecanoic acid	200	C12H24O2	000143-07-7	70
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023132.D
Acq On : 16 Jul 2016 4:56
Operator : UM/SJ
Sample : H4045-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

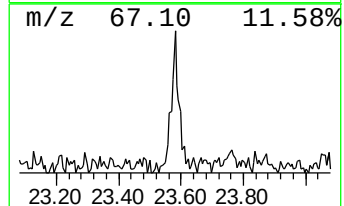
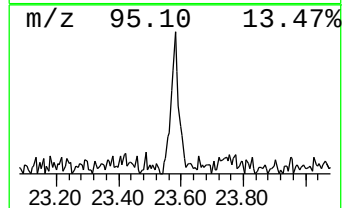
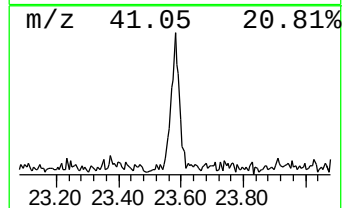
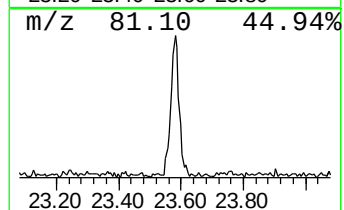
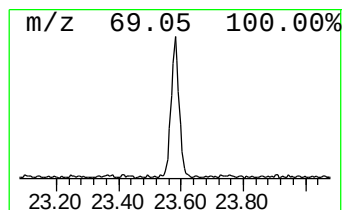
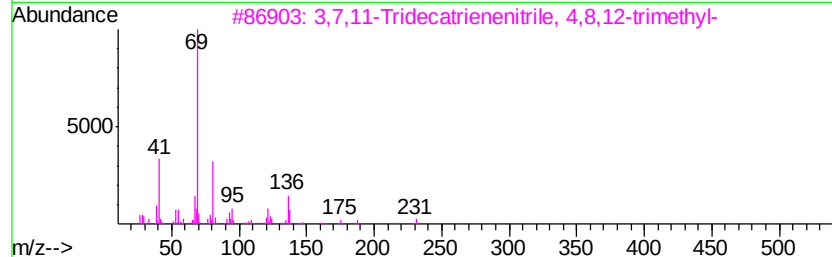
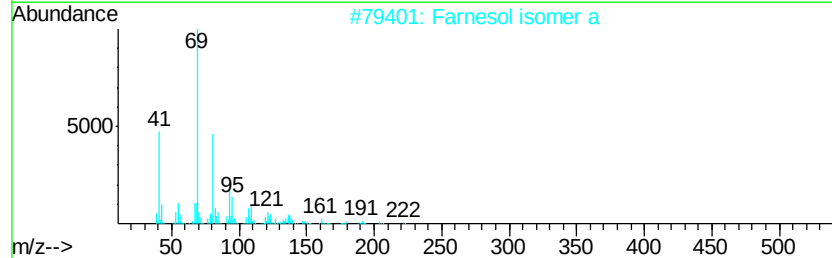
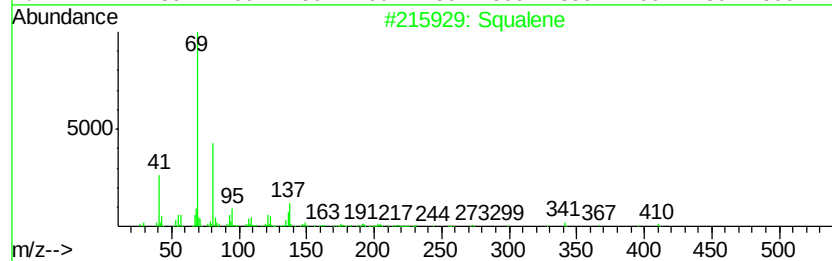
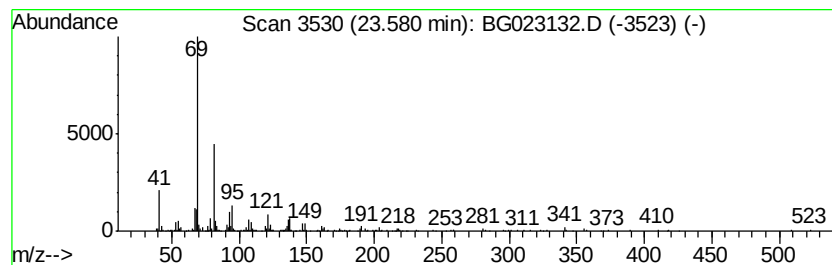
Instrument :
BNA_G
ClientSampleId :
H10-B3(12-18)C

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 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	3.21 ng	370018	Perylene-d12	25.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	91
2	Farnesol isomer a	222 C15H26O	1000108-92-4	64
3	3,7,11-Tridecatrienitrile, 4,8...	231 C16H25N	006006-01-5	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138 C10H18	035387-63-4	59
5	2,6-Octadiene, 4-methyl-	124 C9H16	074498-94-5	59



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023132.D
Acq On : 16 Jul 2016 4:56
Operator : UM/SJ
Sample : H4045-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B3(12-18)C

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
unknown3.04	3.04	314.8	ng	10177300	1	8.15	646524	20.0
unknown5.22	5.22	6.9	ng	222911	1	8.15	646524	20.0
unknown7.68	7.68	118.6	ng	3832530	1	8.15	646524	20.0
n-Hexadecanoic acid	18.42	2.8	ng	301415	4	17.55	2147560	20.0
Squalene	23.58	3.2	ng	370018	6	25.23	2303270	20.0