

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
 Data File : BG023418.D
 Acq On : 3 Aug 2016 5:42
 Operator : UM/SJ
 Sample : H4288-18
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-67-14.0-15.0

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-BG080116.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	2.993	21	26	47	rVB	4491400	7731501	74.53%	12.132%
2	5.184	393	399	410	rVB	618294	969100	9.34%	1.521%
3	5.660	474	480	493	rBV	2088806	3629061	34.99%	5.695%
4	7.275	747	755	767	rBV	2473477	4452654	42.93%	6.987%
5	7.651	810	819	830	rBV	2256447	4017914	38.73%	6.305%
6	8.121	893	899	905	rBV	345232	610772	5.89%	0.958%
7	8.444	947	954	963	rBV	1468278	2573694	24.81%	4.039%
8	9.296	1090	1099	1108	rBV	1440740	2645849	25.51%	4.152%
9	10.952	1372	1381	1388	rBV	559475	1053771	10.16%	1.654%
10	13.396	1788	1797	1805	rBV	3928346	6307785	60.81%	9.898%
11	14.224	1932	1938	1944	rBV	648856	948826	9.15%	1.489%
12	14.782	2026	2033	2043	rBV2	1127001	1801157	17.36%	2.826%
13	15.605	2168	2173	2179	rVB2	80886	109647	1.06%	0.172%
14	16.280	2281	2288	2298	rBV	4877177	7488533	72.19%	11.751%
15	16.468	2315	2320	2330	rBV2	96840	195144	1.88%	0.306%
16	17.543	2495	2503	2516	rVB	1806387	2720300	26.22%	4.269%
17	18.413	2646	2651	2658	rBV	364070	531648	5.13%	0.834%
18	19.682	2863	2867	2873	rBV3	134200	197660	1.91%	0.310%
19	20.152	2941	2947	2953	rBV	7885200	10372983	100.00%	16.277%
20	21.468	3165	3171	3185	rBV5	98249	313324	3.02%	0.492%
21	21.855	3231	3237	3244	rVB2	1499889	2544921	24.53%	3.993%
22	25.233	3801	3812	3825	rBV3	839137	2511104	24.21%	3.940%

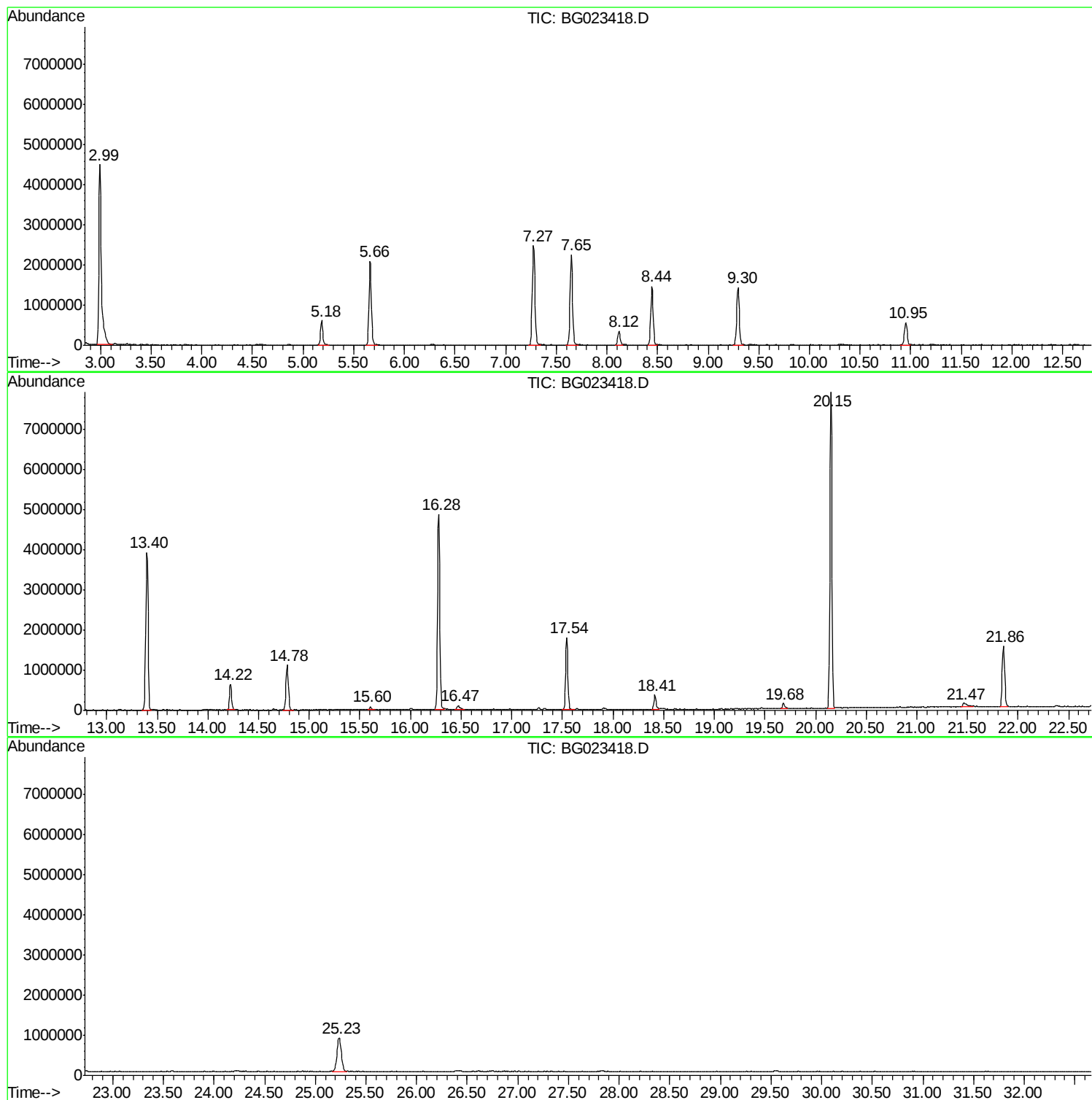
Sum of corrected areas: 63727348

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023418.D
Acq On : 3 Aug 2016 5:42
Operator : UM/SJ
Sample : H4288-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-67-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.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\BG080216\
Data File : BG023418.D
Acq On : 3 Aug 2016 5:42
Operator : UM/SJ
Sample : H4288-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-67-14.0-15.0

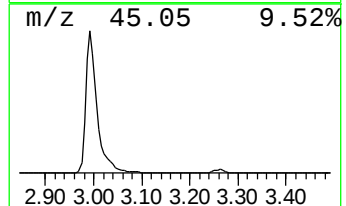
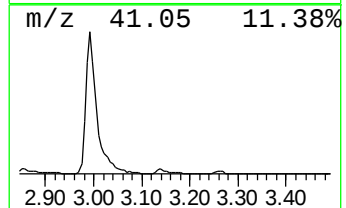
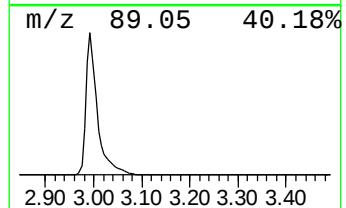
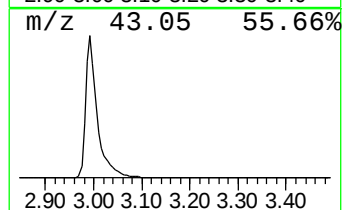
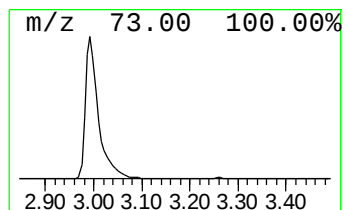
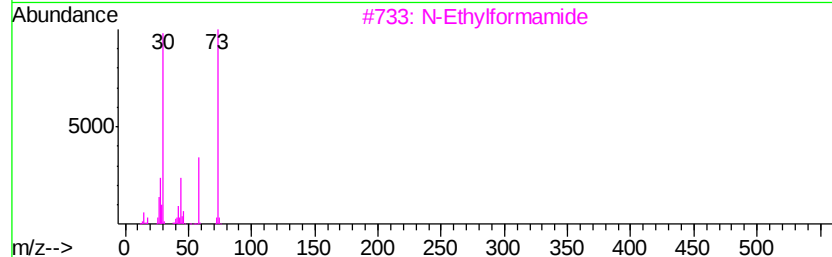
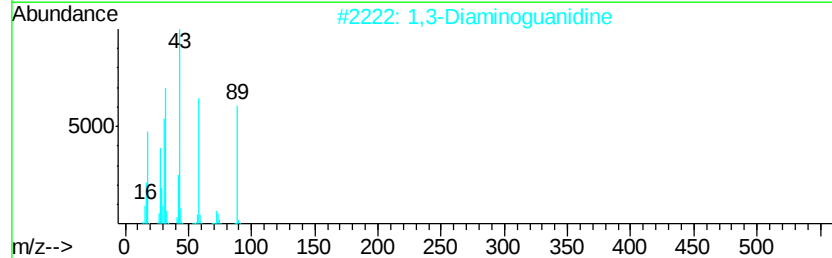
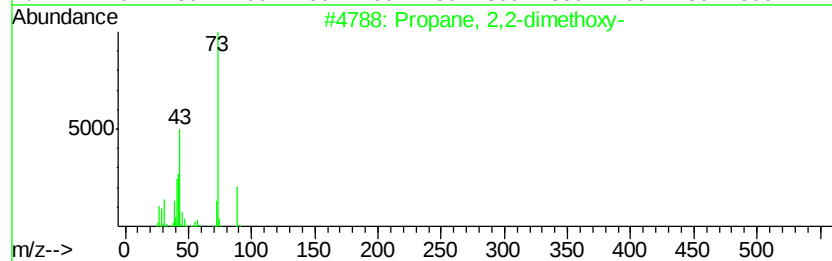
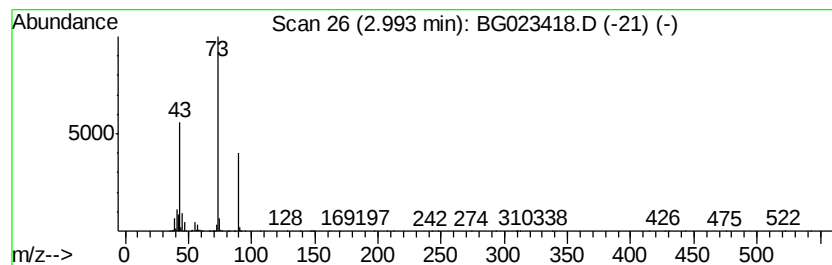
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	253.17 ng	7731500	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023418.D
Acq On : 3 Aug 2016 5:42
Operator : UM/SJ
Sample : H4288-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-67-14.0-15.0

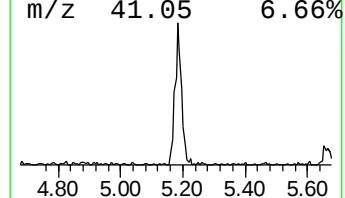
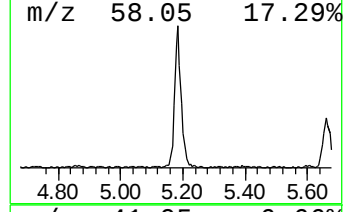
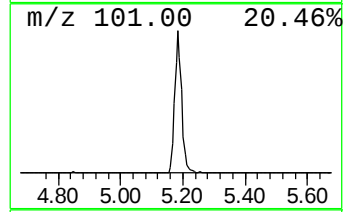
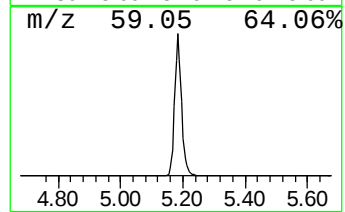
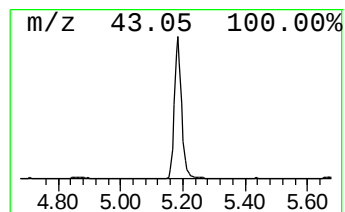
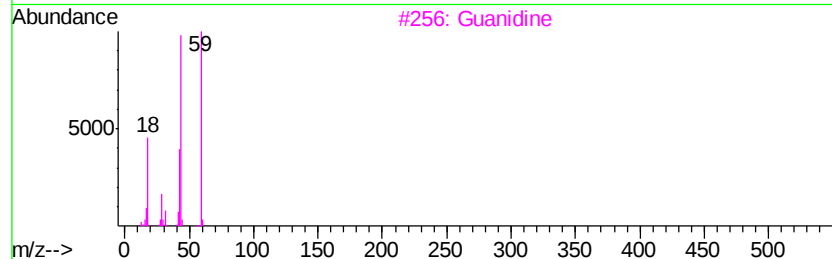
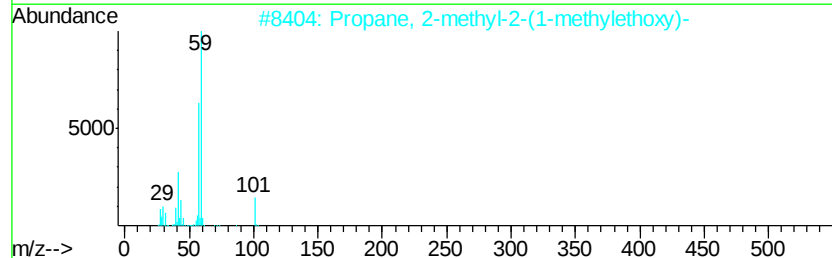
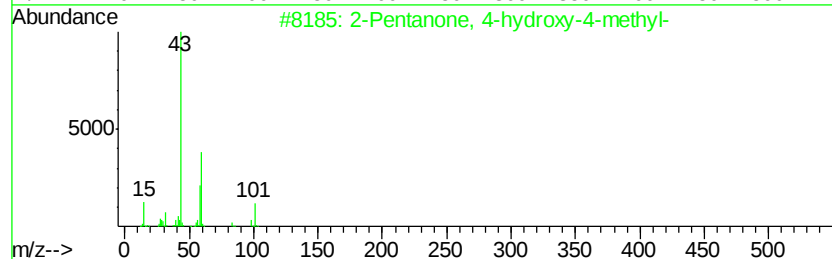
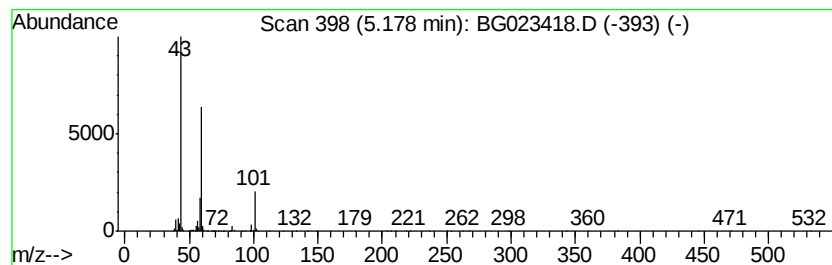
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	31.73 ng	969100	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	53
3		Guanidine	59	CH5N3	000113-00-8	43
4		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023418.D
Acq On : 3 Aug 2016 5:42
Operator : UM/SJ
Sample : H4288-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-67-14.0-15.0

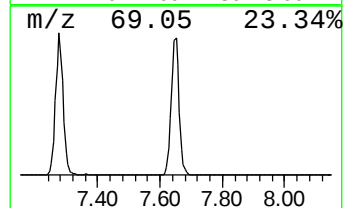
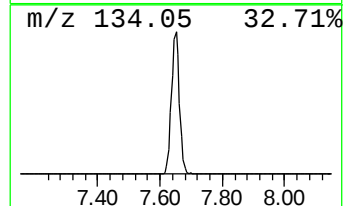
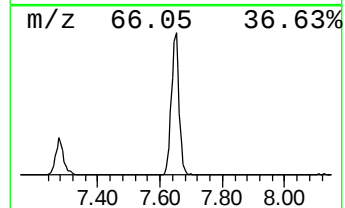
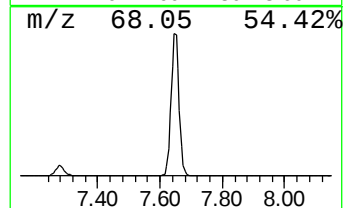
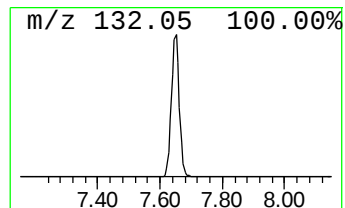
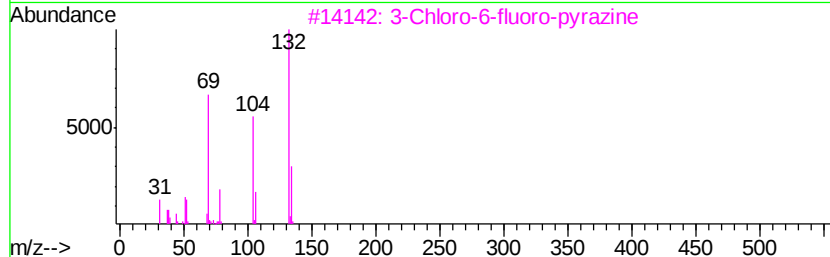
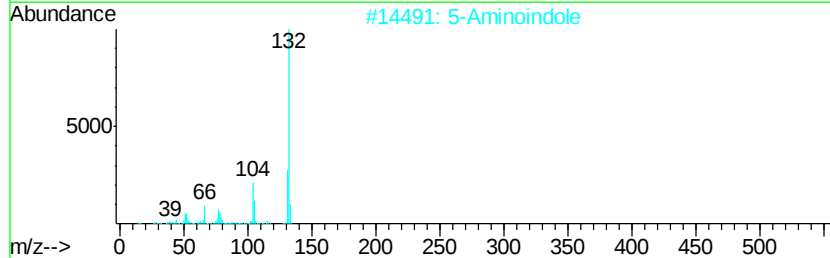
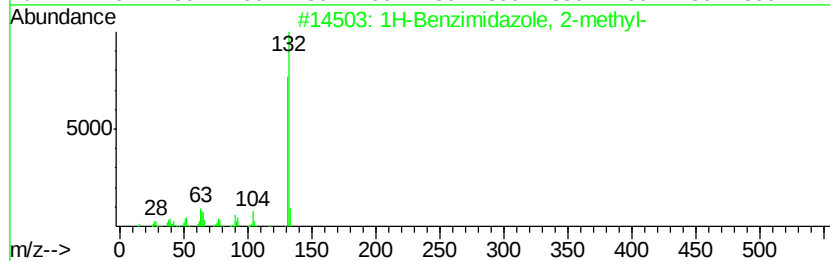
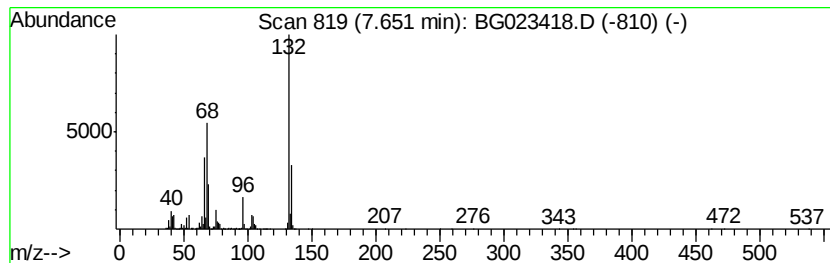
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	131.57 ng	4017910	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023418.D
Acq On : 3 Aug 2016 5:42
Operator : UM/SJ
Sample : H4288-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

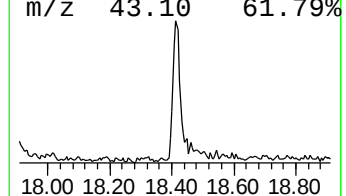
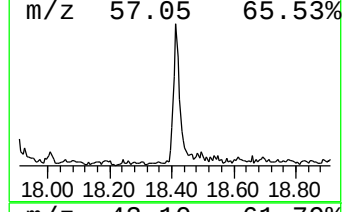
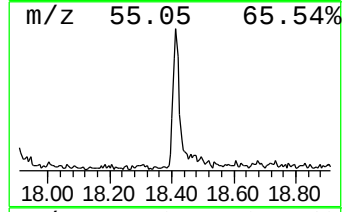
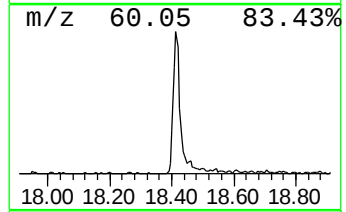
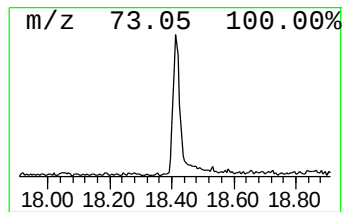
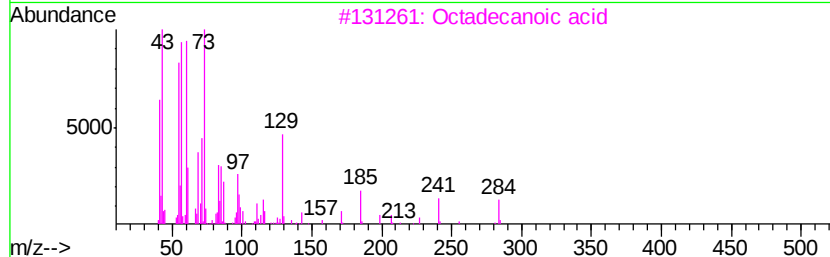
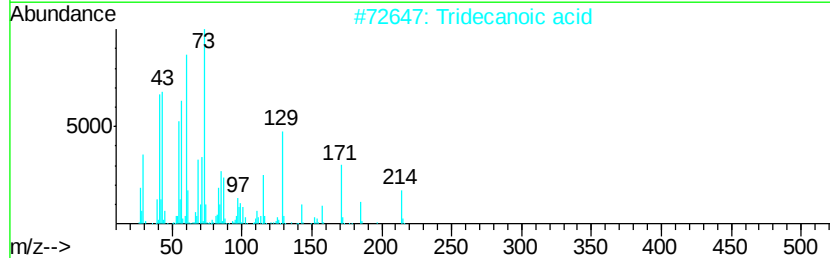
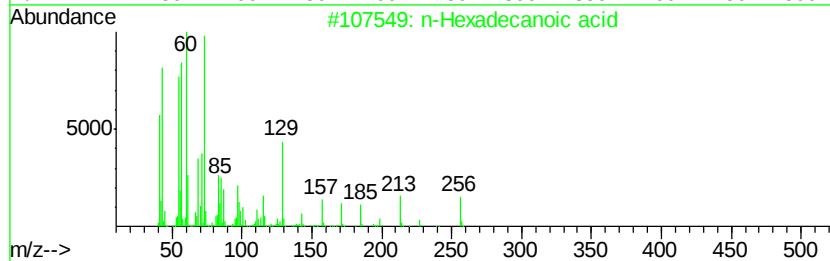
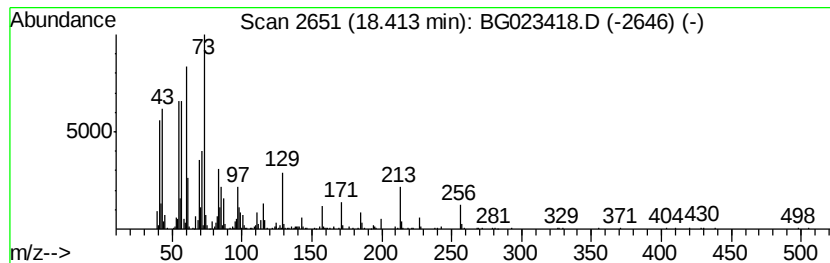
Instrument :
BNA_G
ClientSampleId :
SB-67-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.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 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.41	3.91 ng	531648	Phenanthrene-d10	17.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023418.D
Acq On : 3 Aug 2016 5:42
Operator : UM/SJ
Sample : H4288-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

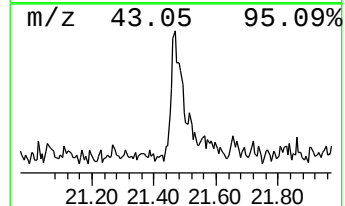
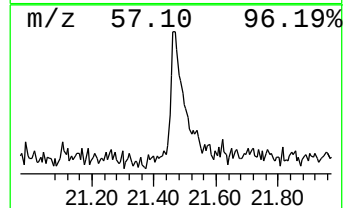
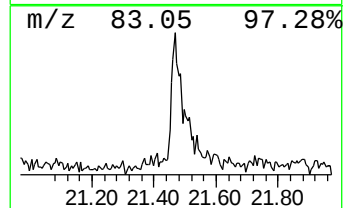
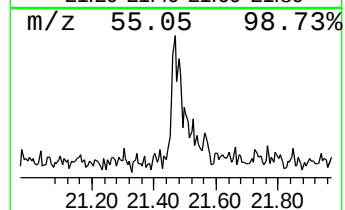
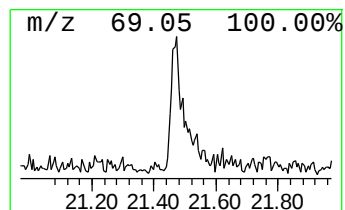
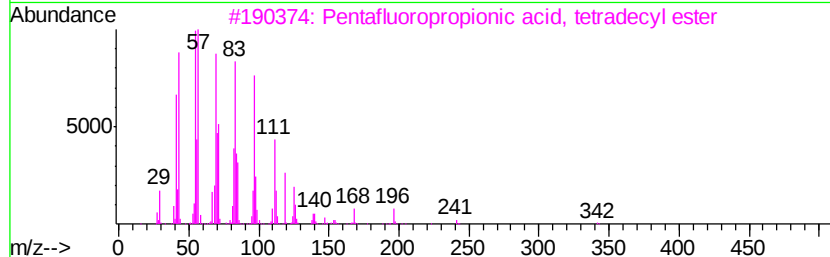
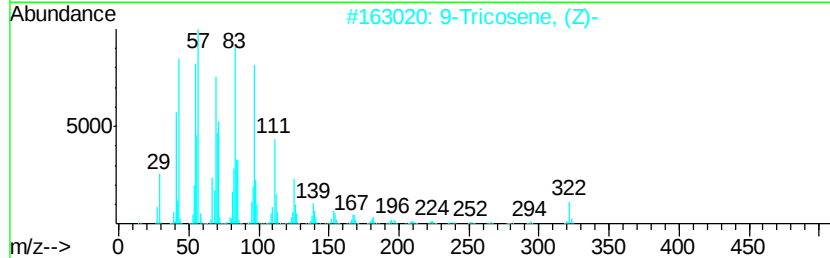
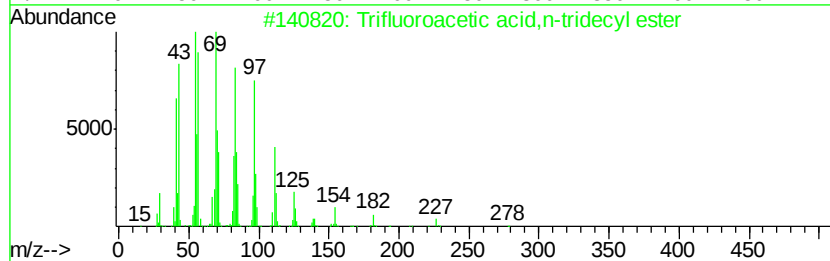
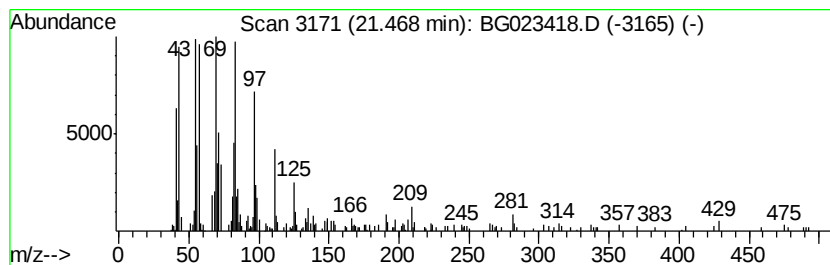
Instrument :
BNA_G
ClientSampleId :
SB-67-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetic acid,n-trid... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.47	2.46 ng	313324	Chrysene-d12	21.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	90
2		9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87
4		1-Octadecanol	270	C18H38O	000112-92-5	87
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080216\
Data File : BG023418.D
Acq On : 3 Aug 2016 5:42
Operator : UM/SJ
Sample : H4288-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-67-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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
Propane, 2,2-dime...	2.99	253.2	ng	7731500	1	8.12	610772	20.0
2-Pentanone, 4-hy...	5.18	31.7	ng	969100	1	8.12	610772	20.0
unknown7.65	7.65	131.6	ng	4017910	1	8.12	610772	20.0
n-Hexadecanoic acid	18.41	3.9	ng	531648	4	17.54	2720300	20.0
Trifluoroacetic a...	21.47	2.5	ng	313324	5	21.86	2544920	20.0