

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
 Data File : BG016234.D
 Acq On : 6 Apr 2015 21:24
 Operator : TP/IZ
 Sample : G1757-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LS-SW04

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-BG040615.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	2.799	14	19	28	rBV	353791	517198	12.15%	2.488%
2	2.875	28	32	38	rVV	374410	411582	9.67%	1.980%
3	4.814	355	362	369	rVB2	35000	50552	1.19%	0.243%
4	5.278	435	441	452	rBV	509240	706185	16.59%	3.397%
5	6.870	705	712	721	rBV	337090	498307	11.71%	2.397%
6	7.229	766	773	785	rBV	934123	1472060	34.58%	7.080%
7	7.699	845	853	860	rBV	224710	339751	7.98%	1.634%
8	8.016	899	907	916	rBV	840935	1345960	31.62%	6.474%
9	8.856	1042	1050	1062	rBV	720629	1153845	27.11%	5.550%
10	10.484	1320	1327	1334	rBV	336933	558695	13.13%	2.687%
11	12.963	1741	1749	1757	rBV	1908364	2843979	66.82%	13.679%
12	14.338	1976	1983	1991	rBV2	546354	816467	19.18%	3.927%
13	15.825	2230	2236	2251	rBV	1221287	1804241	42.39%	8.678%
14	17.076	2443	2449	2455	rBV2	719448	1016888	23.89%	4.891%
15	19.409	2840	2846	2851	rBV	304098	347756	8.17%	1.673%
16	19.708	2891	2897	2908	rBV	3410101	4256445	100.00%	20.472%
17	20.449	3018	3023	3028	rBV	225995	244430	5.74%	1.176%
18	20.971	3107	3112	3121	rBV	52249	79918	1.88%	0.384%
19	21.254	3155	3160	3171	rBV	924602	1134271	26.65%	5.455%
20	21.406	3182	3186	3193	rBV	35323	42885	1.01%	0.206%
21	22.299	3333	3338	3346	rBV	32140	52048	1.22%	0.250%
22	22.811	3419	3425	3430	rBV2	23899	43404	1.02%	0.209%
23	23.498	3534	3542	3553	rBV	557356	1054464	24.77%	5.072%

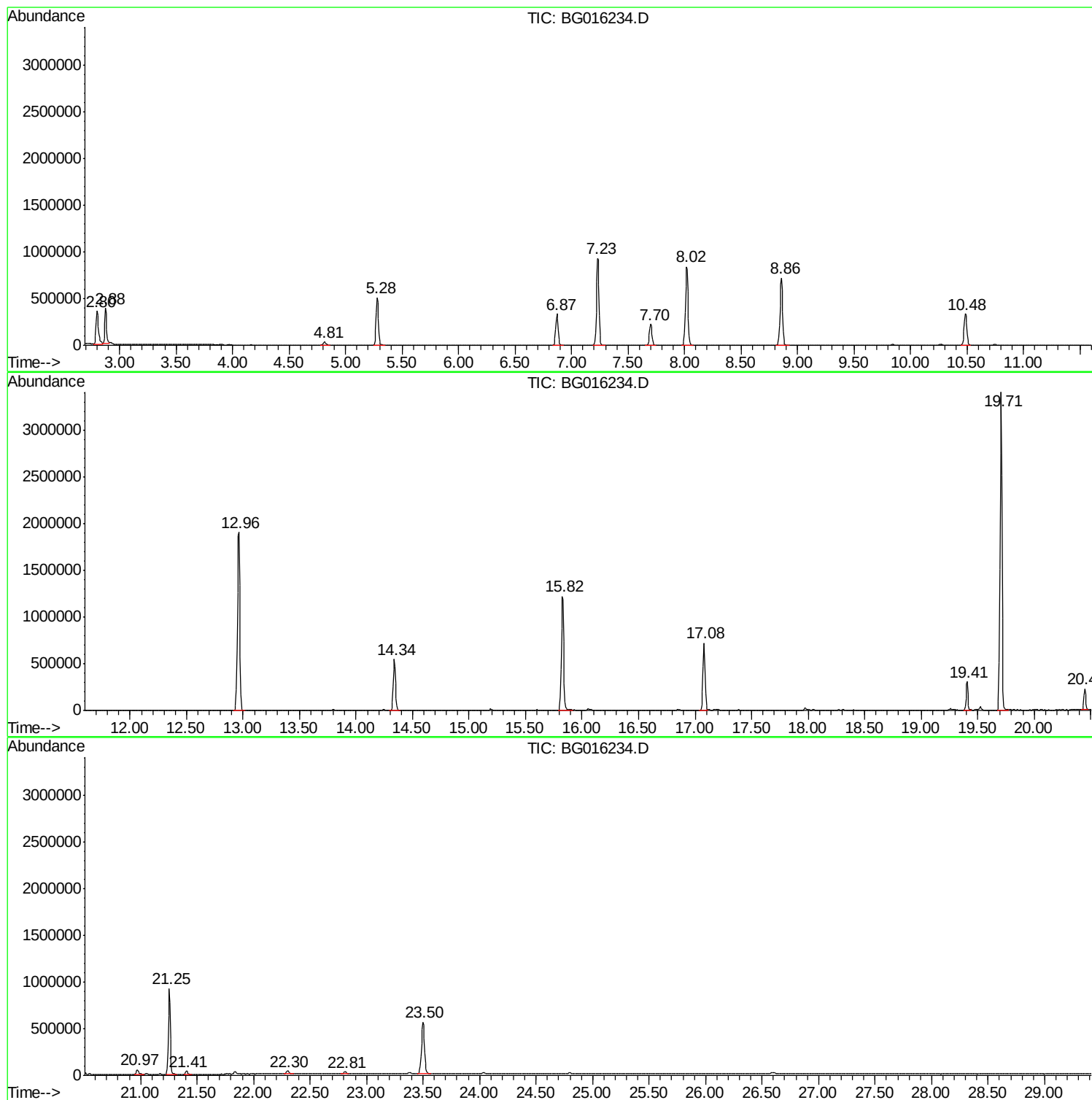
Sum of corrected areas: 20791331

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016234.D
Acq On : 6 Apr 2015 21:24
Operator : TP/IZ
Sample : G1757-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SW04

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016234.D
Acq On : 6 Apr 2015 21:24
Operator : TP/IZ
Sample : G1757-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SW04

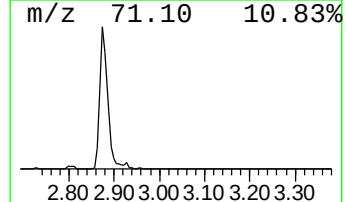
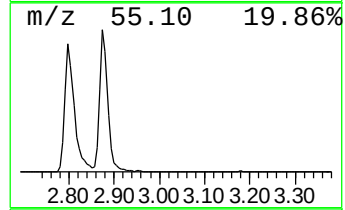
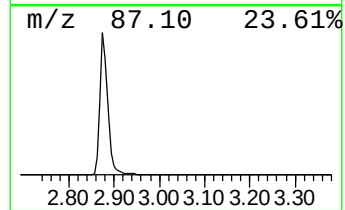
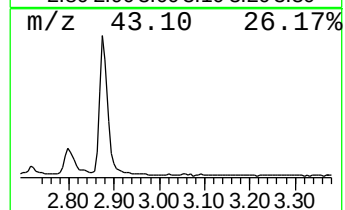
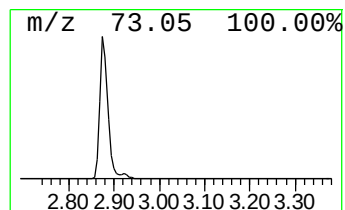
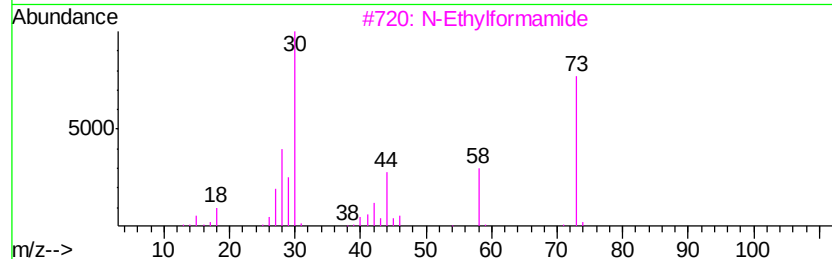
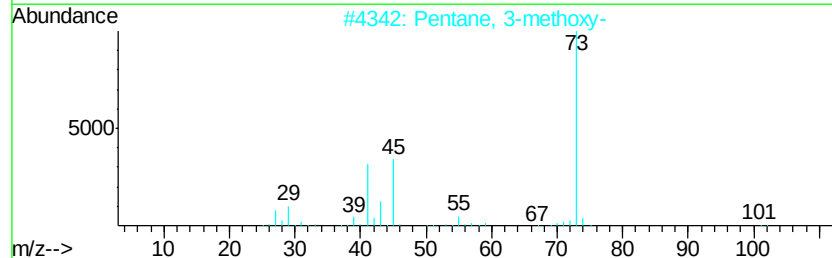
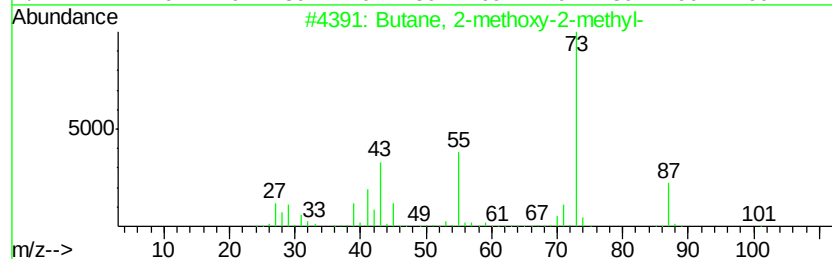
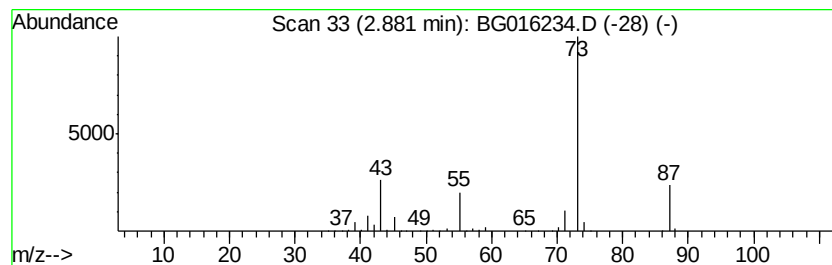
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.88	24.23 ng	411582	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016234.D
Acq On : 6 Apr 2015 21:24
Operator : TP/IZ
Sample : G1757-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SW04

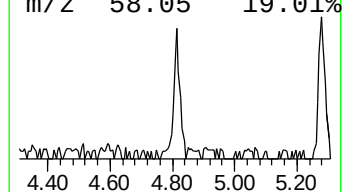
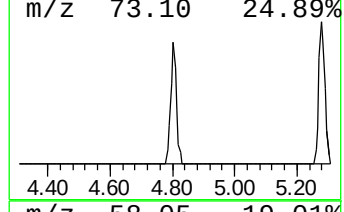
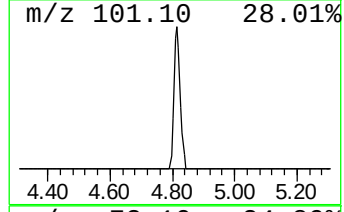
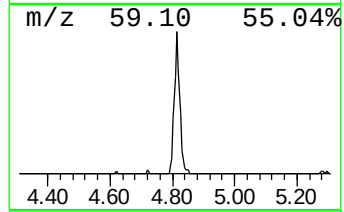
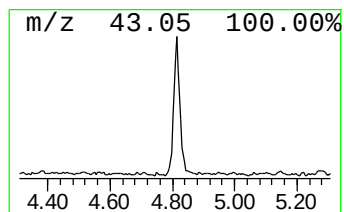
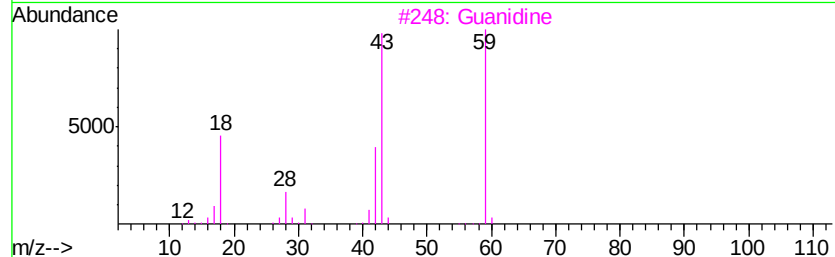
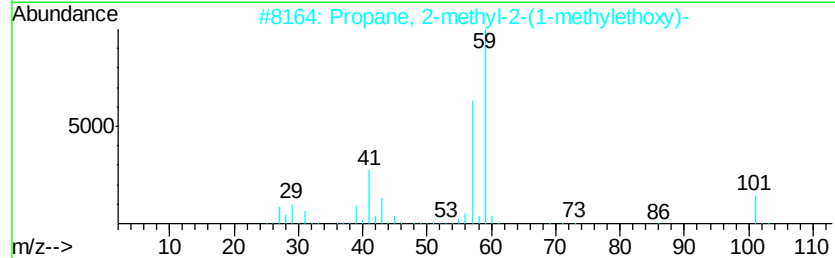
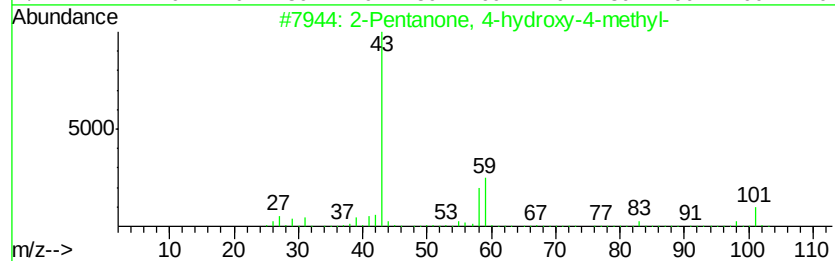
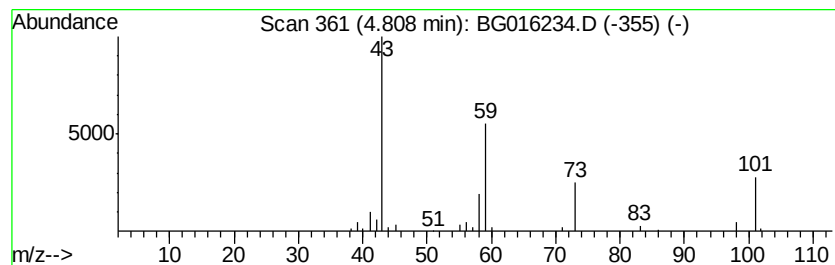
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	2.98 ng	50552	1,4-Dichlorobenzene-d4	7.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	38	
3	Guanidine	59	CH5N3	000113-00-8	38	
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	37	
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016234.D
Acq On : 6 Apr 2015 21:24
Operator : TP/IZ
Sample : G1757-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SW04

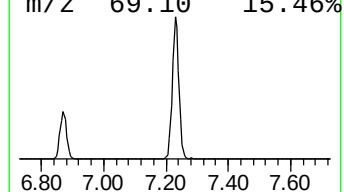
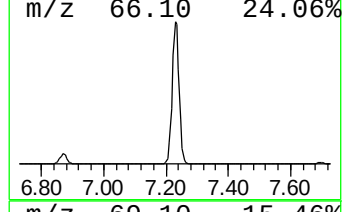
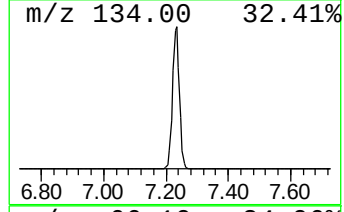
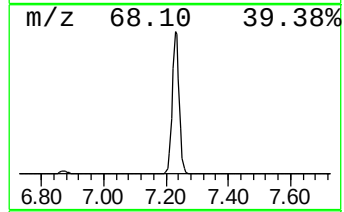
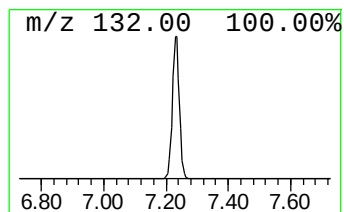
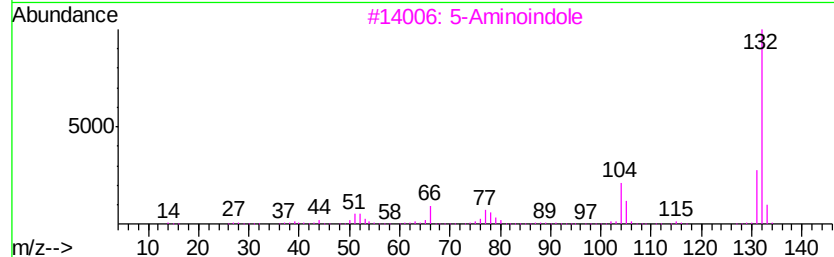
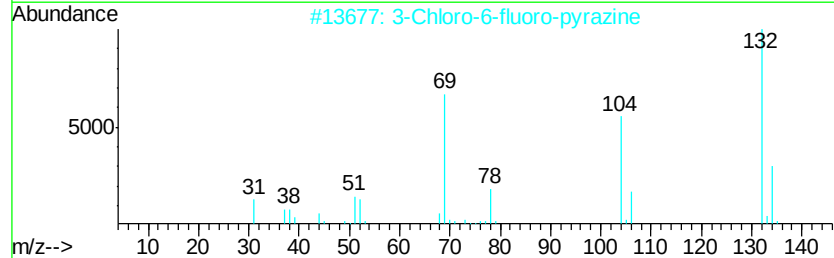
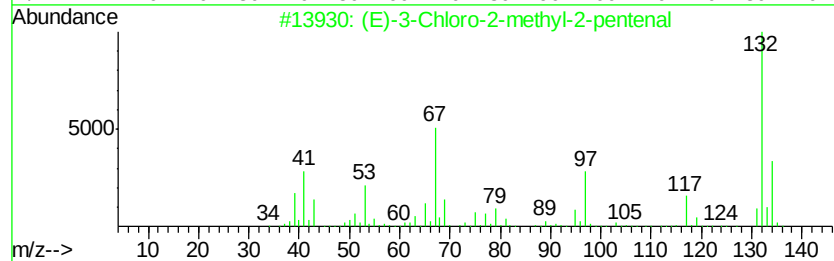
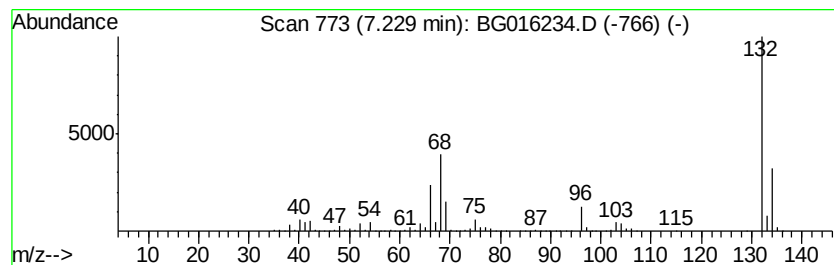
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	86.66 ng	1472060	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016234.D
Acq On : 6 Apr 2015 21:24
Operator : TP/IZ
Sample : G1757-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SW04

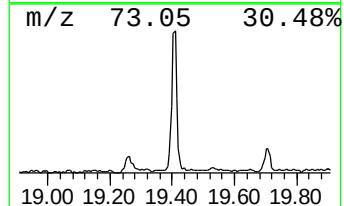
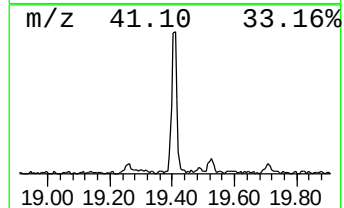
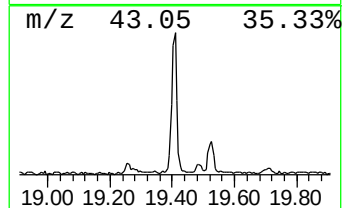
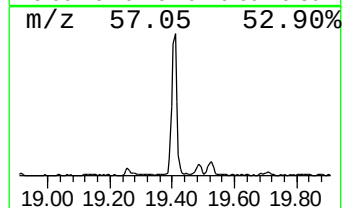
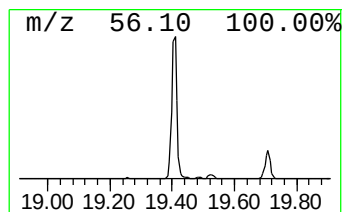
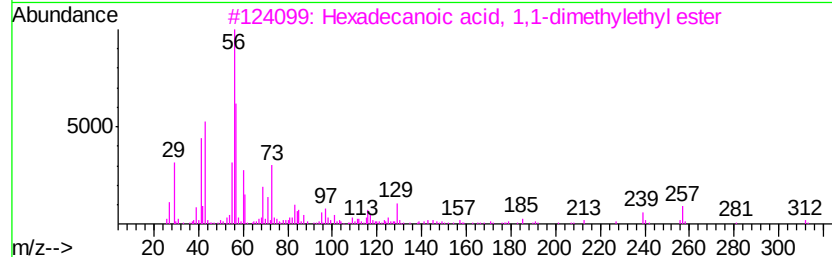
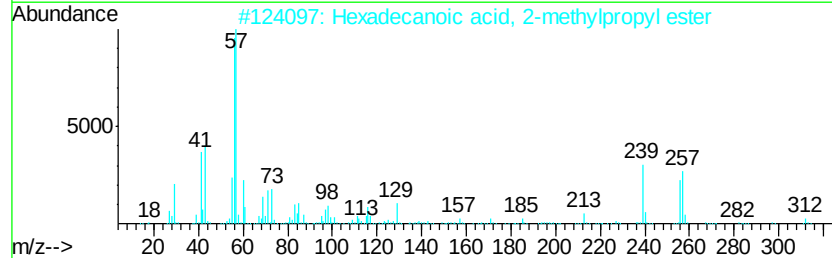
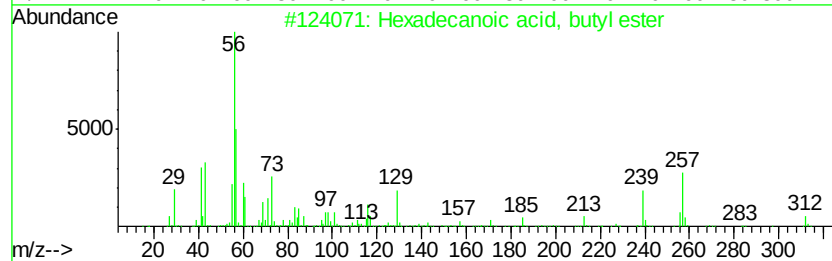
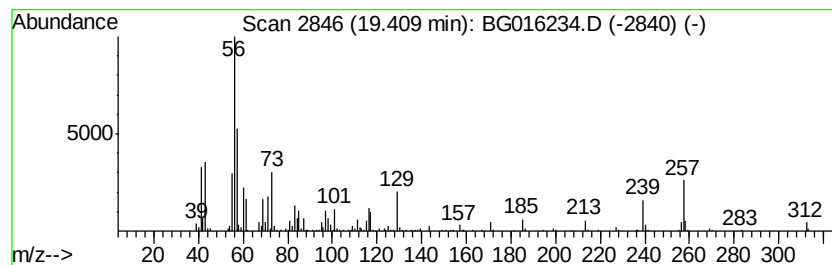
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.41	6.13 ng	347756	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	99
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	81
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	35
4		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
5		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016234.D
Acq On : 6 Apr 2015 21:24
Operator : TP/IZ
Sample : G1757-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SW04

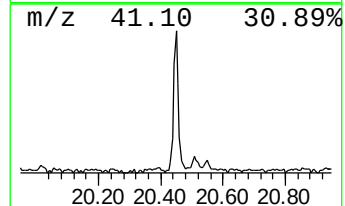
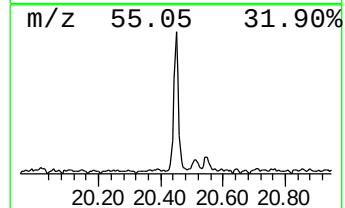
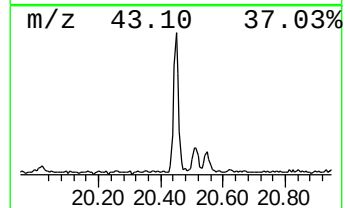
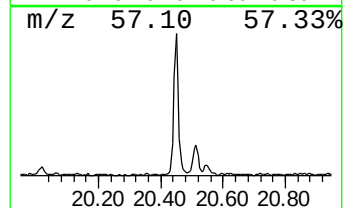
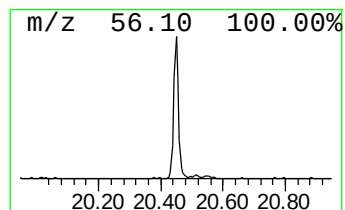
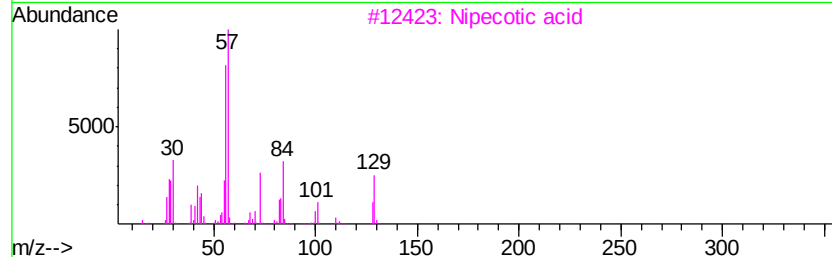
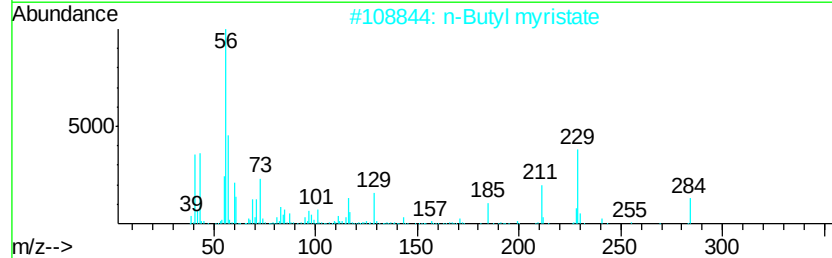
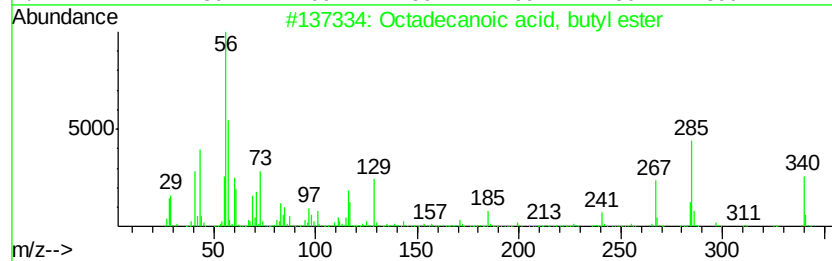
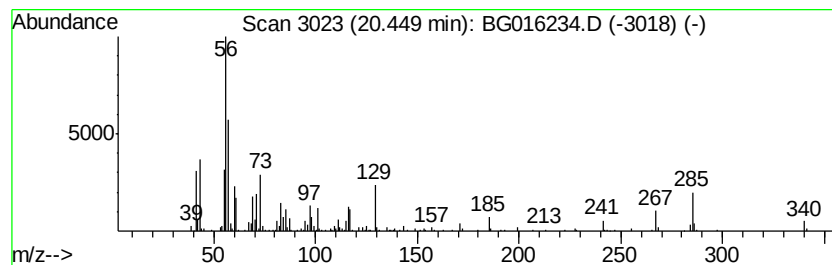
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.45	4.31 ng	244430	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	97
2		n-Butyl myristate	284	C18H36O2	000110-36-1	58
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	45
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016234.D
Acq On : 6 Apr 2015 21:24
Operator : TP/IZ
Sample : G1757-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SW04

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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...	2.88	24.2	ng	411582	1	7.70	339751	20.0
2-Pentanone, 4-hy...	4.81	3.0	ng	50552	1	7.70	339751	20.0
unknown7.23	7.23	86.7	ng	1472060	1	7.70	339751	20.0
Hexadecanoic acid...	19.41	6.1	ng	347756	5	21.25	1134270	20.0
Octadecanoic acid...	20.45	4.3	ng	244430	5	21.25	1134270	20.0