

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG017007.D
 Acq On : 10 May 2015 1:35
 Operator : TP/IZ
 Sample : G2104-05
 Misc :
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-101

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-BG050515.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	2.915	33	38	47	rBV	231688	357658	7.04%	1.272%
2	2.991	47	51	58	rVV	477499	553276	10.89%	1.967%
3	4.906	369	377	386	rBV	65447	97905	1.93%	0.348%
4	5.370	449	456	465	rBV	617132	891781	17.55%	3.170%
5	6.957	717	726	738	rBV	474518	756556	14.89%	2.690%
6	7.321	781	788	795	rBV	1135243	1726106	33.98%	6.137%
7	7.785	859	867	874	rBV	339315	540131	10.63%	1.920%
8	8.108	914	922	929	rBV	840945	1319395	25.97%	4.691%
9	8.949	1057	1065	1072	rBV	876401	1438627	28.32%	5.115%
10	10.582	1335	1343	1351	rBV	539747	893219	17.58%	3.176%
11	12.779	1711	1717	1724	rBV	184091	262512	5.17%	0.933%
12	13.050	1753	1763	1771	rBV	2400637	3739471	73.60%	13.294%
13	13.326	1803	1810	1815	rBV2	54262	93178	1.83%	0.331%
14	14.430	1991	1998	2004	rBV2	870777	1356072	26.69%	4.821%
15	15.241	2130	2136	2140	rBV3	27245	62893	1.24%	0.224%
16	15.788	2225	2229	2235	rVB	43549	61691	1.21%	0.219%
17	15.917	2244	2251	2259	rBV	2200436	3111450	61.24%	11.062%
18	17.168	2458	2464	2473	rBV2	1232345	1668704	32.85%	5.933%
19	18.067	2612	2617	2625	rBV2	270061	395238	7.78%	1.405%
20	19.348	2831	2835	2840	rBV2	209379	261059	5.14%	0.928%
21	19.795	2906	2911	2917	rVB	3900890	5080480	100.00%	18.062%
22	21.058	3123	3126	3132	rVB4	75010	90202	1.78%	0.321%
23	21.346	3170	3175	3181	rBV	1349897	1698158	33.43%	6.037%
24	23.643	3558	3566	3573	rBV	877903	1672392	32.92%	5.946%

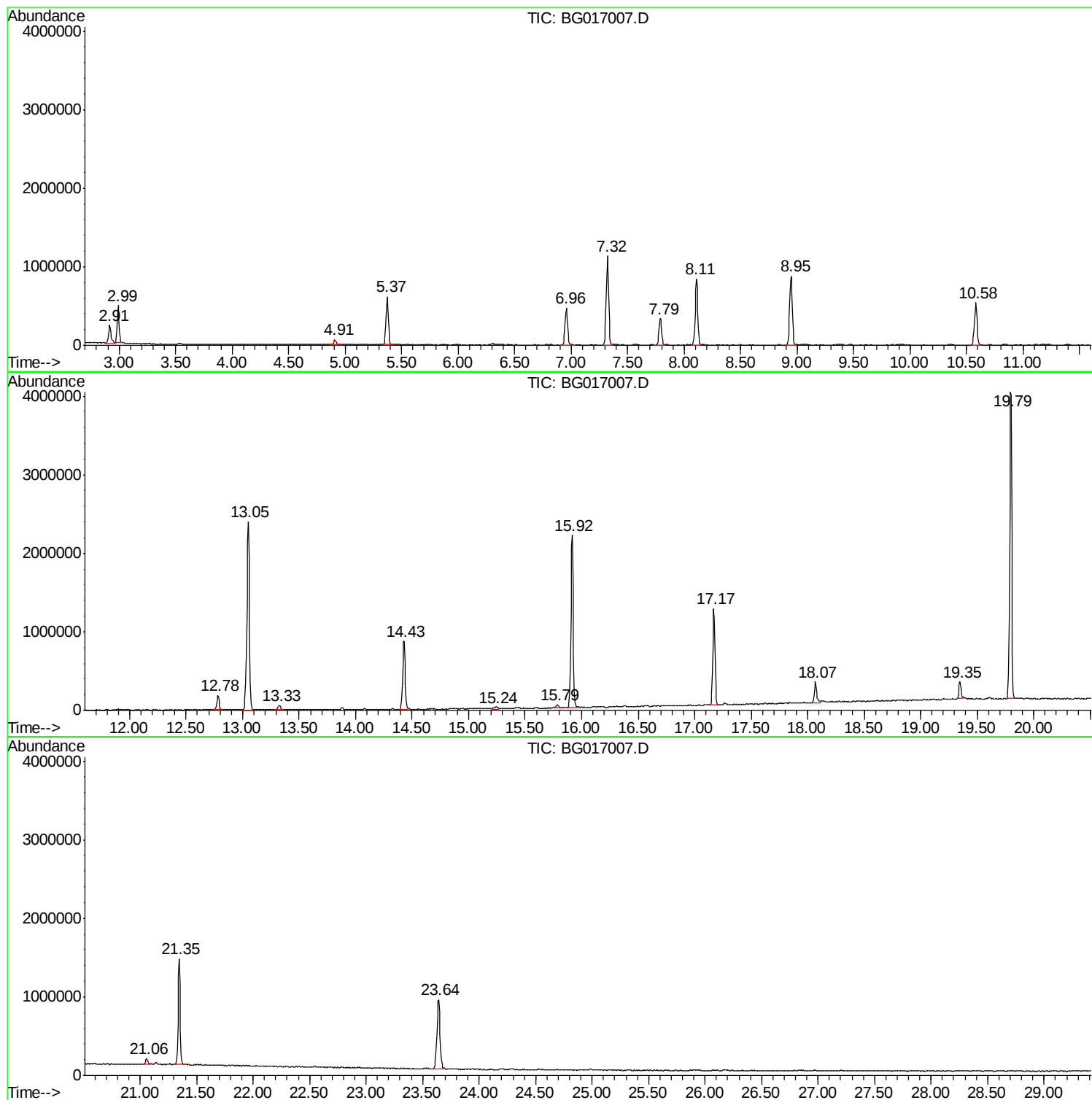
Sum of corrected areas: 28128154

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

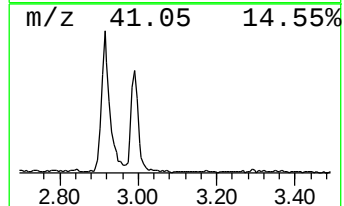
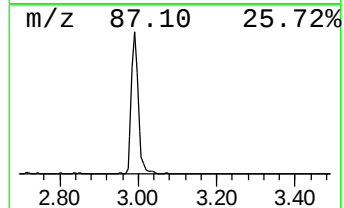
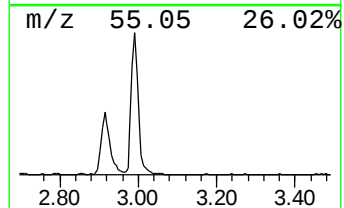
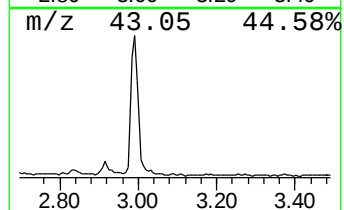
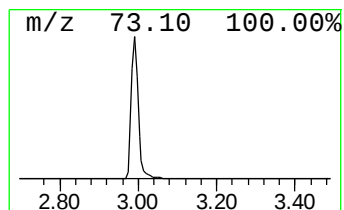
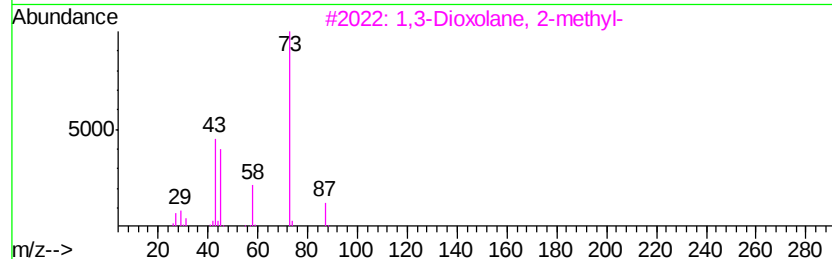
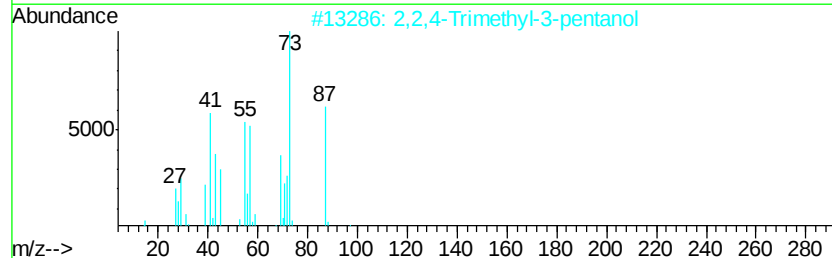
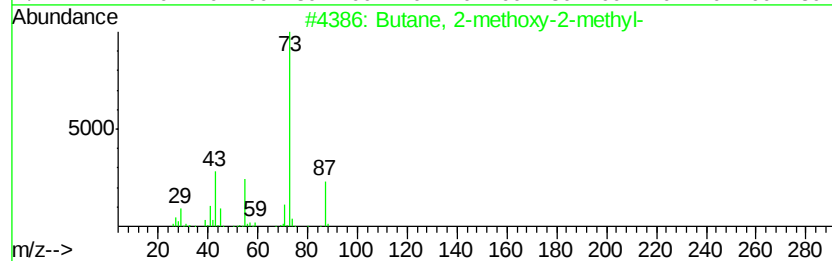
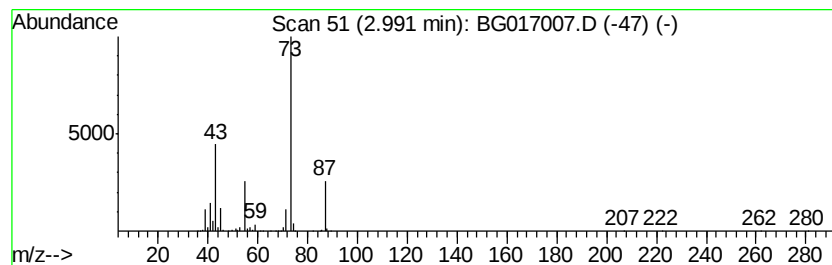
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	20.49 ng	553276	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	42
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

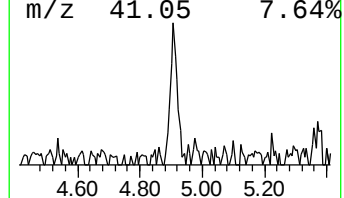
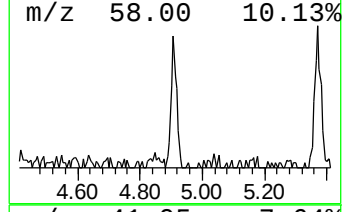
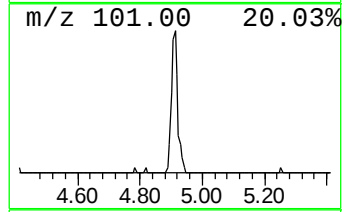
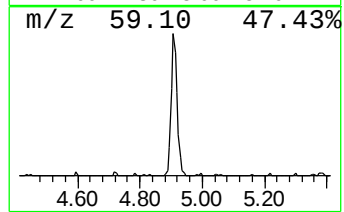
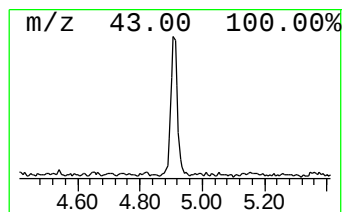
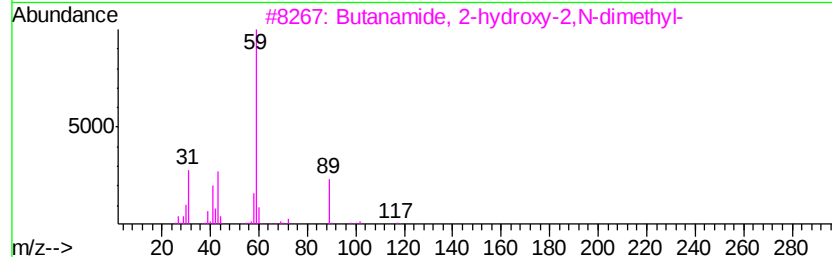
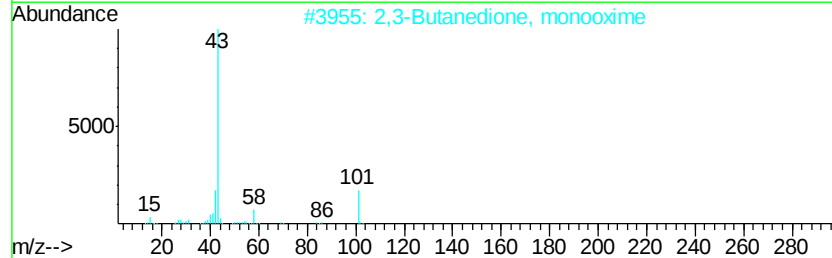
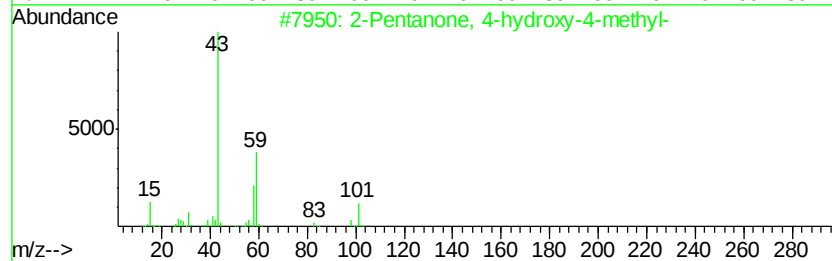
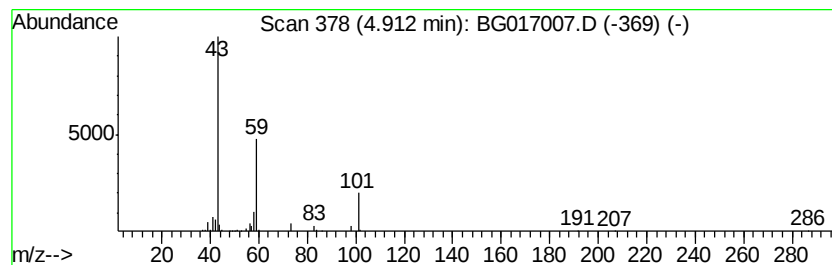
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.91	3.63 ng	97905	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27	
3	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	23	
4	Butane	58	C4H10	000106-97-8	9	
5	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	9	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

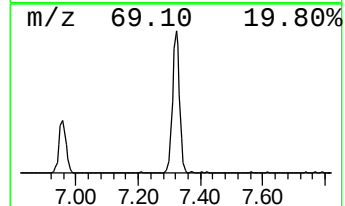
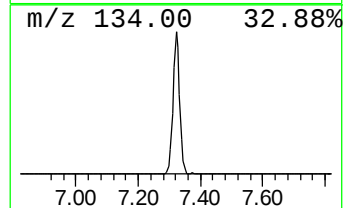
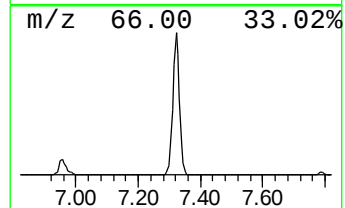
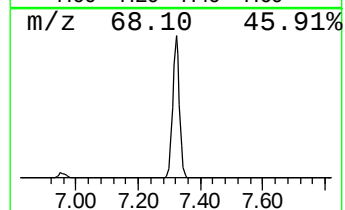
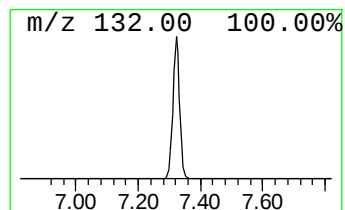
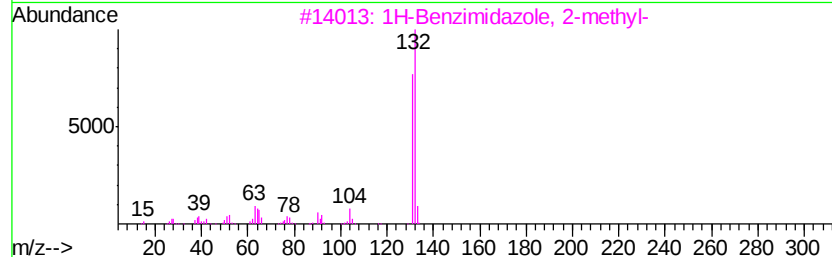
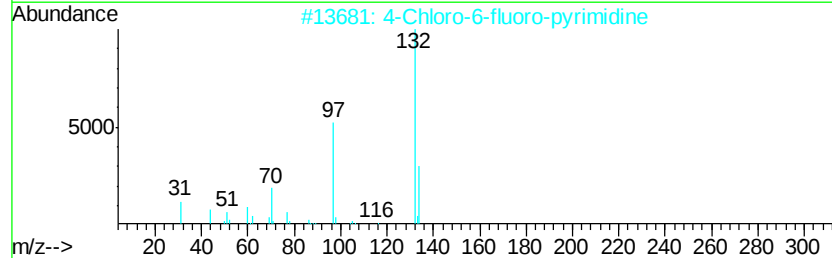
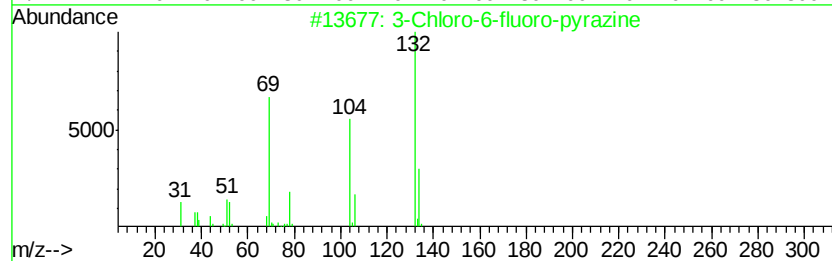
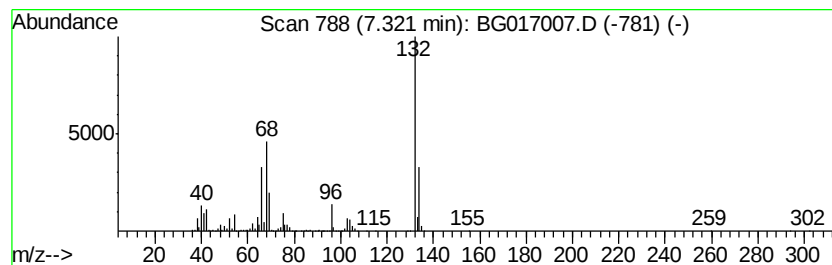
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	63.91 ng	1726110	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

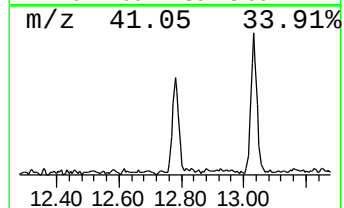
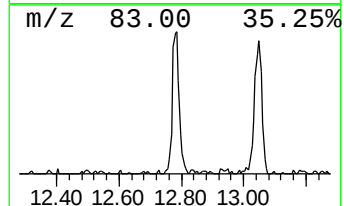
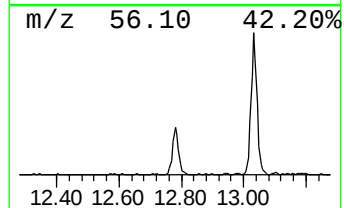
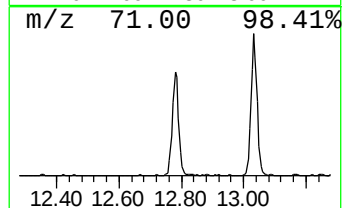
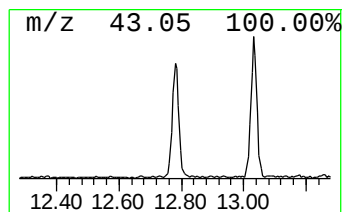
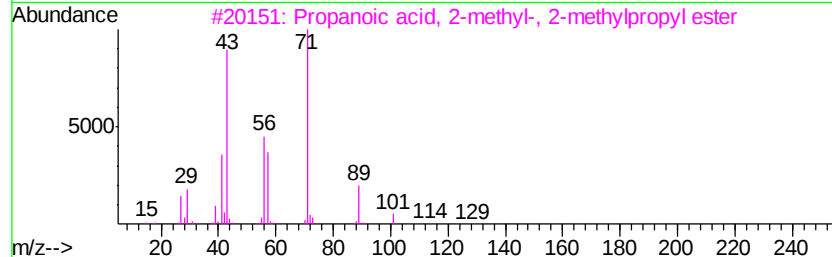
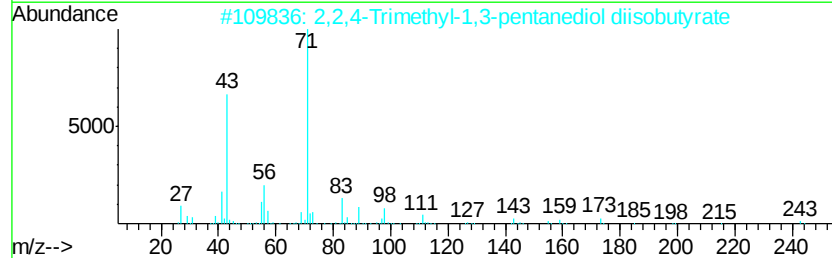
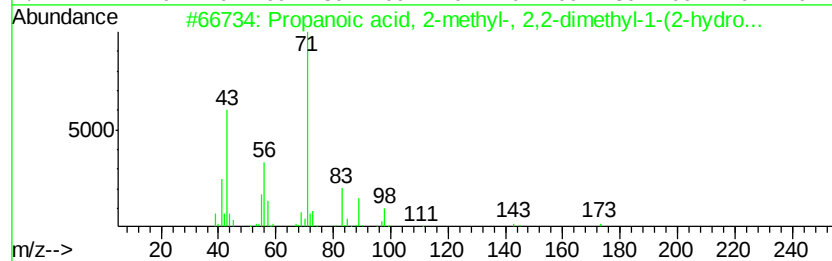
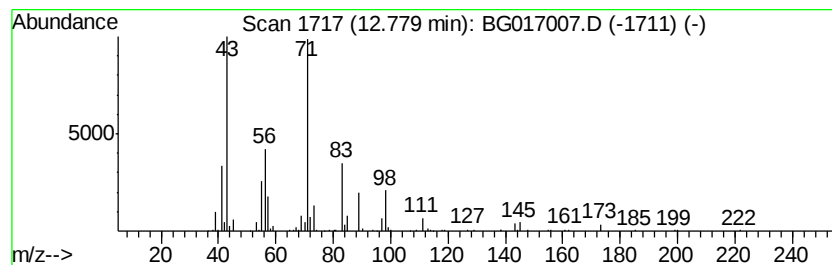
Instrument :
BNA_G
ClientSampleId :
MW-101

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.78	3.87 ng	262512	Acenaphthene-d10	14.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	64
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	40
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40
4	Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	38
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

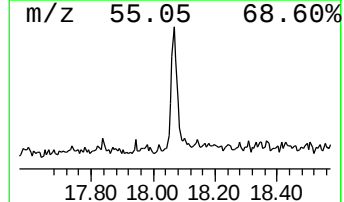
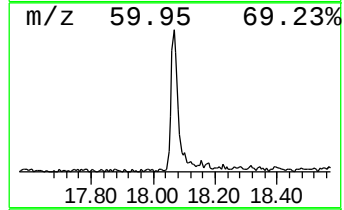
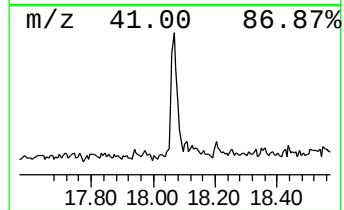
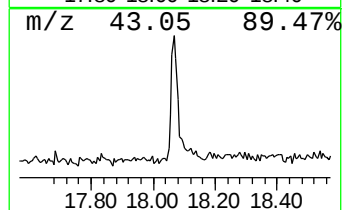
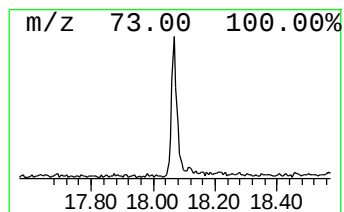
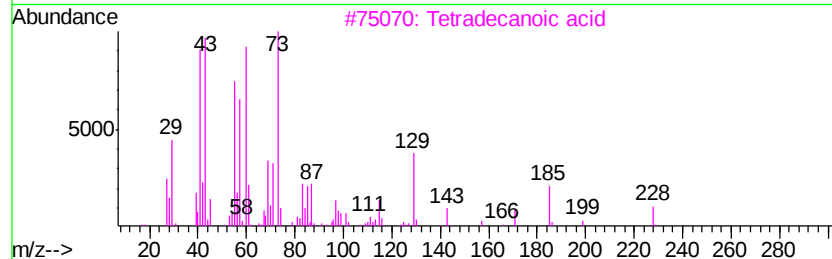
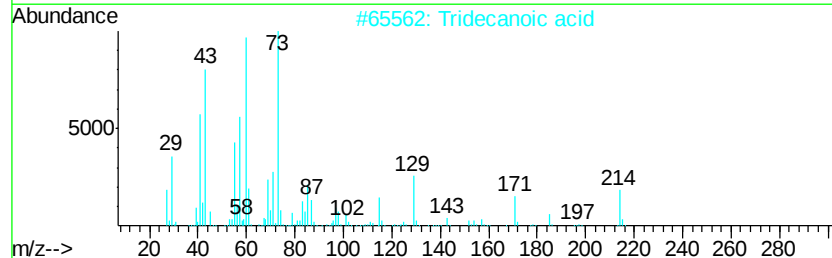
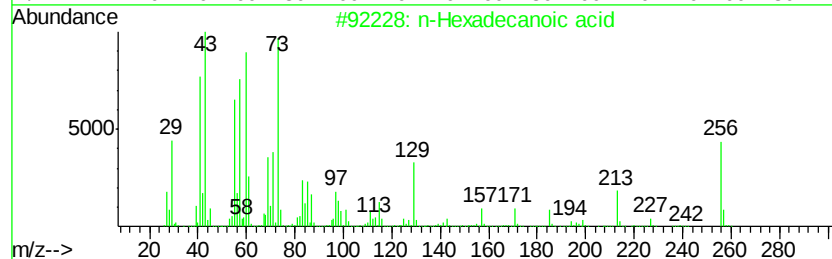
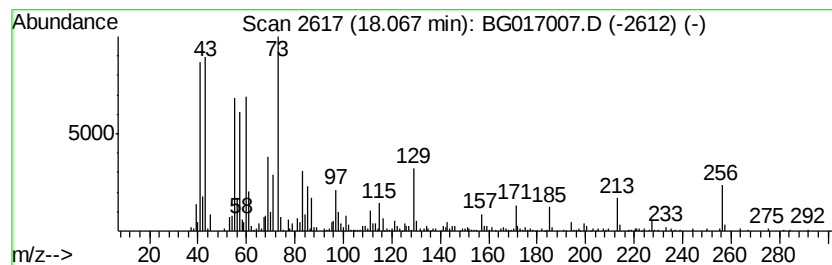
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	4.74 ng	395238	Phenanthrene-d10	17.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	86
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	46



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

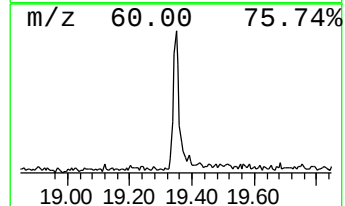
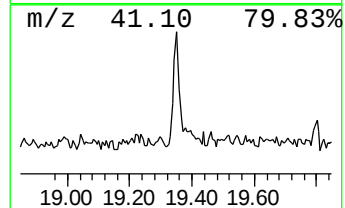
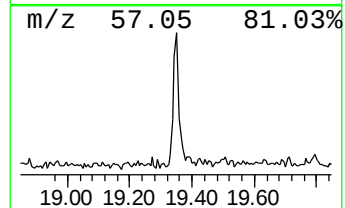
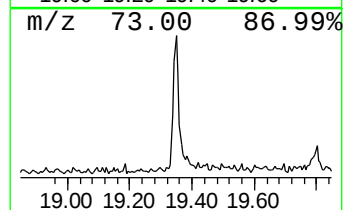
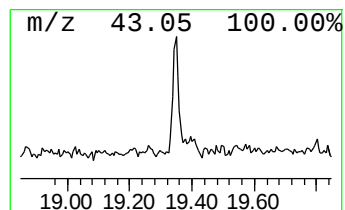
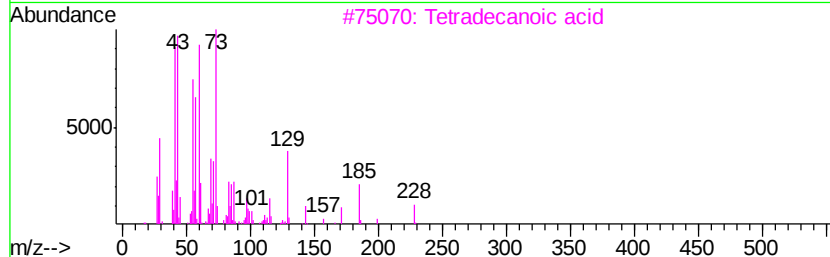
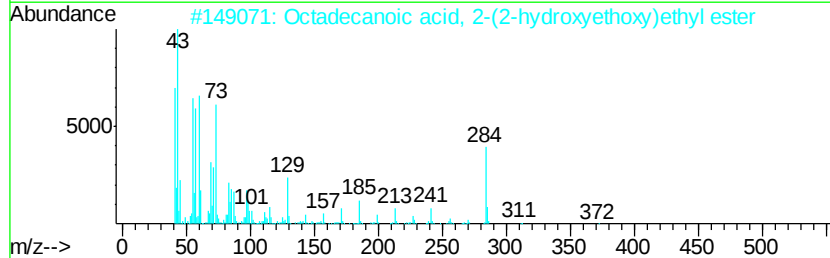
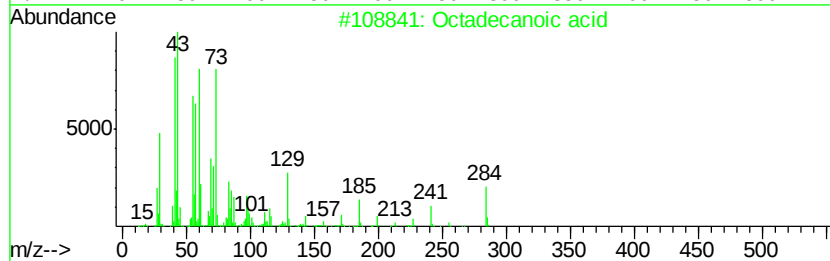
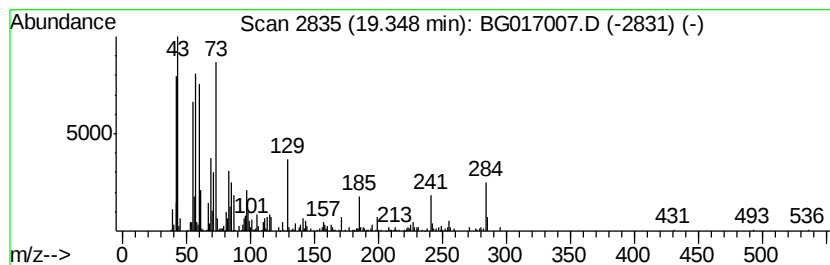
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	3.07 ng	261059	Chrysene-d12	21.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017007.D
Acq On : 10 May 2015 1:35
Operator : TP/IZ
Sample : G2104-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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...	2.99	20.5	ng	553276	1	7.79	540131	20.0
2-Pentanone, 4-hy...	4.91	3.6	ng	97905	1	7.79	540131	20.0
unknown7.32	7.32	63.9	ng	1726110	1	7.79	540131	20.0
Propanoic acid, 2...	12.78	3.9	ng	262512	3	14.43	1356070	20.0
n-Hexadecanoic acid	18.07	4.7	ng	395238	4	17.17	1668700	20.0
Octadecanoic acid	19.35	3.1	ng	261059	5	21.35	1698160	20.0