

Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
 Data File : BG023848.D
 Acq On : 23 Aug 2016 11:52
 Operator : UM/SJ
 Sample : PB93006BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB93006BL

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-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	2.969	15	22	32	rBV	266704	402302	4.94%	0.902%
2	3.233	62	67	77	rVB2	55202	97377	1.20%	0.218%
3	5.154	387	394	403	rBV	700113	1124462	13.81%	2.522%
4	5.636	469	476	498	rBV	2140902	3518522	43.21%	7.891%
5	7.251	744	751	763	rBV	2091543	3732623	45.84%	8.371%
6	7.622	806	814	827	rBV	2139506	3708957	45.55%	8.318%
7	8.092	887	894	906	rBV	422546	733922	9.01%	1.646%
8	8.420	941	950	960	rBV	1567380	2735745	33.60%	6.136%
9	9.272	1088	1095	1107	rBV	1293220	2339588	28.74%	5.247%
10	10.929	1369	1377	1387	rBV	536785	1000846	12.29%	2.245%
11	13.378	1786	1794	1802	rBV	3329314	5187754	63.72%	11.635%
12	14.765	2024	2030	2038	rBV2	823403	1412748	17.35%	3.168%
13	16.263	2278	2285	2303	rBV	2651587	4359501	53.54%	9.777%
14	17.532	2494	2501	2513	rBV2	1091330	1823062	22.39%	4.089%
15	19.805	2885	2888	2893	rVB	73181	86920	1.07%	0.195%
16	20.134	2938	2944	2951	rBV	5919653	8141902	100.00%	18.260%
17	21.838	3228	3234	3244	rBV	1226535	2150831	26.42%	4.824%
18	25.221	3799	3810	3826	rVB2	672647	2031332	24.95%	4.556%

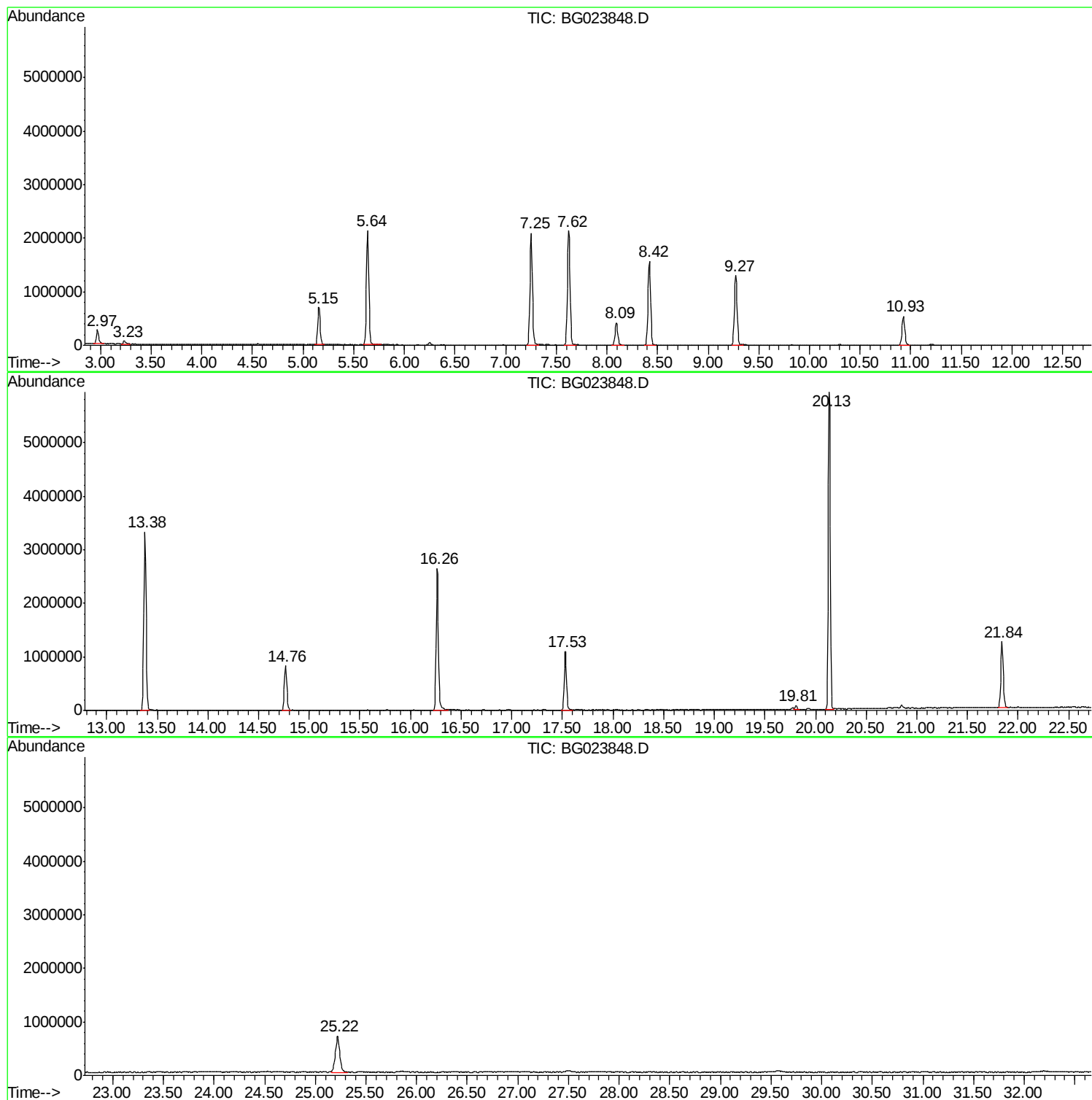
Sum of corrected areas: 44588394

Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
Data File : BG023848.D
Acq On : 23 Aug 2016 11:52
Operator : UM/SJ
Sample : PB93006BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB93006BL

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\BG082316\
Data File : BG023848.D
Acq On : 23 Aug 2016 11:52
Operator : UM/SJ
Sample : PB93006BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB93006BL

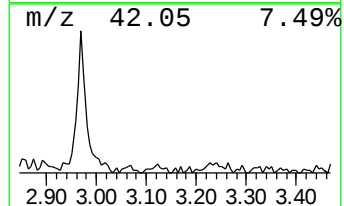
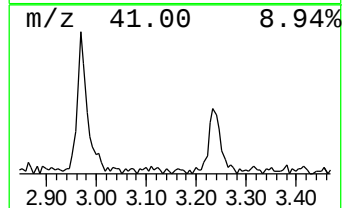
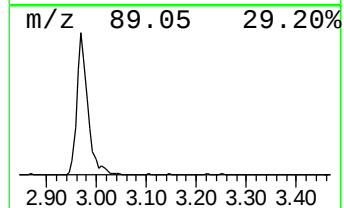
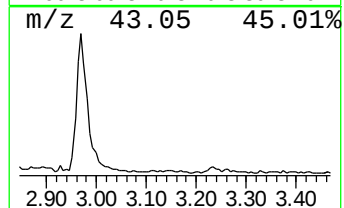
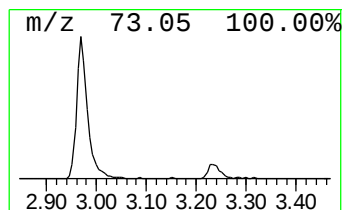
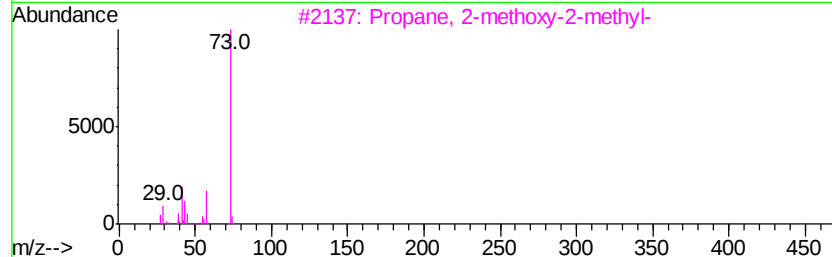
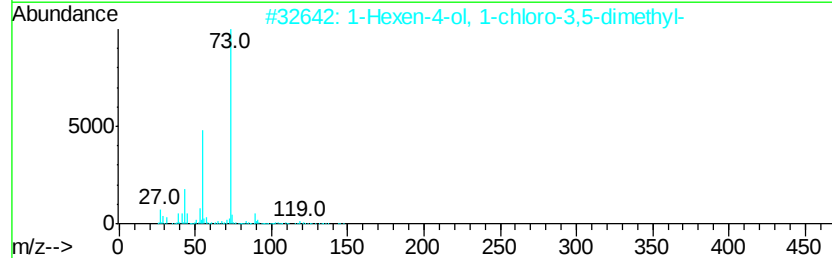
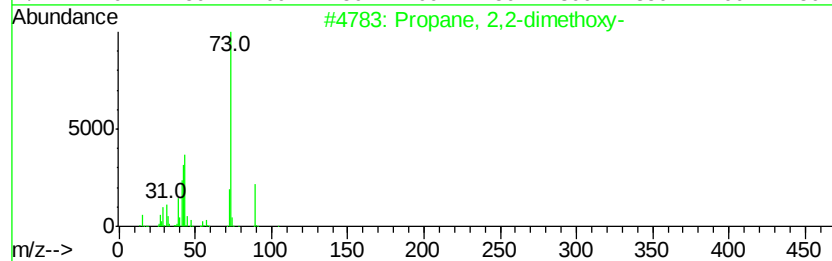
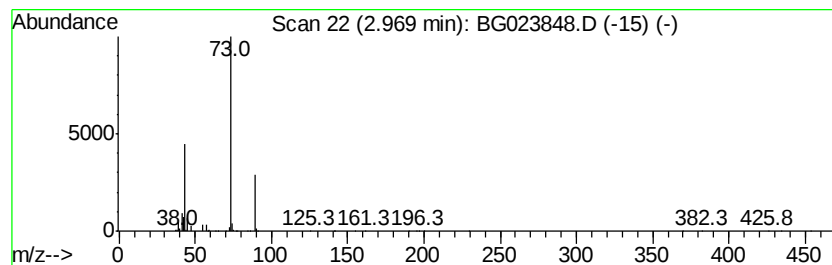
Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	10.96 ng	402302	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	36
2		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
Data File : BG023848.D
Acq On : 23 Aug 2016 11:52
Operator : UM/SJ
Sample : PB93006BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB93006BL

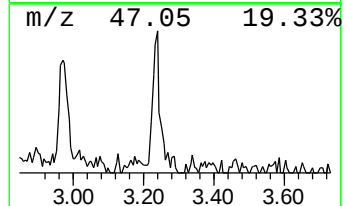
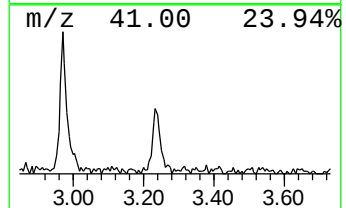
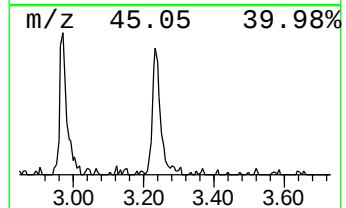
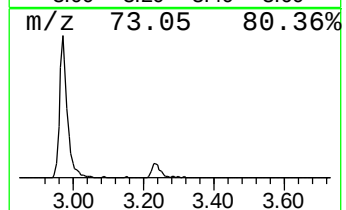
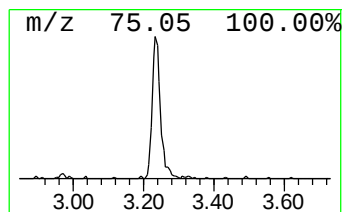
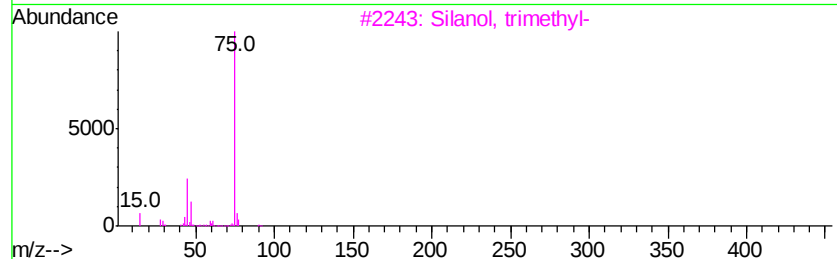
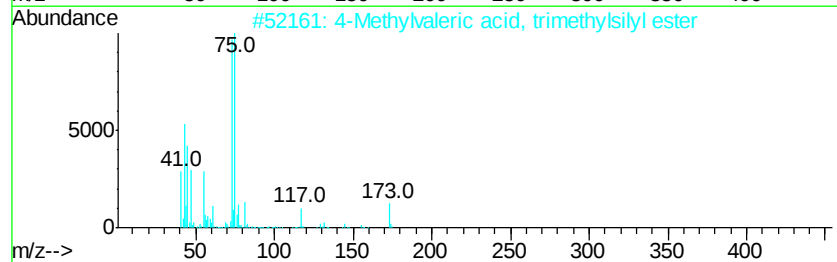
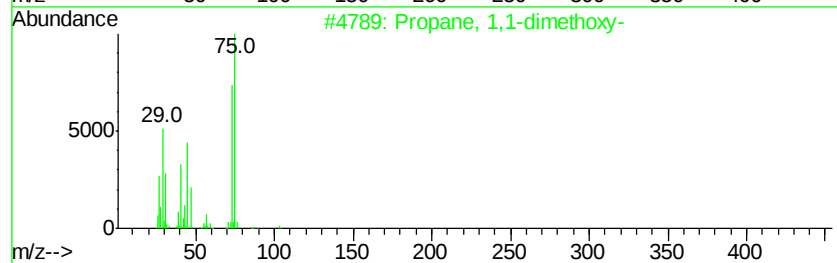
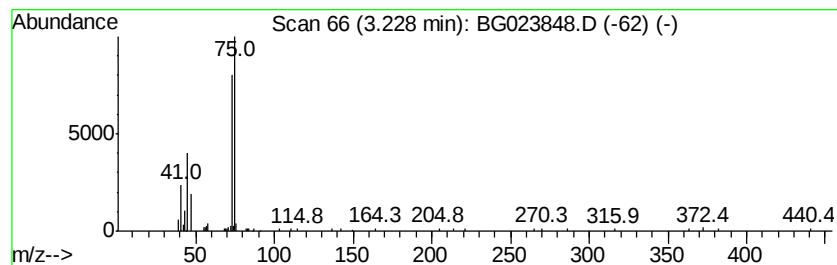
Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	2.65 ng	97377	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		4-Methylvaleric acid, trimethyls...	188	C9H20O2Si	959048-10-3	74
3		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	50
4		Methanamine, N,N-dimethyl-, N-oxide	75	C3H9NO	001184-78-7	37
5		Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	33



Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
Data File : BG023848.D
Acq On : 23 Aug 2016 11:52
Operator : UM/SJ
Sample : PB93006BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB93006BL

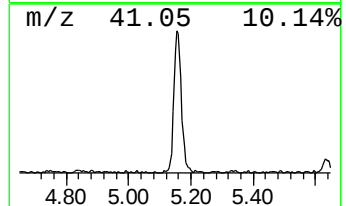
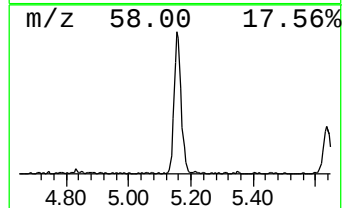
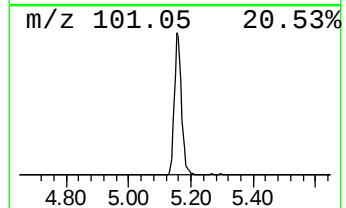
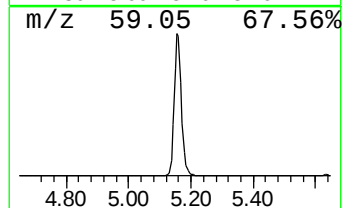
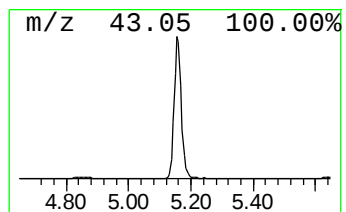
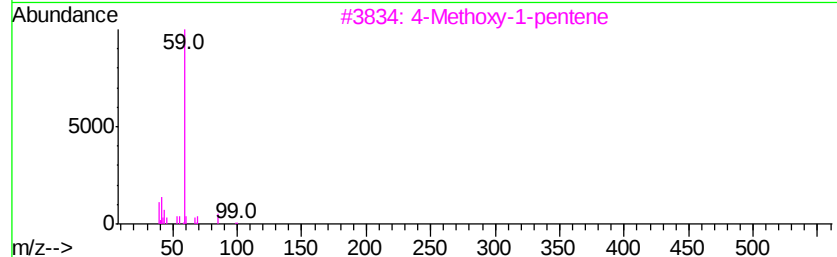
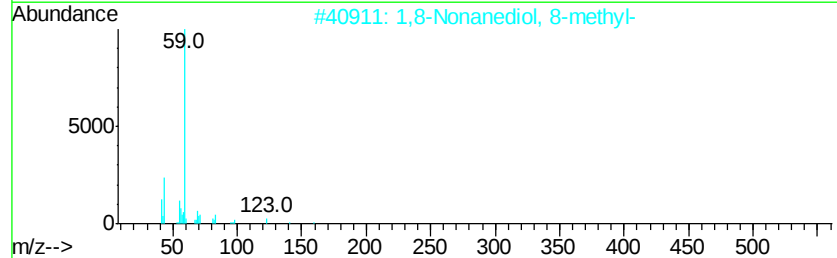
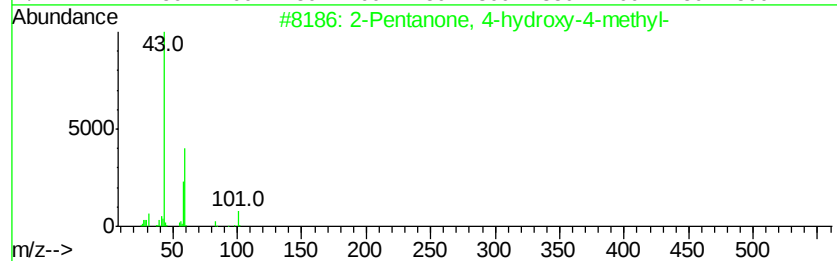
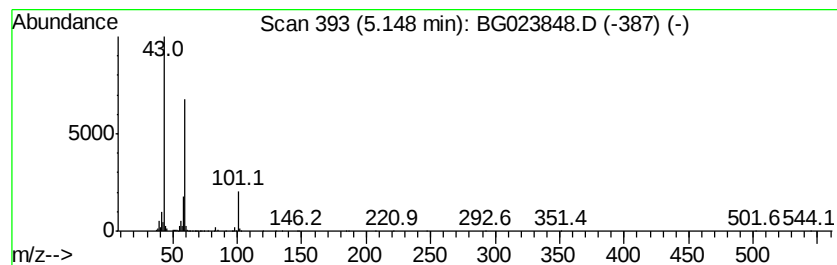
Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	30.64 ng	1124460	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3		4-Methoxy-1-pentene	100	C6H12O	098386-09-5	23
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
Data File : BG023848.D
Acq On : 23 Aug 2016 11:52
Operator : UM/SJ
Sample : PB93006BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB93006BL

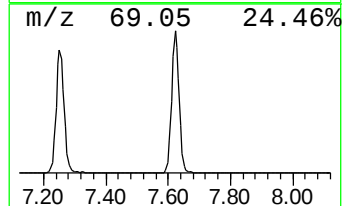
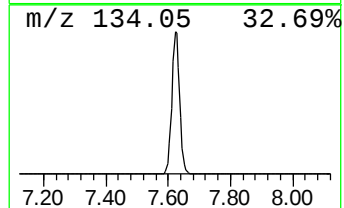
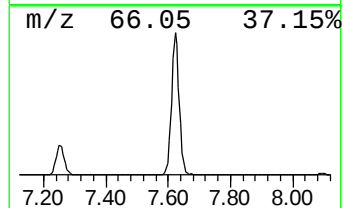
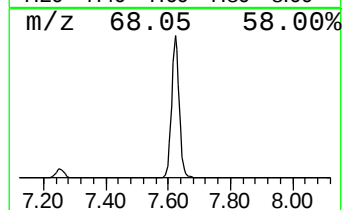
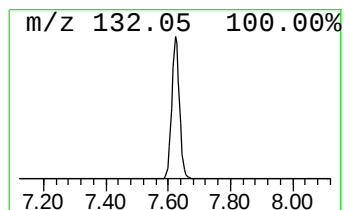
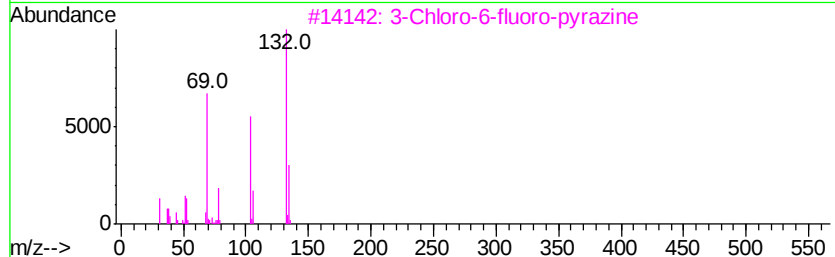
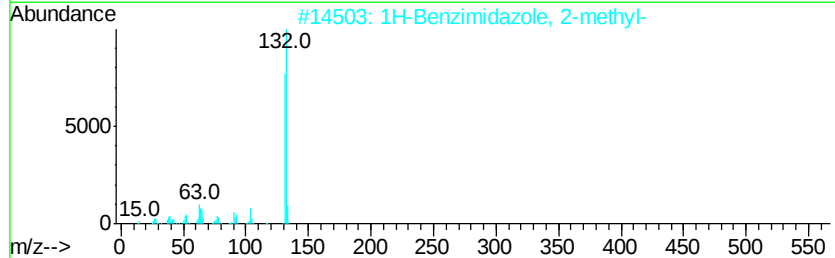
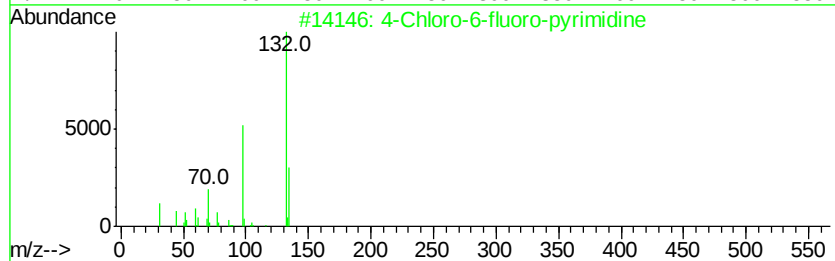
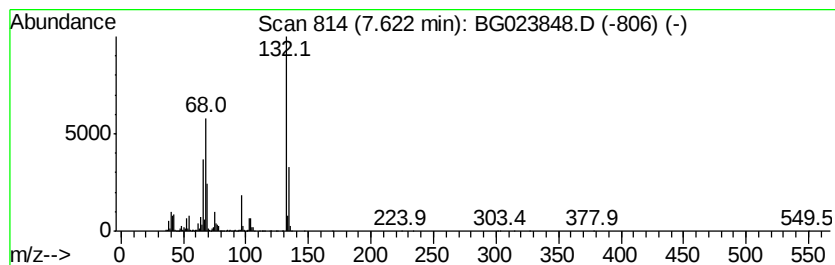
Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	101.07 ng	3708960	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082316\
Data File : BG023848.D
Acq On : 23 Aug 2016 11:52
Operator : UM/SJ
Sample : PB93006BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB93006BL

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
unknown2.97	2.97	11.0	ng	402302	1	8.09	733922	20.0
Propane, 1,1-dime...	3.23	2.6	ng	97377	1	8.09	733922	20.0
2-Pentanone, 4-hy...	5.15	30.6	ng	1124460	1	8.09	733922	20.0
unknown7.62	7.62	101.1	ng	3708960	1	8.09	733922	20.0