

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
 Data File : BG019121.D
 Acq On : 10 Oct 2015 17:27
 Operator : UM/NP
 Sample : PB86017BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB86017BL

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-BG101015.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	2.997	23	27	38	rVB	44375	54123	3.29%	0.754%
2	4.536	283	289	299	rBV	90159	126688	7.71%	1.765%
3	5.135	383	391	403	rBV	240584	350504	21.33%	4.883%
4	5.605	464	471	480	rBV	292799	444125	27.03%	6.187%
5	7.192	734	741	751	rBV	295472	503832	30.66%	7.019%
6	7.568	797	805	813	rBV	274268	466581	28.40%	6.500%
7	8.032	878	884	892	rVB	55187	91831	5.59%	1.279%
8	8.355	932	939	948	rVB	207642	344487	20.97%	4.799%
9	9.189	1073	1081	1088	rBV	177953	313886	19.10%	4.373%
10	10.835	1354	1361	1372	rVB	79059	134843	8.21%	1.878%
11	13.285	1771	1778	1785	rBV	517817	764472	46.53%	10.650%
12	14.659	2006	2012	2019	rVB3	126945	207856	12.65%	2.896%
13	16.146	2259	2265	2280	rBV	452993	678563	41.30%	9.453%
14	17.403	2473	2479	2487	rBV	207242	304525	18.53%	4.242%
15	20.018	2918	2924	2930	rBV	1306902	1643062	100.00%	22.889%
16	21.675	3199	3206	3213	rBV	252681	400323	24.36%	5.577%
17	24.900	3744	3755	3772	rBV4	123586	348668	21.22%	4.857%

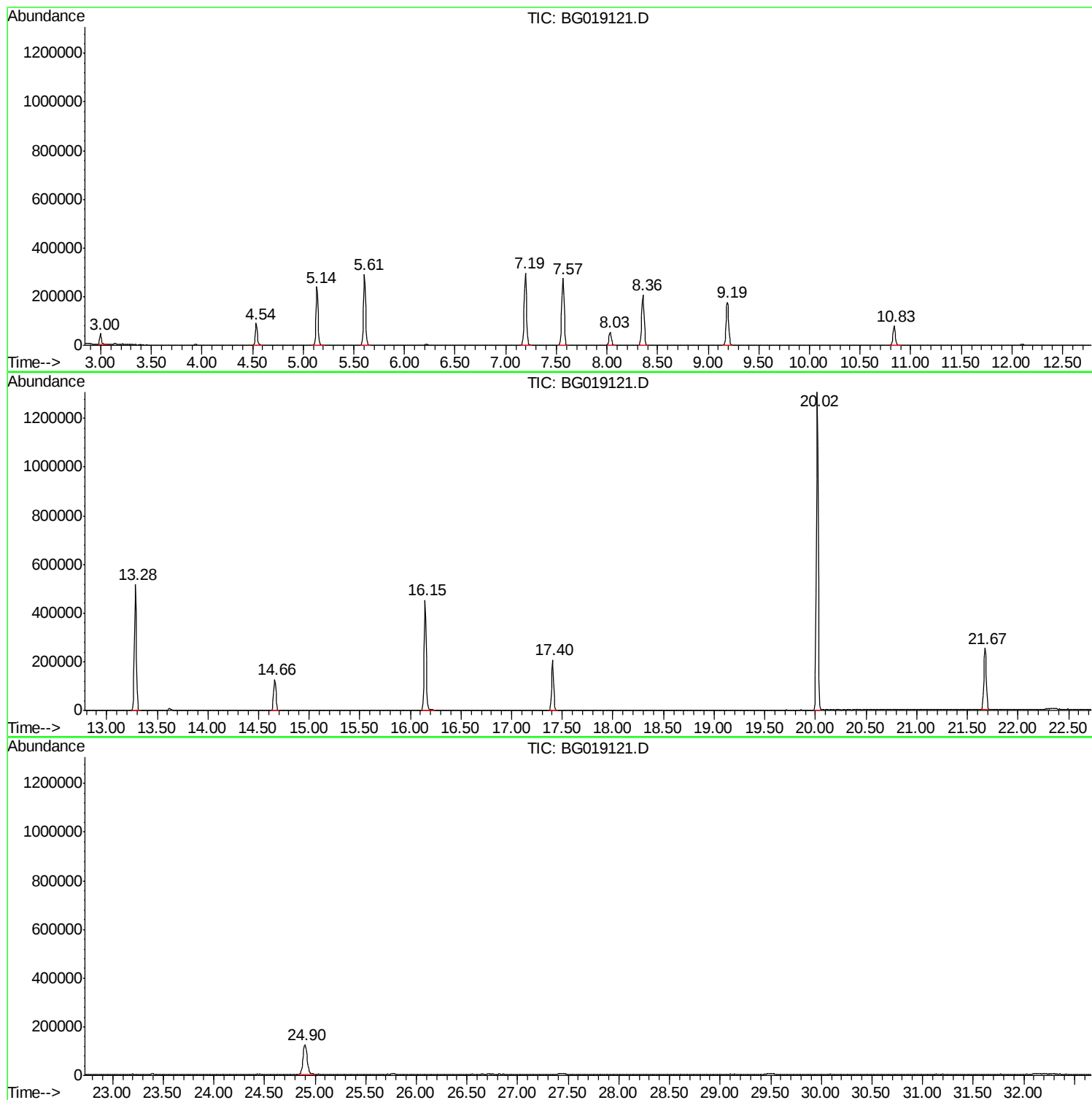
Sum of corrected areas: 7178369

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019121.D
Acq On : 10 Oct 2015 17:27
Operator : UM/NP
Sample : PB86017BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB86017BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.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\BG101015\
Data File : BG019121.D
Acq On : 10 Oct 2015 17:27
Operator : UM/NP
Sample : PB86017BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleID :
PB86017BL

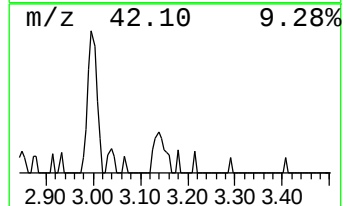
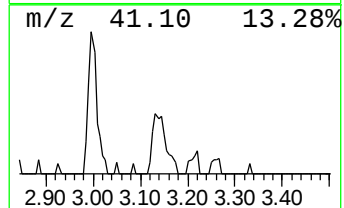
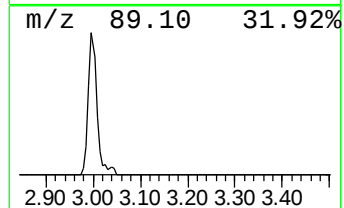
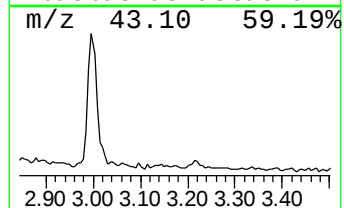
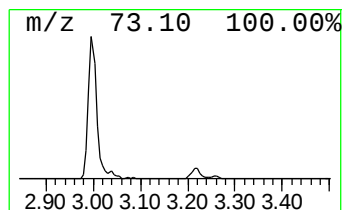
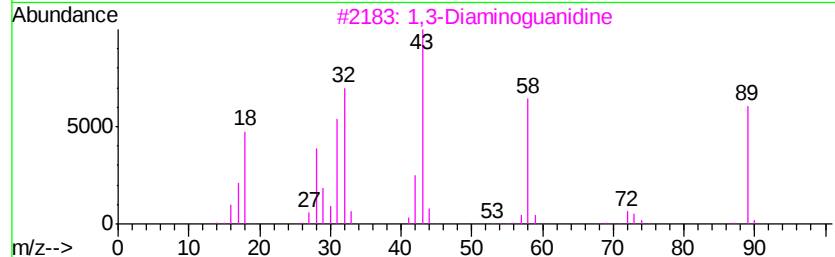
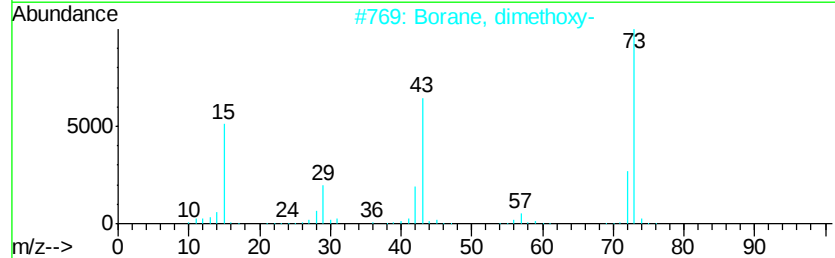
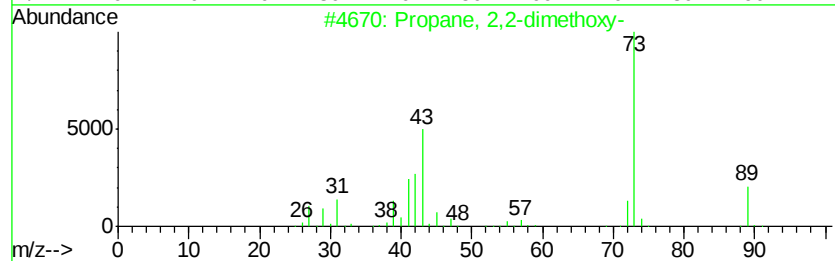
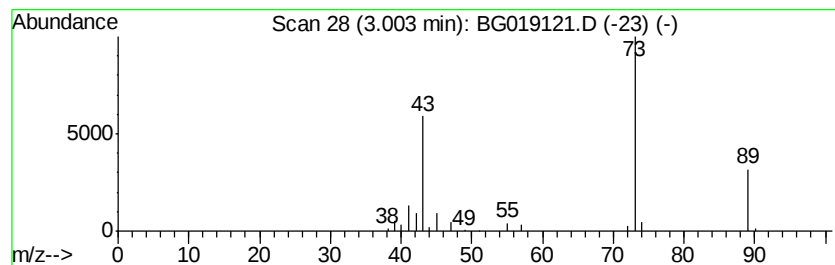
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	11.79 ng	54123	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5		Methylglyoxal	72	C3H4O2	000078-98-8	7



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019121.D
Acq On : 10 Oct 2015 17:27
Operator : UM/NP
Sample : PB86017BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB86017BL

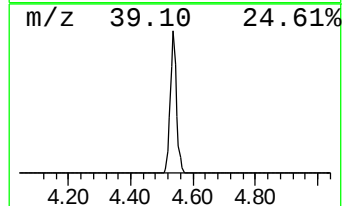
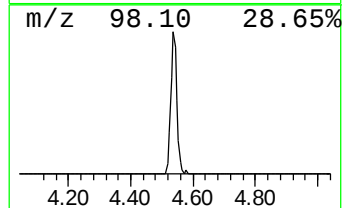
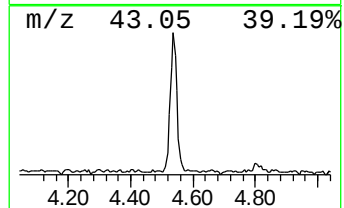
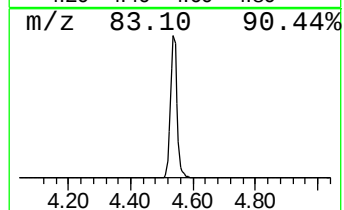
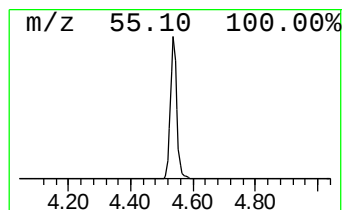
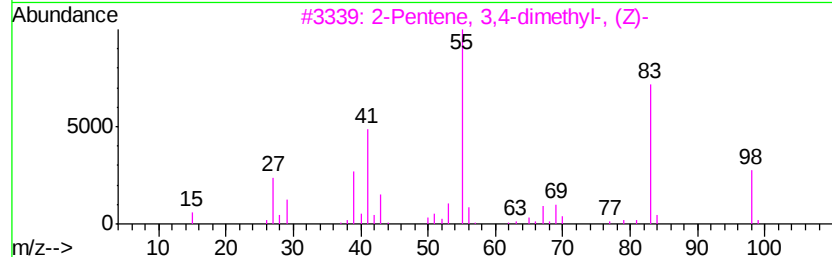
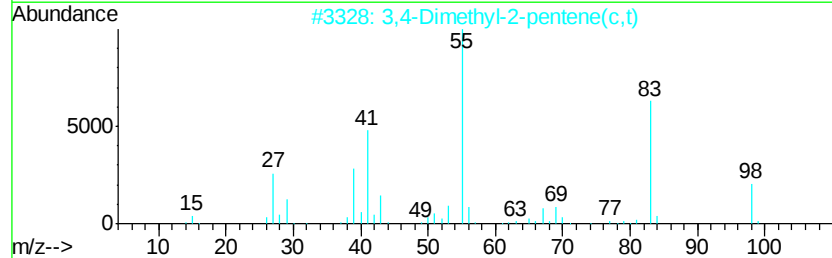
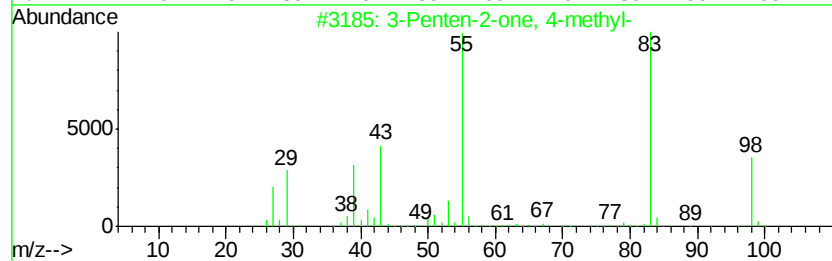
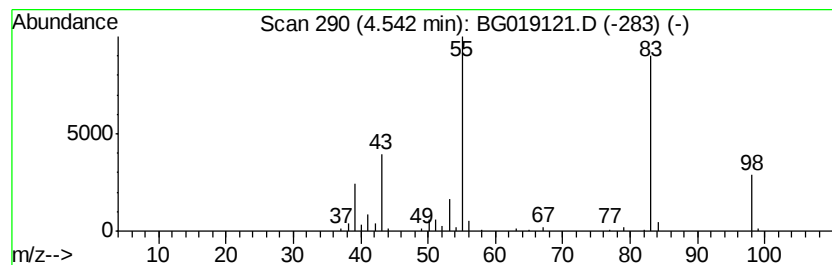
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	27.59 ng	126688	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
5		3-Hexen-2-one	98	C6H10O	000763-93-9	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019121.D
Acq On : 10 Oct 2015 17:27
Operator : UM/NP
Sample : PB86017BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB86017BL

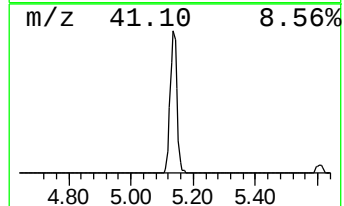
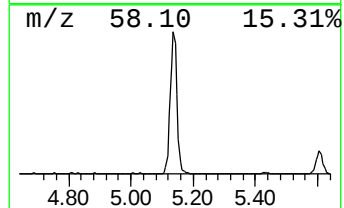
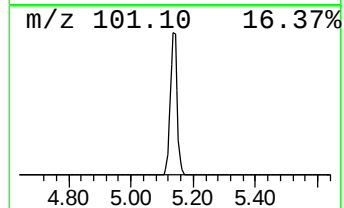
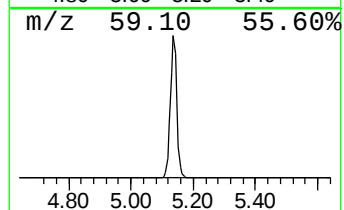
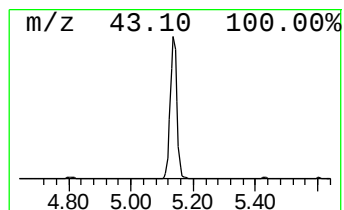
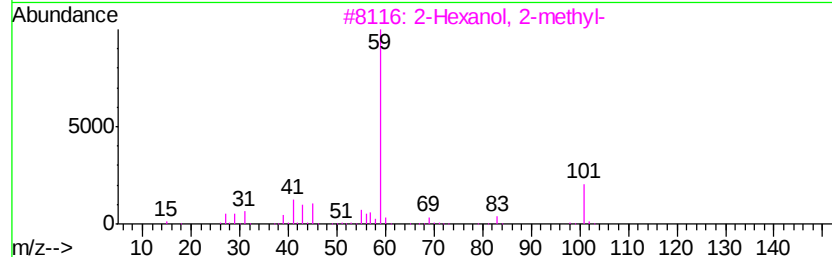
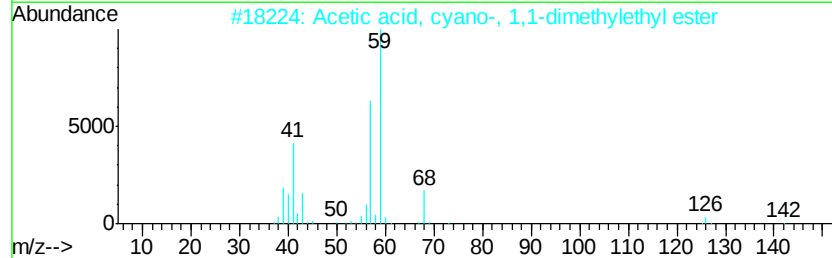
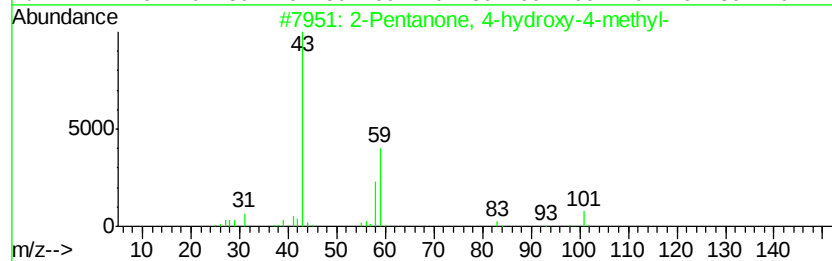
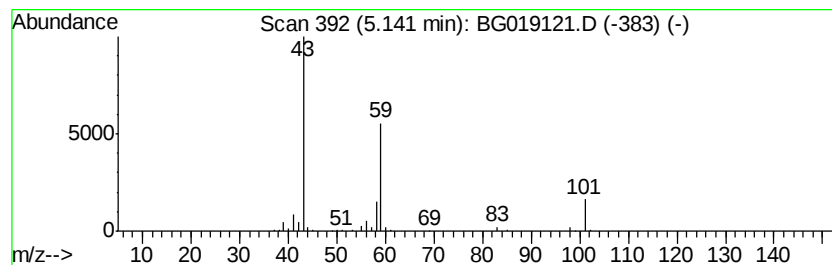
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	76.34 ng	350504	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019121.D
Acq On : 10 Oct 2015 17:27
Operator : UM/NP
Sample : PB86017BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB86017BL

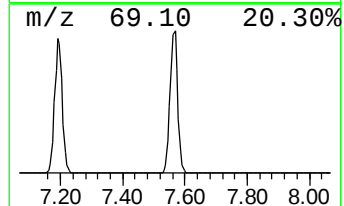
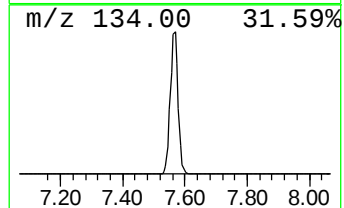
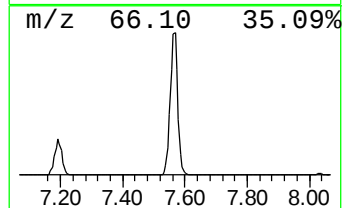
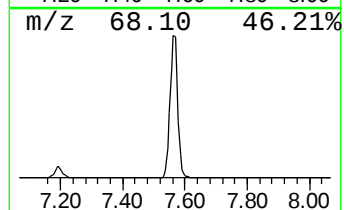
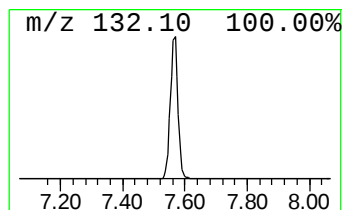
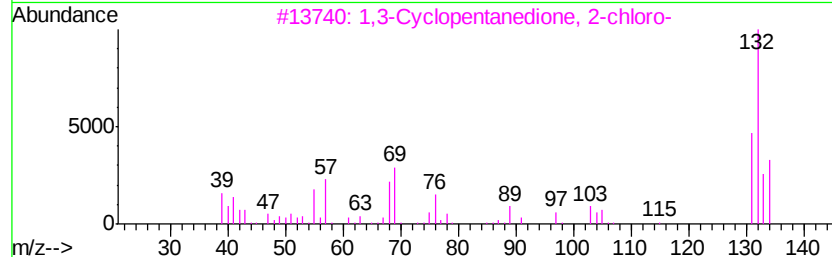
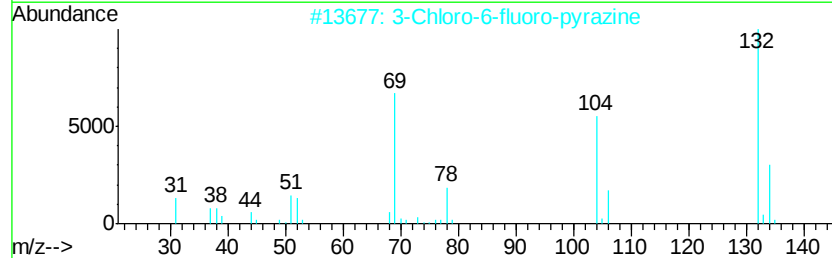
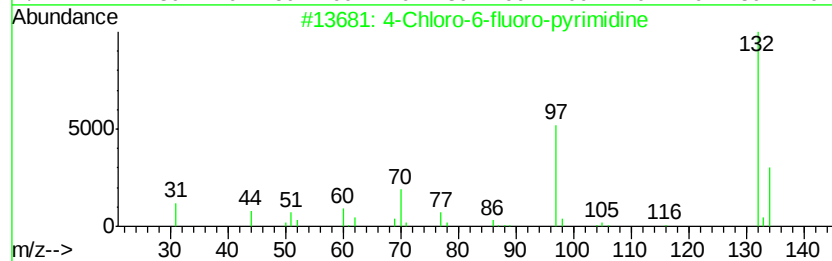
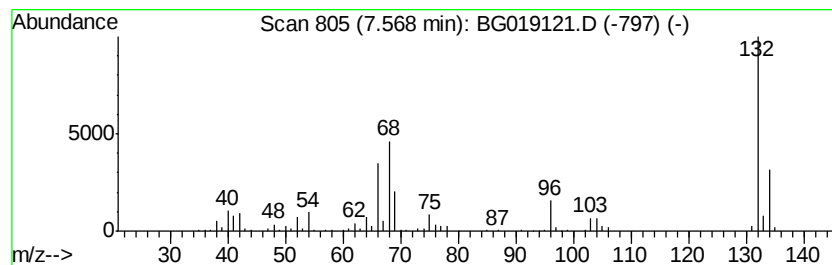
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	101.62 ng	466581	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019121.D
Acq On : 10 Oct 2015 17:27
Operator : UM/NP
Sample : PB86017BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB86017BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.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
Propane, 2,2-dime...	3.00	11.8	ng	54123	1	8.03	91831	20.0
3-Penten-2-one, 4...	4.54	27.6	ng	126688	1	8.03	91831	20.0
2-Pentanone, 4-hy...	5.14	76.3	ng	350504	1	8.03	91831	20.0
unknown7.57	7.57	101.6	ng	466581	1	8.03	91831	20.0