

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
 Data File : BF087661.D
 Acq On : 4 Jun 2016 12:43
 Operator : UM/SJ
 Sample : PB91039BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91039BL

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_F\METHODS\8270-BF060416.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	1.781	14	17	26	rVB	2323243	3203077	72.07%	9.437%
2	1.895	26	27	51	rVB	1793550	4444382	100.00%	13.094%
3	2.192	51	53	87	rVB3	87244	369972	8.32%	1.090%
4	3.850	195	198	201	rVB	29634	46044	1.04%	0.136%
5	5.050	301	303	308	rBV	138267	228196	5.13%	0.672%
6	5.461	336	339	341	rBV	2372340	2580272	58.06%	7.602%
7	6.479	425	428	431	rBV	1782993	2406039	54.14%	7.088%
8	6.627	438	441	443	rBV	2407963	2661732	59.89%	7.842%
9	6.856	459	461	464	rBV	949973	839154	18.88%	2.472%
10	7.016	472	475	477	rBV	2308212	2053684	46.21%	6.050%
11	7.416	507	510	513	rBV	1184663	1525066	34.31%	4.493%
12	8.147	571	574	576	rBV	1071665	1192910	26.84%	3.514%
13	9.222	665	668	671	rBV	2705175	2828794	63.65%	8.334%
14	9.896	724	727	730	rVB	1294380	1272944	28.64%	3.750%
15	10.685	793	796	798	rBV	1769356	1757915	39.55%	5.179%
16	11.382	854	857	859	rBV	1520585	1389905	31.27%	4.095%
17	12.971	993	996	998	rBV	2843340	2934448	66.03%	8.645%
18	14.011	1084	1087	1089	rBV	1407833	1234909	27.79%	3.638%
19	15.440	1209	1212	1215	rBV	805597	973461	21.90%	2.868%

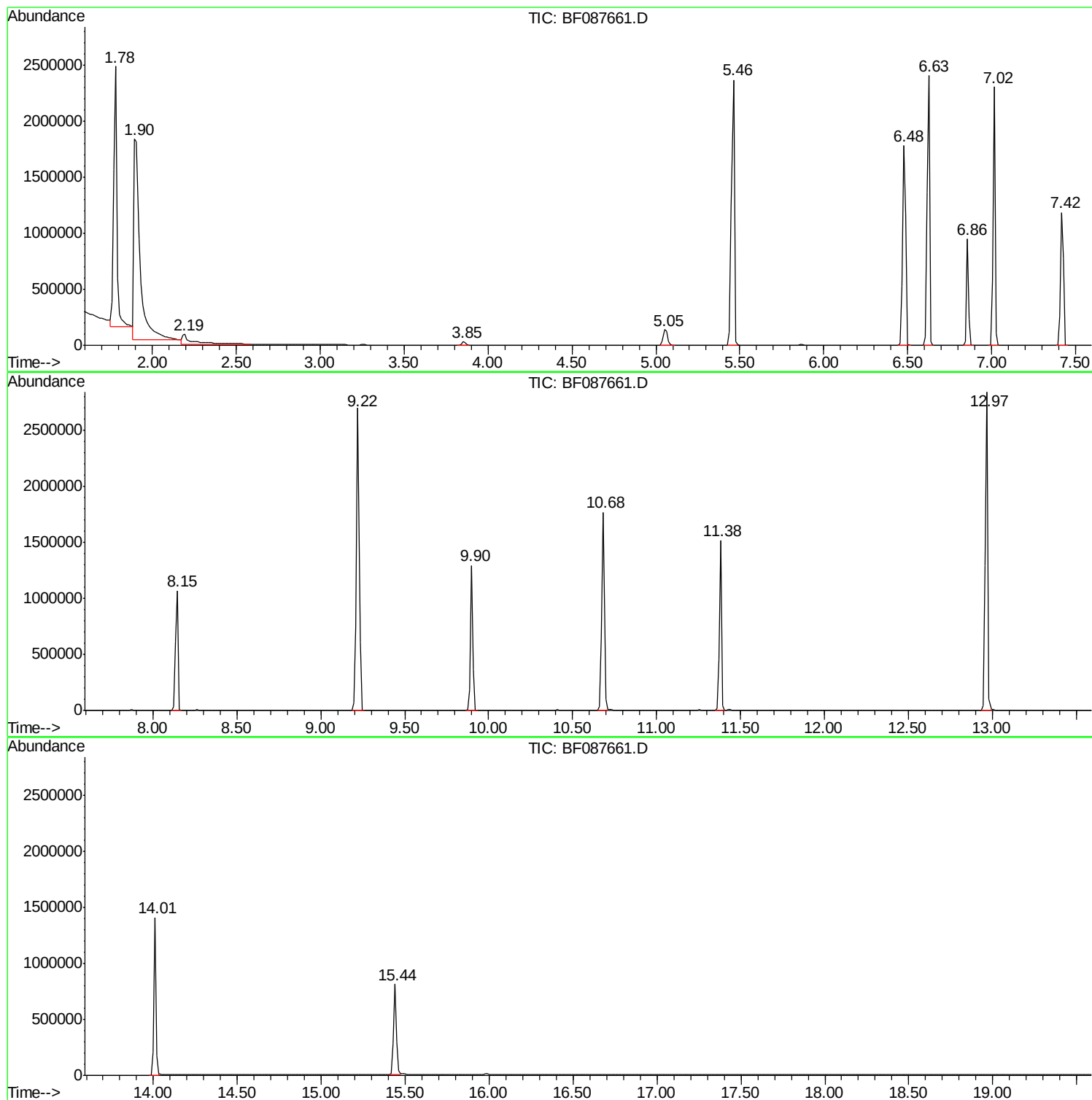
Sum of corrected areas: 33942904

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087661.D
Acq On : 4 Jun 2016 12:43
Operator : UM/SJ
Sample : PB91039BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91039BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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 F\DATA\BF060416\
Data File : BF087661.D
Acq On : 4 Jun 2016 12:43
Operator : UM/SJ
Sample : PB91039BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91039BL

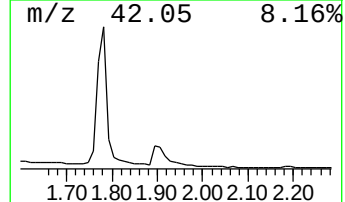
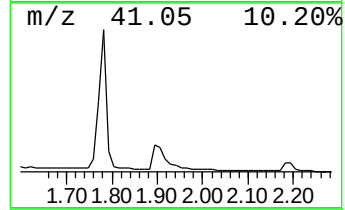
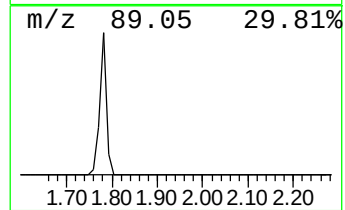
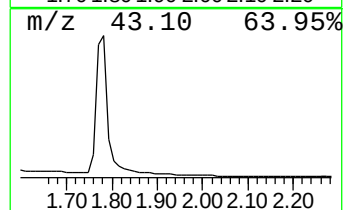
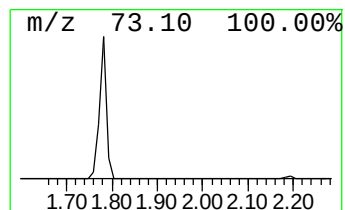
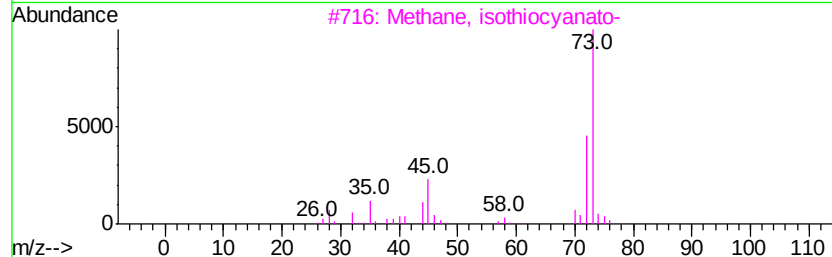
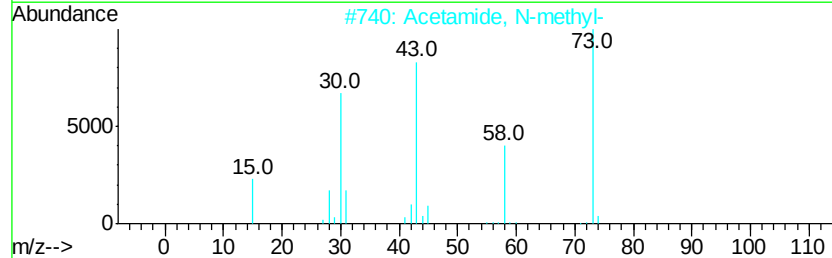
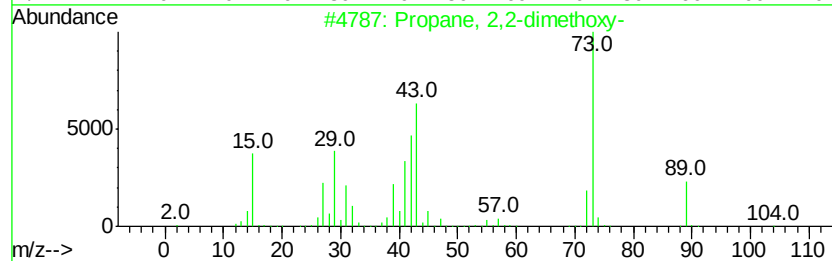
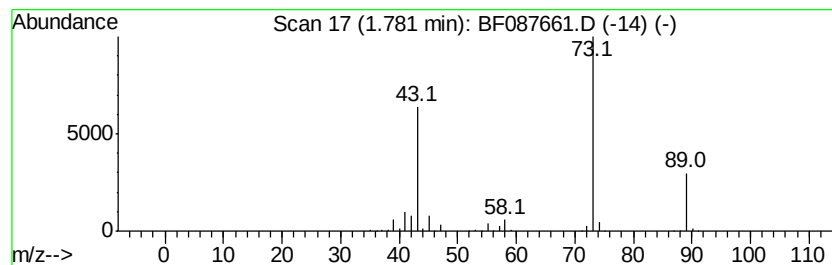
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.78 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	76.34 ng	3203080	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	27
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087661.D
Acq On : 4 Jun 2016 12:43
Operator : UM/SJ
Sample : PB91039BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91039BL

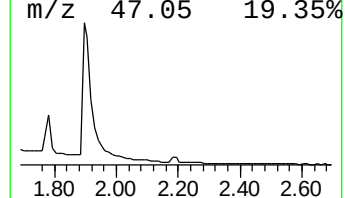
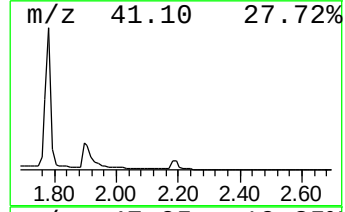
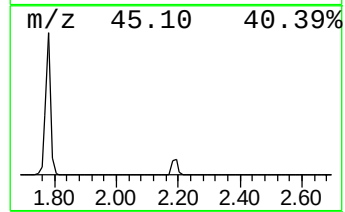
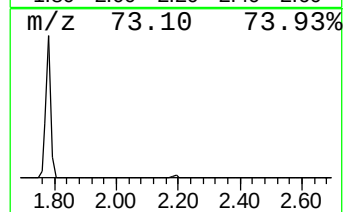
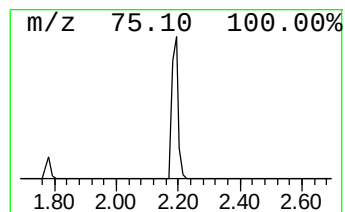
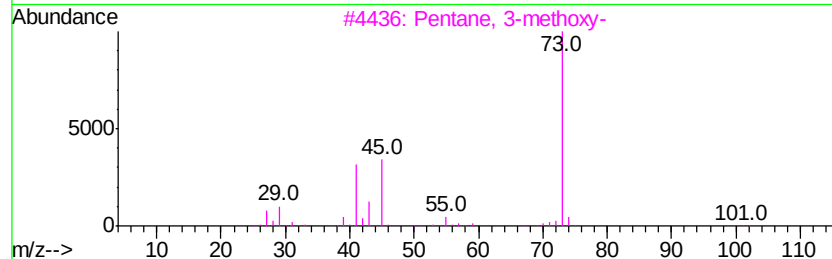
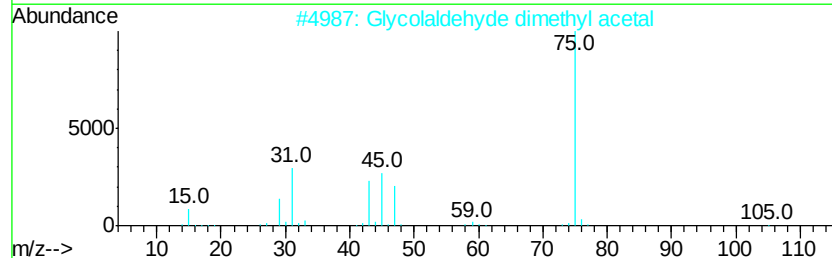
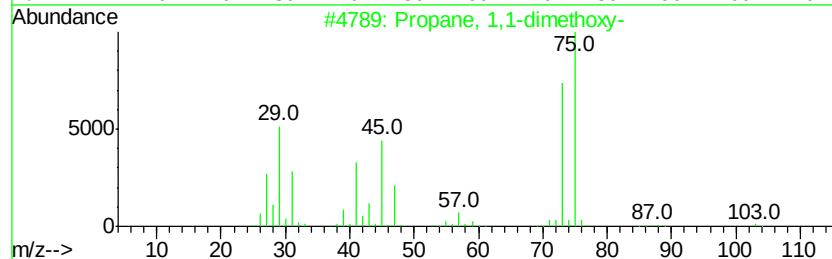
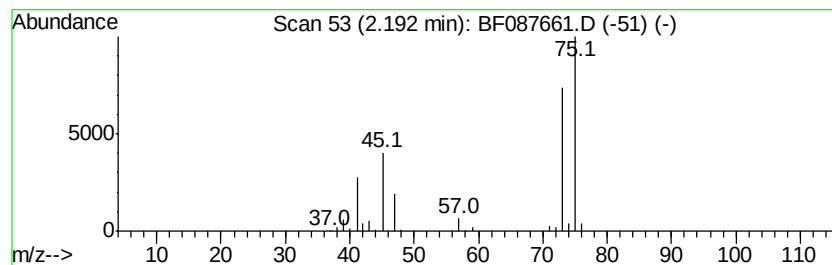
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	8.82 ng	369972	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087661.D
Acq On : 4 Jun 2016 12:43
Operator : UM/SJ
Sample : PB91039BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91039BL

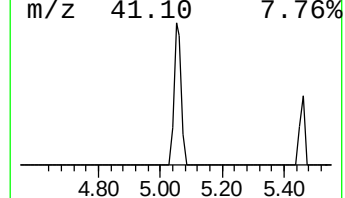
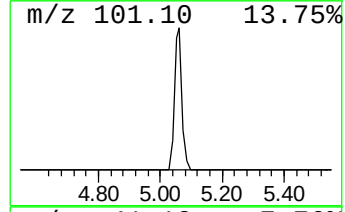
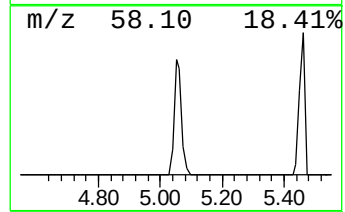
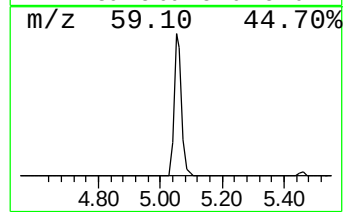
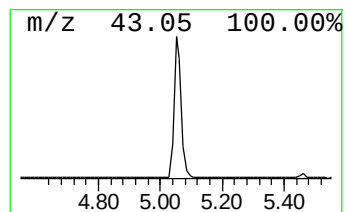
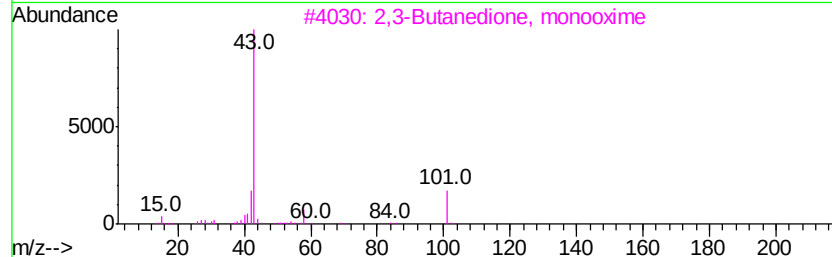
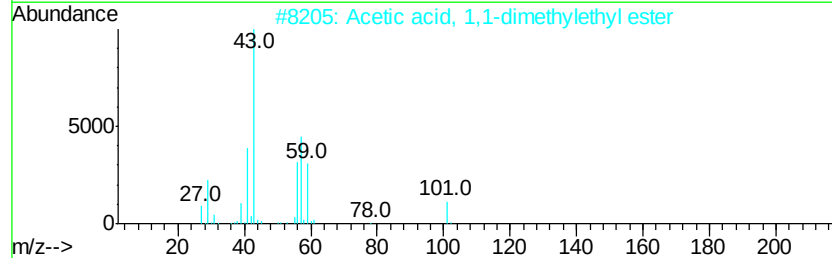
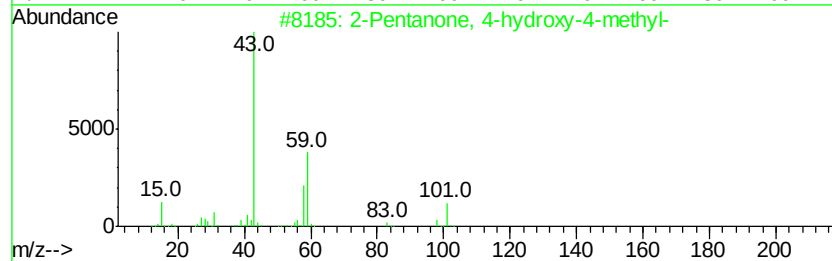
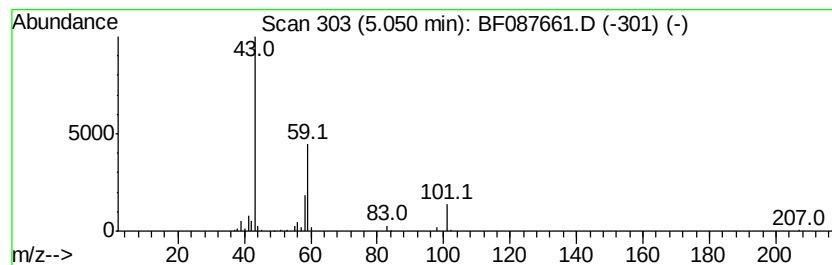
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	5.44 ng	228196	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		Acetone	58	C3H6O	000067-64-1	12
5		Diacetamide	101	C4H7NO2	000625-77-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087661.D
Acq On : 4 Jun 2016 12:43
Operator : UM/SJ
Sample : PB91039BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91039BL

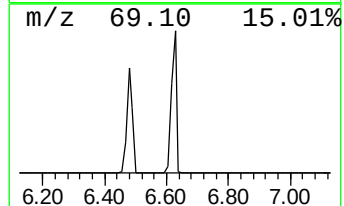
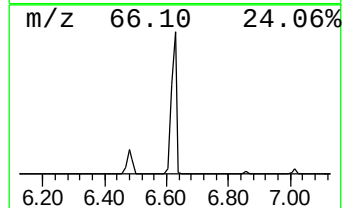
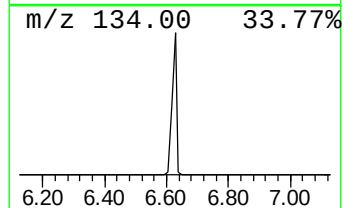
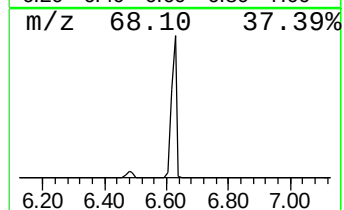
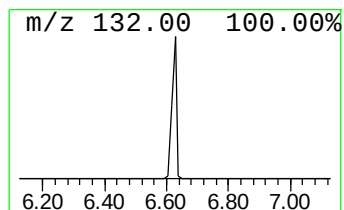
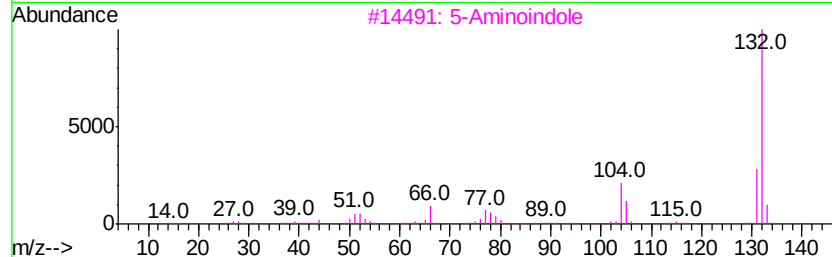
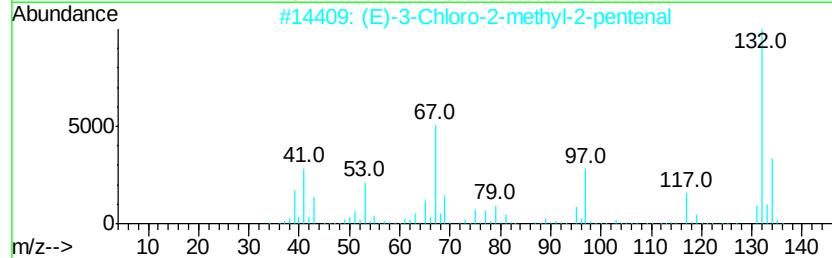
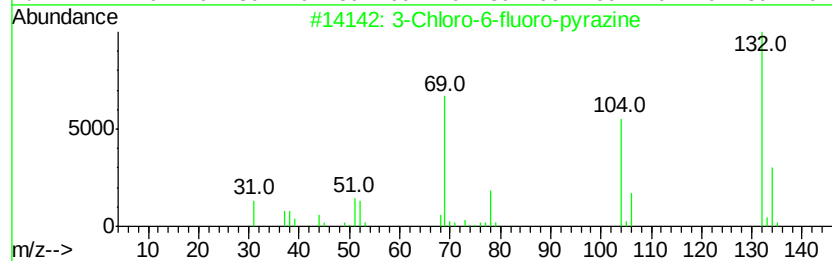
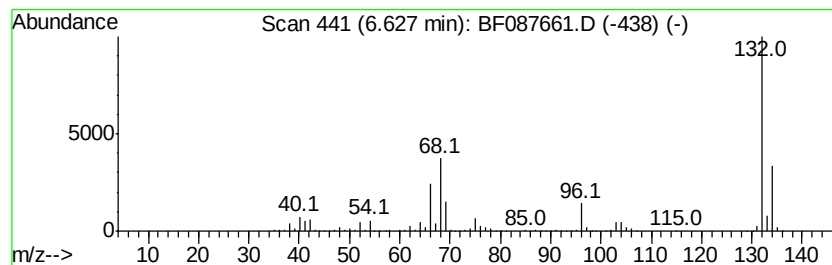
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	63.44 ng	2661730	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	25
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087661.D
Acq On : 4 Jun 2016 12:43
Operator : UM/SJ
Sample : PB91039BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91039BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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
unknown1.78	1.78	76.3	ng	3203080	1	6.86	839154	20.0
Propane, 1,1-dime...	2.19	8.8	ng	369972	1	6.86	839154	20.0
2-Pentanone, 4-hy...	5.05	5.4	ng	228196	1	6.86	839154	20.0
unknown6.63	6.63	63.4	ng	2661730	1	6.86	839154	20.0