

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093630.D
 Acq On : 14 Mar 2017 2:02
 Operator : SJ/MA
 Sample : I2199-22
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-89

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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	2.436	46	48	61	rVB	100090	230541	3.98%	0.477%
2	3.144	108	110	116	rBV	64391	174375	3.01%	0.361%
3	4.184	196	201	218	rBV2	333431	945744	16.31%	1.959%
4	4.401	218	220	224	rBV	81411	136933	2.36%	0.284%
5	4.870	259	261	277	rBV	879769	1646561	28.39%	3.410%
6	5.316	298	300	324	rBV	3717281	5499151	94.82%	11.388%
7	5.716	333	335	347	rVB	41987	91377	1.58%	0.189%
8	6.367	391	392	400	rBV	3278334	5018913	86.54%	10.394%
9	6.482	400	402	405	rVB	4786401	4906703	84.60%	10.162%
10	6.710	420	422	430	rVB	954983	1086822	18.74%	2.251%
11	6.859	433	435	438	rBV	3947542	3941719	67.96%	8.163%
12	7.282	470	472	485	rBV	3030696	3587279	61.85%	7.429%
13	8.002	532	535	544	rBV	1244927	1444332	24.90%	2.991%
14	9.076	626	629	632	rBV	3988572	5799662	100.00%	12.011%
15	9.762	686	689	691	rBV	1154229	1555185	26.82%	3.221%
16	10.551	756	758	761	rBV2	2303491	3088989	53.26%	6.397%
17	11.248	816	819	825	rBV	1663476	1606285	27.70%	3.327%
18	12.837	955	958	961	rBV	4622368	5294071	91.28%	10.964%
19	13.900	1049	1051	1060	rBV	971086	1368990	23.60%	2.835%
20	15.305	1171	1174	1182	rBV	558430	863416	14.89%	1.788%

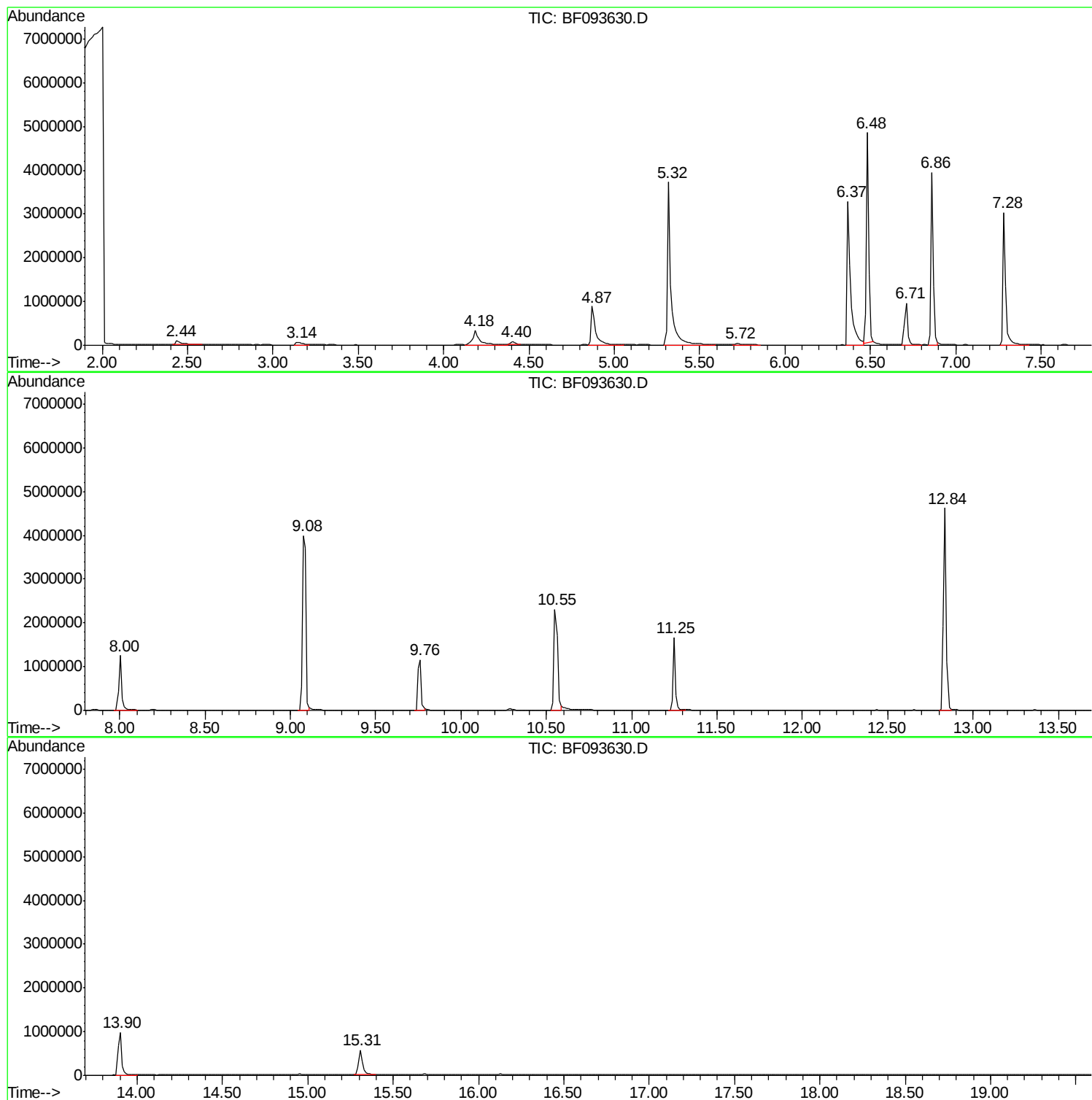
Sum of corrected areas: 48287048

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-89

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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 F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
D-89

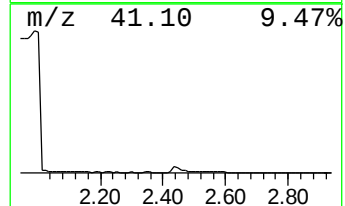
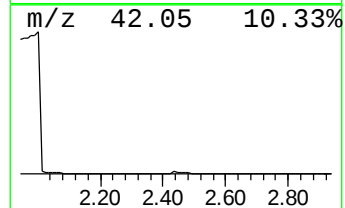
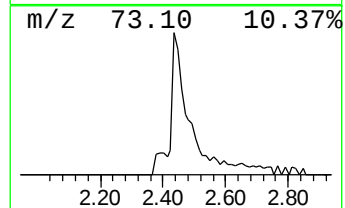
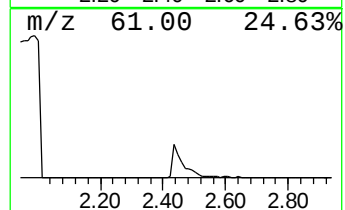
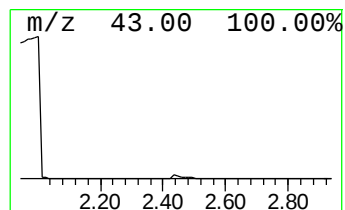
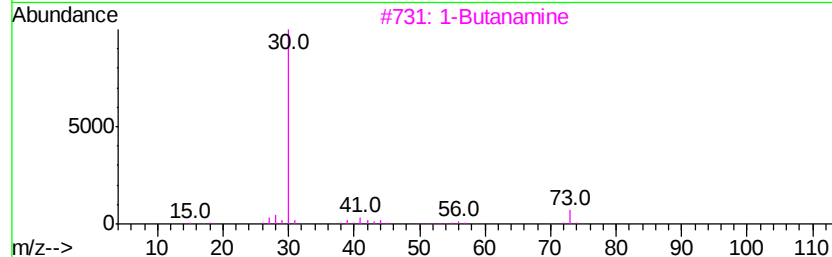
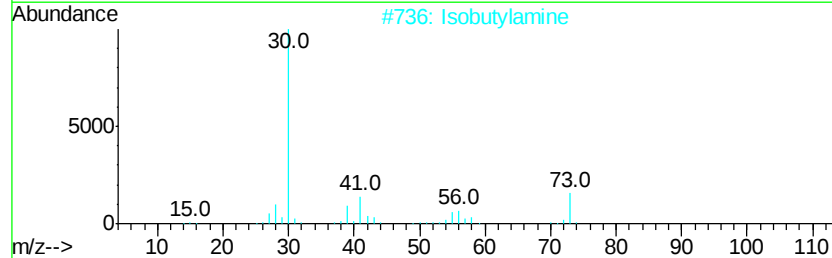
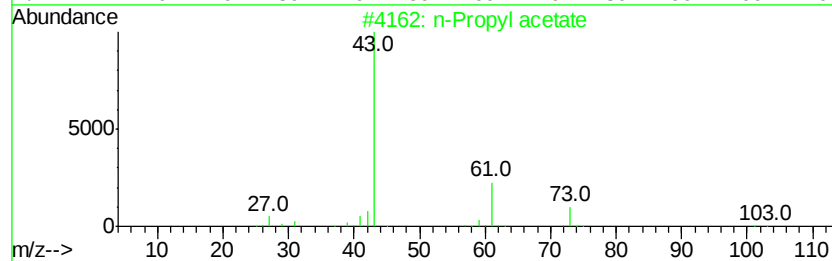
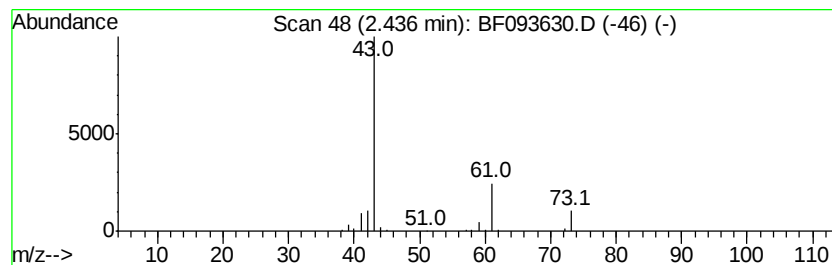
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	4.24 ng	230541	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83	
2	Isobutylamine	73	C4H11N	000078-81-9	5	
3	1-Butanamine	73	C4H11N	000109-73-9	5	
4	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5	
5	Butane, 2-methyl-	72	C5H12	000078-78-4	4	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
D-89

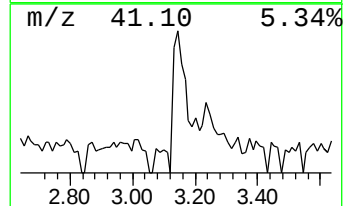
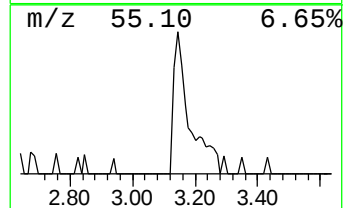
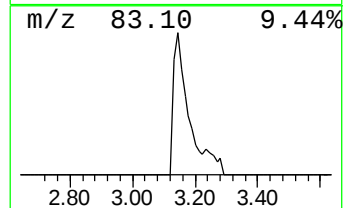
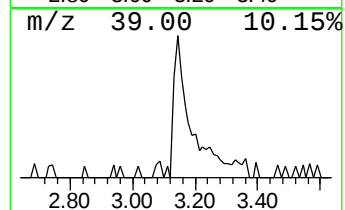
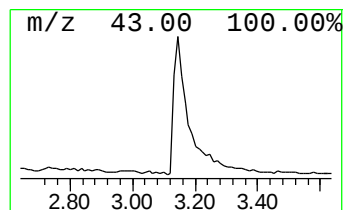
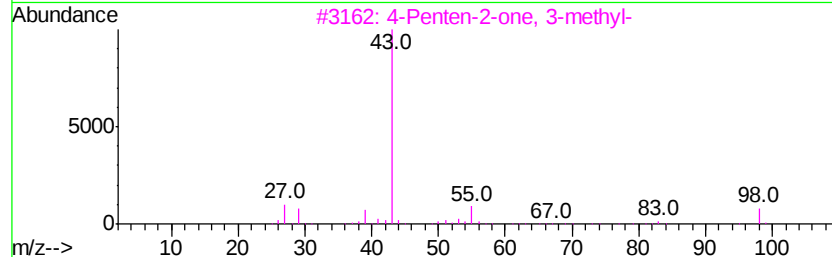
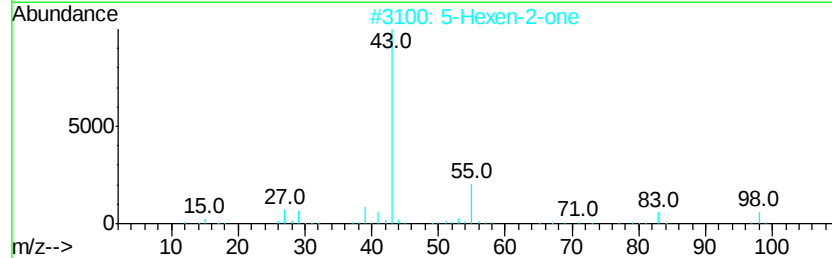
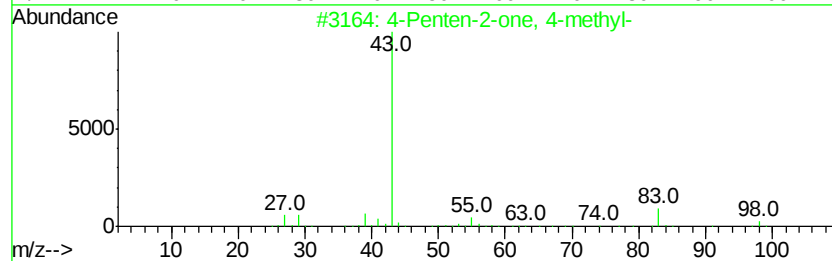
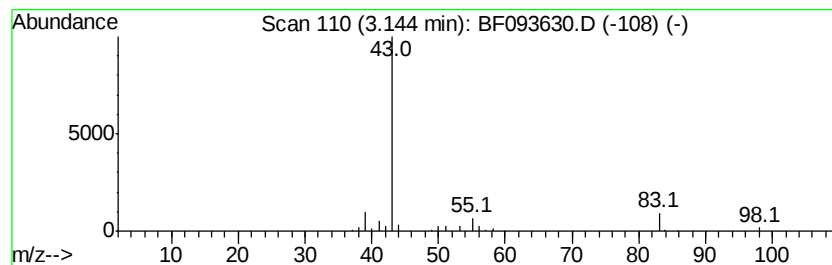
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	3.21 ng	174375	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2		5-Hexen-2-one	98	C6H10O	000109-49-9	37
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	32
4		4-Hexen-2-one	98	C6H10O	025659-22-7	9
5		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-89

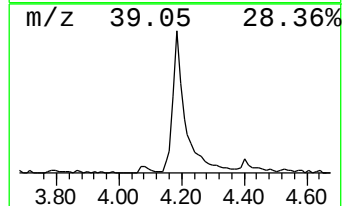
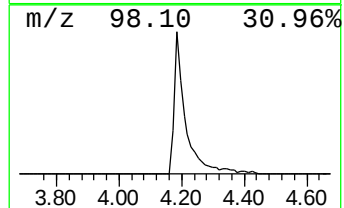
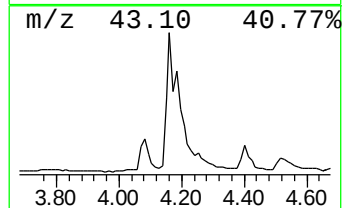
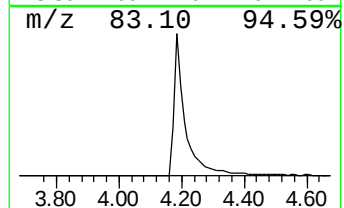
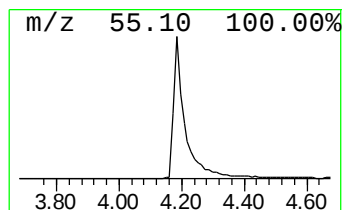
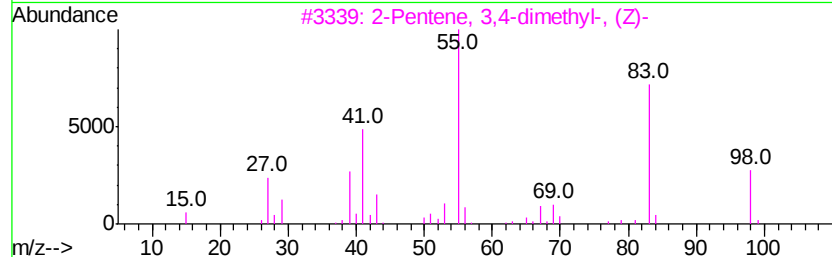
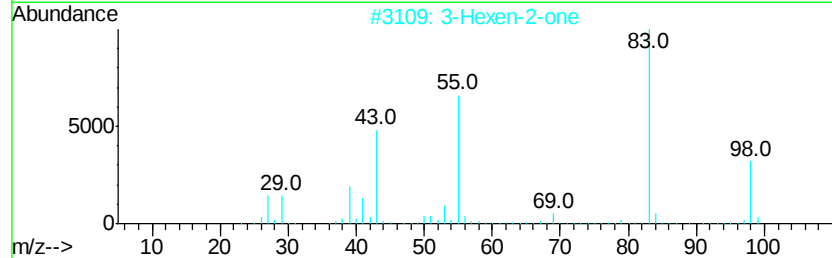
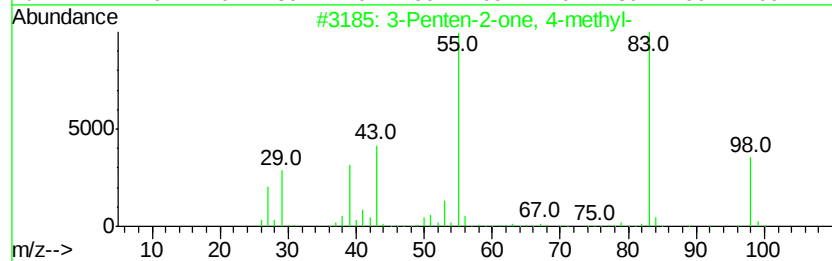
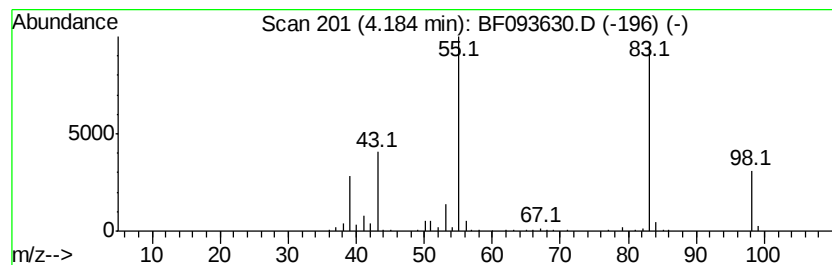
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	17.40 ng	945744	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleID :
D-89

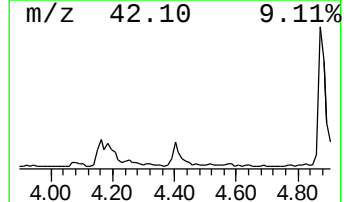
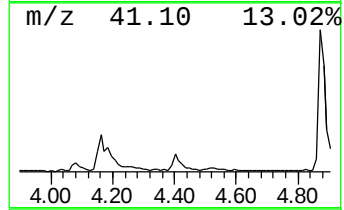
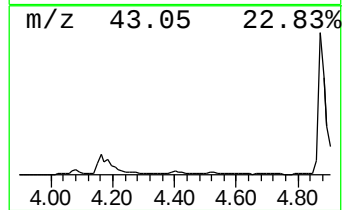
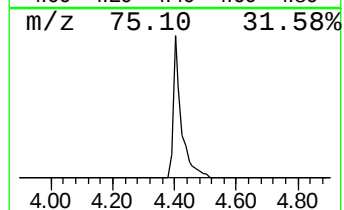
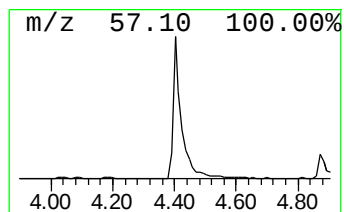
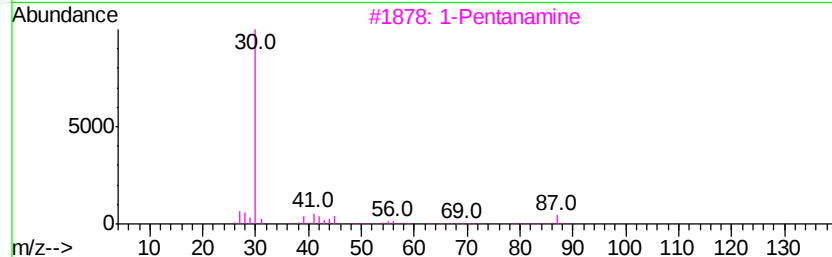
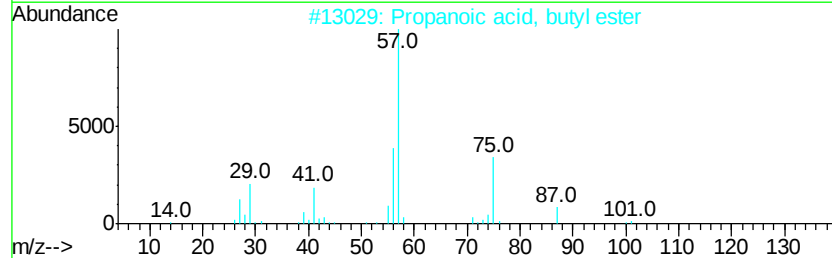
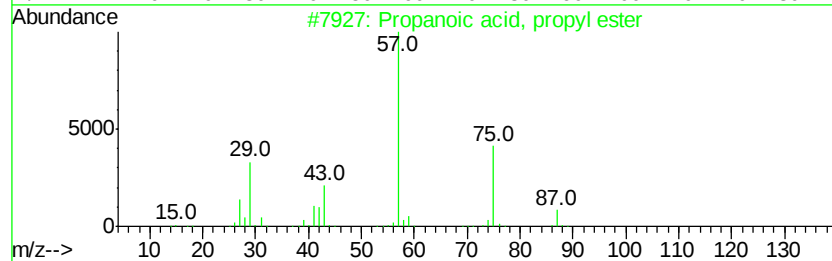
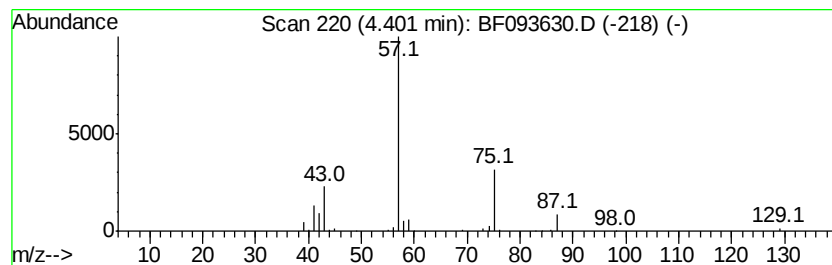
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	2.52 ng	136933	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36
3			1-Pentanamine	87	C5H13N	000110-58-7	9
4			1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	9
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-89

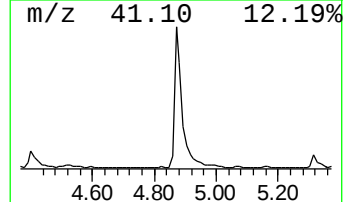
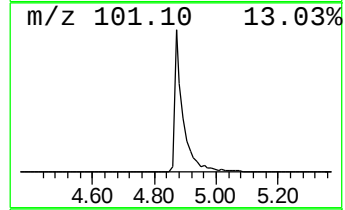
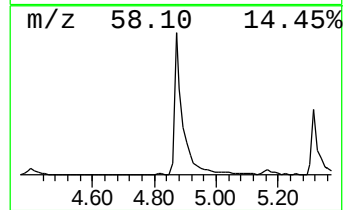
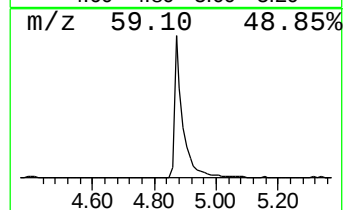
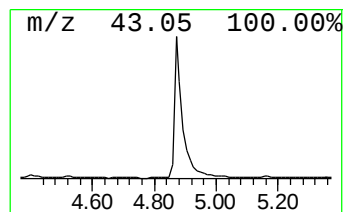
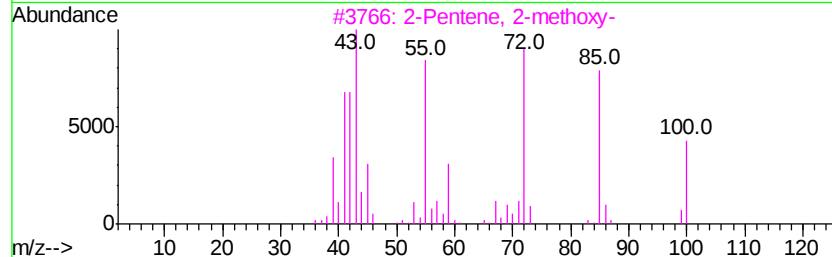
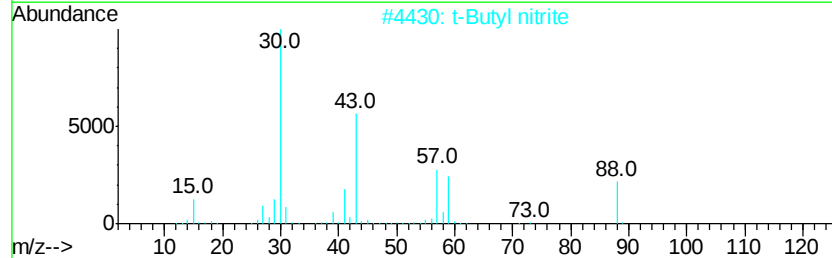
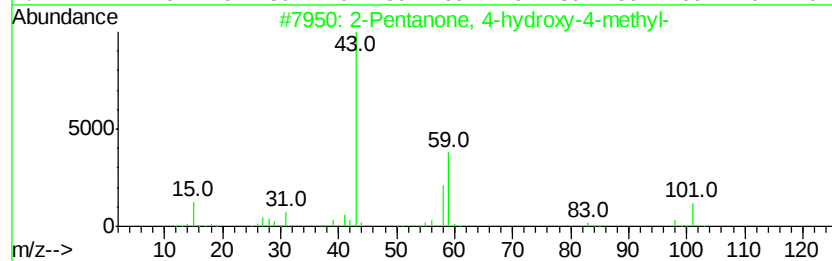
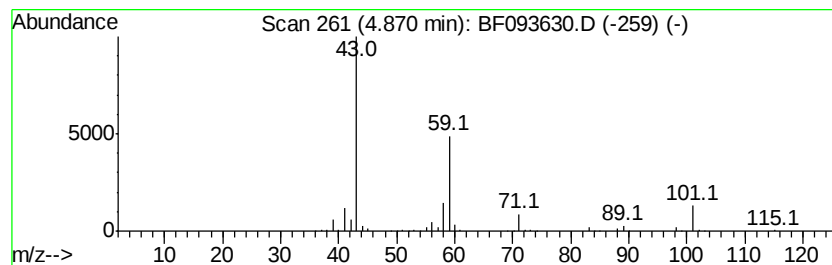
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	30.30 ng	1646560	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	59
2	t-Butyl nitrite	103	C4H9NO2		000540-80-7	38
3	2-Pentene, 2-methoxy-	100	C6H12O		061142-47-0	17
4	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2		000766-15-4	10
5	1,4-Butanediamine	88	C4H12N2		000110-60-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-89

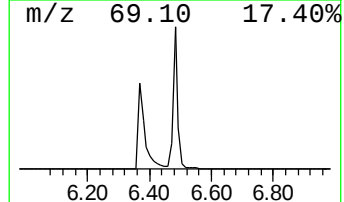
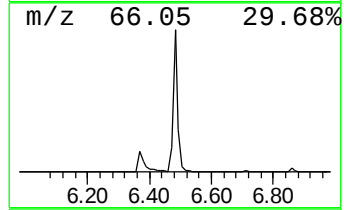
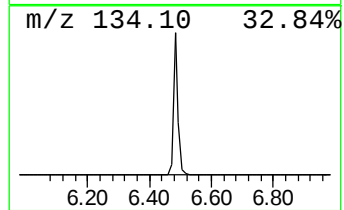
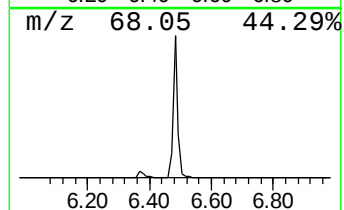
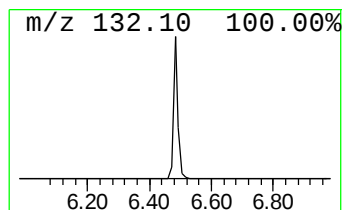
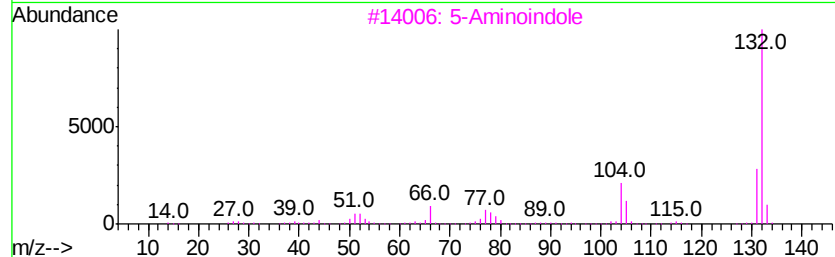
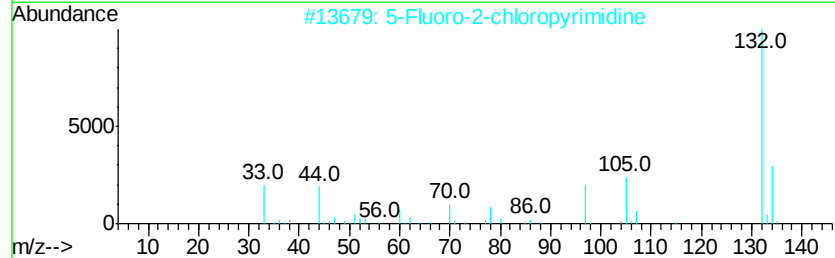
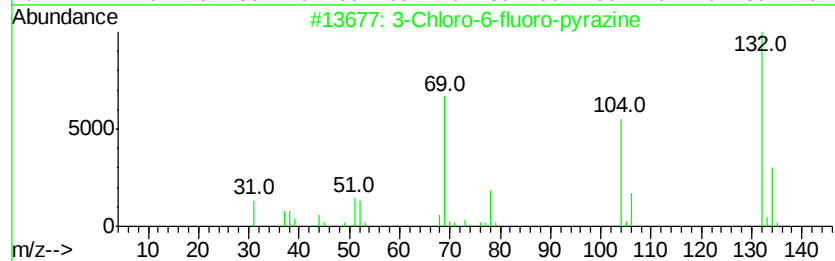
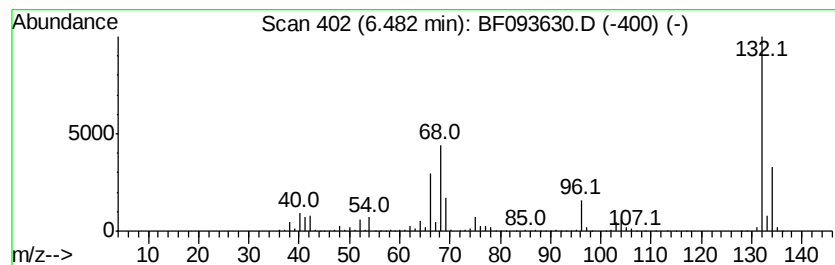
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	90.29 ng	4906700	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093630.D
Acq On : 14 Mar 2017 2:02
Operator : SJ/MA
Sample : I2199-22
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-89

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
n-Propyl acetate	2.44	4.2	ng	230541	1	6.71	1086820	20.0
4-Penten-2-one, 4...	3.14	3.2	ng	174375	1	6.71	1086820	20.0
3-Penten-2-one, 4...	4.18	17.4	ng	945744	1	6.71	1086820	20.0
Propanoic acid, p...	4.40	2.5	ng	136933	1	6.71	1086820	20.0
2-Pentanone, 4-hy...	4.87	30.3	ng	1646560	1	6.71	1086820	20.0
unknown6.48	6.48	90.3	ng	4906700	1	6.71	1086820	20.0