

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093617.D
 Acq On : 13 Mar 2017 19:45
 Operator : SJ/MA
 Sample : I2174-27
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-85

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	2.413	43	46	57	rVB	64286	180685	3.93%	0.464%
2	4.150	196	198	205	rVB	54561	89230	1.94%	0.229%
3	4.401	217	220	228	rBV	40775	85822	1.87%	0.220%
4	4.870	258	261	278	rBV	665377	1395171	30.35%	3.581%
5	5.316	298	300	327	rBV	2666646	4596827	100.00%	11.798%
6	5.716	333	335	349	rVB	48355	101336	2.20%	0.260%
7	6.367	390	392	400	rBV	3215695	4228612	91.99%	10.853%
8	6.482	400	402	405	rVB	4332475	4231704	92.06%	10.861%
9	6.710	419	422	427	rBV	876016	918792	19.99%	2.358%
10	6.859	433	435	438	rBV	3271508	3313544	72.08%	8.505%
11	7.282	470	472	487	rBV	2785809	3066671	66.71%	7.871%
12	8.002	532	535	548	rBV	1115979	1244778	27.08%	3.195%
13	9.076	627	629	632	rBV	3536785	4505825	98.02%	11.565%
14	9.762	686	689	691	rBV	1050002	1295203	28.18%	3.324%
15	10.551	756	758	761	rBV2	2032417	2474142	53.82%	6.350%
16	11.248	817	819	825	rBV	1414924	1345317	29.27%	3.453%
17	12.836	955	958	960	rBV	4057900	4149955	90.28%	10.651%
18	13.899	1048	1051	1060	rBV	700853	989903	21.53%	2.541%
19	15.305	1171	1174	1184	rBV	503289	747857	16.27%	1.919%

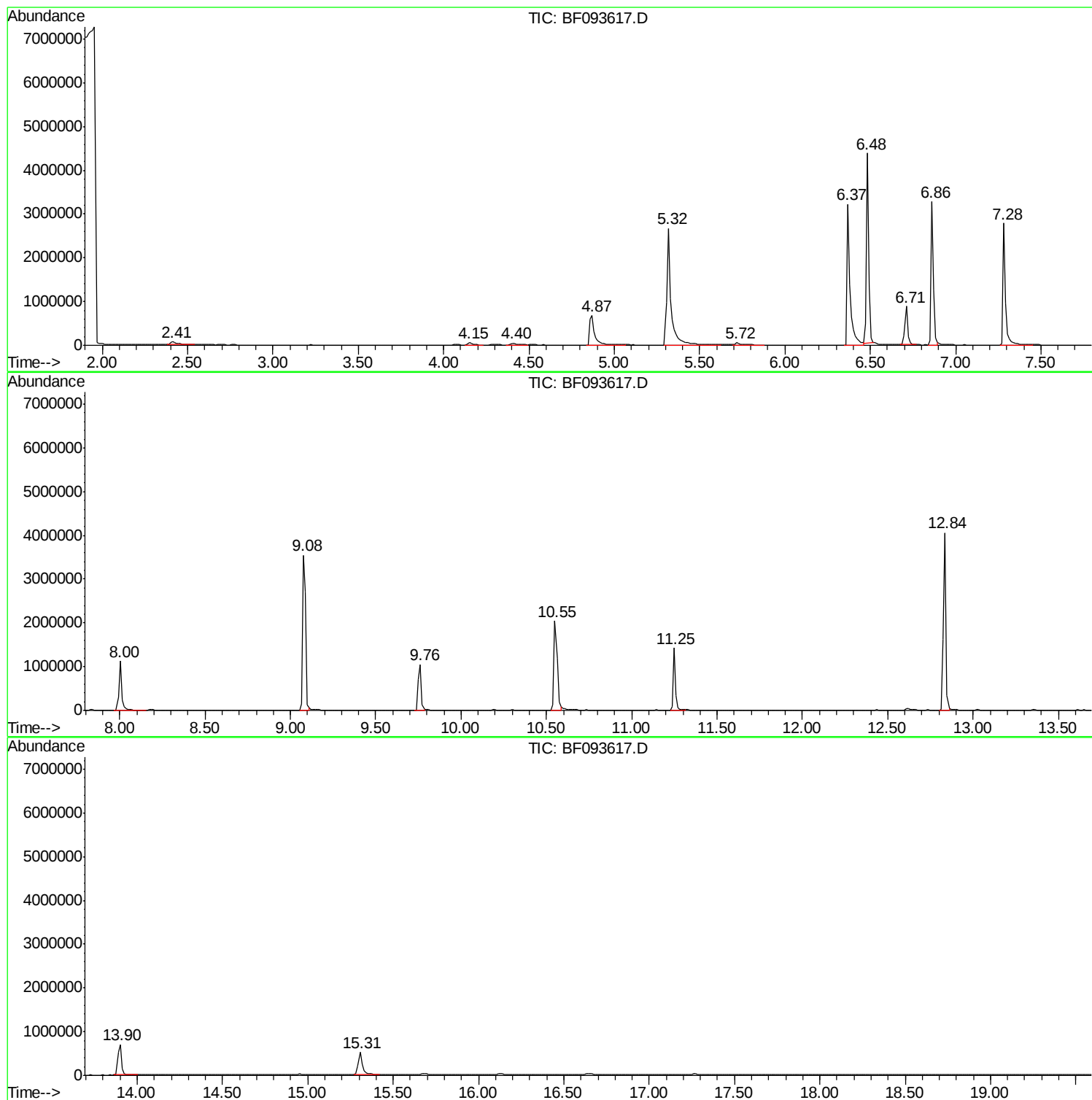
Sum of corrected areas: 38961374

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093617.D
Acq On : 13 Mar 2017 19:45
Operator : SJ/MA
Sample : I2174-27
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-85

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 : BF093617.D
Acq On : 13 Mar 2017 19:45
Operator : SJ/MA
Sample : I2174-27
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
D-85

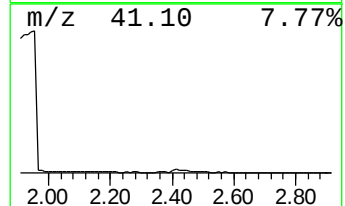
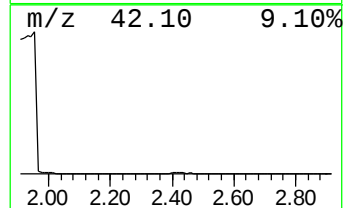
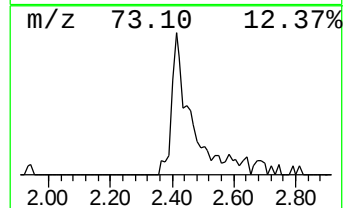
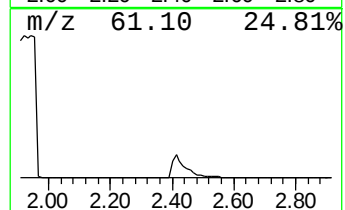
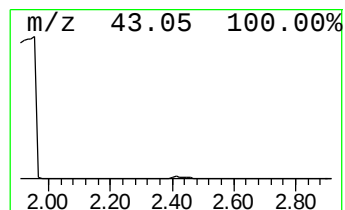
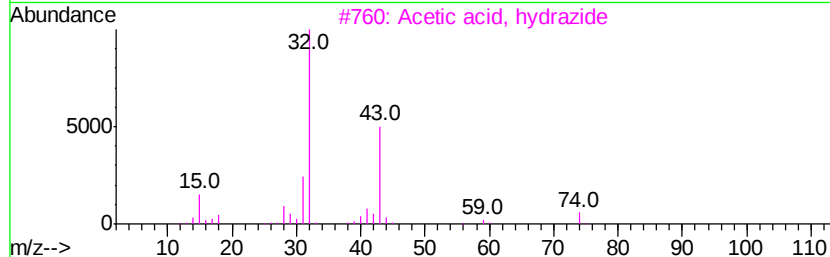
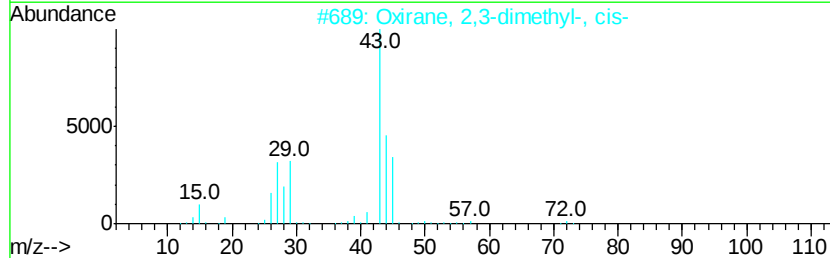
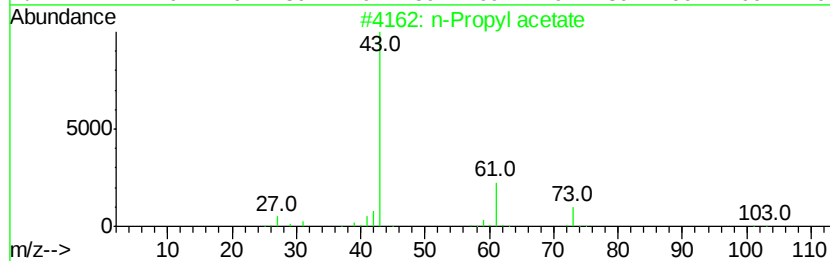
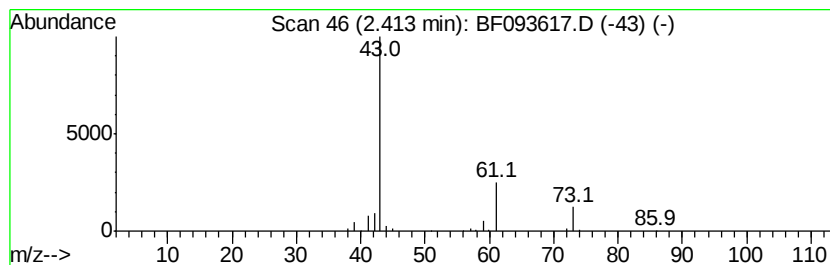
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.41	3.93 ng	180685	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	9
3		Acetic acid, hvdrazide	74	C2H6N2O	001068-57-1	9
4		1-Butanamine	73	C4H11N	000109-73-9	7
5		Isobutylamine	73	C4H11N	000078-81-9	7



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093617.D
Acq On : 13 Mar 2017 19:45
Operator : SJ/MA
Sample : I2174-27
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-85

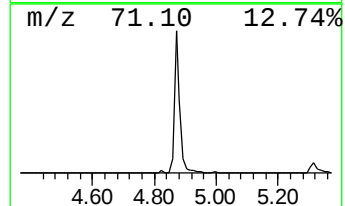
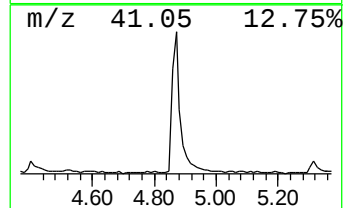
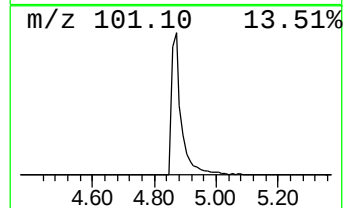
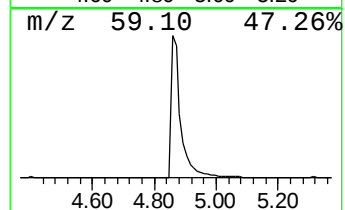
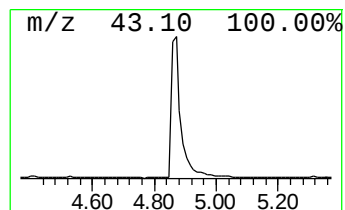
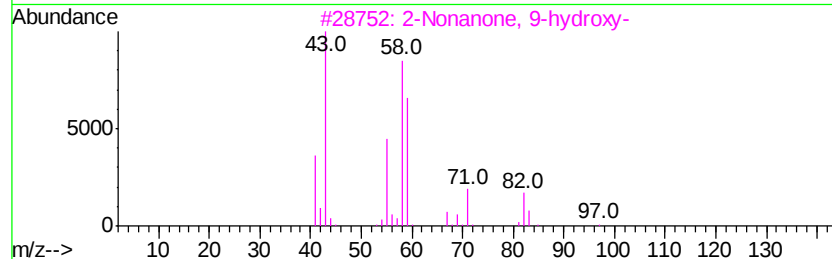
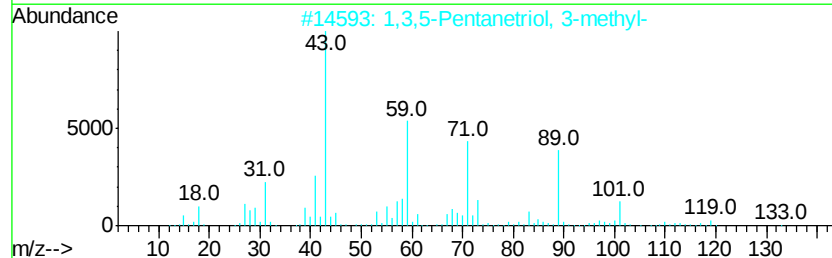
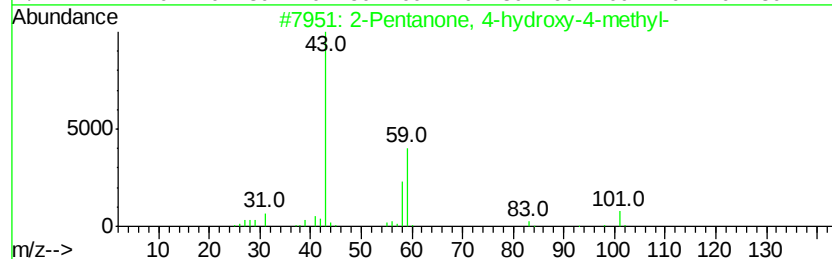
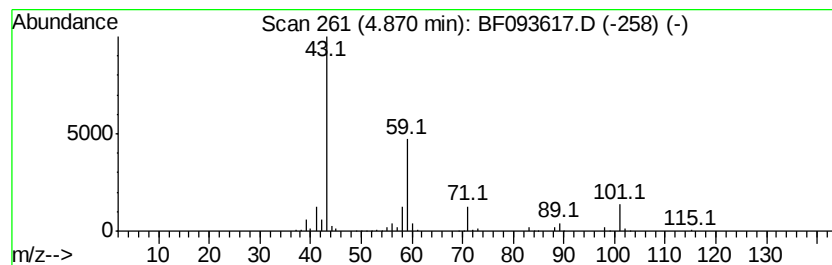
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	30.37 ng	1395170	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
3		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
4		1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093617.D
Acq On : 13 Mar 2017 19:45
Operator : SJ/MA
Sample : I2174-27
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-85

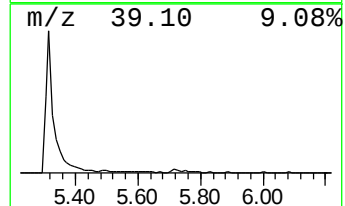
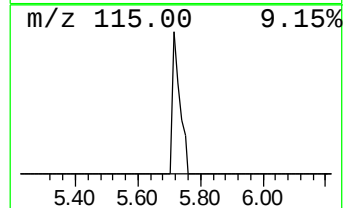
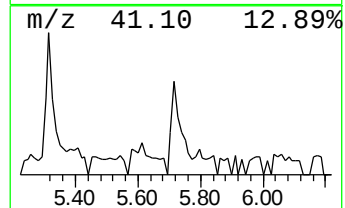
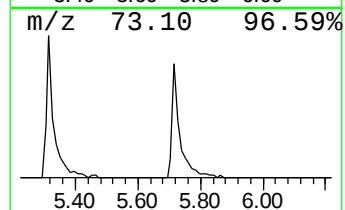
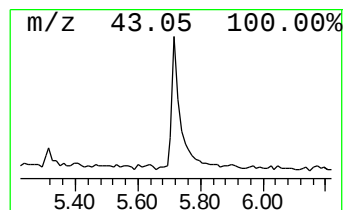
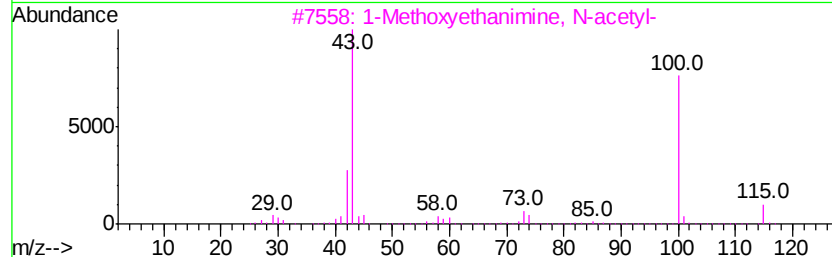
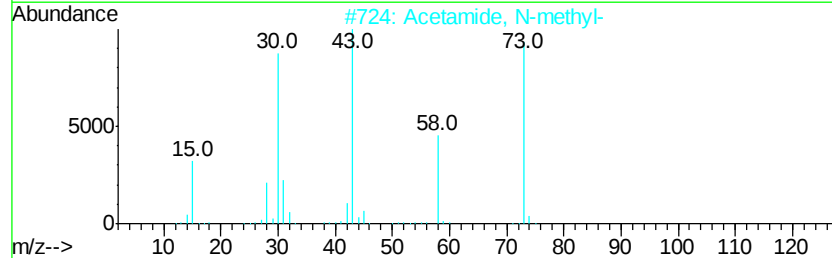
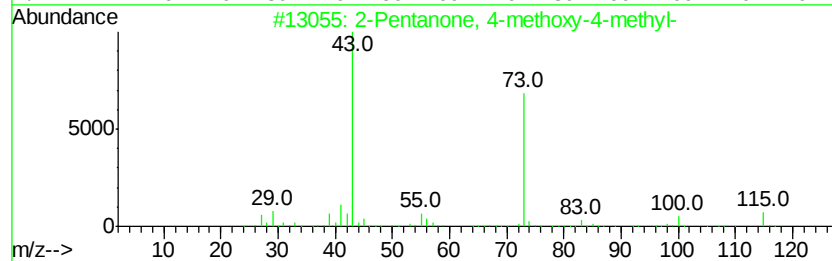
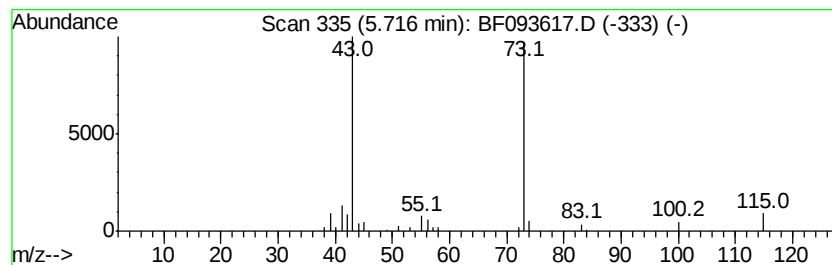
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.21 ng	101336	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	32
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
5		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093617.D
Acq On : 13 Mar 2017 19:45
Operator : SJ/MA
Sample : I2174-27
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-85

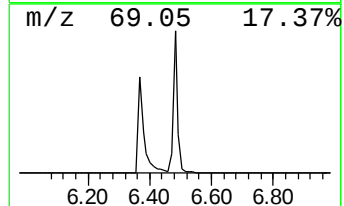
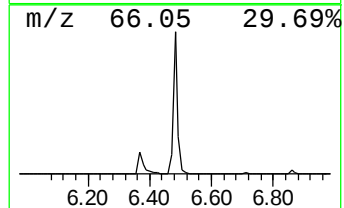
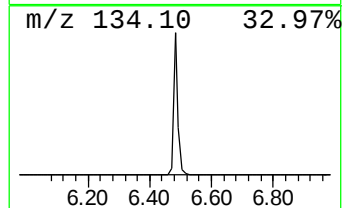
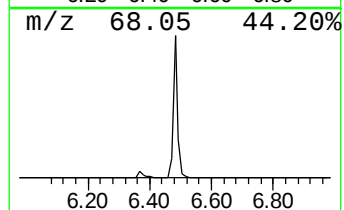
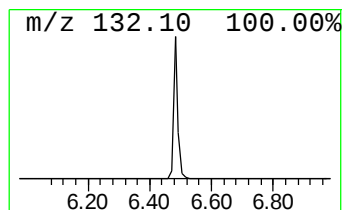
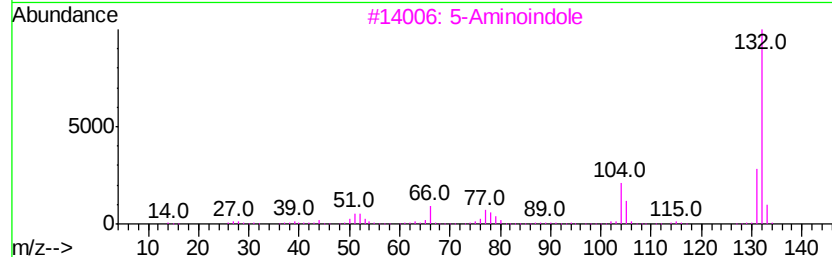
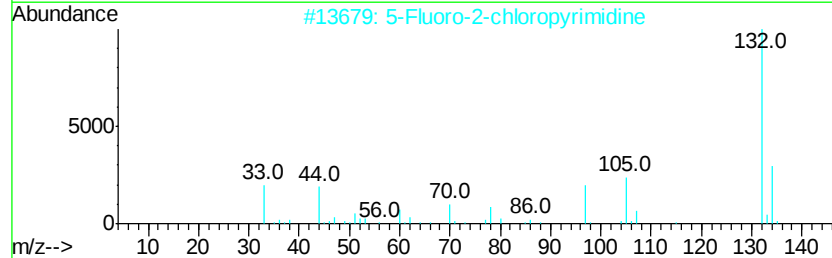
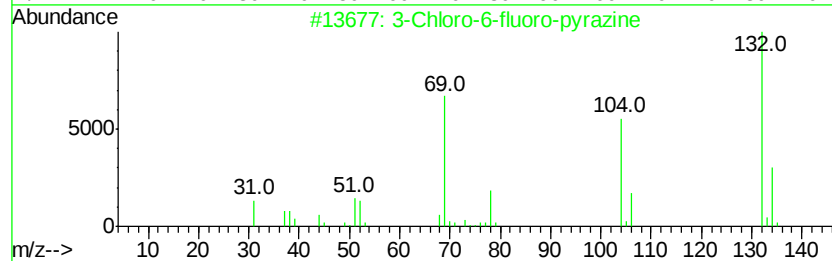
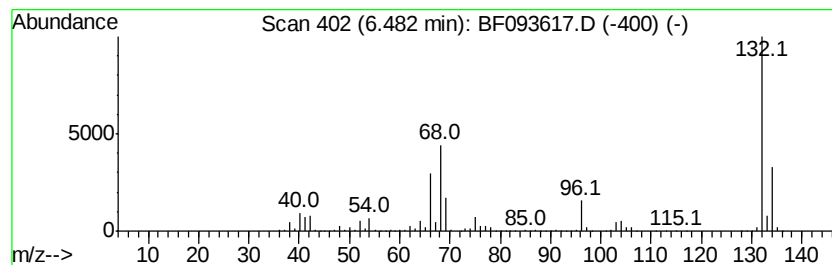
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	92.11 ng	4231700	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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093617.D
Acq On : 13 Mar 2017 19:45
Operator : SJ/MA
Sample : I2174-27
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-85

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	2.41	3.9	ng	180685	1	6.71	918792	20.0
2-Pentanone, 4-hy...	4.87	30.4	ng	1395170	1	6.71	918792	20.0
2-Pentanone, 4-me...	5.72	2.2	ng	101336	1	6.71	918792	20.0
unknown6.48	6.48	92.1	ng	4231700	1	6.71	918792	20.0