

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070715\
 Data File : BF080375.D
 Acq On : 7 Jul 2015 16:49
 Operator : TP/UM
 Sample : PB84384BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84384BL

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-BF070615.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	2.213	8	11	29	rVB	344425	793066	63.74%	8.535%
2	2.441	29	31	41	rVB	14265	35004	2.81%	0.377%
3	4.841	239	241	247	rVB	22782	24633	1.98%	0.265%
4	5.436	290	293	295	rBV	540047	517552	41.59%	5.570%
5	5.836	325	328	330	rBV	925997	798609	64.18%	8.595%
6	6.236	361	363	365	rBV	49980	40593	3.26%	0.437%
7	6.830	413	415	418	rBV	823567	755495	60.72%	8.131%
8	6.990	427	429	432	rBV	960683	834370	67.06%	8.980%
9	7.230	448	450	452	rBB	212013	175392	14.10%	1.888%
10	7.390	462	464	466	rBV	676852	659102	52.97%	7.093%
11	7.779	496	498	501	rBV	368773	444790	35.75%	4.787%
12	8.522	561	563	565	rBV	223966	220844	17.75%	2.377%
13	9.596	655	657	659	rBV	1360294	1077514	86.60%	11.596%
14	10.282	716	717	720	rBB	180443	244990	19.69%	2.637%
15	11.082	785	787	789	rBV	674358	579819	46.60%	6.240%
16	11.814	848	851	853	rBV	336695	280678	22.56%	3.021%
17	13.619	1006	1009	1011	rBV	1118983	1244289	100.00%	13.391%
18	14.991	1126	1129	1132	rBV	239518	291812	23.45%	3.141%
19	16.968	1299	1302	1305	rBV	183164	273276	21.96%	2.941%

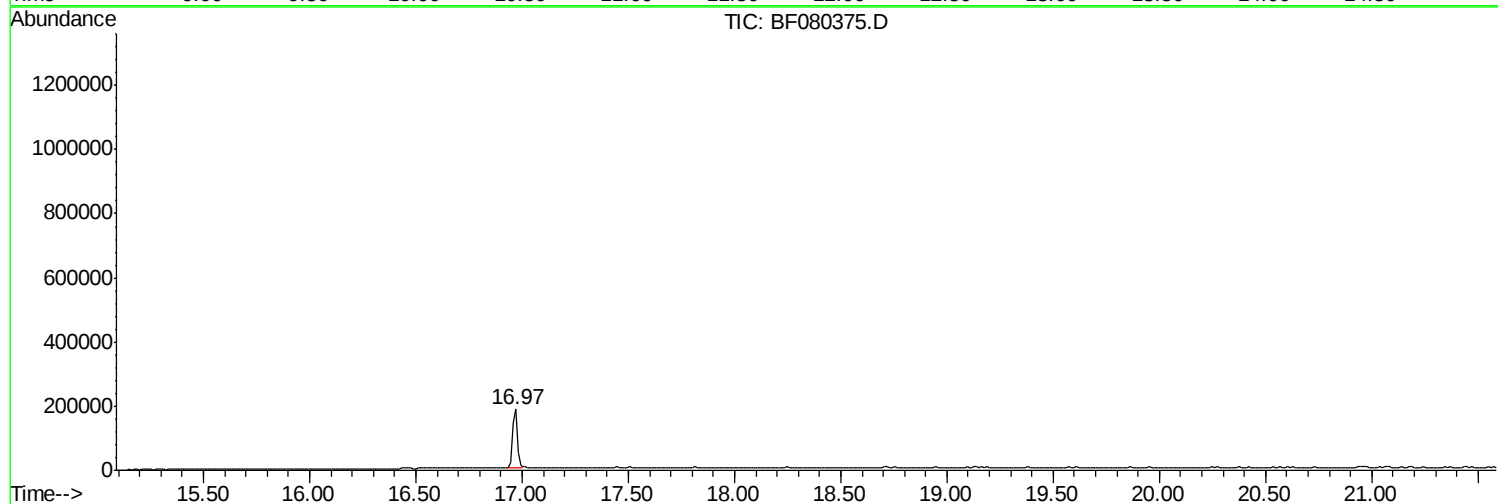
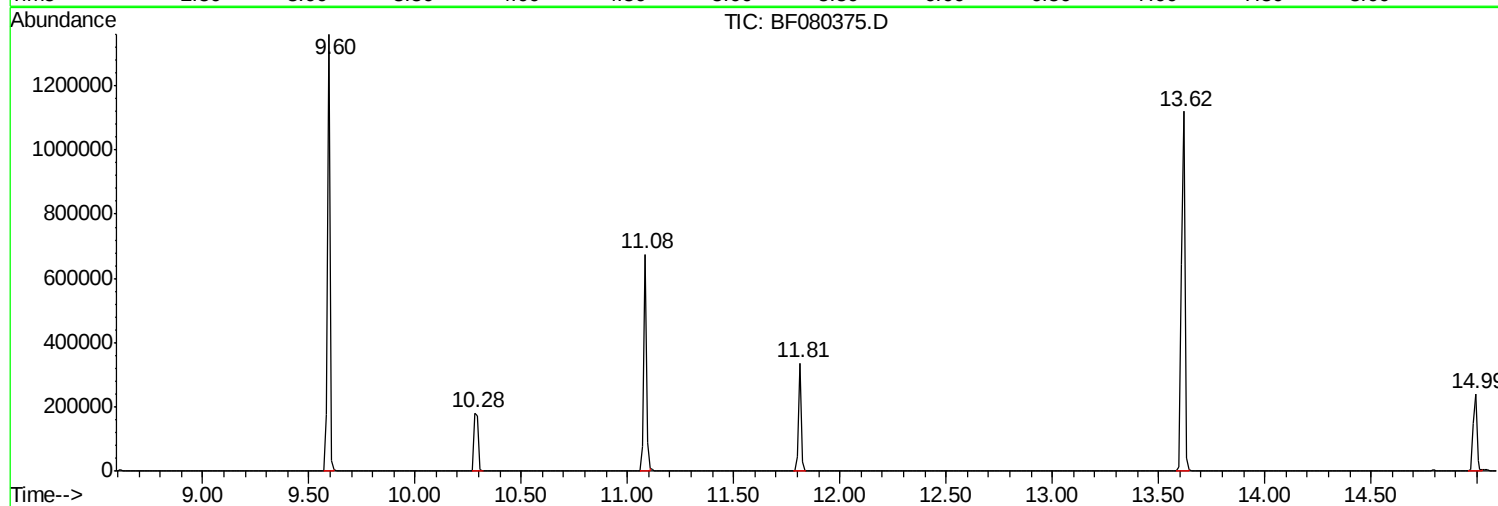
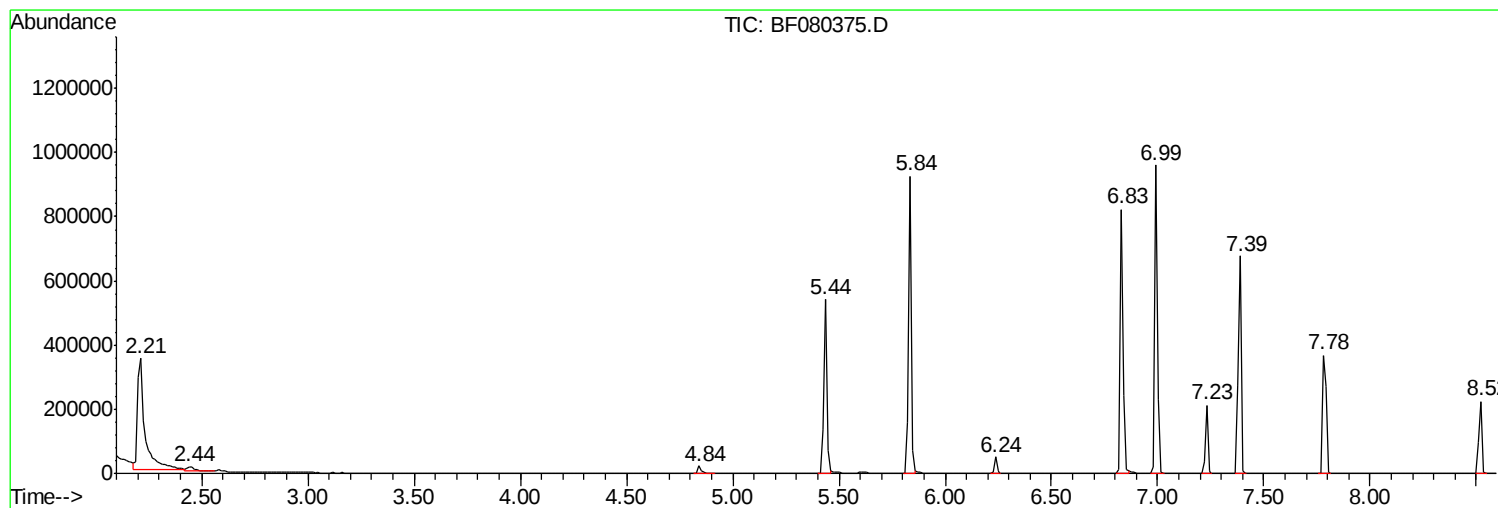
Sum of corrected areas: 9291828

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070715\
Data File : BF080375.D
Acq On : 7 Jul 2015 16:49
Operator : TP/UM
Sample : PB84384BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84384BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.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\BF070715\
Data File : BF080375.D
Acq On : 7 Jul 2015 16:49
Operator : TP/UM
Sample : PB84384BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB84384BL

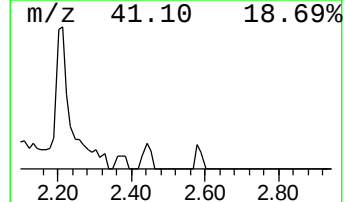
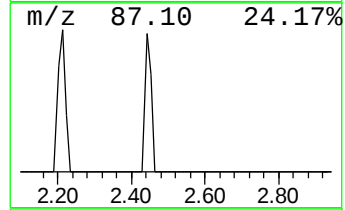
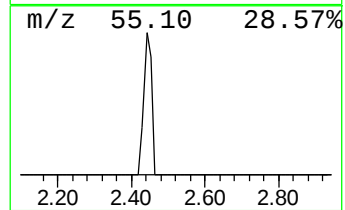
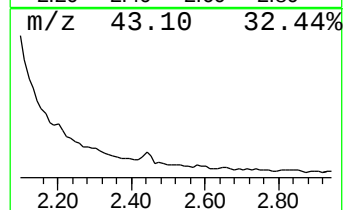
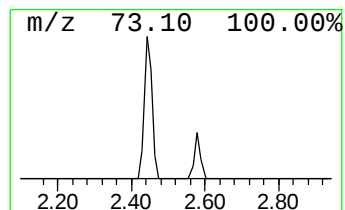
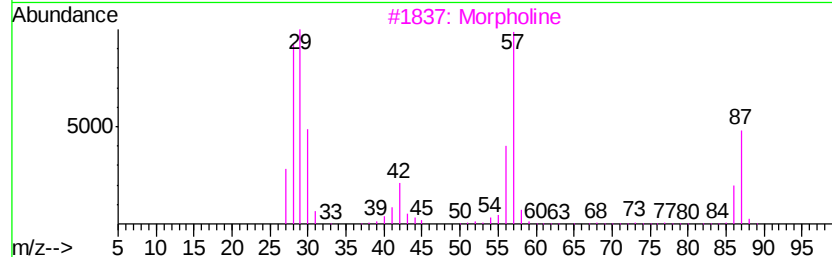
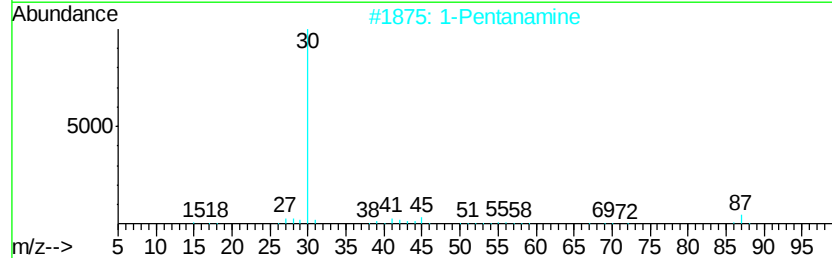
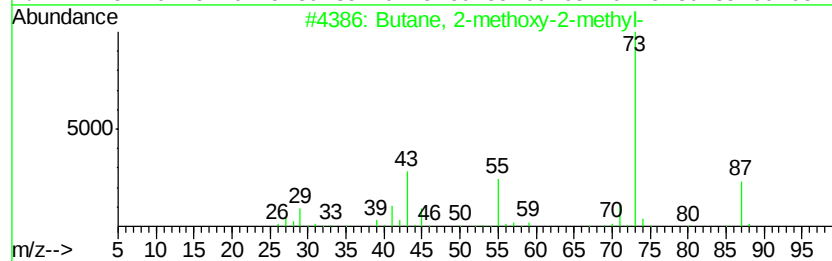
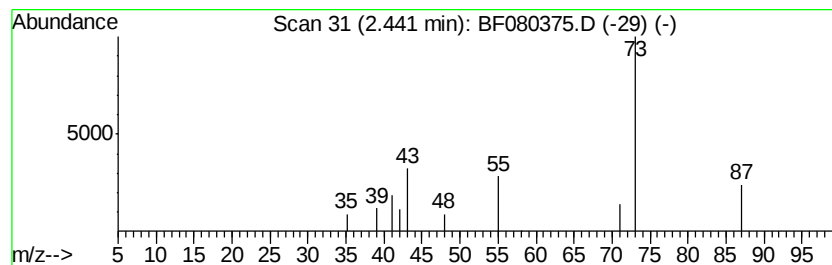
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	3.99 ng	35004	1,4-Dichlorobenzene-d4	7.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	33
2	1-Pentanamine	87	C5H13N	000110-58-7	5
3	Morpholine	87	C4H9NO	000110-91-8	4
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	4



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070715\
Data File : BF080375.D
Acq On : 7 Jul 2015 16:49
Operator : TP/UM
Sample : PB84384BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84384BL

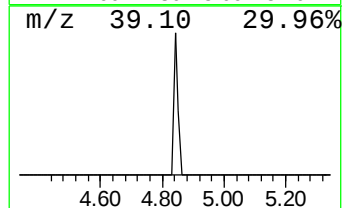
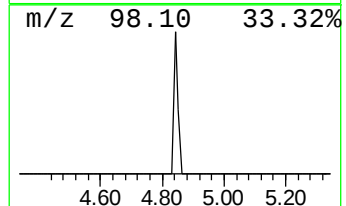
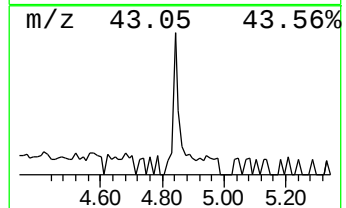
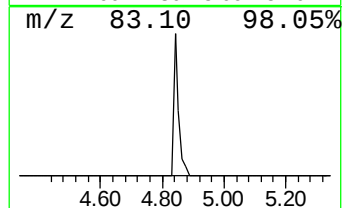
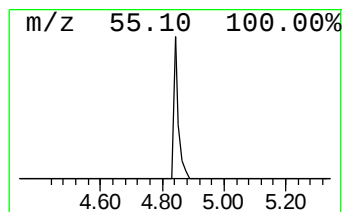
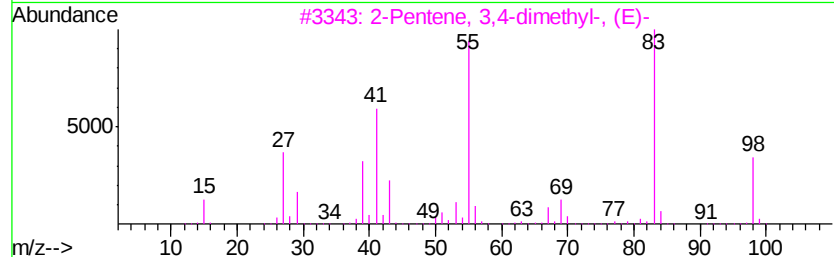
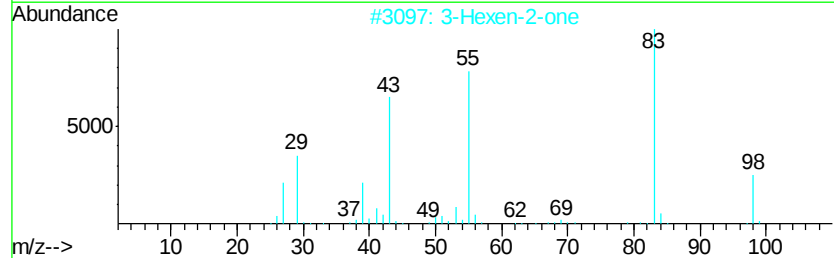
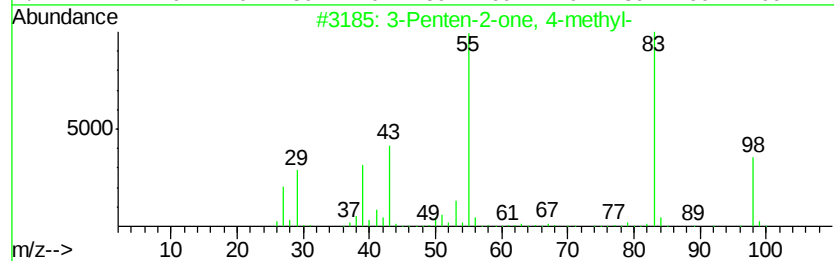
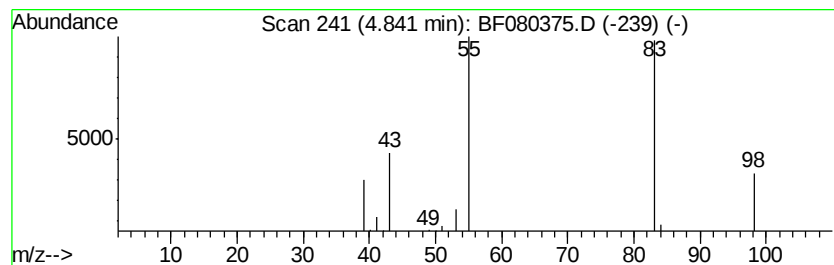
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	2.81 ng	24633	1,4-Dichlorobenzene-d4	7.23

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-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070715\
Data File : BF080375.D
Acq On : 7 Jul 2015 16:49
Operator : TP/UM
Sample : PB84384BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84384BL

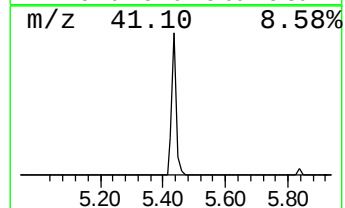
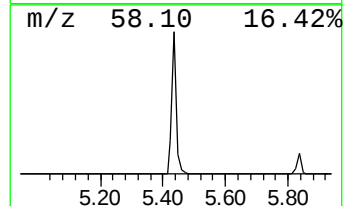
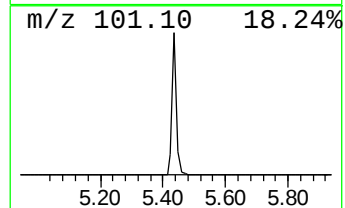
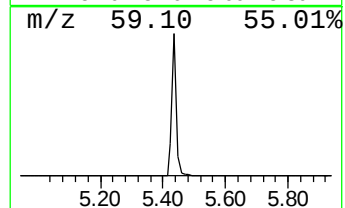
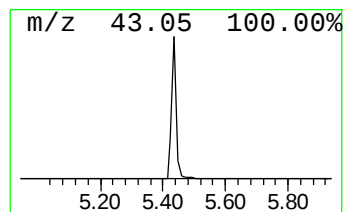
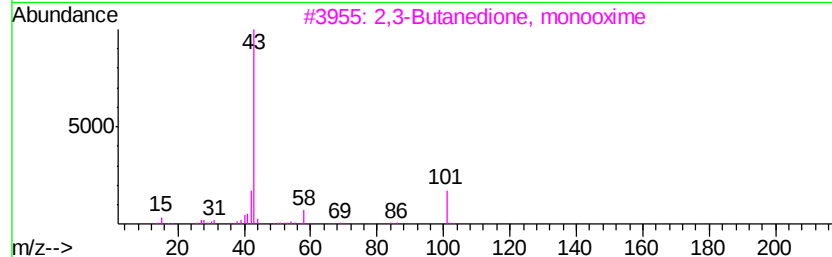
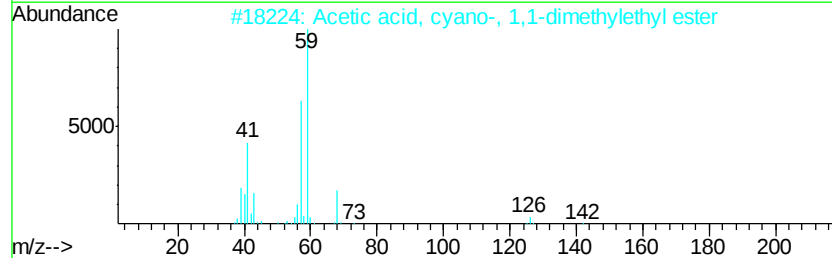
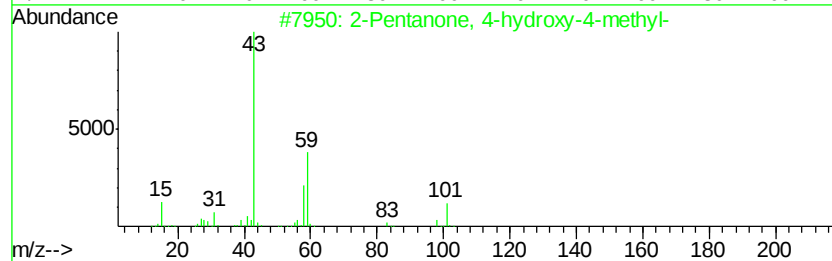
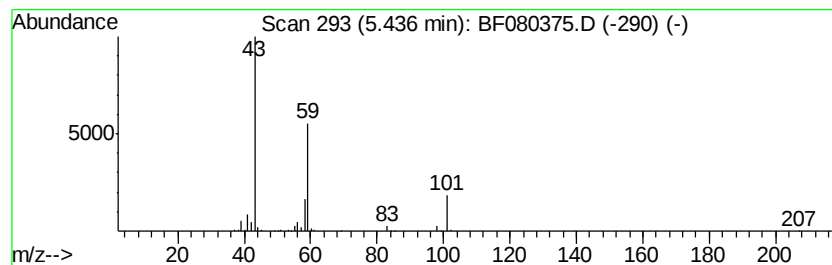
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.44	59.02 ng	517552	1,4-Dichlorobenzene-d4	7.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070715\
Data File : BF080375.D
Acq On : 7 Jul 2015 16:49
Operator : TP/UM
Sample : PB84384BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84384BL

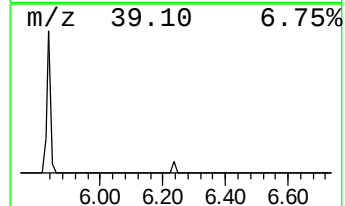
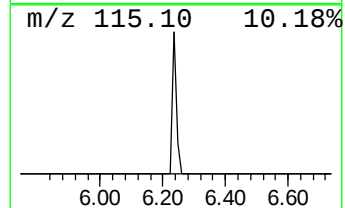
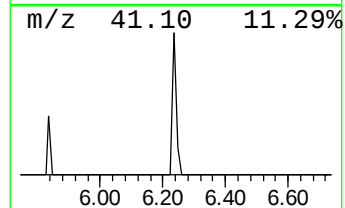
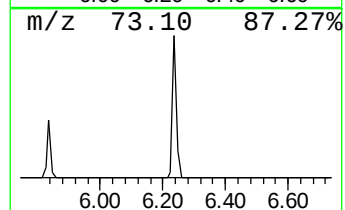
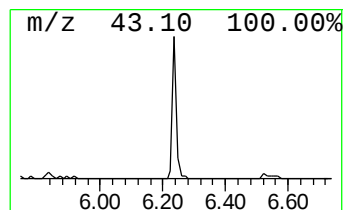
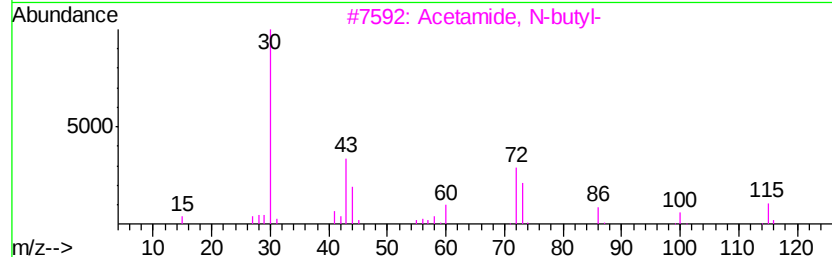
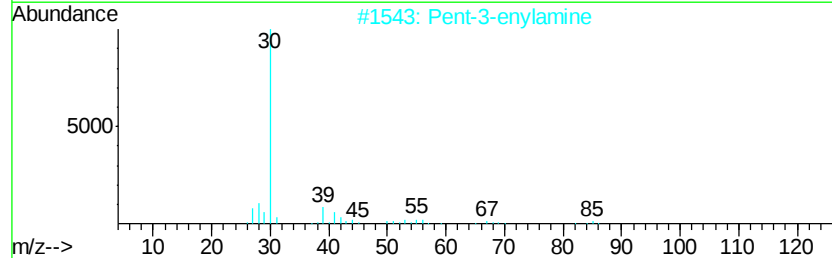
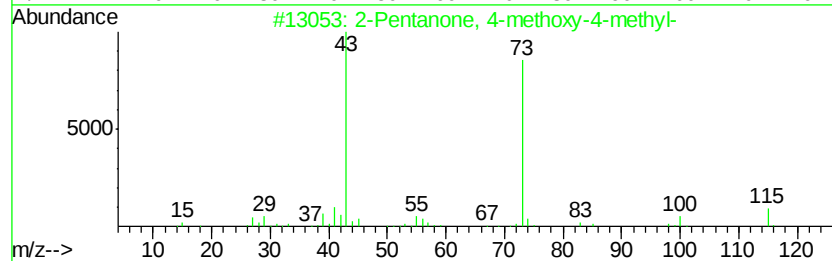
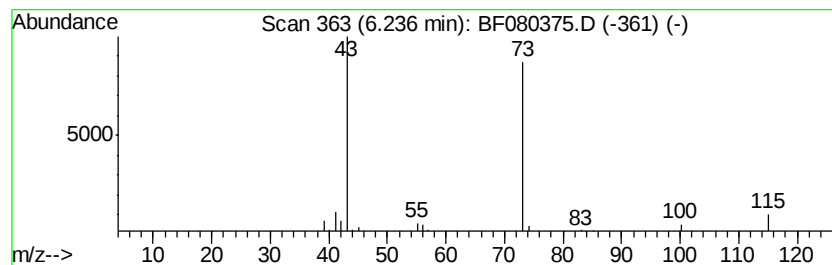
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	4.63 ng	40593	1,4-Dichlorobenzene-d4	7.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Pent-3-enylamine	85	C5H11N	087156-70-5	9
3		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070715\
Data File : BF080375.D
Acq On : 7 Jul 2015 16:49
Operator : TP/UM
Sample : PB84384BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84384BL

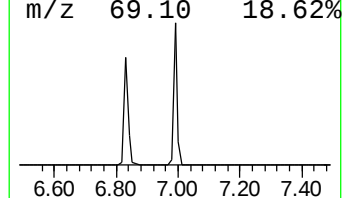
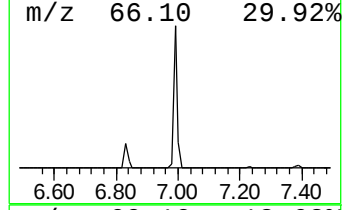
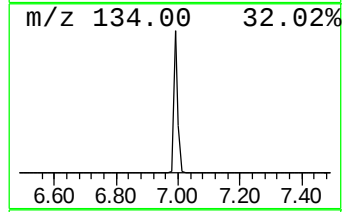
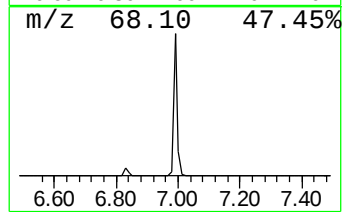
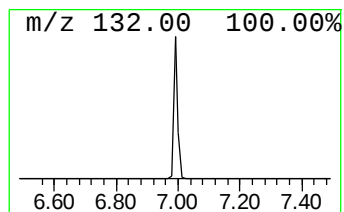
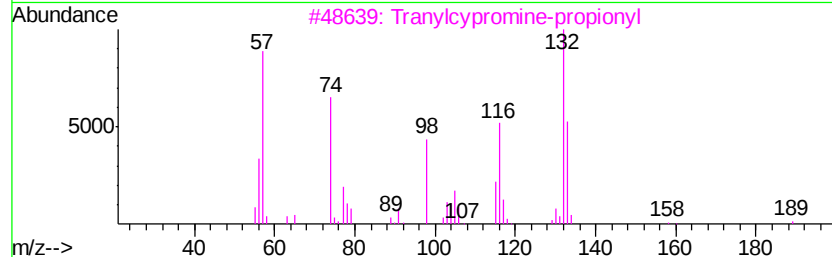
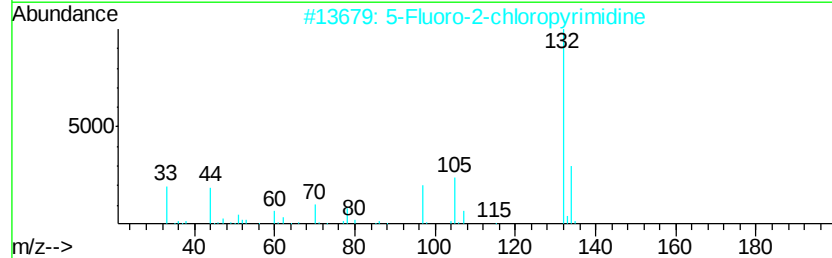
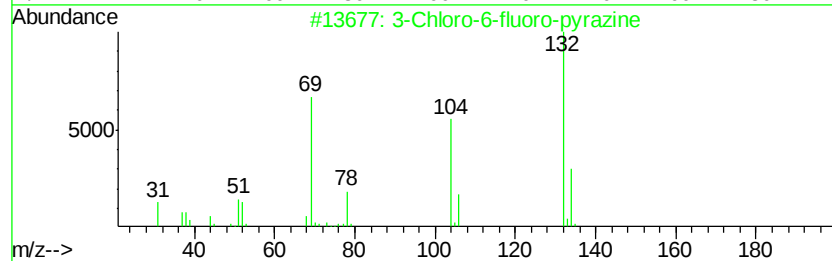
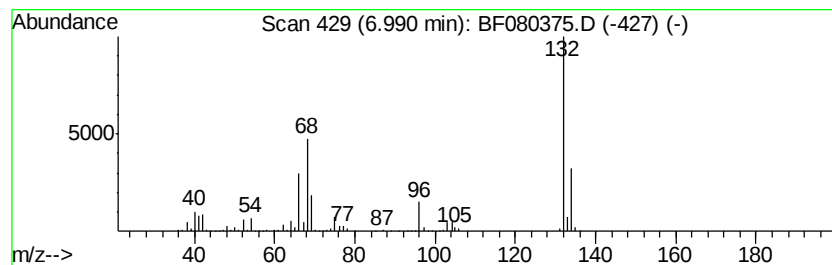
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	95.14 ng	834370	1,4-Dichlorobenzene-d4	7.23

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	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070715\
Data File : BF080375.D
Acq On : 7 Jul 2015 16:49
Operator : TP/UM
Sample : PB84384BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84384BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.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
unknown2.44	2.44	4.0	ng	35004	1	7.23	175392	20.0
3-Penten-2-one, 4...	4.84	2.8	ng	24633	1	7.23	175392	20.0
2-Pentanone, 4-hy...	5.44	59.0	ng	517552	1	7.23	175392	20.0
2-Pentanone, 4-me...	6.24	4.6	ng	40593	1	7.23	175392	20.0
unknown6.99	6.99	95.1	ng	834370	1	7.23	175392	20.0