

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031715\
 Data File : BF077776.D
 Acq On : 17 Mar 2015 17:21
 Operator : TP/IZ
 Sample : PB82148BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB82148BL

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-BF031115.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	1.333	36	39	41	rBV	893135	1031484	38.84%	5.647%
2	1.435	45	48	52	rVB	11806	28118	1.06%	0.154%
3	1.790	77	79	84	rBV	30171	43849	1.65%	0.240%
4	4.213	279	291	305	rBV3	218137	1374595	51.76%	7.525%
5	4.922	351	353	356	rBV	600926	751859	28.31%	4.116%
6	5.447	396	399	401	rBV	655900	695850	26.20%	3.809%
7	5.493	401	403	408	rVB	105730	213283	8.03%	1.168%
8	5.984	441	446	450	rBV	414267	758636	28.57%	4.153%
9	6.727	508	511	513	rBV	754161	684512	25.78%	3.747%
10	6.865	521	523	526	rBV	556286	693465	26.11%	3.796%
11	7.116	542	545	547	rBV	407795	514262	19.37%	2.815%
12	7.162	547	549	551	rVB	261654	244388	9.20%	1.338%
13	7.345	563	565	568	rBV	848967	750793	28.27%	4.110%
14	7.848	607	609	612	rBV	423731	535857	20.18%	2.933%
15	8.419	656	659	661	rBV	243960	325776	12.27%	1.783%
16	8.739	685	687	689	rBV	346019	328891	12.39%	1.800%
17	10.019	797	799	802	rBV	1273105	1142524	43.02%	6.254%
18	10.088	802	805	807	rVB	1163734	1195554	45.02%	6.545%
19	10.876	872	874	875	rBV	359727	371319	13.98%	2.033%
20	10.911	875	877	879	rVB	336897	369693	13.92%	2.024%
21	11.882	959	962	965	rBV	759185	990243	37.29%	5.421%
22	12.739	1035	1037	1040	rBV	579828	785059	29.56%	4.298%
23	14.751	1210	1213	1215	rBV	1868437	2655556	100.00%	14.537%
24	16.054	1324	1327	1330	rBV	811005	884755	33.32%	4.843%
25	17.871	1483	1486	1489	rBV	715204	897036	33.78%	4.911%

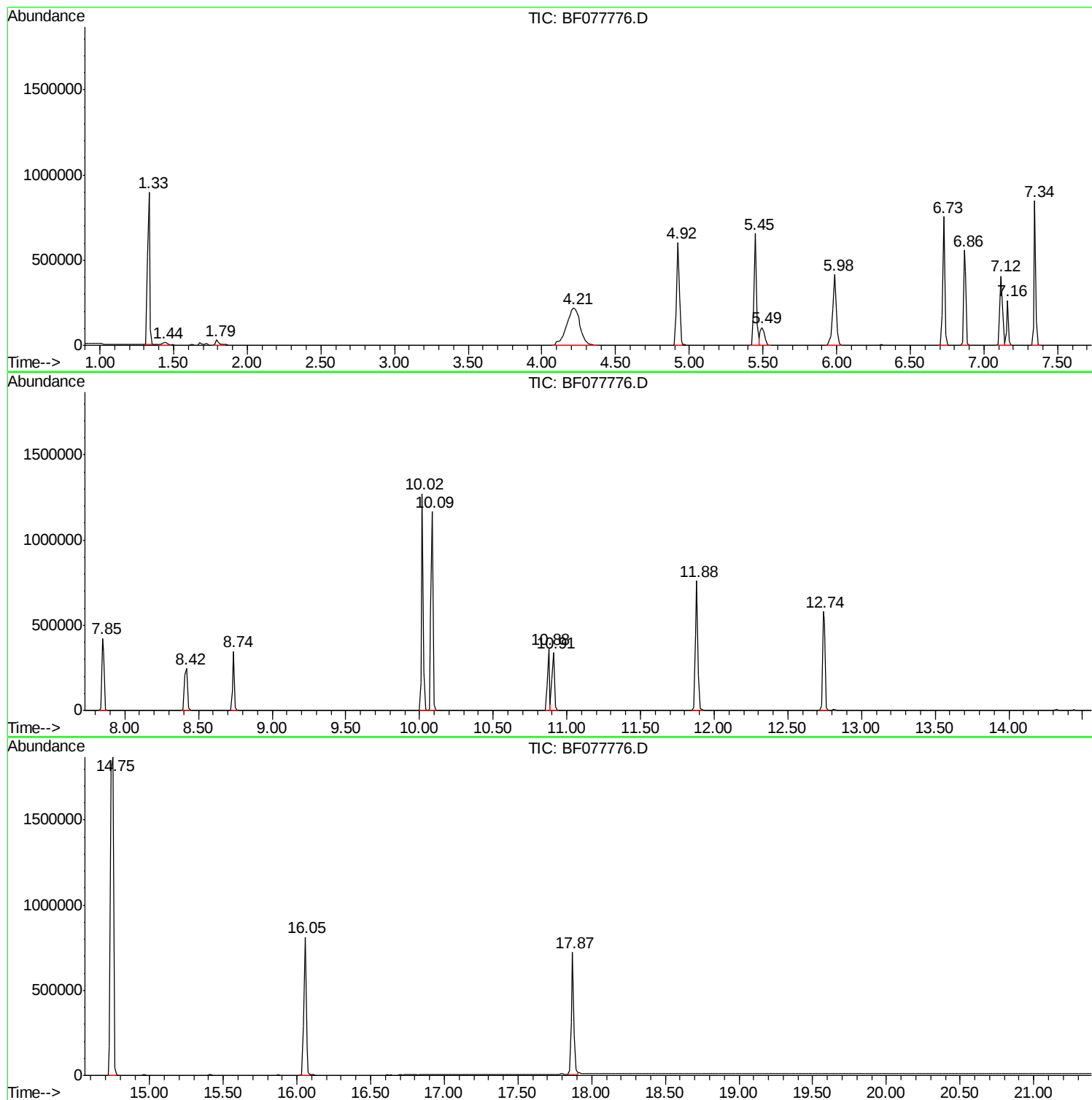
Sum of corrected areas: 18267357

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031715\
Data File : BF077776.D
Acq On : 17 Mar 2015 17:21
Operator : TP/IZ
Sample : PB82148BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB82148BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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\BF031715\
Data File : BF077776.D
Acq On : 17 Mar 2015 17:21
Operator : TP/IZ
Sample : PB82148BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB82148BL

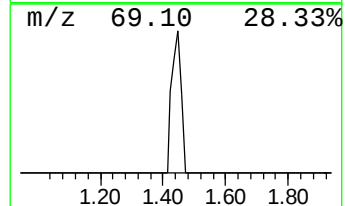
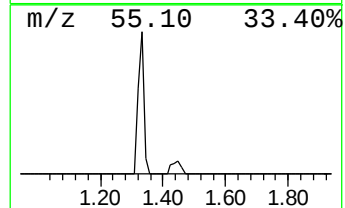
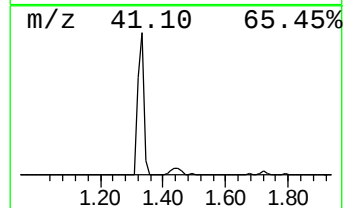
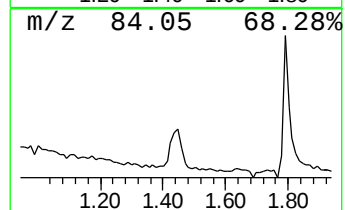
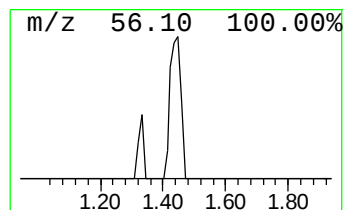
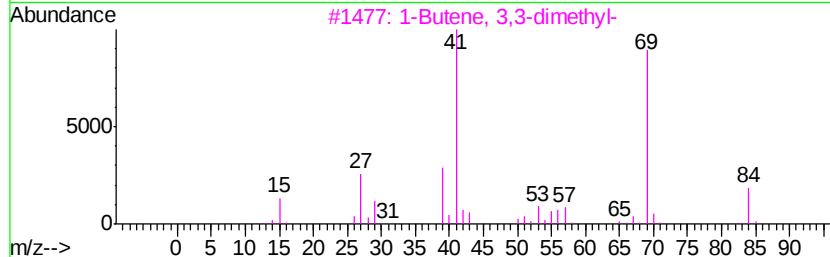
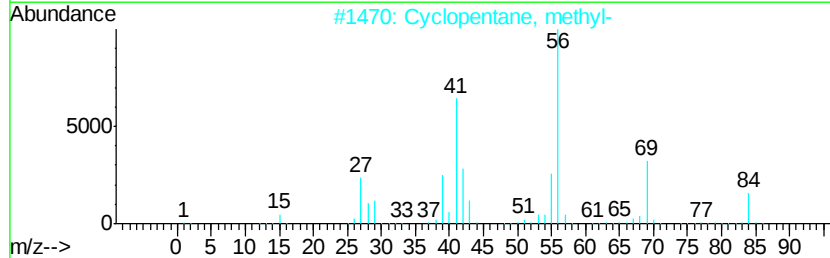
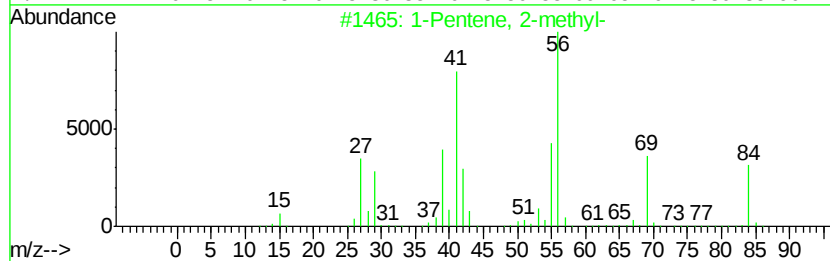
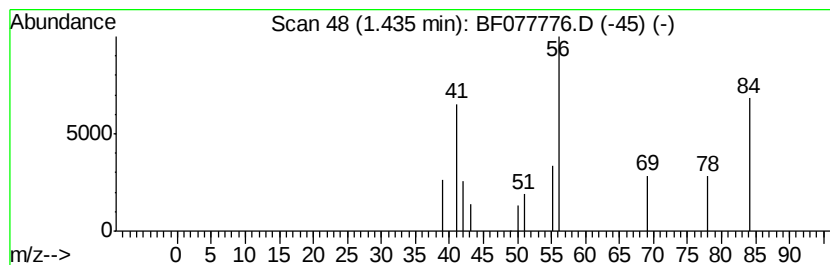
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown1.44 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.44	2.30 ng	28118	1,4-Dichlorobenzene-d4	7.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	45
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	33
3			1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	9
4			2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	9
5			2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031715\
Data File : BF077776.D
Acq On : 17 Mar 2015 17:21
Operator : TP/IZ
Sample : PB82148BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB82148BL

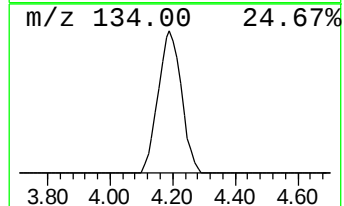
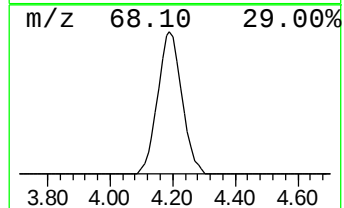
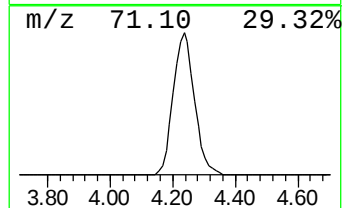
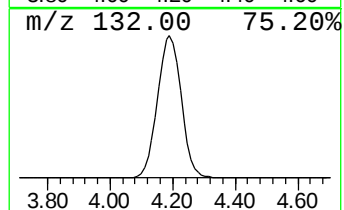
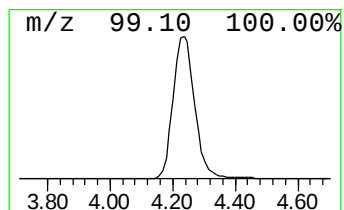
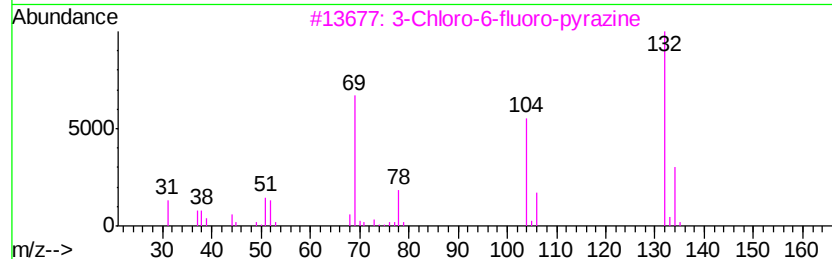
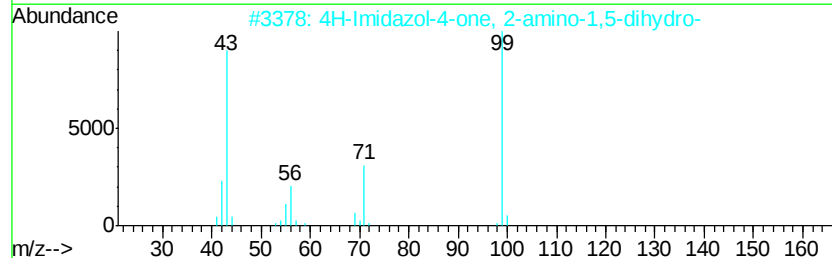
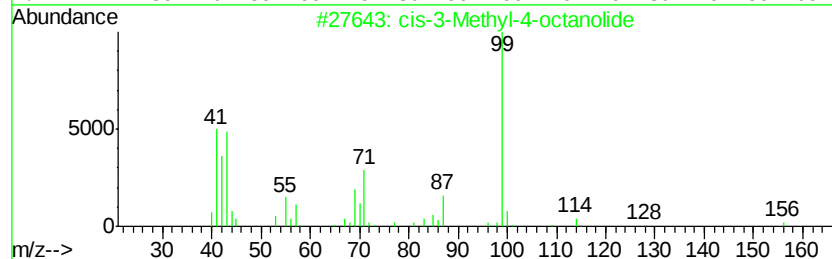
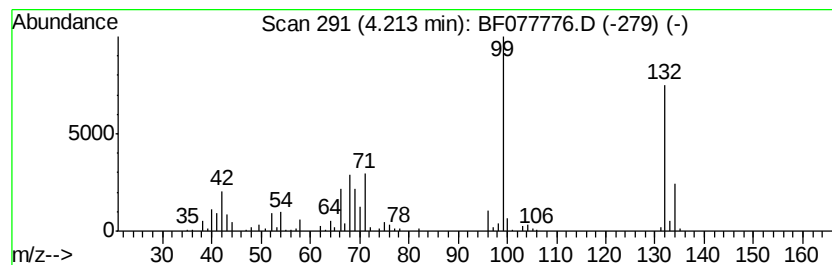
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown4.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.21	112.49 ng	1374600	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	22
2		4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	18
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	18
5		Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031715\
Data File : BF077776.D
Acq On : 17 Mar 2015 17:21
Operator : TP/IZ
Sample : PB82148BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB82148BL

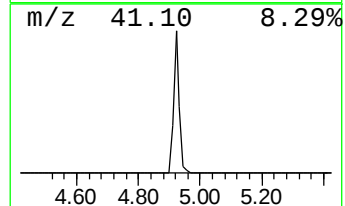
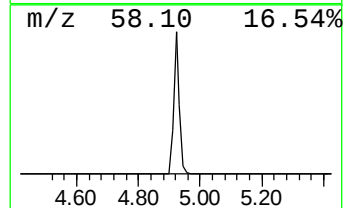
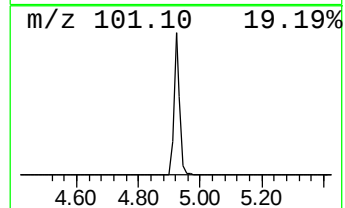
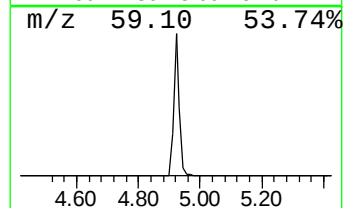
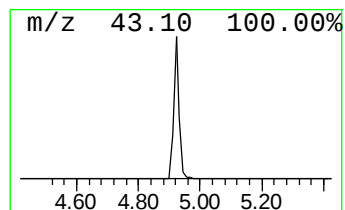
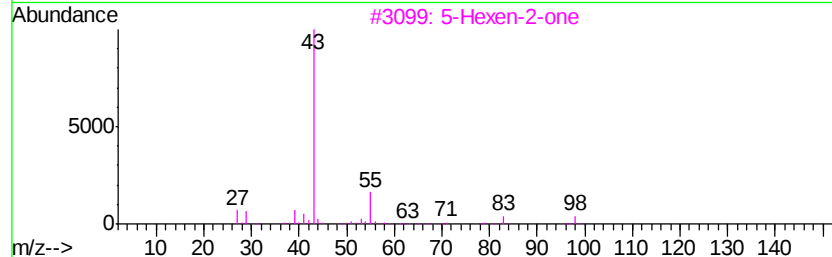
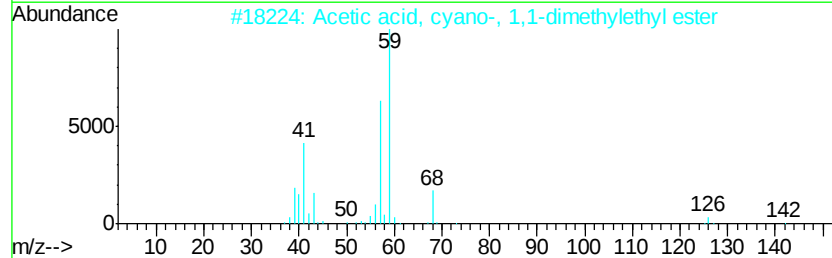
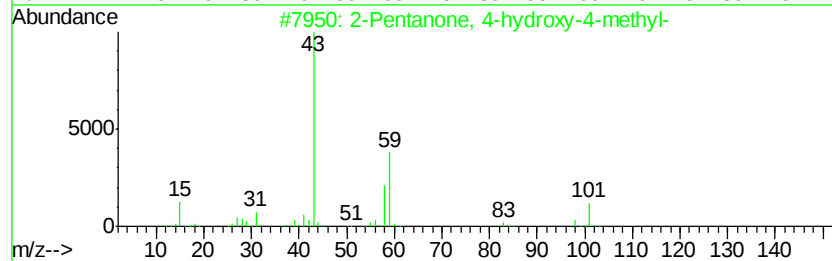
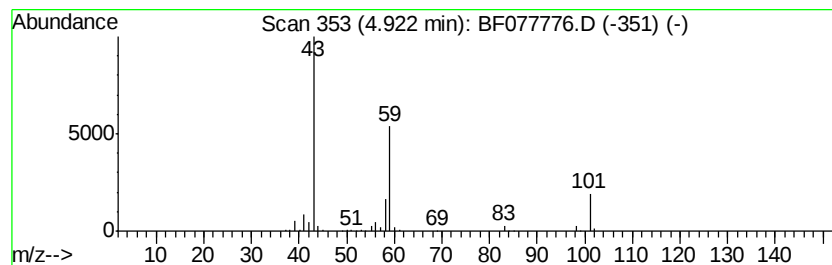
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	61.53 ng	751859	1,4-Dichlorobenzene-d4	7.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031715\
Data File : BF077776.D
Acq On : 17 Mar 2015 17:21
Operator : TP/IZ
Sample : PB82148BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB82148BL

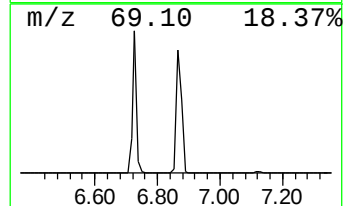
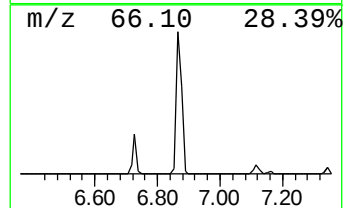
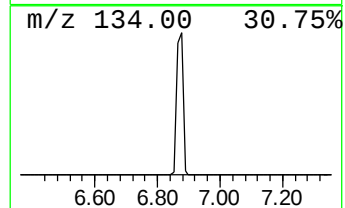
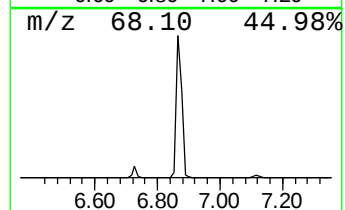
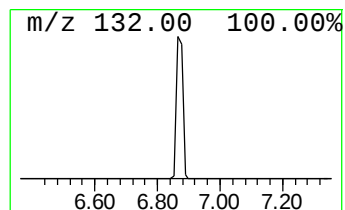
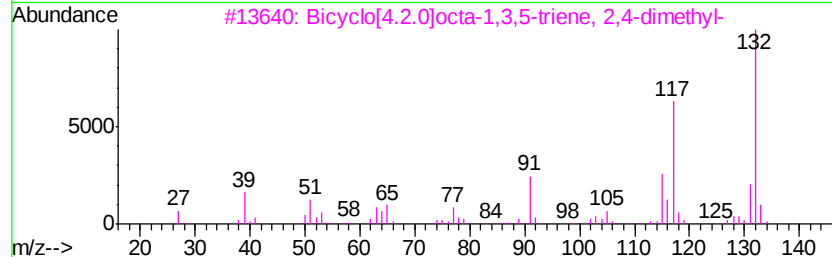
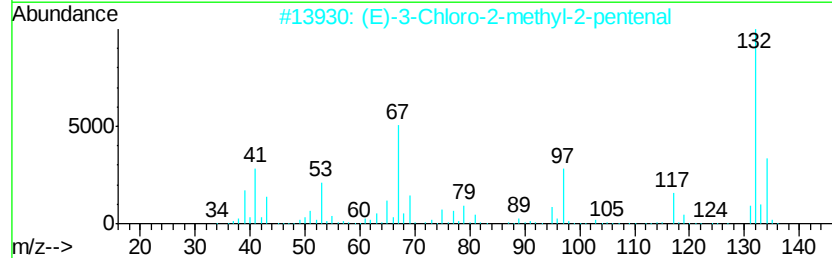
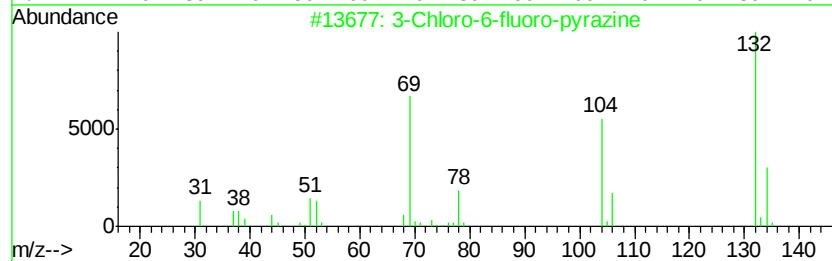
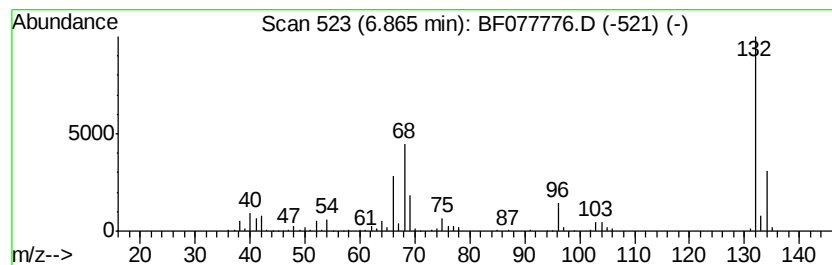
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.86 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.86	56.75 ng	693465	1,4-Dichlorobenzene-d4	7.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...			132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-			132	C10H12	005379-20-4	9
5	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031715\
Data File : BF077776.D
Acq On : 17 Mar 2015 17:21
Operator : TP/IZ
Sample : PB82148BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

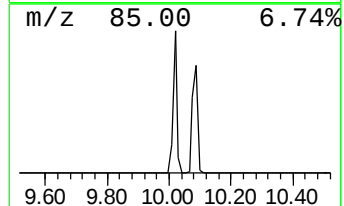
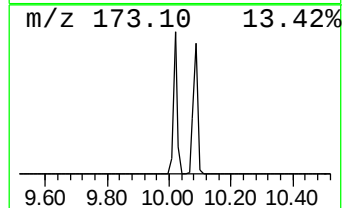
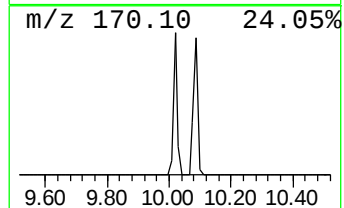
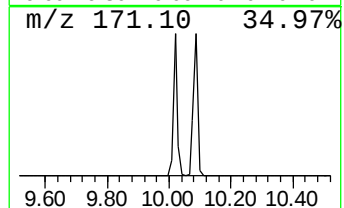
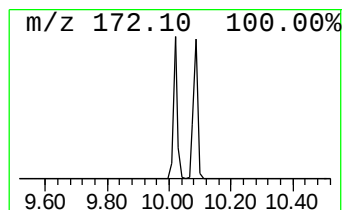
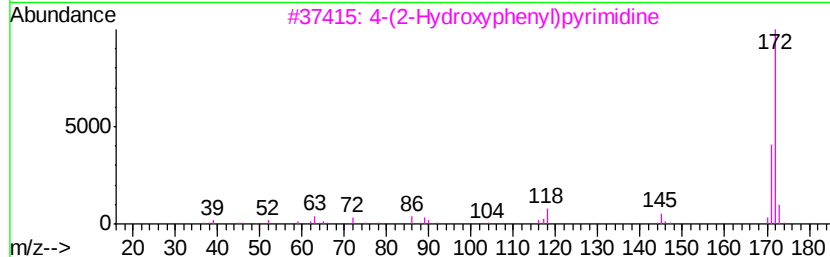
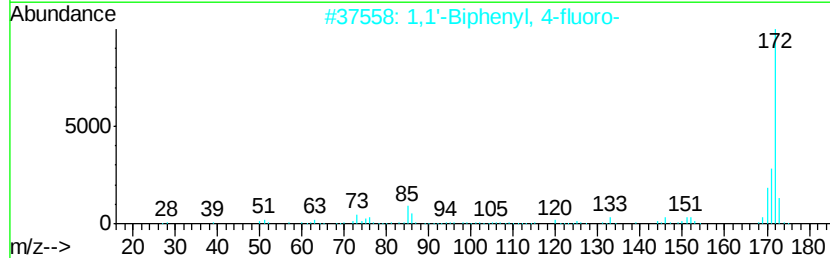
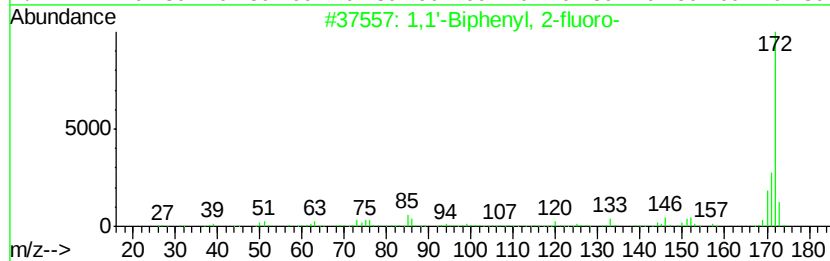
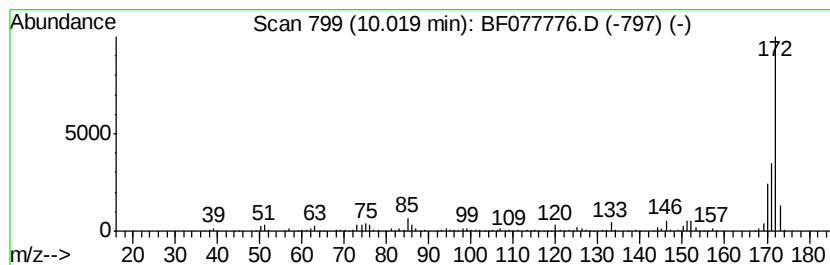
Instrument :
BNA_F
ClientSampleId :
PB82148BL

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,1'-Biphenyl, 2-fluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.02	61.81 ng	1142520	Acenaphthene-d10	10.91	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	000321-60-8	96
2	1,1'-Biphenyl, 4-fluoro-	172	C12H9F	000324-74-3	87
3	4-(2-Hydroxyphenyl)pyrimidine	172	C10H8N2O	068535-55-7	42
4	4-Pyrimidinol, 5-phenyl-	172	C10H8N2O	022433-69-8	42
5	5-(4-Hydroxyphenyl)pyrimidine	172	C10H8N2O	069491-51-6	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031715\
Data File : BF077776.D
Acq On : 17 Mar 2015 17:21
Operator : TP/IZ
Sample : PB82148BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB82148BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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
unknown1.44	1.44	2.3	ng	28118	1	7.16	244388	20.0
unknown4.21	4.21	112.5	ng	1374600	1	7.16	244388	20.0
2-Pentanone, 4-hy...	4.92	61.5	ng	751859	1	7.16	244388	20.0
unknown6.86	6.86	56.8	ng	693465	1	7.16	244388	20.0
1,1'-Biphenyl, 2-...	10.02	61.8	ng	1142520	3	10.91	369693	20.0