

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
 Data File : BM009925.D
 Acq On : 06 May 2017 04:54
 Operator : SJ/MA
 Sample : I2893-13
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3072-PA3

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_M\METHODS\8270-BM050517.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	4.904	304	309	320	rVB	413675	616441	5.47%	1.308%
2	5.369	381	388	399	rBV	1300717	2007171	17.82%	4.258%
3	5.969	483	490	499	rBV	87659	141468	1.26%	0.300%
4	6.963	652	659	669	rBV	830436	1346936	11.96%	2.858%
5	7.316	711	719	731	rBV	2562872	4056448	36.01%	8.606%
6	7.775	790	797	803	rBV	474407	762244	6.77%	1.617%
7	8.092	844	851	859	rBV	2053162	3356473	29.80%	7.121%
8	8.951	989	997	1007	rBV	2196751	3541344	31.44%	7.513%
9	10.575	1266	1273	1284	rBV	627373	1051922	9.34%	2.232%
10	11.239	1381	1386	1394	rBV2	87678	165463	1.47%	0.351%
11	13.045	1686	1693	1702	rVB	4794010	6706715	59.54%	14.229%
12	14.433	1919	1929	1935	rBV2	859495	1372068	12.18%	2.911%
13	15.933	2177	2184	2194	rBV	4257760	5802502	51.51%	12.311%
14	16.151	2217	2221	2233	rVB3	98466	181626	1.61%	0.385%
15	17.186	2392	2397	2404	rBV	1177389	1642834	14.59%	3.485%
16	19.815	2838	2844	2849	rBV	9628223	11263813	100.00%	23.898%
17	21.374	3105	3109	3114	rBV	1493837	1802083	16.00%	3.823%
18	23.680	3496	3501	3508	rVB2	718046	1315896	11.68%	2.792%

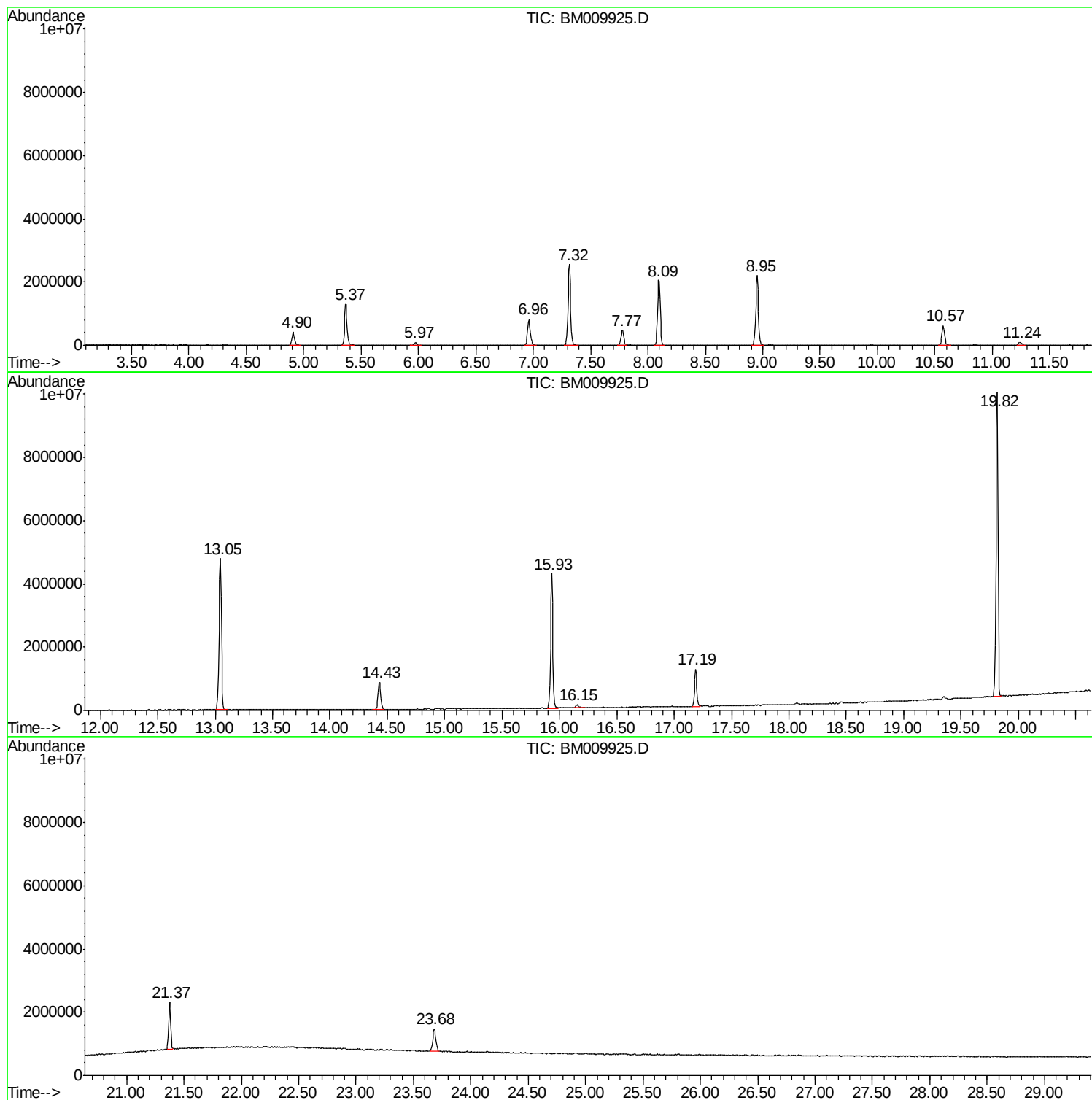
Sum of corrected areas: 47133447

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009925.D
Acq On : 06 May 2017 04:54
Operator : SJ/MA
Sample : I2893-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3072-PA3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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_M\DATA\BM050517\
Data File : BM009925.D
Acq On : 06 May 2017 04:54
Operator : SJ/MA
Sample : I2893-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3072-PA3

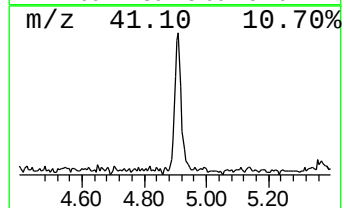
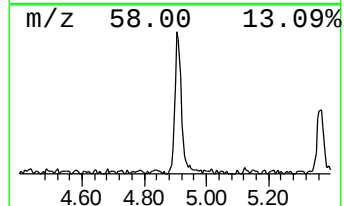
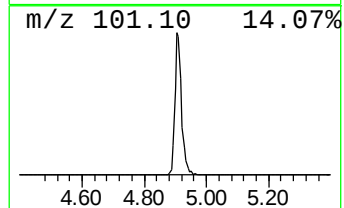
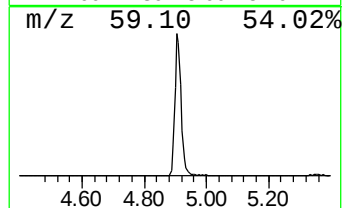
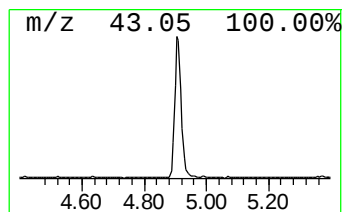
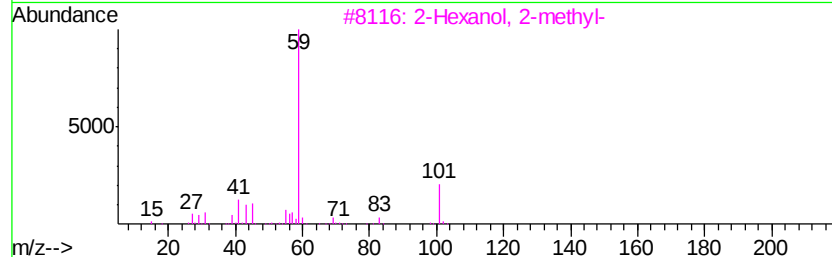
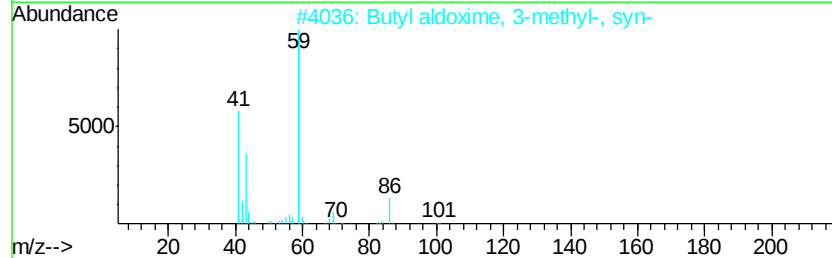
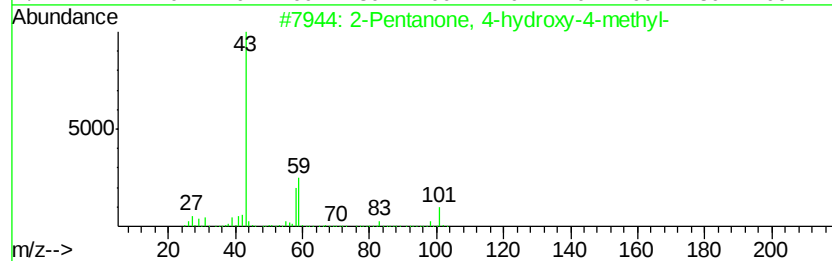
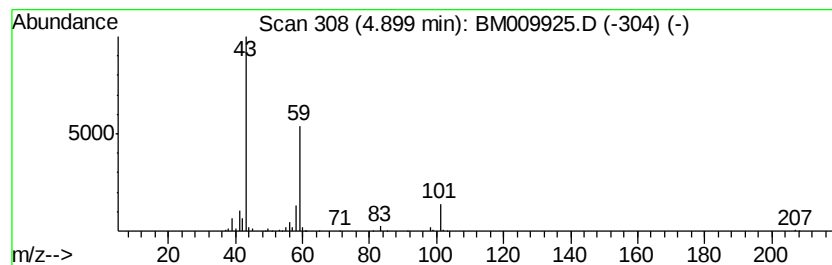
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	16.17 ng	616441	1,4-Dichlorobenzene-d4	7.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009925.D
Acq On : 06 May 2017 04:54
Operator : SJ/MA
Sample : I2893-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3072-PA3

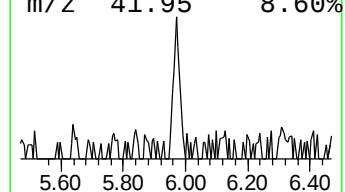
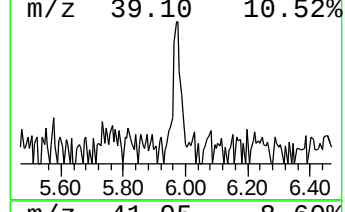
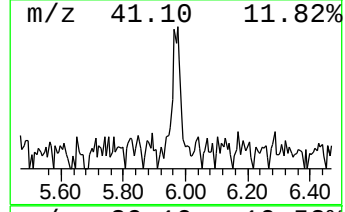
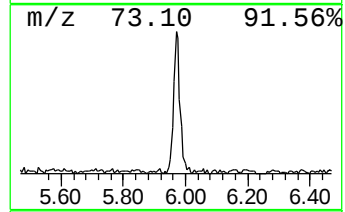
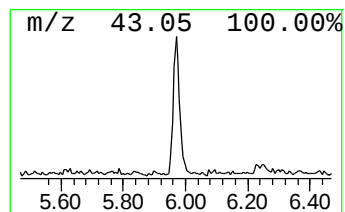
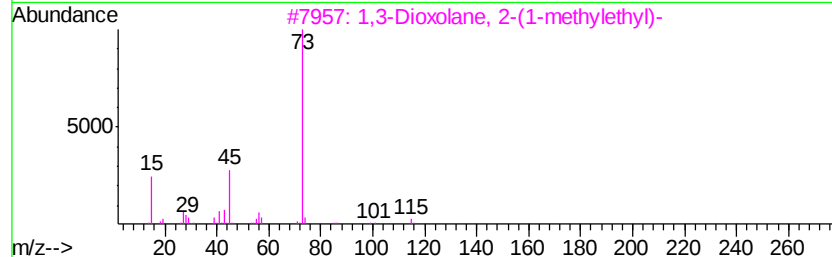
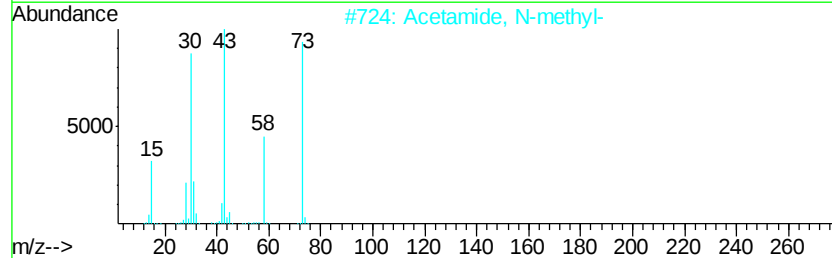
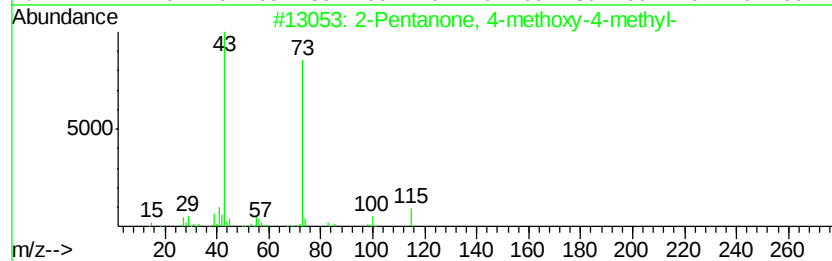
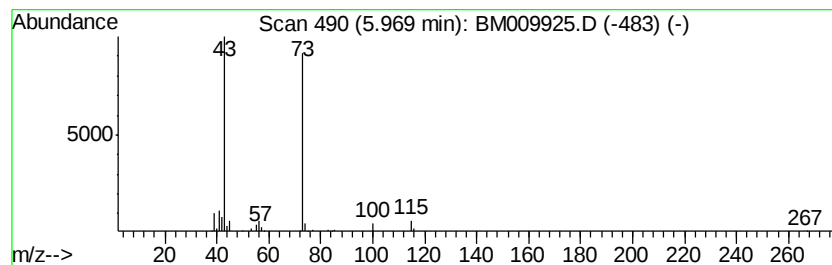
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	3.71 ng	141468	1,4-Dichlorobenzene-d4	7.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	59
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	50
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	23
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	17
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	10



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009925.D
Acq On : 06 May 2017 04:54
Operator : SJ/MA
Sample : I2893-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3072-PA3

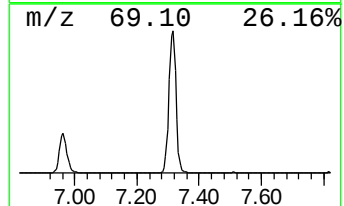
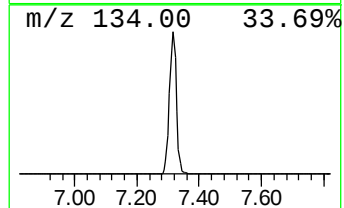
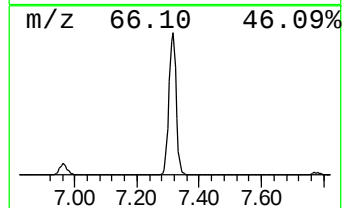
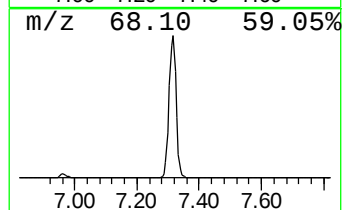
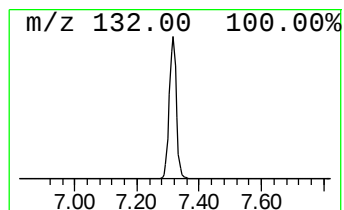
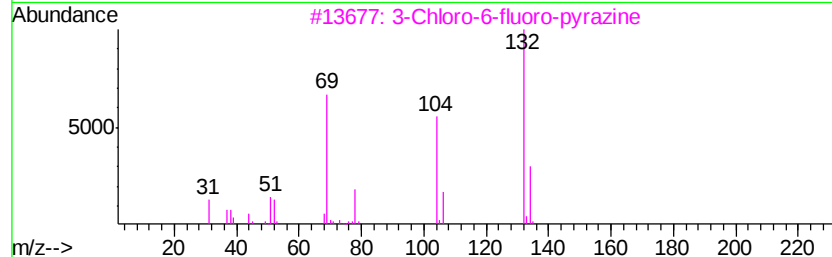
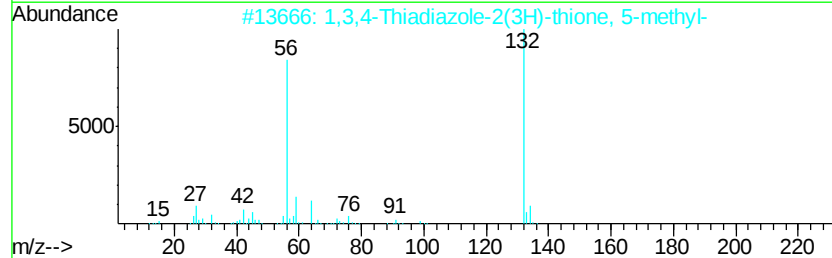
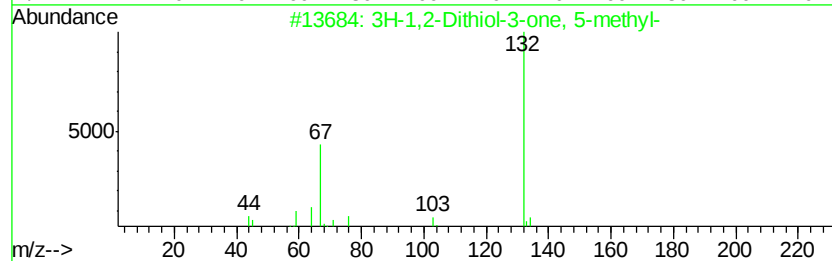
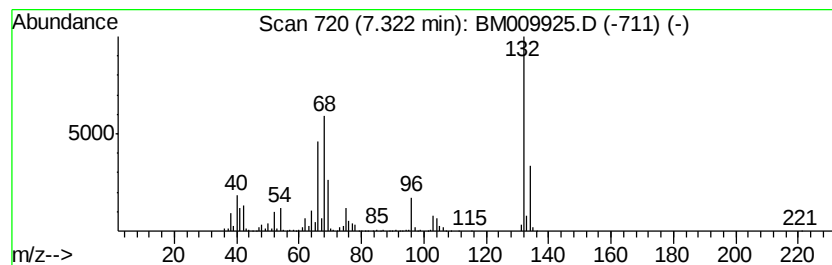
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	106.43 ng	4056450	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009925.D
Acq On : 06 May 2017 04:54
Operator : SJ/MA
Sample : I2893-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3072-PA3

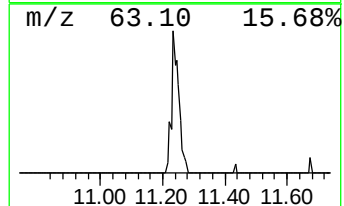
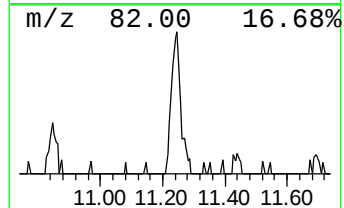
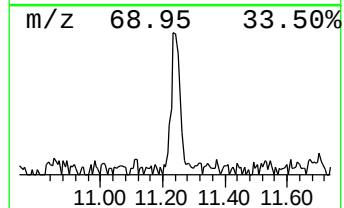
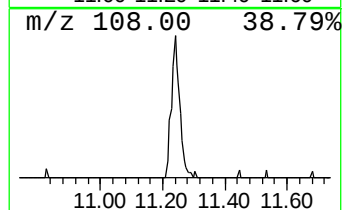
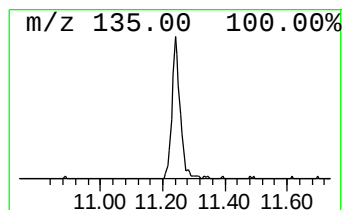
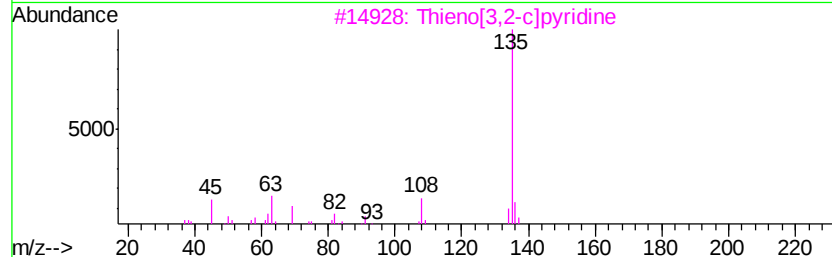
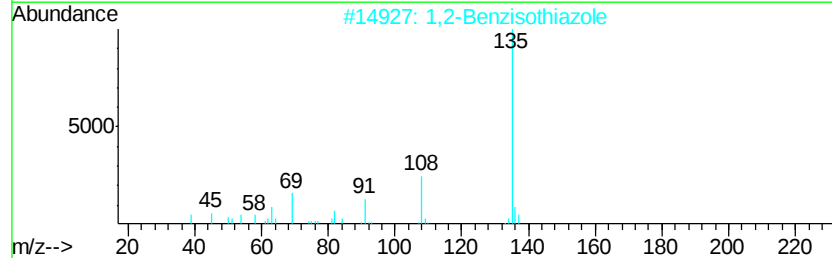
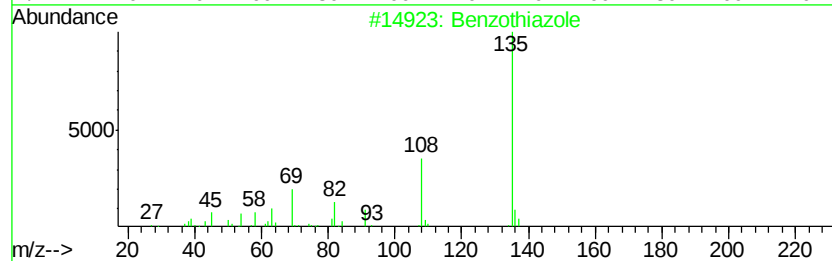
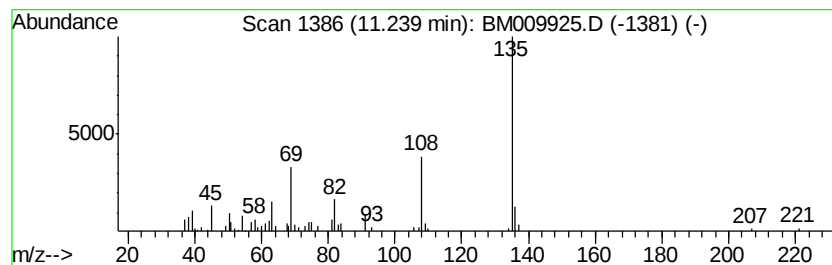
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	3.15 ng	165463	Naphthalene-d8	10.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	94
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3		Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	76
4		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
5		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	68



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009925.D
Acq On : 06 May 2017 04:54
Operator : SJ/MA
Sample : I2893-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

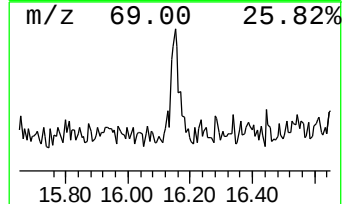
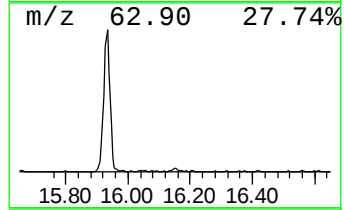
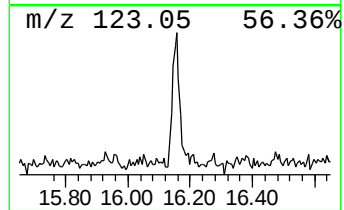
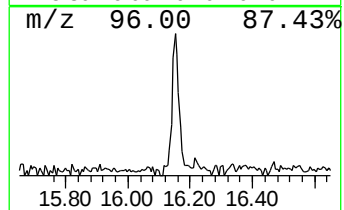
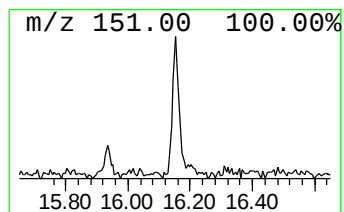
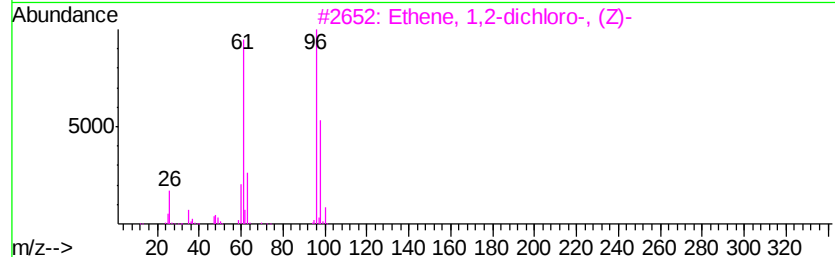
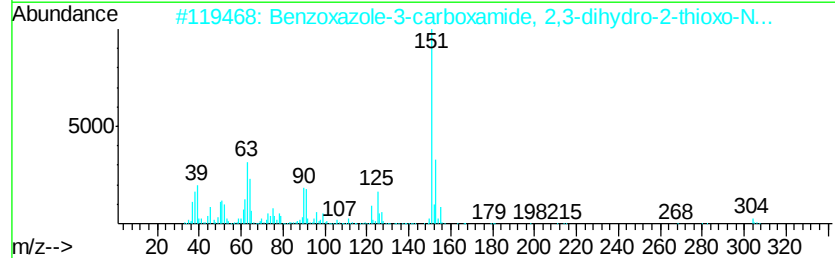
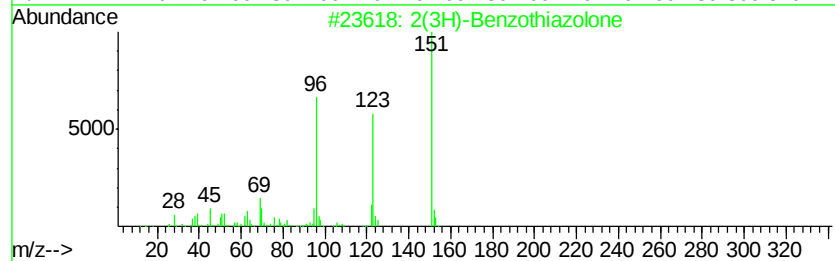
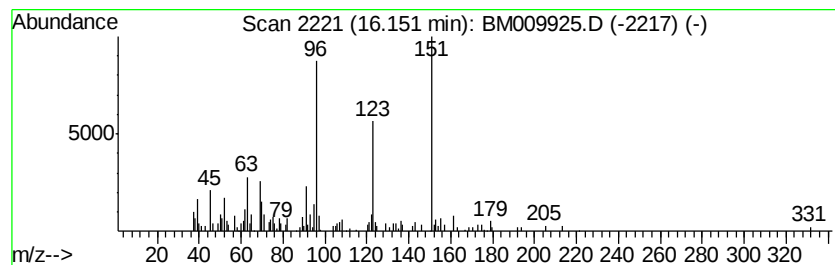
Instrument :
BNA_M
ClientSampleId :
3072-PA3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.15	2.21 ng	181626	Phenanthrene-d10	17.19		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	89
2		Benzoxazole-3-carboxamide, 2,3-d...	304	C14H9ClN2O2S	1000264-58-7	43
3		Ethene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
4		6-Methyltetrazolo[1,5-c]pyrimidi...	151	C5H5N5O	144877-40-7	32
5		Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	32



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009925.D
Acq On : 06 May 2017 04:54
Operator : SJ/MA
Sample : I2893-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3072-PA3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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
2-Pentanone, 4-hy...	4.90	16.2	ng	616441	1	7.77	762244	20.0
2-Pentanone, 4-me...	5.97	3.7	ng	141468	1	7.77	762244	20.0
unknown7.32	7.32	106.4	ng	4056450	1	7.77	762244	20.0
Benzothiazole	11.24	3.1	ng	165463	2	10.57	1051920	20.0
2(3H)-Benzothiazo...	16.15	2.2	ng	181626	4	17.19	1642830	20.0