

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099459.D
 Acq On : 14 Oct 2017 00:25
 Operator : SJ/JU
 Sample : I5819-10
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3911-SPP4

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-BF092317.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	2.134	3	8	17	rVB	189918	254015	8.45%	1.269%
2	5.081	506	509	525	rVB	154317	197151	6.56%	0.985%
3	5.481	573	577	592	rBV	1517109	1473235	49.01%	7.360%
4	6.487	744	748	758	rBV	1010135	886488	29.49%	4.429%
5	6.628	767	772	775	rBV	2632518	2421771	80.56%	12.099%
6	6.851	807	810	817	rBV	691203	572630	19.05%	2.861%
7	7.010	833	837	840	rBV	2609086	2395498	79.69%	11.968%
8	7.422	902	907	910	rBV	1895764	1815868	60.41%	9.072%
9	8.133	1024	1028	1036	rBV	878840	717374	23.86%	3.584%
10	8.416	1072	1076	1091	rBV	824868	711291	23.66%	3.554%
11	9.210	1206	1211	1214	rBV	3274821	3006035	100.00%	15.018%
12	9.886	1323	1326	1337	rVB	730889	668591	22.24%	3.340%
13	10.680	1457	1461	1472	rBV	1418616	1314313	43.72%	6.566%
14	11.374	1576	1579	1588	rBV	626503	532843	17.73%	2.662%
15	12.963	1844	1849	1852	rBV	2003664	1991643	66.25%	9.950%
16	14.015	2025	2028	2037	rVB	516969	496053	16.50%	2.478%
17	15.492	2274	2279	2289	rBV	457495	560860	18.66%	2.802%

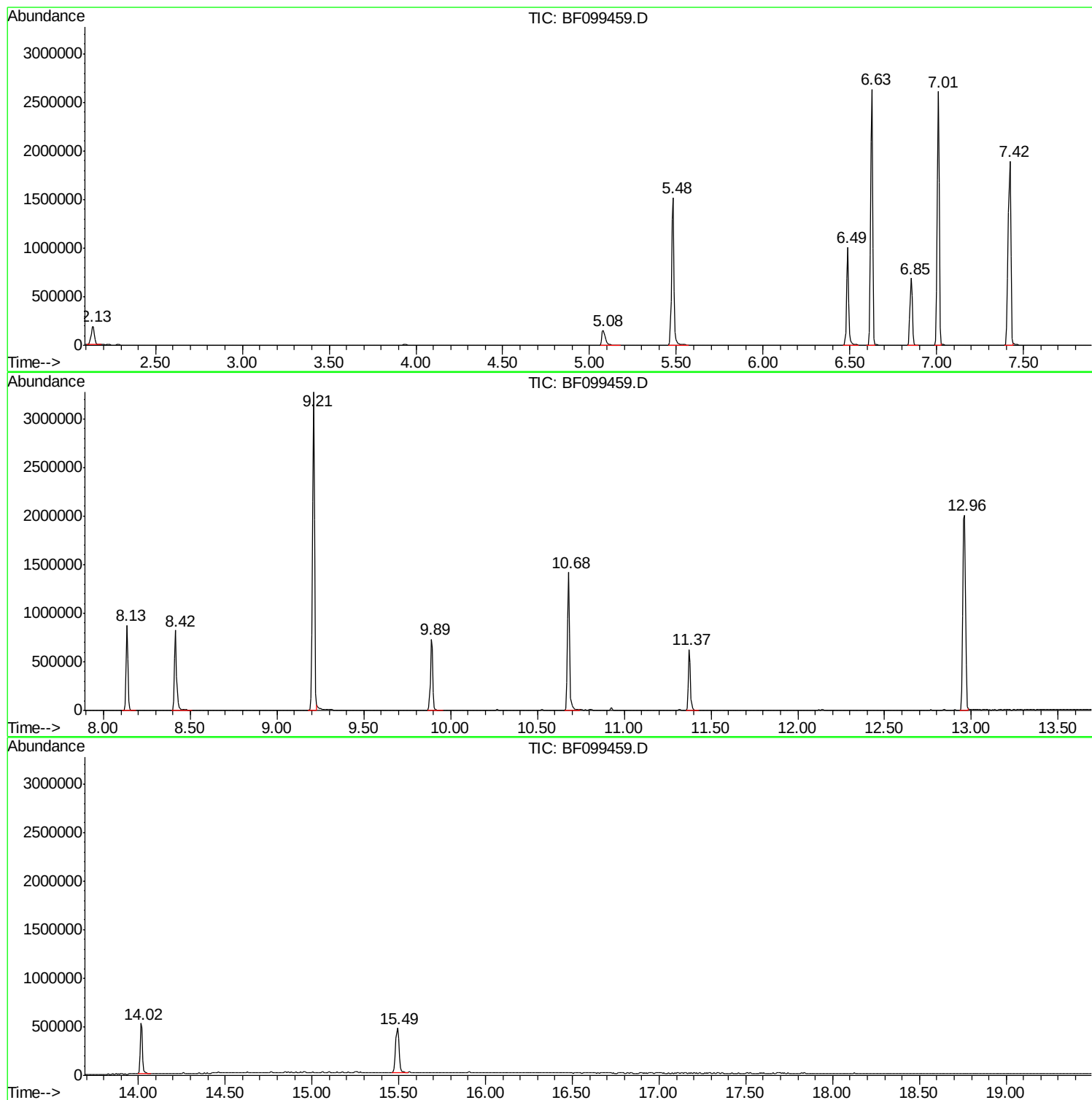
Sum of corrected areas: 20015659

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099459.D
Acq On : 14 Oct 2017 00:25
Operator : SJ/JU
Sample : I5819-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3911-SPP4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099459.D
Acq On : 14 Oct 2017 00:25
Operator : SJ/JU
Sample : I5819-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3911-SPP4

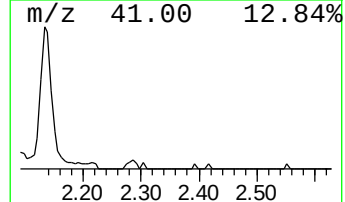
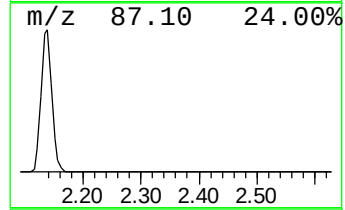
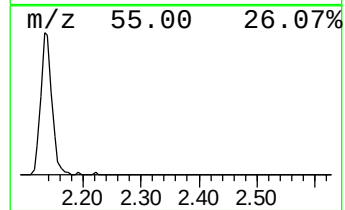
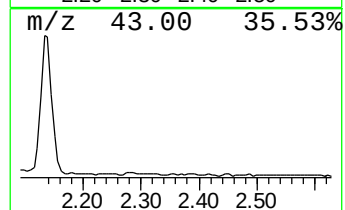
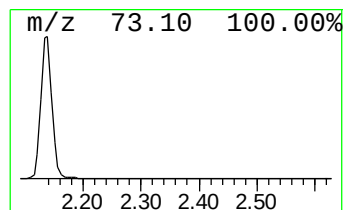
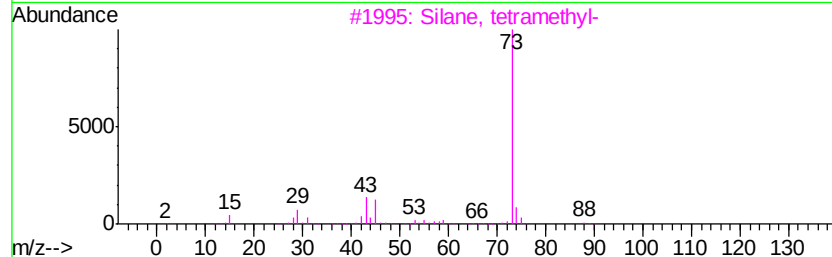
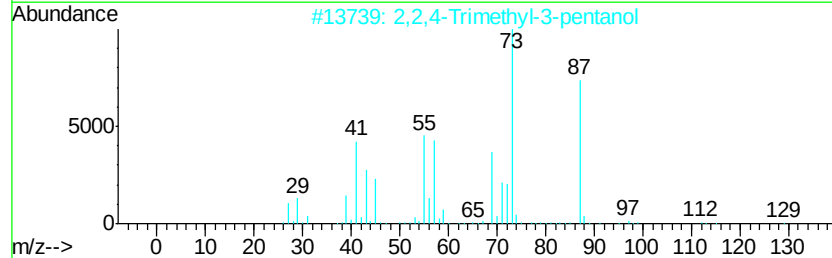
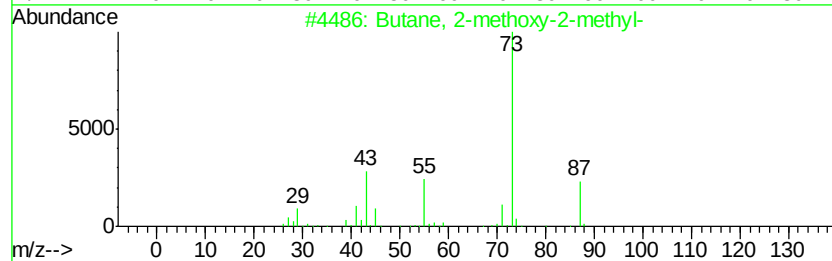
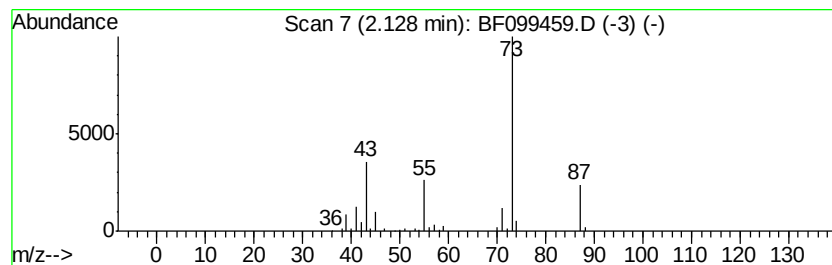
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	8.87 ng	254015	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099459.D
Acq On : 14 Oct 2017 00:25
Operator : SJ/JU
Sample : I5819-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3911-SPP4

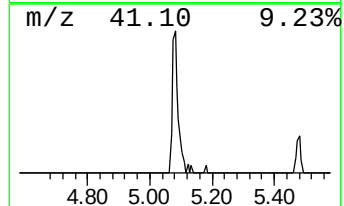
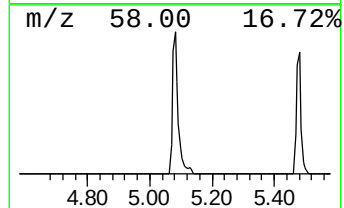
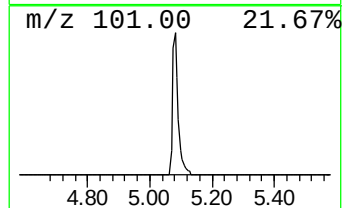
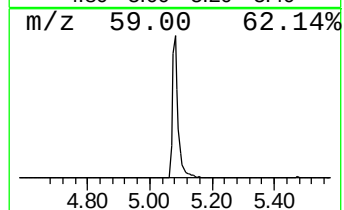
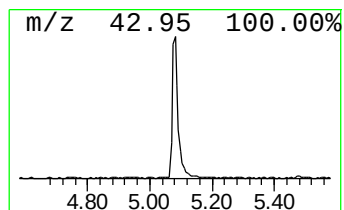
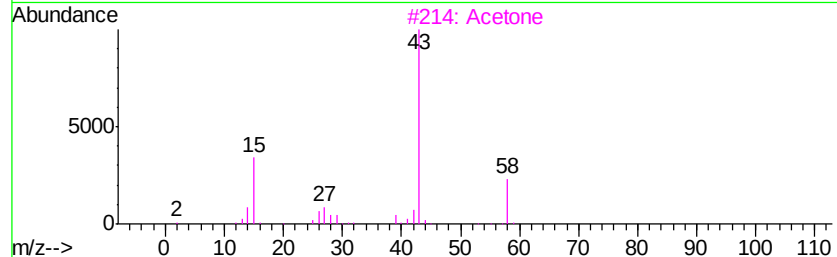
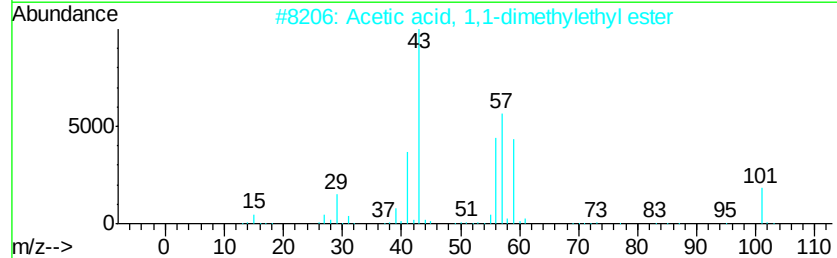
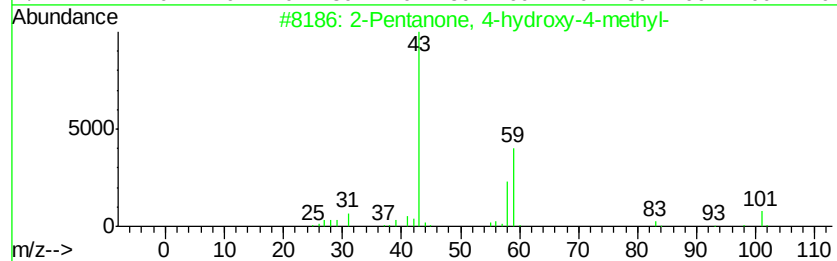
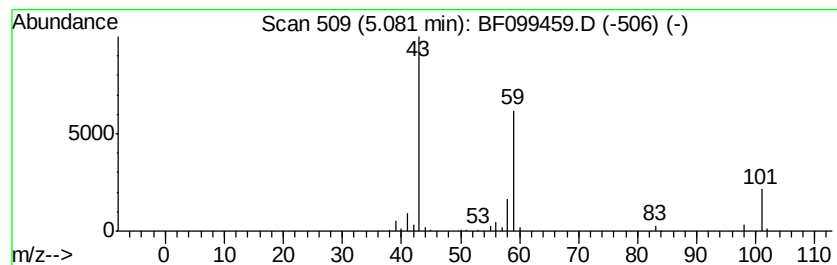
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	6.89 ng	197151	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetone	58	C3H6O	000067-64-1	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099459.D
Acq On : 14 Oct 2017 00:25
Operator : SJ/JU
Sample : I5819-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3911-SPP4

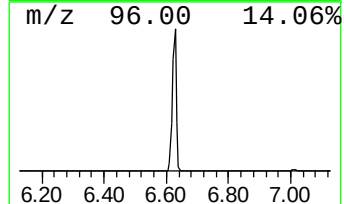
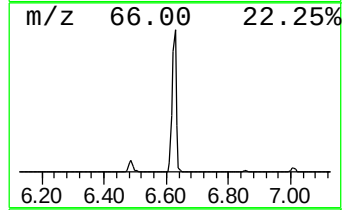
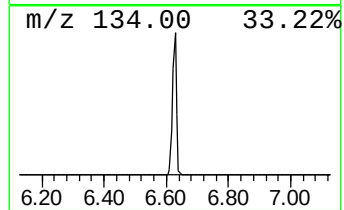
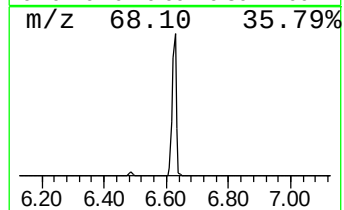
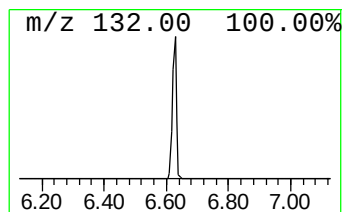
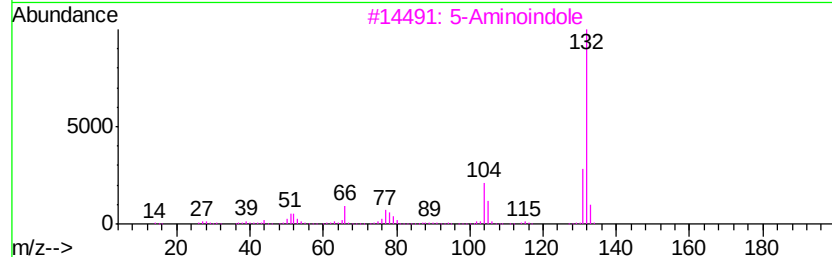
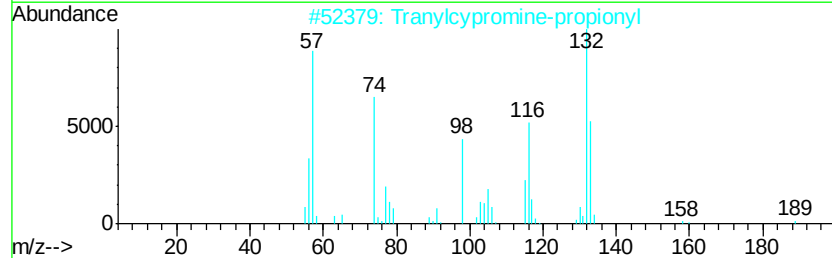
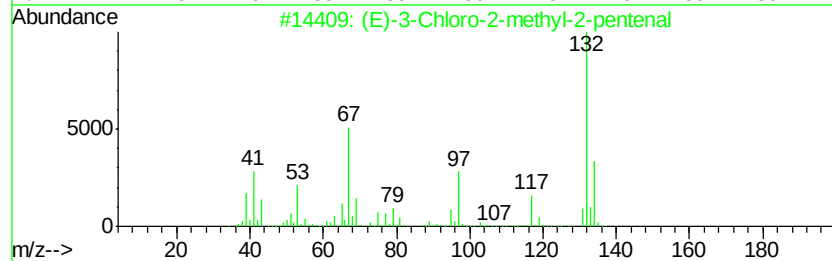
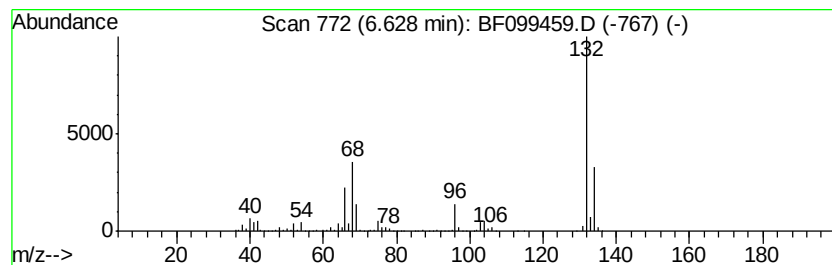
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (E)-3-Chloro-2-methyl-2-pen... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.58 ng	2421770	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Xenon	132	Xe	007440-63-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099459.D
Acq On : 14 Oct 2017 00:25
Operator : SJ/JU
Sample : I5819-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3911-SPP4

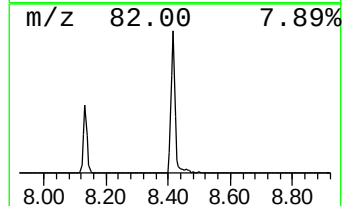
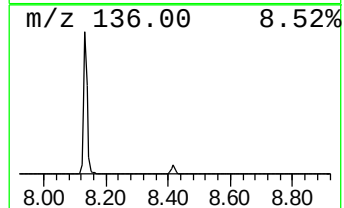
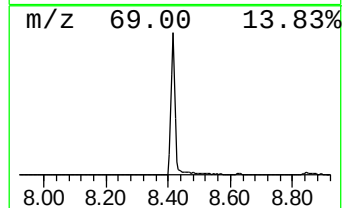
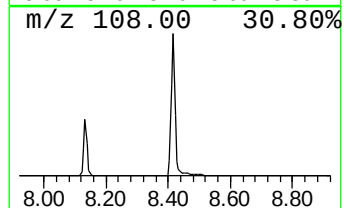
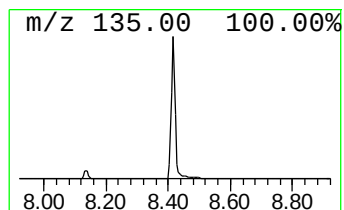
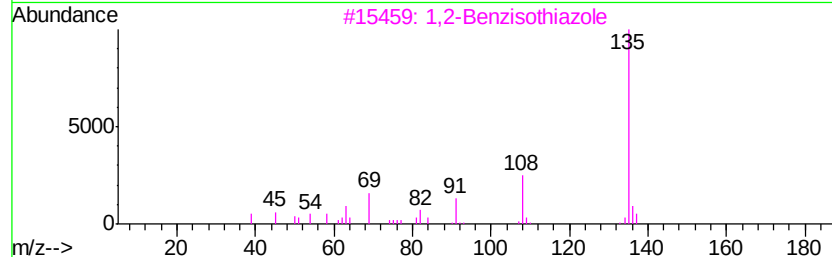
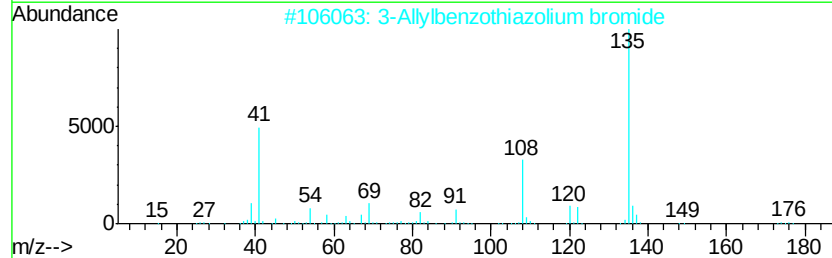
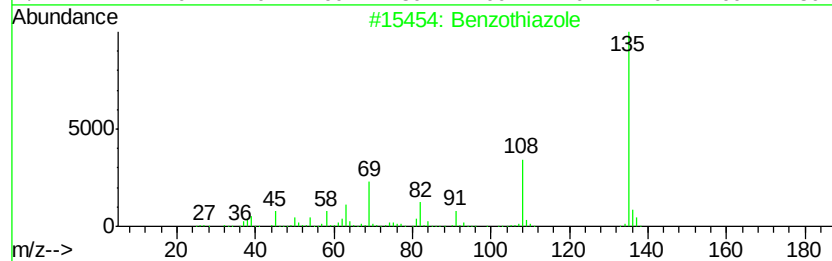
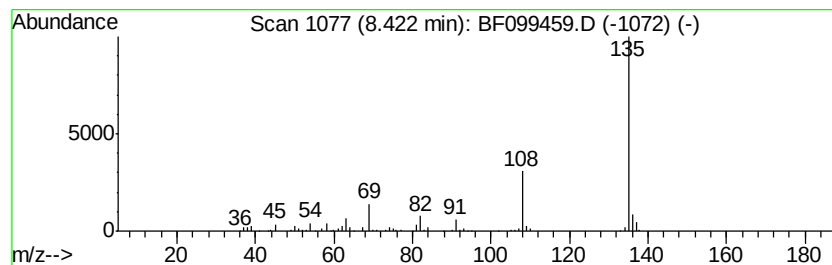
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	19.83 ng	711291	Naphthalene-d8	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	95
2		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
3		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	78
4		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
5		Adenine	135	C5H5N5	000073-24-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099459.D
Acq On : 14 Oct 2017 00:25
Operator : SJ/JU
Sample : I5819-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3911-SPP4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	8.9	ng	254015	1	6.85	572630	20.0
2-Pentanone, 4-hy...	5.08	6.9	ng	197151	1	6.85	572630	20.0
(E)-3-Chloro-2-me...	6.63	84.6	ng	2421770	1	6.85	572630	20.0
Benzothiazole	8.42	19.8	ng	711291	2	8.13	717374	20.0