

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099460.D
 Acq On : 14 Oct 2017 00:53
 Operator : SJ/JU
 Sample : I5819-11
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3914-PA3

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	2.128	3	7	14	rVB	171072	222347	7.98%	1.234%
2	5.075	505	508	520	rBV	158504	186056	6.67%	1.033%
3	5.475	573	576	591	rBV	1368834	1374992	49.33%	7.632%
4	6.487	744	748	758	rBV	928736	820911	29.45%	4.557%
5	6.628	767	772	775	rBV	2489445	2231955	80.07%	12.389%
6	6.851	807	810	814	rBV	635815	514456	18.46%	2.856%
7	7.010	833	837	840	rBV	2539024	2211336	79.33%	12.274%
8	7.422	902	907	910	rBV	1777421	1668272	59.85%	9.260%
9	8.134	1024	1028	1034	rBV	810715	646709	23.20%	3.590%
10	8.416	1073	1076	1082	rBV	98550	92195	3.31%	0.512%
11	9.210	1206	1211	1214	rBV	3153994	2787394	100.00%	15.472%
12	9.886	1323	1326	1330	rBV	678483	597260	21.43%	3.315%
13	10.680	1457	1461	1471	rBV	1318692	1218561	43.72%	6.764%
14	11.375	1576	1579	1583	rBV	549065	486546	17.46%	2.701%
15	12.963	1844	1849	1852	rBV	1935565	1904262	68.32%	10.570%
16	13.980	2020	2022	2025	rBV	86136	78611	2.82%	0.436%
17	14.021	2025	2029	2033	rBV	502307	454592	16.31%	2.523%
18	15.498	2275	2280	2286	rVB	422802	519250	18.63%	2.882%

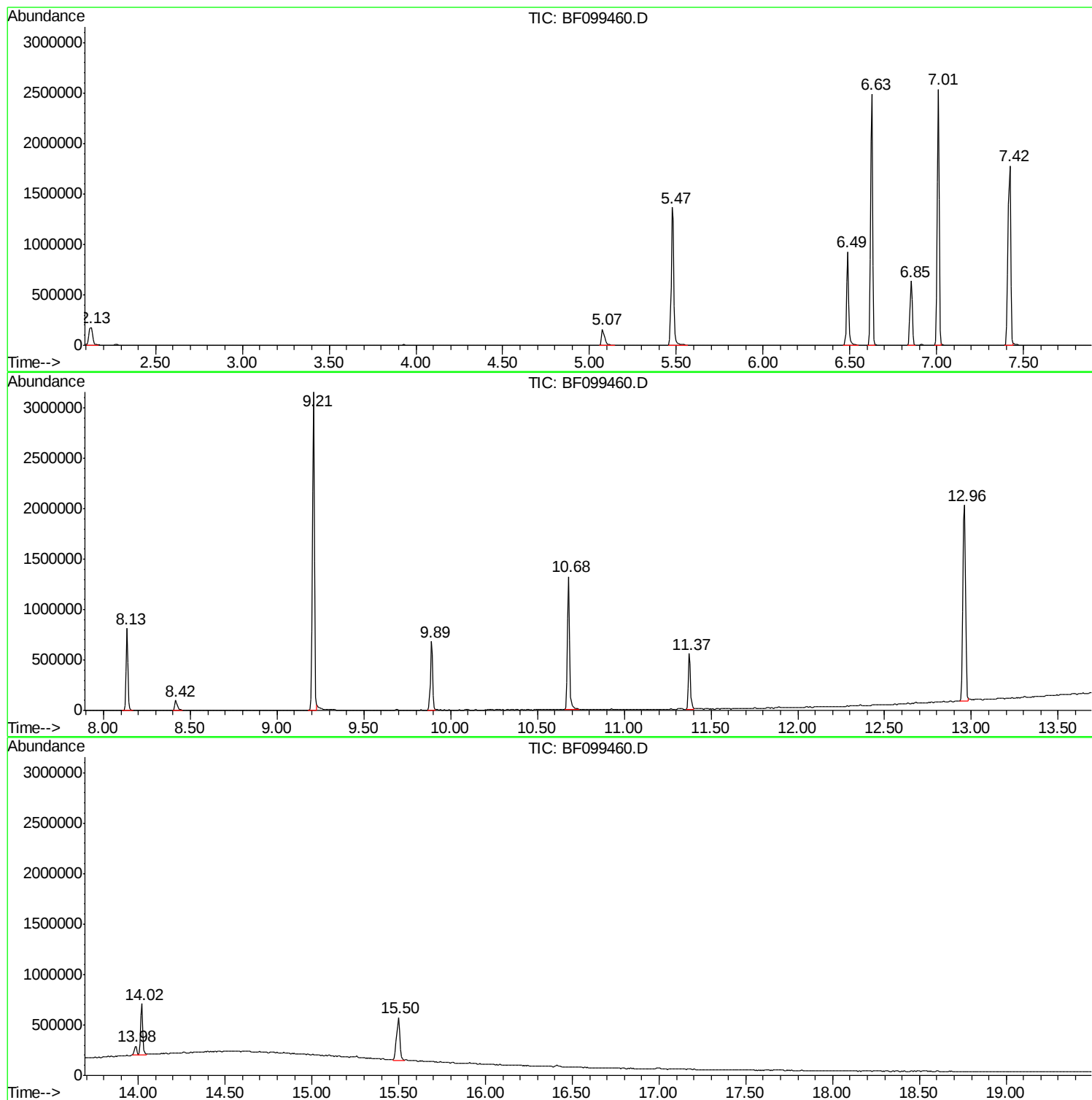
Sum of corrected areas: 18015705

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099460.D
Acq On : 14 Oct 2017 00:53
Operator : SJ/JU
Sample : I5819-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3914-PA3

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 : BF099460.D
Acq On : 14 Oct 2017 00:53
Operator : SJ/JU
Sample : I5819-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3914-PA3

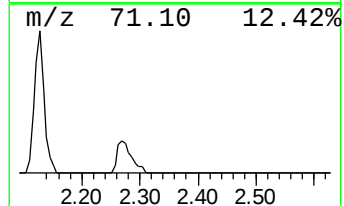
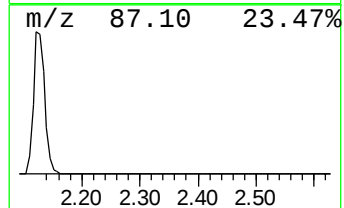
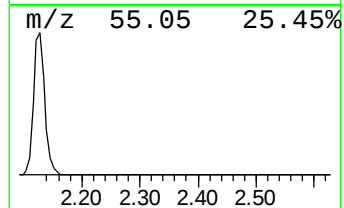
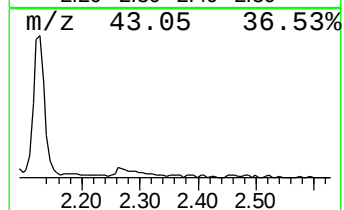
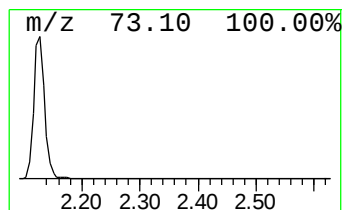
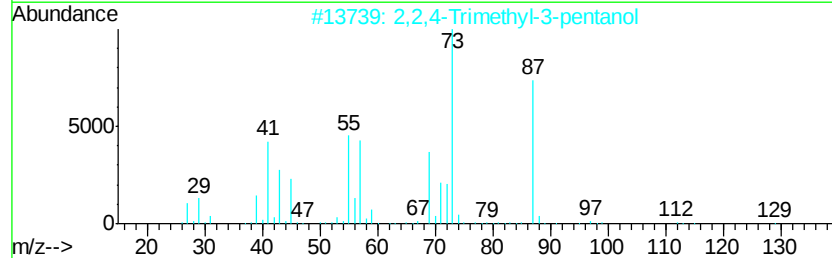
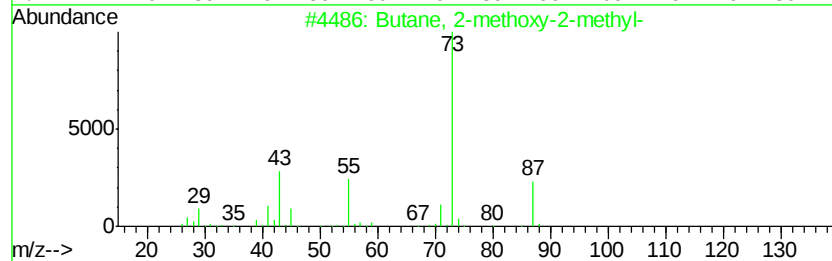
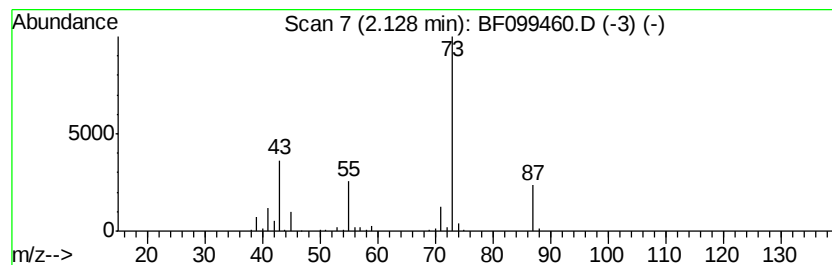
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	8.64 ng	222347	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5			1,4-Butanediamine	88	C4H12N2	000110-60-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099460.D
Acq On : 14 Oct 2017 00:53
Operator : SJ/JU
Sample : I5819-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3914-PA3

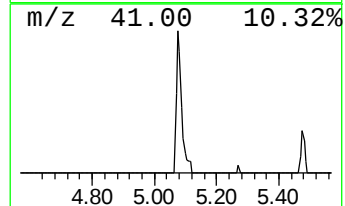
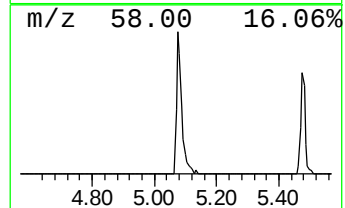
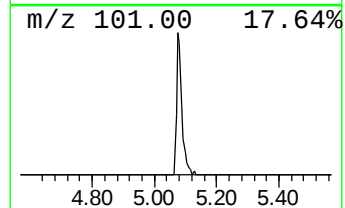
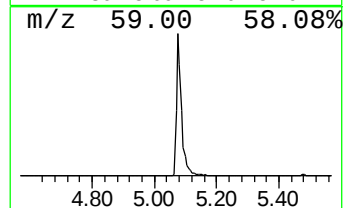
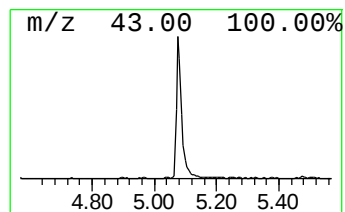
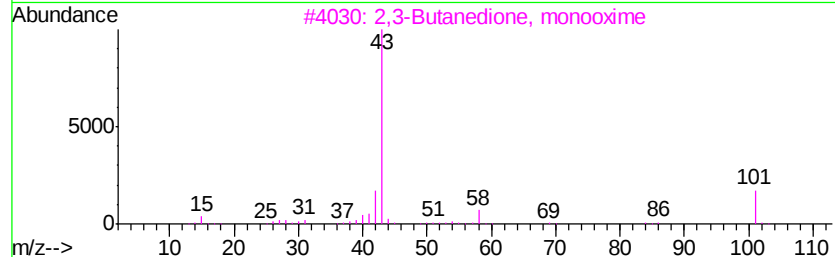
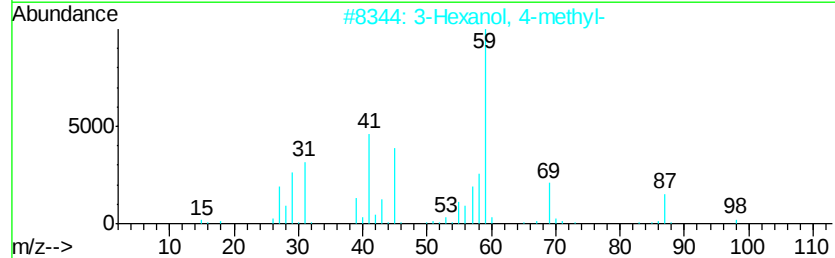
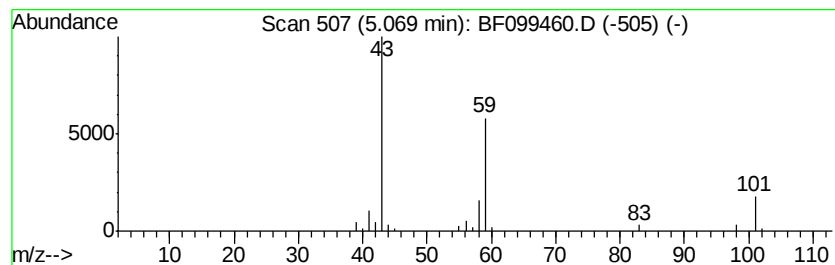
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	7.23 ng	186056	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	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099460.D
Acq On : 14 Oct 2017 00:53
Operator : SJ/JU
Sample : I5819-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3914-PA3

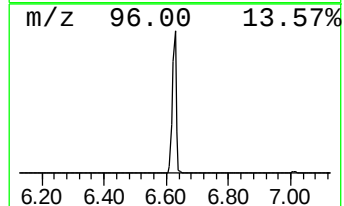
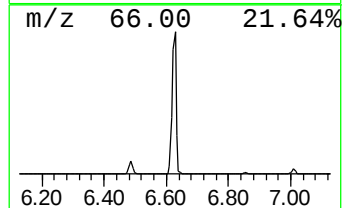
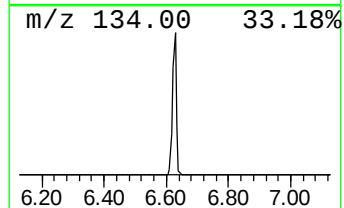
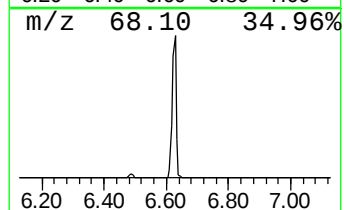
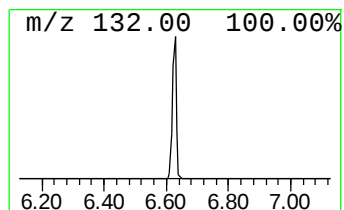
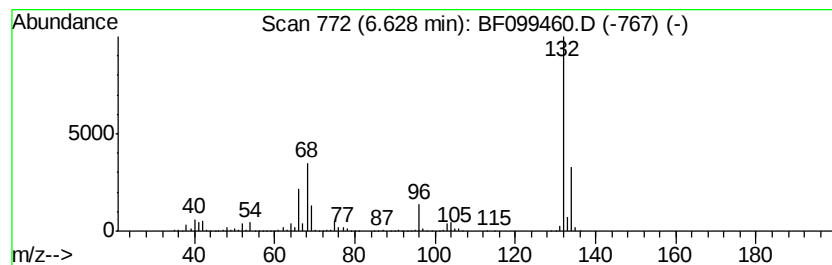
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	86.77 ng	2231960	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099460.D
Acq On : 14 Oct 2017 00:53
Operator : SJ/JU
Sample : I5819-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3914-PA3

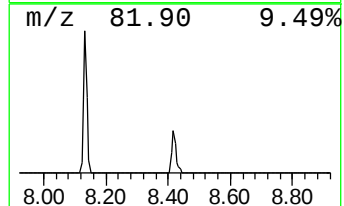
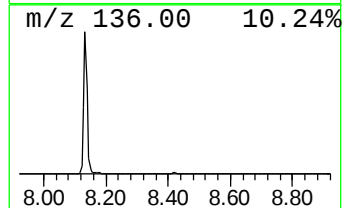
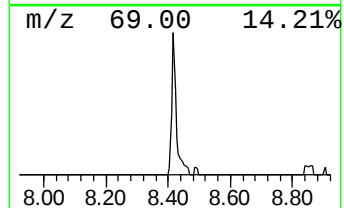
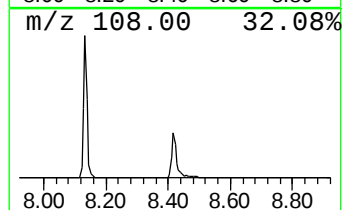
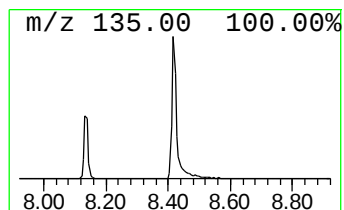
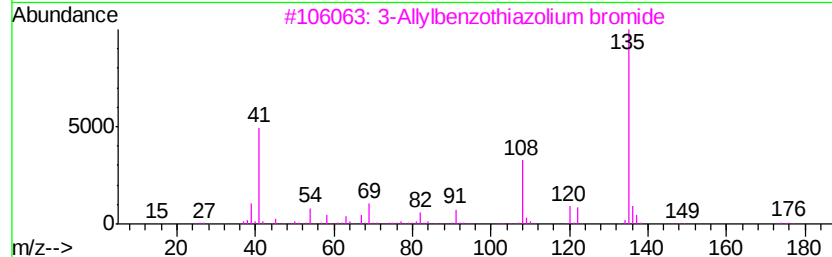
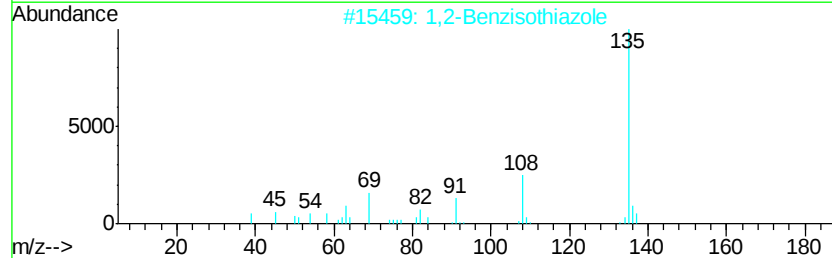
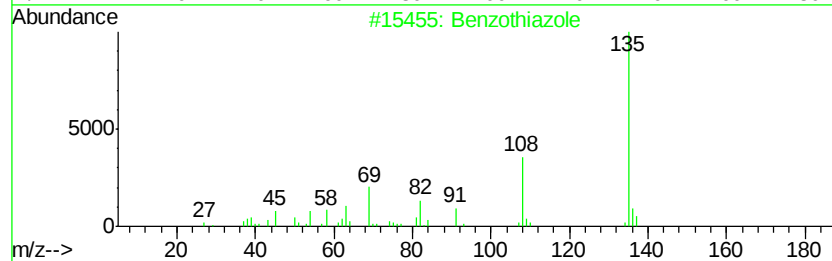
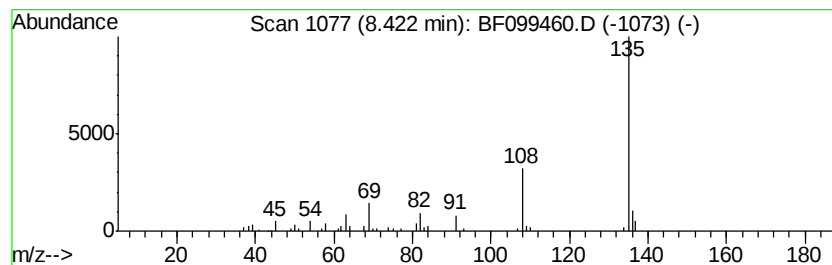
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	2.85 ng	92195	Naphthalene-d8	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	95
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	83
4		Thiocyanic acid, phenyl ester	135	C7H5NS	005285-87-0	64
5		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099460.D
Acq On : 14 Oct 2017 00:53
Operator : SJ/JU
Sample : I5819-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3914-PA3

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	8.6	ng	222347	1	6.85	514456	20.0
2-Pentanone, 4-hy...	5.07	7.2	ng	186056	1	6.85	514456	20.0
unknown6.63	6.63	86.8	ng	2231960	1	6.85	514456	20.0
Benzothiazole	8.42	2.9	ng	92195	2	8.13	646709	20.0