

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099457.D
 Acq On : 13 Oct 2017 23:29
 Operator : SJ/JU
 Sample : I5819-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3909-SPP2-DUP

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-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	4	8	15	rVB	183768	240362	7.79%	1.205%
2	5.075	505	508	523	rBV	162693	203748	6.60%	1.022%
3	5.475	573	576	599	rVB	1428876	1427967	46.26%	7.161%
4	6.487	744	748	760	rBV	960189	851936	27.60%	4.272%
5	6.628	767	772	775	rBV	2651908	2417349	78.32%	12.123%
6	6.851	807	810	814	rBV	684774	550719	17.84%	2.762%
7	7.010	833	837	840	rBV	2629685	2386104	77.31%	11.966%
8	7.422	902	907	910	rBV	1881245	1834518	59.44%	9.200%
9	8.134	1024	1028	1032	rBV	873403	705589	22.86%	3.538%
10	8.416	1072	1076	1082	rBV	594734	520620	16.87%	2.611%
11	9.210	1206	1211	1214	rBV	3328091	3086592	100.00%	15.479%
12	9.886	1323	1326	1330	rBV2	757863	655464	21.24%	3.287%
13	10.680	1457	1461	1470	rBV	1471264	1404949	45.52%	7.046%
14	10.792	1477	1480	1488	rVB	44438	52783	1.71%	0.265%
15	11.375	1576	1579	1583	rBV	623777	527084	17.08%	2.643%
16	12.963	1844	1849	1852	rBV	2097212	2050747	66.44%	10.284%
17	14.016	2024	2028	2034	rBV	497136	482916	15.65%	2.422%
18	15.492	2274	2279	2290	rVB	440071	541494	17.54%	2.715%

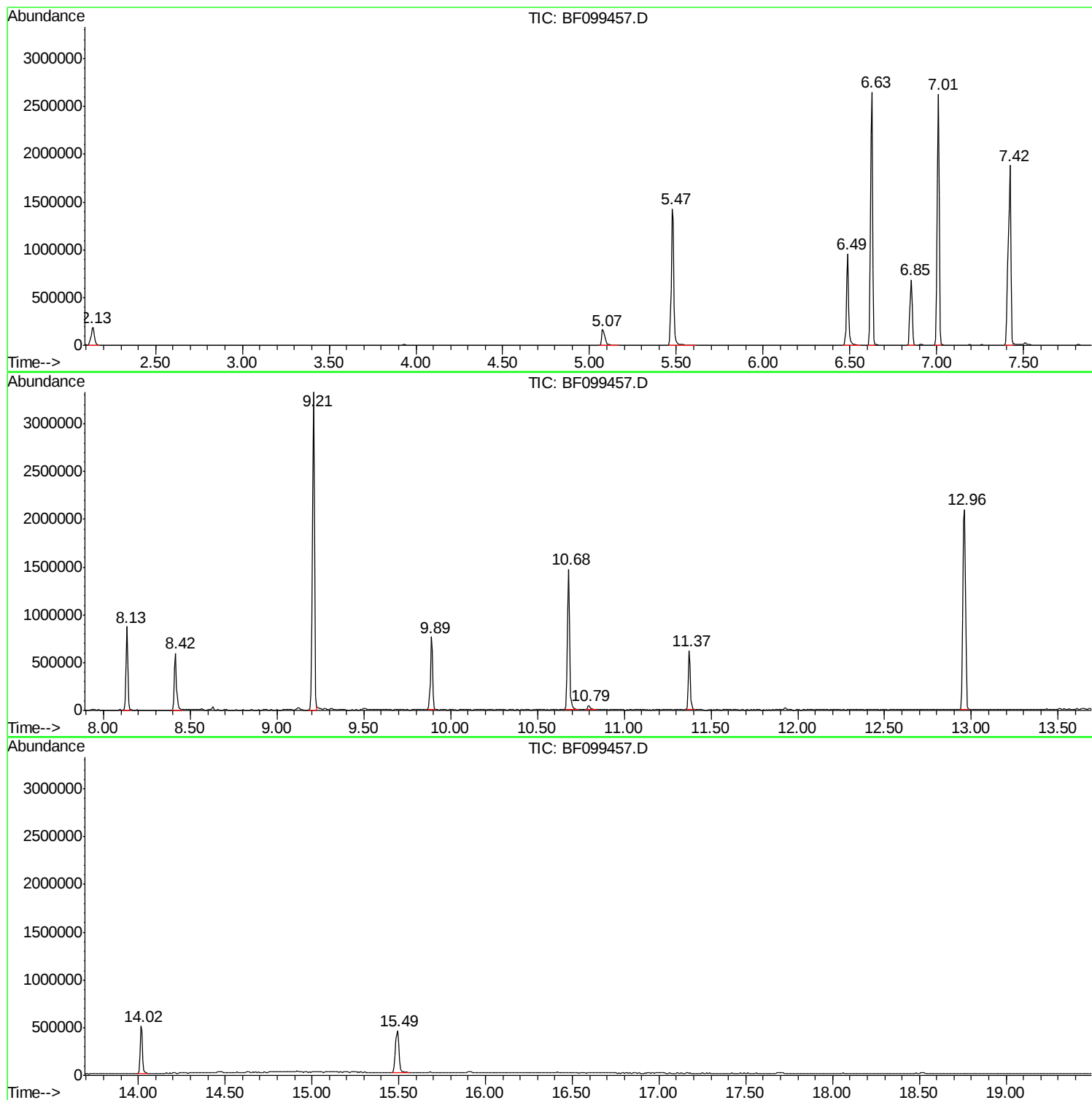
Sum of corrected areas: 19940941

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099457.D
Acq On : 13 Oct 2017 23:29
Operator : SJ/JU
Sample : I5819-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3909-SPP2-DUP

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 : BF099457.D
Acq On : 13 Oct 2017 23:29
Operator : SJ/JU
Sample : I5819-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3909-SPP2-DUP

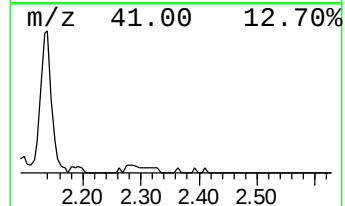
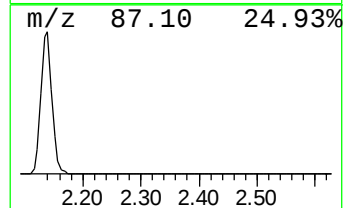
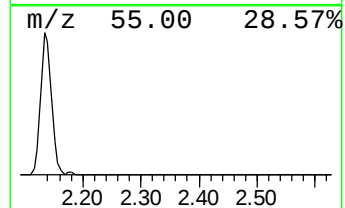
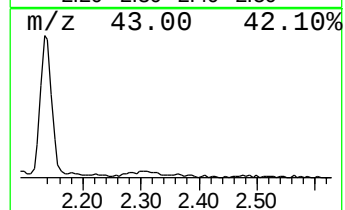
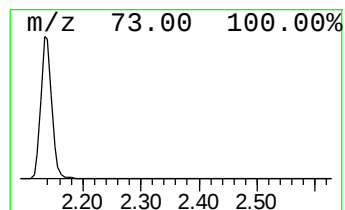
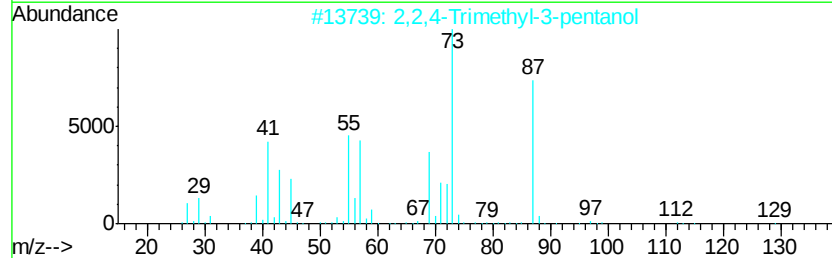
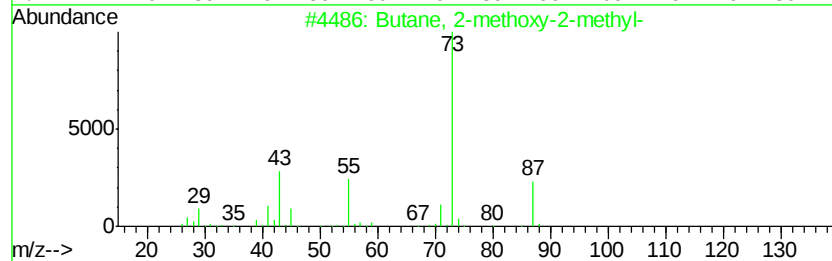
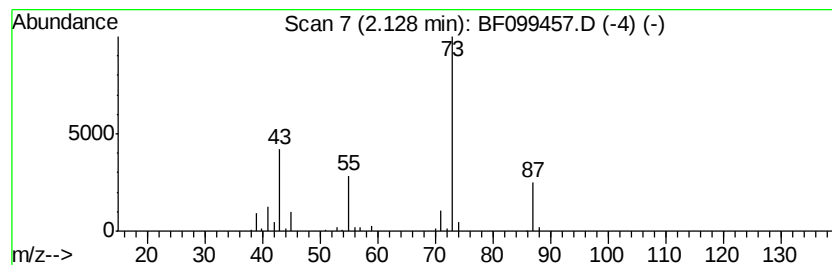
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	8.73 ng	240362	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	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099457.D
Acq On : 13 Oct 2017 23:29
Operator : SJ/JU
Sample : I5819-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3909-SPP2-DUP

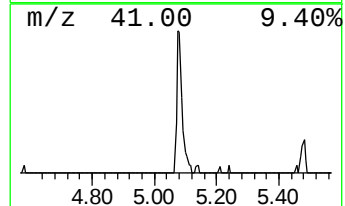
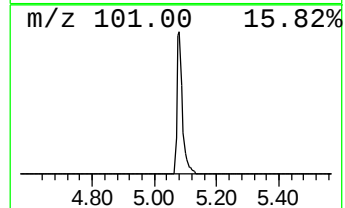
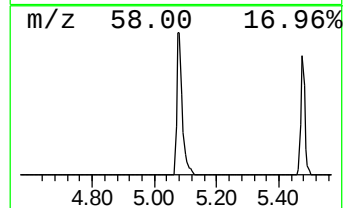
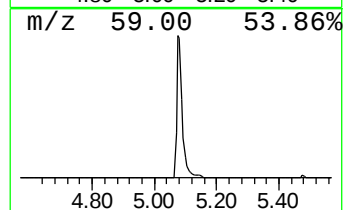
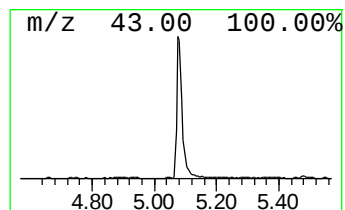
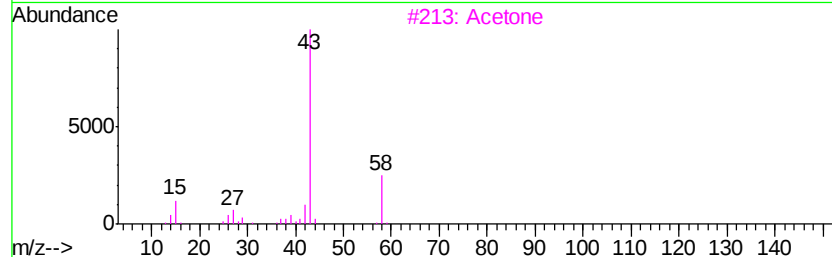
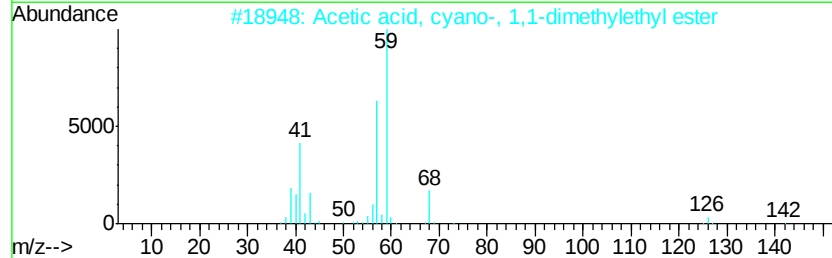
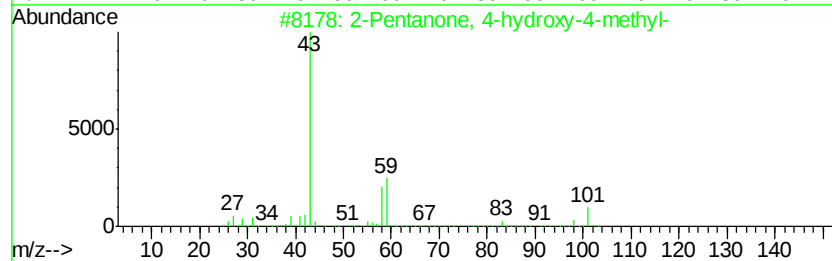
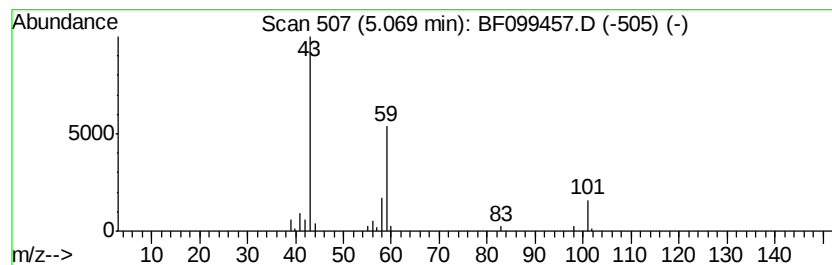
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.07	7.40 ng	203748	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Acetone	58	C3H6O	000067-64-1	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099457.D
Acq On : 13 Oct 2017 23:29
Operator : SJ/JU
Sample : I5819-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3909-SPP2-DUP

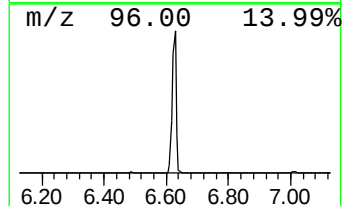
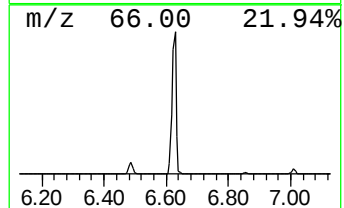
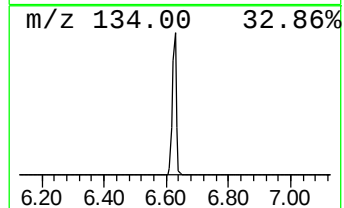
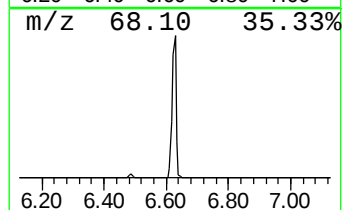
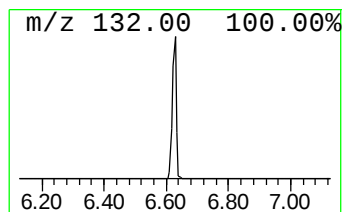
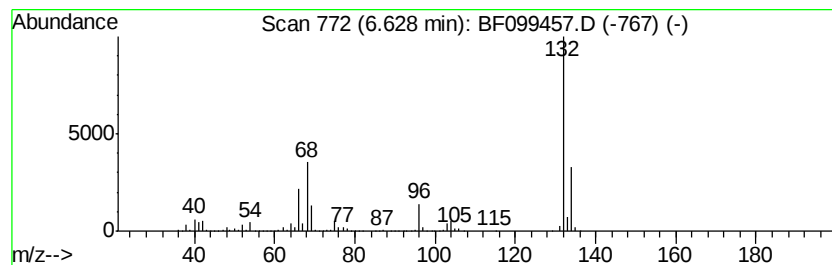
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	87.79 ng	2417350	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	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		Xenon	132	Xe	007440-63-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099457.D
Acq On : 13 Oct 2017 23:29
Operator : SJ/JU
Sample : I5819-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3909-SPP2-DUP

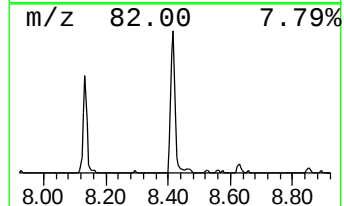
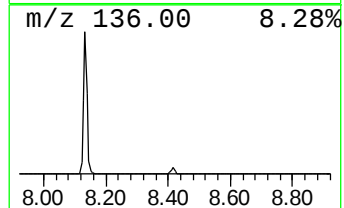
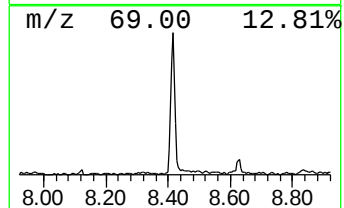
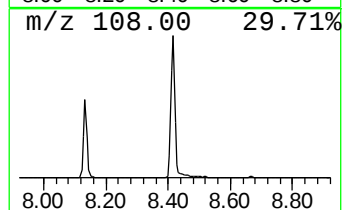
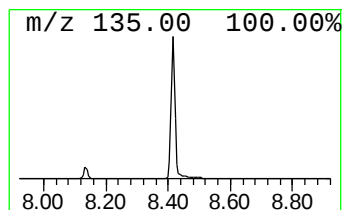
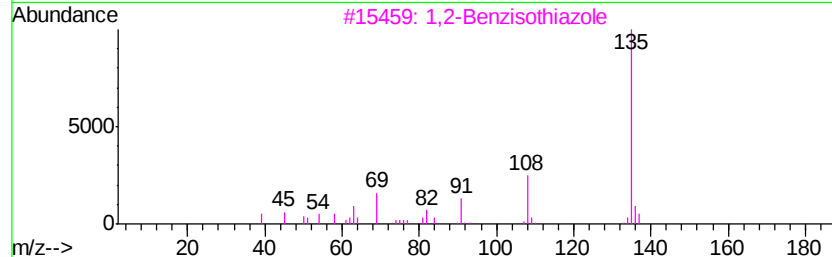
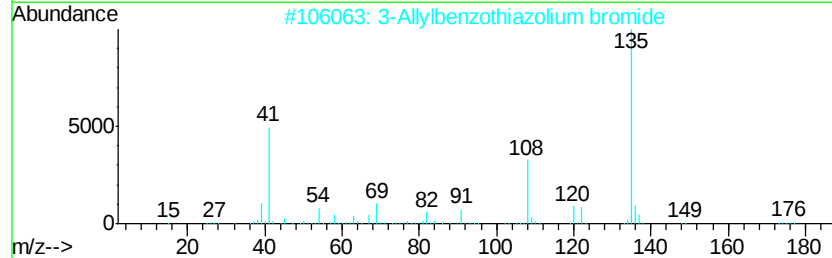
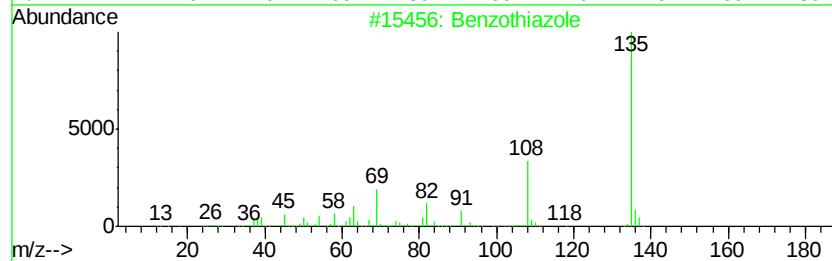
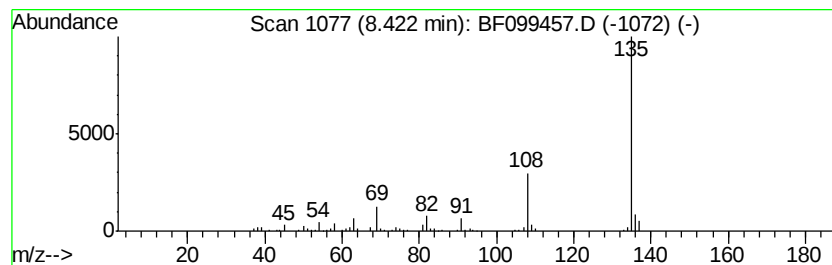
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	14.76 ng	520620	Naphthalene-d8	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	94
2		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
3		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	86
4		Adenine	135	C5H5N5	000073-24-5	64
5		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099457.D
Acq On : 13 Oct 2017 23:29
Operator : SJ/JU
Sample : I5819-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

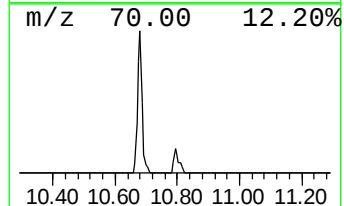
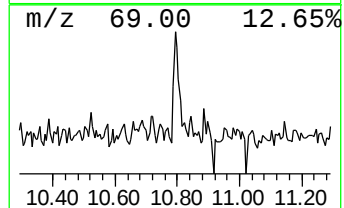
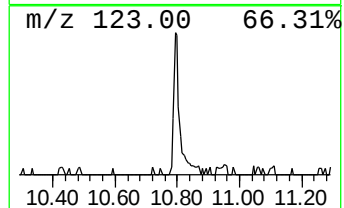
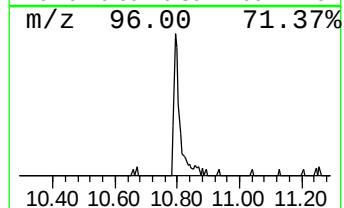
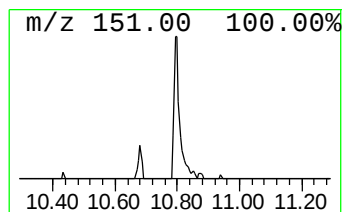
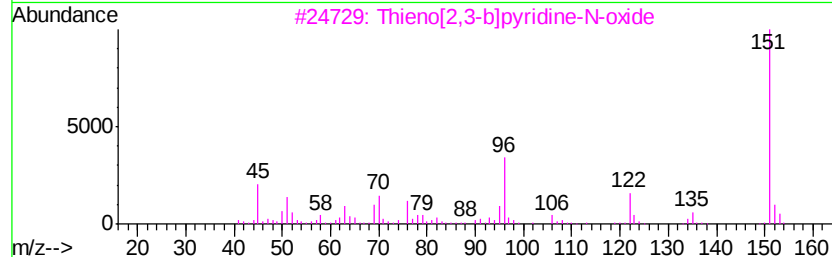
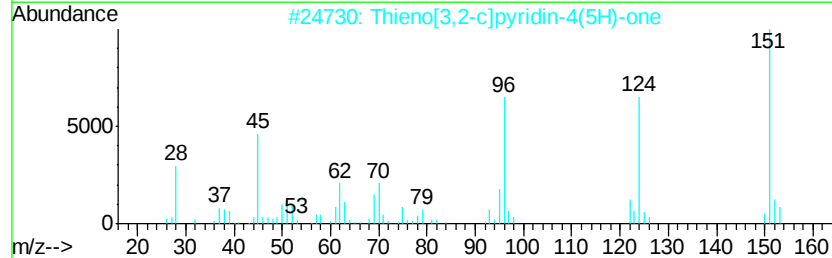
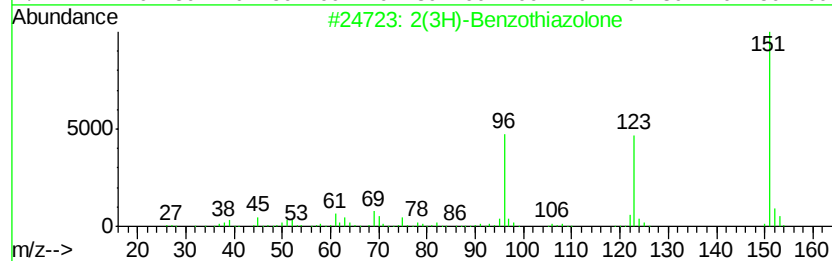
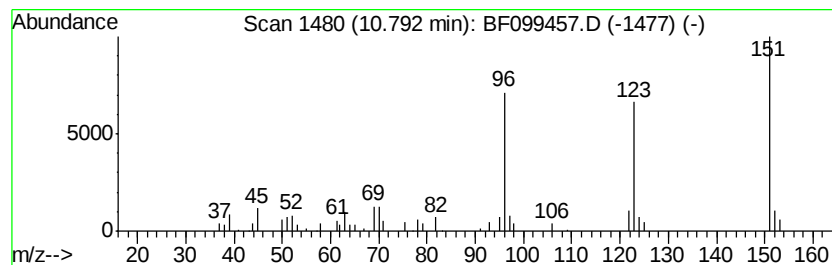
Instrument :
BNA_F
ClientSampleId :
3909-SPP2-DUP

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 6 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.79	2.00 ng	52783	Phenanthrene-d10		11.37	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2		Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	64
3		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	50
4		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	49
5		4-Methoxyformanilide	151	C8H9NO2	005470-34-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099457.D
Acq On : 13 Oct 2017 23:29
Operator : SJ/JU
Sample : I5819-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3909-SPP2-DUP

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	8.7	ng	240362	1	6.85	550719	20.0
2-Pentanone, 4-hy...	5.07	7.4	ng	203748	1	6.85	550719	20.0
unknown6.63	6.63	87.8	ng	2417350	1	6.85	550719	20.0
Benzothiazole	8.42	14.8	ng	520620	2	8.13	705589	20.0
2(3H)-Benzothiazo...	10.79	2.0	ng	52783	4	11.37	527084	20.0