

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
 Data File : BF096840.D
 Acq On : 18 Jul 2017 11:39
 Operator : SJ/JU
 Sample : I4199-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3573-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-BF071317.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	4.757	467	471	479	rBV	93393	110633	3.83%	0.559%
2	5.198	542	546	561	rVB	1213060	1123965	38.90%	5.676%
3	6.239	719	723	734	rVB	849236	707781	24.50%	3.574%
4	6.369	740	745	748	rBV	2123274	2028995	70.22%	10.247%
5	6.598	780	784	787	rBV	739012	660800	22.87%	3.337%
6	6.751	806	810	814	rBV	1921816	1903400	65.87%	9.612%
7	7.163	874	880	883	rBV	1965881	1855501	64.22%	9.370%
8	7.881	997	1002	1005	rBV	1153705	1014400	35.11%	5.123%
9	7.957	1009	1015	1022	rBV3	37130	94867	3.28%	0.479%
10	8.151	1045	1048	1053	rVB	229671	203079	7.03%	1.026%
11	8.957	1179	1185	1188	rBV	2833496	2889456	100.00%	14.592%
12	9.392	1256	1259	1263	rVB	31949	31234	1.08%	0.158%
13	9.627	1294	1299	1303	rBV	1160900	990876	34.29%	5.004%
14	10.251	1402	1405	1408	rVB2	33151	29502	1.02%	0.149%
15	10.416	1427	1433	1436	rBV	1549834	1560824	54.02%	7.882%
16	11.104	1546	1550	1553	rBV	982871	846552	29.30%	4.275%
17	11.651	1640	1643	1646	rBV	167718	172321	5.96%	0.870%
18	12.439	1773	1777	1785	rVB	320121	320607	11.10%	1.619%
19	12.692	1815	1820	1823	rBV	1990985	2138175	74.00%	10.798%
20	13.727	1992	1996	2002	rBV	666157	566747	19.61%	2.862%
21	14.374	2104	2106	2109	rVB	61018	50477	1.75%	0.255%
22	15.098	2225	2229	2234	rVB	447154	501619	17.36%	2.533%

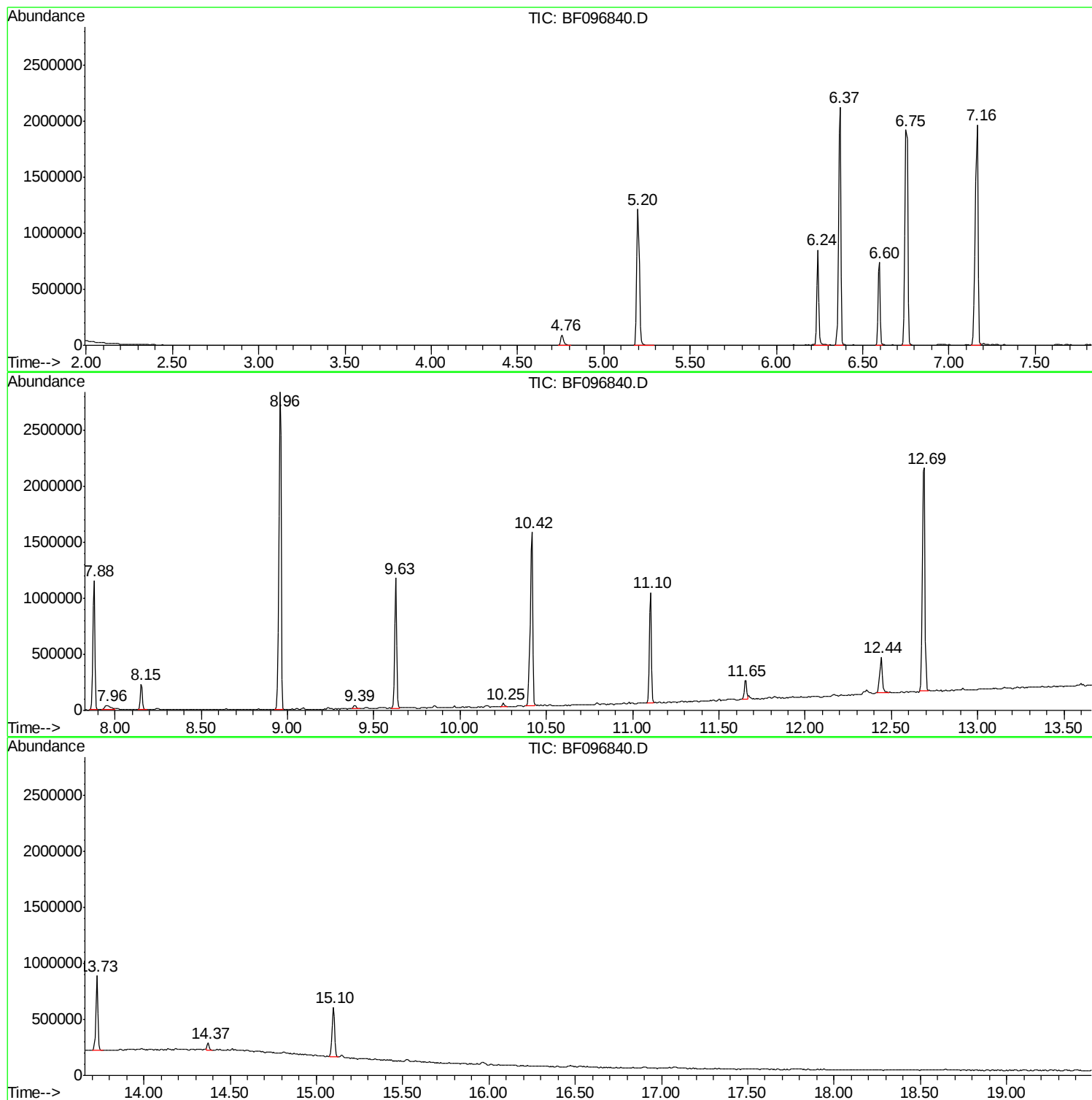
Sum of corrected areas: 19801811

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
Data File : BF096840.D
Acq On : 18 Jul 2017 11:39
Operator : SJ/JU
Sample : I4199-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3573-PA3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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\BF071817\
Data File : BF096840.D
Acq On : 18 Jul 2017 11:39
Operator : SJ/JU
Sample : I4199-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3573-PA3

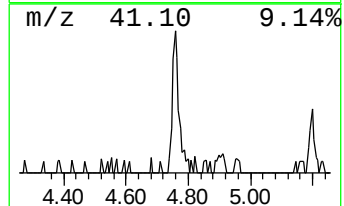
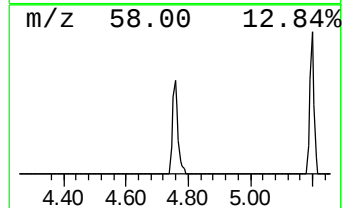
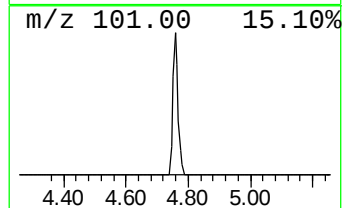
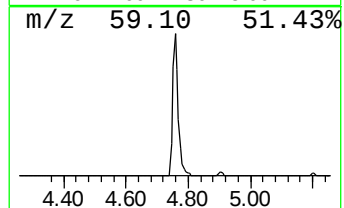
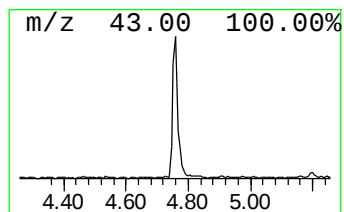
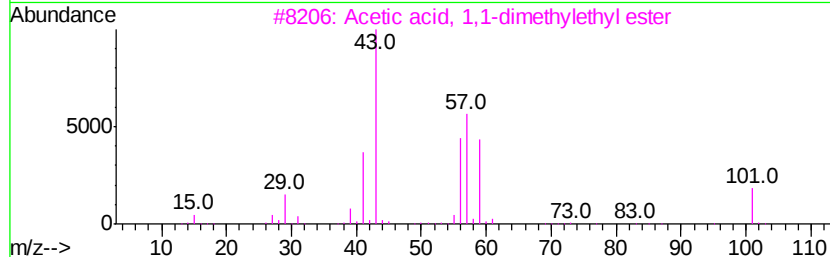
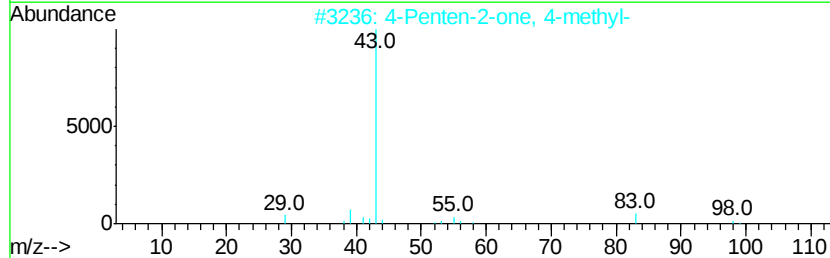
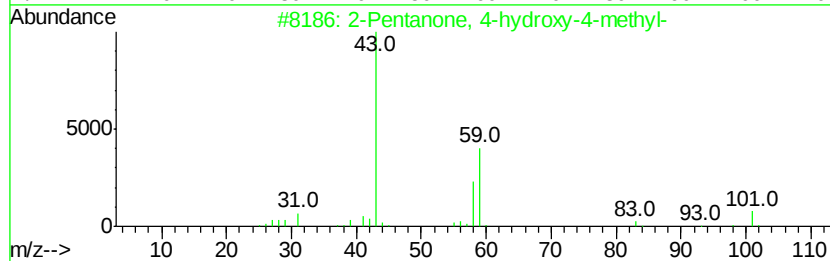
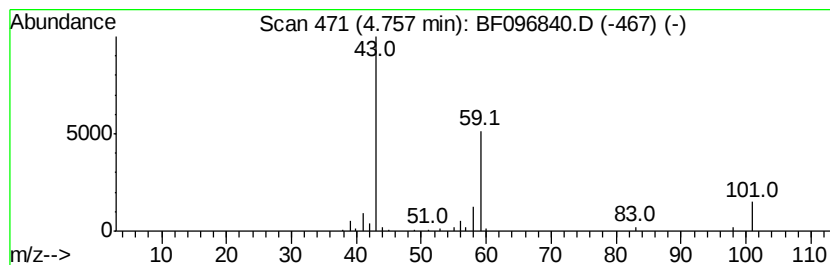
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.76 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	3.35 ng	110633	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			1,2-Butanediol	90	C4H10O2	000584-03-2	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096840.D
Acq On : 18 Jul 2017 11:39
Operator : SJ/JU
Sample : I4199-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3573-PA3

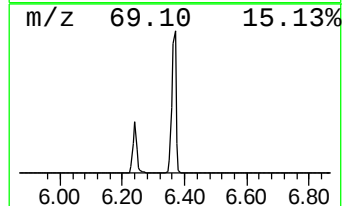
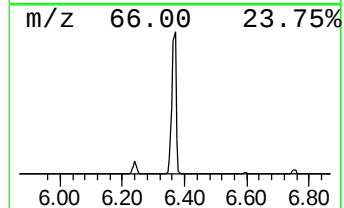
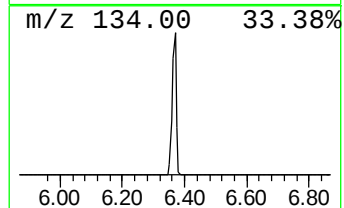
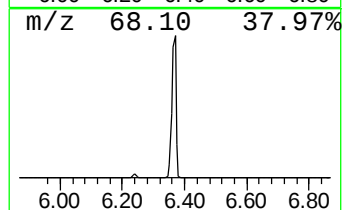
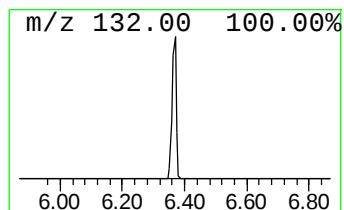
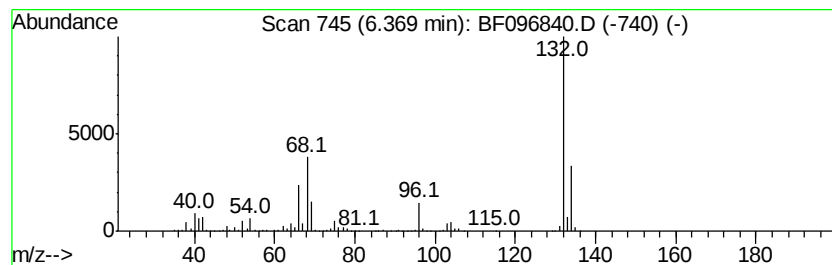
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	61.41 ng	2029000	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096840.D
Acq On : 18 Jul 2017 11:39
Operator : SJ/JU
Sample : I4199-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3573-PA3

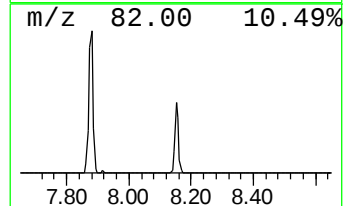
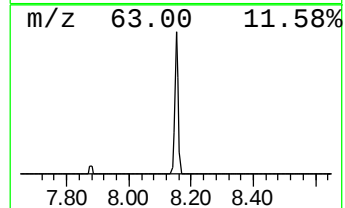
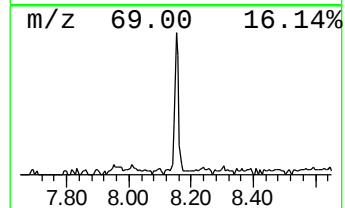
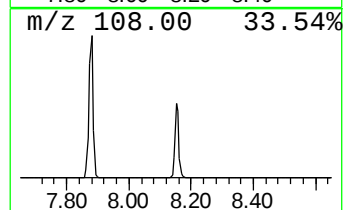
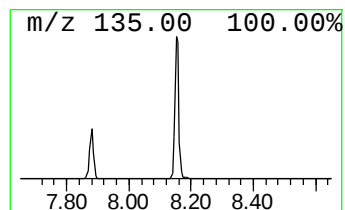
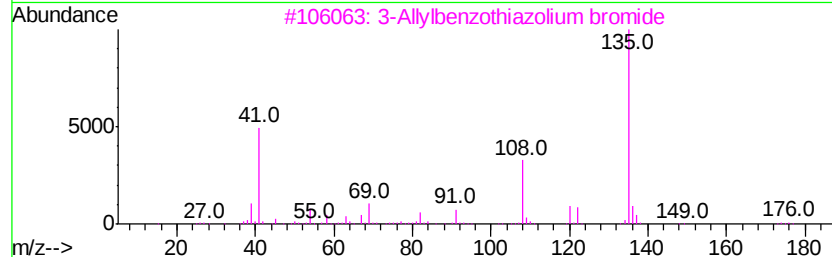
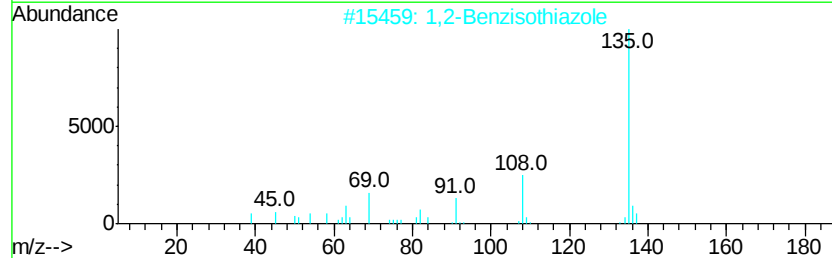
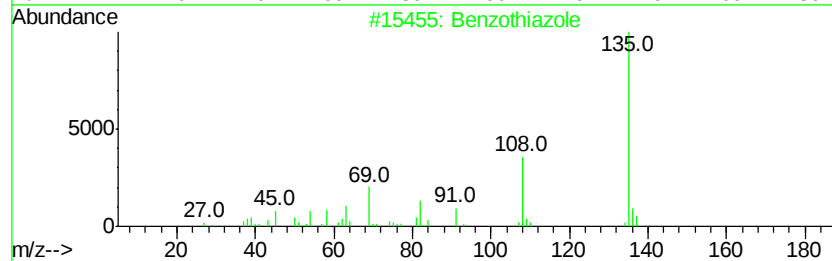
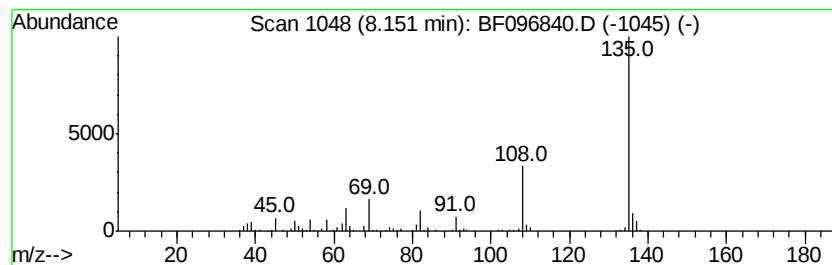
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	4.00 ng	203079	Naphthalene-d8	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	97
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	64
4		2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	59
5		Adenine	135	C5H5N5	000073-24-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
Data File : BF096840.D
Acq On : 18 Jul 2017 11:39
Operator : SJ/JU
Sample : I4199-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3573-PA3

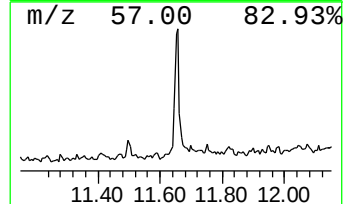
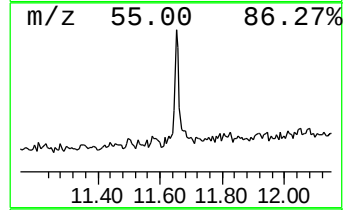
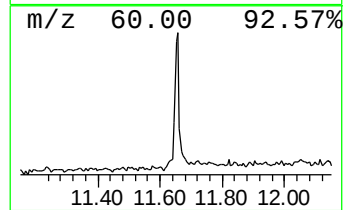
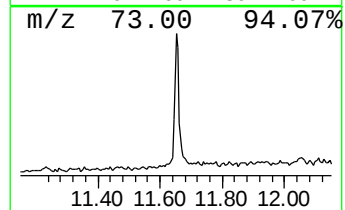
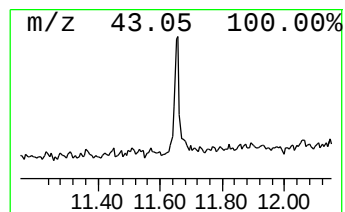
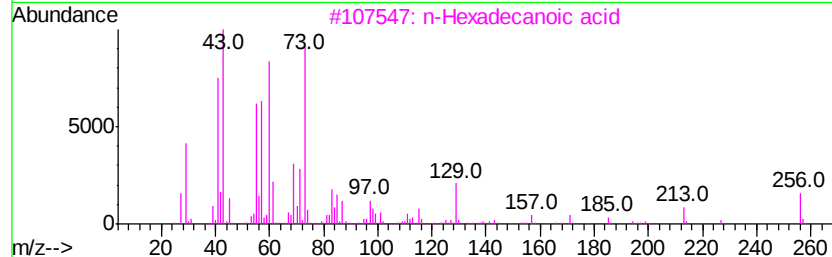
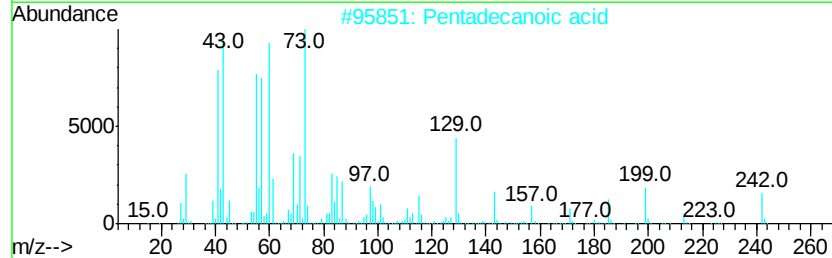
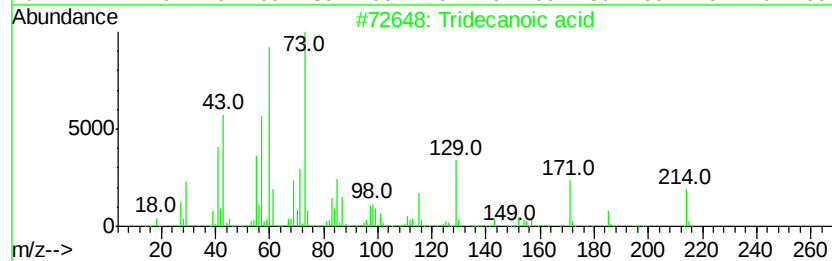
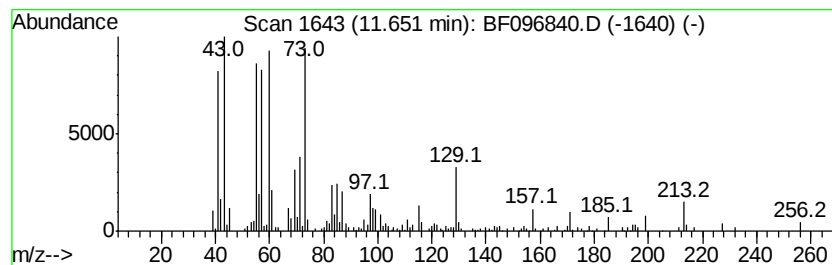
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	4.07 ng	172321	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Undecanoic acid	186	C11H22O2	000112-37-8	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
Data File : BF096840.D
Acq On : 18 Jul 2017 11:39
Operator : SJ/JU
Sample : I4199-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3573-PA3

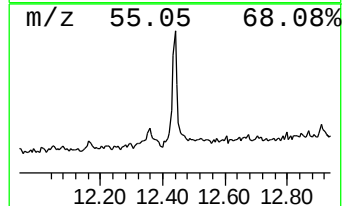
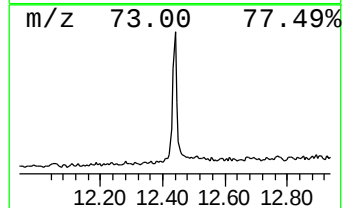
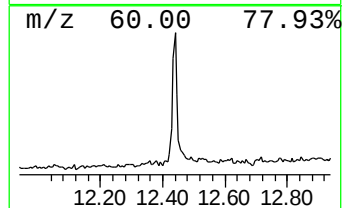
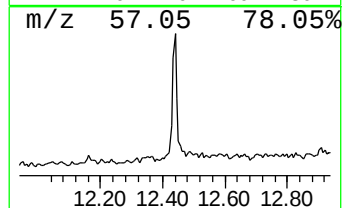
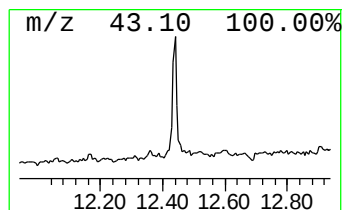
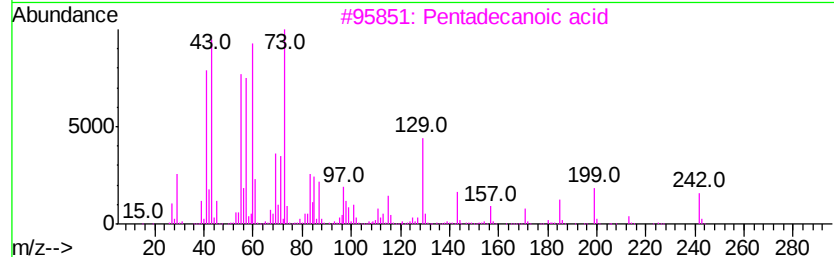
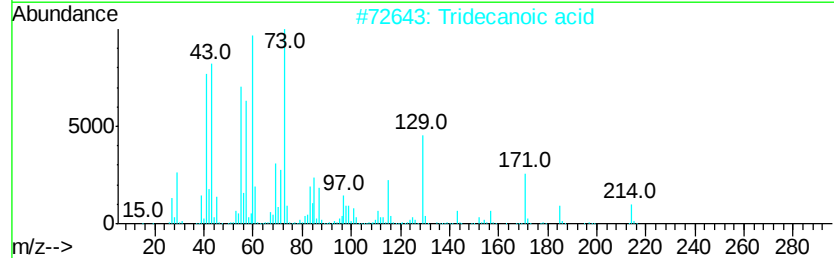
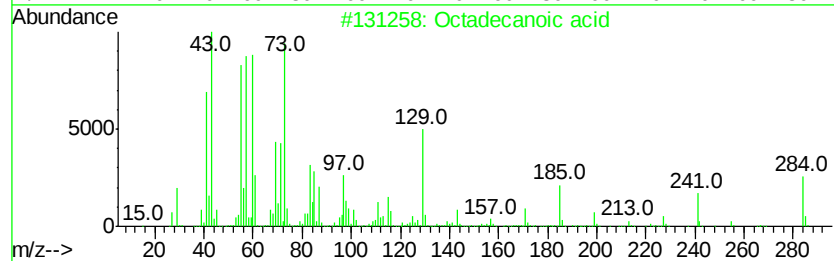
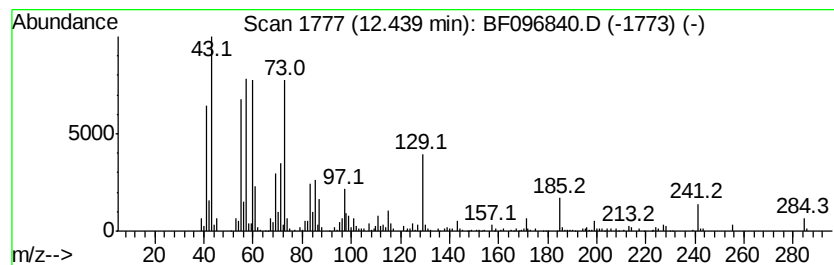
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	11.31 ng	320607	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	74
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
Data File : BF096840.D
Acq On : 18 Jul 2017 11:39
Operator : SJ/JU
Sample : I4199-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3573-PA3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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
unknown4.76	4.76	3.4	ng	110633	1	6.60	660800	20.0
unknown6.37	6.37	61.4	ng	2029000	1	6.60	660800	20.0
Benzothiazole	8.15	4.0	ng	203079	2	7.88	1014400	20.0
Tridecanoic acid	11.65	4.1	ng	172321	4	11.10	846552	20.0
Octadecanoic acid	12.44	11.3	ng	320607	5	13.73	566747	20.0