

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
 Data File : BM009926.D
 Acq On : 06 May 2017 05:30
 Operator : SJ/MA
 Sample : I2893-14
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3073-PA4

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	4.910	304	310	320	rBV	208723	303673	2.74%	0.619%
2	5.369	381	388	397	rBV	1396167	2094447	18.88%	4.267%
3	6.963	652	659	671	rBV2	881170	1435566	12.94%	2.925%
4	7.316	711	719	729	rBV	2710163	4260122	38.39%	8.679%
5	7.775	790	797	804	rBV	501964	824548	7.43%	1.680%
6	8.098	843	852	860	rBV	2248509	3673251	33.11%	7.483%
7	8.951	989	997	1005	rBV	2310982	3778967	34.06%	7.699%
8	10.575	1264	1273	1281	rBV	697088	1148378	10.35%	2.340%
9	11.239	1381	1386	1394	rBV	80346	143278	1.29%	0.292%
10	13.045	1683	1693	1701	rBV	5208365	7319391	65.97%	14.912%
11	14.433	1922	1929	1936	rBV2	975725	1499358	13.51%	3.055%
12	15.933	2177	2184	2194	rBV	4535131	6139206	55.33%	12.507%
13	16.151	2218	2221	2228	rVB4	84376	130815	1.18%	0.267%
14	17.186	2391	2397	2408	rBV	1253561	1795987	16.19%	3.659%
15	18.068	2543	2547	2553	rBV2	128573	190502	1.72%	0.388%
16	19.351	2761	2765	2769	rBV4	118292	187942	1.69%	0.383%
17	19.815	2838	2844	2849	rBV	9272628	11095754	100.00%	22.605%
18	21.374	3105	3109	3115	rBV	1366717	1689033	15.22%	3.441%
19	23.680	3496	3501	3509	rVB	706704	1374774	12.39%	2.801%

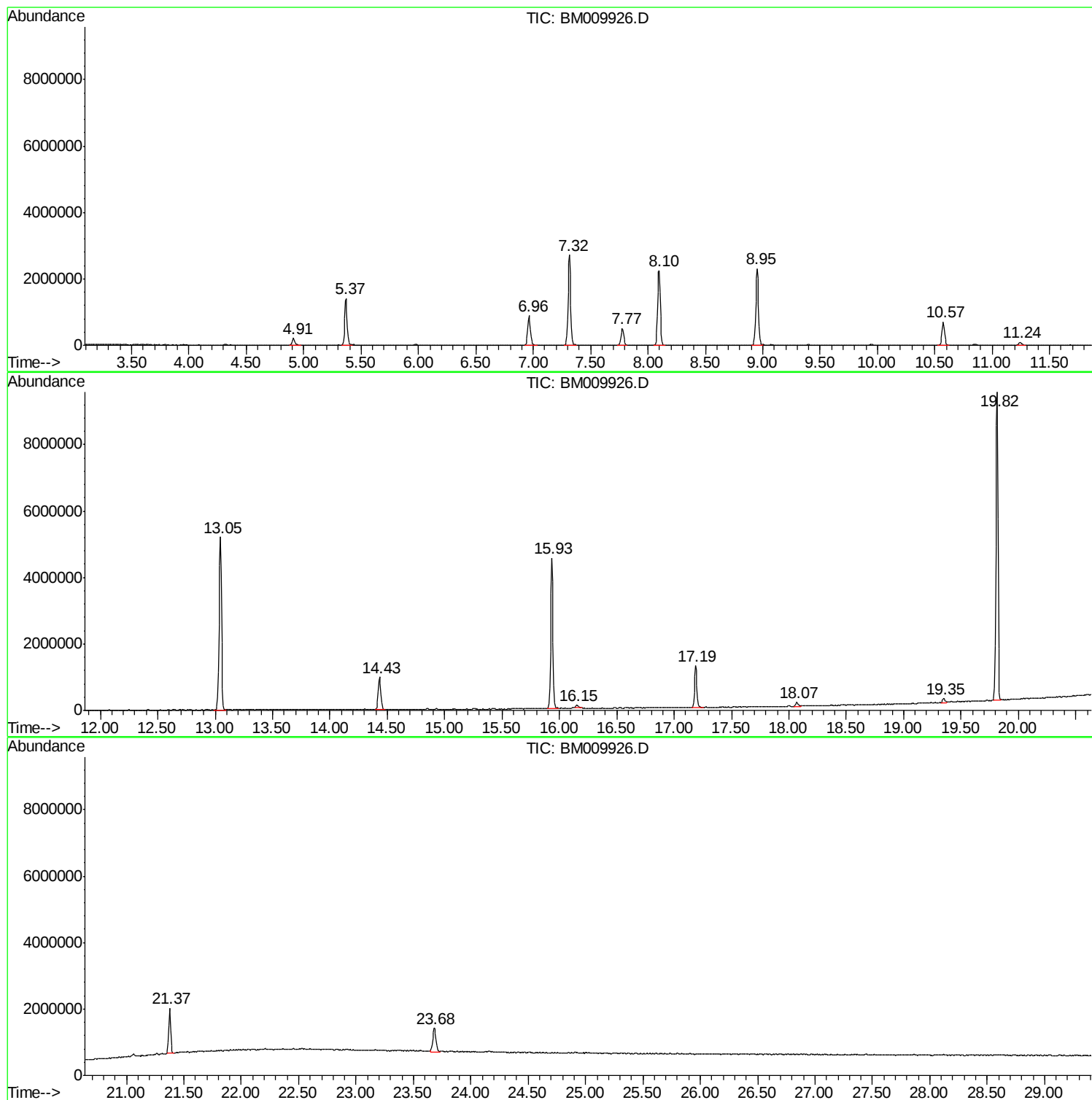
Sum of corrected areas: 49084992

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009926.D
Acq On : 06 May 2017 05:30
Operator : SJ/MA
Sample : I2893-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3073-PA4

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 : BM009926.D
Acq On : 06 May 2017 05:30
Operator : SJ/MA
Sample : I2893-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3073-PA4

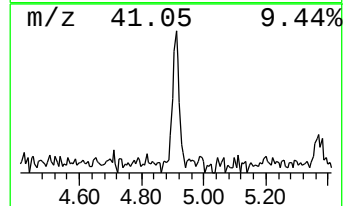
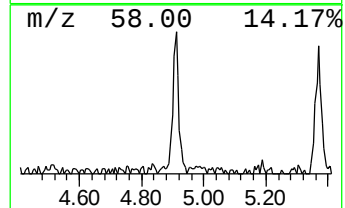
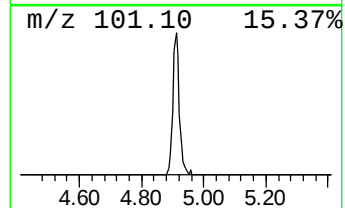
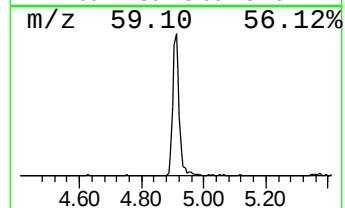
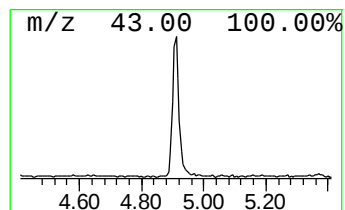
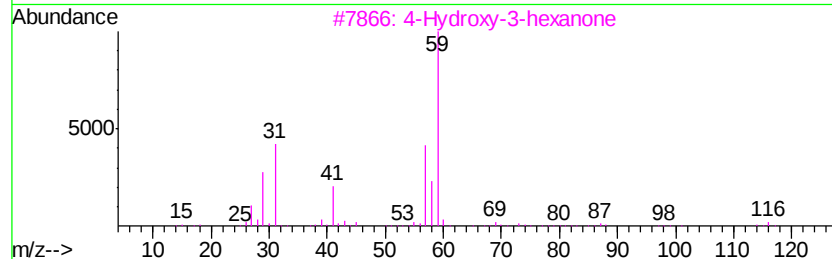
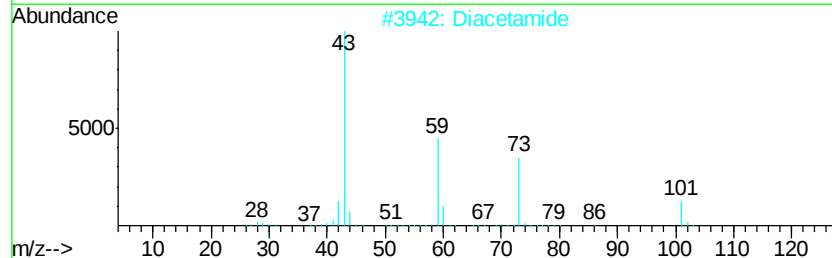
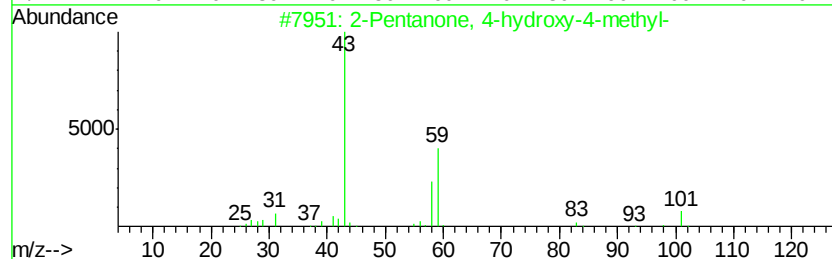
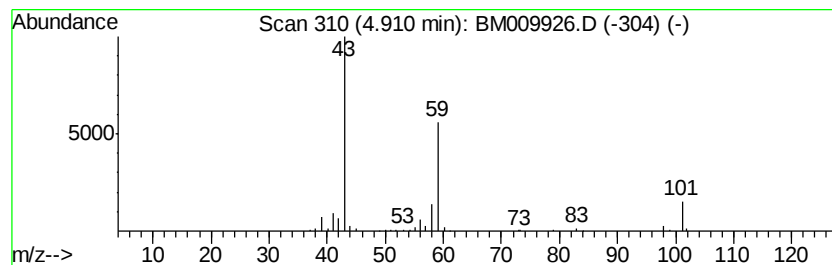
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.91	7.37 ng	303673	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Diacetamide	101	C4H7NO2	000625-77-4	36
3		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009926.D
Acq On : 06 May 2017 05:30
Operator : SJ/MA
Sample : I2893-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3073-PA4

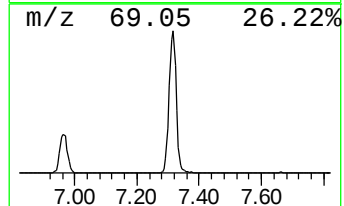
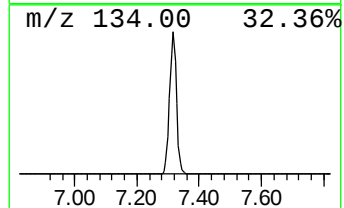
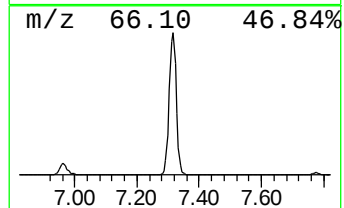
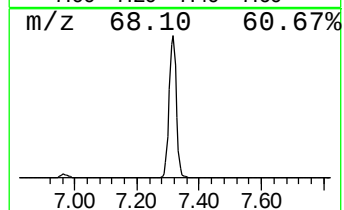
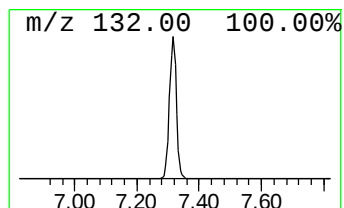
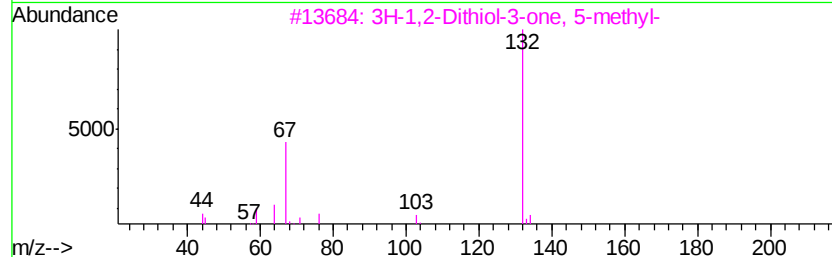
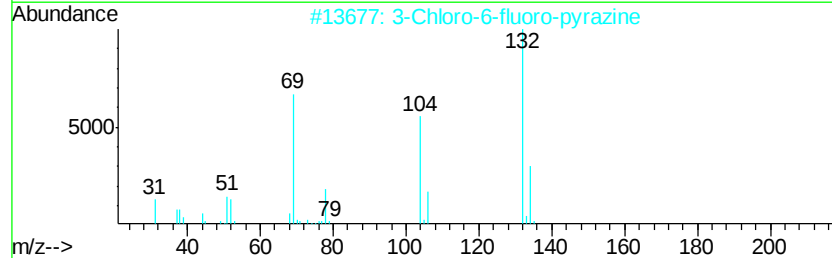
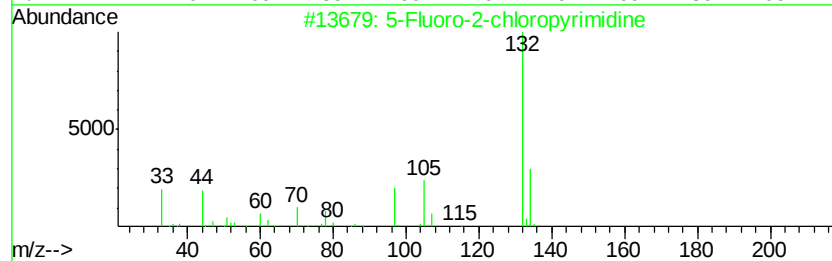
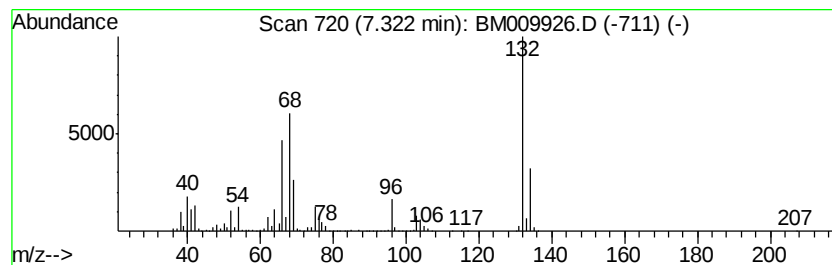
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	103.33 ng	4260120	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009926.D
Acq On : 06 May 2017 05:30
Operator : SJ/MA
Sample : I2893-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3073-PA4

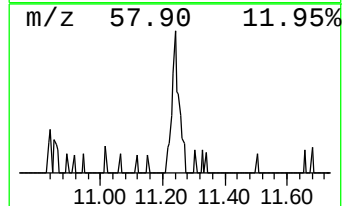
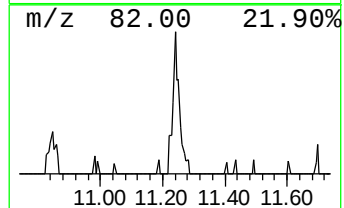
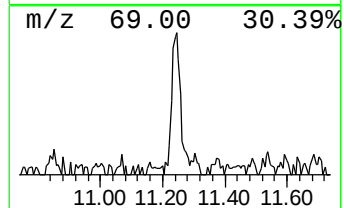
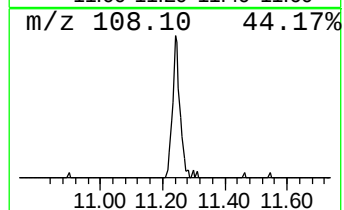
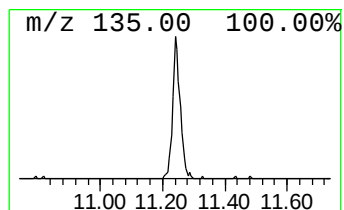
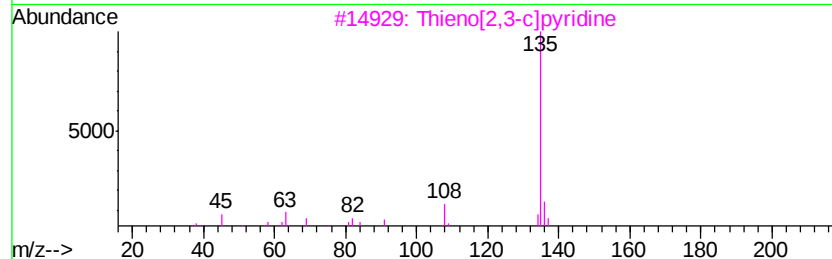
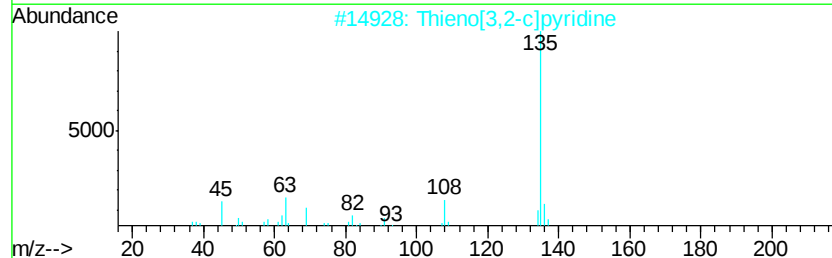
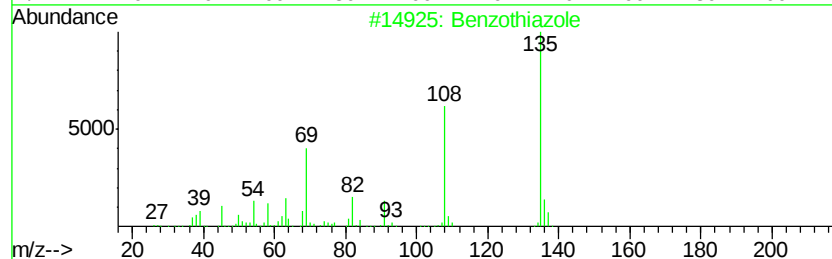
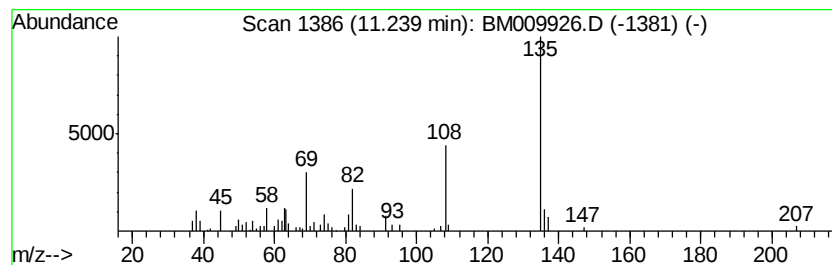
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	2.50 ng	143278	Napthalene-d8	10.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	87
2		Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	60
3		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	56
4		Adenine	135	C5H5N5	000073-24-5	50
5		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	50



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009926.D
Acq On : 06 May 2017 05:30
Operator : SJ/MA
Sample : I2893-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3073-PA4

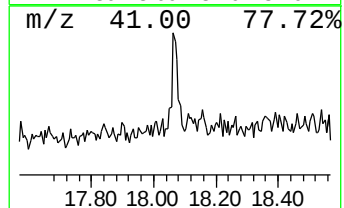
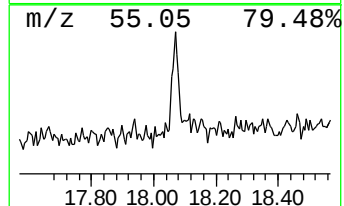
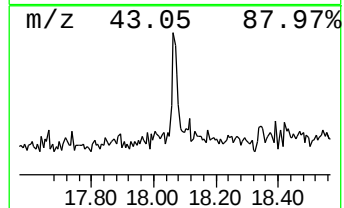
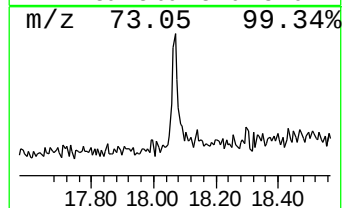
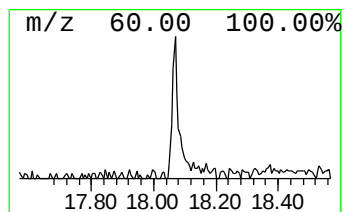
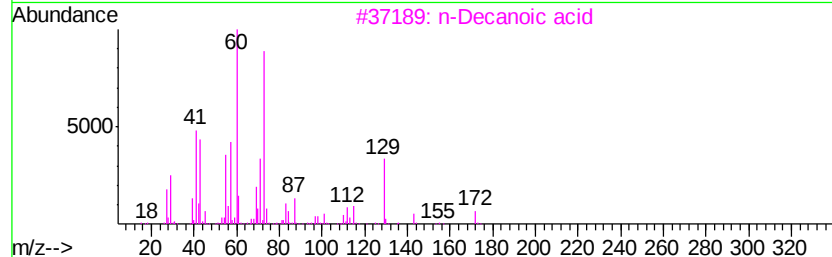
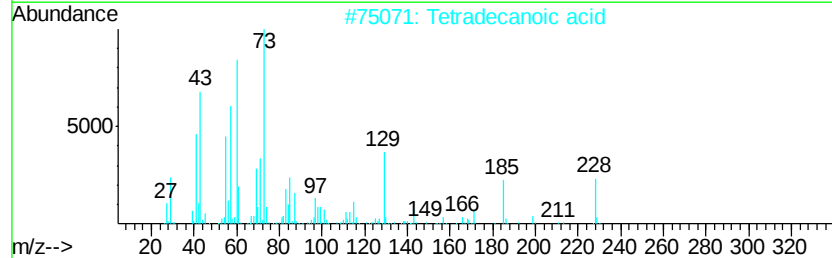
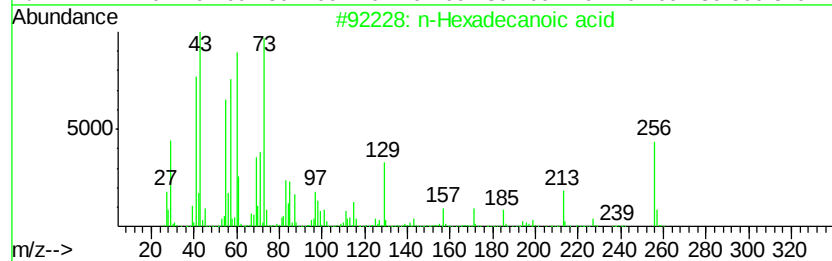
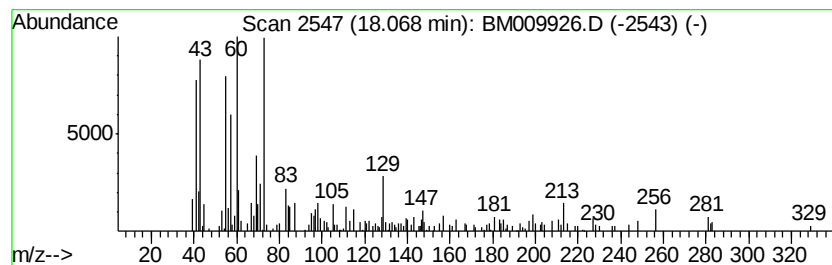
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	2.12 ng	190502	Phenanthrene-d10	17.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3		n-Decanoic acid	172	C10H20O2	000334-48-5	62
4		Tridecanoic acid	214	C13H26O2	000638-53-9	59
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009926.D
Acq On : 06 May 2017 05:30
Operator : SJ/MA
Sample : I2893-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3073-PA4

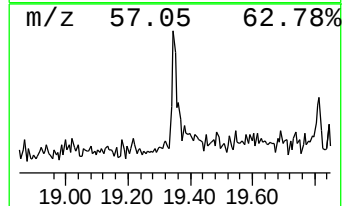
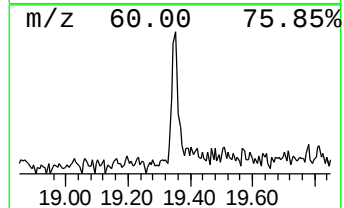
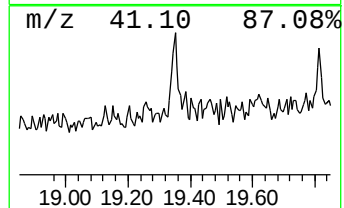
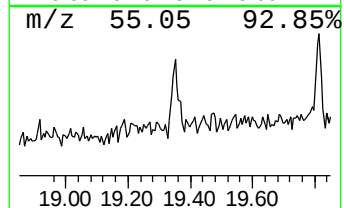
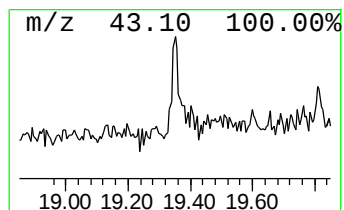
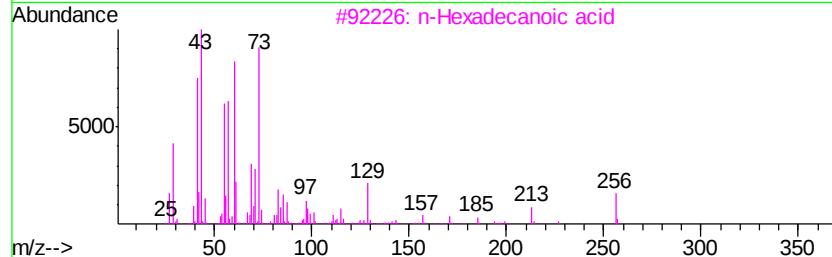
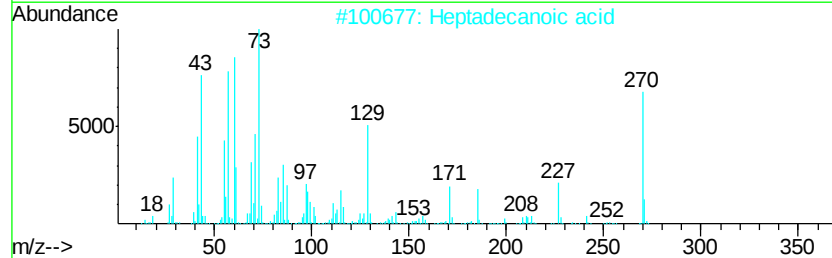
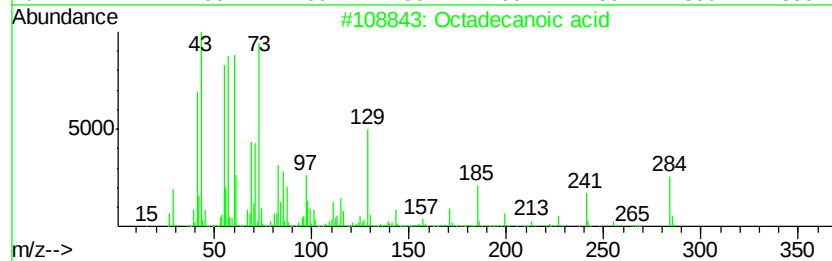
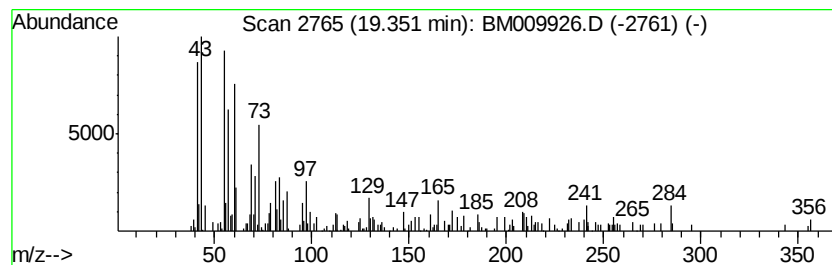
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	2.23 ng	187942	Chrysene-d12	21.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	86
2		Heptadecanoic acid	270	C17H34O2	000506-12-7	60
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5		.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	43



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009926.D
Acq On : 06 May 2017 05:30
Operator : SJ/MA
Sample : I2893-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3073-PA4

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...	4.91	7.4	ng	303673	1	7.77	824548	20.0
unknown7.32	7.32	103.3	ng	4260120	1	7.77	824548	20.0
Benzothiazole	11.24	2.5	ng	143278	2	10.57	1148380	20.0
n-Hexadecanoic acid	18.07	2.1	ng	190502	4	17.19	1795990	20.0
Octadecanoic acid	19.35	2.2	ng	187942	5	21.37	1689030	20.0