

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
 Data File : BM011390.D
 Acq On : 01 Sep 2017 02:09
 Operator : SJ/JU
 Sample : I4963-08
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3827-SPP4

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-BM083117.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	3.057	41	46	56	rBV	1100258	2092110	5.51%	1.157%
2	3.134	56	59	77	rVB	510639	739707	1.95%	0.409%
3	5.087	383	391	399	rBV	385949	588677	1.55%	0.326%
4	5.545	461	469	478	rBV	5141602	7507194	19.79%	4.152%
5	7.134	729	739	748	rBV	3090562	4760906	12.55%	2.633%
6	7.516	796	804	816	rBV	9398430	14945764	39.39%	8.266%
7	7.987	877	884	892	rBV	2024055	3268548	8.61%	1.808%
8	8.310	930	939	949	rBV	8111817	13464171	35.48%	7.446%
9	9.151	1074	1082	1094	rBV	7032154	11460627	30.20%	6.338%
10	10.798	1352	1362	1370	rBV	2949841	4954876	13.06%	2.740%
11	11.445	1465	1472	1481	rVB	430648	777165	2.05%	0.430%
12	13.245	1767	1778	1786	rBV	18508517	26659333	70.26%	14.744%
13	14.621	2003	2012	2020	rBV2	4350557	6492231	17.11%	3.590%
14	16.104	2257	2264	2284	rBV	13070944	19470572	51.31%	10.768%
15	16.292	2289	2296	2308	rVB2	205149	413391	1.09%	0.229%
16	17.356	2471	2477	2485	rBV2	5300471	7633722	20.12%	4.222%
17	19.968	2915	2921	2927	rBV	28502523	37943625	100.00%	20.984%
18	21.521	3180	3185	3191	rBV	7539210	9387122	24.74%	5.191%
19	23.903	3583	3590	3599	rBV	4183425	8257936	21.76%	4.567%

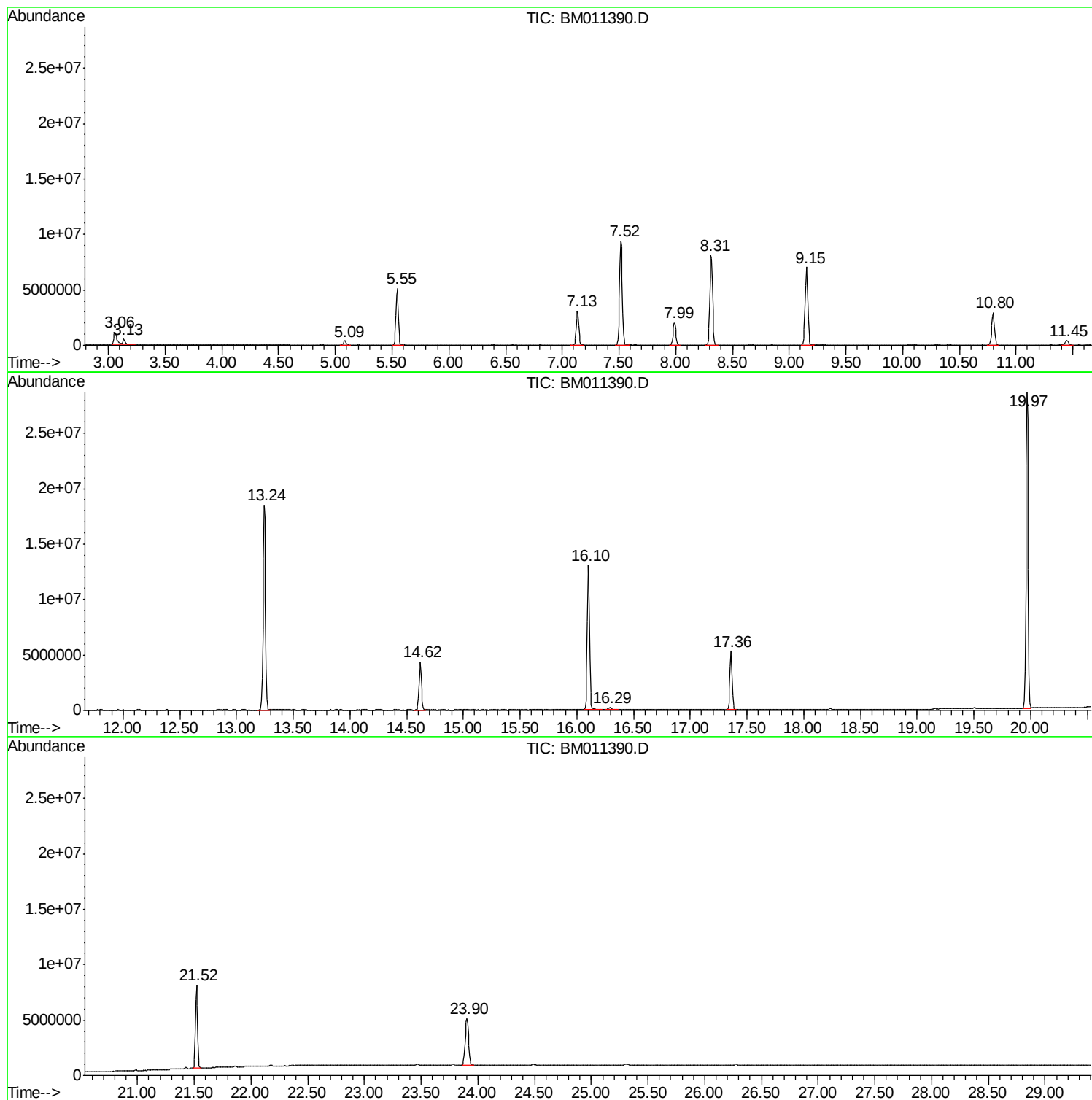
Sum of corrected areas: 180817677

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011390.D
Acq On : 01 Sep 2017 02:09
Operator : SJ/JU
Sample : I4963-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3827-SPP4

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.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\BM083117\
Data File : BM011390.D
Acq On : 01 Sep 2017 02:09
Operator : SJ/JU
Sample : I4963-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3827-SPP4

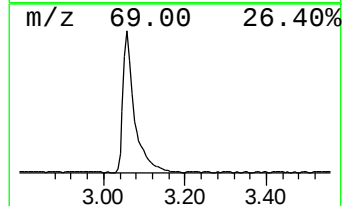
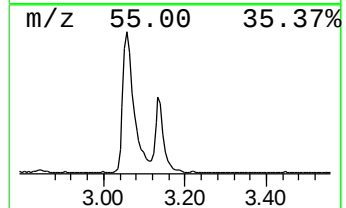
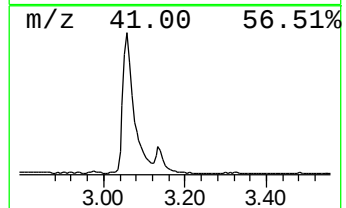
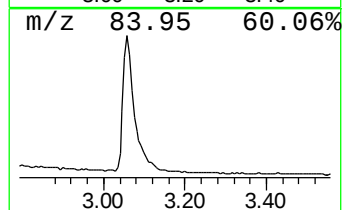
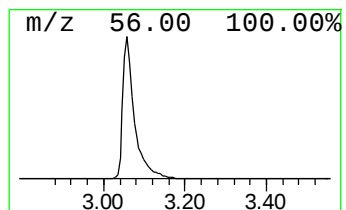
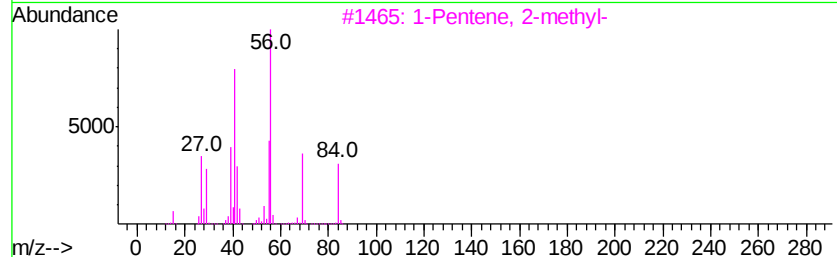
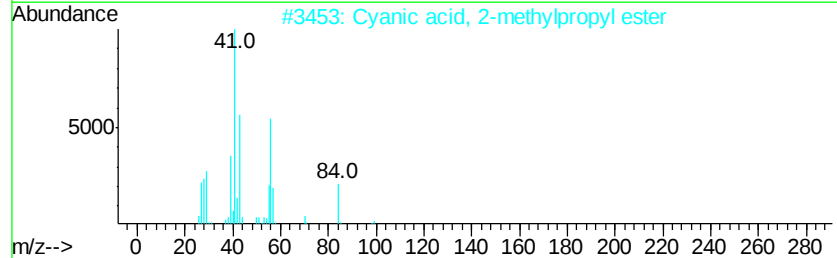
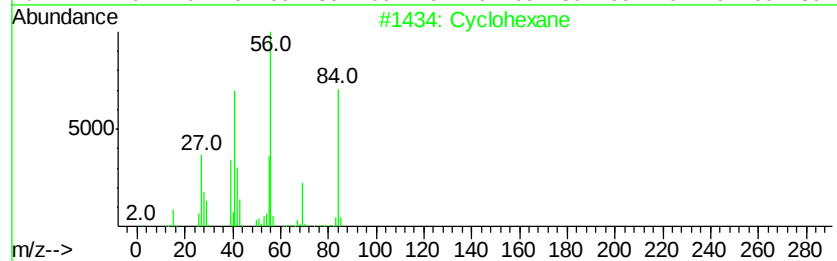
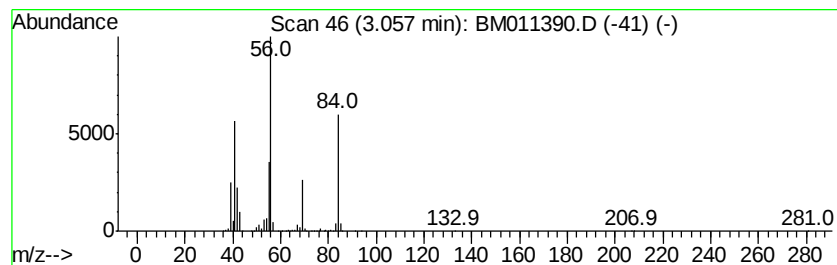
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	12.80 ng	2092110	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane	84	C6H12	000110-82-7	91
2		Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	64
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
4		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47
5		Cyclopentane, methyl-	84	C6H12	000096-37-7	45



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011390.D
Acq On : 01 Sep 2017 02:09
Operator : SJ/JU
Sample : I4963-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3827-SPP4

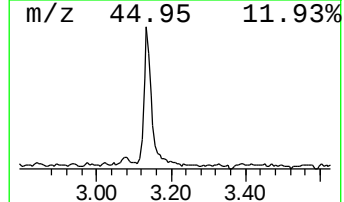
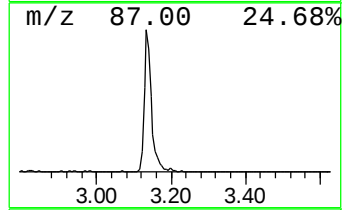
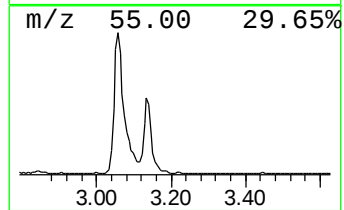
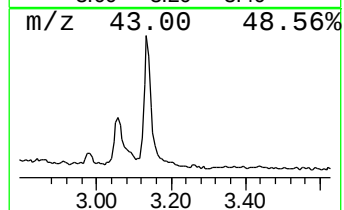
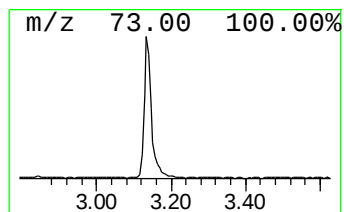
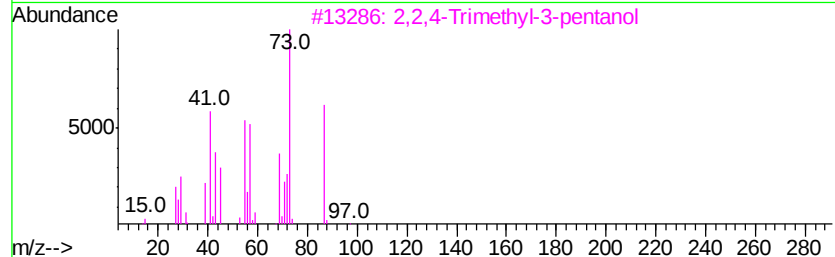
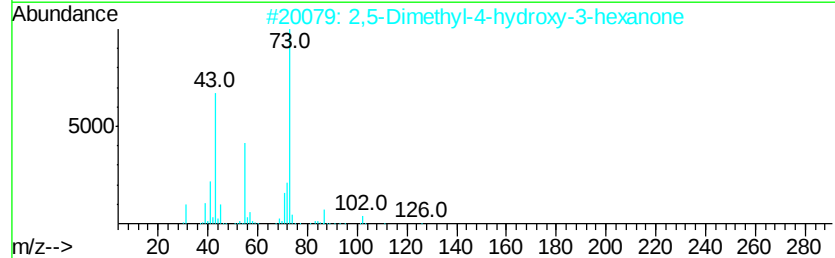
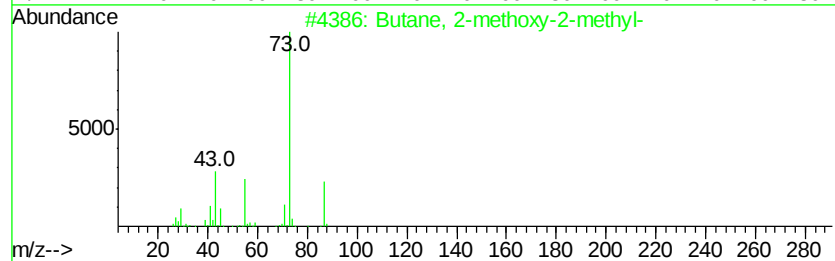
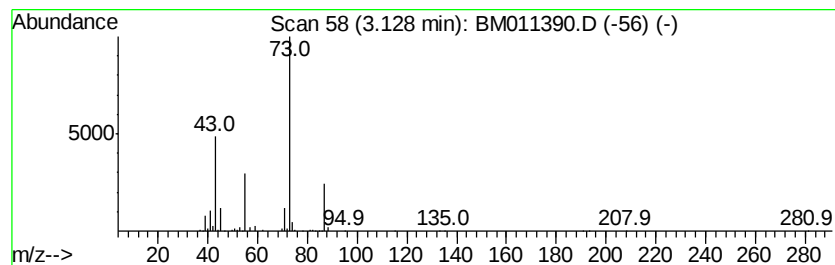
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	4.53 ng	739707	1,4-Dichlorobenzene-d4	7.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	40
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	16



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011390.D
Acq On : 01 Sep 2017 02:09
Operator : SJ/JU
Sample : I4963-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

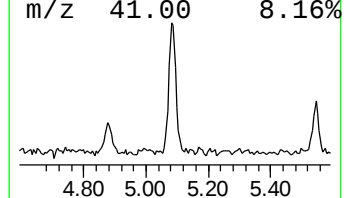
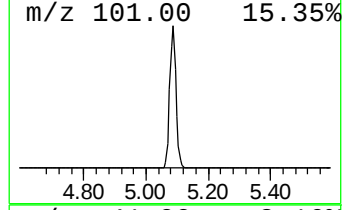
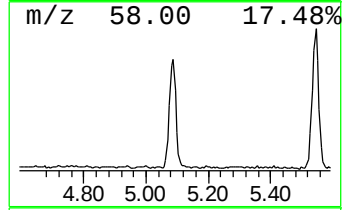
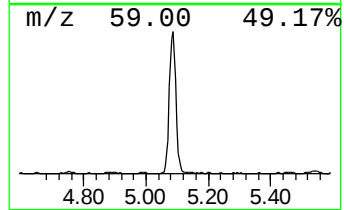
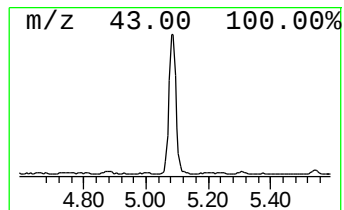
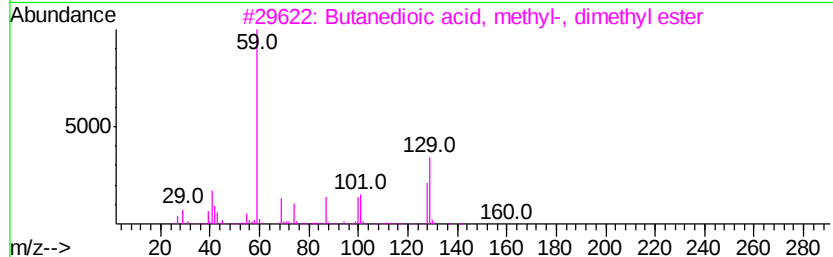
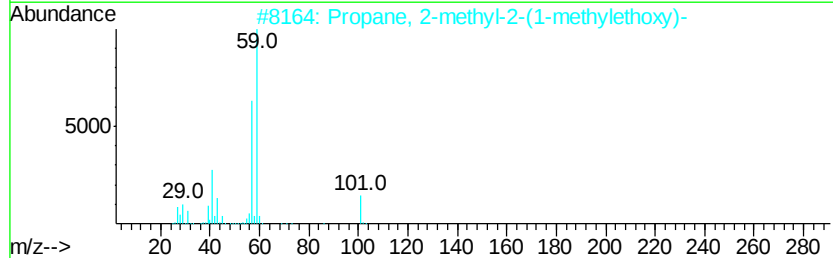
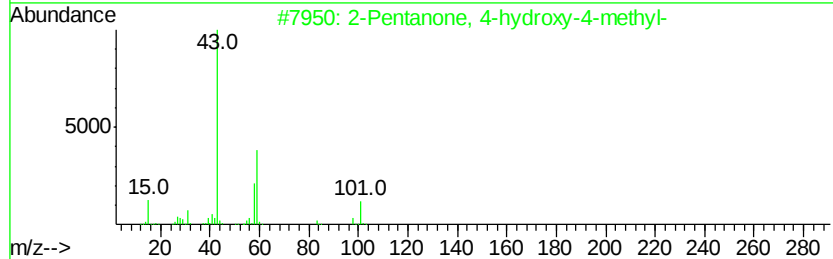
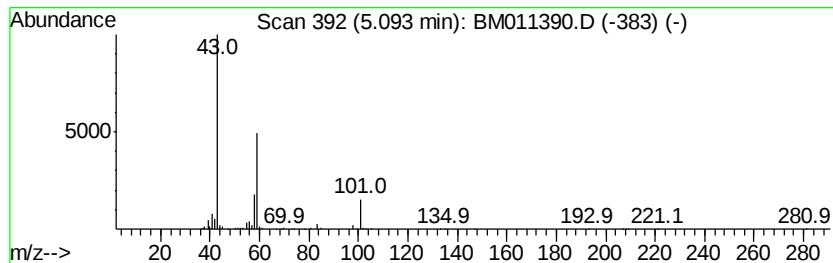
Instrument :
BNA_M
ClientSampleId :
3827-SPP4

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.09	3.60 ng	588677	1,4-Dichlorobenzene-d4	7.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011390.D
Acq On : 01 Sep 2017 02:09
Operator : SJ/JU
Sample : I4963-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3827-SPP4

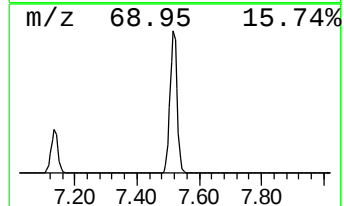
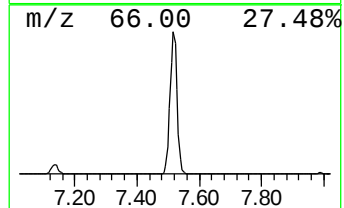
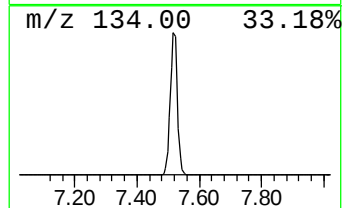
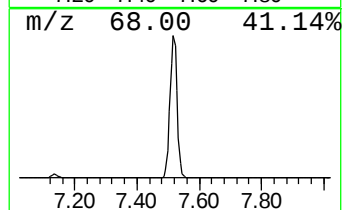
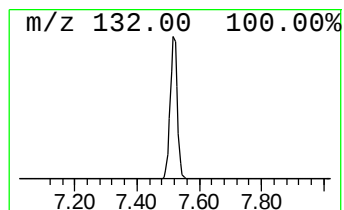
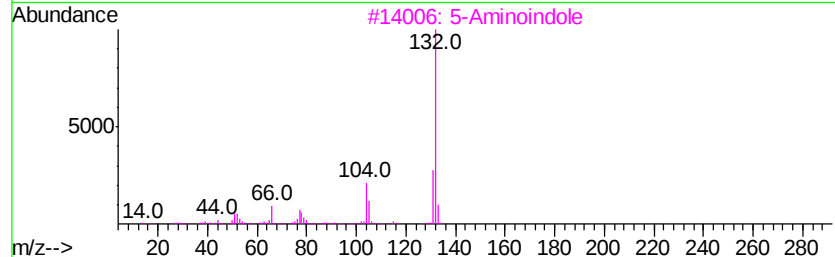
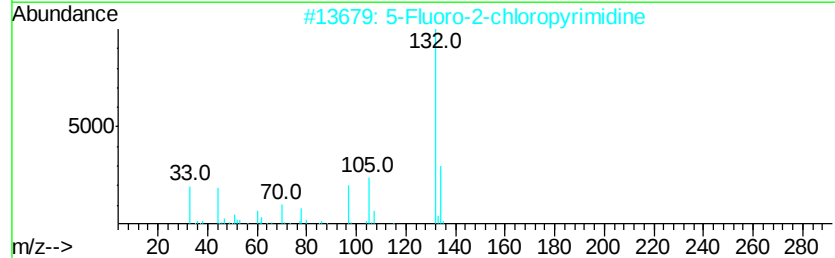
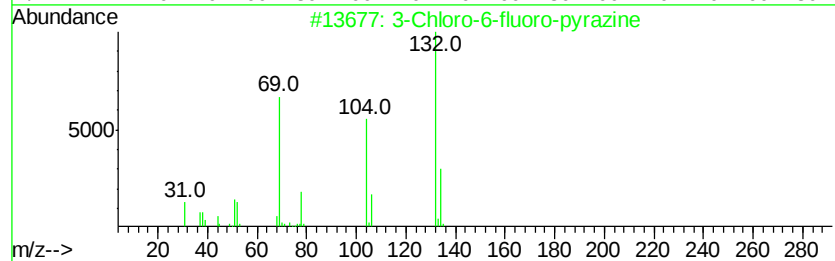
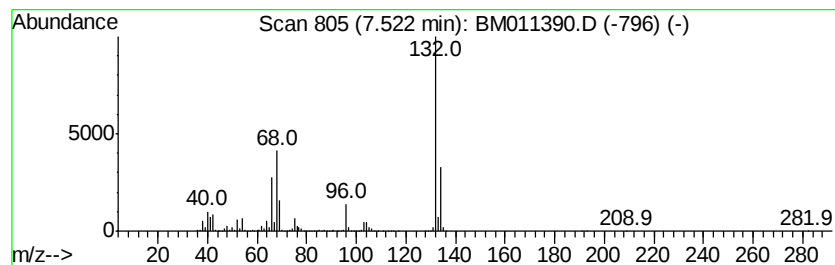
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	91.45 ng	14945800	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011390.D
Acq On : 01 Sep 2017 02:09
Operator : SJ/JU
Sample : I4963-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

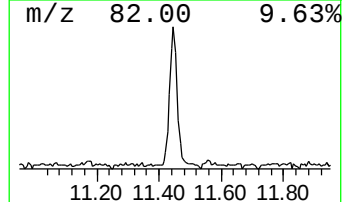
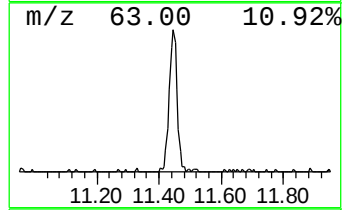
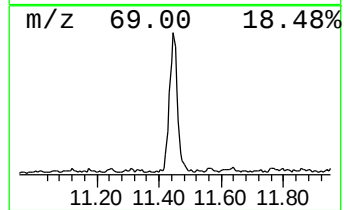
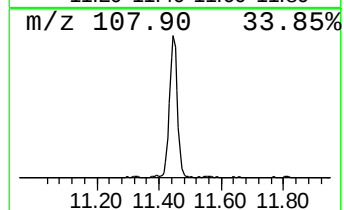
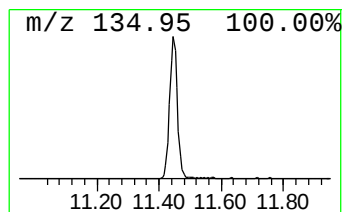
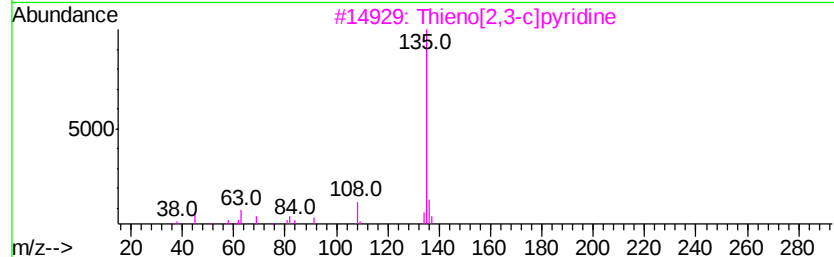
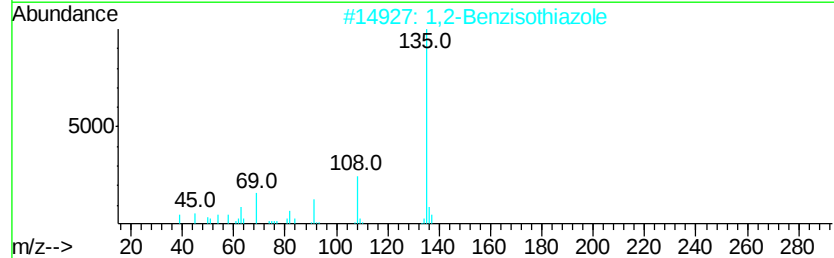
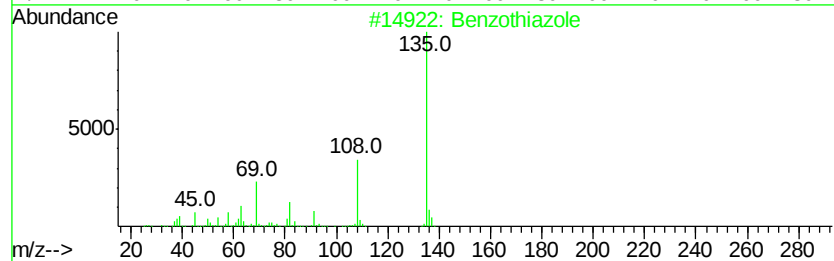
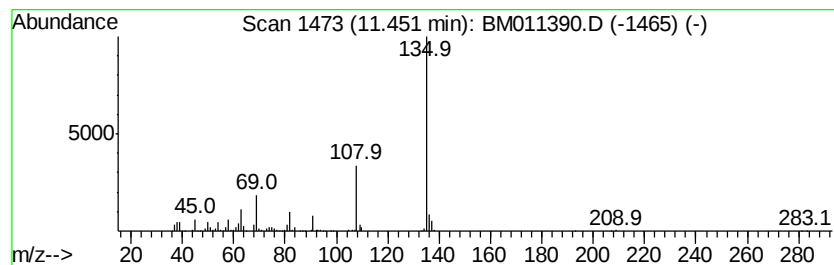
Instrument :
BNA_M
ClientSampled :
3827-SPP4

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.45	3.14 ng	777165	Naphthalene-d8	10.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	94
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	78
4	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
5	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM083117\
Data File : BM011390.D
Acq On : 01 Sep 2017 02:09
Operator : SJ/JU
Sample : I4963-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3827-SPP4

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.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
Cyclohexane	3.06	12.8	ng	2092110	1	7.99	3268550	20.0
Butane, 2-methoxy...	3.13	4.5	ng	739707	1	7.99	3268550	20.0
2-Pentanone, 4-hy...	5.09	3.6	ng	588677	1	7.99	3268550	20.0
unknown7.52	7.52	91.5	ng	14945800	1	7.99	3268550	20.0
Benzothiazole	11.45	3.1	ng	777165	2	10.80	4954880	20.0