

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
 Data File : BM011387.D
 Acq On : 01 Sep 2017 00:21
 Operator : SJ/JU
 Sample : I4963-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3826-SPP3

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_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	40	46	56	rBV	1223357	2221345	6.46%	1.350%
2	3.134	56	59	73	rVB	547853	736108	2.14%	0.447%
3	5.081	383	390	400	rVB	476209	711446	2.07%	0.432%
4	5.546	462	469	480	rBV	4552003	6568205	19.10%	3.991%
5	7.134	732	739	749	rBV	2621935	4113260	11.96%	2.499%
6	7.516	796	804	816	rBV	8326244	13238823	38.51%	8.044%
7	7.987	876	884	891	rBV	1834783	2972310	8.65%	1.806%
8	8.310	931	939	953	rBV	7298757	12207604	35.51%	7.418%
9	9.151	1074	1082	1092	rBV	6262896	10330020	30.05%	6.277%
10	10.798	1353	1362	1370	rBV	2650751	4422278	12.86%	2.687%
11	11.445	1465	1472	1483	rVB	923240	1629347	4.74%	0.990%
12	13.245	1767	1778	1788	rBV	16411574	23909564	69.55%	14.528%
13	14.621	2005	2012	2025	rBV2	3794748	5810893	16.90%	3.531%
14	16.104	2256	2264	2284	rBV	11944686	17261452	50.21%	10.488%
15	16.298	2289	2297	2304	rVB2	307288	546444	1.59%	0.332%
16	17.357	2471	2477	2485	rBV	4770179	6848699	19.92%	4.161%
17	18.562	2677	2682	2691	rBV	235824	386911	1.13%	0.235%
18	19.968	2915	2921	2928	rBV	25851852	34379783	100.00%	20.890%
19	21.521	3180	3185	3191	rBV	6975095	8507780	24.75%	5.169%
20	23.903	3583	3590	3602	rVB2	3726945	7775931	22.62%	4.725%

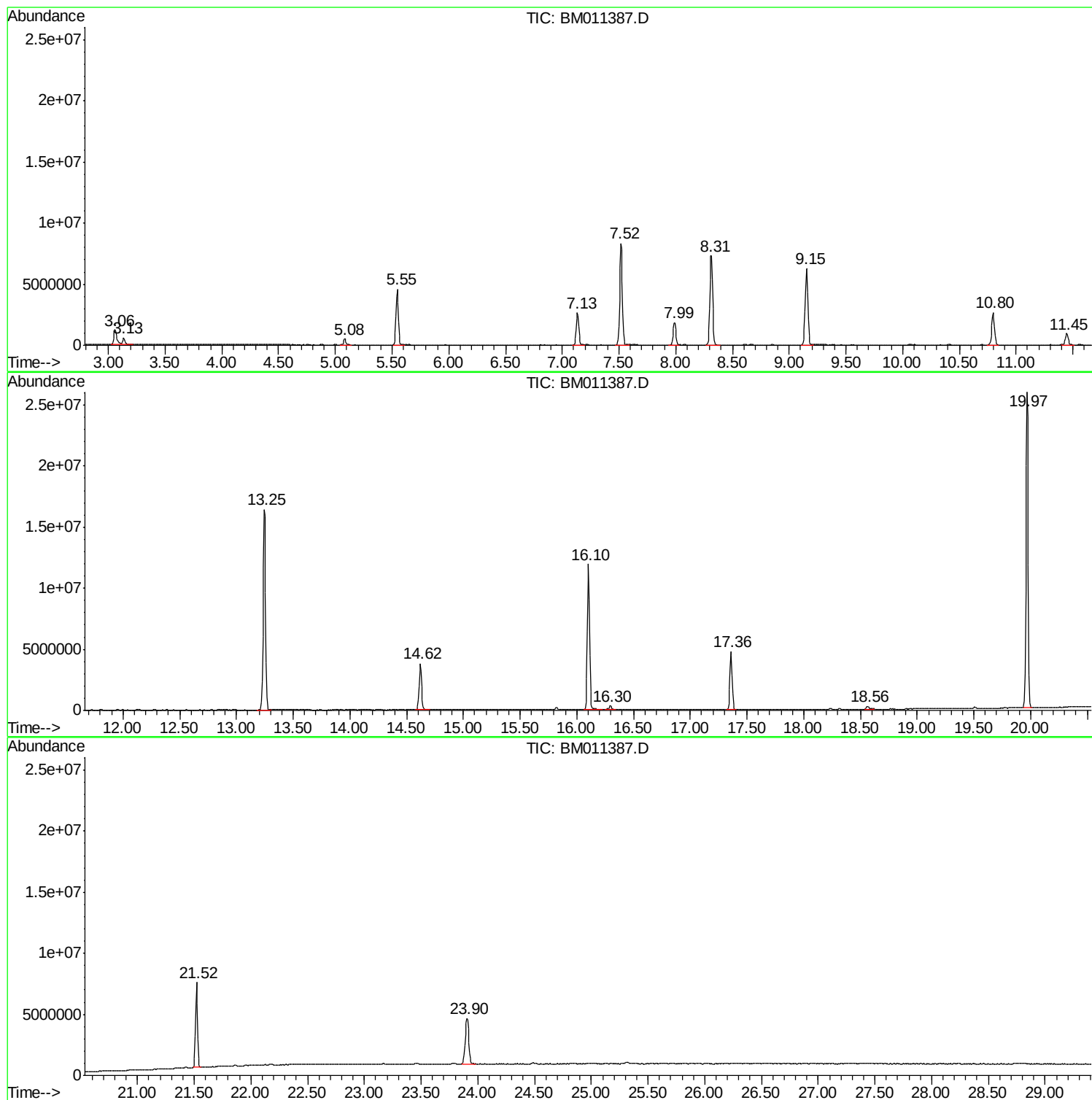
Sum of corrected areas: 164578203

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011387.D
Acq On : 01 Sep 2017 00:21
Operator : SJ/JU
Sample : I4963-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3826-SPP3

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 : BM011387.D
Acq On : 01 Sep 2017 00:21
Operator : SJ/JU
Sample : I4963-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3826-SPP3

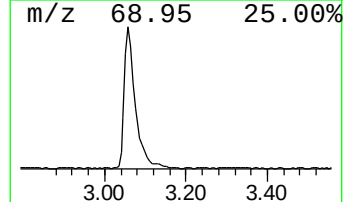
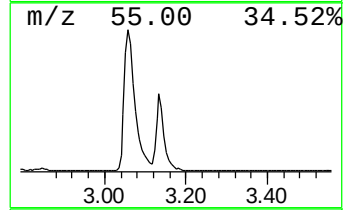
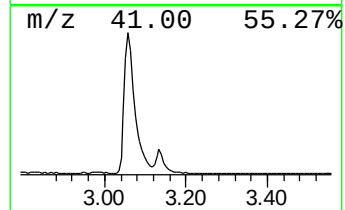
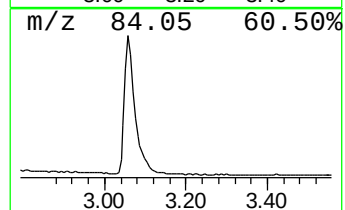
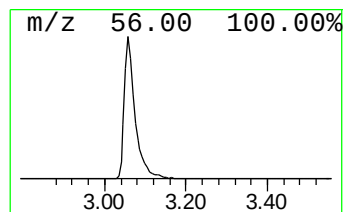
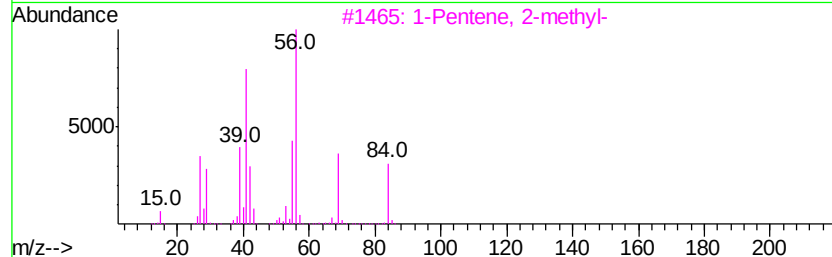
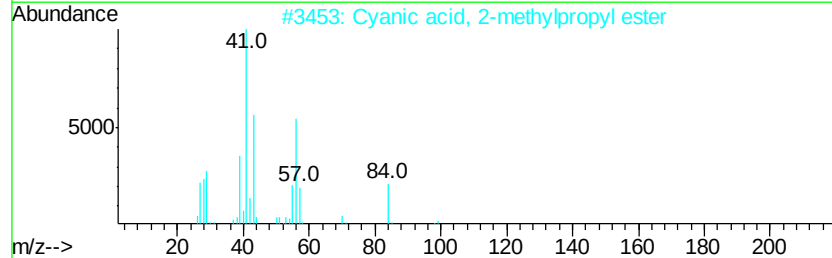
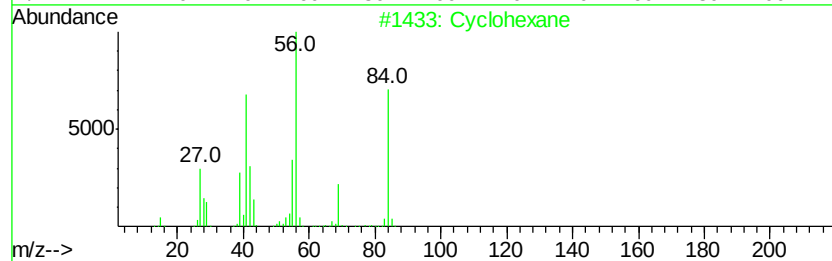
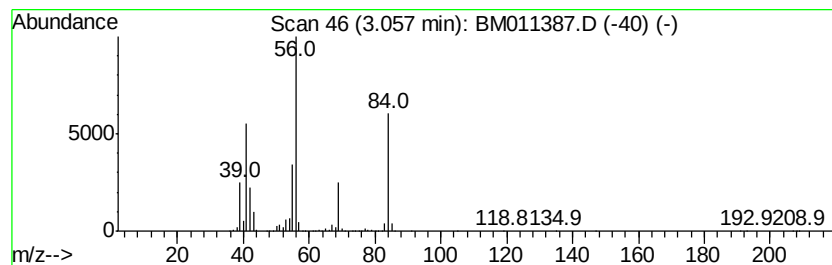
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	14.95 ng	2221350	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	56
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	50
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	47



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011387.D
Acq On : 01 Sep 2017 00:21
Operator : SJ/JU
Sample : I4963-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3826-SPP3

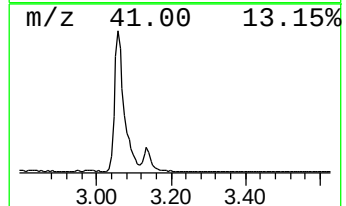
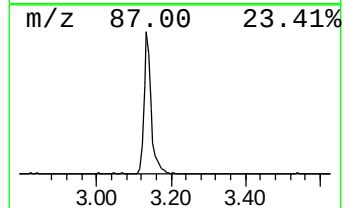
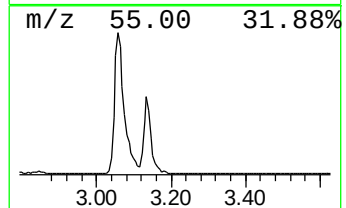
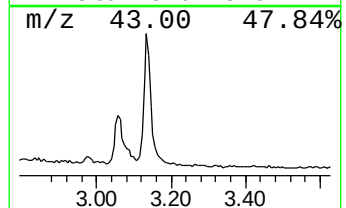
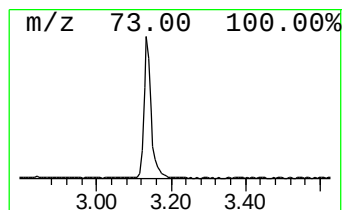
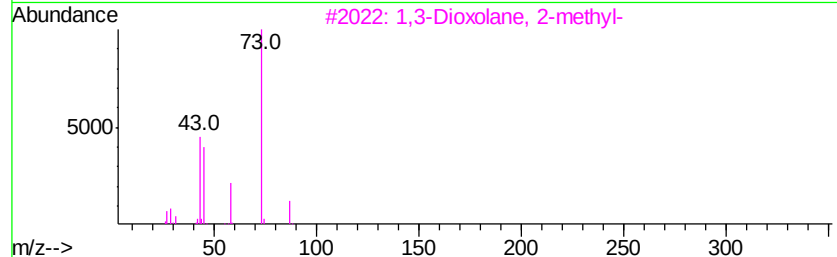
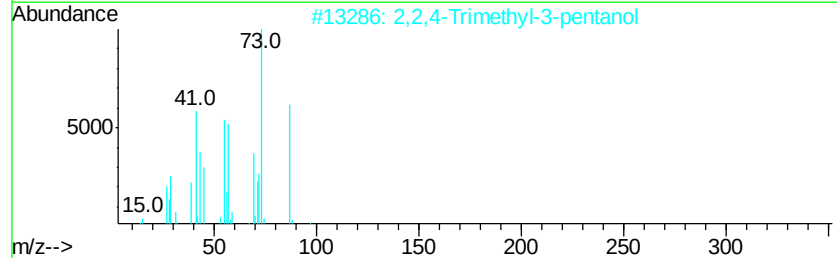
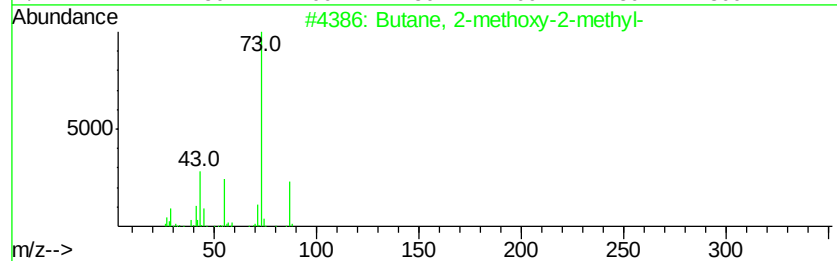
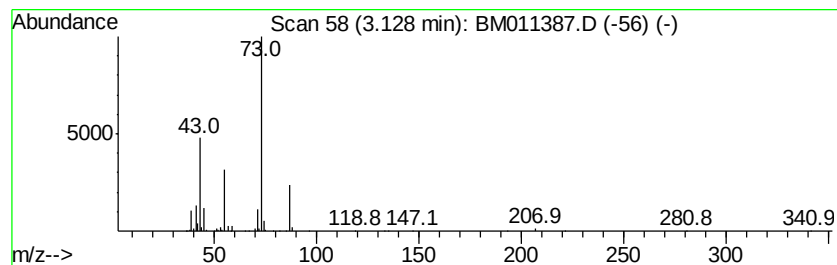
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	4.95 ng	736108	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011387.D
Acq On : 01 Sep 2017 00:21
Operator : SJ/JU
Sample : I4963-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3826-SPP3

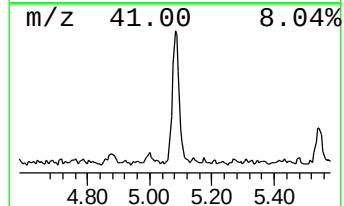
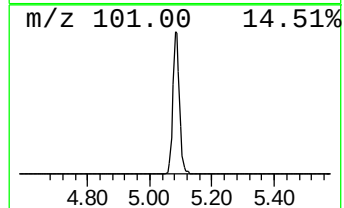
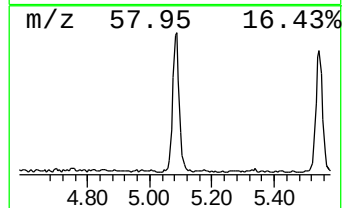
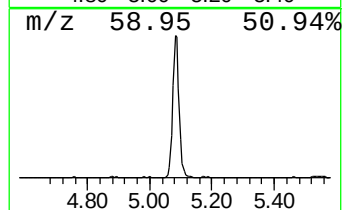
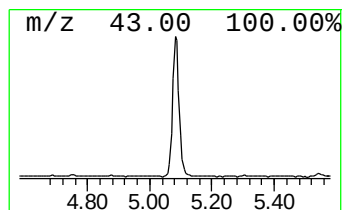
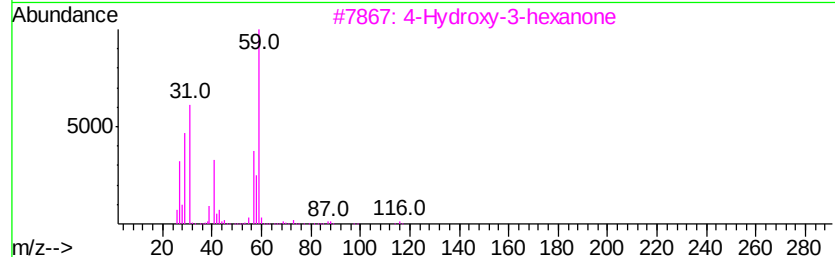
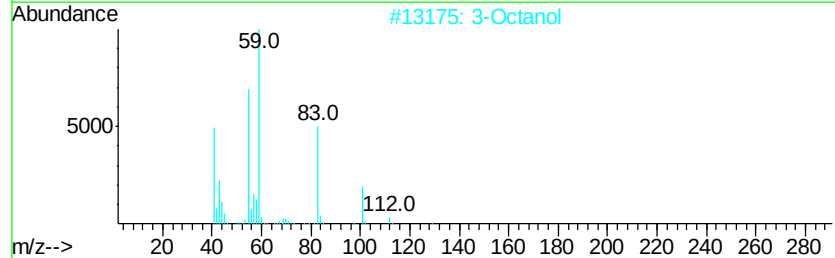
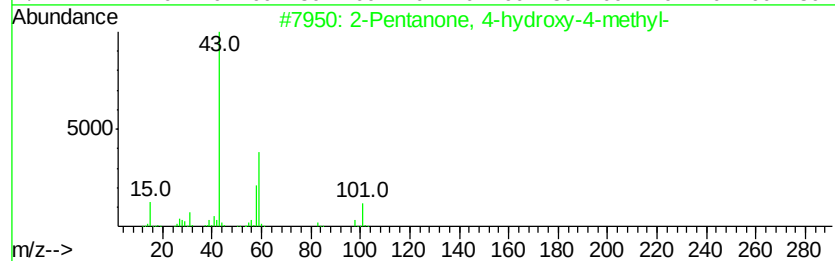
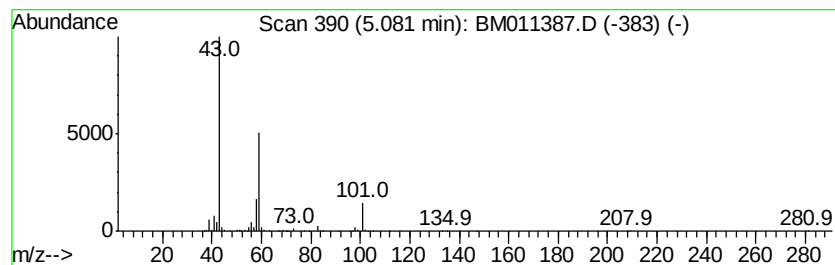
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	4.79 ng	711446	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Octanol	130	C8H18O	020296-29-1	33
3		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	28
4		3-Octanol	130	C8H18O	000589-98-0	28
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011387.D
Acq On : 01 Sep 2017 00:21
Operator : SJ/JU
Sample : I4963-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3826-SPP3

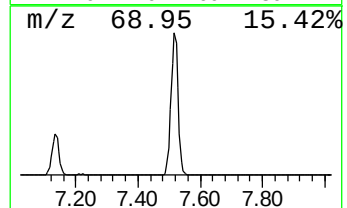
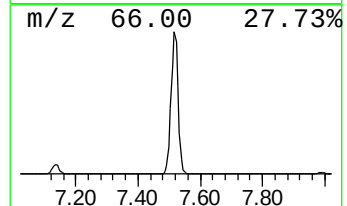
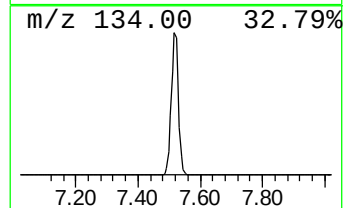
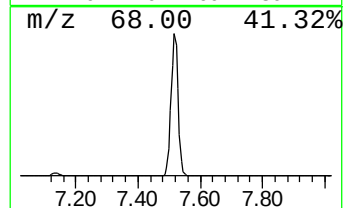
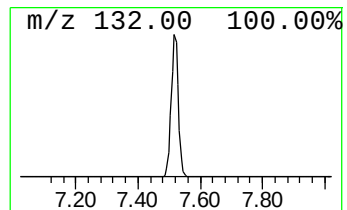
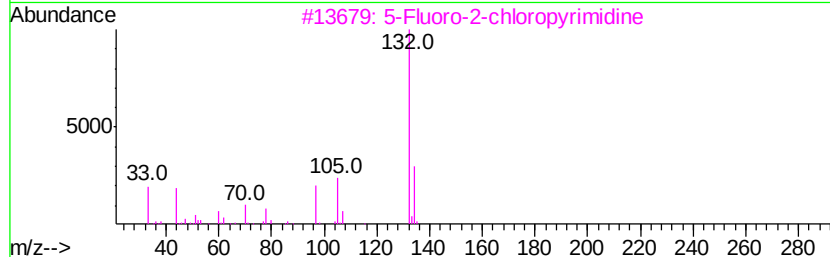
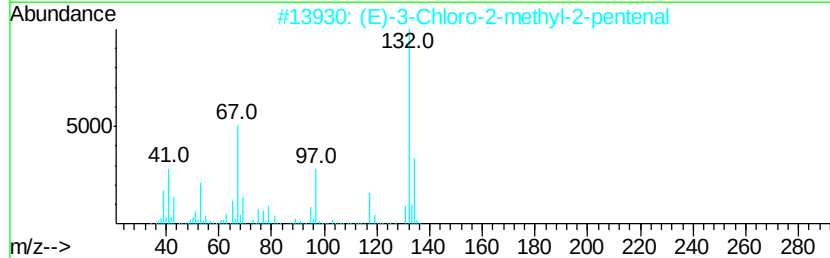
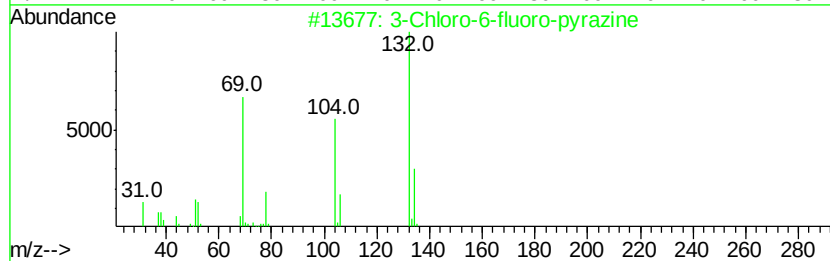
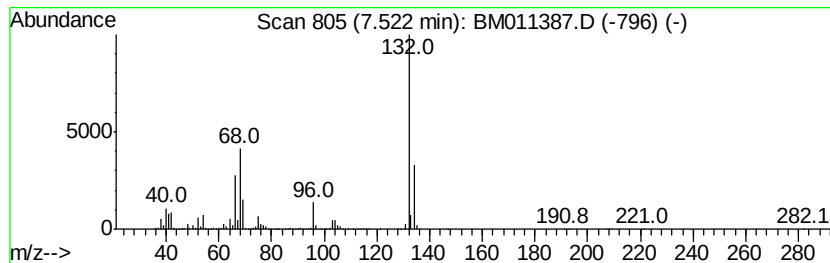
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	89.08 ng	13238800	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Amphetaminil	250	C17H18N2	017590-01-1	10



Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011387.D
Acq On : 01 Sep 2017 00:21
Operator : SJ/JU
Sample : I4963-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

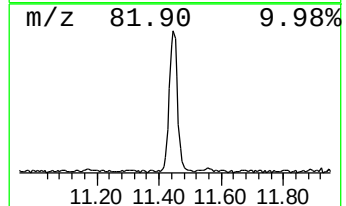
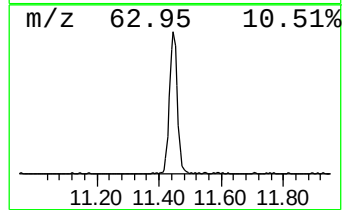
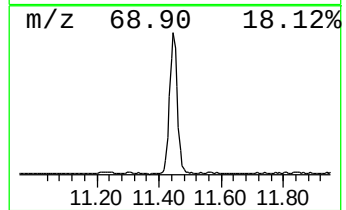
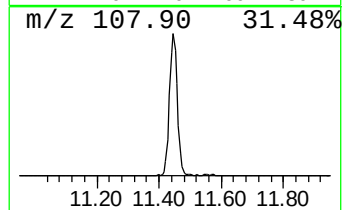
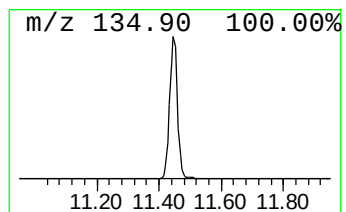
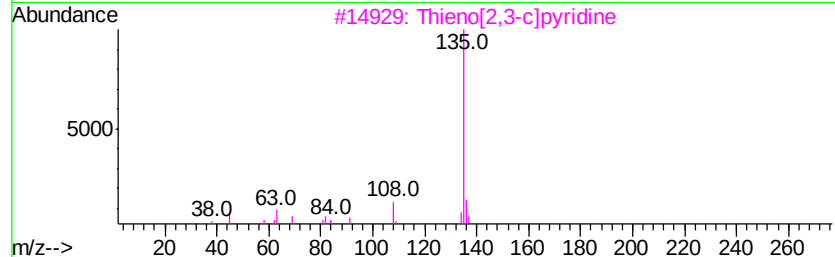
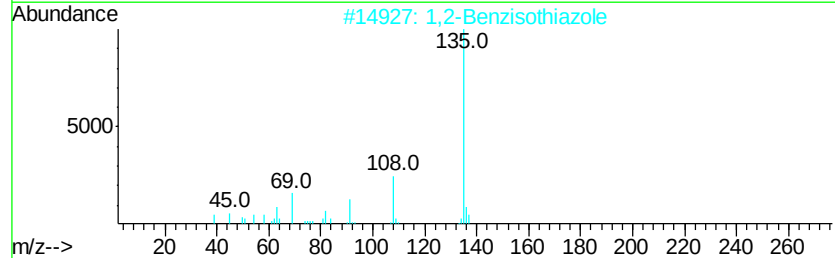
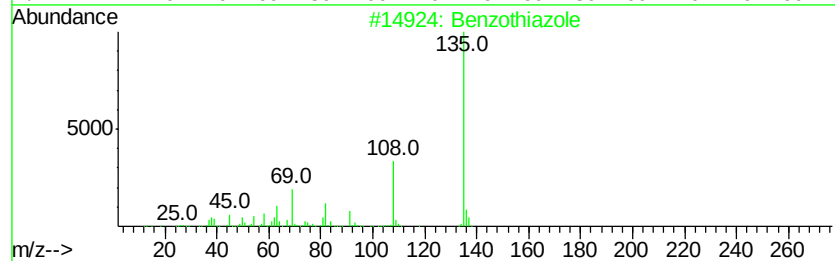
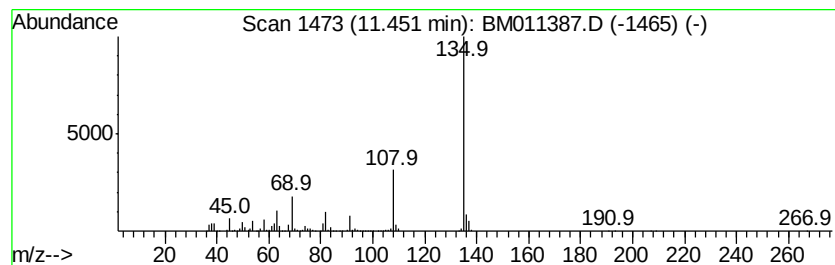
Instrument :
BNA_M
ClientSampleId :
3826-SPP3

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 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	7.37 ng	1629350	Napthalene-d8	10.80
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzothiazole	135 C7H5NS	000095-16-9 97
2		1,2-Benzisothiazole	135 C7H5NS	000272-16-2 90
3		Thieno[2,3-c]pyridine	135 C7H5NS	000272-12-8 72
4		2-Fluoro-4-cyanotoluene	135 C8H6FN	170572-49-3 64
5		4-Aminopyrazolo(3,4-d)pyrimidine	135 C5H5N5	020289-44-5 53



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM083117\
Data File : BM011387.D
Acq On : 01 Sep 2017 00:21
Operator : SJ/JU
Sample : I4963-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3826-SPP3

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	14.9	ng	2221350	1	7.99	2972310	20.0
Butane, 2-methoxy...	3.13	5.0	ng	736108	1	7.99	2972310	20.0
2-Pentanone, 4-hy...	5.08	4.8	ng	711446	1	7.99	2972310	20.0
unknown7.52	7.52	89.1	ng	13238800	1	7.99	2972310	20.0
Benzothiazole	11.45	7.4	ng	1629350	2	10.80	4422280	20.0