

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
 Data File : BM009452.D
 Acq On : 30 Mar 2017 15:57
 Operator : SJ/MA
 Sample : PB97931BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB97931BL

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-BM032217.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	4.375	215	219	231	rVB	173895	252186	3.41%	0.657%
2	4.975	315	321	333	rBV	2056564	2795540	37.84%	7.278%
3	5.428	391	398	406	rBV	1808077	2582656	34.96%	6.724%
4	6.040	497	502	509	rBV	102948	153379	2.08%	0.399%
5	7.011	658	667	678	rBV	1660110	2619173	35.45%	6.819%
6	7.381	723	730	743	rBV	1612289	2536054	34.33%	6.603%
7	7.852	803	810	820	rBV	484245	776082	10.50%	2.021%
8	8.175	858	865	873	rVB	1881299	2956779	40.02%	7.698%
9	9.022	1001	1009	1021	rBV	1450647	2466109	33.38%	6.421%
10	10.651	1278	1286	1297	rBV	553552	932980	12.63%	2.429%
11	13.116	1697	1705	1717	rBV	3142049	4717665	63.86%	12.282%
12	14.498	1934	1940	1949	rVB2	690714	1062968	14.39%	2.767%
13	15.986	2186	2193	2207	rBV	1498462	2109319	28.55%	5.492%
14	17.245	2401	2407	2413	rBV2	908140	1315506	17.81%	3.425%
15	19.863	2846	2852	2857	rBV	6183019	7388042	100.00%	19.235%
16	21.421	3112	3117	3124	rBV	1514915	1912280	25.88%	4.979%
17	23.745	3506	3512	3522	rVB2	901538	1833042	24.81%	4.772%

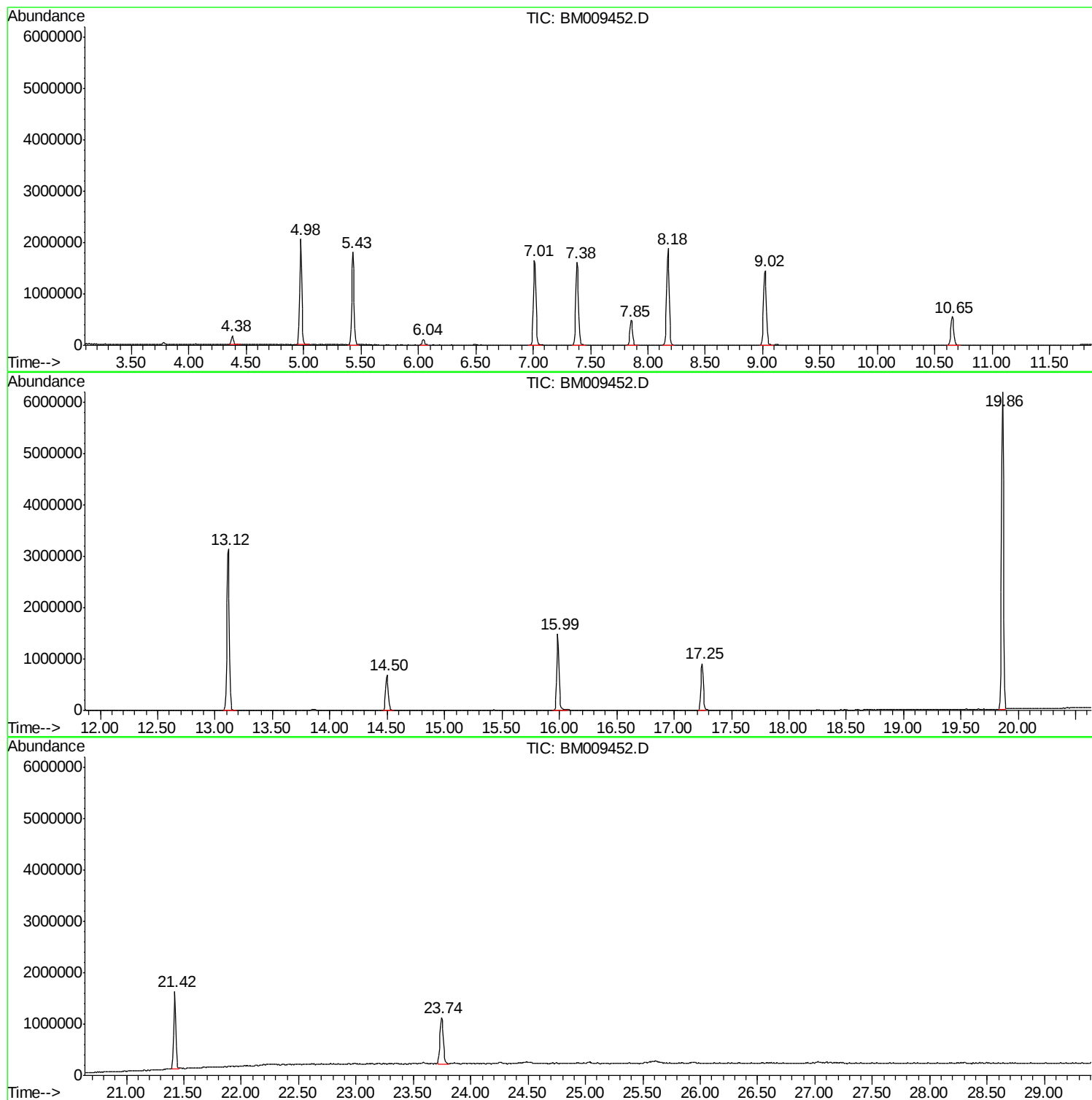
Sum of corrected areas: 38409760

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009452.D
Acq On : 30 Mar 2017 15:57
Operator : SJ/MA
Sample : PB97931BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB97931BL

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM032217.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\BM033017\
Data File : BM009452.D
Acq On : 30 Mar 2017 15:57
Operator : SJ/MA
Sample : PB97931BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampled :
PB97931BL

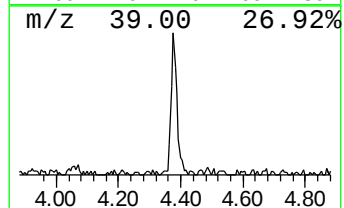
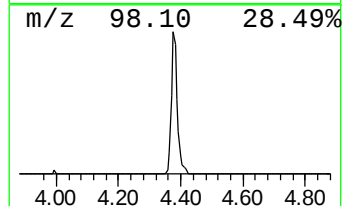
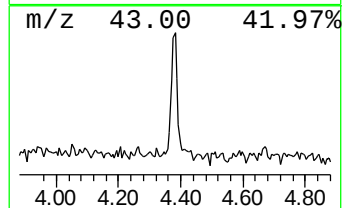
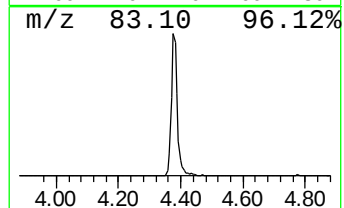
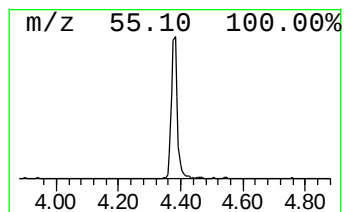
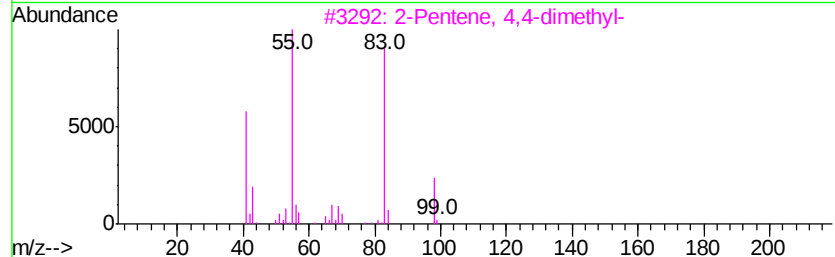
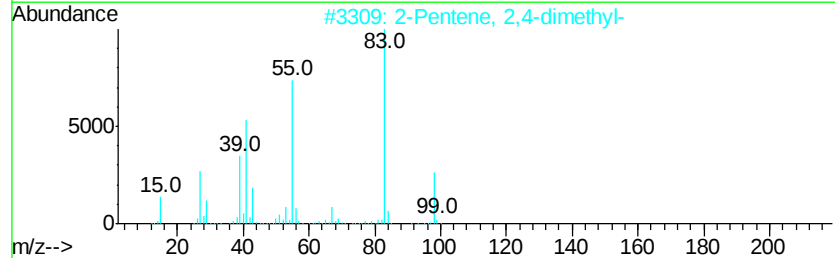
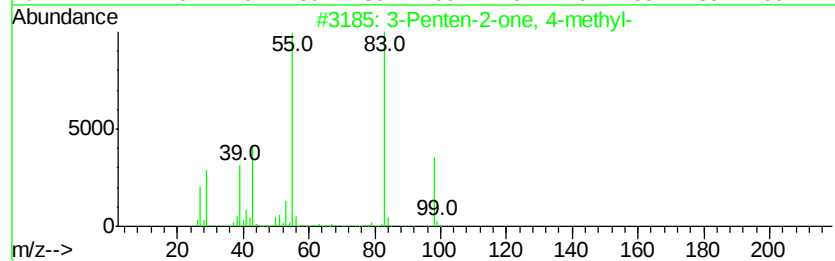
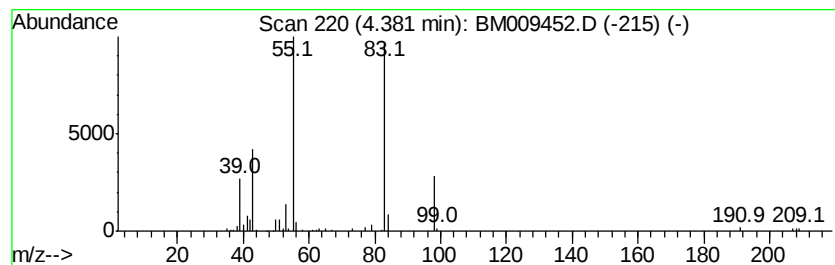
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	6.50 ng	252186	1,4-Dichlorobenzene-d4	7.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
3			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86
4			3-Hexen-2-one	98	C6H10O	000763-93-9	86
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009452.D
Acq On : 30 Mar 2017 15:57
Operator : SJ/MA
Sample : PB97931BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB97931BL

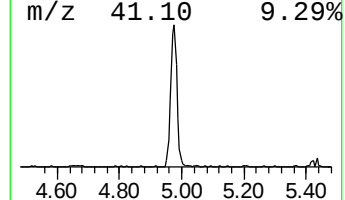
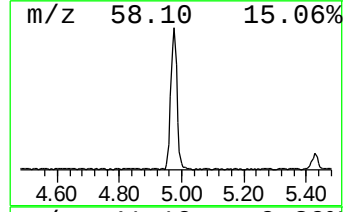
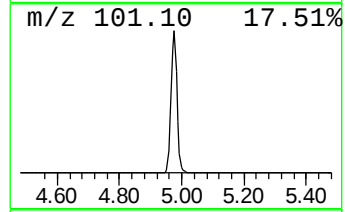
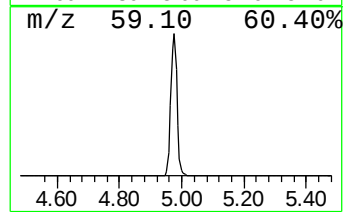
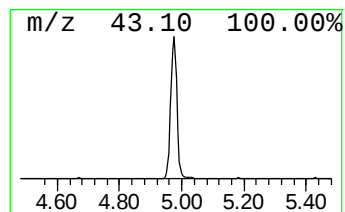
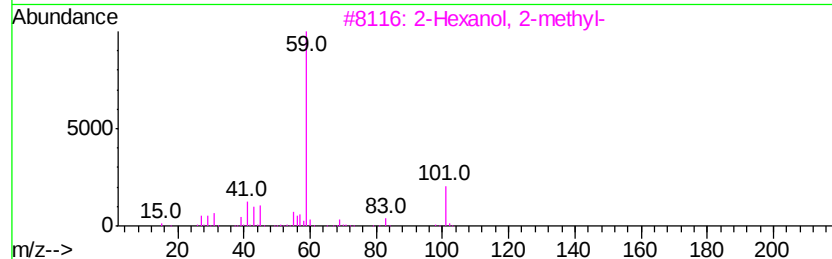
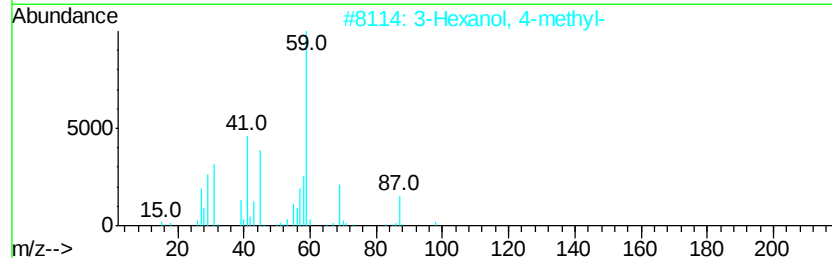
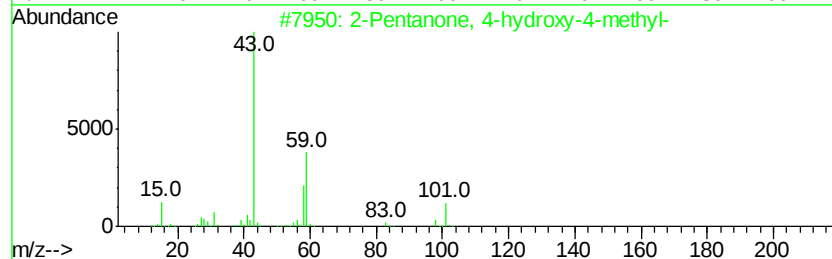
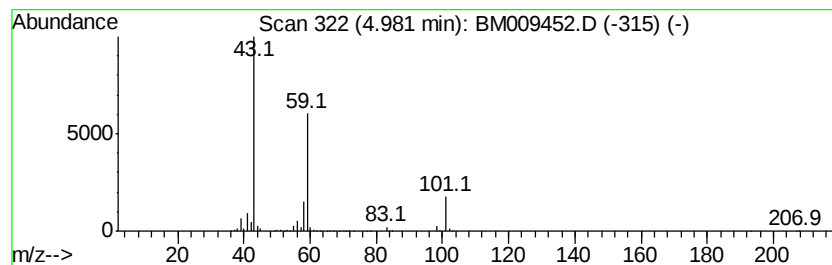
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	72.04 ng	2795540	1,4-Dichlorobenzene-d4	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009452.D
Acq On : 30 Mar 2017 15:57
Operator : SJ/MA
Sample : PB97931BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampled :
PB97931BL

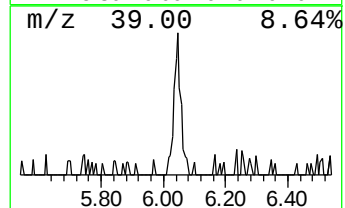
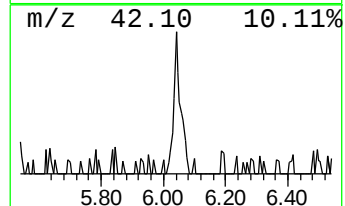
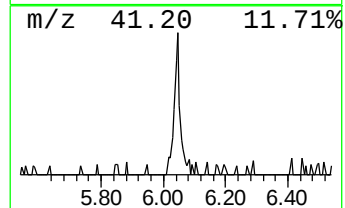
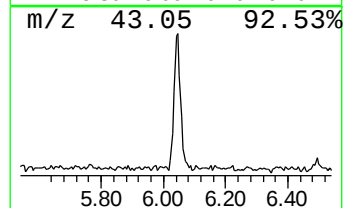
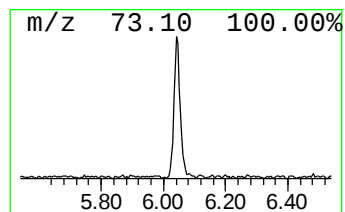
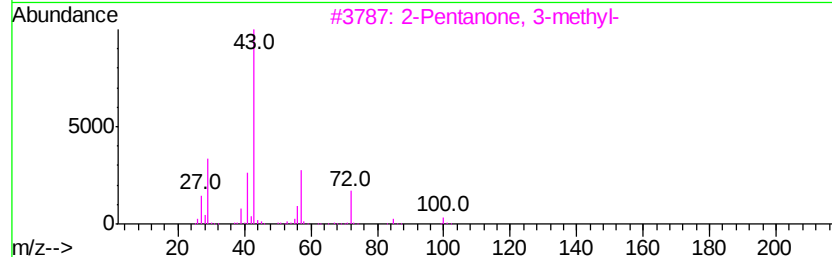
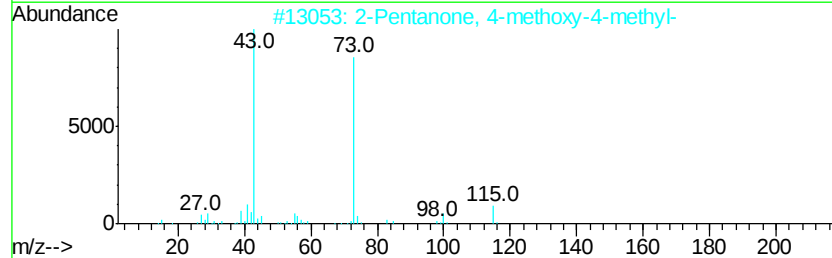
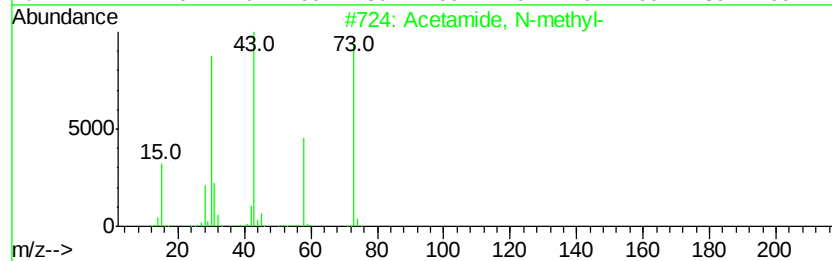
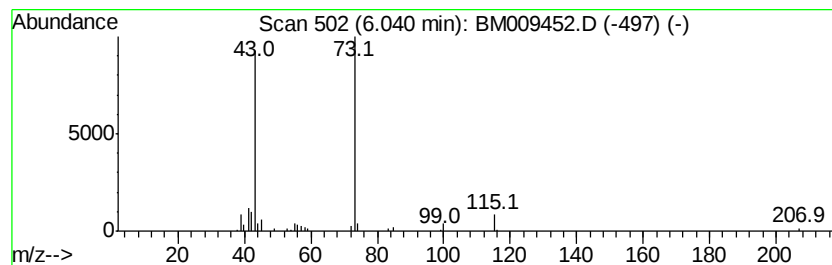
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Acetamide, N-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.04	3.95 ng	153379	1,4-Dichlorobenzene-d4	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	58
2		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	53
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	27
4		N-Ethylformamide	73	C3H7NO	000627-45-2	23
5		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	23



Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009452.D
Acq On : 30 Mar 2017 15:57
Operator : SJ/MA
Sample : PB97931BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB97931BL

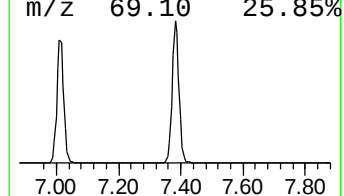
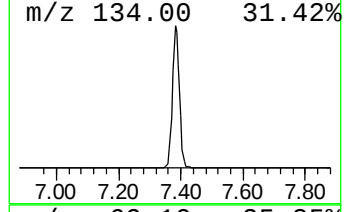
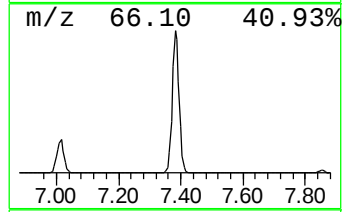
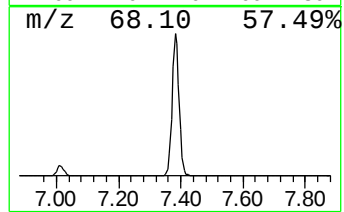
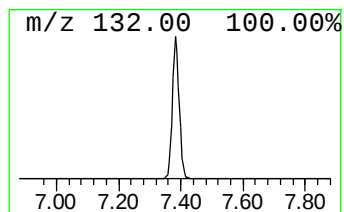
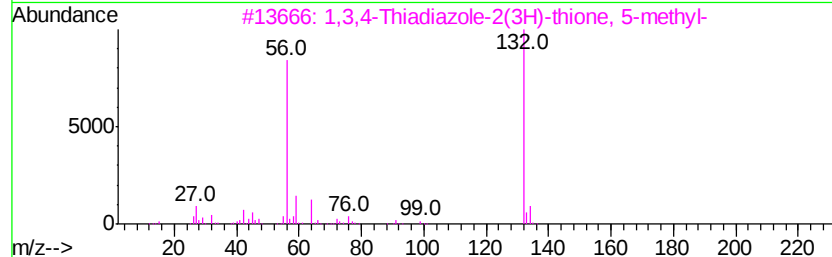
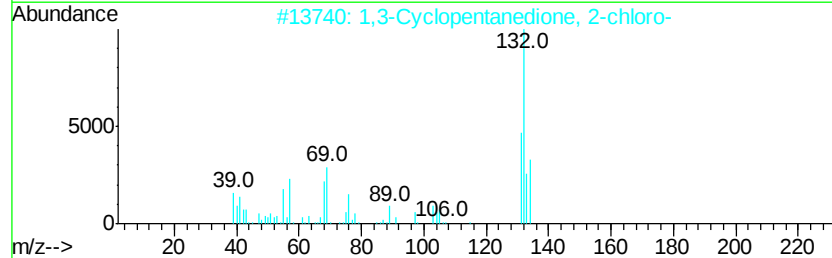
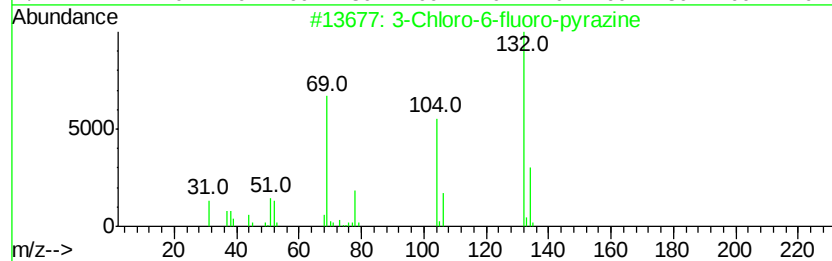
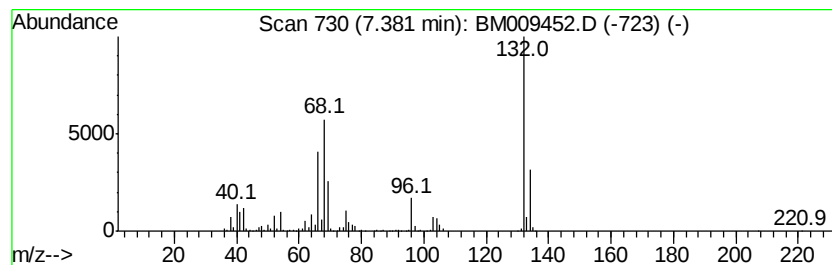
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.38 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	65.36 ng	2536050	1,4-Dichlorobenzene-d4	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM033017\
Data File : BM009452.D
Acq On : 30 Mar 2017 15:57
Operator : SJ/MA
Sample : PB97931BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB97931BL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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
3-Penten-2-one, 4...	4.38	6.5	ng	252186	1	7.86	776082	20.0
2-Pentanone, 4-hy...	4.98	72.0	ng	2795540	1	7.86	776082	20.0
Acetamide, N-methyl-	6.04	4.0	ng	153379	1	7.86	776082	20.0
unknown7.38	7.38	65.4	ng	2536050	1	7.86	776082	20.0