

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\  
 Data File : BM010057.D  
 Acq On : 16 May 2017 17:27  
 Operator : SJ/MA  
 Sample : PB99002BL  
 Misc :  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PB99002BL

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-BM051117.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 3.693       | 99            | 103         | 111          | rBV      | 95681          | 134819        | 2.19%           | 0.494%        |
| 2         | 4.287       | 199           | 204         | 216          | rBV      | 1192318        | 1623251       | 26.39%          | 5.944%        |
| 3         | 4.899       | 301           | 308         | 322          | rBV      | 4402351        | 6150632       | 100.00%         | 22.521%       |
| 4         | 5.346       | 377           | 384         | 395          | rBV      | 877307         | 1332037       | 21.66%          | 4.877%        |
| 5         | 5.951       | 482           | 487         | 495          | rBV      | 255539         | 388547        | 6.32%           | 1.423%        |
| 6         | 6.934       | 648           | 654         | 670          | rBV      | 881873         | 1465087       | 23.82%          | 5.365%        |
| 7         | 7.292       | 708           | 715         | 728          | rBV      | 854430         | 1403718       | 22.82%          | 5.140%        |
| 8         | 7.757       | 787           | 794         | 806          | rBV2     | 216299         | 353628        | 5.75%           | 1.295%        |
| 9         | 8.075       | 841           | 848         | 860          | rVB      | 897509         | 1481918       | 24.09%          | 5.426%        |
| 10        | 8.928       | 986           | 993         | 1007         | rBV      | 772137         | 1371036       | 22.29%          | 5.020%        |
| 11        | 10.551      | 1262          | 1269        | 1281         | rBV      | 245244         | 434385        | 7.06%           | 1.591%        |
| 12        | 13.022      | 1682          | 1689        | 1704         | rBV      | 1764121        | 2536408       | 41.24%          | 9.287%        |
| 13        | 14.410      | 1919          | 1925        | 1934         | rBV3     | 334360         | 541622        | 8.81%           | 1.983%        |
| 14        | 15.910      | 2174          | 2180        | 2195         | rBV      | 883807         | 1399543       | 22.75%          | 5.125%        |
| 15        | 17.168      | 2388          | 2394        | 2405         | rBV2     | 423690         | 691963        | 11.25%          | 2.534%        |
| 16        | 19.792      | 2834          | 2840        | 2850         | rBV      | 3810821        | 4565428       | 74.23%          | 16.717%       |
| 17        | 21.356      | 3101          | 3106        | 3116         | rBV      | 586055         | 813301        | 13.22%          | 2.978%        |
| 18        | 23.650      | 3489          | 3496        | 3504         | rBV2     | 275543         | 622976        | 10.13%          | 2.281%        |

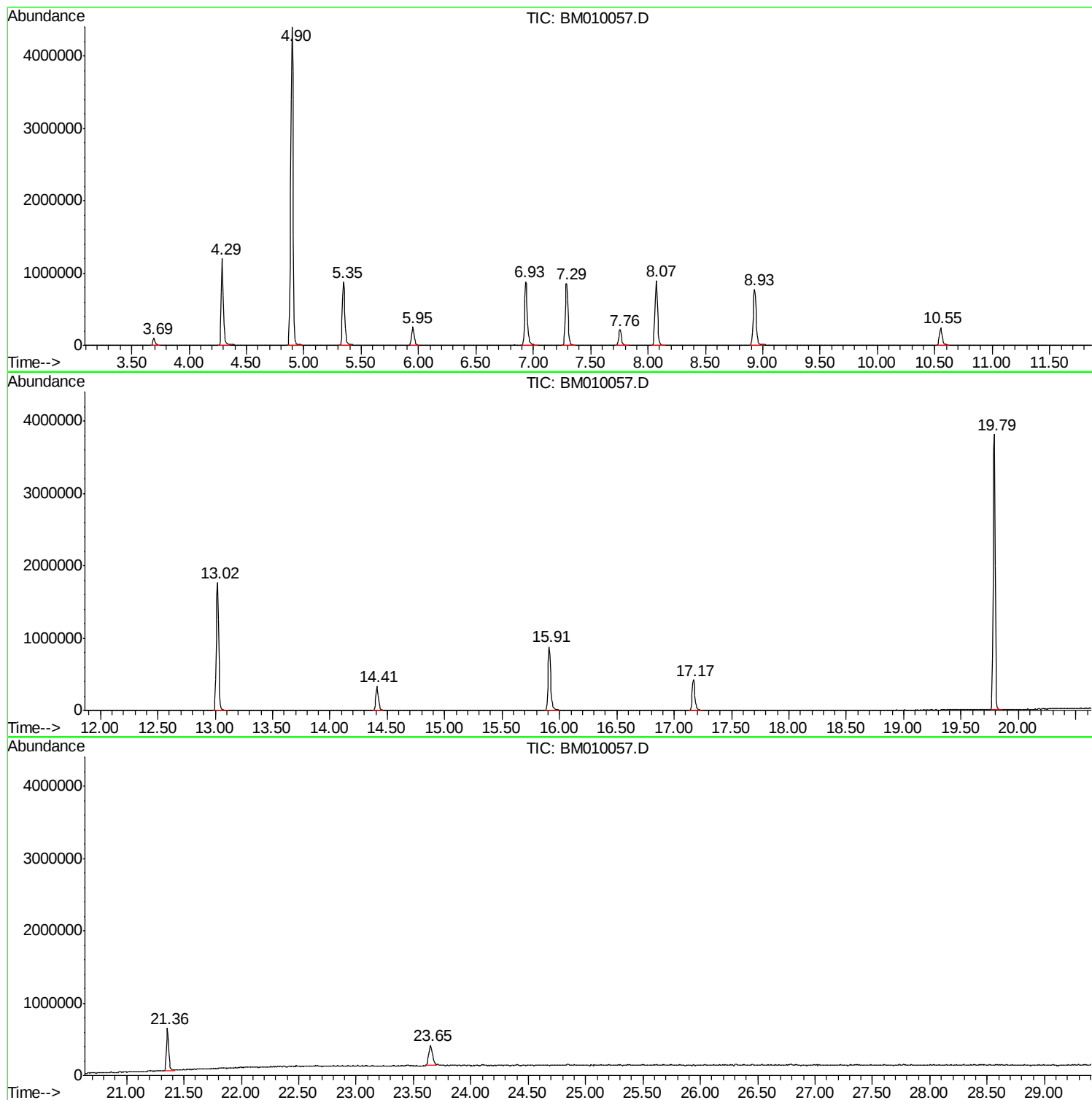
Sum of corrected areas: 27310299

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\  
Data File : BM010057.D  
Acq On : 16 May 2017 17:27  
Operator : SJ/MA  
Sample : PB99002BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB99002BL

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.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\BM051617\  
Data File : BM010057.D  
Acq On : 16 May 2017 17:27  
Operator : SJ/MA  
Sample : PB99002BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampled :  
PB99002BL

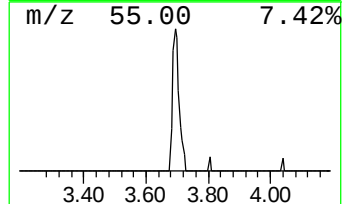
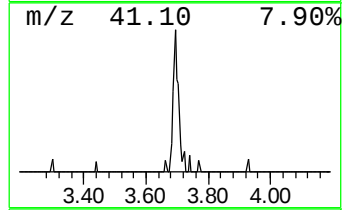
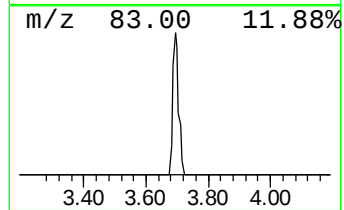
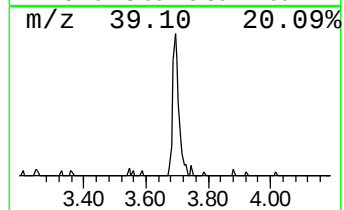
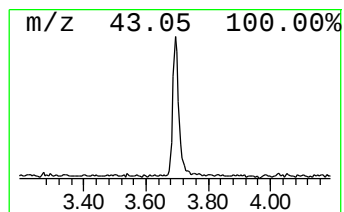
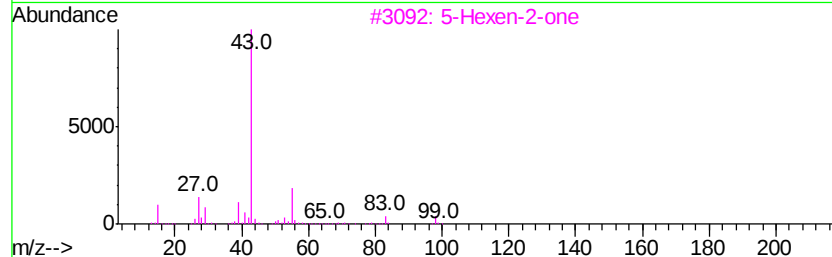
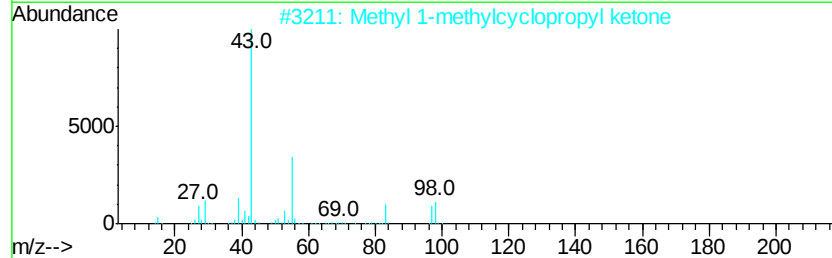
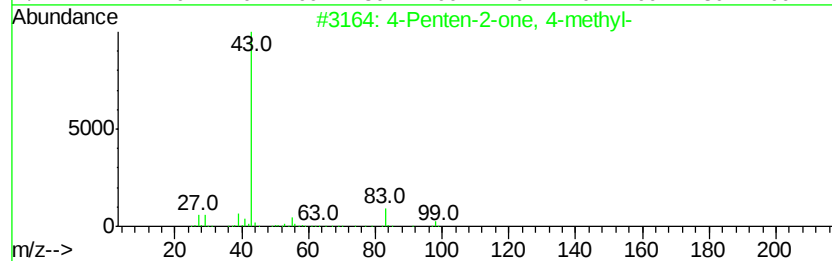
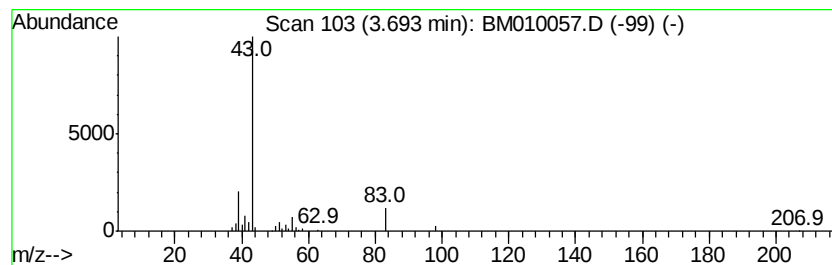
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 3.69 | 7.62 ng | 134819 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm  | CAS#         | Qual |
|------|----|---|------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 4-Penten-2-one, 4-methyl-          | 98  | C6H10O   | 003744-02-3  | 58   |
| 2    |    |   | Methyl 1-methylcyclopropyl ketone  | 98  | C6H10O   | 001567-75-5  | 43   |
| 3    |    |   | 5-Hexen-2-one                      | 98  | C6H10O   | 000109-49-9  | 37   |
| 4    |    |   | Imidazo[1,2-a]pyrimidine-2,3-d...  | 225 | C11H7N5O | 1000260-39-7 | 28   |
| 5    |    |   | Ethanone, 1-(2-methylcyclopropyl)- | 98  | C6H10O   | 000930-56-3  | 9    |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\  
Data File : BM010057.D  
Acq On : 16 May 2017 17:27  
Operator : SJ/MA  
Sample : PB99002BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB99002BL

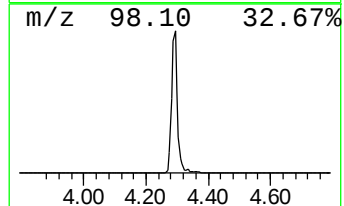
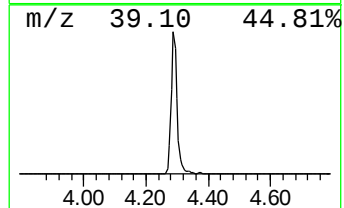
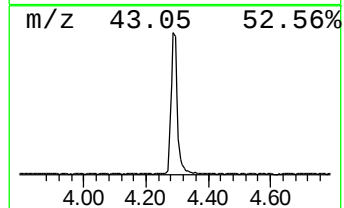
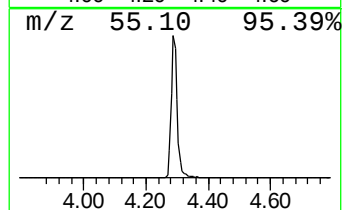
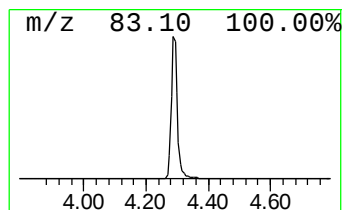
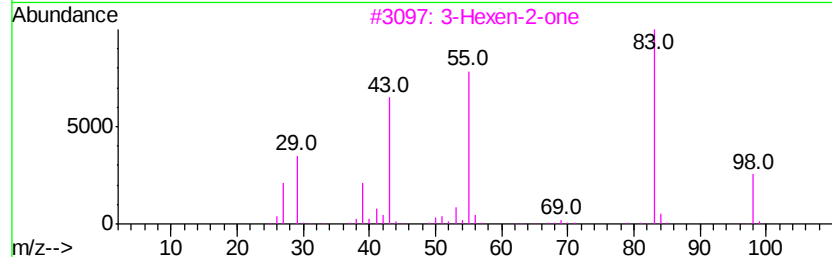
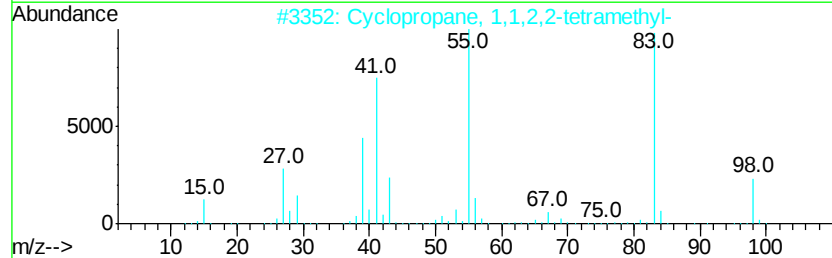
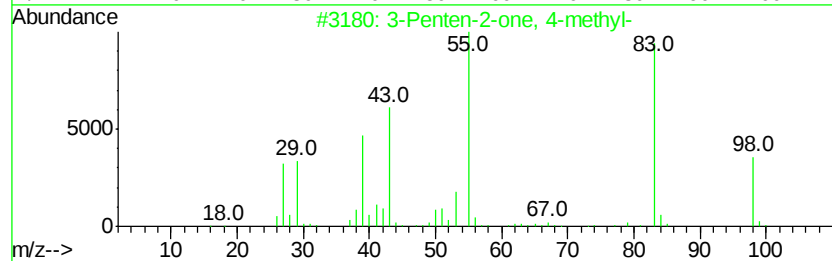
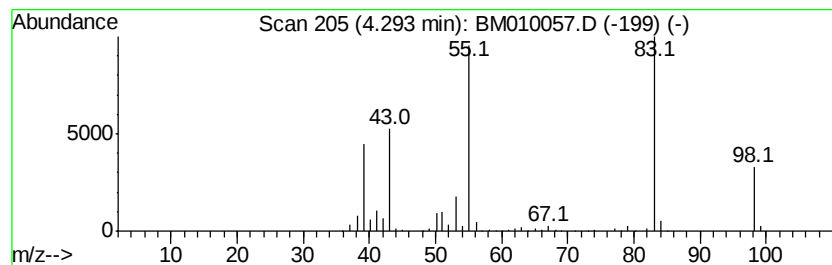
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.29 | 91.81 ng | 1623250 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | 5 | Tentative ID                       | MW | MolForm | CAS#        | Qual |
|------|----|---|------------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-          | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |    |   | Cyclopropane, 1,1,2,2-tetramethyl- | 98 | C7H14   | 004127-47-3 | 80   |
| 3    |    |   | 3-Hexen-2-one                      | 98 | C6H10O  | 000763-93-9 | 58   |
| 4    |    |   | 2-Pentene, 2,3-dimethyl-           | 98 | C7H14   | 010574-37-5 | 53   |
| 5    |    |   | 2-Pentene, 2,4-dimethyl-           | 98 | C7H14   | 000625-65-0 | 53   |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\  
Data File : BM010057.D  
Acq On : 16 May 2017 17:27  
Operator : SJ/MA  
Sample : PB99002BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB99002BL

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

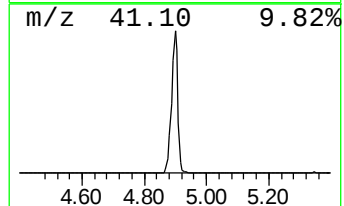
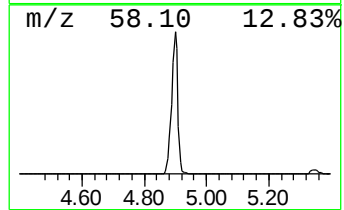
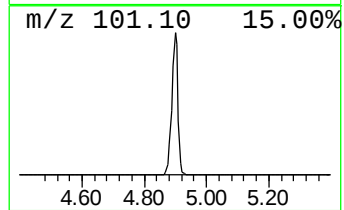
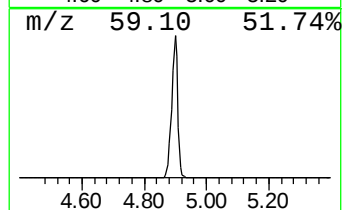
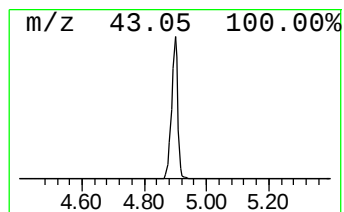
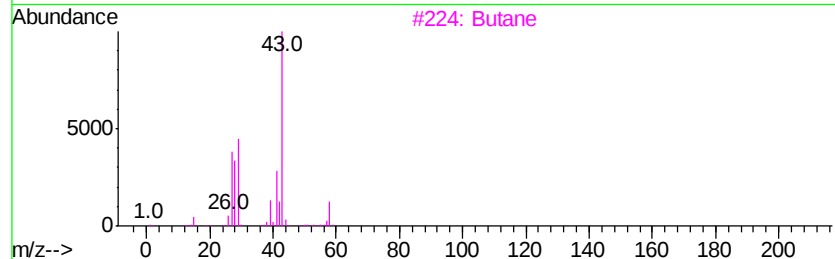
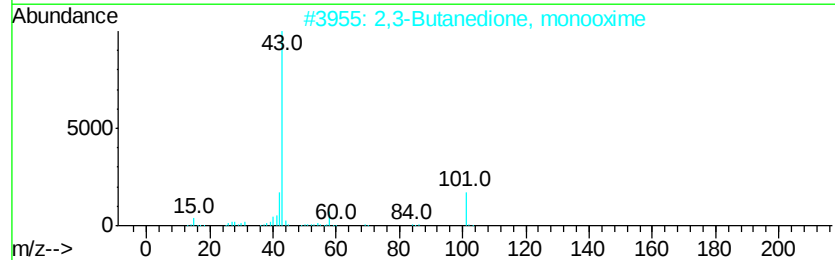
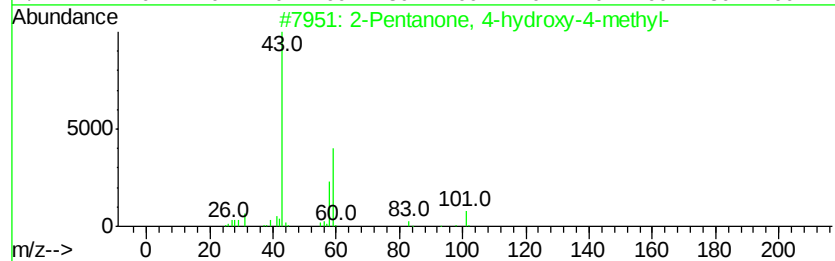
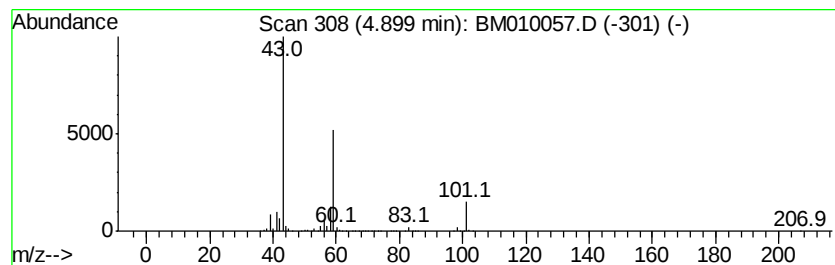
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 4.90 | 347.86 ng | 6150630 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64   |
| 2    |    | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6 | 27   |
| 3    |    | Butane                           | 58  | C4H10   | 000106-97-8 | 9    |
| 4    |    | 2-Propanone, 1-(1-methylethoxy)- | 116 | C6H12O2 | 042781-12-4 | 9    |
| 5    |    | 2-Hexanol, 2-methyl-             | 116 | C7H16O  | 000625-23-0 | 9    |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\  
Data File : BM010057.D  
Acq On : 16 May 2017 17:27  
Operator : SJ/MA  
Sample : PB99002BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampled :  
PB99002BL

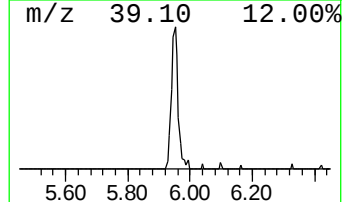
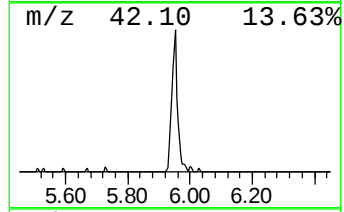
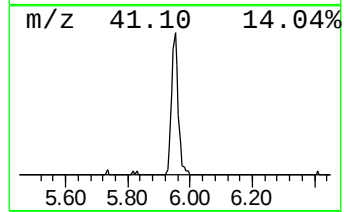
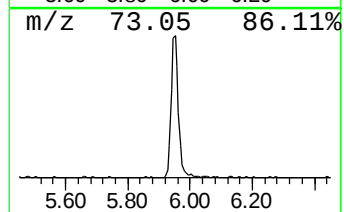
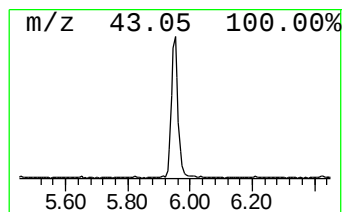
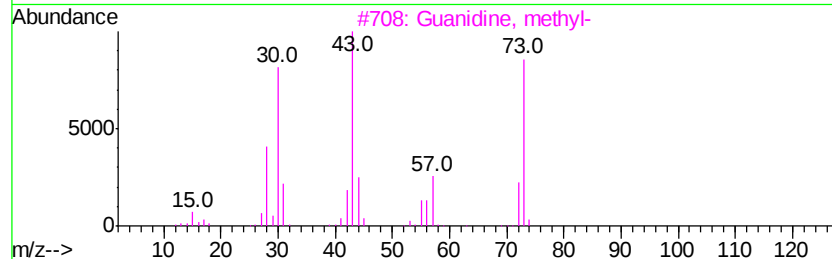
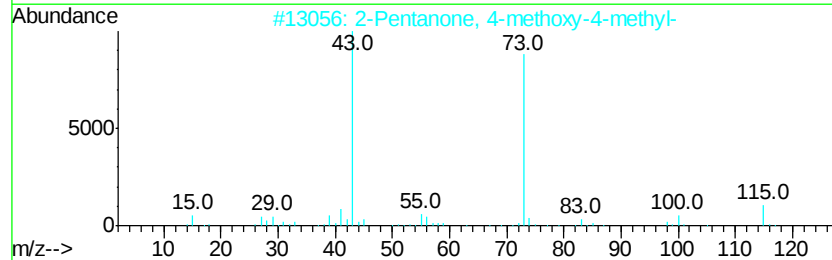
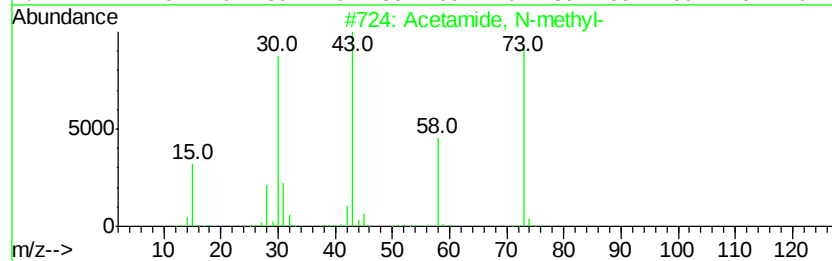
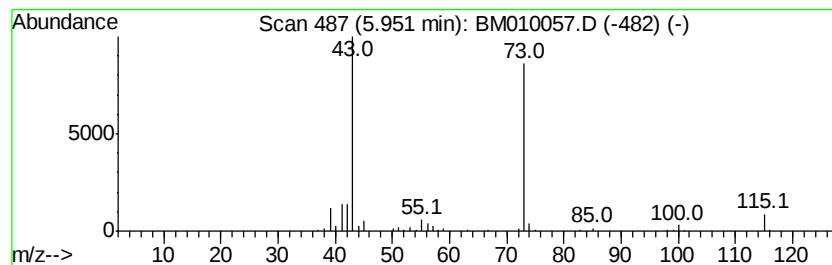
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 4 Acetamide, N-methyl- Concentration Rank 5

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.95 | 21.97 ng | 388547 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------|-----|---------|-------------|------|
| 1    | 5  | Acetamide, N-methyl-             | 73  | C3H7NO  | 000079-16-3 | 64   |
| 2    |    | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 64   |
| 3    |    | Guanidine, methyl-               | 73  | C2H7N3  | 000471-29-4 | 53   |
| 4    |    | N-Ethylformamide                 | 73  | C3H7NO  | 000627-45-2 | 37   |
| 5    |    | 2-Butanone, 3-methoxy-3-methyl-  | 116 | C6H12O2 | 036687-98-6 | 28   |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\  
Data File : BM010057.D  
Acq On : 16 May 2017 17:27  
Operator : SJ/MA  
Sample : PB99002BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampled :  
PB99002BL

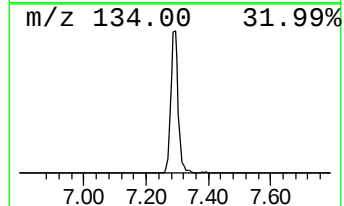
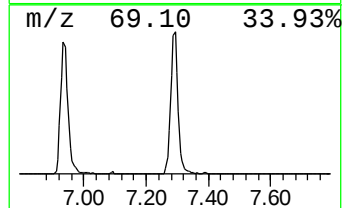
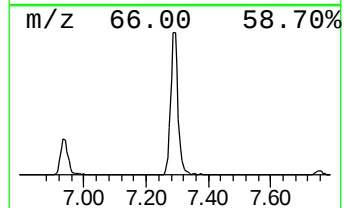
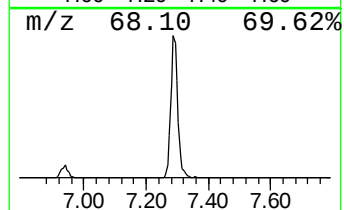
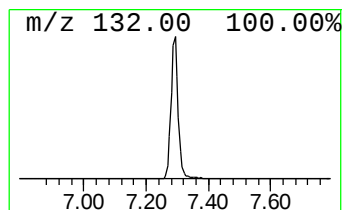
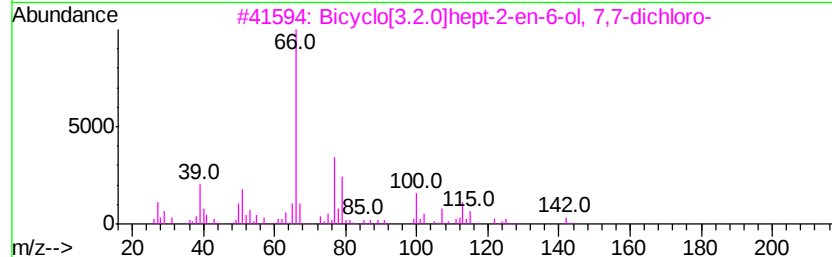
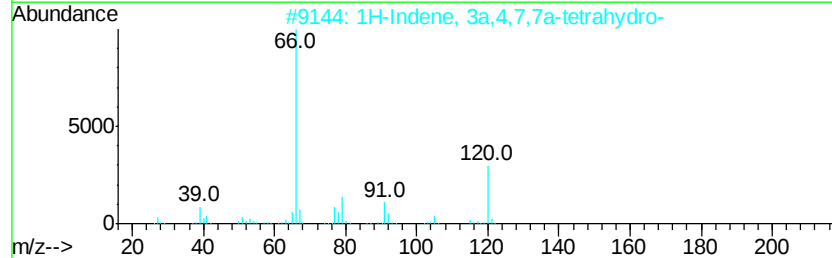
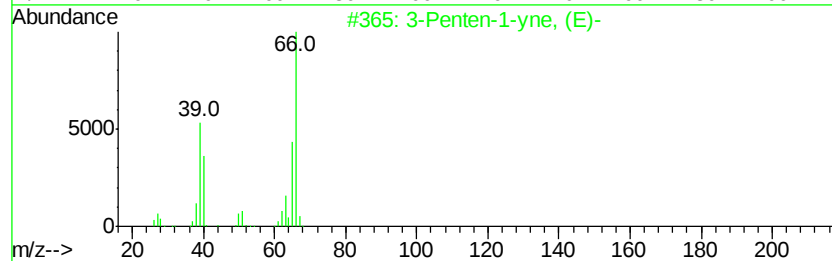
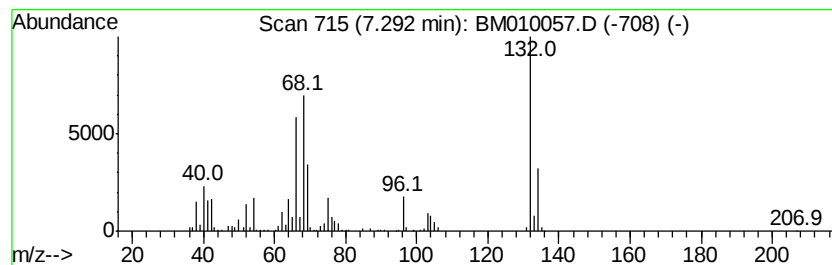
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 unknown7.29 Concentration Rank 4

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.29 | 79.39 ng | 1403720 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of                                  | Tentative ID | MW  | MolForm  | CAS#        | Qual |
|------|-------------------------------------|--------------|-----|----------|-------------|------|
| 1    | 3-Penten-1-yne, (E)-                |              | 66  | C5H6     | 002004-69-5 | 27   |
| 2    | 1H-Indene, 3a,4,7,7a-tetrahydro-    |              | 120 | C9H12    | 003048-65-5 | 16   |
| 3    | Bicyclo[3.2.0]hept-2-en-6-ol, 7,... |              | 178 | C7H8Cl2O | 092998-64-6 | 16   |
| 4    | 5-Ethyl bicyclo[2.2.1]-2-heptene    |              | 122 | C9H14    | 015403-89-1 | 16   |
| 5    | 3-Penten-1-yne, (Z)-                |              | 66  | C5H6     | 001574-40-9 | 16   |



Data Path : Z:\HPCHEM1\BNA\_M\DATA\BM051617\  
Data File : BM010057.D  
Acq On : 16 May 2017 17:27  
Operator : SJ/MA  
Sample : PB99002BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB99002BL

Quant Method : Z:\HPCHEM1\BNA\_M\METHODS\8270-BM051117.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 |
| 4-Penten-2-one, 4... | 3.69 | 7.6     | ng    | 134819   | 1                     | 7.76 | 353628 | 20.0 |
| 3-Penten-2-one, 4... | 4.29 | 91.8    | ng    | 1623250  | 1                     | 7.76 | 353628 | 20.0 |
| 2-Pentanone, 4-hy... | 4.90 | 347.9   | ng    | 6150630  | 1                     | 7.76 | 353628 | 20.0 |
| Acetamide, N-methyl- | 5.95 | 22.0    | ng    | 388547   | 1                     | 7.76 | 353628 | 20.0 |
| unknown7.29          | 7.29 | 79.4    | ng    | 1403720  | 1                     | 7.76 | 353628 | 20.0 |