

Data Path : Z:\HPCHEM1\BNA\_G\DATA\BG120215\  
 Data File : BG019848.D  
 Acq On : 2 Dec 2015 23:52  
 Operator : UM/NP  
 Sample : G4585-13  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-P3WC-16(0-4)

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\_G\METHODS\8270-BG120215.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         | 2.875       | 4             | 6           | 8            | rVB      | 2571292        | 1795888       | 67.81%          | 13.912%       |
| 2         | 3.145       | 46            | 52          | 62           | rBV2     | 57157          | 122749        | 4.64%           | 0.951%        |
| 3         | 3.239       | 63            | 68          | 77           | rVB      | 195057         | 280651        | 10.60%          | 2.174%        |
| 4         | 5.207       | 393           | 403         | 411          | rBV      | 104986         | 161761        | 6.11%           | 1.253%        |
| 5         | 5.671       | 475           | 482         | 490          | rBV      | 412360         | 638771        | 24.12%          | 4.948%        |
| 6         | 7.269       | 747           | 754         | 764          | rVB      | 396055         | 670102        | 25.30%          | 5.191%        |
| 7         | 7.657       | 812           | 820         | 827          | rBV      | 435507         | 732967        | 27.68%          | 5.678%        |
| 8         | 8.127       | 894           | 900         | 907          | rVB      | 85560          | 143056        | 5.40%           | 1.108%        |
| 9         | 8.456       | 947           | 956         | 964          | rBV      | 321806         | 563982        | 21.30%          | 4.369%        |
| 10        | 9.296       | 1090          | 1099        | 1108         | rBV      | 280942         | 489711        | 18.49%          | 3.793%        |
| 11        | 10.947      | 1372          | 1380        | 1385         | rBV      | 113080         | 202047        | 7.63%           | 1.565%        |
| 12        | 11.000      | 1385          | 1389        | 1399         | rVB      | 50048          | 82544         | 3.12%           | 0.639%        |
| 13        | 13.386      | 1788          | 1795        | 1802         | rBV      | 820918         | 1217917       | 45.99%          | 9.434%        |
| 14        | 14.761      | 2023          | 2029        | 2035         | rBV2     | 189350         | 303859        | 11.47%          | 2.354%        |
| 15        | 16.241      | 2274          | 2281        | 2288         | rBV      | 793030         | 1174079       | 44.33%          | 9.095%        |
| 16        | 17.504      | 2489          | 2496        | 2501         | rBV2     | 302904         | 469845        | 17.74%          | 3.640%        |
| 17        | 20.113      | 2933          | 2940        | 2945         | rBV      | 1927511        | 2648230       | 100.00%         | 20.514%       |
| 18        | 21.782      | 3218          | 3224        | 3231         | rBV      | 399176         | 644022        | 24.32%          | 4.989%        |
| 19        | 25.090      | 3778          | 3787        | 3797         | rVB      | 202931         | 567150        | 21.42%          | 4.393%        |

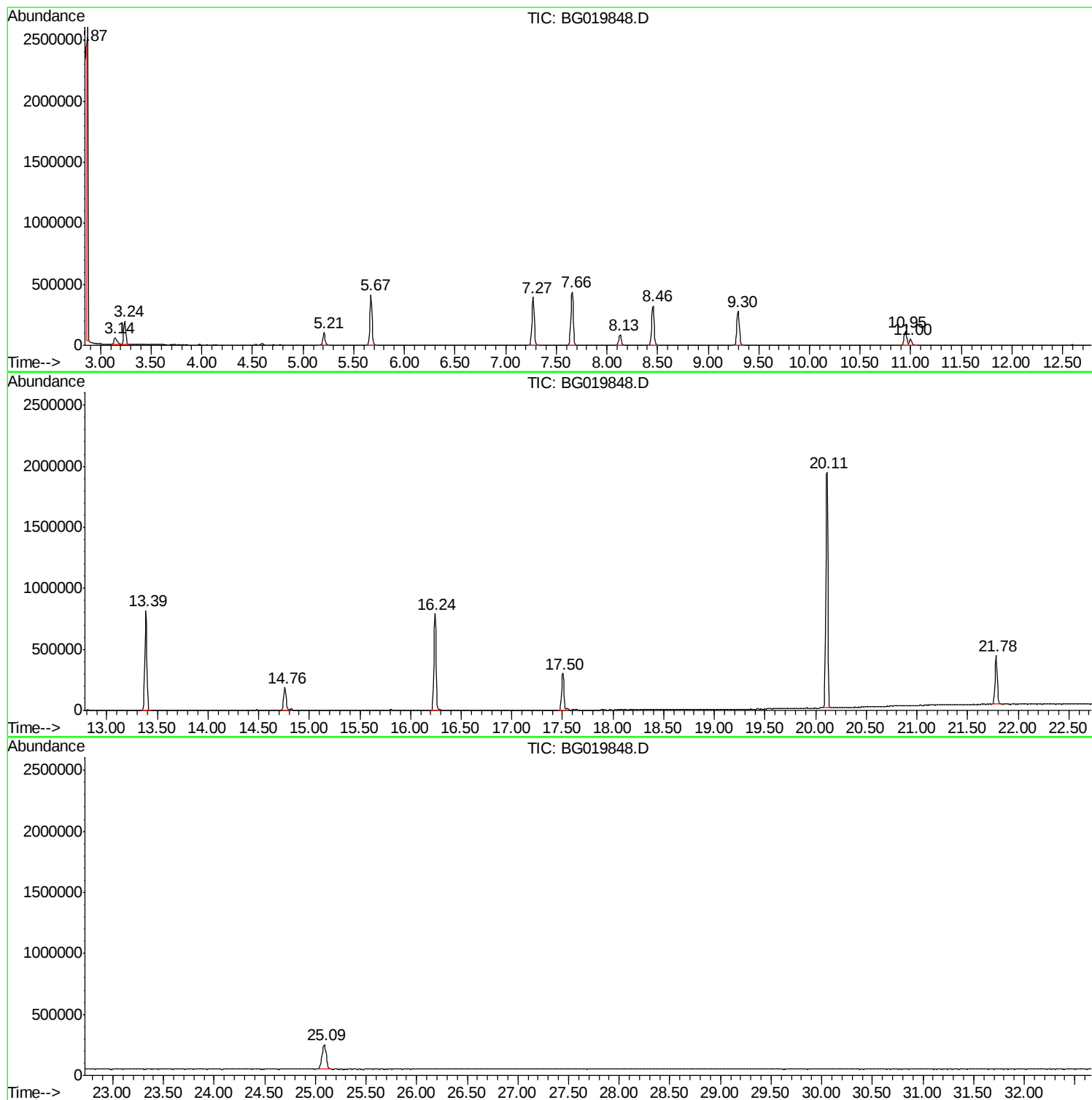
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ClientSampleId :  
SB-P3WC-16(0-4)

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG120215.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

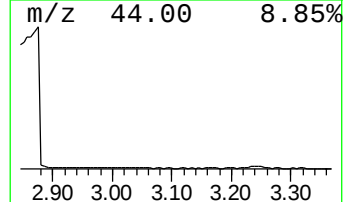
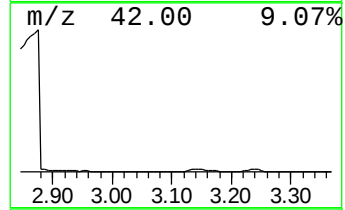
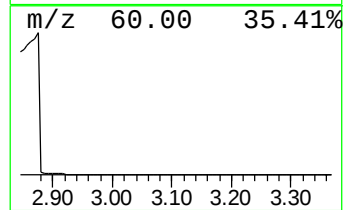
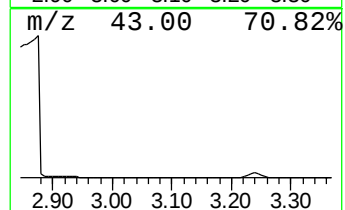
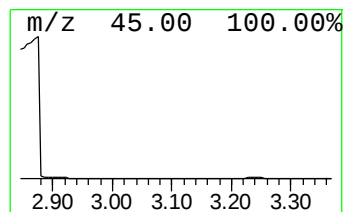
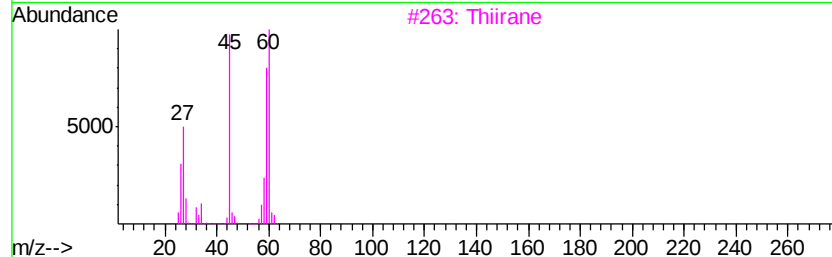
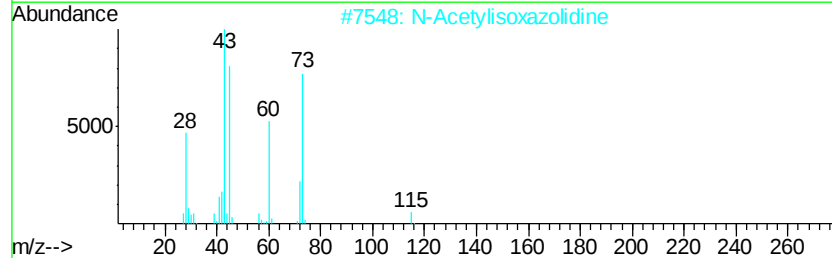
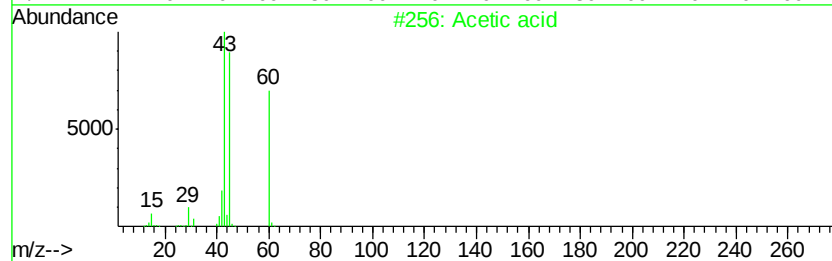
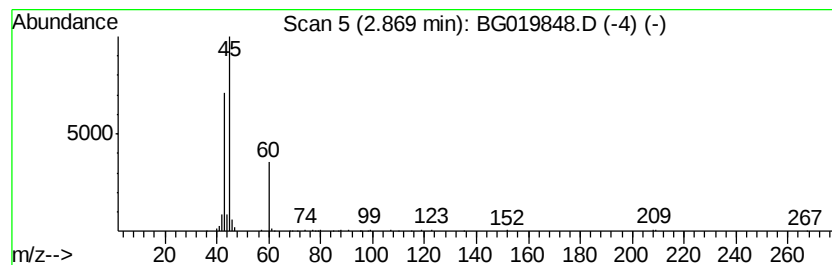
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Acetic acid Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 2.87 | 251.08 ng | 1795890 | 1,4-Dichlorobenzene-d4 | 8.13 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Acetic acid                         | 60  | C2H4O2  | 000064-19-7 | 90   |
| 2    |    | N-Acetylisoaxazolidine              | 115 | C5H9N02 | 115615-36-6 | 50   |
| 3    |    | Thiirane                            | 60  | C2H4S   | 000420-12-2 | 28   |
| 4    |    | Thiazole, 4,5-dihydro-2-methyl-     | 101 | C4H7NS  | 002346-00-1 | 25   |
| 5    |    | Ethanone, 1-(4,5-dihydro-2-thiaz... | 129 | C5H7NOS | 029926-41-8 | 23   |



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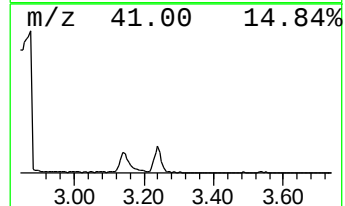
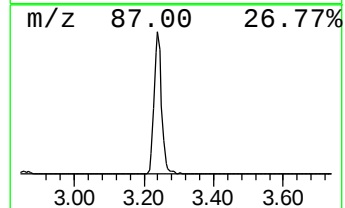
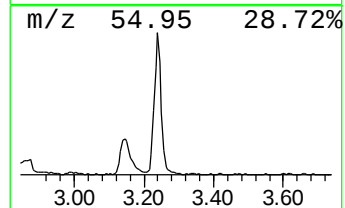
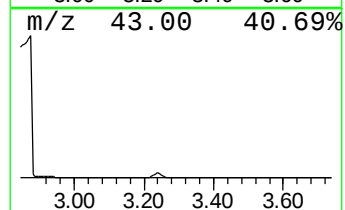
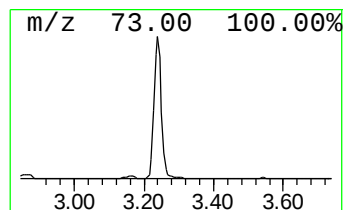
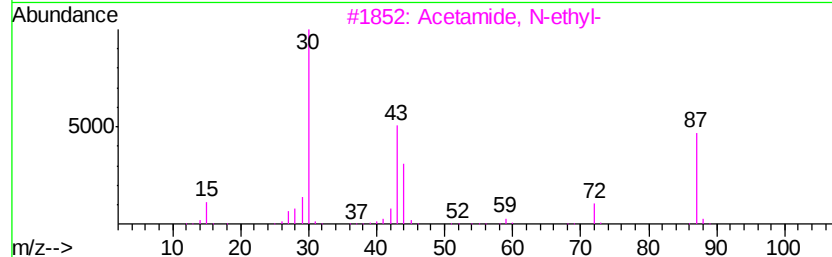
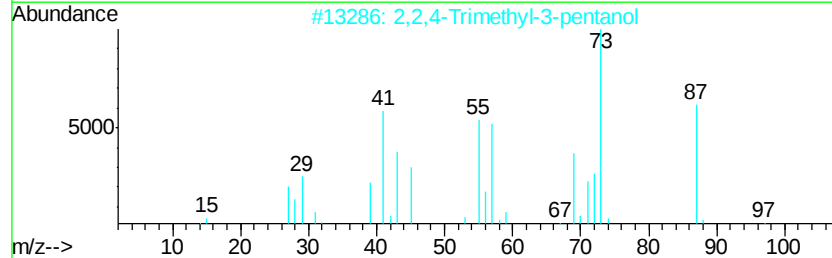
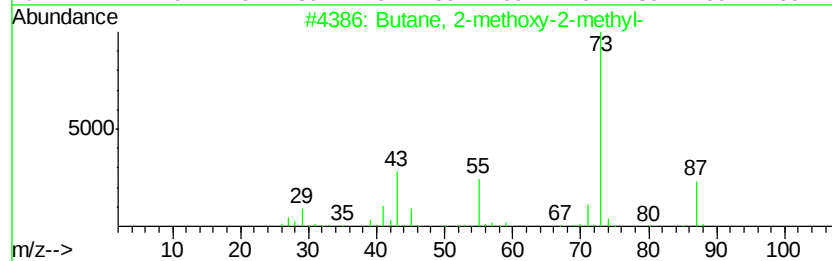
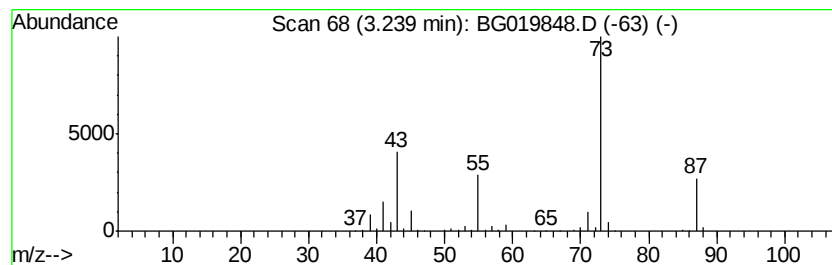
Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG120215.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 3.24 | 39.24 ng | 280651 | 1,4-Dichlorobenzene-d4 | 8.13 |

| Hit# | of | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------|-----|---------|-------------|------|
| 1    | 5  | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 78   |
| 2    |    | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 22   |
| 4    |    | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |
| 5    |    | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-P3WC-16(0-4)

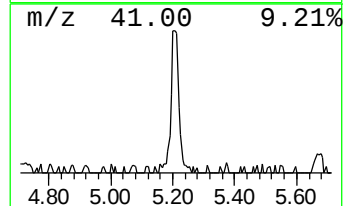
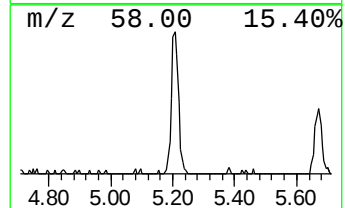
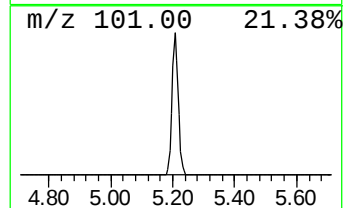
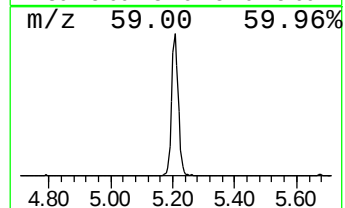
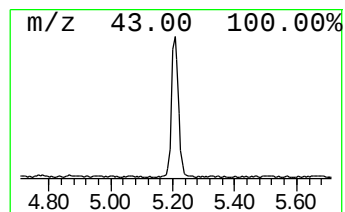
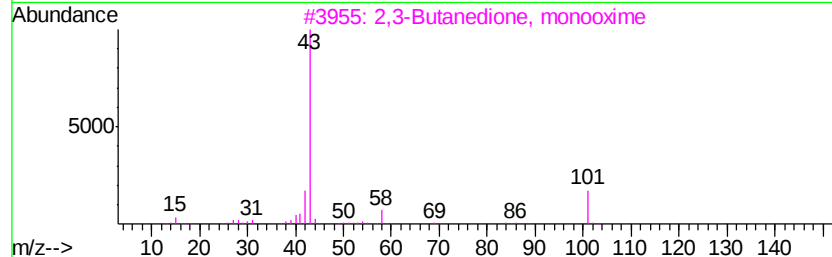
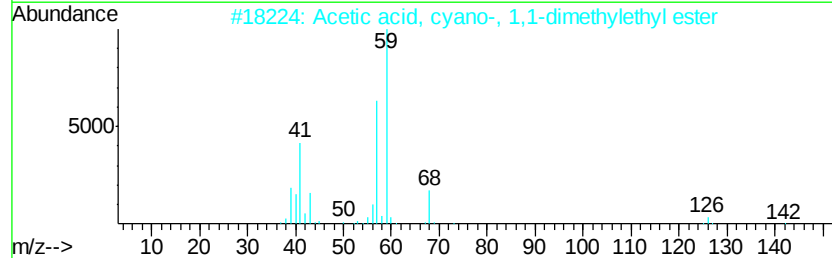
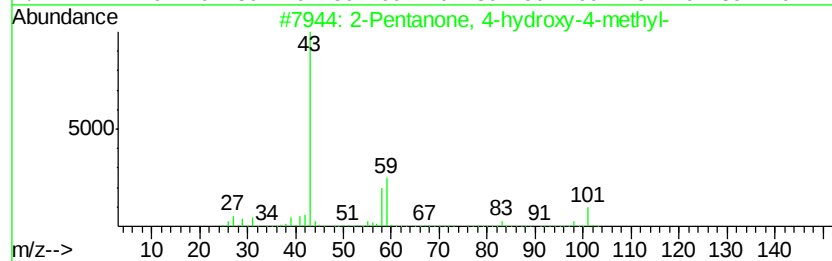
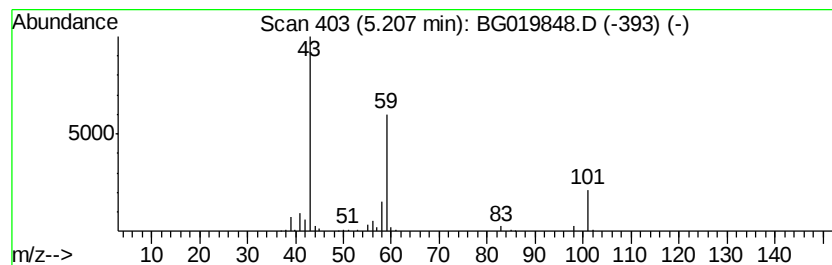
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.21 | 22.62 ng | 161761 | 1,4-Dichlorobenzene-d4 | 8.13 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 3    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 4    |    | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    | (+)-4-Amino-4,5-dihydro-2(3H)-f...  | 101 | C4H7NO2  | 016504-58-8 | 9    |



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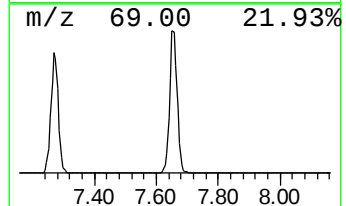
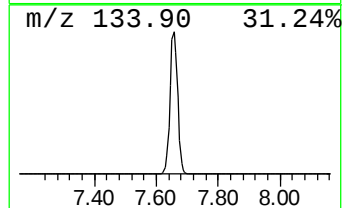
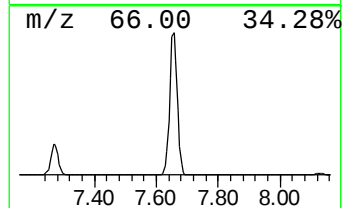
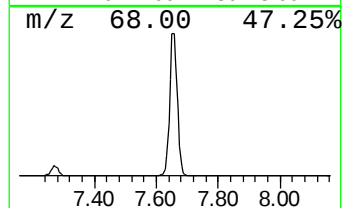
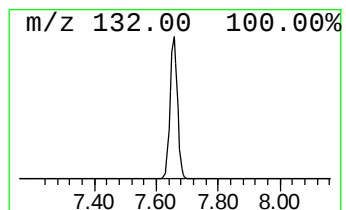
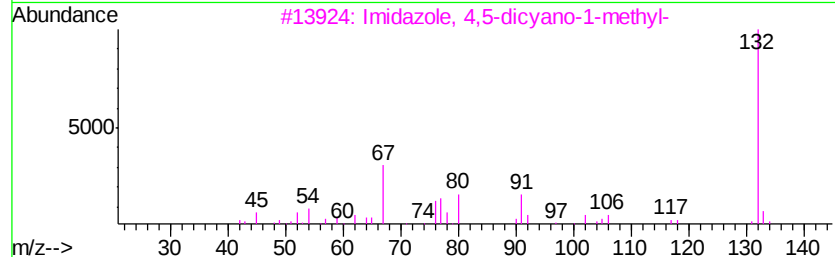
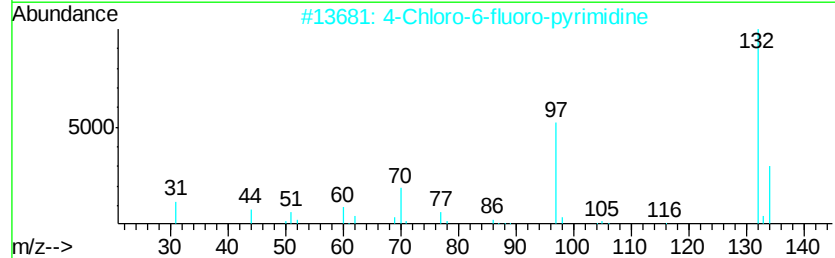
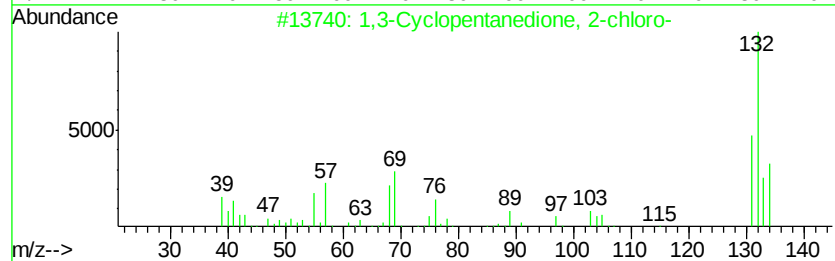
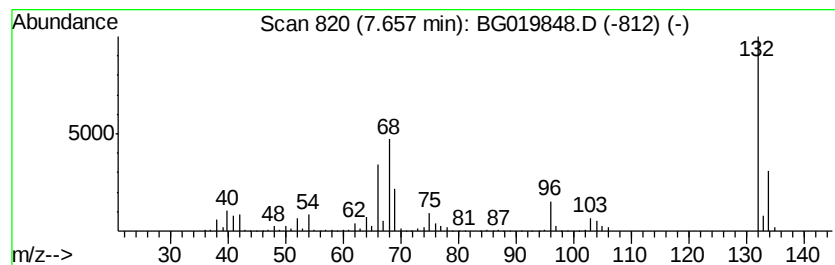
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TIC Library : C:\DATABASE\NIST02.L  
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\*\*\*\*\*  
Peak Number 5 unknown7.66 Concentration Rank 2

| R.T. | EstConc   | Area   | Relative to ISTD       | R.T. |
|------|-----------|--------|------------------------|------|
| 7.66 | 102.47 ng | 732967 | 1,4-Dichlorobenzene-d4 | 8.13 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#        | Qual |
|------|----|----------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2  | 014203-19-1 | 32   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6 | 27   |
| 3    |    | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4    | 019485-35-9 | 25   |
| 4    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6 | 22   |
| 5    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0 | 22   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Acetic acid          | 2.87 | 251.1   | ng    | 1795890  | 1                     | 8.13 | 143056 | 20.0 |
| Butane, 2-methoxy... | 3.24 | 39.2    | ng    | 280651   | 1                     | 8.13 | 143056 | 20.0 |
| 2-Pentanone, 4-hy... | 5.21 | 22.6    | ng    | 161761   | 1                     | 8.13 | 143056 | 20.0 |
| unknown7.66          | 7.66 | 102.5   | ng    | 732967   | 1                     | 8.13 | 143056 | 20.0 |