

Data Path : Z:\HPCHEM1\BNA\_G\DATA\BG071616\  
 Data File : BG023143.D  
 Acq On : 16 Jul 2016 12:19  
 Operator : UM/SJ  
 Sample : H4016-18  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 C5-15

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-BG070816.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         | 2.896       | 4             | 10          | 29           | rVB      | 271310         | 671605        | 8.32%           | 1.303%        |
| 2         | 3.037       | 29            | 34          | 53           | rVV      | 5403512        | 8069455       | 100.00%         | 15.660%       |
| 3         | 3.184       | 53            | 59          | 72           | rVB      | 217073         | 465855        | 5.77%           | 0.904%        |
| 4         | 5.217       | 400           | 405         | 412          | rBV      | 241751         | 376427        | 4.66%           | 0.730%        |
| 5         | 5.693       | 476           | 486         | 498          | rBV      | 1700248        | 2762130       | 34.23%          | 5.360%        |
| 6         | 7.303       | 748           | 760         | 770          | rBV      | 1954902        | 3432086       | 42.53%          | 6.660%        |
| 7         | 7.679       | 817           | 824         | 835          | rBV      | 1783755        | 3072952       | 38.08%          | 5.963%        |
| 8         | 8.149       | 897           | 904         | 911          | rBV      | 372441         | 632499        | 7.84%           | 1.227%        |
| 9         | 8.472       | 953           | 959         | 966          | rVB      | 1188117        | 2061770       | 25.55%          | 4.001%        |
| 10        | 9.318       | 1094          | 1103        | 1110         | rBV      | 1153567        | 2121358       | 26.29%          | 4.117%        |
| 11        | 10.975      | 1377          | 1385        | 1396         | rBV      | 549311         | 1006311       | 12.47%          | 1.953%        |
| 12        | 13.413      | 1793          | 1800        | 1820         | rVB      | 2787784        | 4435028       | 54.96%          | 8.607%        |
| 13        | 14.236      | 1934          | 1940        | 1947         | rBV      | 1014188        | 1471265       | 18.23%          | 2.855%        |
| 14        | 14.794      | 2026          | 2035        | 2043         | rBV2     | 975651         | 1644013       | 20.37%          | 3.190%        |
| 15        | 15.616      | 2170          | 2175        | 2181         | rVB      | 55478          | 86199         | 1.07%           | 0.167%        |
| 16        | 16.286      | 2283          | 2289        | 2299         | rBV      | 2940786        | 4732491       | 58.65%          | 9.184%        |
| 17        | 16.480      | 2318          | 2322        | 2325         | rBV      | 69717          | 99448         | 1.23%           | 0.193%        |
| 18        | 17.273      | 2452          | 2457        | 2463         | rBV3     | 87380          | 128394        | 1.59%           | 0.249%        |
| 19        | 17.549      | 2495          | 2504        | 2510         | rBV      | 1380016        | 2162923       | 26.80%          | 4.197%        |
| 20        | 18.419      | 2647          | 2652        | 2656         | rBV5     | 63782          | 106583        | 1.32%           | 0.207%        |
| 21        | 19.600      | 2846          | 2853        | 2859         | rBV      | 100224         | 182395        | 2.26%           | 0.354%        |
| 22        | 19.958      | 2909          | 2914        | 2921         | rVB2     | 99581          | 166029        | 2.06%           | 0.322%        |
| 23        | 20.152      | 2941          | 2947        | 2953         | rBV      | 4950062        | 6535854       | 80.99%          | 12.684%       |
| 24        | 21.468      | 3167          | 3171        | 3175         | rBV7     | 65429          | 117795        | 1.46%           | 0.229%        |
| 25        | 21.850      | 3228          | 3236        | 3243         | rBV      | 1516737        | 2680601       | 33.22%          | 5.202%        |
| 26        | 25.229      | 3800          | 3811        | 3822         | rVB3     | 785691         | 2308900       | 28.61%          | 4.481%        |

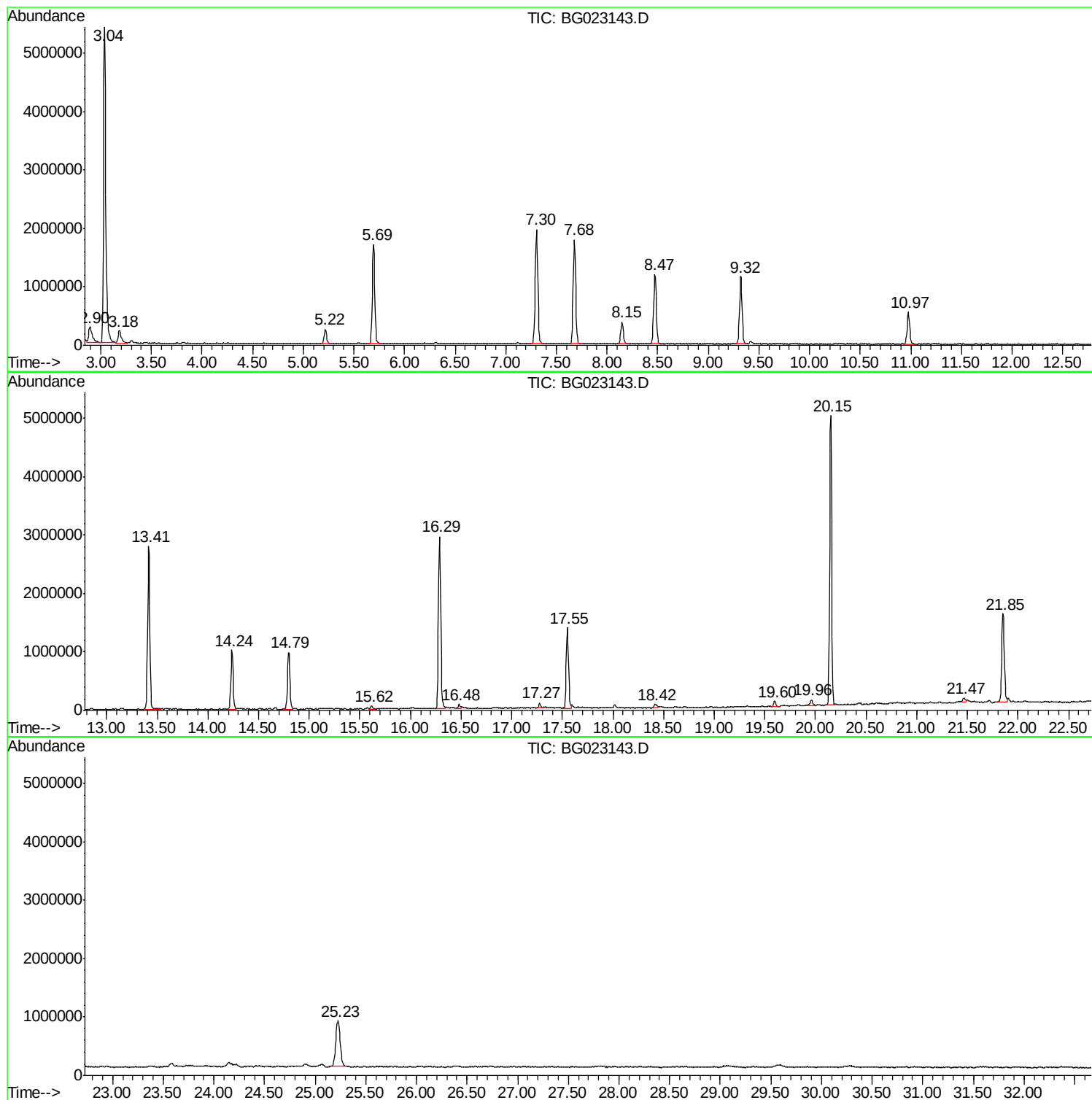
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BNA\_G  
ClientSampleId :  
C5-15

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG070816.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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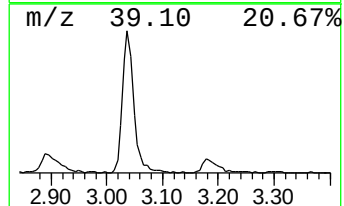
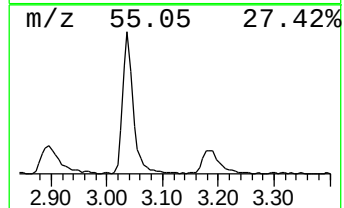
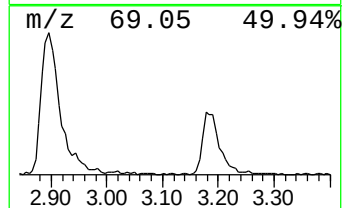
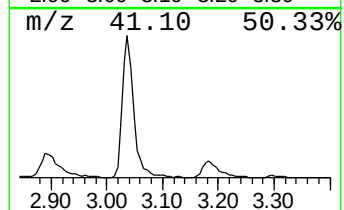
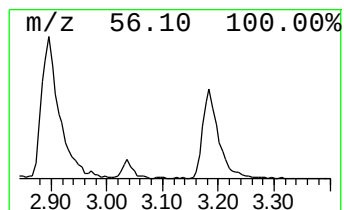
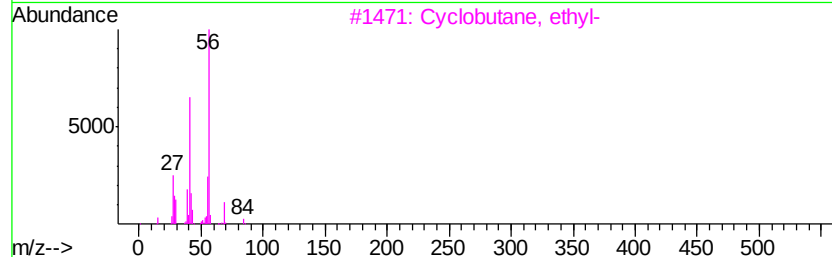
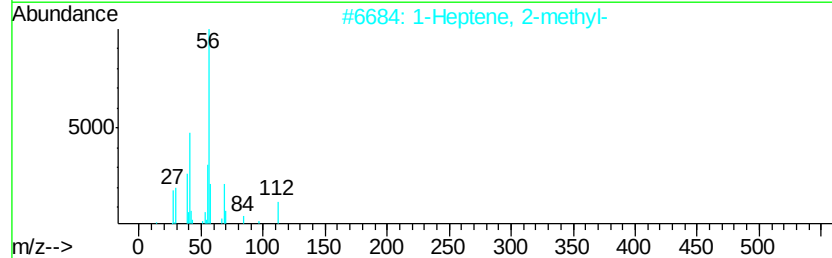
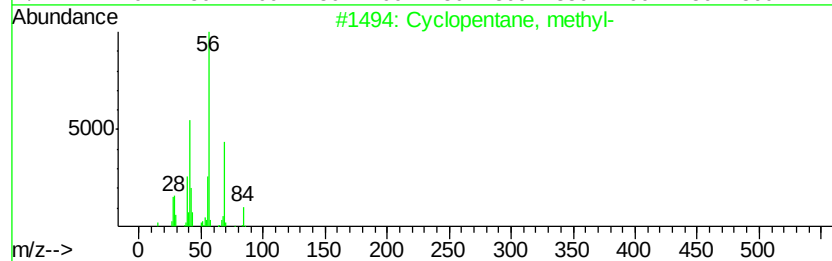
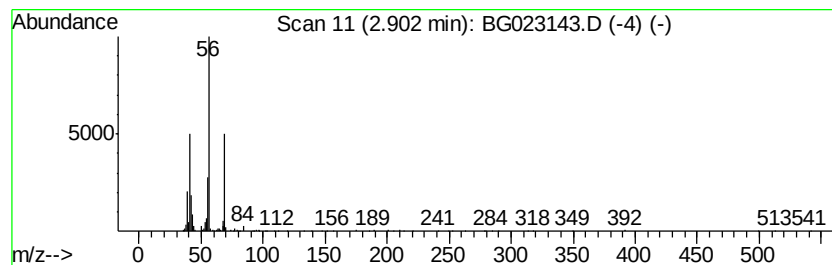
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 2.90 | 21.24 ng | 671605 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------|-----|---------|-------------|------|
| 1    | 5  | Cyclopentane, methyl- | 84  | C6H12   | 000096-37-7 | 72   |
| 2    |    | 1-Heptene, 2-methyl-  | 112 | C8H16   | 015870-10-7 | 64   |
| 3    |    | Cyclobutane, ethyl-   | 84  | C6H12   | 004806-61-5 | 56   |
| 4    |    | Cyclopropane, propyl- | 84  | C6H12   | 002415-72-7 | 50   |
| 5    |    | 1-Hexene, 2-methyl-   | 98  | C7H14   | 006094-02-6 | 50   |



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Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG070816.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

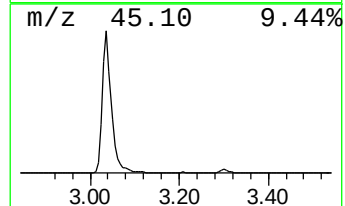
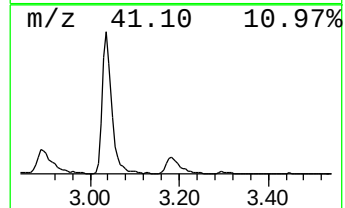
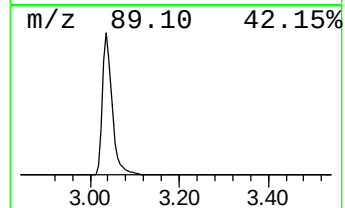
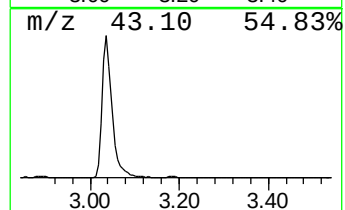
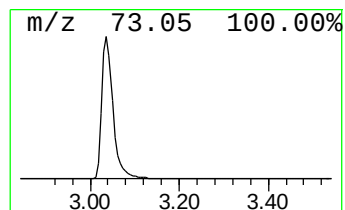
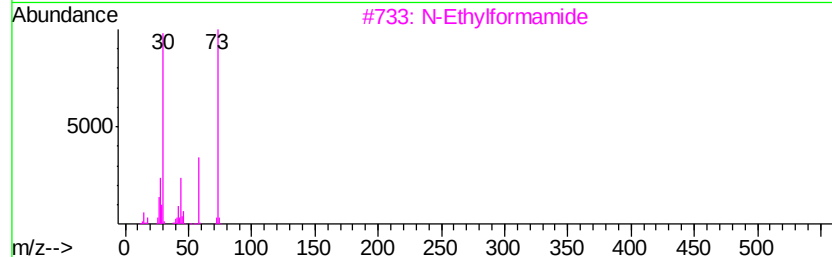
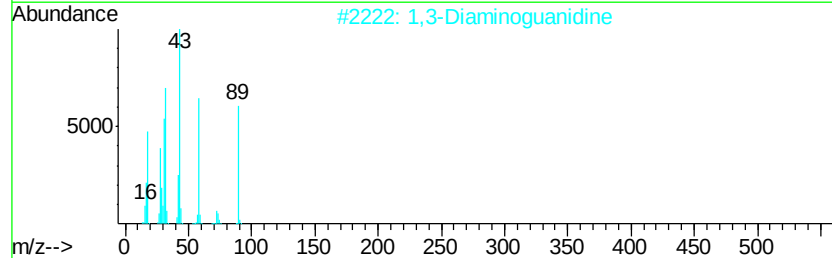
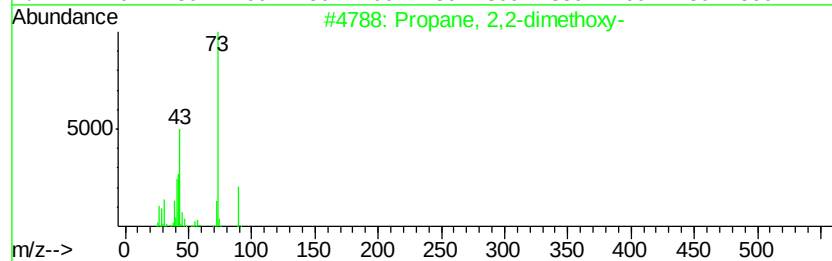
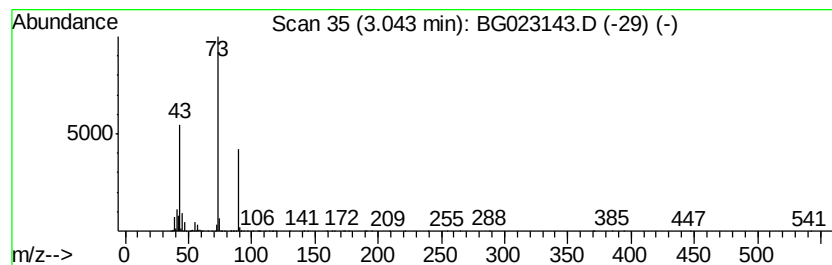
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown3.04 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 3.04 | 255.16 ng | 8069460 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-             | 104 | C5H12O2  | 000077-76-9 | 39   |
| 2    |    | 1,3-Diaminoguanidine                | 89  | CH7N5    | 004364-78-7 | 23   |
| 3    |    | N-Ethylformamide                    | 73  | C3H7NO   | 000627-45-2 | 9    |
| 4    |    | Acetamide, N-methyl-                | 73  | C3H7NO   | 000079-16-3 | 9    |
| 5    |    | 1-Hexen-4-ol, 1-chloro-3,5-dimet... | 162 | C8H15ClO | 100244-09-5 | 9    |



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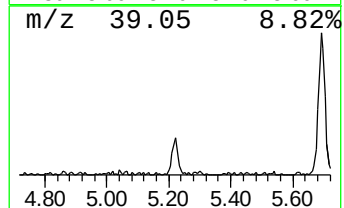
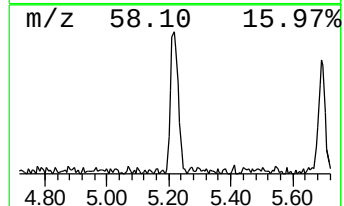
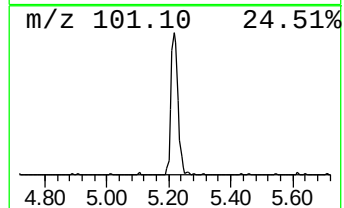
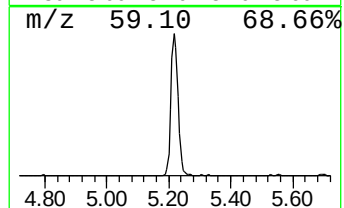
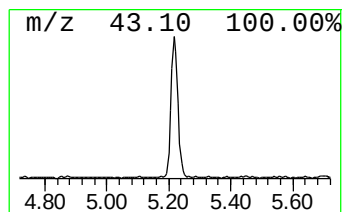
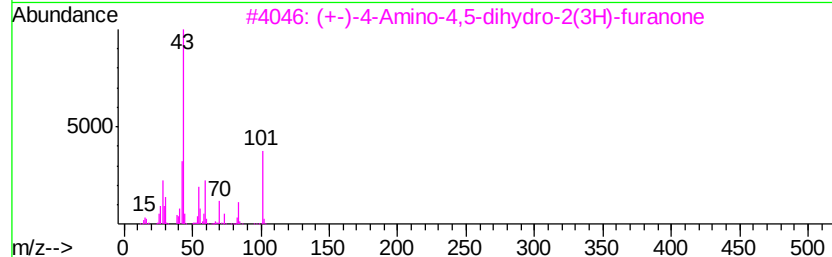
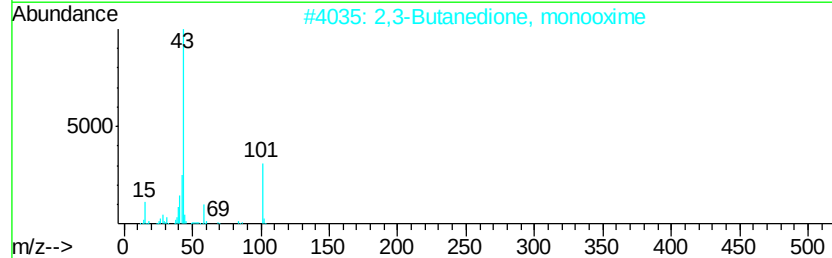
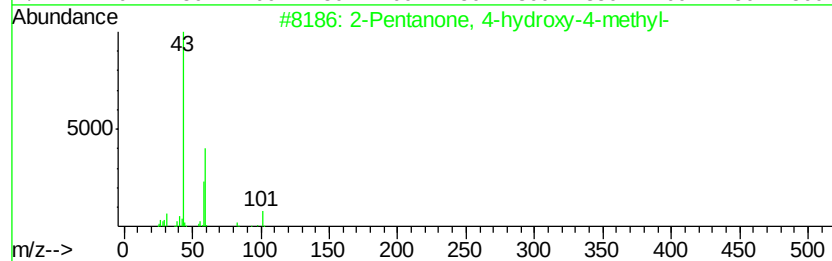
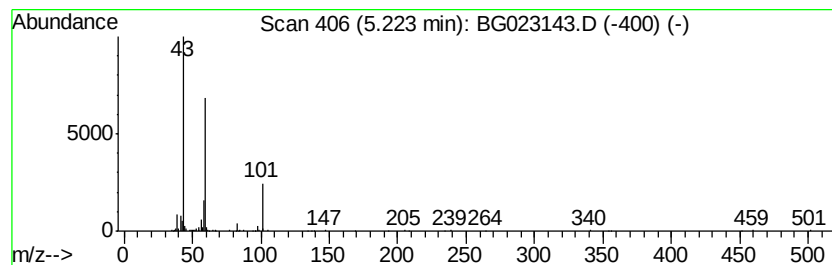
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown5.22 Concentration Rank 6

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.22 | 11.90 ng | 376427 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2 | 000123-42-2 | 47   |
| 2    |    | 2,3-Butanedione, monooxime         | 101 | C4H7NO2 | 000057-71-6 | 17   |
| 3    |    | (+)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9    |
| 4    |    | Morpholine, 4-methyl-              | 101 | C5H11NO | 000109-02-4 | 9    |
| 5    |    | Guanidine                          | 59  | CH5N3   | 000113-00-8 | 9    |



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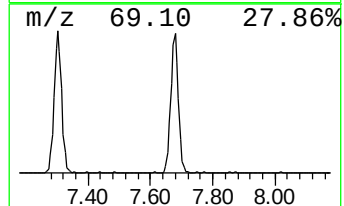
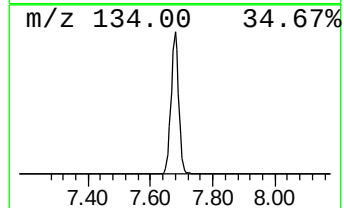
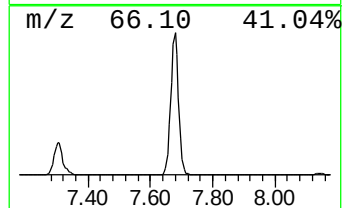
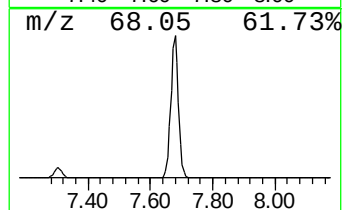
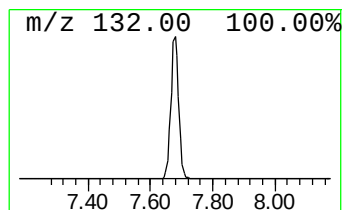
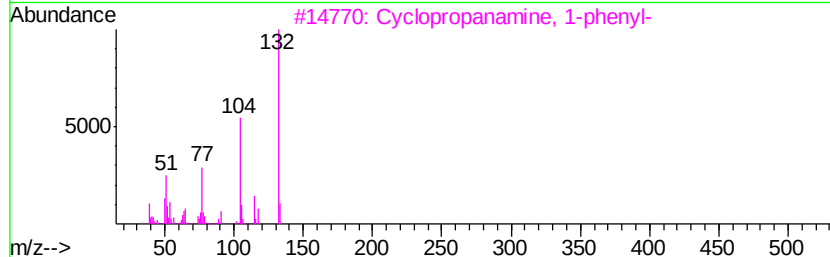
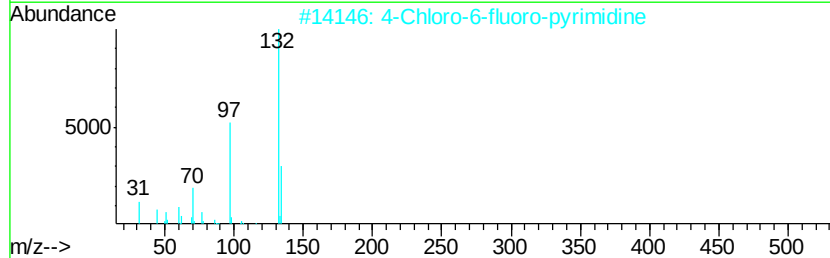
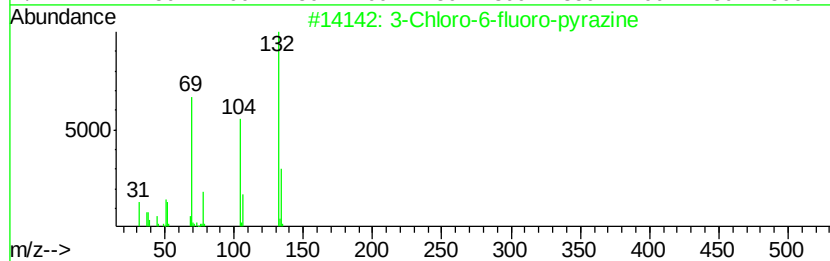
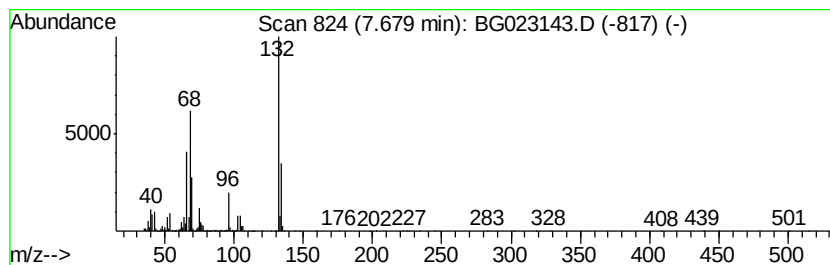
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 unknown7.68 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.68 | 97.17 ng | 3072950 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID                 | MW  | MolForm   | CAS#         | Qual |
|------|----|------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine   | 132 | C4H2ClFN2 | 1000146-10-7 | 14   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6  | 14   |
| 3    |    | Cyclopropanamine, 1-phenyl-  | 133 | C9H11N    | 1000351-26-2 | 10   |
| 4    |    | 1H-Benzimidazole, 2-methyl-  | 132 | C8H8N2    | 000615-15-6  | 10   |
| 5    |    | 5-Fluoro-2-chloropyrimidine  | 132 | C4H2ClFN2 | 062802-42-0  | 10   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Cyclopentane, met... | 2.90 | 21.2    | ng    | 671605   | 1                     | 8.15 | 632499 | 20.0 |
| unknown3.04          | 3.04 | 255.2   | ng    | 8069460  | 1                     | 8.15 | 632499 | 20.0 |
| unknown5.22          | 5.22 | 11.9    | ng    | 376427   | 1                     | 8.15 | 632499 | 20.0 |
| unknown7.68          | 7.68 | 97.2    | ng    | 3072950  | 1                     | 8.15 | 632499 | 20.0 |