

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF070516\  
 Data File : BF088713.D  
 Acq On : 5 Jul 2016 20:10  
 Operator : UM/SJ  
 Sample : PB91868BL  
 Misc :  
 ALS Vial : 36 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB91868BL

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\_F\METHODS\8270-BF063016.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         | 1.655       | 3             | 6           | 8            | rVB      | 2787189        | 3931957       | 100.00%         | 14.281%       |
| 2         | 1.712       | 10            | 11          | 20           | rVV      | 422314         | 621478        | 15.81%          | 2.257%        |
| 3         | 1.838       | 20            | 22          | 37           | rVB      | 1329739        | 2209257       | 56.19%          | 8.024%        |
| 4         | 2.032       | 37            | 39          | 68           | rVB4     | 52909          | 236345        | 6.01%           | 0.858%        |
| 5         | 4.947       | 291           | 294         | 299          | rBV      | 93175          | 135937        | 3.46%           | 0.494%        |
| 6         | 5.370       | 328           | 331         | 334          | rBV      | 1745791        | 1962263       | 49.91%          | 7.127%        |
| 7         | 6.410       | 419           | 422         | 424          | rBV      | 2035453        | 2087305       | 53.09%          | 7.581%        |
| 8         | 6.536       | 431           | 433         | 436          | rBV      | 1738398        | 2089849       | 53.15%          | 7.590%        |
| 9         | 6.776       | 452           | 454         | 456          | rBV      | 608822         | 622840        | 15.84%          | 2.262%        |
| 10        | 6.924       | 465           | 467         | 470          | rVB      | 1472214        | 1635542       | 41.60%          | 5.940%        |
| 11        | 7.336       | 500           | 503         | 505          | rBV      | 1379919        | 1403746       | 35.70%          | 5.098%        |
| 12        | 8.056       | 563           | 566         | 568          | rBV      | 961042         | 876547        | 22.29%          | 3.184%        |
| 13        | 9.130       | 657           | 660         | 663          | rBV      | 2114099        | 2500775       | 63.60%          | 9.083%        |
| 14        | 9.805       | 716           | 719         | 722          | rBB      | 1060741        | 995488        | 25.32%          | 3.616%        |
| 15        | 10.593      | 785           | 788         | 790          | rBV      | 1103948        | 1214471       | 30.89%          | 4.411%        |
| 16        | 11.279      | 846           | 848         | 851          | rBV      | 994550         | 1001714       | 25.48%          | 3.638%        |
| 17        | 12.868      | 984           | 987         | 990          | rBV      | 2538297        | 2484523       | 63.19%          | 9.024%        |
| 18        | 13.908      | 1075          | 1078        | 1080         | rBV      | 974573         | 928898        | 23.62%          | 3.374%        |
| 19        | 15.291      | 1196          | 1199        | 1202         | rBV      | 461887         | 593865        | 15.10%          | 2.157%        |

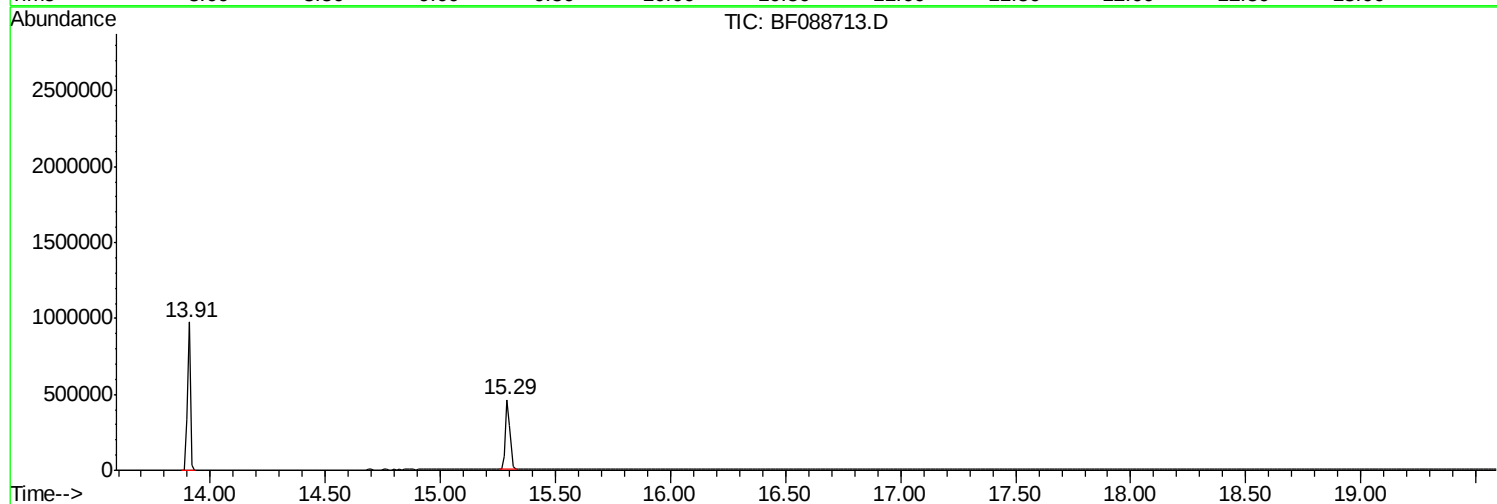
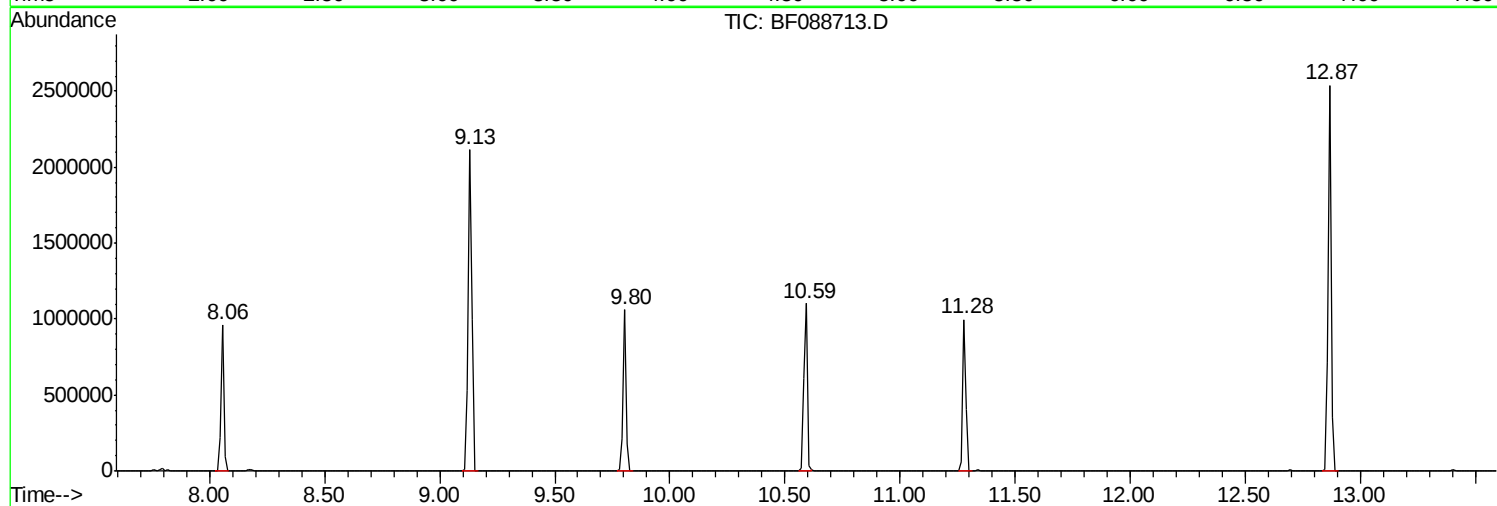
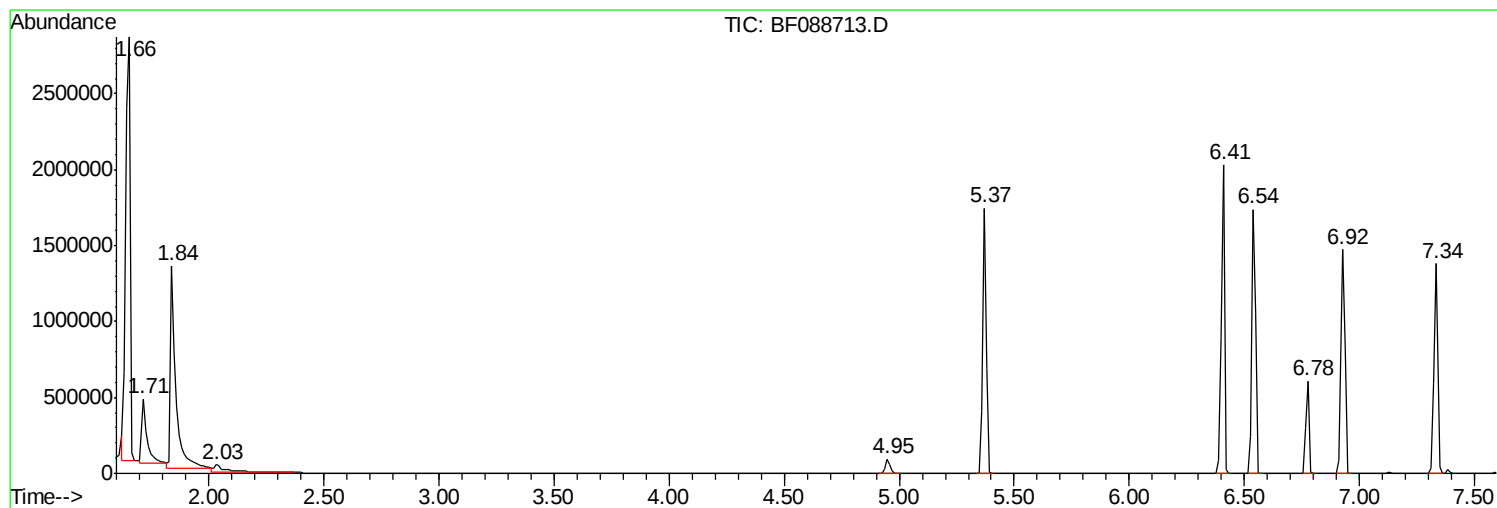
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ALS Vial : 36 Sample Multiplier: 1

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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.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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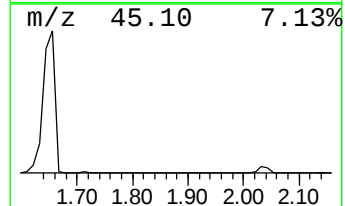
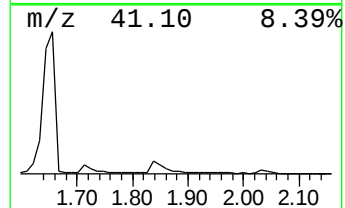
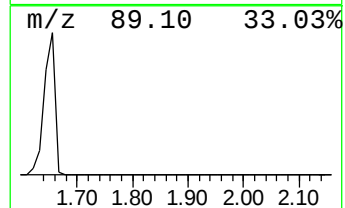
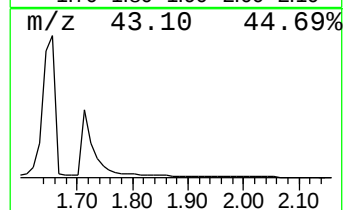
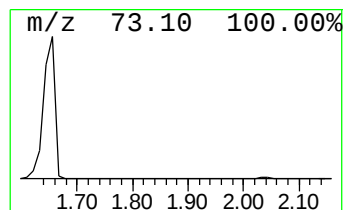
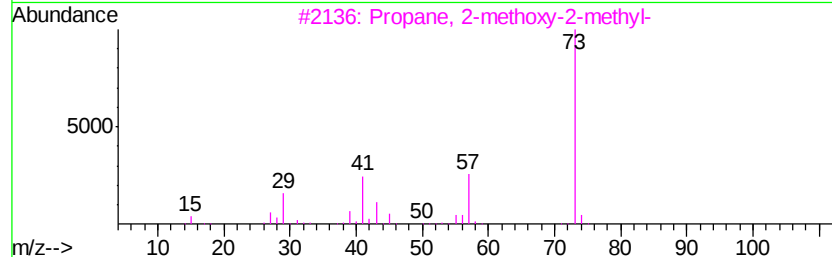
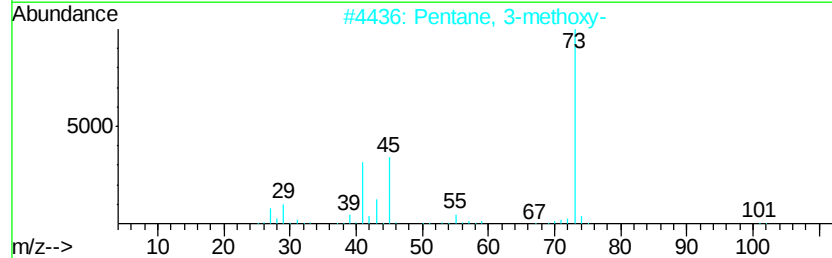
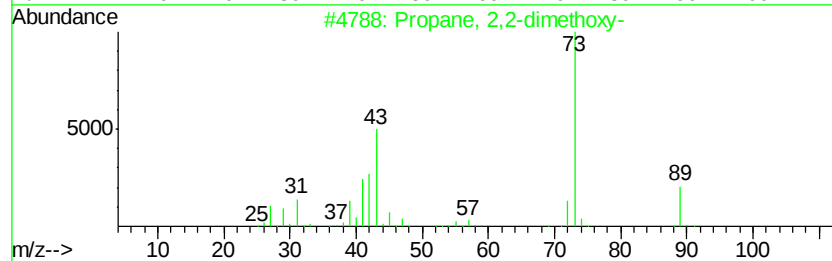
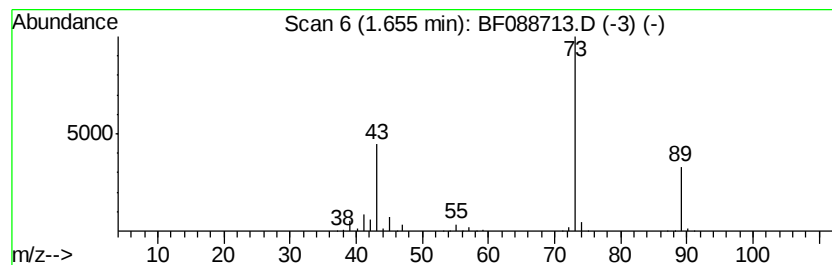
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown1.66 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 1.66 | 126.26 ng | 3931960 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-        | 104 | C5H12O2 | 000077-76-9 | 45   |
| 2    |    | Pentane, 3-methoxy-            | 102 | C6H14O  | 036839-67-5 | 17   |
| 3    |    | Propane, 2-methoxy-2-methyl-   | 88  | C5H12O  | 001634-04-4 | 9    |
| 4    |    | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9    |
| 5    |    | Methane, isothiocyanato-       | 73  | C2H3NS  | 000556-61-6 | 7    |



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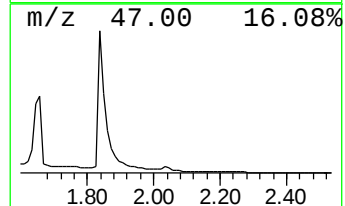
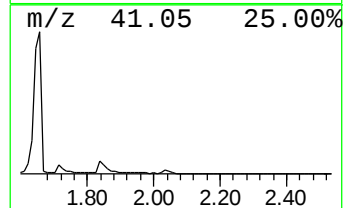
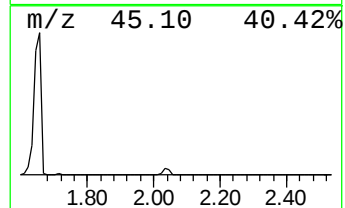
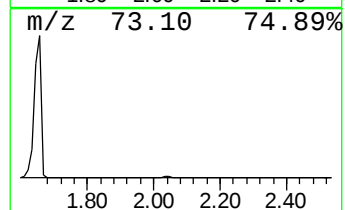
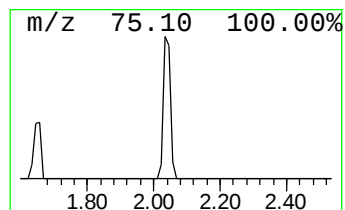
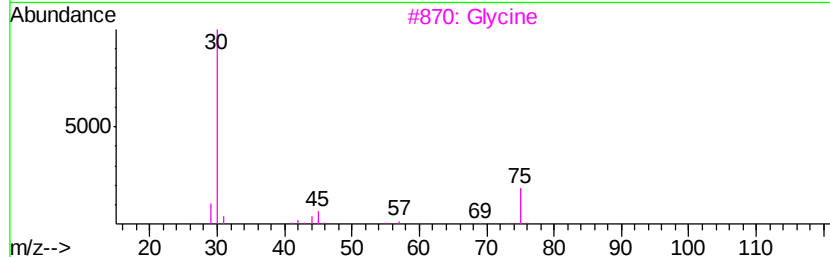
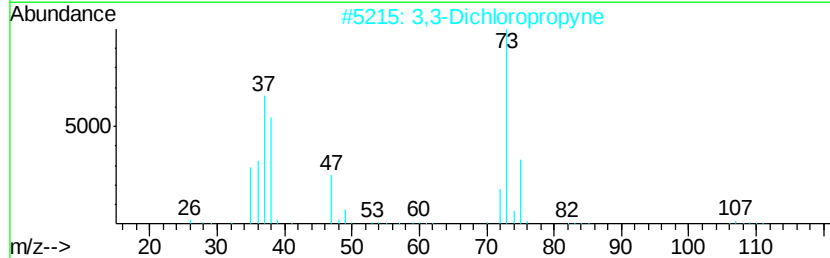
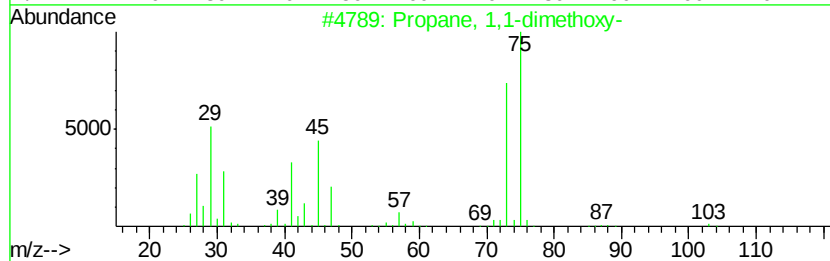
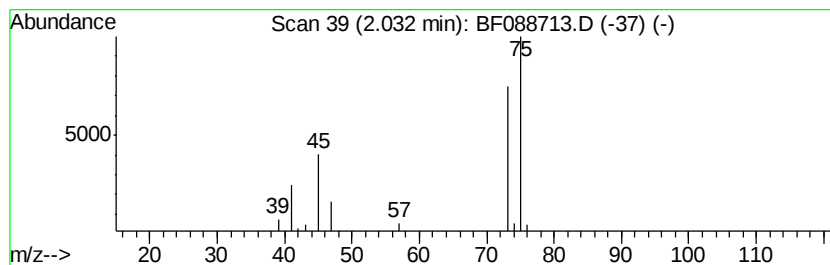
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
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Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 2.03 | 7.59 ng | 236345 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------|-----|----------|-------------|------|
| 1    |    |   | Propane, 1,1-dimethoxy-        | 104 | C5H12O2  | 004744-10-9 | 83   |
| 2    |    |   | 3,3-Dichloropropyne            | 108 | C3H2Cl2  | 025523-14-2 | 9    |
| 3    |    |   | Glycine                        | 75  | C2H5NO2  | 000056-40-6 | 5    |
| 4    |    |   | Silanol, trimethyl-            | 90  | C3H10OSi | 001066-40-6 | 4    |
| 5    |    |   | Glycolaldehyde dimethyl acetal | 106 | C4H10O3  | 030934-97-5 | 4    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M  
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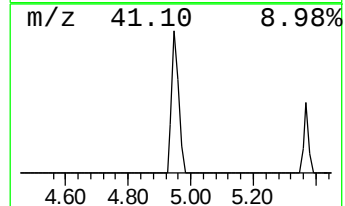
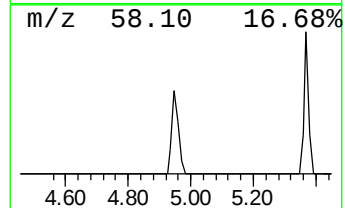
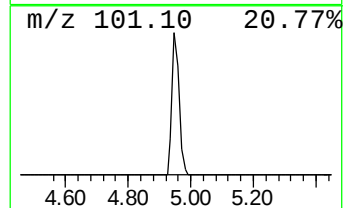
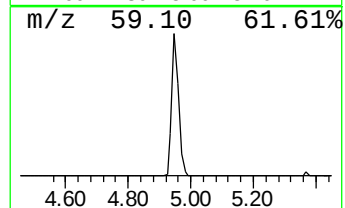
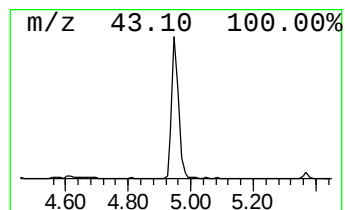
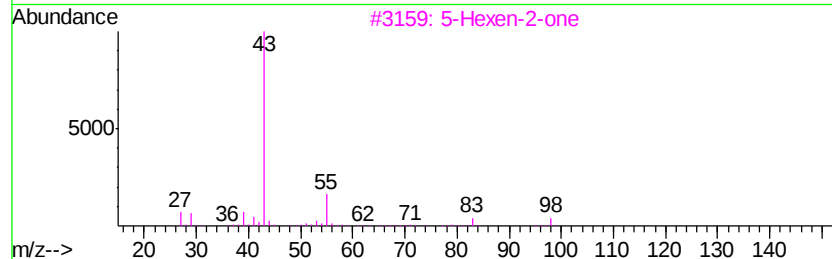
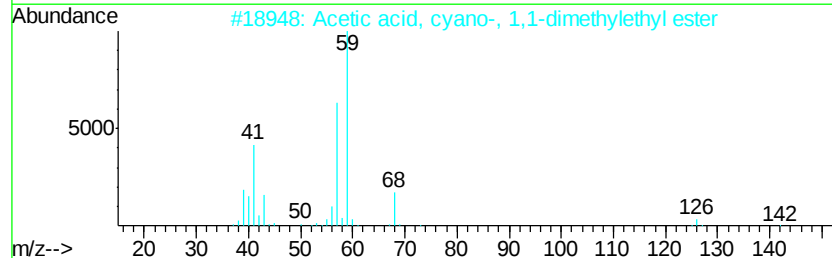
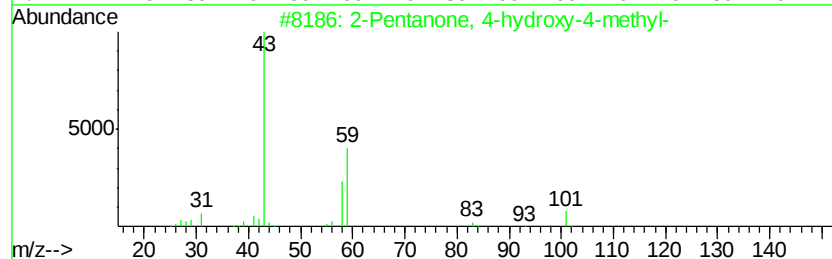
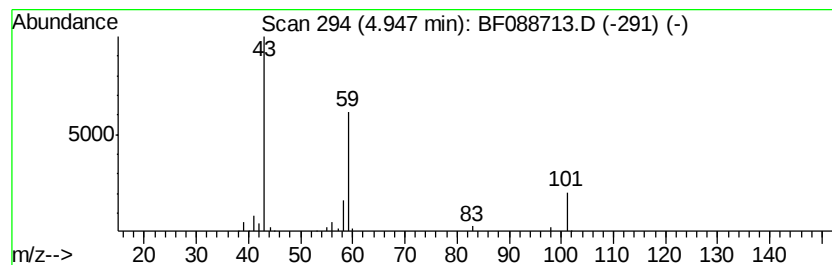
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.95 | 4.37 ng | 135937 | 1,4-Dichlorobenzene-d4 | 6.78 |

| 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-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 3    |    | 5-Hexen-2-one                        | 98  | C6H10O   | 000109-49-9 | 9    |
| 4    |    | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |



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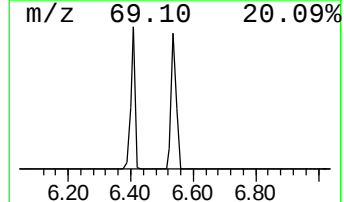
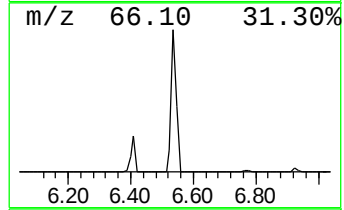
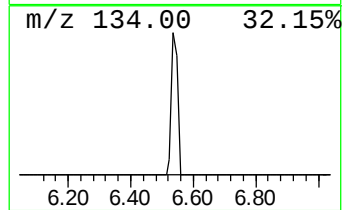
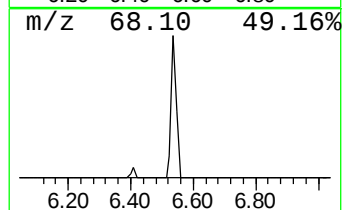
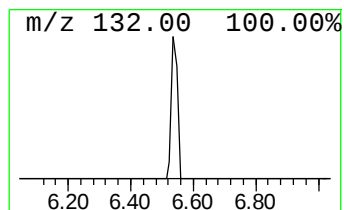
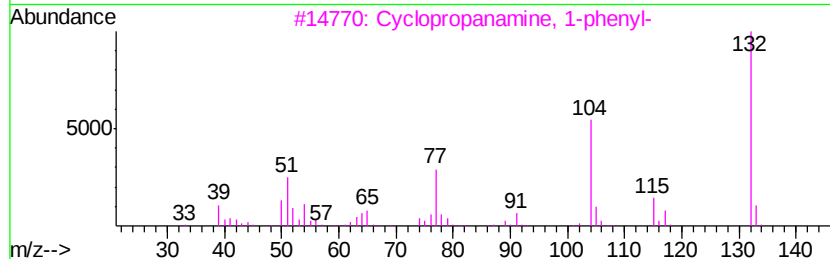
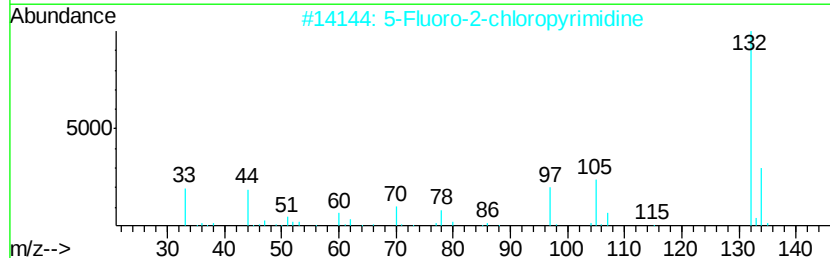
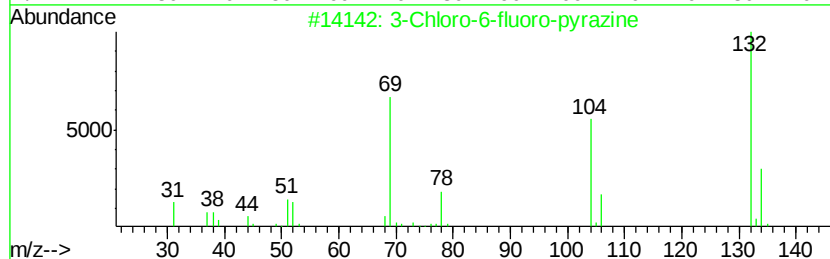
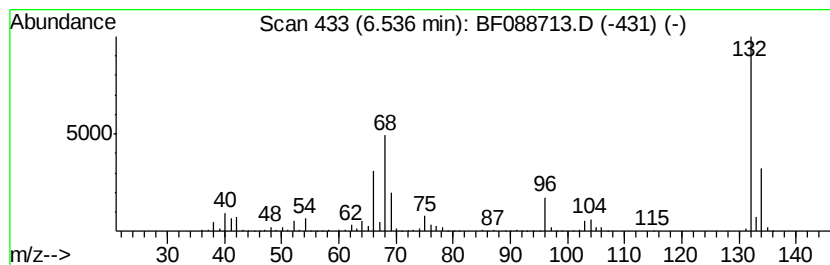
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Peak Number 6 unknown6.54 Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.54 | 67.11 ng | 2089850 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | Cyclopropanamine, 1-phenyl-      | 133 | C9H11N    | 1000351-26-2 | 10   |
| 4    |    | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2    | 1000241-93-9 | 10   |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| unknown1.66          | 1.66 | 126.3   | ng    | 3931960  | 1                     | 6.78 | 622840 | 20.0 |
| Propane, 1,1-dime... | 2.03 | 7.6     | ng    | 236345   | 1                     | 6.78 | 622840 | 20.0 |
| 2-Pentanone, 4-hy... | 4.95 | 4.4     | ng    | 135937   | 1                     | 6.78 | 622840 | 20.0 |
| unknown6.54          | 6.54 | 67.1    | ng    | 2089850  | 1                     | 6.78 | 622840 | 20.0 |