

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF082118\  
 Data File : BF108338.D  
 Acq On : 21 Aug 2018 14:50  
 Operator : JU/SJ  
 Sample : J4521-24  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 72-11979

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:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF080818.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         | 3.190       | 140           | 145         | 152          | rVB      | 72487          | 108429        | 1.47%           | 0.221%        |
| 2         | 5.272       | 494           | 499         | 509          | rVB      | 586963         | 807333        | 10.94%          | 1.644%        |
| 3         | 5.648       | 558           | 563         | 566          | rBV      | 4295696        | 4550981       | 61.69%          | 9.267%        |
| 4         | 6.630       | 724           | 730         | 733          | rBV      | 3921142        | 4258436       | 57.72%          | 8.671%        |
| 5         | 6.778       | 750           | 755         | 759          | rBV      | 4759127        | 5203558       | 70.53%          | 10.595%       |
| 6         | 7.007       | 790           | 794         | 797          | rBV      | 1162027        | 1026003       | 13.91%          | 2.089%        |
| 7         | 7.166       | 816           | 821         | 824          | rBV      | 3899790        | 3937858       | 53.38%          | 8.018%        |
| 8         | 7.572       | 884           | 890         | 893          | rBV      | 3150428        | 3599527       | 48.79%          | 7.329%        |
| 9         | 8.289       | 1007          | 1012        | 1014         | rBV      | 1308902        | 1460229       | 19.79%          | 2.973%        |
| 10        | 8.307       | 1014          | 1015        | 1019         | rVB      | 746744         | 520637        | 7.06%           | 1.060%        |
| 11        | 9.366       | 1188          | 1195        | 1198         | rBV      | 5909771        | 6173428       | 83.68%          | 12.570%       |
| 12        | 10.048      | 1306          | 1311        | 1315         | rBV      | 1712226        | 1548675       | 20.99%          | 3.153%        |
| 13        | 10.848      | 1440          | 1447        | 1450         | rBV      | 4413242        | 4417407       | 59.88%          | 8.995%        |
| 14        | 11.548      | 1560          | 1566        | 1569         | rBV      | 1783202        | 1718426       | 23.29%          | 3.499%        |
| 15        | 13.136      | 1830          | 1836        | 1839         | rBV      | 6493535        | 7377283       | 100.00%         | 15.022%       |
| 16        | 14.201      | 2012          | 2017        | 2020         | rBV      | 1454081        | 1442512       | 19.55%          | 2.937%        |
| 17        | 15.753      | 2275          | 2281        | 2287         | rVB      | 721548         | 960561        | 13.02%          | 1.956%        |

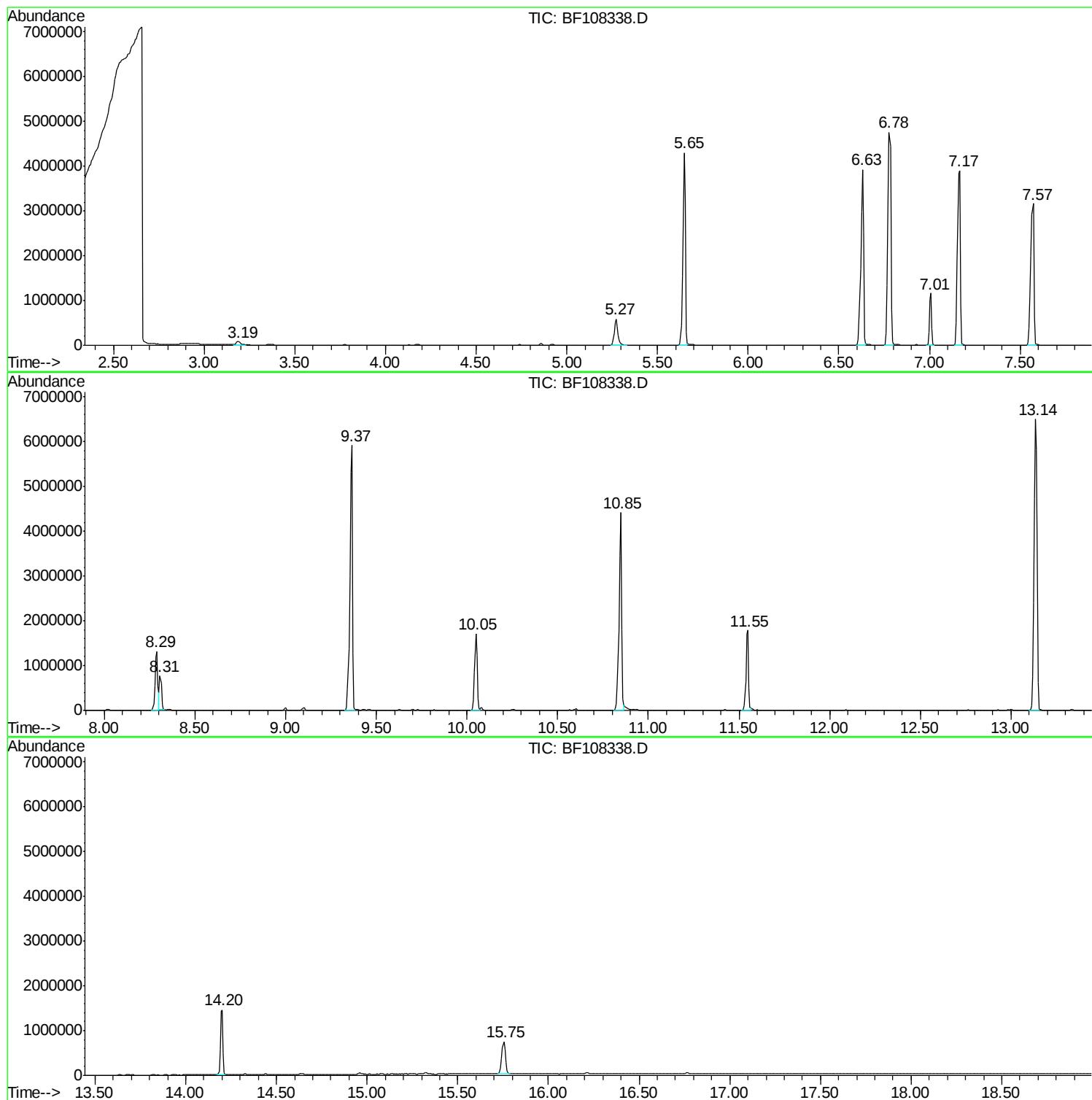
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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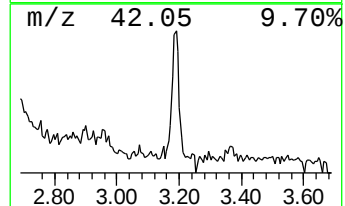
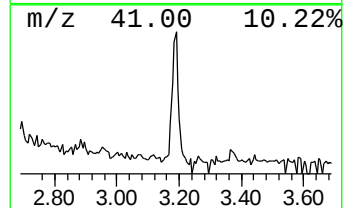
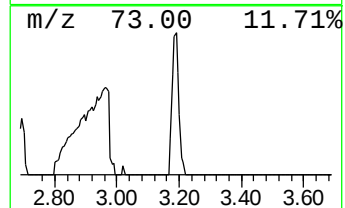
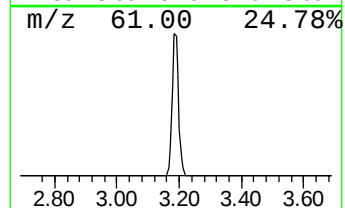
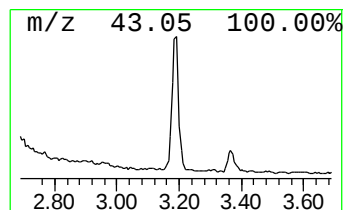
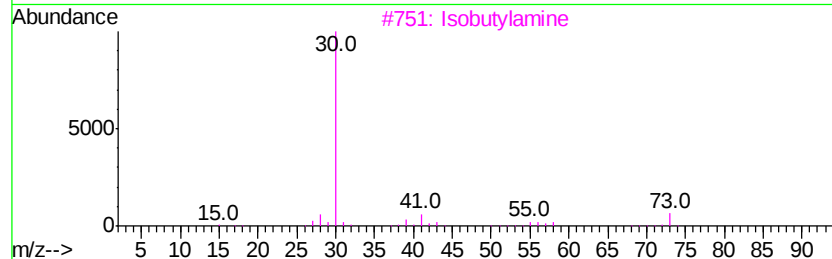
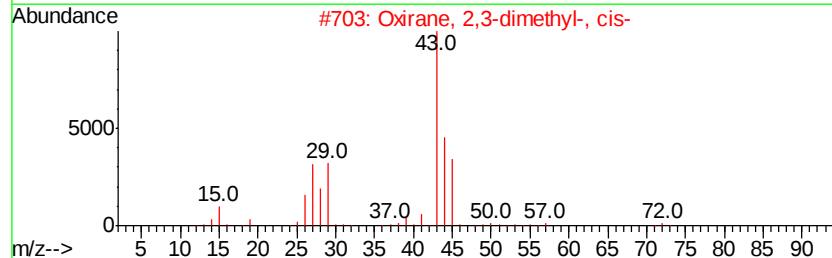
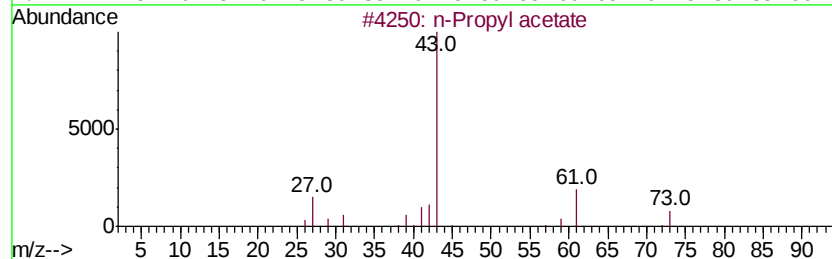
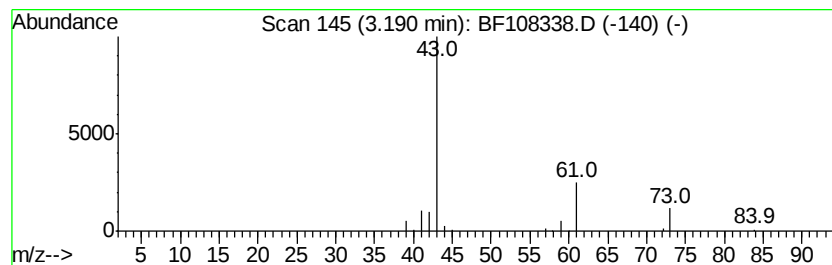
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Propyl acetate Concentration Rank 4

| R.T.      | EstConc                        | Area   | Relative to ISTD       | R.T.        |      |
|-----------|--------------------------------|--------|------------------------|-------------|------|
| 3.19      | 2.11 ng                        | 108429 | 1,4-Dichlorobenzene-d4 | 7.01        |      |
| Hit# of 5 | Tentative ID                   | MW     | MolForm                | CAS#        | Qual |
| 1         | n-Propyl acetate               | 102    | C5H10O2                | 000109-60-4 | 78   |
| 2         | Oxirane, 2,3-dimethyl-, cis-   | 72     | C4H8O                  | 001758-33-4 | 7    |
| 3         | Isobutylamine                  | 73     | C4H11N                 | 000078-81-9 | 7    |
| 4         | 1-Butanamine                   | 73     | C4H11N                 | 000109-73-9 | 5    |
| 5         | Sulfurous acid, dipropyl ester | 166    | C6H14O3S               | 000623-98-3 | 4    |



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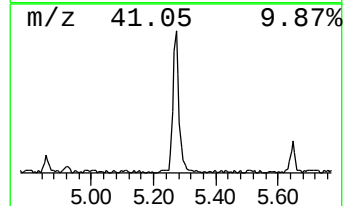
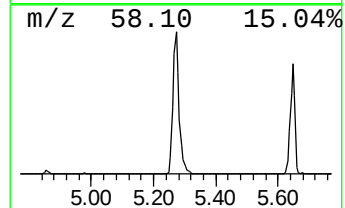
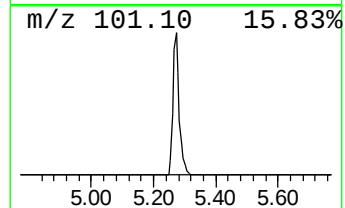
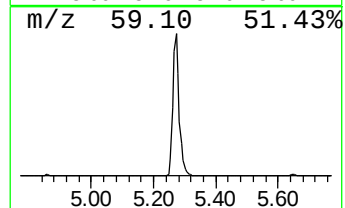
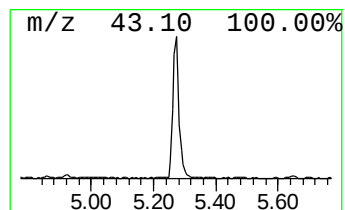
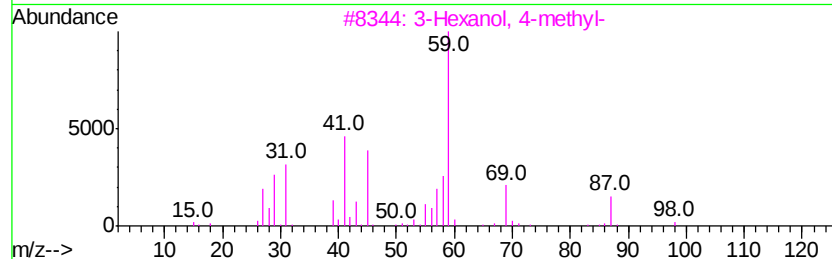
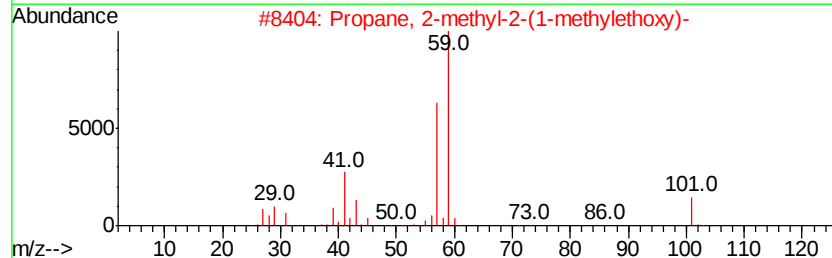
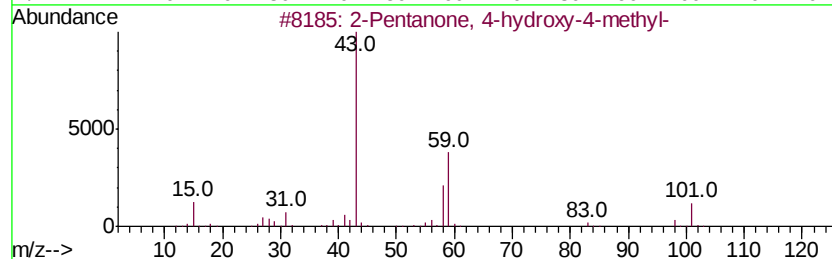
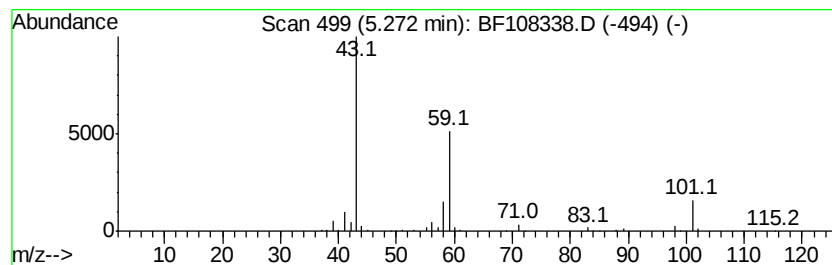
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.27 | 15.74 ng | 807333 | 1,4-Dichlorobenzene-d4 | 7.01 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 53   |
| 2    |    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 36   |
| 3    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 4    |    | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 28   |
| 5    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |



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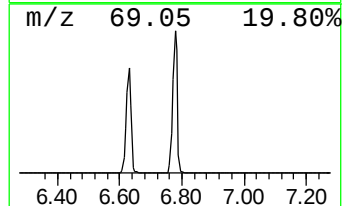
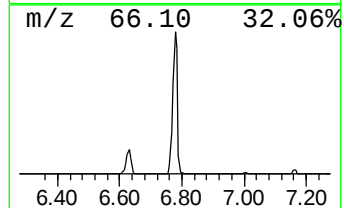
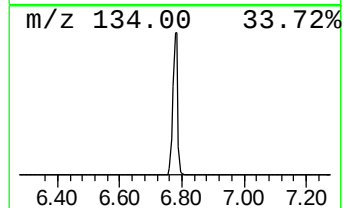
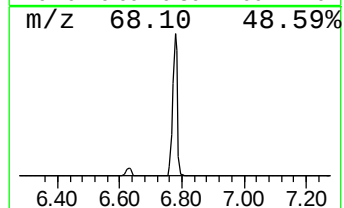
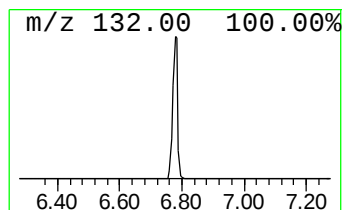
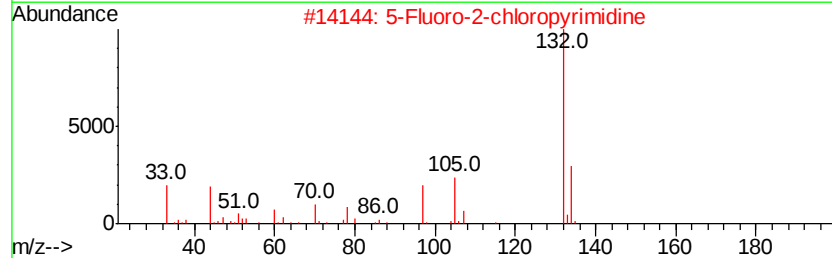
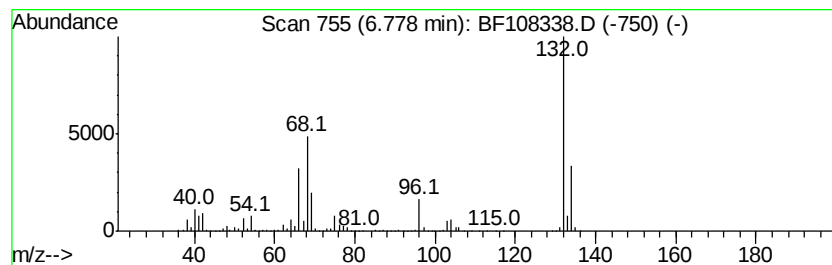
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Peak Number 3 unknown6.78 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 6.78 | 101.43 ng | 5203560 | 1,4-Dichlorobenzene-d4 | 7.01 |

| 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    |    | Tranvlcyproline-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2    | 1000241-93-9 | 10   |
| 5    |    | Cyclopropanamine, 1-phenyl-      | 133 | C9H11N    | 1000351-26-2 | 10   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| n-Propyl acetate     | 3.19 | 2.1     | ng    | 108429   | 1                     | 7.01 | 1026000 | 20.0 |
| 2-Pentanone, 4-hy... | 5.27 | 15.7    | ng    | 807333   | 1                     | 7.01 | 1026000 | 20.0 |
| unknown6.78          | 6.78 | 101.4   | ng    | 5203560  | 1                     | 7.01 | 1026000 | 20.0 |