

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF061021\  
 Data File : BF124226.D  
 Acq On : 10 Jun 2021 10:21  
 Operator : JU/CG  
 Sample : PB136946BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB136946BL

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-BF060321.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124226.D\data.ms

| 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         | 2.205       | 12            | 20          | 26           | rVB      | 41499          | 54175         | 2.95%           | 0.522%        |
| 2         | 2.310       | 33            | 38          | 43           | rBB2     | 27124          | 34644         | 1.89%           | 0.334%        |
| 3         | 5.099       | 508           | 512         | 518          | rBV2     | 33492          | 45801         | 2.50%           | 0.441%        |
| 4         | 5.493       | 574           | 579         | 582          | rBV      | 1535251        | 1306521       | 71.23%          | 12.589%       |
| 5         | 6.493       | 744           | 749         | 752          | rBV      | 1208994        | 1282723       | 69.94%          | 12.360%       |
| 6         | 6.845       | 806           | 809         | 813          | rBV      | 312276         | 272354        | 14.85%          | 2.624%        |
| 7         | 7.416       | 900           | 906         | 909          | rBV      | 842067         | 875589        | 47.74%          | 8.437%        |
| 8         | 8.134       | 1023          | 1028        | 1031         | rBV      | 344145         | 335545        | 18.29%          | 3.233%        |
| 9         | 9.210       | 1205          | 1211        | 1214         | rBV      | 2088892        | 1719239       | 93.74%          | 16.566%       |
| 10        | 9.886       | 1321          | 1326        | 1330         | rBV      | 517651         | 424224        | 23.13%          | 4.088%        |
| 11        | 10.681      | 1456          | 1461        | 1464         | rBV      | 1374714        | 1166998       | 63.63%          | 11.244%       |
| 12        | 11.375      | 1575          | 1579        | 1583         | rBV      | 538685         | 433824        | 23.65%          | 4.180%        |
| 13        | 12.963      | 1844          | 1849        | 1852         | rBV      | 1911258        | 1834101       | 100.00%         | 17.672%       |
| 14        | 14.016      | 2025          | 2028        | 2032         | rBV      | 368814         | 331705        | 18.09%          | 3.196%        |
| 15        | 15.498      | 2275          | 2280        | 2286         | rVB      | 191084         | 260970        | 14.23%          | 2.515%        |

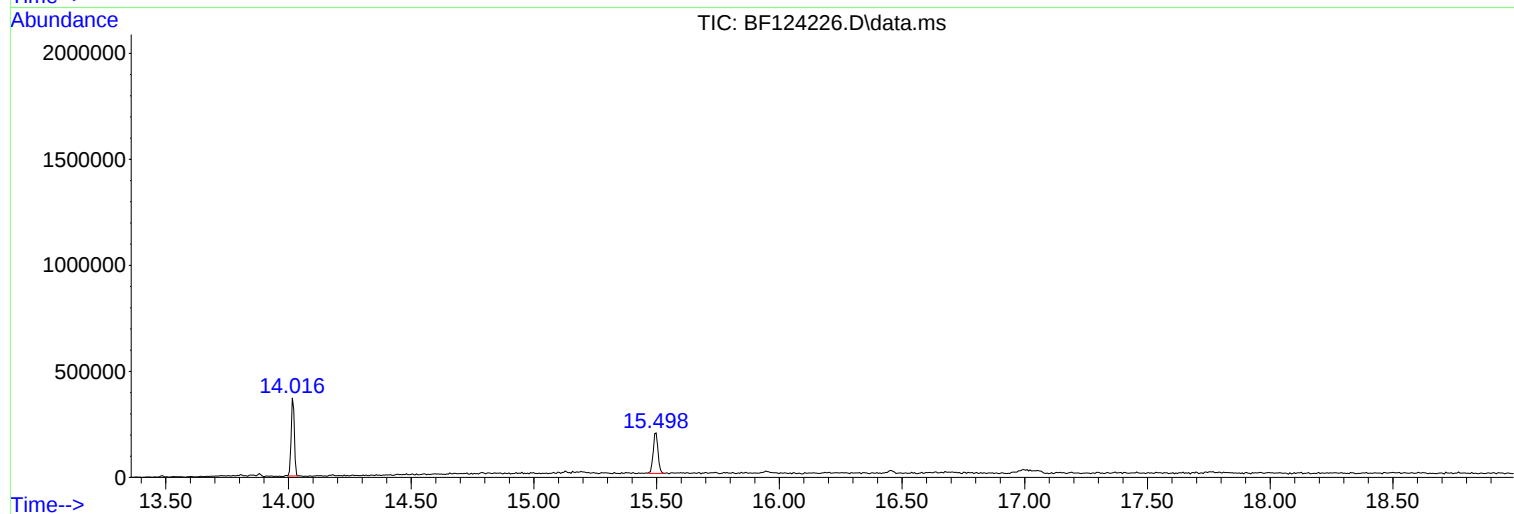
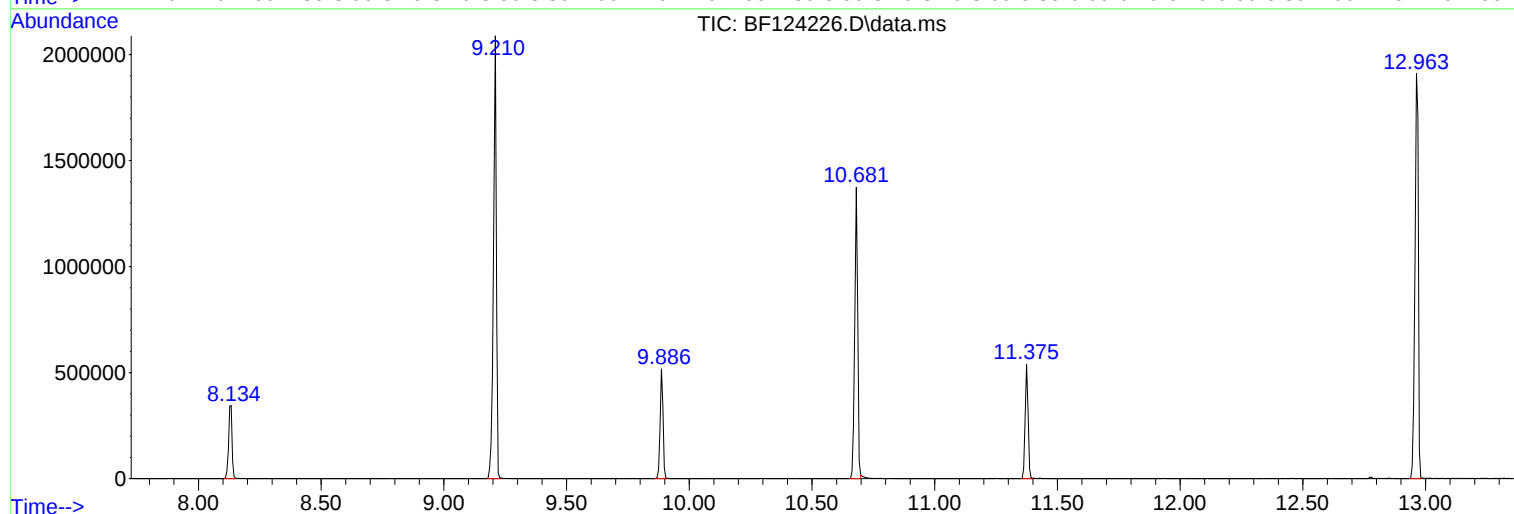
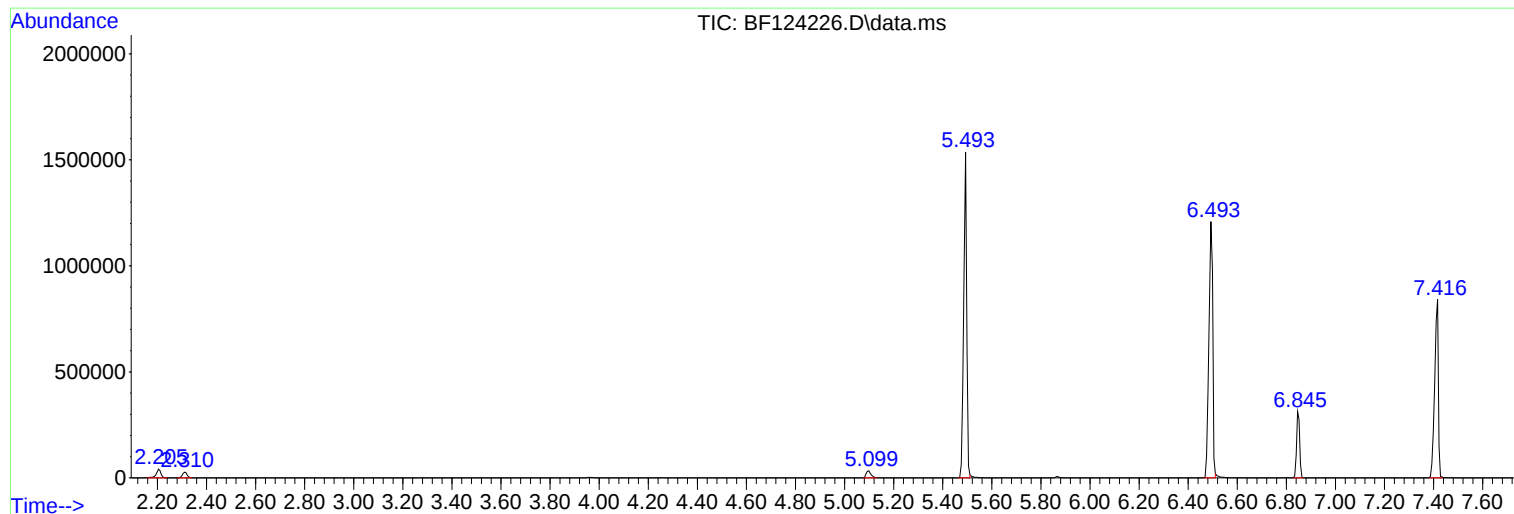
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF060321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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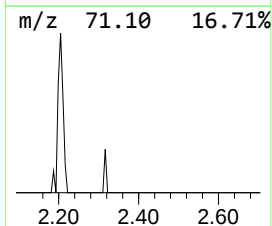
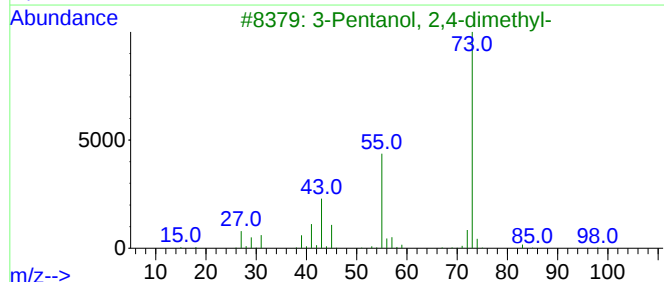
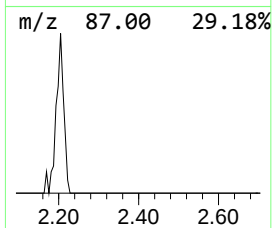
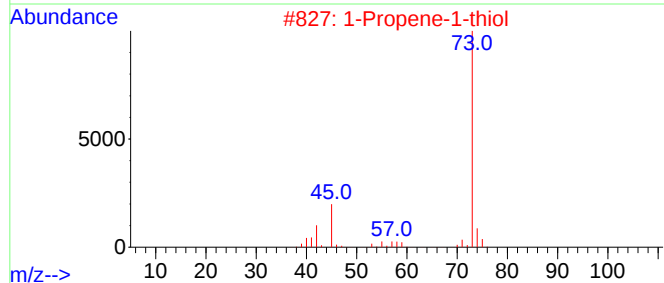
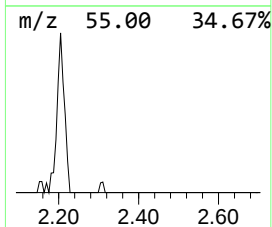
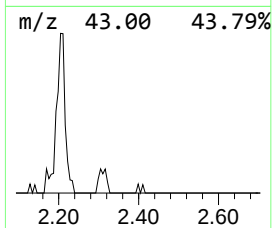
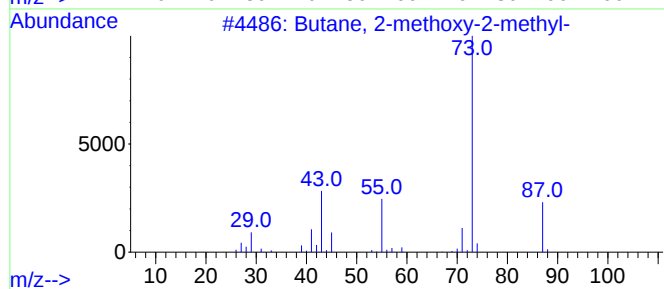
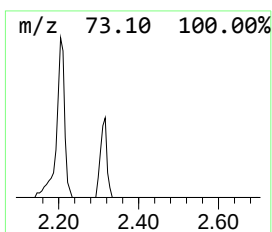
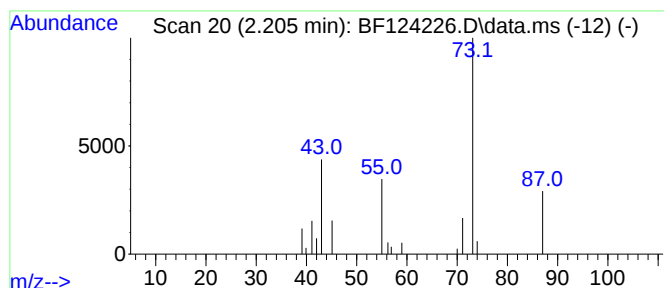
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 2.205 | 3.98 ng | 54175 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 1-Propene-1-thiol           | 74  | C3H6S   | 000925-89-3 | 25   |
| 3    |    |   | 3-Pentanol, 2,4-dimethyl-   | 116 | C7H16O  | 000600-36-2 | 25   |
| 4    |    |   | 2-Methyl-5-hexen-3-ol       | 114 | C7H14O  | 032815-70-6 | 25   |
| 5    |    |   | 1-Pentanamine               | 87  | C5H13N  | 000110-58-7 | 5    |



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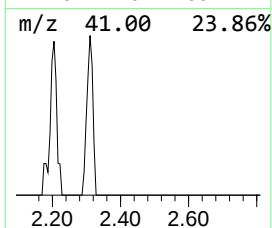
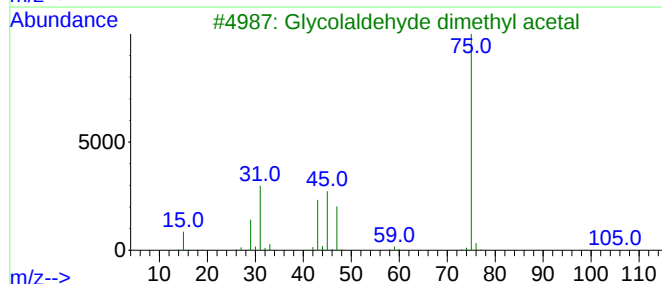
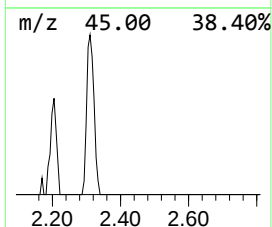
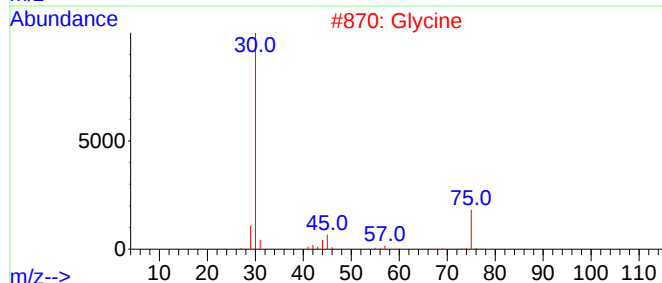
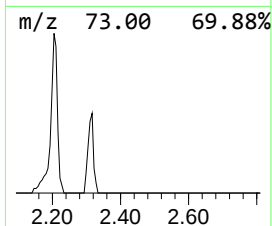
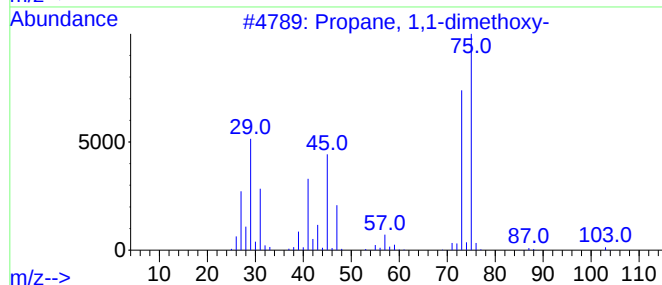
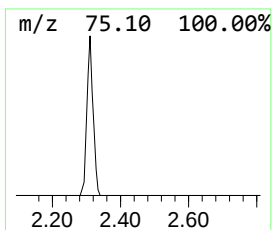
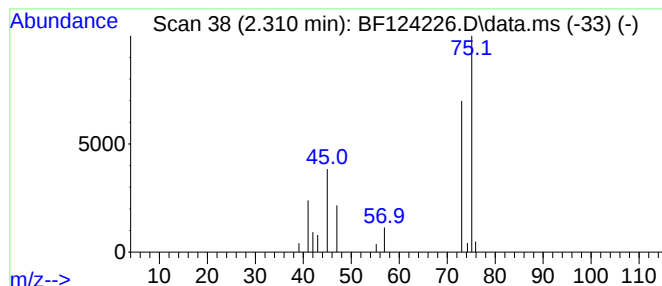
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF060321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 2.310 | 2.54 ng | 34644 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|---|----------------------------------|-----|----------|-------------|------|
| 1    |    |   | Propane, 1,1-dimethoxy-          | 104 | C5H12O2  | 004744-10-9 | 74   |
| 2    |    |   | Glycine                          | 75  | C2H5NO2  | 000056-40-6 | 64   |
| 3    |    |   | Glycolaldehyde dimethyl acetal   | 106 | C4H10O3  | 030934-97-5 | 9    |
| 4    |    |   | 1-Propene-1-thiol                | 74  | C3H6S    | 000925-89-3 | 4    |
| 5    |    |   | 1,3-Dioxolane, 2-(chloromethyl)- | 122 | C4H7ClO2 | 002568-30-1 | 4    |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF060321.M  
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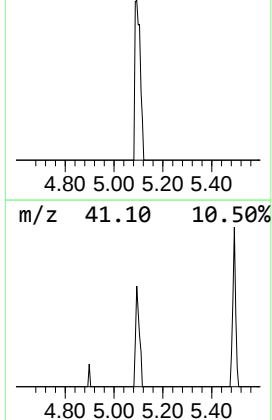
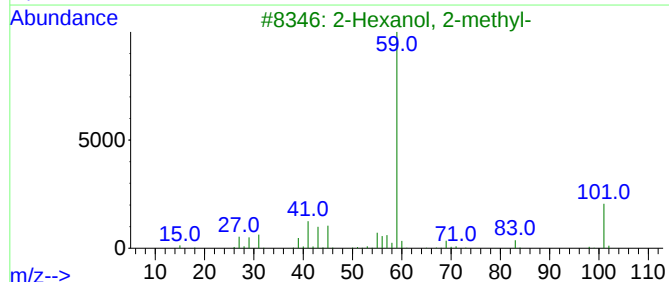
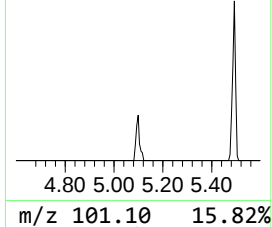
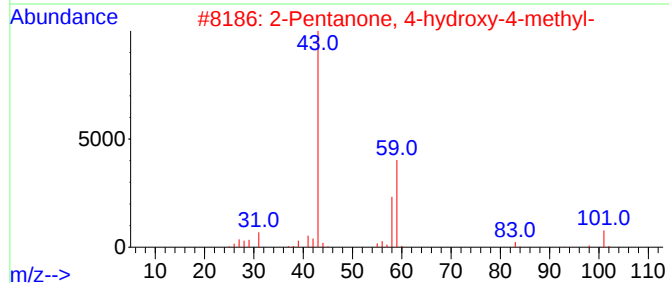
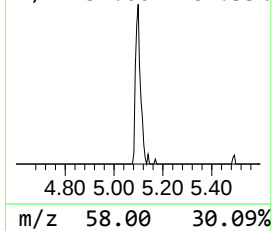
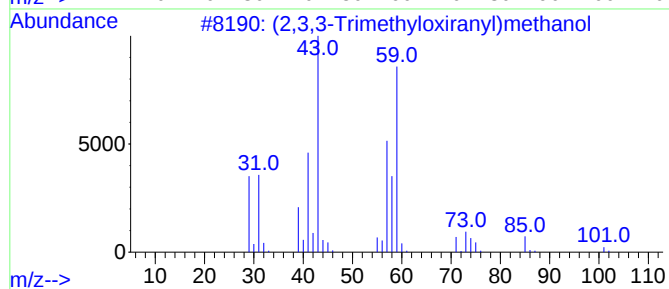
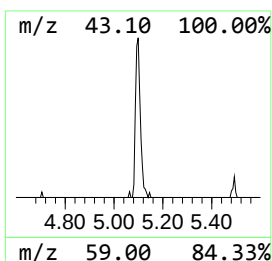
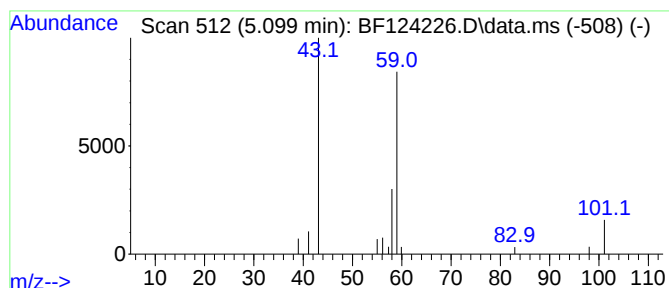
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown5.099 Concentration Rank 2

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.099 | 3.36 ng | 45801 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# | of                                | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-----------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | (2,3,3-Trimethyloxiranyl)methanol | 116 | C6H12O2      | 1000306-64-7 | 43      |      |      |
| 2    | 2-Pentanone, 4-hydroxy-4-methyl-  | 116 | C6H12O2      | 000123-42-2  | 40      |      |      |
| 3    | 2-Hexanol, 2-methyl-              | 116 | C7H16O       | 000625-23-0  | 36      |      |      |
| 4    | Guanidine                         | 59  | CH5N3        | 000113-00-8  | 9       |      |      |
| 5    | Formamide, N-butyl-               | 101 | C5H11NO      | 000871-71-6  | 9       |      |      |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Butane, 2-metho... | 2.205 | 4.0     | ng    | 54175    | 1                     | 6.845 | 272354 | 20.0 |
| Propane, 1,1-di... | 2.310 | 2.5     | ng    | 34644    | 1                     | 6.845 | 272354 | 20.0 |
| unknown5.099       | 5.099 | 3.4     | ng    | 45801    | 1                     | 6.845 | 272354 | 20.0 |