

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX032421\  
 Data File : VX021445.D  
 Acq On : 24 Mar 2021 18:46  
 Operator : JC/MD  
 Sample : M1774-04  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 30808

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:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032421W.M  
 Title : SW846 8260

Signal : TIC: VX021445.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         | 1.164       | 10            | 13          | 19           | rVB      | 12365          | 12876         | 2.99%           | 0.470%        |
| 2         | 1.375       | 46            | 49          | 54           | rVB3     | 3473           | 4368          | 1.01%           | 0.160%        |
| 3         | 1.593       | 80            | 86          | 89           | rVB4     | 3491           | 6403          | 1.49%           | 0.234%        |
| 4         | 2.093       | 164           | 171         | 177          | rBV      | 6705           | 9860          | 2.29%           | 0.360%        |
| 5         | 2.334       | 206           | 212         | 219          | rVB      | 4358           | 7735          | 1.80%           | 0.282%        |
| 6         | 2.423       | 220           | 227         | 240          | rVB      | 23703          | 40443         | 9.39%           | 1.477%        |
| 7         | 2.587       | 250           | 255         | 262          | rVB3     | 2868           | 6040          | 1.40%           | 0.221%        |
| 8         | 3.917       | 470           | 481         | 497          | rBV      | 56293          | 145458        | 33.79%          | 5.312%        |
| 9         | 4.305       | 536           | 547         | 557          | rBV3     | 7855           | 22159         | 5.15%           | 0.809%        |
| 10        | 4.635       | 594           | 603         | 616          | rBV2     | 2523           | 8226          | 1.91%           | 0.300%        |
| 11        | 5.464       | 733           | 744         | 759          | rBV2     | 51702          | 148533        | 34.50%          | 5.424%        |
| 12        | 5.629       | 761           | 772         | 788          | rVB      | 79166          | 219261        | 50.93%          | 8.007%        |
| 13        | 6.029       | 829           | 840         | 851          | rBV      | 58753          | 153845        | 35.73%          | 5.618%        |
| 14        | 6.829       | 966           | 976         | 989          | rBV      | 133285         | 312067        | 72.49%          | 11.396%       |
| 15        | 7.270       | 1044          | 1051        | 1058         | rBV5     | 1903           | 5201          | 1.21%           | 0.190%        |
| 16        | 8.694       | 1286          | 1293        | 1301         | rBV      | 276231         | 430524        | 100.00%         | 15.722%       |
| 17        | 8.765       | 1301          | 1305        | 1311         | rVB      | 6994           | 11870         | 2.76%           | 0.433%        |
| 18        | 10.094      | 1525          | 1531        | 1545         | rBV      | 297532         | 405414        | 94.17%          | 14.805%       |
| 19        | 11.118      | 1700          | 1705        | 1711         | rBV      | 242166         | 314726        | 73.10%          | 11.493%       |
| 20        | 11.171      | 1711          | 1714        | 1719         | rVB2     | 5803           | 7017          | 1.63%           | 0.256%        |
| 21        | 11.318      | 1735          | 1739        | 1748         | rBV3     | 5270           | 8656          | 2.01%           | 0.316%        |
| 22        | 11.718      | 1801          | 1807        | 1814         | rBV      | 17380          | 21691         | 5.04%           | 0.792%        |
| 23        | 11.906      | 1835          | 1839        | 1845         | rBV2     | 7424           | 9766          | 2.27%           | 0.357%        |
| 24        | 11.995      | 1849          | 1854        | 1860         | rBV2     | 4517           | 6188          | 1.44%           | 0.226%        |
| 25        | 12.059      | 1860          | 1865        | 1872         | rVV      | 303400         | 379716        | 88.20%          | 13.867%       |
| 26        | 13.812      | 2158          | 2163        | 2170         | rBV      | 7260           | 9865          | 2.29%           | 0.360%        |
| 27        | 13.883      | 2170          | 2175        | 2181         | rVV2     | 11548          | 15789         | 3.67%           | 0.577%        |
| 28        | 13.954      | 2182          | 2187        | 2194         | rVB2     | 10201          | 14669         | 3.41%           | 0.536%        |

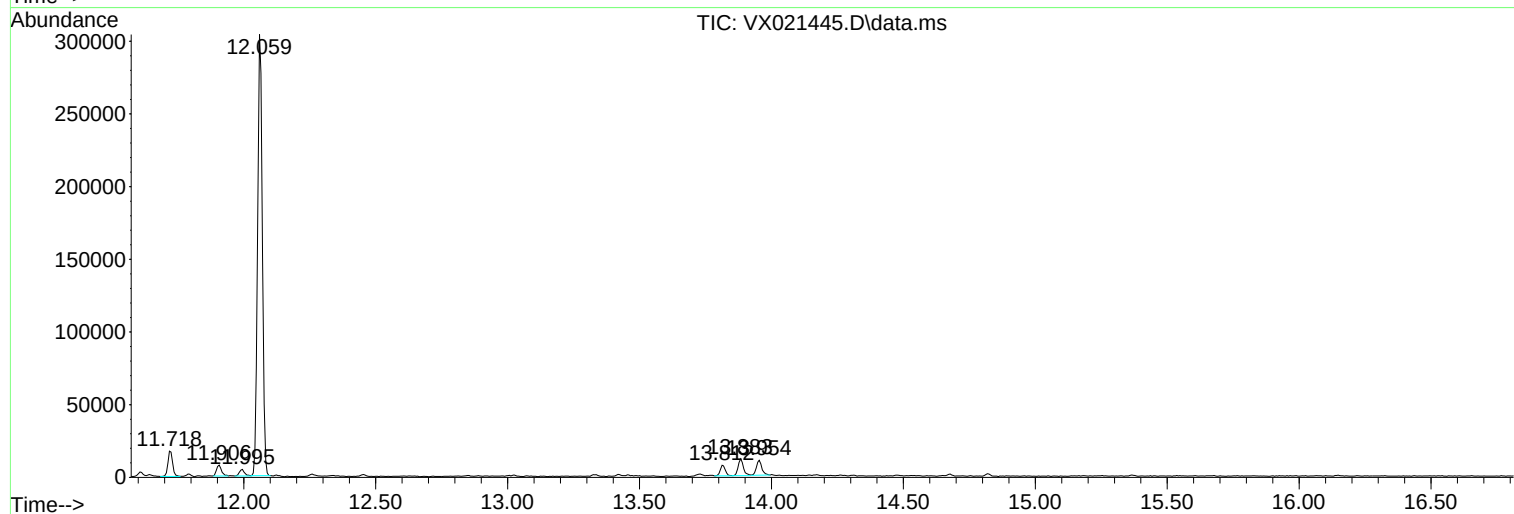
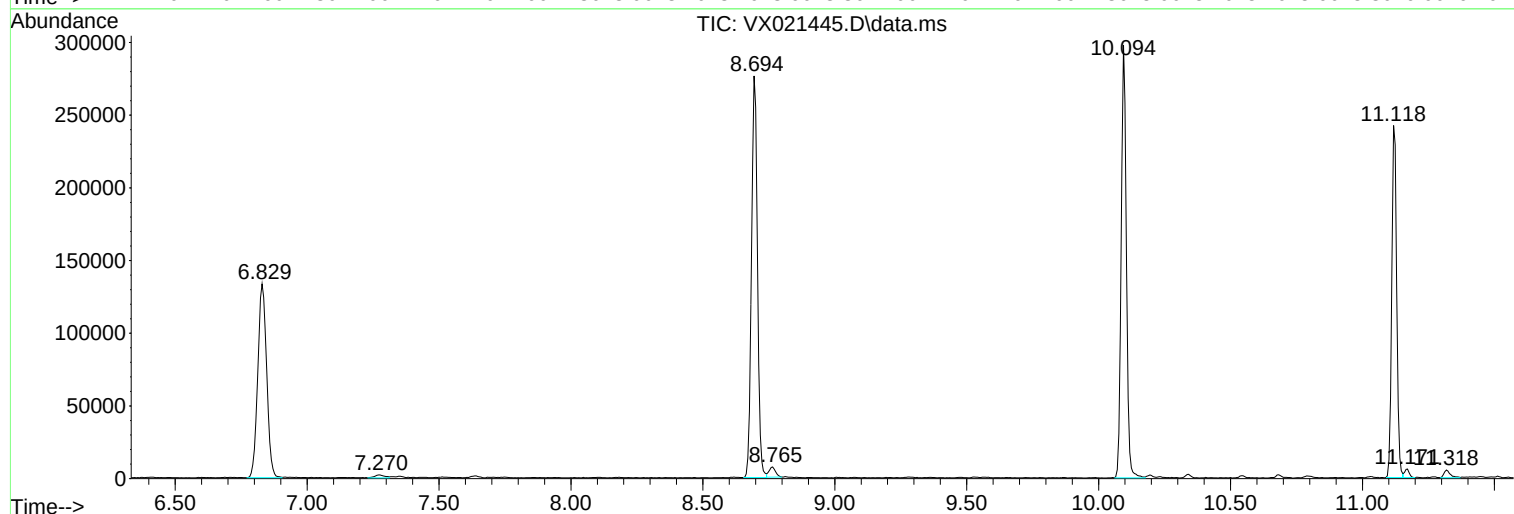
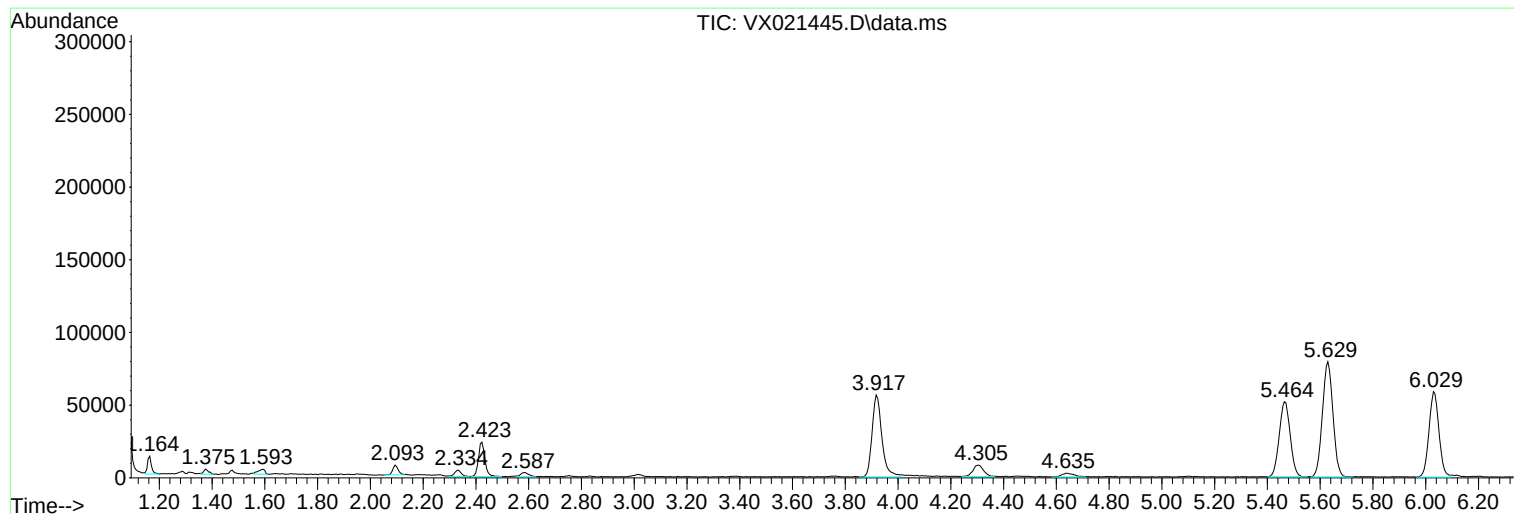
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032421W.M  
Quant Title : SW846 8260

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



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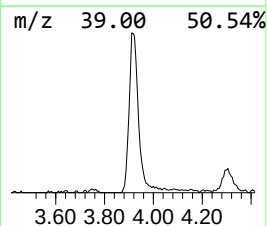
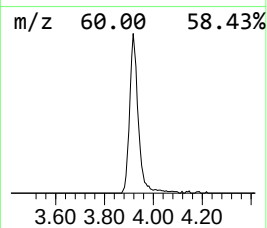
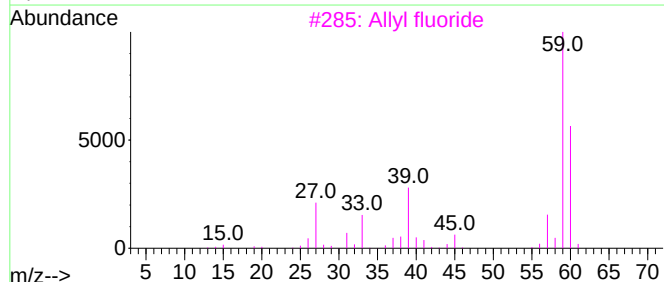
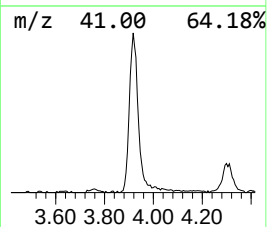
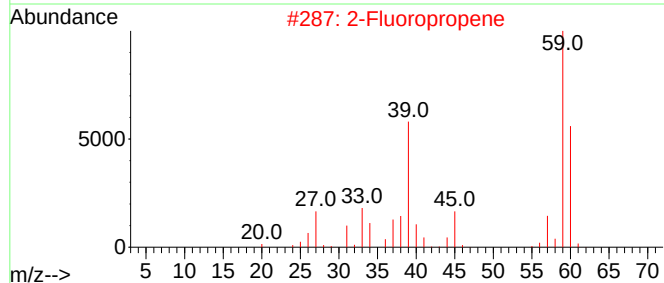
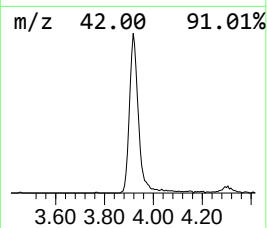
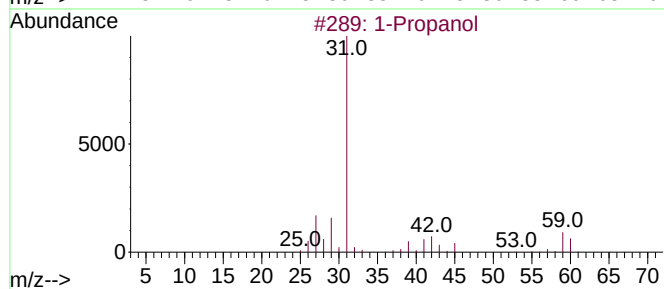
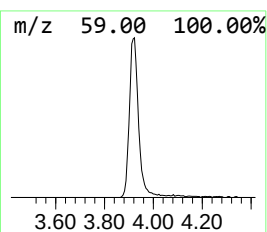
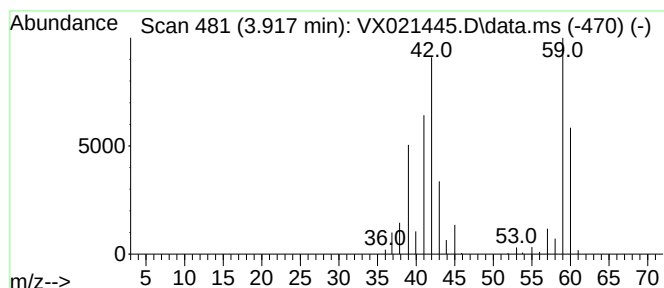
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Peak Number 1 1-Propanol Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 3.917 | 33.17 ug/l | 145458 | Pentafluorobenzene | 5.629 |

| Hit# | of              | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|-----------------|---|--------------|----|---------|-------------|------|
| 1    | 1-Propanol      |   |              | 60 | C3H8O   | 000071-23-8 | 59   |
| 2    | 2-Fluoropropene |   |              | 60 | C3H5F   | 001184-60-7 | 49   |
| 3    | Allyl fluoride  |   |              | 60 | C3H5F   | 000818-92-8 | 35   |
| 4    | Cyclopropane    |   |              | 42 | C3H6    | 000075-19-4 | 32   |
| 5    | Propene         |   |              | 42 | C3H6    | 000115-07-1 | 23   |



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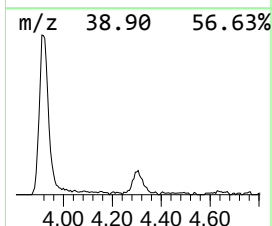
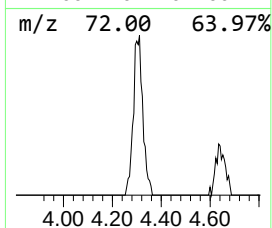
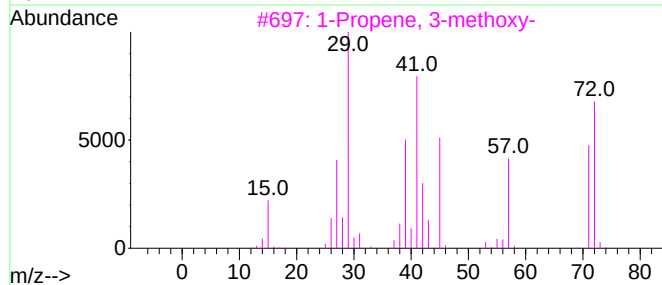
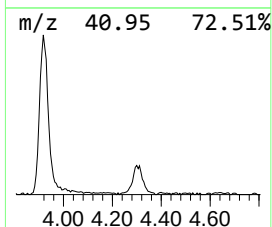
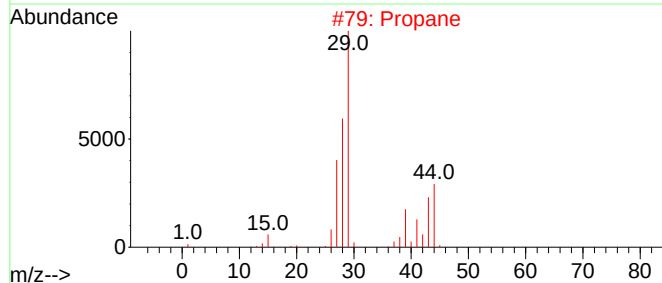
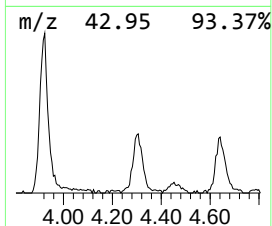
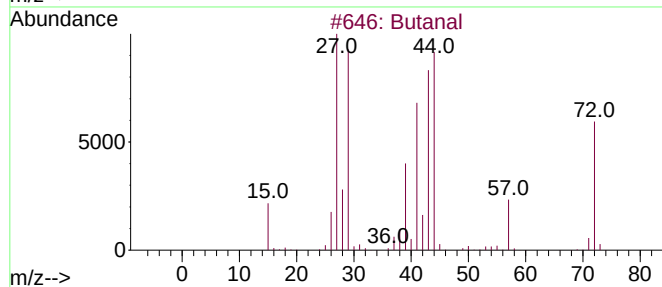
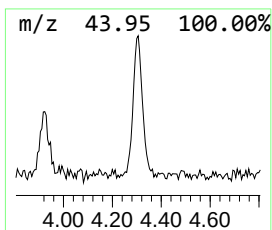
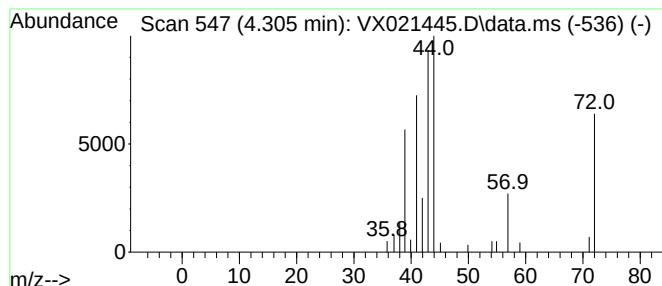
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Peak Number 2 Butanal Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 4.305 | 5.05 ug/l | 22159 | Pentafluorobenzene | 5.629 |

| Hit# | of | 5 | Tentative ID          | MW | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|----|---------|-------------|------|
| 1    |    |   | Butanal               | 72 | C4H8O   | 000123-72-8 | 91   |
| 2    |    |   | Propane               | 44 | C3H8    | 000074-98-6 | 45   |
| 3    |    |   | 1-Propene, 3-methoxy- | 72 | C4H8O   | 000627-40-7 | 35   |
| 4    |    |   | Propanal, 2-methyl-   | 72 | C4H8O   | 000078-84-2 | 9    |
| 5    |    |   | Ethene, ethoxy-       | 72 | C4H8O   | 000109-92-2 | 9    |



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Quant Title : SW846 8260

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

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| 1-Propanol       | 3.917 | 33.2    | ug/l  | 145458   | 1                     | 5.629 | 219261 | 50.0 |
| Butanal          | 4.305 | 5.0     | ug/l  | 22159    | 1                     | 5.629 | 219261 | 50.0 |