

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091224\  
 Data File : VN083864.D  
 Acq On : 13 Sep 2024 09:24  
 Operator : JC\MD  
 Sample : P3957-08  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 52 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW179D-20240910

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\_N\methods\82N091024W.M  
 Title : SW846 8260

Signal : TIC: VN083864.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         | 2.295       | 53            | 58          | 68           | rBV4     | 19647          | 41823         | 2.73%           | 0.605%        |
| 2         | 2.847       | 141           | 152         | 153          | rBV5     | 10110          | 30128         | 1.97%           | 0.436%        |
| 3         | 2.900       | 153           | 161         | 167          | rVB6     | 16423          | 57485         | 3.76%           | 0.831%        |
| 4         | 4.441       | 413           | 423         | 437          | rBV      | 62751          | 176608        | 11.54%          | 2.553%        |
| 5         | 5.788       | 643           | 652         | 663          | rBV3     | 7605           | 24769         | 1.62%           | 0.358%        |
| 6         | 7.482       | 928           | 940         | 954          | rBV      | 130680         | 337949        | 22.09%          | 4.885%        |
| 7         | 8.165       | 1046          | 1056        | 1060         | rBV      | 109619         | 249814        | 16.33%          | 3.611%        |
| 8         | 8.218       | 1060          | 1065        | 1076         | rVB      | 163653         | 366971        | 23.99%          | 5.305%        |
| 9         | 8.576       | 1116          | 1126        | 1137         | rBV      | 111048         | 249490        | 16.31%          | 3.606%        |
| 10        | 9.100       | 1206          | 1215        | 1225         | rBV      | 298372         | 589582        | 38.54%          | 8.523%        |
| 11        | 9.353       | 1248          | 1258        | 1273         | rBV      | 736633         | 1529888       | 100.00%         | 22.115%       |
| 12        | 10.565      | 1456          | 1464        | 1477         | rBV      | 431756         | 767594        | 50.17%          | 11.096%       |
| 13        | 11.106      | 1548          | 1556        | 1563         | rVB      | 67347          | 125145        | 8.18%           | 1.809%        |
| 14        | 11.865      | 1677          | 1685        | 1695         | rVB      | 506703         | 875414        | 57.22%          | 12.654%       |
| 15        | 12.847      | 1843          | 1852        | 1867         | rVB      | 380934         | 640481        | 41.86%          | 9.258%        |
| 16        | 13.788      | 2003          | 2012        | 2021         | rBV      | 496586         | 854724        | 55.87%          | 12.355%       |

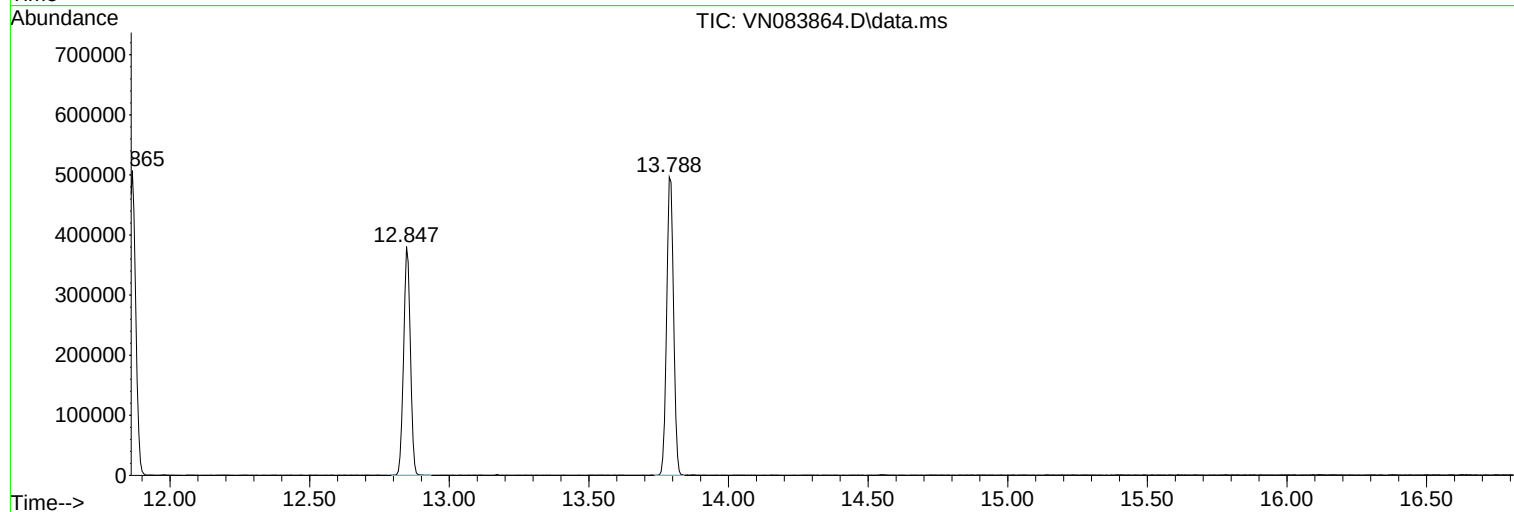
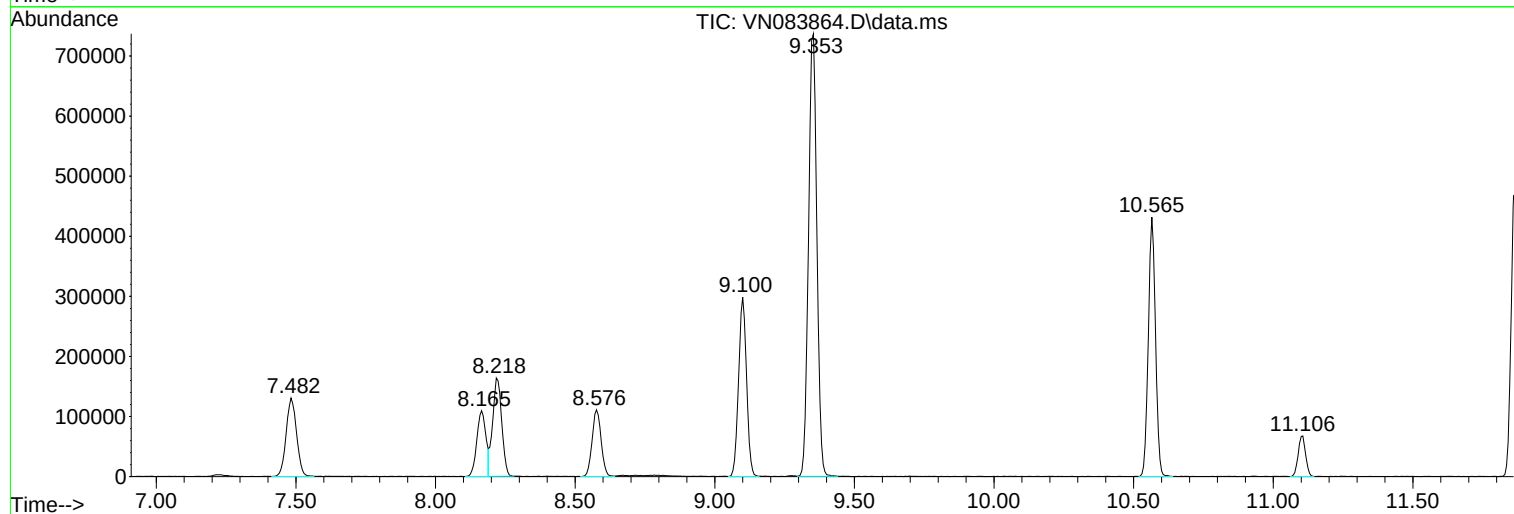
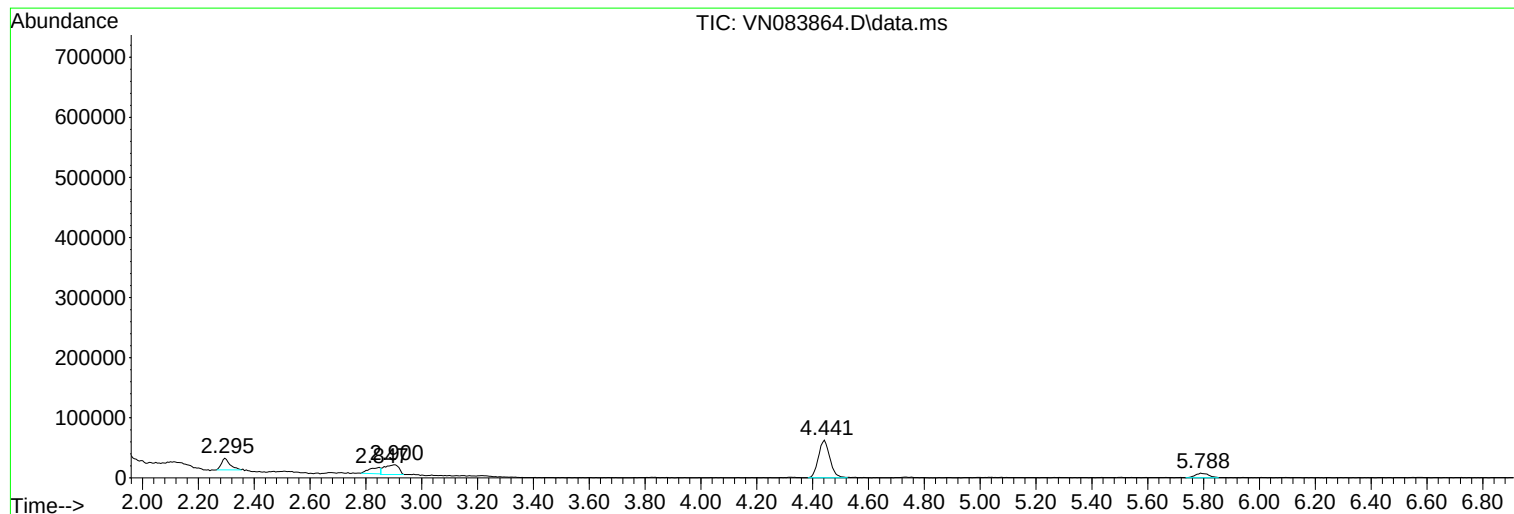
Sum of corrected areas: 6917865

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ClientSampleId :  
MW179D-20240910

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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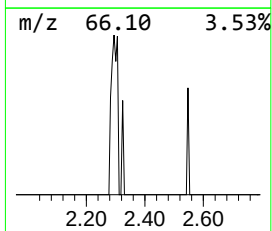
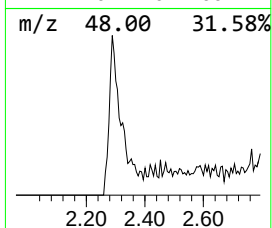
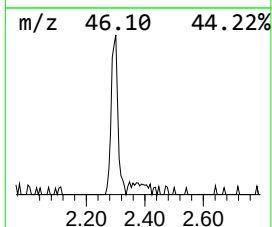
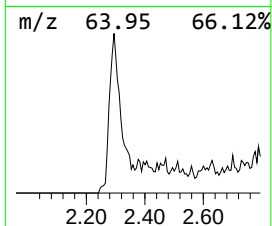
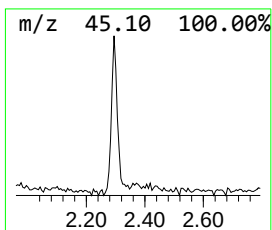
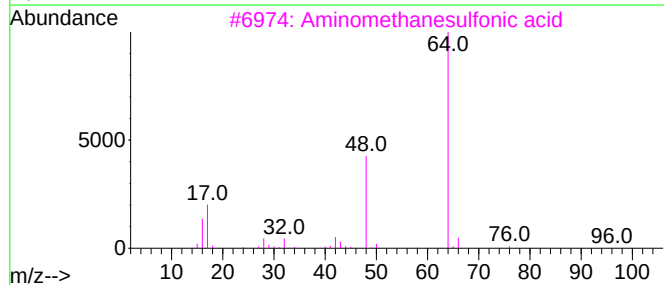
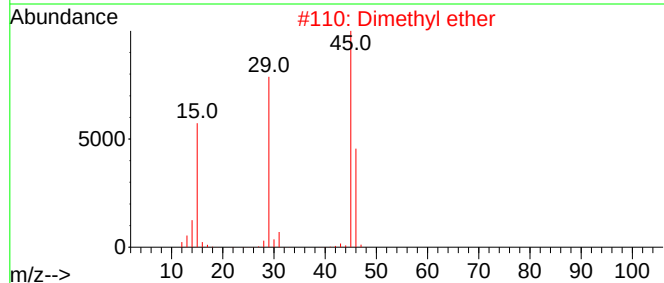
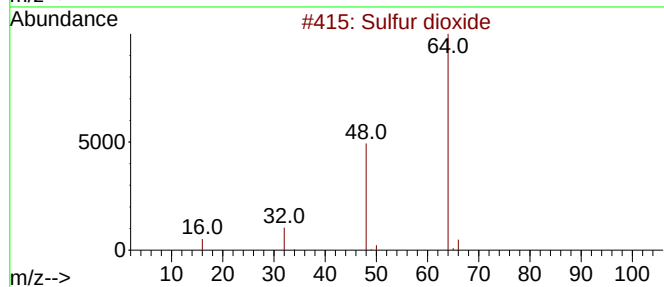
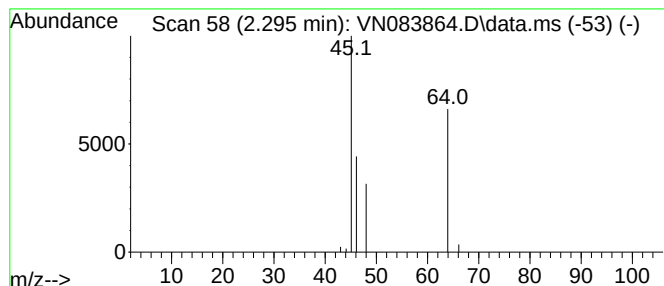
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown2.295 Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.295 | 5.70 ug/l | 41823 | Pentafluorobenzene | 8.224 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 38   |
| 2    |    |   | Dimethyl ether            | 46  | C2H6O    | 000115-10-6 | 9    |
| 3    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 4    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 5    |    |   | Ethanol                   | 46  | C2H6O    | 000064-17-5 | 5    |



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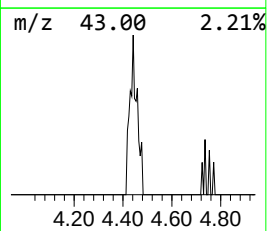
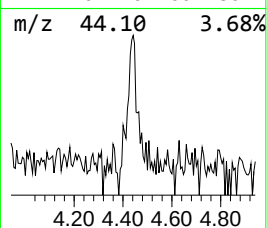
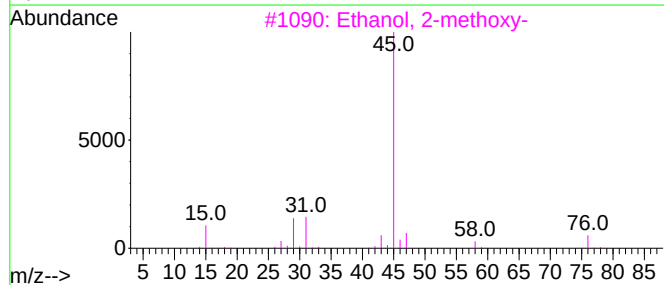
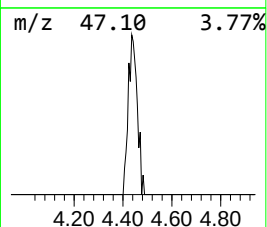
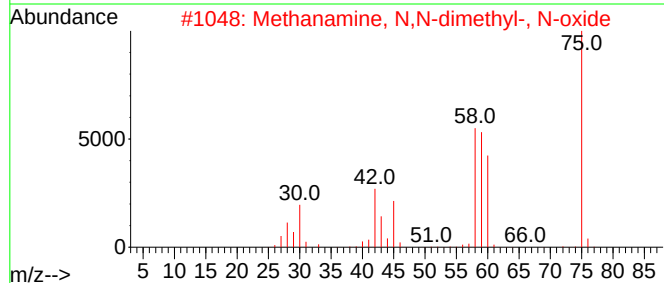
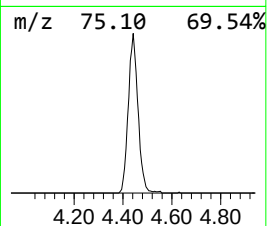
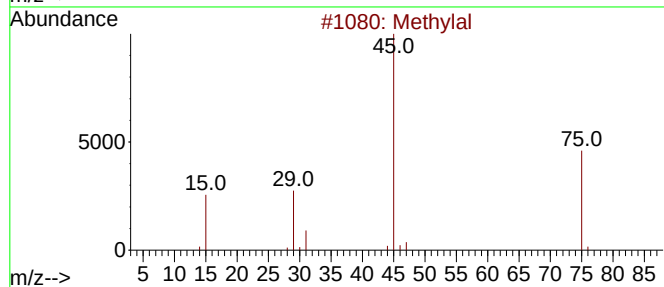
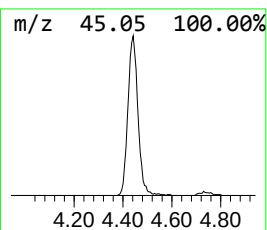
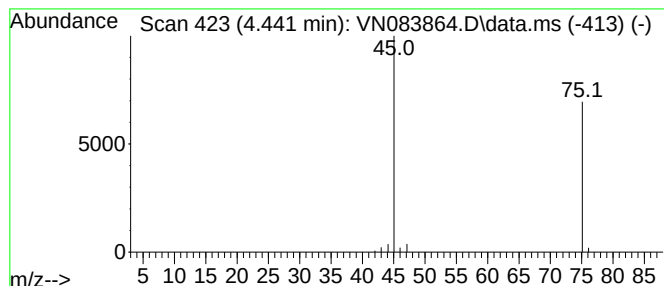
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Peak Number 3 Methylal Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 4.441 | 24.06 ug/l | 176608 | Pentafluorobenzene | 8.224 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Methylal                            | 76  | C3H8O2  | 000109-87-5 | 90   |
| 2    |    |   | Methanamine, N,N-dimethyl-, N-oxide | 75  | C3H9NO  | 001184-78-7 | 7    |
| 3    |    |   | Ethanol, 2-methoxy-                 | 76  | C3H8O2  | 000109-86-4 | 5    |
| 4    |    |   | Glycolaldehyde dimethyl acetal      | 106 | C4H10O3 | 030934-97-5 | 4    |
| 5    |    |   | Formamide                           | 45  | CH3NO   | 000075-12-7 | 4    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown2.295     | 2.295 | 5.7     | ug/l  | 41823    | 1                     | 8.224 | 366971 | 50.0 |
| Methylal         | 4.441 | 24.1    | ug/l  | 176608   | 1                     | 8.224 | 366971 | 50.0 |