

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN100722\  
 Data File : VN074812.D  
 Acq On : 07 Oct 2022 15:31  
 Operator : JC\MD  
 Sample : N4977-01  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 251032-3

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\82N100522W.M

Title : SW846 8260

Signal : TIC: VN074812.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         | 2.312       | 38            | 44          | 52           | rBV      | 258927         | 477590        | 15.22%          | 3.549%        |
| 2         | 2.406       | 55            | 60          | 61           | rBV2     | 34702          | 43868         | 1.40%           | 0.326%        |
| 3         | 2.771       | 118           | 122         | 125          | rBV2     | 95264          | 136977        | 4.37%           | 1.018%        |
| 4         | 2.830       | 129           | 132         | 133          | rBV2     | 55491          | 61264         | 1.95%           | 0.455%        |
| 5         | 7.453       | 912           | 918         | 929          | rVB      | 29206          | 70524         | 2.25%           | 0.524%        |
| 6         | 8.177       | 1031          | 1041        | 1046         | rBV      | 409333         | 988703        | 31.51%          | 7.347%        |
| 7         | 8.236       | 1046          | 1051        | 1061         | rVB      | 414562         | 928833        | 29.60%          | 6.902%        |
| 8         | 8.588       | 1100          | 1111        | 1121         | rBV      | 497102         | 1166380       | 37.17%          | 8.667%        |
| 9         | 9.106       | 1189          | 1199        | 1209         | rBV      | 608641         | 1286618       | 41.00%          | 9.561%        |
| 10        | 10.571      | 1437          | 1448        | 1459         | rBV      | 1679576        | 3137785       | 100.00%         | 23.316%       |
| 11        | 11.871      | 1661          | 1669        | 1686         | rBV      | 958043         | 1760897       | 56.12%          | 13.085%       |
| 12        | 12.853      | 1829          | 1836        | 1844         | rBV      | 966707         | 1628805       | 51.91%          | 12.103%       |
| 13        | 13.794      | 1986          | 1996        | 2007         | rBV      | 1018246        | 1769202       | 56.38%          | 13.147%       |

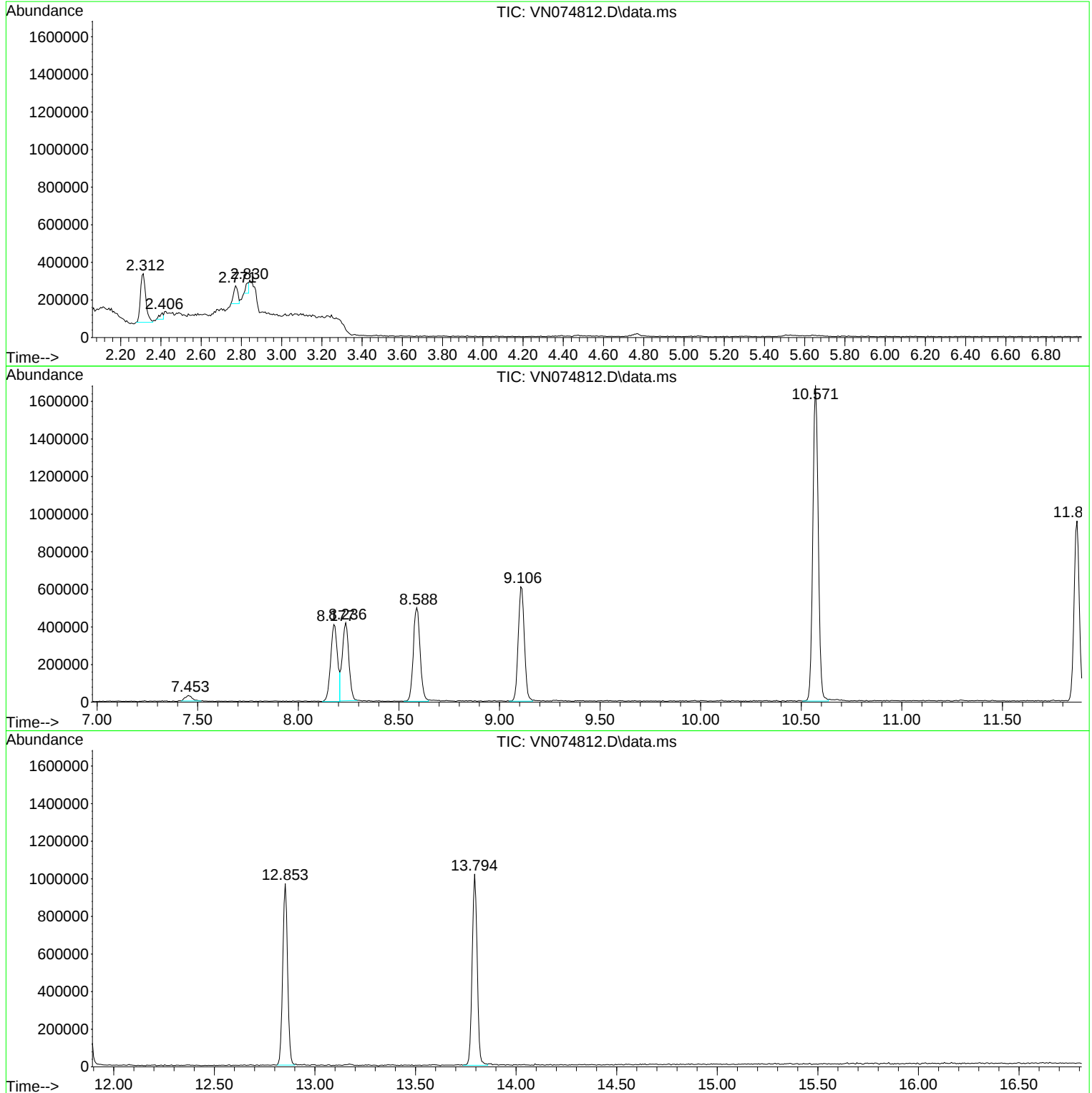
Sum of corrected areas: 13457446

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N100522W.M  
Quant Title : SW846 8260

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



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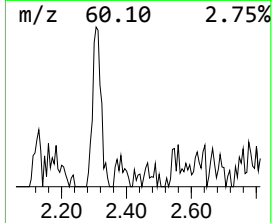
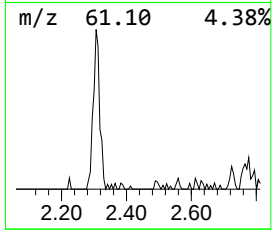
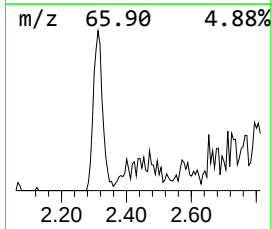
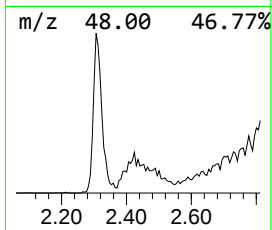
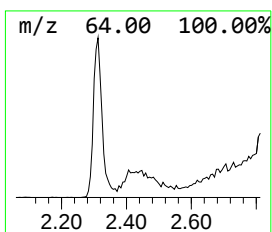
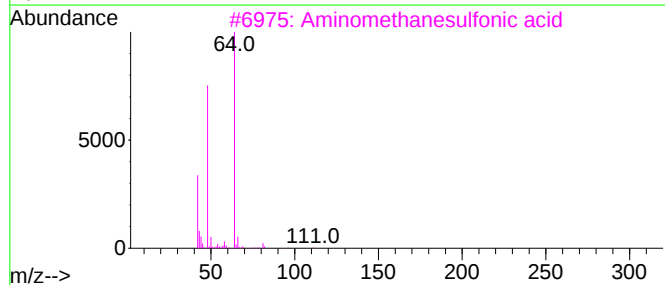
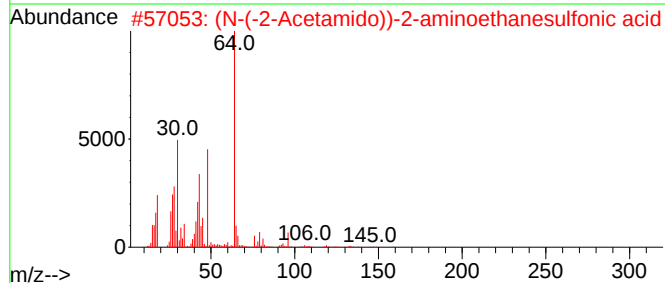
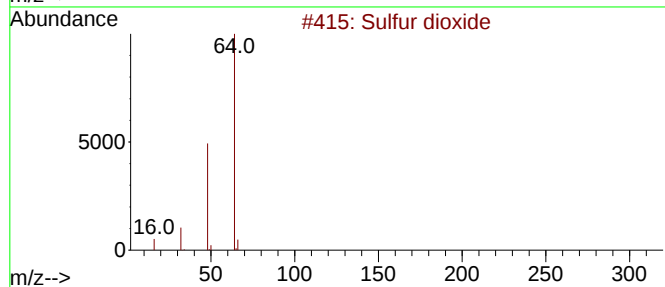
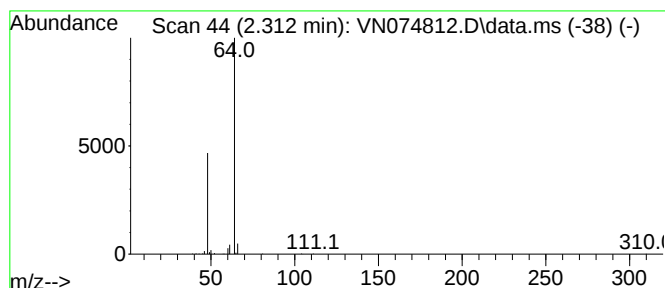
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N100522W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Sulfur dioxide Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 2.312 | 25.71 ug/l | 477590 | Pentafluorobenzene | 8.236 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Sulfur dioxide                      | 64  | O2S        | 007446-09-5 | 90   |
| 2    |    |   | (N-(-2-Acetamido))-2-aminoethane... | 182 | C4H10N2O4S | 007365-82-4 | 64   |
| 3    |    |   | Aminomethanesulfonic acid           | 111 | CH5NO3S    | 013881-91-9 | 9    |
| 4    |    |   | L-Alanine, 3-sulfo-                 | 169 | C3H7NO5S   | 000498-40-8 | 9    |
| 5    |    |   | 2-Aminoethyl hydrogen sulfate       | 141 | C2H7NO4S   | 000926-39-6 | 9    |



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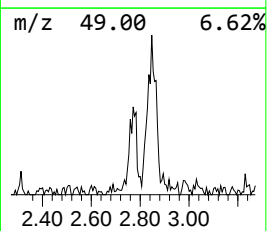
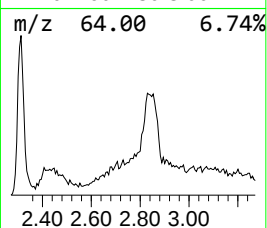
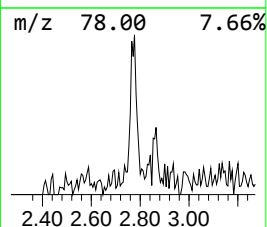
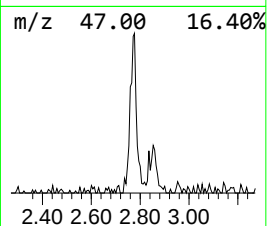
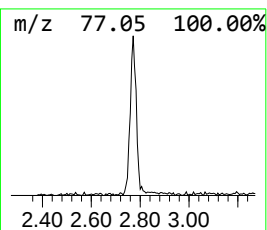
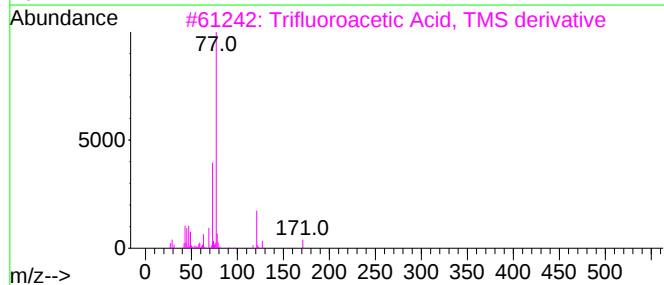
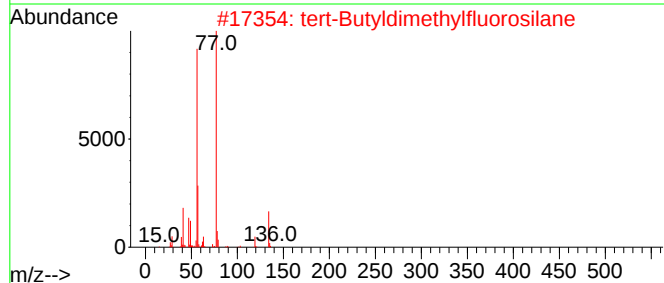
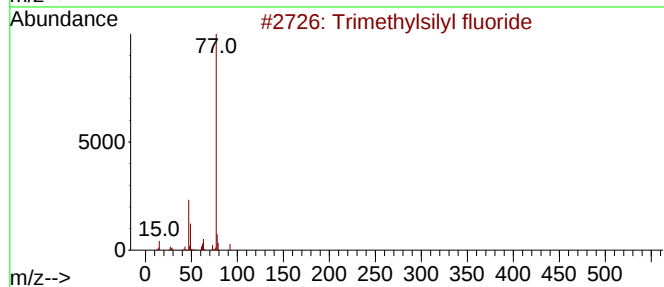
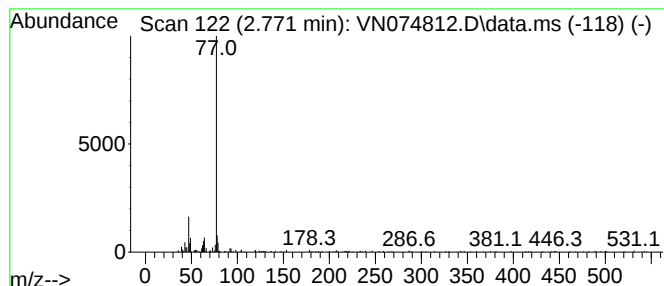
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Peak Number 2 unknown2.771 Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD   | R.T.  |
|-------|-----------|--------|--------------------|-------|
| 2.771 | 7.37 ug/l | 136977 | Pentafluorobenzene | 8.236 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Trimethylsilyl fluoride             | 92  | C3H9FSi    | 000420-56-4  | 43   |
| 2    |    |   | tert-Butyldimethylfluorosilane      | 134 | C6H15FSi   | 1000366-62-3 | 39   |
| 3    |    |   | Trifluoroacetic Acid, TMS deriva... | 186 | C5H9F3O2Si | 000400-53-3  | 39   |
| 4    |    |   | Perfluoropropionic acid, TMS der... | 236 | C6H9F5O2Si | 024930-02-7  | 9    |
| 5    |    |   | Silanediol, dimethyl-               | 92  | C2H8O2Si   | 001066-42-8  | 9    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 2.312 | 25.7    | ug/l  | 477590   | 1                     | 8.236 | 928833 | 50.0 |
| unknown2.771     | 2.771 | 7.4     | ug/l  | 136977   | 1                     | 8.236 | 928833 | 50.0 |