

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN101022\  
 Data File : VN074826.D  
 Acq On : 10 Oct 2022 12:28  
 Operator : JC\MD  
 Sample : VN1010MBL01  
 Misc : 5.0g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 VN1010MBL01

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: VN074826.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       | 39            | 44          | 50           | rBV      | 113020         | 213702        | 5.88%           | 1.421%        |
| 2         | 2.830       | 125           | 132         | 133          | rBV2     | 148945         | 226183        | 6.23%           | 1.504%        |
| 3         | 7.447       | 910           | 917         | 924          | rBV      | 17872          | 44479         | 1.22%           | 0.296%        |
| 4         | 8.177       | 1030          | 1041        | 1046         | rBV      | 462836         | 1115980       | 30.73%          | 7.420%        |
| 5         | 8.235       | 1046          | 1051        | 1061         | rVB      | 517548         | 1129418       | 31.10%          | 7.510%        |
| 6         | 8.588       | 1101          | 1111        | 1122         | rBV2     | 590612         | 1296230       | 35.69%          | 8.619%        |
| 7         | 9.106       | 1190          | 1199        | 1208         | rBV      | 718251         | 1495896       | 41.19%          | 9.947%        |
| 8         | 10.571      | 1437          | 1448        | 1457         | rBV      | 1993042        | 3631441       | 100.00%         | 24.146%       |
| 9         | 11.871      | 1661          | 1669        | 1681         | rBV      | 1102039        | 1998769       | 55.04%          | 13.290%       |
| 10        | 12.853      | 1828          | 1836        | 1848         | rBV      | 1067532        | 1850965       | 50.97%          | 12.308%       |
| 11        | 13.794      | 1989          | 1996        | 2005         | rVV      | 1182116        | 1958833       | 53.94%          | 13.025%       |
| 12        | 15.647      | 2309          | 2311        | 2317         | rVB5     | 26623          | 39116         | 1.08%           | 0.260%        |
| 13        | 15.841      | 2338          | 2344        | 2348         | rVB7     | 18820          | 38282         | 1.05%           | 0.255%        |

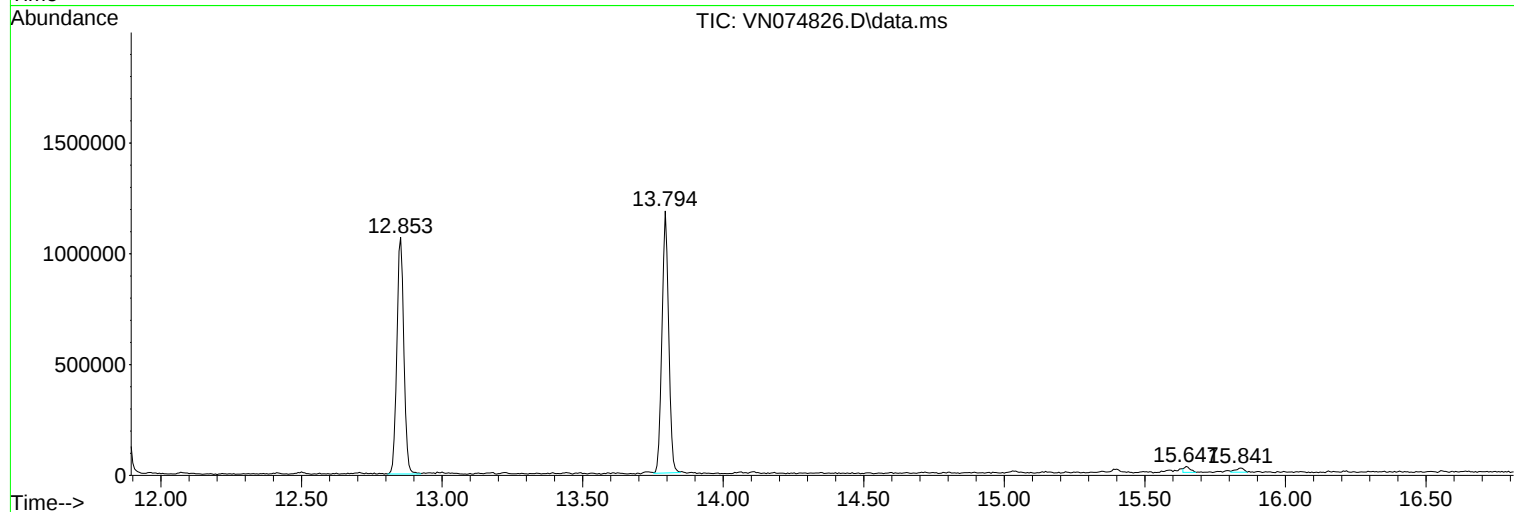
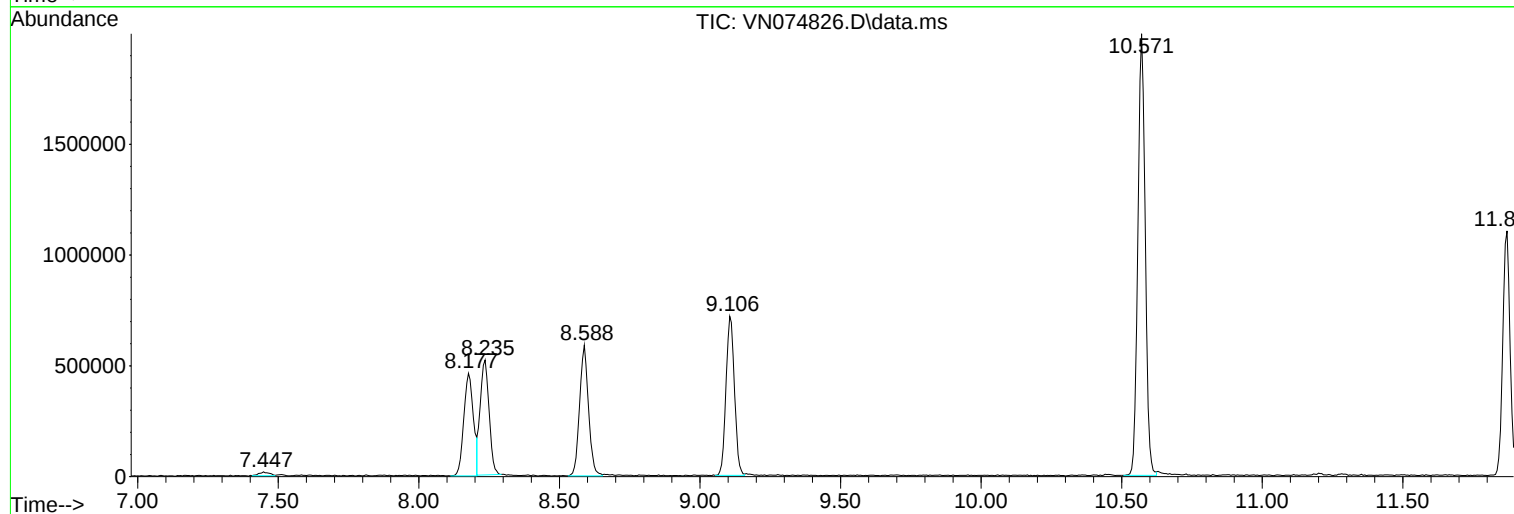
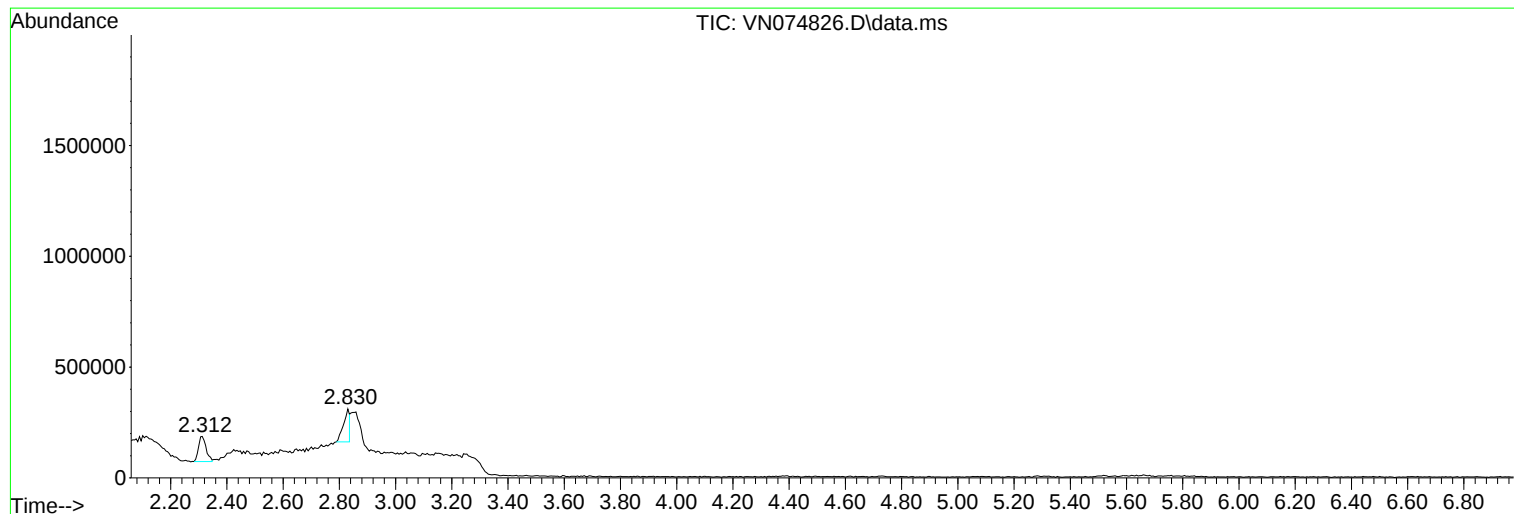
Sum of corrected areas: 15039294

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Quant Title : SW846 8260

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



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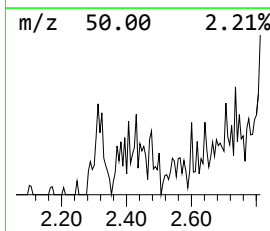
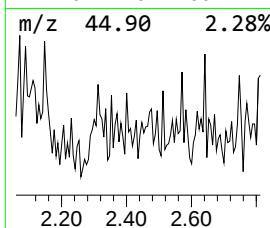
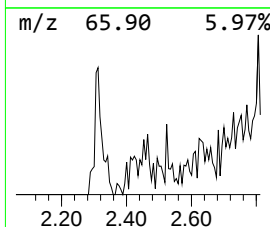
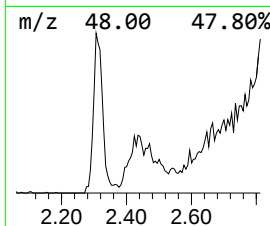
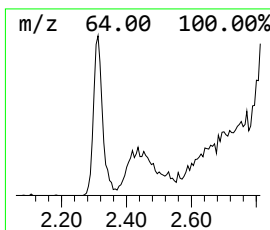
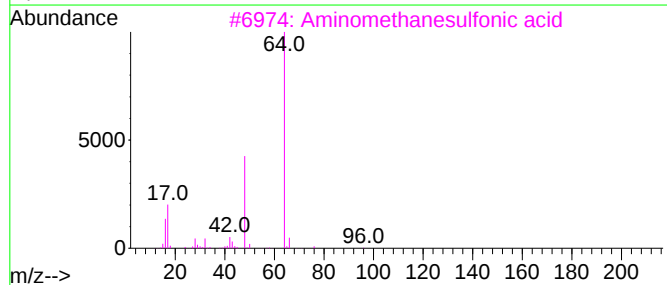
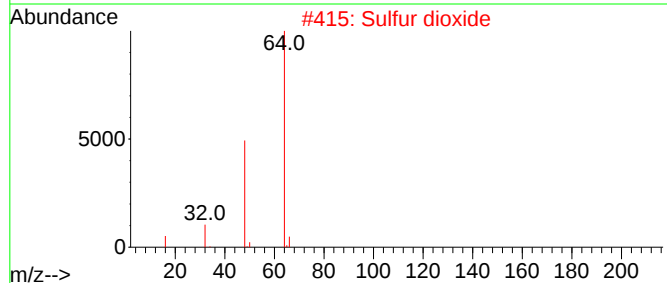
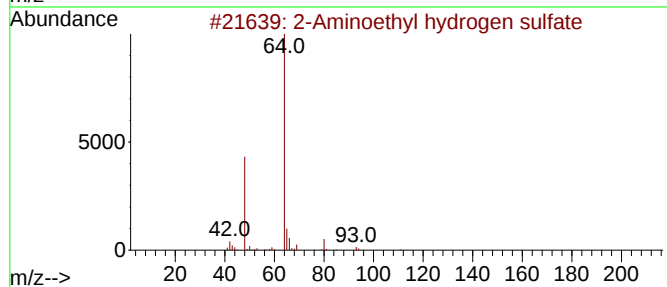
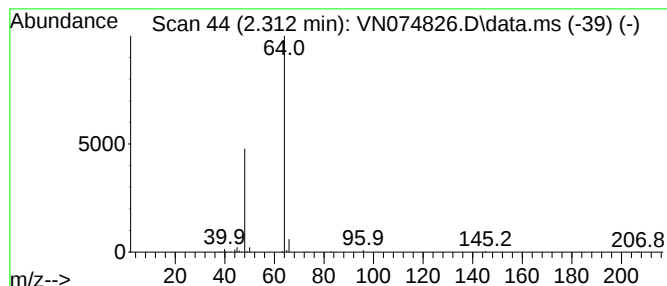
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Aminoethyl hydrogen sulfate Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD   | R.T.  |
|-------|-----------|--------|--------------------|-------|
| 2.312 | 9.46 ug/l | 213702 | Pentafluorobenzene | 8.235 |

| Hit# | of | 5 | Tentative ID                             | MW  | MolForm   | CAS#         | Qual |
|------|----|---|------------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 2-Aminoethyl hydrogen sulfate            | 141 | C2H7NO4S  | 000926-39-6  | 83   |
| 2    |    |   | Sulfur dioxide                           | 64  | O2S       | 007446-09-5  | 83   |
| 3    |    |   | Aminomethanesulfonic acid                | 111 | CH5NO3S   | 013881-91-9  | 74   |
| 4    |    |   | 1,1,1,2,2,3,3,4,4,5,5-Undecafluorooctane | 602 | C10F22O2S | 1000486-78-5 | 64   |
| 5    |    |   | Benzenesulfonic acid, 2,5-diamino-       | 188 | C6H8N2O3S | 000088-45-9  | 9    |



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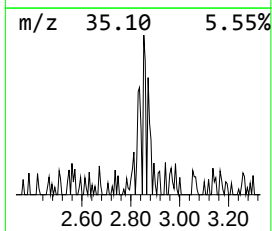
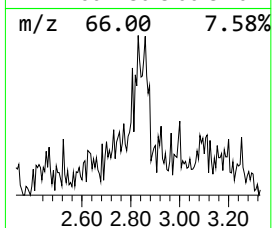
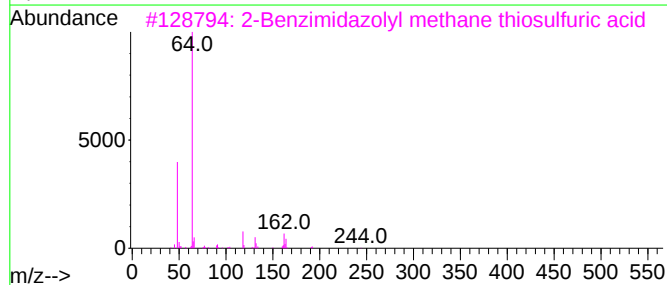
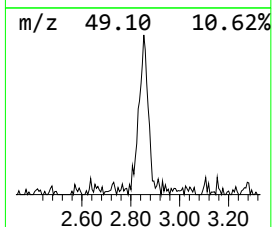
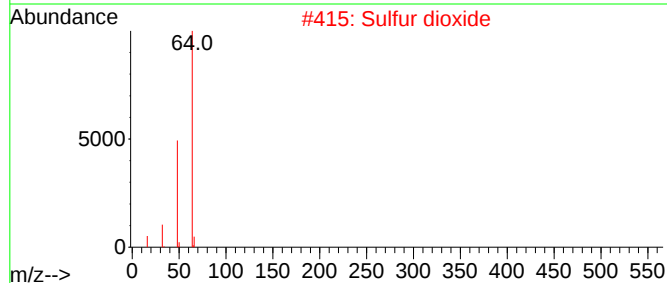
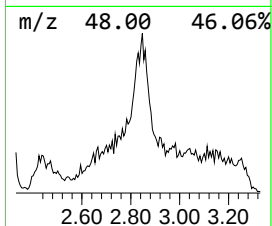
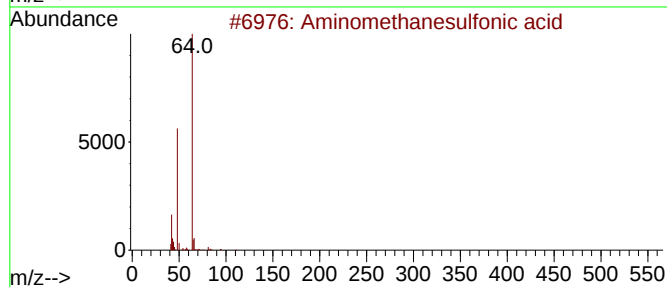
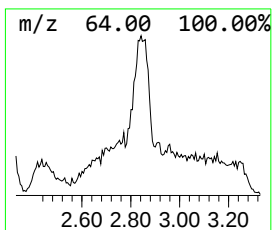
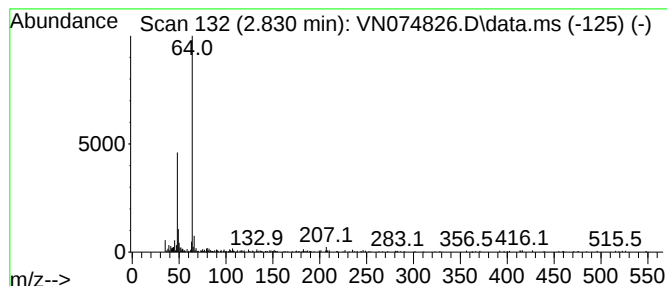
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Peak Number 2 Aminomethanesulfonic acid Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 2.830 | 10.01 ug/l | 226183 | Pentafluorobenzene | 8.235 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Aminomethanesulfonic acid           | 111 | CH5NO3S     | 013881-91-9  | 78   |
| 2    |    |   | Sulfur dioxide                      | 64  | O2S         | 007446-09-5  | 64   |
| 3    |    |   | 2-Benzimidazolyl methane thiosul... | 244 | C8H8N2O3S2  | 1010256-39-2 | 64   |
| 4    |    |   | 2-Aminoethyl hydrogen sulfate       | 141 | C2H7NO4S    | 000926-39-6  | 64   |
| 5    |    |   | 2,6-Dichloro-4-nitrobenzene-1-su... | 289 | C6H2Cl3NO4S | 074875-17-5  | 64   |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                    |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Aminoethyl hy... | 2.312 | 9.5     | ug/l  | 213702   | 1                     | 8.235 | 1129420 | 50.0 |
| Aminomethanesul... | 2.830 | 10.0    | ug/l  | 226183   | 1                     | 8.235 | 1129420 | 50.0 |