

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX041222\  
Data File : VX028076.D  
Acq On : 12 Apr 2022 22:59  
Operator : JC/MD  
Sample : N2334-11  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-26

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041222W.M

Title : SW846 8260

Signal : TIC: VX028076.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         | 1.246       | 22            | 26          | 38           | rBV      | 144698         | 247443        | 21.09%          | 3.786%        |
| 2         | 1.563       | 70            | 78          | 83           | rVB3     | 33754          | 70704         | 6.03%           | 1.082%        |
| 3         | 5.391       | 694           | 706         | 719          | rBV      | 138445         | 405959        | 34.60%          | 6.211%        |
| 4         | 5.556       | 721           | 733         | 748          | rVB      | 214535         | 604481        | 51.53%          | 9.249%        |
| 5         | 5.958       | 787           | 799         | 813          | rBV2     | 146585         | 402954        | 34.35%          | 6.165%        |
| 6         | 6.763       | 921           | 931         | 946          | rBV      | 356116         | 829407        | 70.70%          | 12.690%       |
| 7         | 8.653       | 1233          | 1241        | 1251         | rBV      | 741284         | 1173140       | 100.00%         | 17.949%       |
| 8         | 10.055      | 1465          | 1471        | 1482         | rBV      | 786562         | 1038275       | 88.50%          | 15.886%       |
| 9         | 11.085      | 1634          | 1640        | 1649         | rBV      | 599864         | 781813        | 66.64%          | 11.962%       |
| 10        | 12.024      | 1788          | 1794        | 1807         | rBV      | 798582         | 981757        | 83.69%          | 15.021%       |

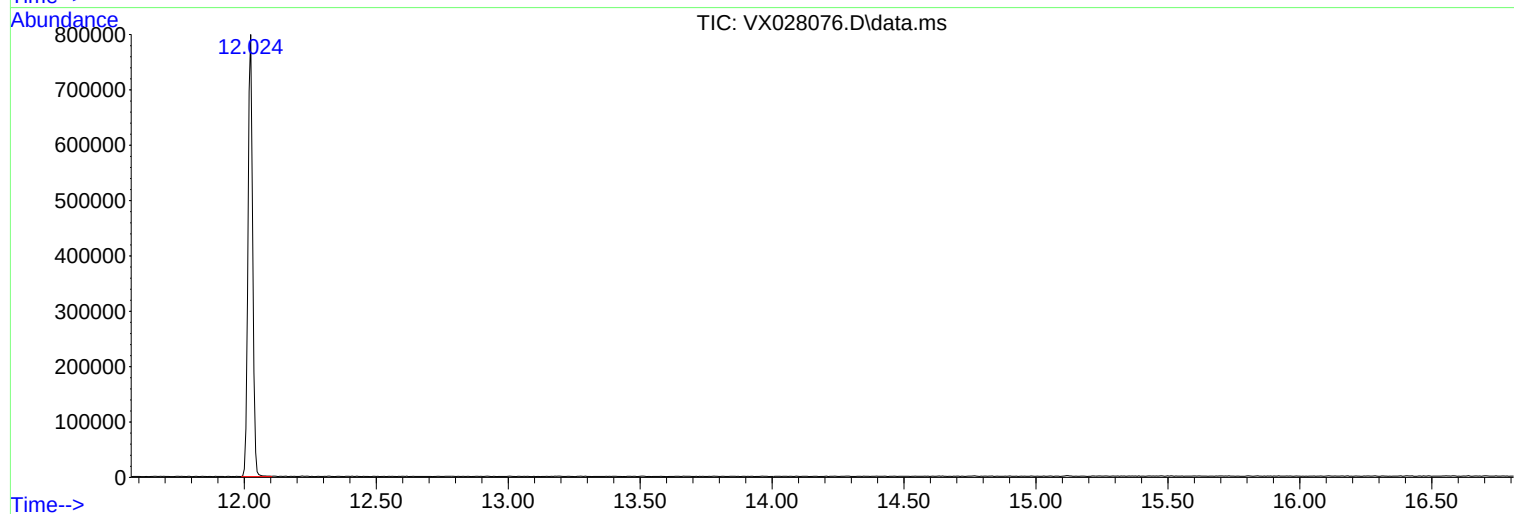
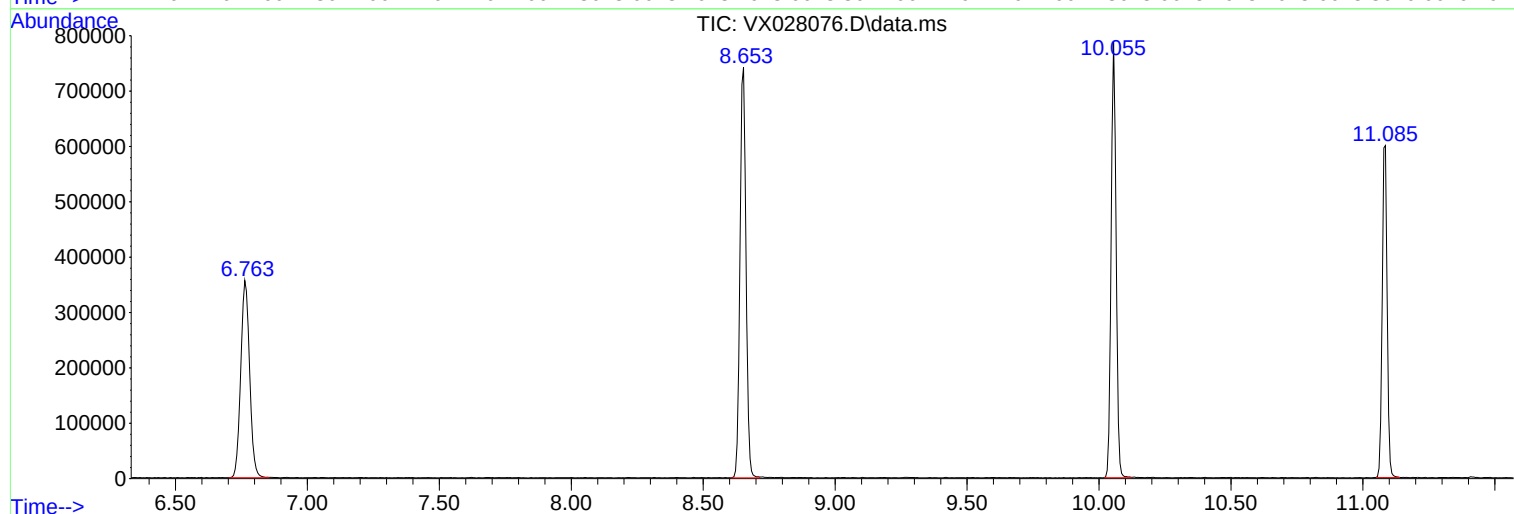
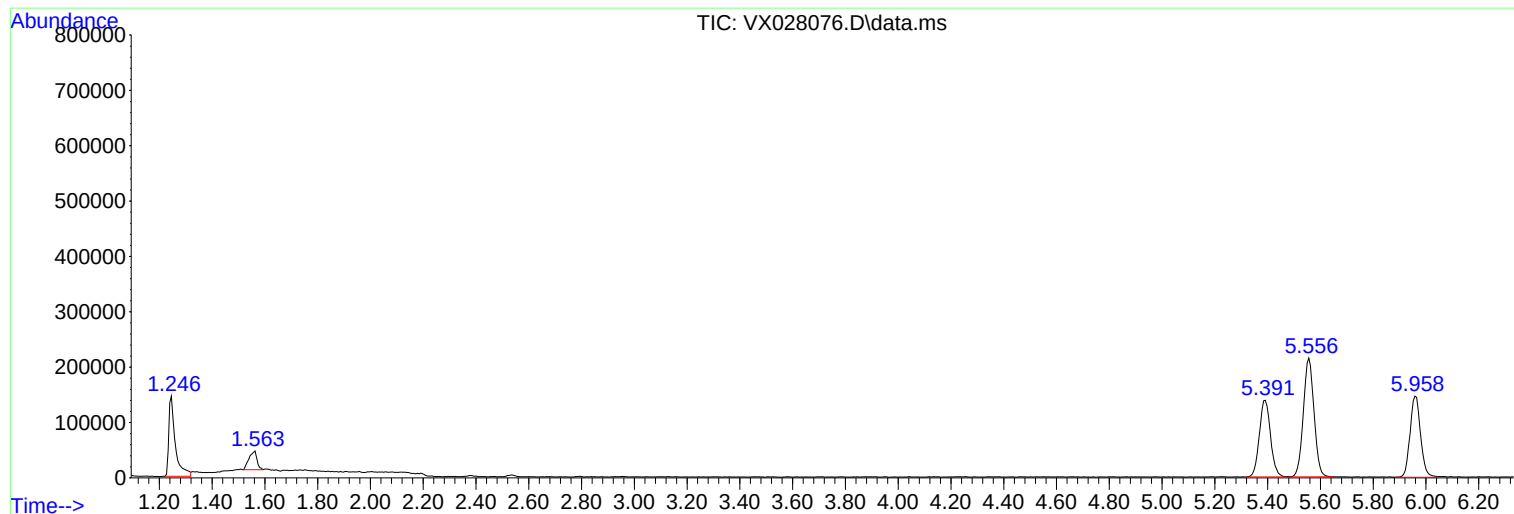
Sum of corrected areas: 6535933

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ClientSampleId :  
MW-26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041222W.M  
Quant Title : SW846 8260

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



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MSVOA\_X  
ClientSampleId :  
MW-26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041222W.M  
Quant Title : SW846 8260

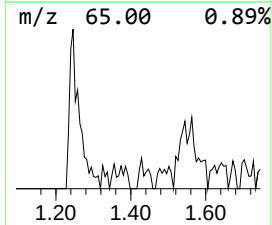
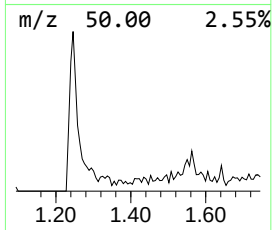
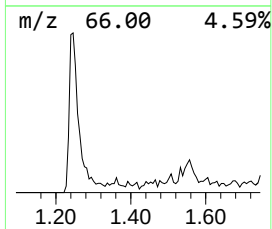
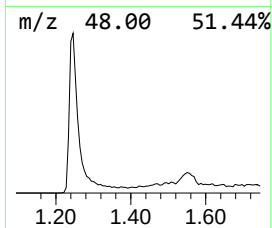
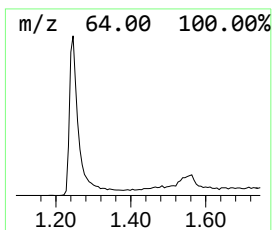
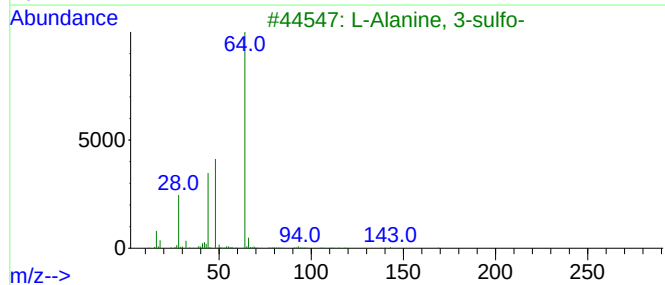
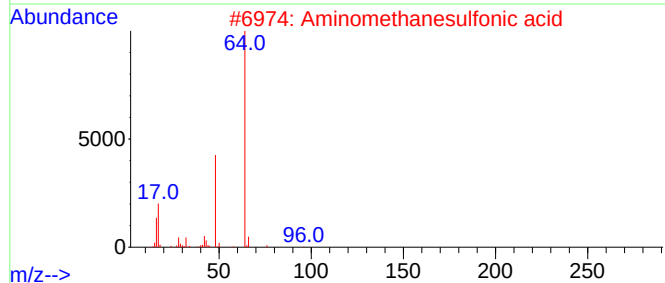
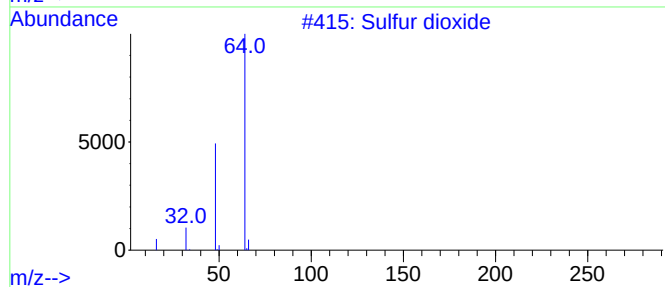
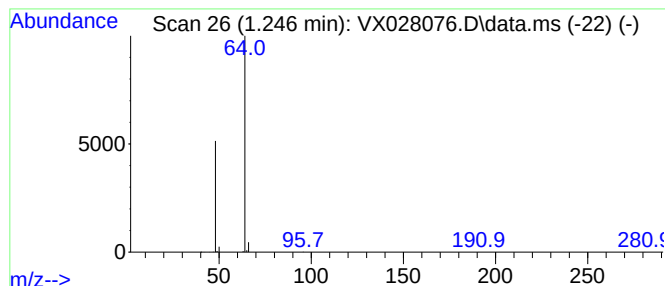
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Sulfur dioxide Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 1.246 | 20.47 ug/l | 247443 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 83   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |
| 5    |    |   | Ethyl Chloride            | 64  | C2H5Cl   | 000075-00-3 | 4    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\WX041222\  
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Sample : N2334-11  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-26

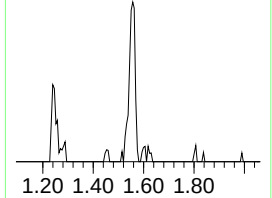
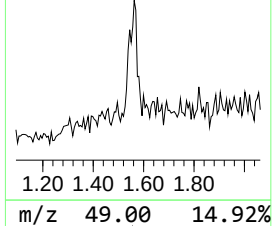
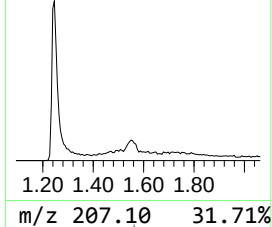
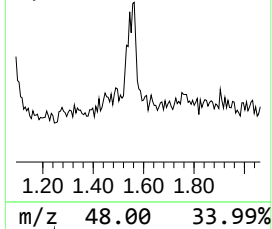
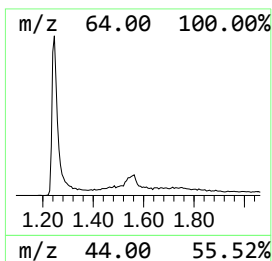
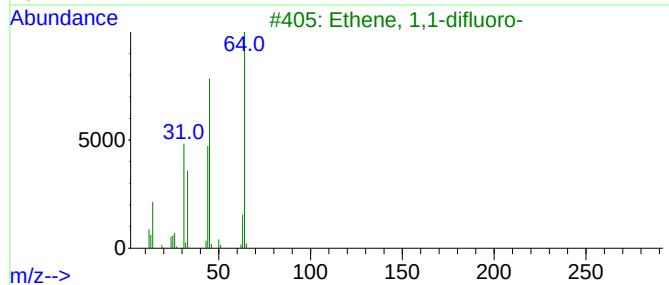
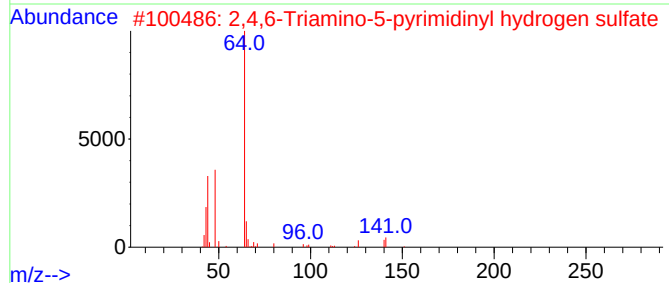
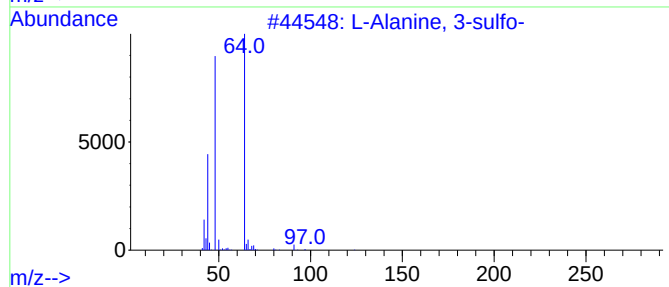
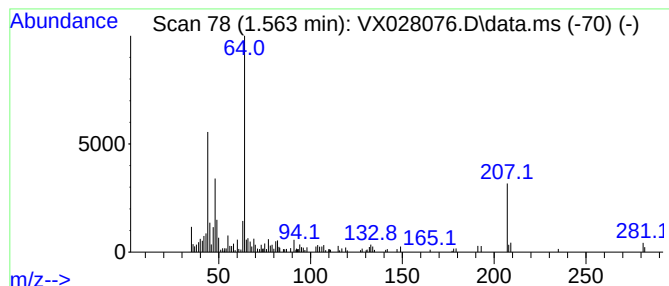
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041222W.M  
Quant Title : SW846 8260

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

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Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.563 | 5.85 ug/l | 70704 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm      | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|--------------|-------------|------|
| 1    |    |   | L-Alanine, 3-sulfo-                 | 169 | C3H7NO5S     | 000498-40-8 | 50   |
| 2    |    |   | 2,4,6-Triamino-5-pyrimidinyl hyd... | 221 | C4H7N5O4S    | 071552-23-3 | 50   |
| 3    |    |   | Ethene, 1,1-difluoro-               | 64  | C2H2F2       | 000075-38-7 | 50   |
| 4    |    |   | N,N'-Nonamethylenebis[-S-3-amino... | 466 | C15H34N2O6S4 | 035871-58-0 | 50   |
| 5    |    |   | Sulfur dioxide                      | 64  | O2S          | 007446-09-5 | 45   |



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ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041222W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide     | 1.246 | 20.5    | ug/l  | 247443   | 1                     | 5.556 | 604481 | 50.0 |
| L-Alanine, 3-su... | 1.563 | 5.8     | ug/l  | 70704    | 1                     | 5.556 | 604481 | 50.0 |