

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX100821\  
 Data File : VX024680.D  
 Acq On : 08 Oct 2021 19:07  
 Operator : JC/MD  
 Sample : M4154-05RE  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 SW-CB-32

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\82X092321W.M  
 Title : SW846 8260

Signal : TIC: VX024680.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         | 1.160       | 7             | 12          | 15           | rBV      | 6055           | 8268          | 1.05%           | 0.164%        |
| 2         | 1.276       | 23            | 31          | 43           | rBV      | 160121         | 524194        | 66.55%          | 10.368%       |
| 3         | 1.544       | 73            | 75          | 89           | rVB2     | 35061          | 66030         | 8.38%           | 1.306%        |
| 4         | 2.386       | 206           | 213         | 218          | rBV      | 17065          | 28413         | 3.61%           | 0.562%        |
| 5         | 2.550       | 229           | 240         | 249          | rBV2     | 16193          | 47789         | 6.07%           | 0.945%        |
| 6         | 3.337       | 363           | 369         | 376          | rVB3     | 4403           | 9881          | 1.25%           | 0.195%        |
| 7         | 4.574       | 563           | 572         | 581          | rBV2     | 3677           | 10380         | 1.32%           | 0.205%        |
| 8         | 5.391       | 691           | 706         | 719          | rBV2     | 95114          | 274114        | 34.80%          | 5.422%        |
| 9         | 5.562       | 723           | 734         | 752          | rVB      | 148550         | 417173        | 52.96%          | 8.251%        |
| 10        | 5.964       | 789           | 800         | 814          | rBV      | 101735         | 267135        | 33.91%          | 5.284%        |
| 11        | 6.769       | 921           | 932         | 949          | rBV      | 238322         | 566323        | 71.90%          | 11.201%       |
| 12        | 8.653       | 1234          | 1241        | 1248         | rVV      | 515681         | 787695        | 100.00%         | 15.579%       |
| 13        | 8.726       | 1248          | 1253        | 1260         | rVB      | 27575          | 44442         | 5.64%           | 0.879%        |
| 14        | 8.848       | 1268          | 1273        | 1280         | rVB      | 9431           | 15129         | 1.92%           | 0.299%        |
| 15        | 10.055      | 1465          | 1471        | 1485         | rVB      | 513363         | 710135        | 90.15%          | 14.045%       |
| 16        | 11.085      | 1631          | 1640        | 1652         | rVB      | 467396         | 588956        | 74.77%          | 11.649%       |
| 17        | 12.024      | 1788          | 1794        | 1802         | rBV      | 522014         | 660114        | 83.80%          | 13.056%       |
| 18        | 12.219      | 1820          | 1826        | 1833         | rBV      | 19427          | 29831         | 3.79%           | 0.590%        |

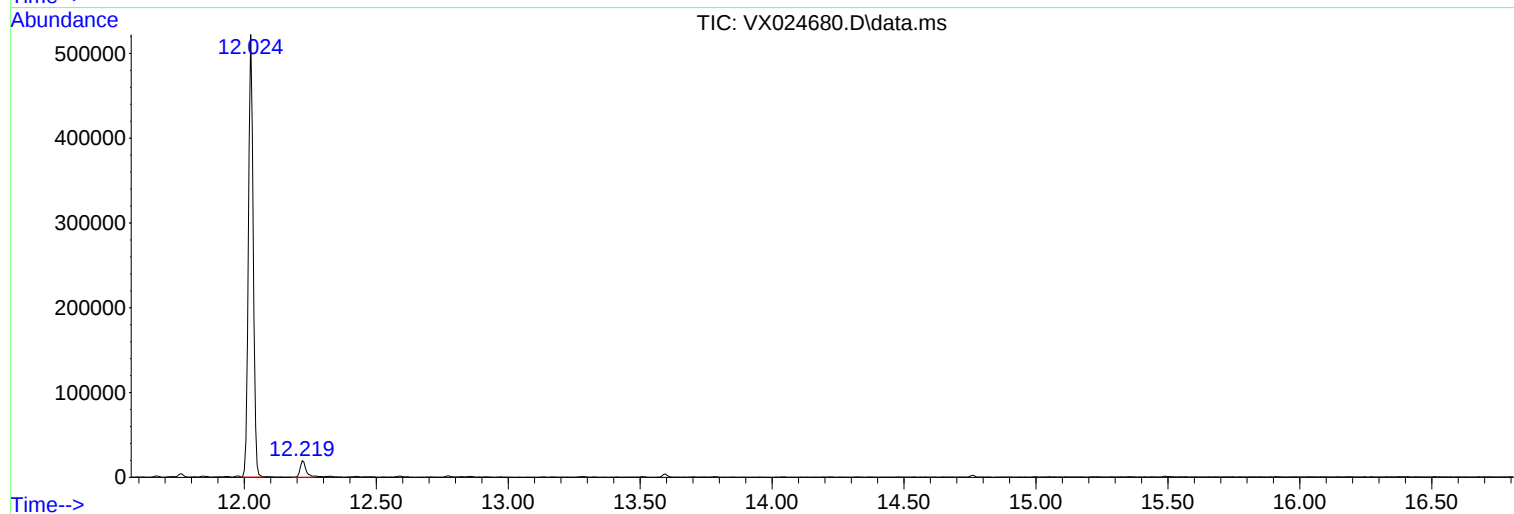
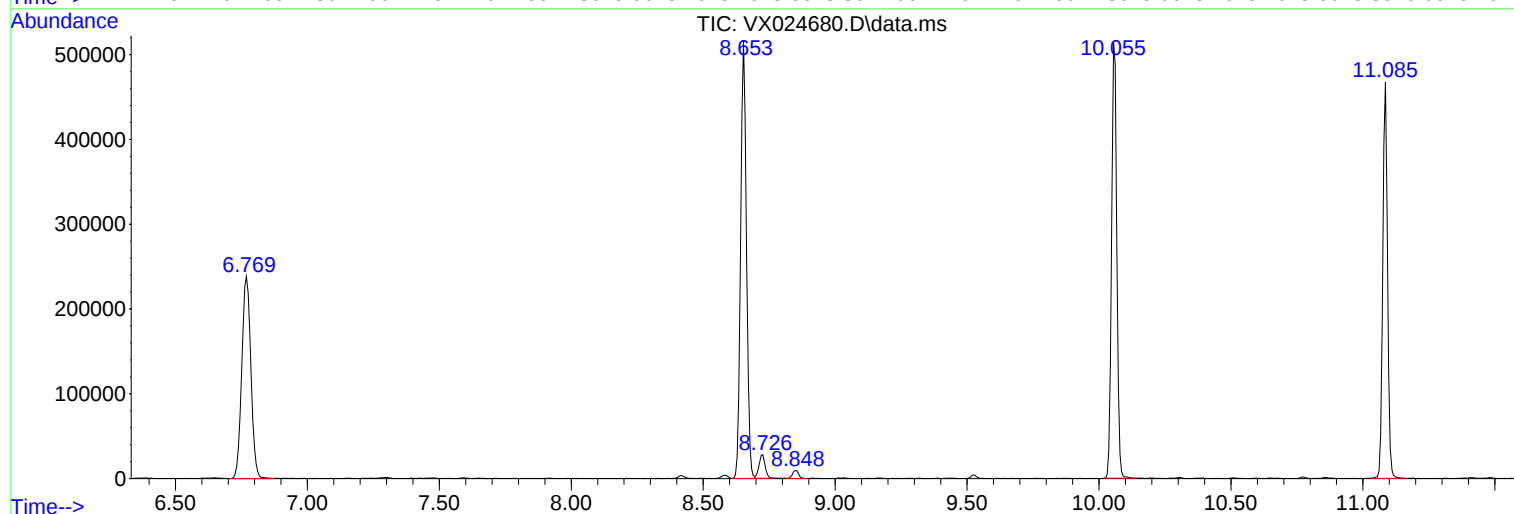
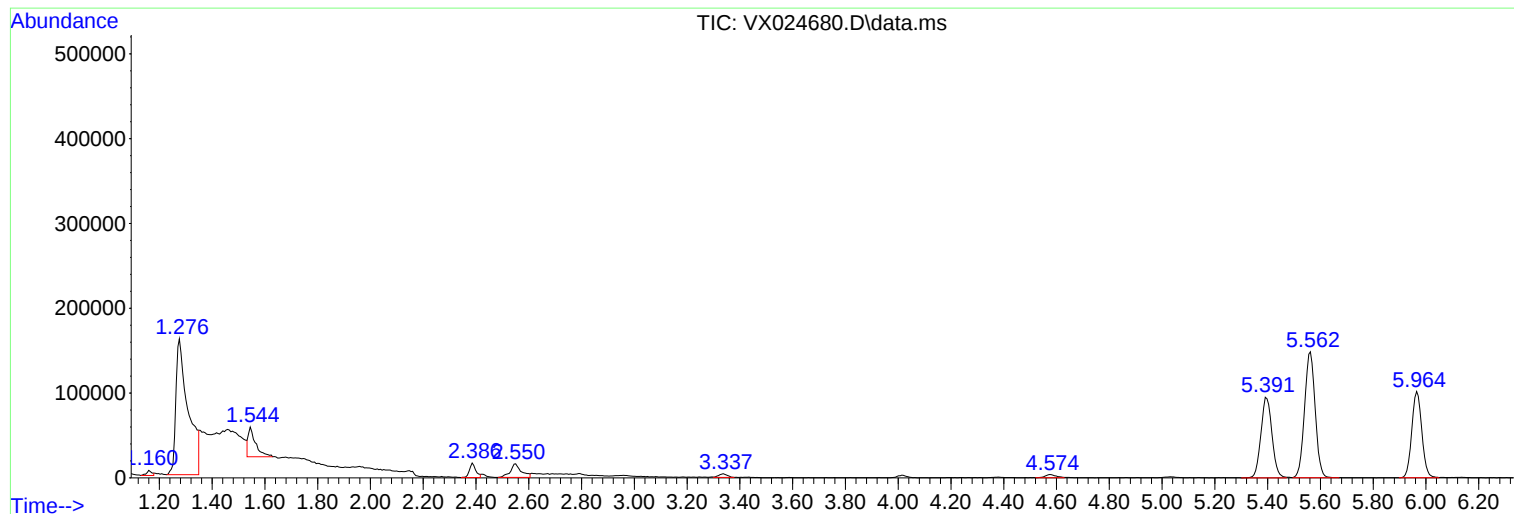
Sum of corrected areas: 5056002

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX100821\  
Data File : VX024680.D  
Acq On : 08 Oct 2021 19:07  
Operator : JC/MD  
Sample : M4154-05RE  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
SW-CB-32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X092321W.M  
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX100821\  
Data File : VX024680.D  
Acq On : 08 Oct 2021 19:07  
Operator : JC/MD  
Sample : M4154-05RE  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
SW-CB-32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X092321W.M  
Quant Title : SW846 8260

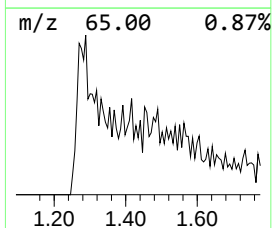
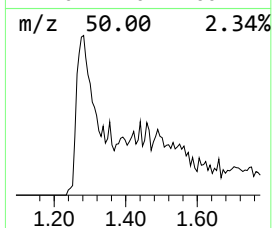
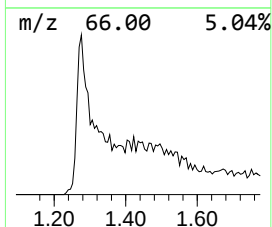
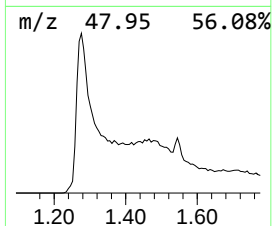
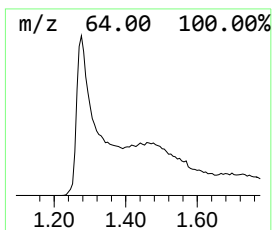
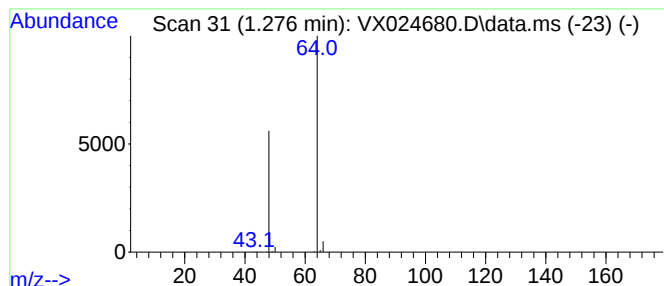
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 1 Sulfur dioxide Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 1.276 | 62.83 ug/l | 524194 | Pentafluorobenzene | 5.562 |

| 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 | 3    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX100821\  
Data File : VX024680.D  
Acq On : 08 Oct 2021 19:07  
Operator : JC/MD  
Sample : M4154-05RE  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
SW-CB-32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X092321W.M  
Quant Title : SW846 8260

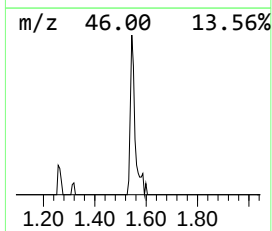
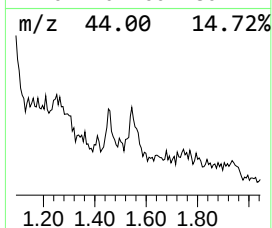
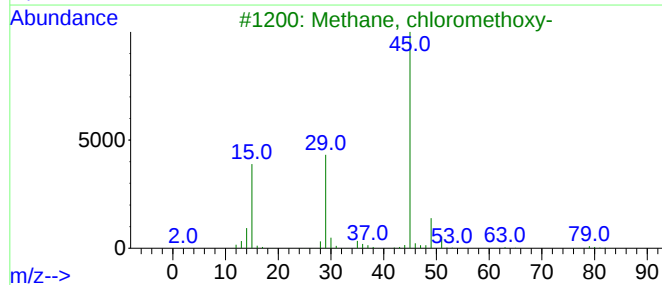
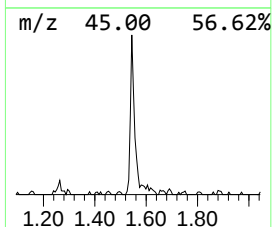
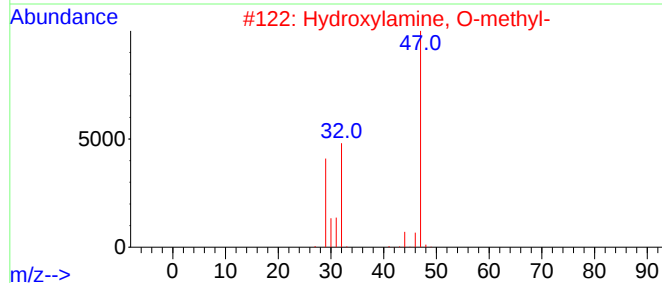
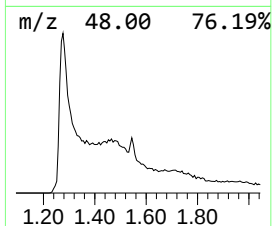
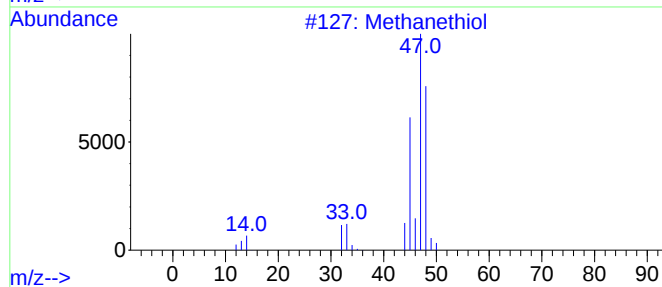
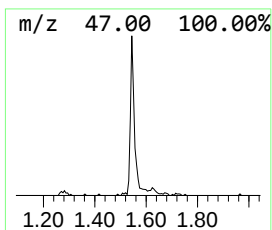
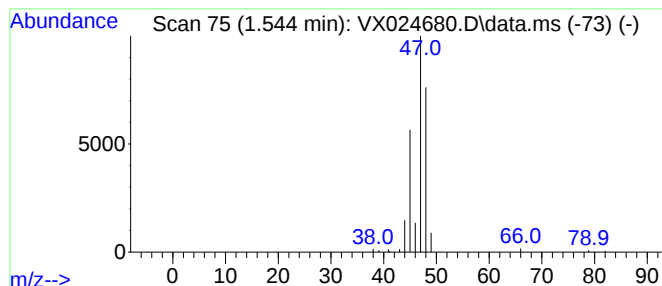
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 2 Methanethiol Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.544 | 7.91 ug/l | 66030 | Pentafluorobenzene | 5.562 |

| Hit# | of | 5 | Tentative ID             | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|----|---------|-------------|------|
| 1    |    |   | Methanethiol             | 48 | CH4S    | 000074-93-1 | 90   |
| 2    |    |   | Hydroxylamine, O-methyl- | 47 | CH5NO   | 000067-62-9 | 7    |
| 3    |    |   | Methane, chloromethoxy-  | 80 | C2H5ClO | 000107-30-2 | 4    |
| 4    |    |   | Formamide                | 45 | CH3NO   | 000075-12-7 | 4    |
| 5    |    |   | Nitrous acid             | 47 | HN02    | 007782-77-6 | 4    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX100821\  
Data File : VX024680.D  
Acq On : 08 Oct 2021 19:07  
Operator : JC/MD  
Sample : M4154-05RE  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
SW-CB-32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X092321W.M  
Quant Title : SW846 8260

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

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.276 | 62.8    | ug/l  | 524194   | 1                     | 5.562 | 417173 | 50.0 |
| Methanethiol     | 1.544 | 7.9     | ug/l  | 66030    | 1                     | 5.562 | 417173 | 50.0 |