

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU061622\  
 Data File : VU049226.D  
 Acq On : 16 Jun 2022 23:56  
 Operator : SY/MD  
 Sample : N3320-08  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 37 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGJ83

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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\_U\Method\SFAMUTR061422WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU049226.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         | 1.359       | 3             | 6           | 22           | rVB4     | 5938           | 7517          | 1.20%           | 0.164%        |
| 2         | 1.507       | 41            | 52          | 66           | rBV2     | 33284          | 113061        | 18.03%          | 2.460%        |
| 3         | 1.597       | 74            | 80          | 90           | rBV      | 56503          | 63227         | 10.08%          | 1.376%        |
| 4         | 1.912       | 171           | 178         | 194          | rVB      | 45830          | 62887         | 10.03%          | 1.369%        |
| 5         | 2.568       | 369           | 382         | 400          | rBV2     | 89954          | 156270        | 24.91%          | 3.401%        |
| 6         | 3.366       | 613           | 630         | 652          | rBV      | 83569          | 197565        | 31.50%          | 4.299%        |
| 7         | 4.639       | 1011          | 1026        | 1072         | rBV2     | 84098          | 278049        | 44.33%          | 6.051%        |
| 8         | 5.063       | 1143          | 1158        | 1179         | rBV      | 86526          | 194969        | 31.08%          | 4.243%        |
| 9         | 5.317       | 1225          | 1237        | 1249         | rBV4     | 3115           | 6894          | 1.10%           | 0.150%        |
| 10        | 5.726       | 1341          | 1364        | 1389         | rBV2     | 171208         | 451251        | 71.94%          | 9.820%        |
| 11        | 6.250       | 1512          | 1527        | 1550         | rBV      | 146204         | 279292        | 44.53%          | 6.078%        |
| 12        | 6.542       | 1602          | 1618        | 1636         | rBV      | 144757         | 275437        | 43.91%          | 5.994%        |
| 13        | 6.690       | 1650          | 1664        | 1683         | rBV      | 113498         | 218396        | 34.82%          | 4.753%        |
| 14        | 7.568       | 1923          | 1937        | 1952         | rBV      | 49069          | 87828         | 14.00%          | 1.911%        |
| 15        | 7.899       | 2024          | 2040        | 2054         | rBV      | 207093         | 357538        | 57.00%          | 7.781%        |
| 16        | 7.970       | 2055          | 2062        | 2074         | rVB2     | 9163           | 16141         | 2.57%           | 0.351%        |
| 17        | 8.182       | 2117          | 2128        | 2143         | rBV2     | 29443          | 51337         | 8.18%           | 1.117%        |
| 18        | 8.555       | 2236          | 2244        | 2253         | rBV4     | 4656           | 6892          | 1.10%           | 0.150%        |
| 19        | 8.636       | 2257          | 2269        | 2302         | rBV2     | 315838         | 627229        | 100.00%         | 13.650%       |
| 20        | 9.417       | 2497          | 2512        | 2533         | rBV      | 196616         | 332206        | 52.96%          | 7.229%        |
| 21        | 9.693       | 2587          | 2598        | 2608         | rBV3     | 6390           | 10810         | 1.72%           | 0.235%        |
| 22        | 10.758      | 2917          | 2929        | 2946         | rVB      | 91177          | 145963        | 23.27%          | 3.176%        |
| 23        | 11.812      | 3244          | 3257        | 3274         | rBV      | 205541         | 327886        | 52.28%          | 7.135%        |
| 24        | 12.192      | 3363          | 3375        | 3397         | rVB      | 200969         | 326607        | 52.07%          | 7.107%        |

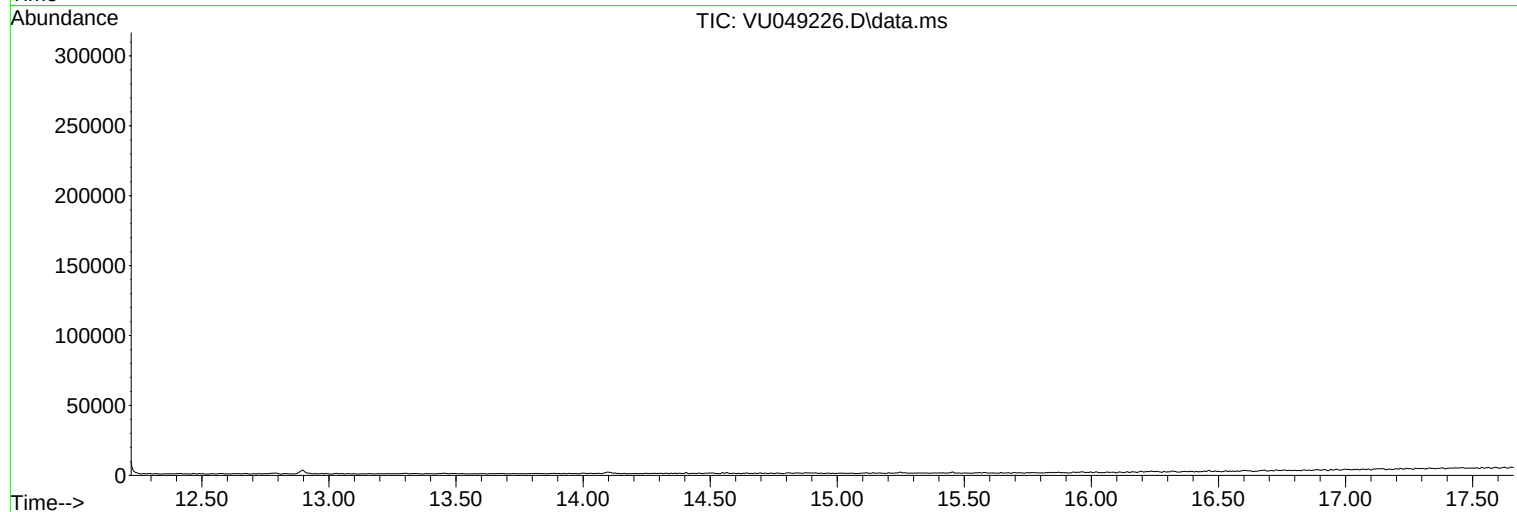
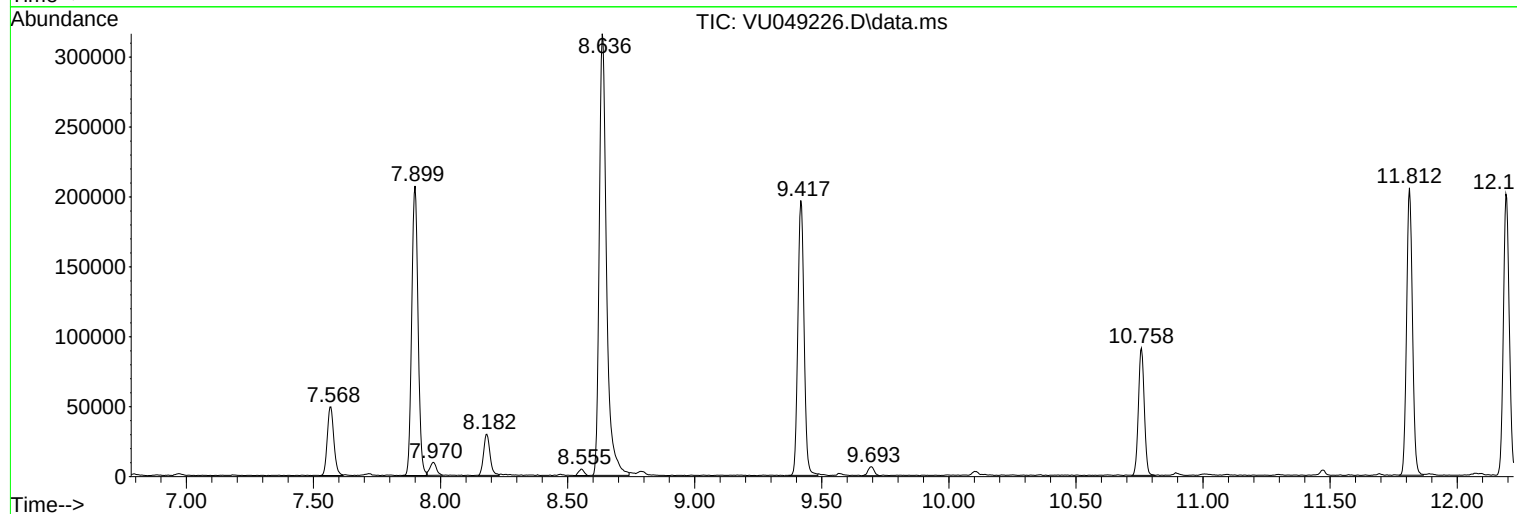
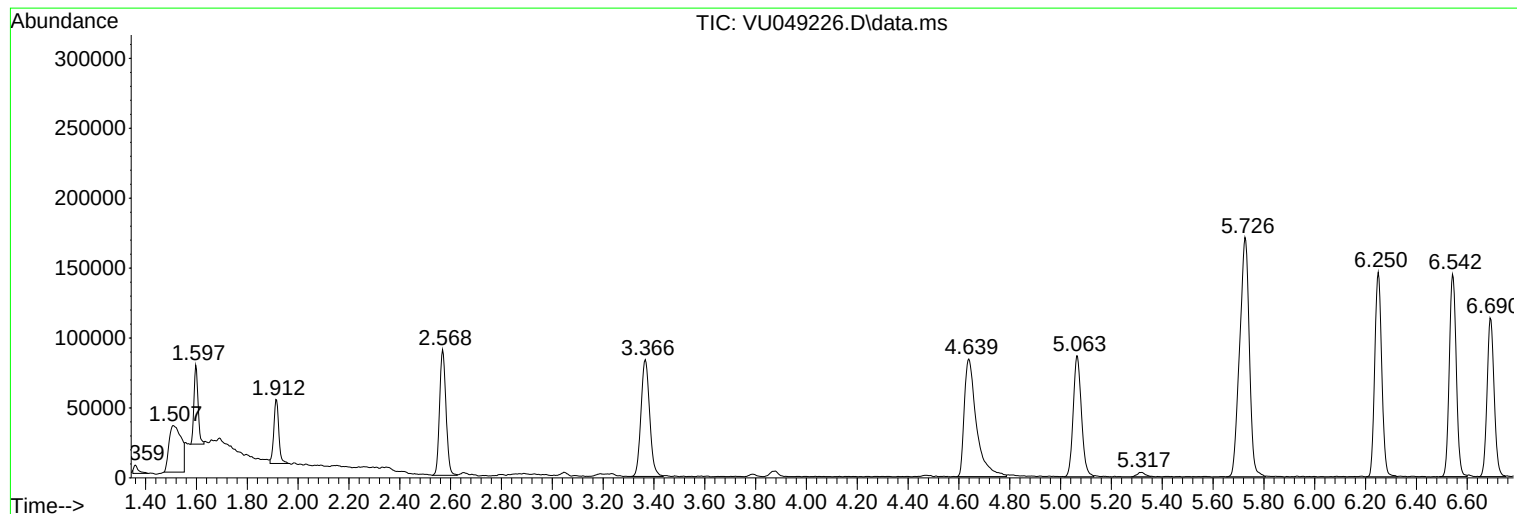
Sum of corrected areas: 4595252

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MSVOA\_U  
ClientSampleId :  
BGJ83

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR061422WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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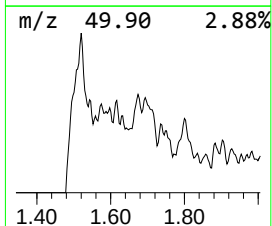
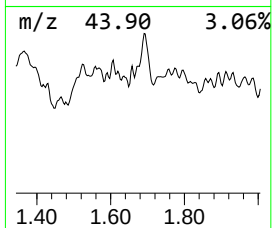
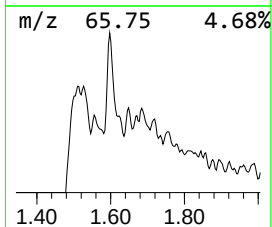
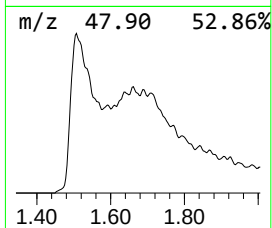
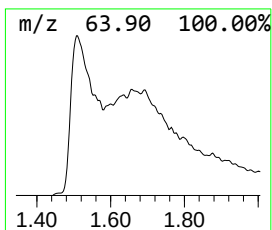
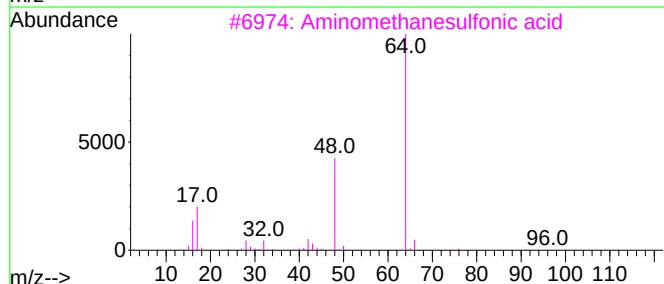
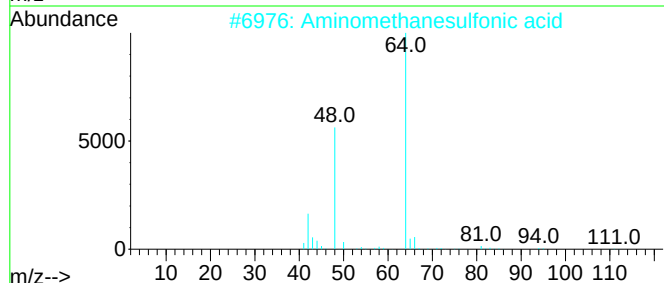
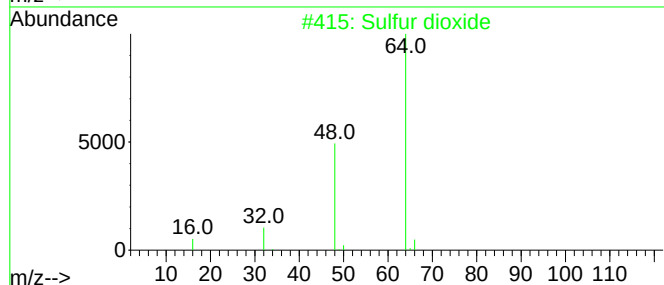
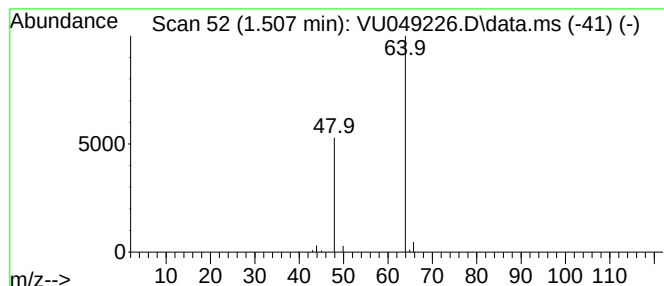
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR061422WMA.M  
Quant Title : TRACE VOA SFAM1.0

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.  |
|-------|-----------|--------|---------------------|-------|
| 1.507 | 2.02 ug/L | 113061 | 1,4-Difluorobenzene | 6.250 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 90   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 64   |
| 4    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 5    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.507 | 2.0     | ug/L  | 113061   | 1                     | 6.250 | 279292 | 5.0  |