

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051823\  
 Data File : VU054180.D  
 Acq On : 18 May 2023 21:18  
 Operator : JC/MD  
 Sample : 02844-14  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 27 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 GBX08

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\SFAMUTR051823WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054180.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         | 1.356       | 3             | 5           | 16           | rVB4     | 23553          | 22479         | 4.32%           | 0.496%        |
| 2         | 1.488       | 37            | 46          | 69           | rBV2     | 33442          | 108704        | 20.89%          | 2.399%        |
| 3         | 1.597       | 70            | 80          | 96           | rVB2     | 66704          | 111751        | 21.48%          | 2.466%        |
| 4         | 1.912       | 170           | 178         | 194          | rBV      | 45268          | 63454         | 12.20%          | 1.400%        |
| 5         | 2.565       | 367           | 381         | 393          | rBV      | 106800         | 175163        | 33.66%          | 3.865%        |
| 6         | 2.642       | 393           | 405         | 438          | rVB      | 77552          | 226662        | 43.56%          | 5.002%        |
| 7         | 3.851       | 772           | 781         | 808          | rVB5     | 8314           | 27368         | 5.26%           | 0.604%        |
| 8         | 4.629       | 1011          | 1023        | 1065         | rBV2     | 44072          | 146955        | 28.24%          | 3.243%        |
| 9         | 4.809       | 1071          | 1079        | 1097         | rVB3     | 7033           | 16205         | 3.11%           | 0.358%        |
| 10        | 5.057       | 1139          | 1156        | 1177         | rBV      | 86305          | 200643        | 38.56%          | 4.427%        |
| 11        | 5.719       | 1343          | 1362        | 1388         | rBV3     | 168737         | 433907        | 83.39%          | 9.575%        |
| 12        | 6.243       | 1512          | 1525        | 1544         | rBV      | 221642         | 430377        | 82.71%          | 9.497%        |
| 13        | 6.687       | 1647          | 1663        | 1685         | rBV      | 99277          | 197783        | 38.01%          | 4.364%        |
| 14        | 7.562       | 1924          | 1935        | 1955         | rBV      | 49738          | 88534         | 17.02%          | 1.954%        |
| 15        | 7.893       | 2025          | 2038        | 2054         | rBV      | 213890         | 372398        | 71.57%          | 8.217%        |
| 16        | 7.970       | 2054          | 2062        | 2072         | rVB3     | 6648           | 12016         | 2.31%           | 0.265%        |
| 17        | 8.176       | 2116          | 2126        | 2139         | rBV3     | 28591          | 50389         | 9.68%           | 1.112%        |
| 18        | 8.629       | 2253          | 2267        | 2303         | rBV2     | 175778         | 340076        | 65.36%          | 7.504%        |
| 19        | 8.928       | 2349          | 2360        | 2376         | rBV5     | 2875           | 6681          | 1.28%           | 0.147%        |
| 20        | 9.414       | 2498          | 2511        | 2530         | rBV      | 307720         | 520328        | 100.00%         | 11.482%       |
| 21        | 9.501       | 2532          | 2538        | 2547         | rVB5     | 4860           | 7551          | 1.45%           | 0.167%        |
| 22        | 10.751      | 2916          | 2927        | 2946         | rVB2     | 70390          | 115275        | 22.15%          | 2.544%        |
| 23        | 11.806      | 3243          | 3255        | 3273         | rBV      | 327739         | 515029        | 98.98%          | 11.365%       |
| 24        | 12.073      | 3325          | 3338        | 3355         | rBV7     | 4156           | 11731         | 2.25%           | 0.259%        |
| 25        | 12.189      | 3362          | 3374        | 3393         | rBV      | 188867         | 311272        | 59.82%          | 6.869%        |
| 26        | 12.883      | 3582          | 3590        | 3602         | rVB7     | 3963           | 6030          | 1.16%           | 0.133%        |
| 27        | 17.282      | 4951          | 4958        | 4968         | rBV4     | 8972           | 13075         | 2.51%           | 0.289%        |

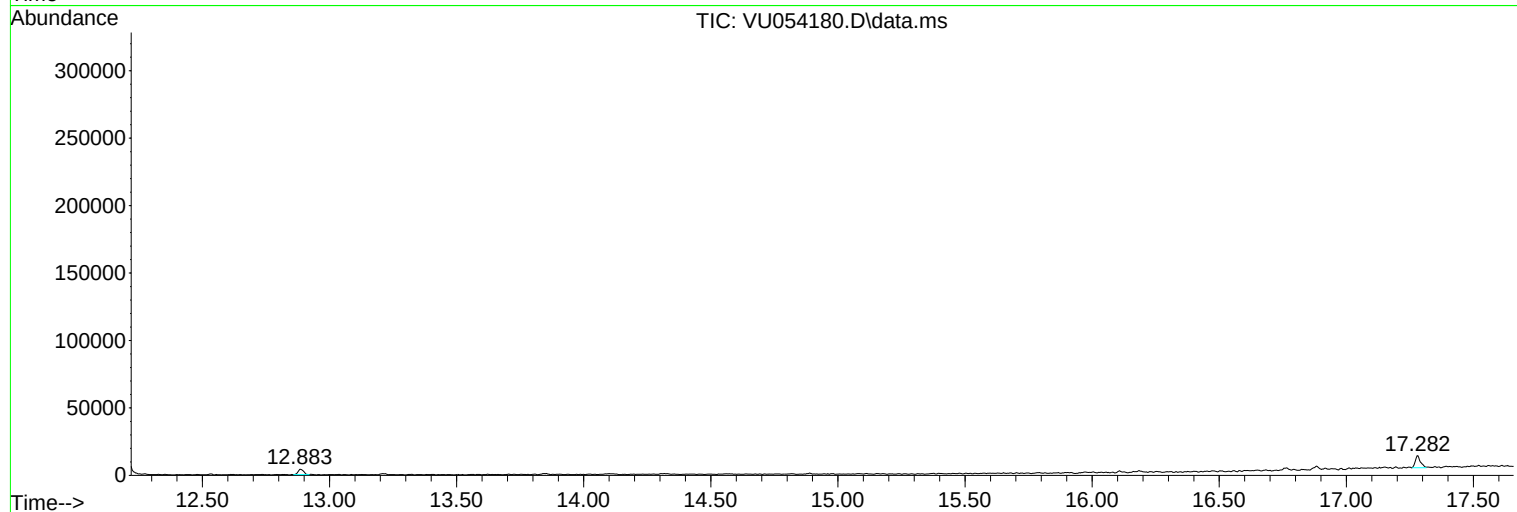
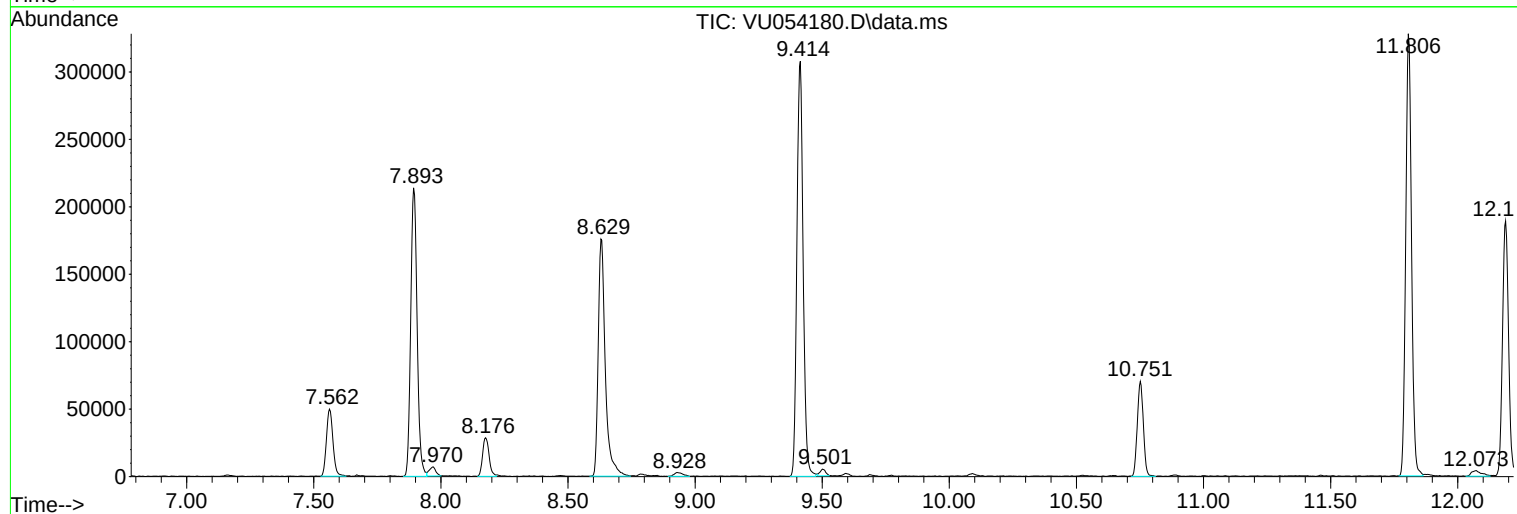
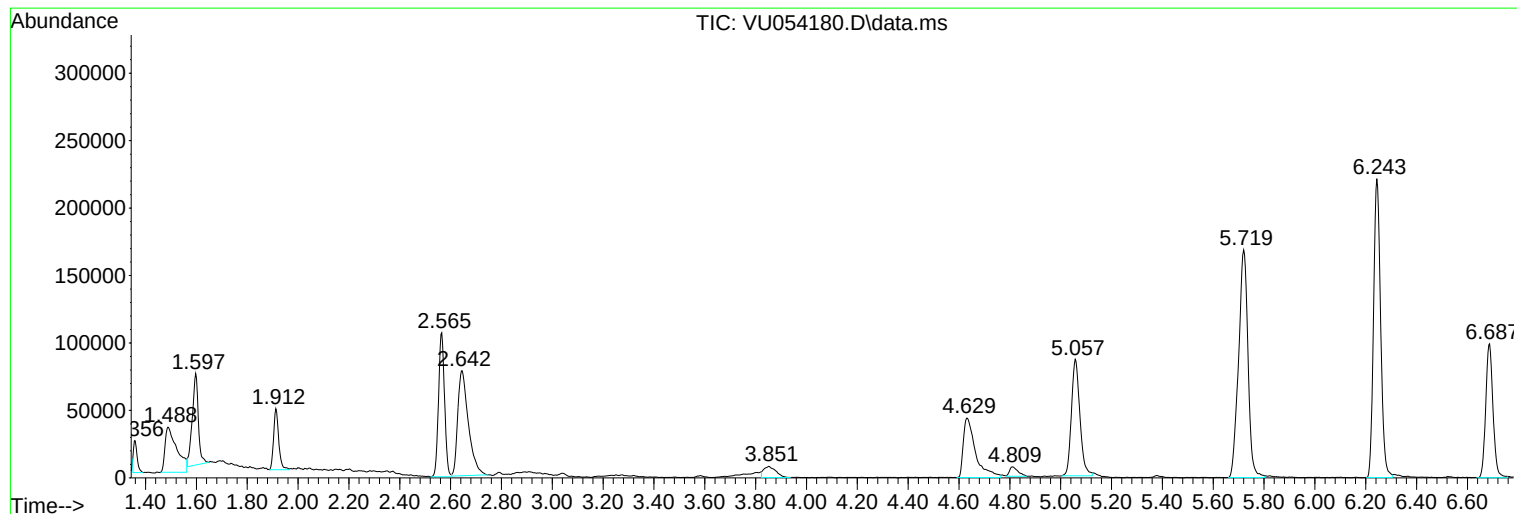
Sum of corrected areas: 4531836

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR051823WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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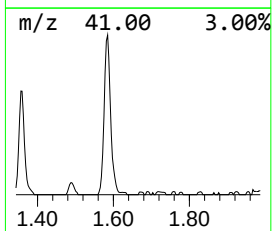
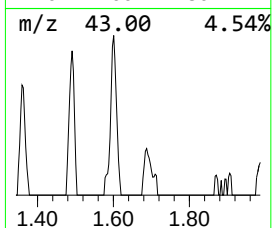
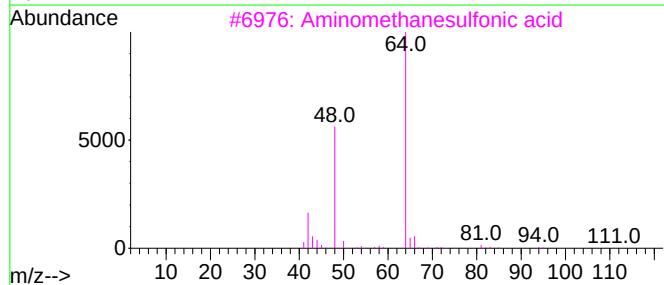
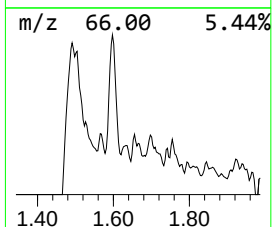
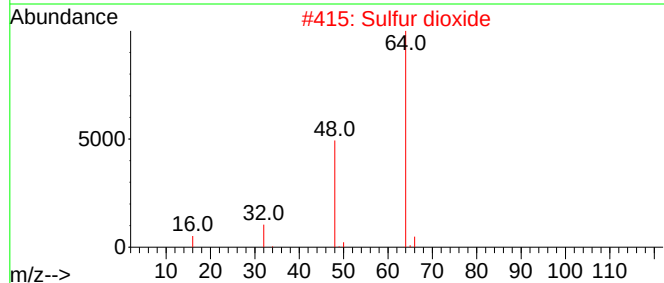
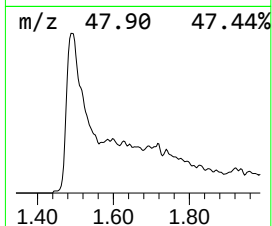
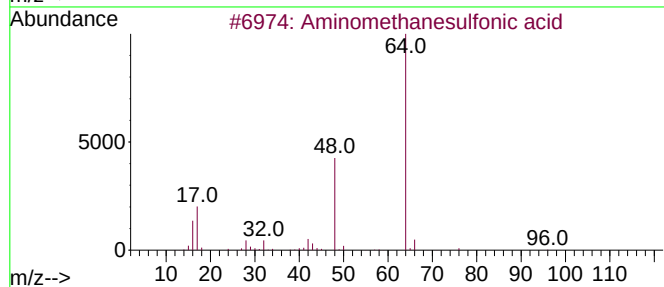
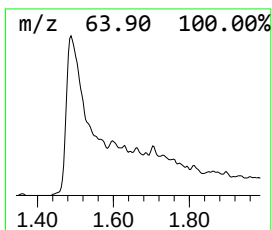
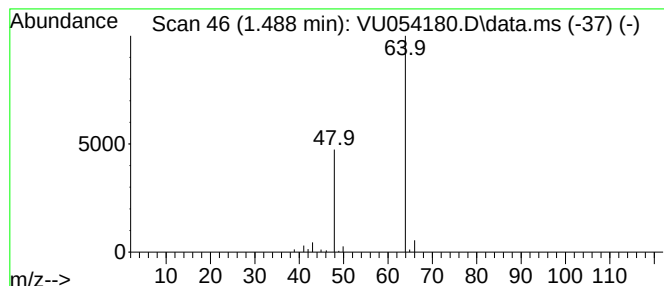
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR051823WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.488 | 1.26 ug/L | 108704 | 1,4-Difluorobenzene | 6.243 |

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



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Aminomethanesul... | 1.488 | 1.3     | ug/L  | 108704   | 1                     | 6.243 | 430377 | 5.0  |