

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121222\  
 Data File : VU052364.D  
 Acq On : 12 Dec 2022 19:41  
 Operator : JC/MD  
 Sample : N5961-07  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F5N46

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\SFAMUTR111822WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052364.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         | 1.469       | 31            | 40          | 73           | rBV      | 672822         | 1279969       | 100.00%         | 13.200%       |
| 2         | 1.601       | 75            | 81          | 90           | rVB      | 122142         | 146832        | 11.47%          | 1.514%        |
| 3         | 1.916       | 172           | 179         | 193          | rBV      | 105821         | 141995        | 11.09%          | 1.464%        |
| 4         | 2.568       | 370           | 382         | 400          | rBV      | 194633         | 317288        | 24.79%          | 3.272%        |
| 5         | 2.723       | 420           | 430         | 445          | rVB3     | 8098           | 15199         | 1.19%           | 0.157%        |
| 6         | 3.279       | 585           | 603         | 618          | rVB      | 4255           | 14806         | 1.16%           | 0.153%        |
| 7         | 4.633       | 1011          | 1024        | 1057         | rBV      | 154375         | 478092        | 37.35%          | 4.931%        |
| 8         | 5.060       | 1141          | 1157        | 1179         | rBV2     | 199277         | 444477        | 34.73%          | 4.584%        |
| 9         | 5.723       | 1341          | 1363        | 1397         | rBV2     | 374708         | 988922        | 77.26%          | 10.199%       |
| 10        | 6.247       | 1513          | 1526        | 1555         | rBV      | 297029         | 571228        | 44.63%          | 5.891%        |
| 11        | 6.687       | 1648          | 1663        | 1688         | rBV      | 236847         | 465122        | 36.34%          | 4.797%        |
| 12        | 7.562       | 1923          | 1935        | 1952         | rBV2     | 102153         | 177714        | 13.88%          | 1.833%        |
| 13        | 7.896       | 2025          | 2039        | 2054         | rBV      | 417825         | 730180        | 57.05%          | 7.530%        |
| 14        | 7.967       | 2054          | 2061        | 2076         | rVB2     | 26323          | 47865         | 3.74%           | 0.494%        |
| 15        | 8.176       | 2117          | 2126        | 2145         | rBV      | 63688          | 107776        | 8.42%           | 1.112%        |
| 16        | 8.632       | 2255          | 2268        | 2301         | rBV      | 622827         | 1197877       | 93.59%          | 12.354%       |
| 17        | 8.784       | 2309          | 2315        | 2327         | rVB5     | 8861           | 14451         | 1.13%           | 0.149%        |
| 18        | 9.414       | 2498          | 2511        | 2535         | rBV      | 453716         | 751332        | 58.70%          | 7.749%        |
| 19        | 9.690       | 2588          | 2597        | 2607         | rBV2     | 9753           | 16480         | 1.29%           | 0.170%        |
| 20        | 10.095      | 2711          | 2723        | 2739         | rBV8     | 6836           | 14237         | 1.11%           | 0.147%        |
| 21        | 10.751      | 2911          | 2927        | 2946         | rBV      | 212815         | 354250        | 27.68%          | 3.653%        |
| 22        | 11.809      | 3243          | 3256        | 3275         | rBV      | 404530         | 656171        | 51.26%          | 6.767%        |
| 23        | 12.057      | 3325          | 3333        | 3348         | rBV5     | 11061          | 22788         | 1.78%           | 0.235%        |
| 24        | 12.189      | 3361          | 3374        | 3395         | rBV      | 432530         | 700480        | 54.73%          | 7.224%        |
| 25        | 12.883      | 3579          | 3590        | 3599         | rBV5     | 15314          | 24462         | 1.91%           | 0.252%        |
| 26        | 16.764      | 4787          | 4797        | 4807         | rBV10    | 9865           | 16402         | 1.28%           | 0.169%        |

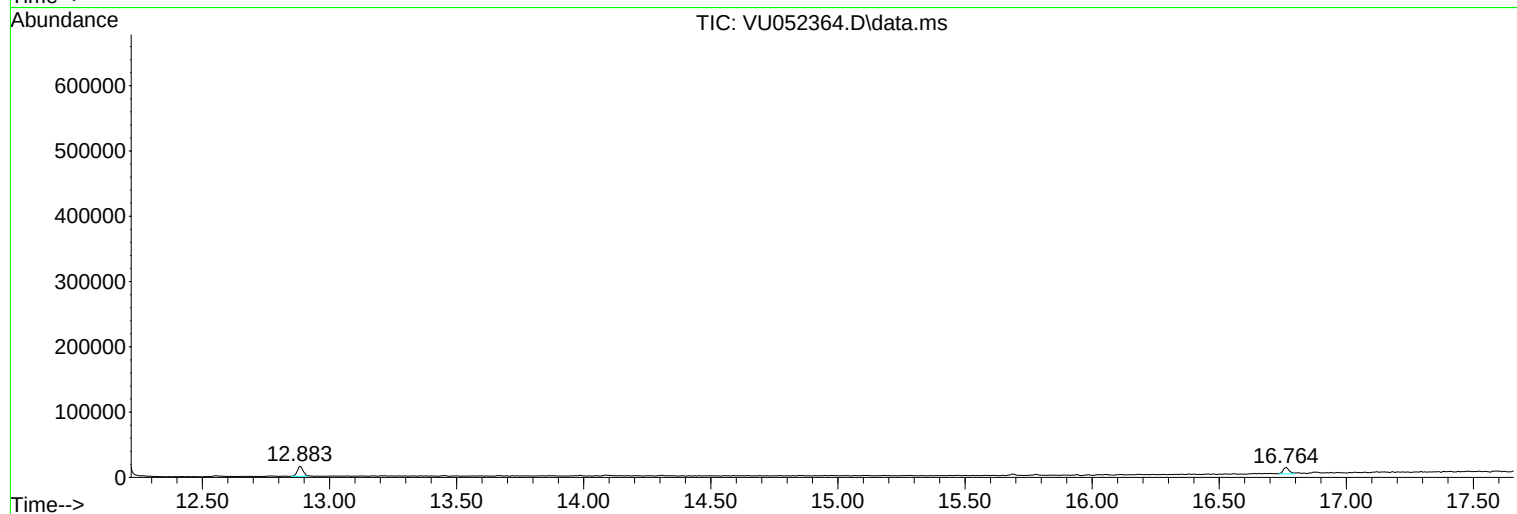
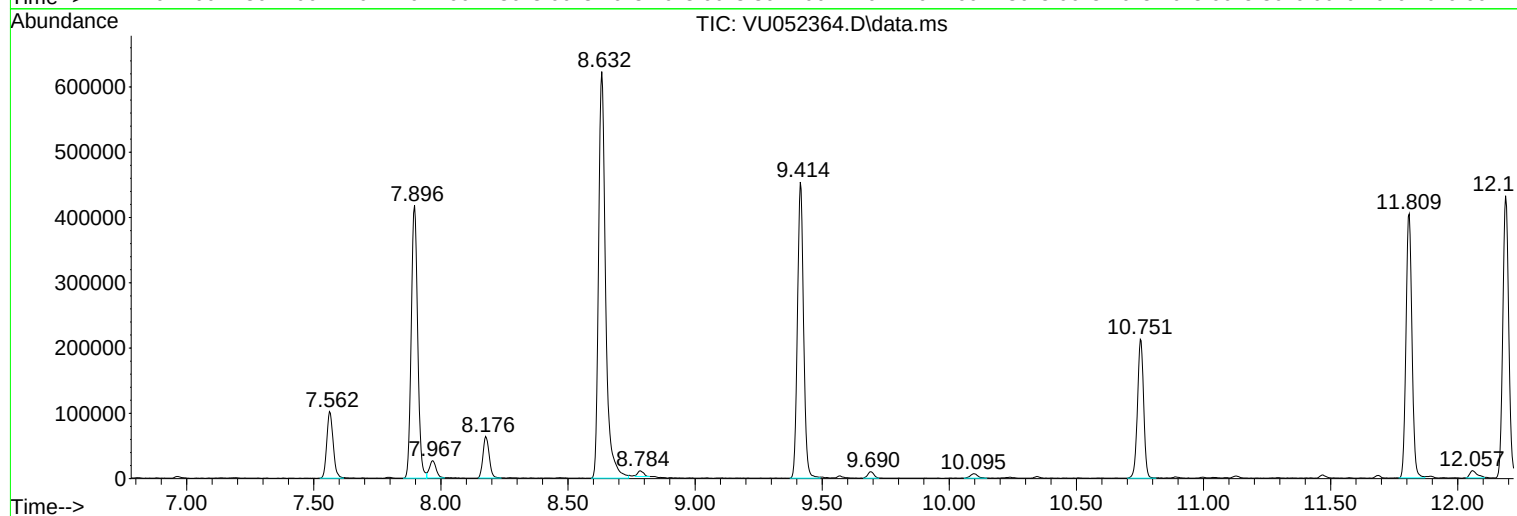
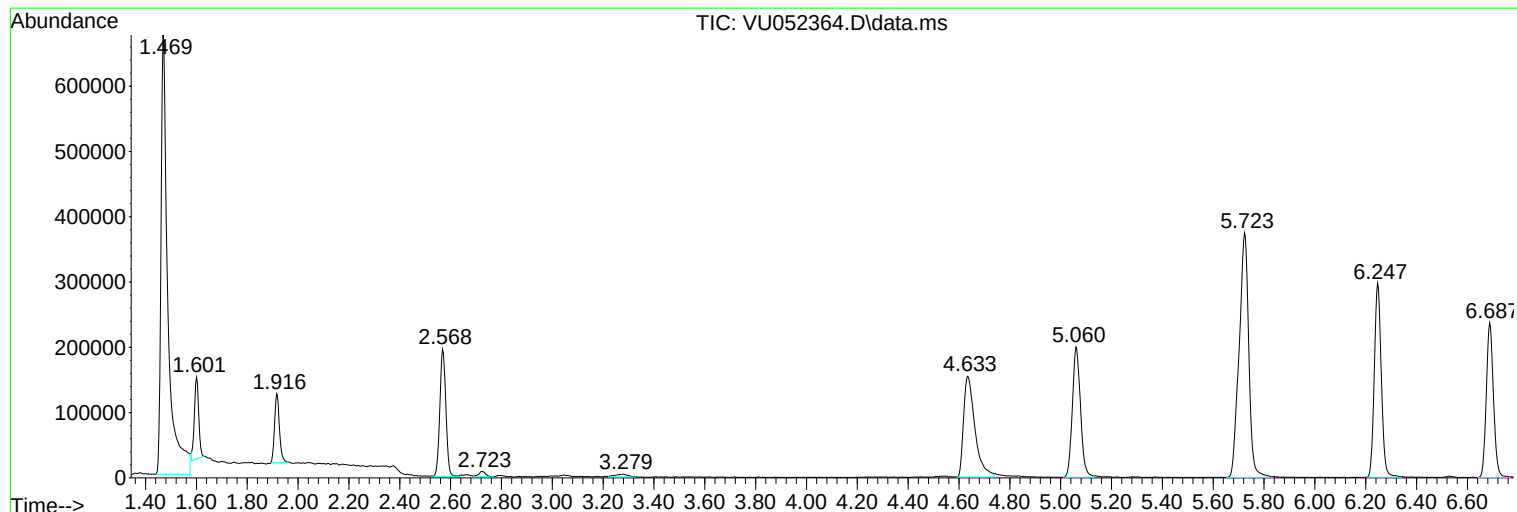
Sum of corrected areas: 9696395

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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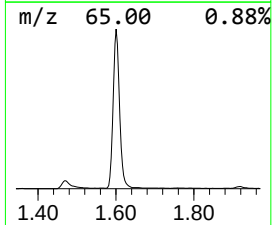
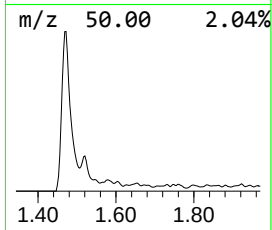
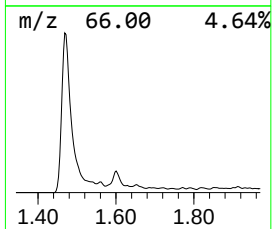
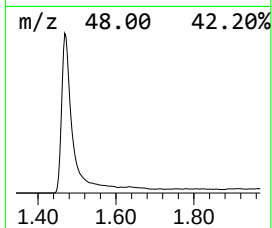
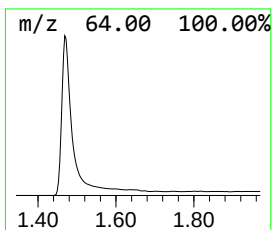
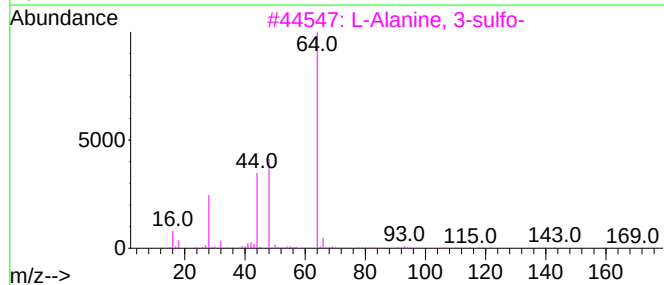
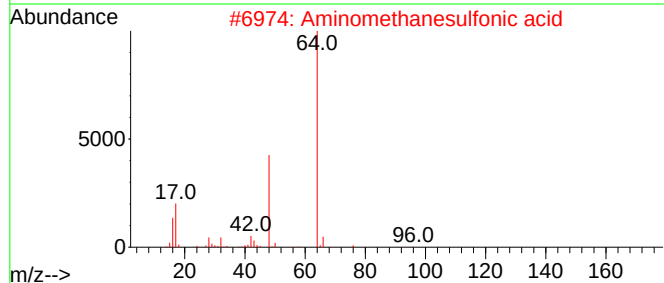
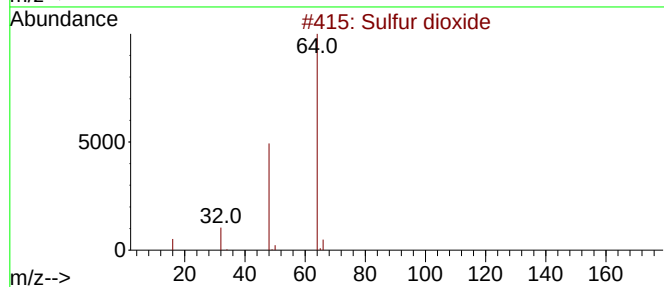
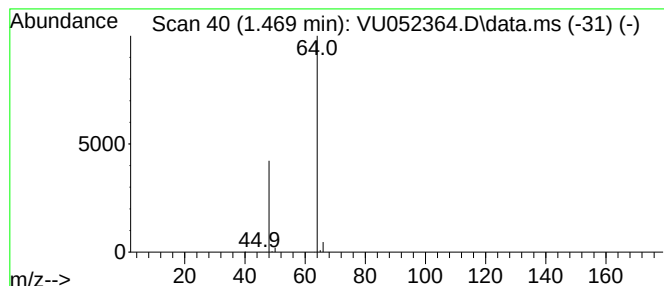
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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.  |
|-------|------------|---------|---------------------|-------|
| 1.469 | 11.20 ug/L | 1279970 | 1,4-Difluorobenzene | 6.247 |

| 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    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |
| 5    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.469 | 11.2    | ug/L  | 1279970  | 1                     | 6.247 | 571228 | 5.0  |