

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU103122\  
 Data File : VU051627.D  
 Acq On : 31 Oct 2022 22:08  
 Operator : JC/MD  
 Sample : VU1031WBL02  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 26 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK124

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\SFAMUTR102822WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051627.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          | 53           | rBV      | 155365         | 283676        | 26.76%          | 4.316%        |
| 2         | 1.597       | 74            | 80          | 87           | rBV      | 70251          | 79244         | 7.48%           | 1.206%        |
| 3         | 1.729       | 114           | 121         | 128          | rVB      | 68115          | 74531         | 7.03%           | 1.134%        |
| 4         | 1.912       | 170           | 178         | 196          | rVB      | 75919          | 107215        | 10.12%          | 1.631%        |
| 5         | 2.565       | 369           | 381         | 392          | rBV      | 102302         | 169170        | 15.96%          | 2.574%        |
| 6         | 2.623       | 392           | 399         | 420          | rVB      | 10566          | 20164         | 1.90%           | 0.307%        |
| 7         | 3.183       | 558           | 573         | 587          | rBV2     | 8786           | 18980         | 1.79%           | 0.289%        |
| 8         | 3.855       | 760           | 782         | 783          | rBV      | 11139          | 21597         | 2.04%           | 0.329%        |
| 9         | 4.617       | 1004          | 1019        | 1050         | rBV      | 191360         | 490317        | 46.26%          | 7.459%        |
| 10        | 5.063       | 1142          | 1158        | 1187         | rBV      | 157825         | 365219        | 34.46%          | 5.556%        |
| 11        | 5.723       | 1343          | 1363        | 1387         | rBV2     | 263019         | 736774        | 69.51%          | 11.209%       |
| 12        | 6.247       | 1513          | 1526        | 1552         | rBV      | 215028         | 418508        | 39.49%          | 6.367%        |
| 13        | 6.543       | 1603          | 1618        | 1634         | rVB7     | 10679          | 21040         | 1.99%           | 0.320%        |
| 14        | 6.690       | 1649          | 1664        | 1681         | rBV      | 195653         | 383263        | 36.16%          | 5.831%        |
| 15        | 7.565       | 1923          | 1936        | 1958         | rBV2     | 69957          | 129099        | 12.18%          | 1.964%        |
| 16        | 7.896       | 2026          | 2039        | 2054         | rBV      | 238959         | 419050        | 39.54%          | 6.375%        |
| 17        | 7.970       | 2054          | 2062        | 2074         | rVB      | 12344          | 23374         | 2.21%           | 0.356%        |
| 18        | 8.179       | 2116          | 2127        | 2145         | rBV2     | 43586          | 75757         | 7.15%           | 1.153%        |
| 19        | 8.632       | 2253          | 2268        | 2297         | rBV      | 575422         | 1059911       | 100.00%         | 16.125%       |
| 20        | 9.417       | 2498          | 2512        | 2532         | rBV      | 325255         | 554256        | 52.29%          | 8.432%        |
| 21        | 10.755      | 2916          | 2928        | 2945         | rBV      | 187066         | 302131        | 28.51%          | 4.596%        |
| 22        | 11.809      | 3245          | 3256        | 3279         | rBV      | 262154         | 432630        | 40.82%          | 6.582%        |
| 23        | 12.192      | 3361          | 3375        | 3396         | rBV      | 233923         | 387179        | 36.53%          | 5.890%        |

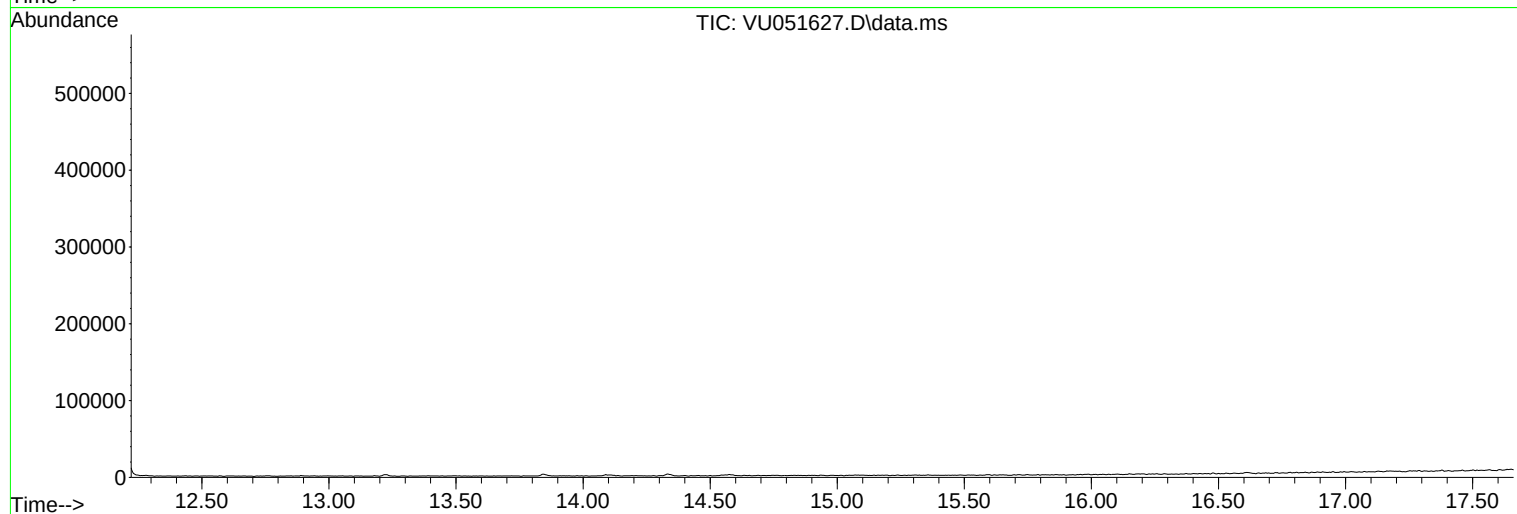
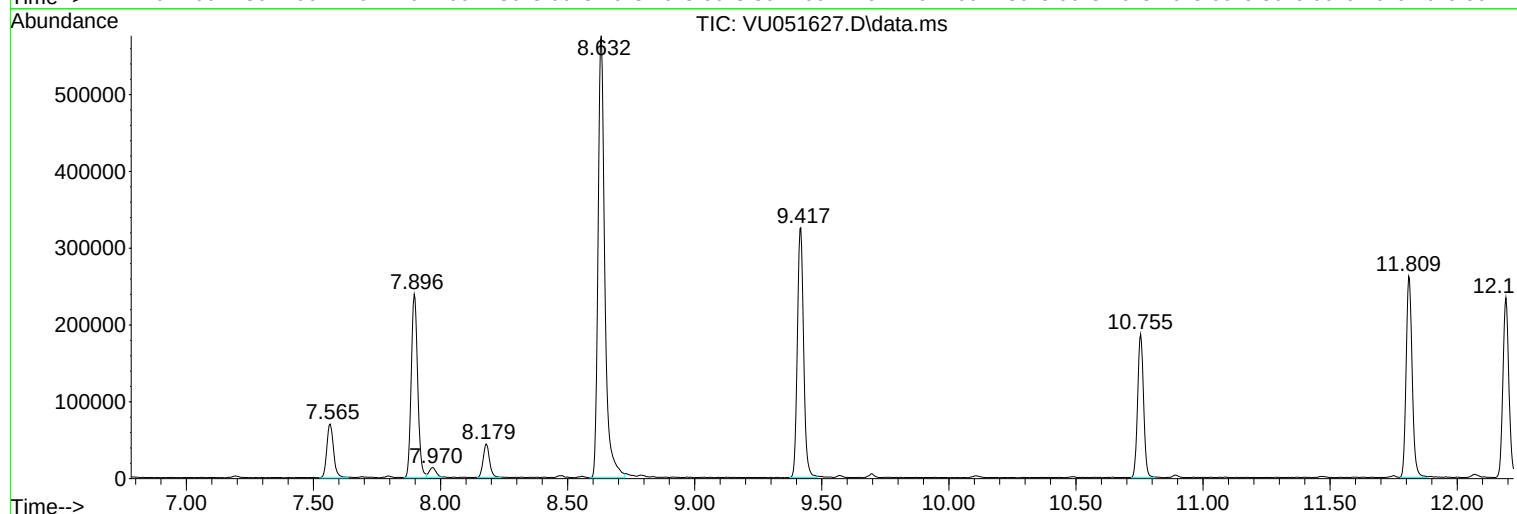
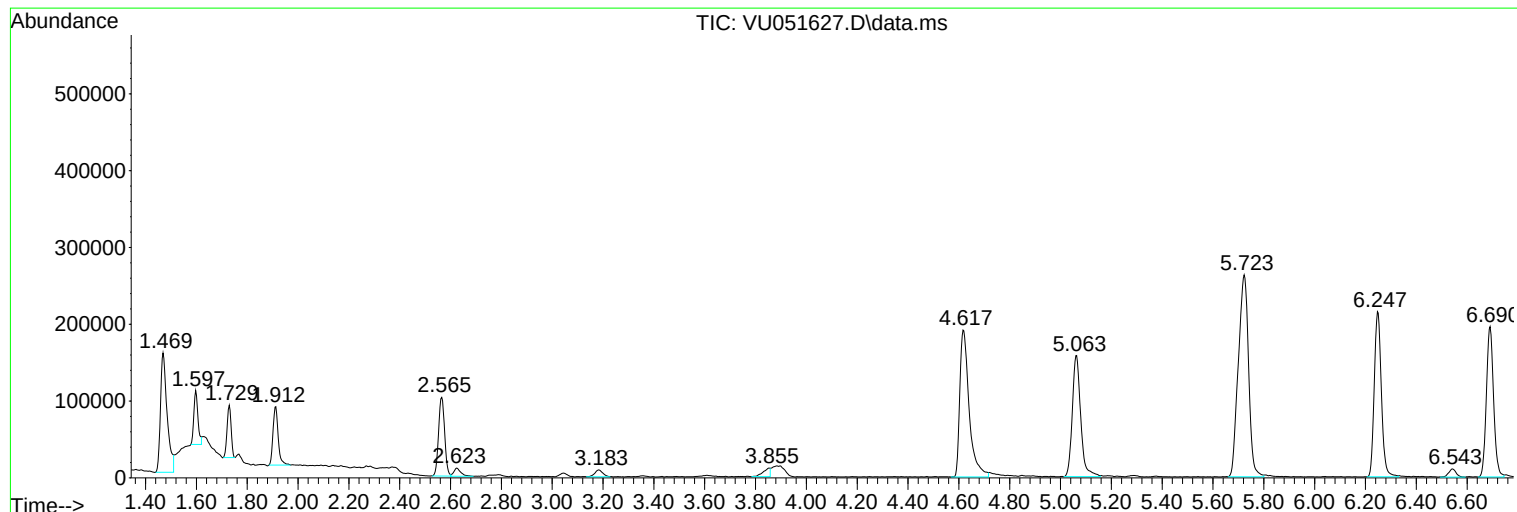
Sum of corrected areas: 6573085

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Instrument :  
MSVOA\_U  
ClientSampleId :  
VBLK124

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR102822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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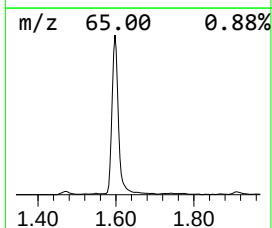
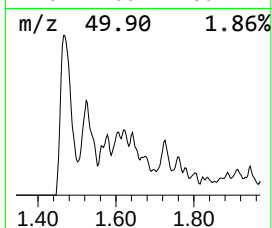
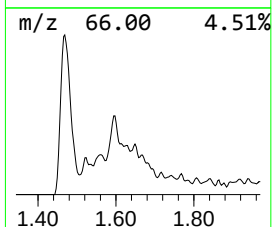
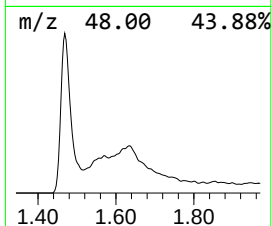
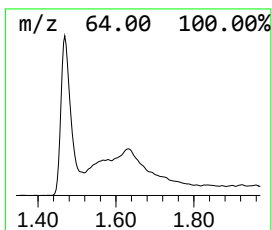
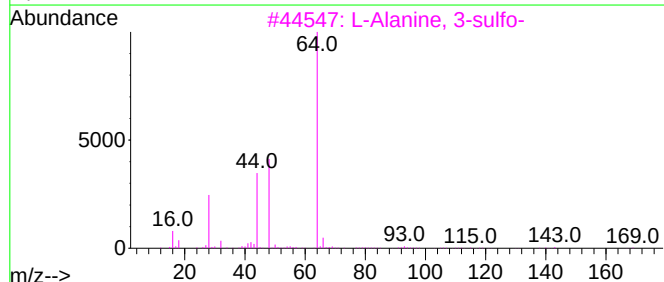
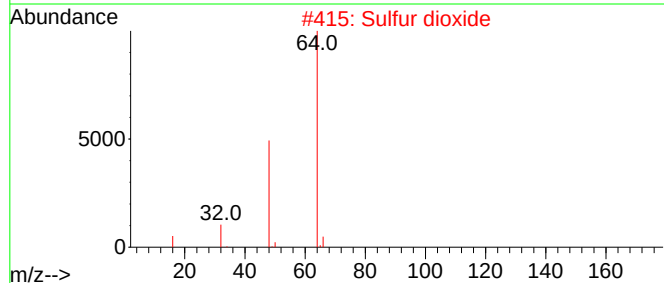
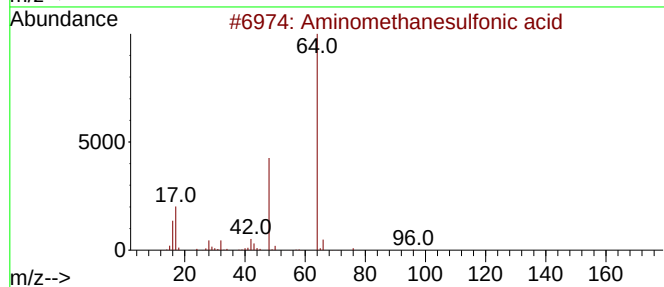
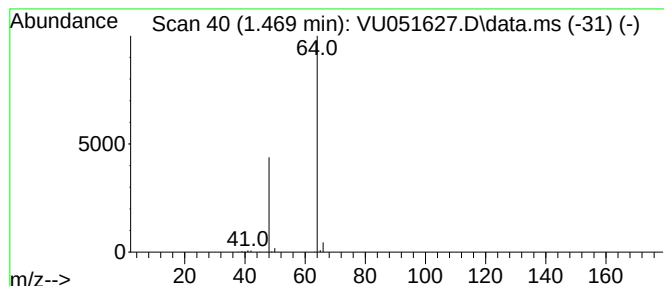
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR102822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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.  |
|-------|-----------|--------|---------------------|-------|
| 1.469 | 3.39 ug/L | 283676 | 1,4-Difluorobenzene | 6.247 |

| 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    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |
| 5    |    |   | Ethyl Chloride            | 64  | C2H5Cl   | 000075-00-3 | 3    |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Aminomethanesul... | 1.469 | 3.4     | ug/L  | 283676   | 1                     | 6.247 | 418508 | 5.0  |