

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011725\  
 Data File : VU062865.D  
 Acq On : 17 Jan 2025 12:34  
 Operator : MD/SY  
 Sample : Q1072-13  
 Misc : 25mL/MSVOA\_U/WATER  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 GCQ95

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\SFAMUTR010225WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU062865.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         | 1.461       | 44            | 53          | 72           | rBV      | 38642          | 66024         | 17.11%          | 1.961%        |
| 2         | 1.596       | 87            | 95          | 107          | rVB      | 36822          | 41945         | 10.87%          | 1.246%        |
| 3         | 1.901       | 182           | 190         | 209          | rVB      | 30646          | 39987         | 10.36%          | 1.188%        |
| 4         | 2.557       | 380           | 394         | 403          | rBV      | 68035          | 112869        | 29.24%          | 3.353%        |
| 5         | 2.612       | 403           | 411         | 437          | rVB      | 78131          | 134177        | 34.76%          | 3.986%        |
| 6         | 2.740       | 437           | 451         | 476          | rBV      | 197846         | 385974        | 100.00%         | 11.465%       |
| 7         | 3.171       | 571           | 585         | 600          | rBV2     | 7371           | 16352         | 4.24%           | 0.486%        |
| 8         | 3.853       | 782           | 797         | 818          | rBV2     | 37493          | 91336         | 23.66%          | 2.713%        |
| 9         | 4.605       | 1021          | 1031        | 1041         | rBV      | 44427          | 100430        | 26.02%          | 2.983%        |
| 10        | 4.985       | 1139          | 1149        | 1154         | rBV5     | 2103           | 3921          | 1.02%           | 0.116%        |
| 11        | 5.049       | 1154          | 1169        | 1191         | rVB      | 68964          | 156980        | 40.67%          | 4.663%        |
| 12        | 5.711       | 1356          | 1375        | 1401         | rBV3     | 122364         | 324348        | 84.03%          | 9.635%        |
| 13        | 6.238       | 1527          | 1539        | 1555         | rBV      | 110603         | 213322        | 55.27%          | 6.337%        |
| 14        | 6.679       | 1664          | 1676        | 1697         | rBV3     | 74794          | 145802        | 37.78%          | 4.331%        |
| 15        | 7.557       | 1938          | 1949        | 1965         | rBV2     | 40793          | 72497         | 18.78%          | 2.154%        |
| 16        | 7.888       | 2040          | 2052        | 2073         | rBV      | 153677         | 271021        | 70.22%          | 8.051%        |
| 17        | 8.171       | 2131          | 2140        | 2164         | rVB      | 25610          | 44760         | 11.60%          | 1.330%        |
| 18        | 8.621       | 2270          | 2280        | 2311         | rBV      | 146170         | 286473        | 74.22%          | 8.510%        |
| 19        | 9.409       | 2513          | 2525        | 2550         | rBV      | 154482         | 264113        | 68.43%          | 7.845%        |
| 20        | 10.746      | 2929          | 2941        | 2957         | rBV      | 61986          | 101457        | 26.29%          | 3.014%        |
| 21        | 11.804      | 3259          | 3270        | 3293         | rBV      | 147287         | 245665        | 63.65%          | 7.297%        |
| 22        | 12.184      | 3376          | 3388        | 3406         | rBV      | 145754         | 247012        | 64.00%          | 7.337%        |

Sum of corrected areas: 3366465

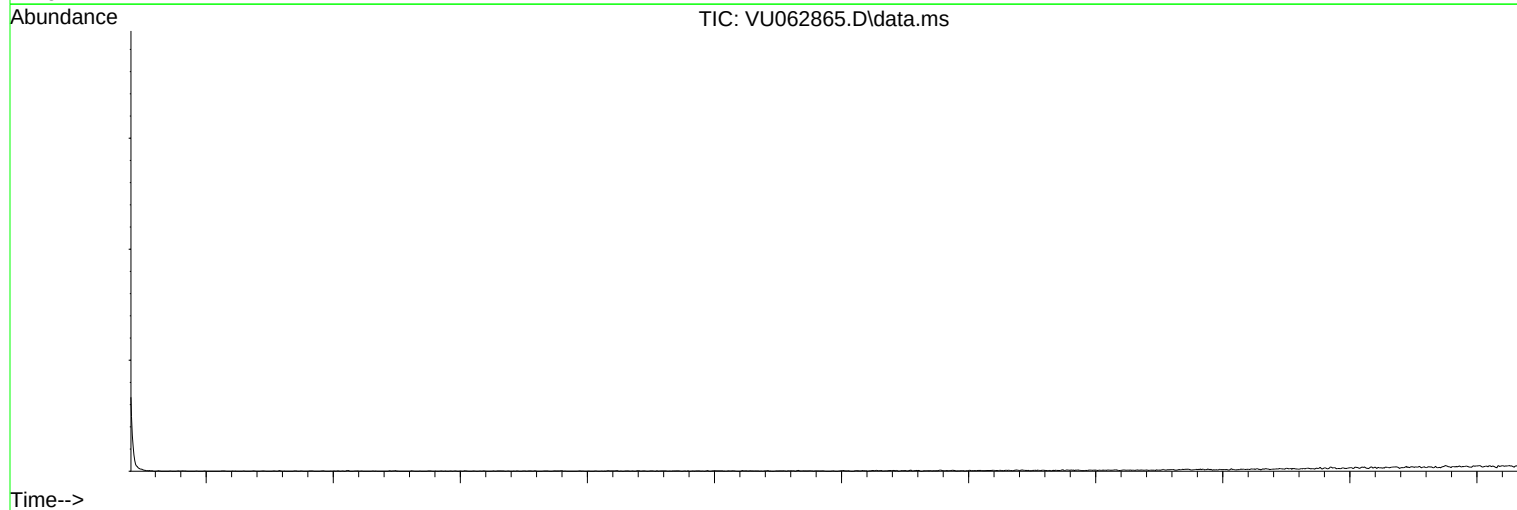
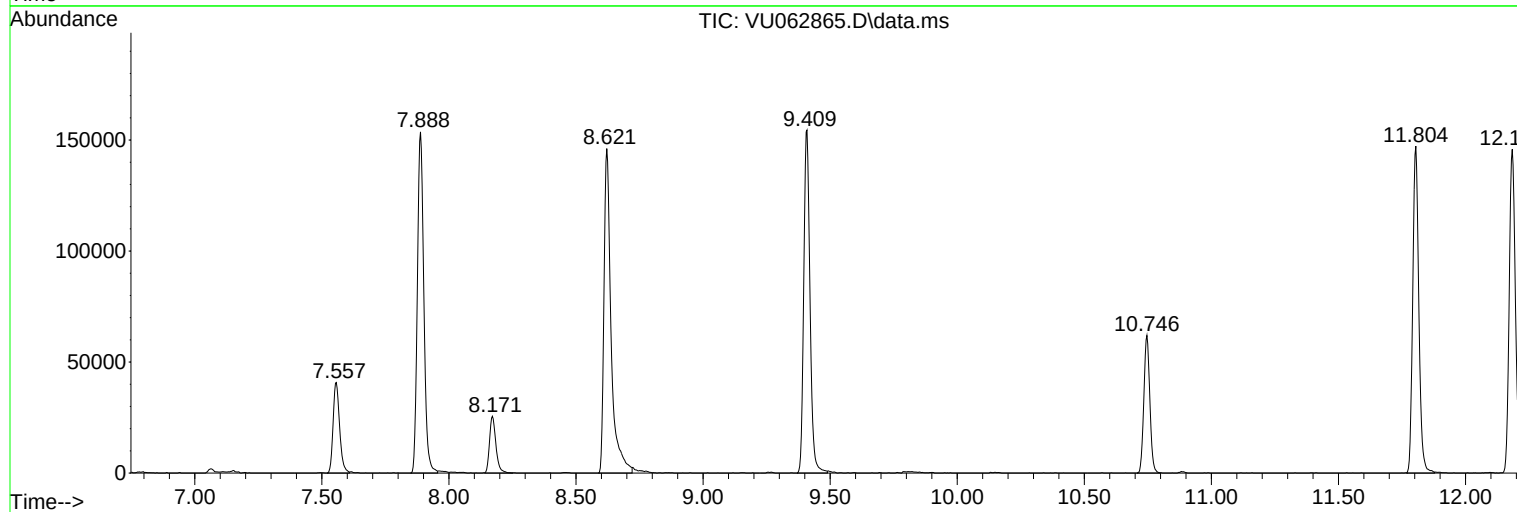
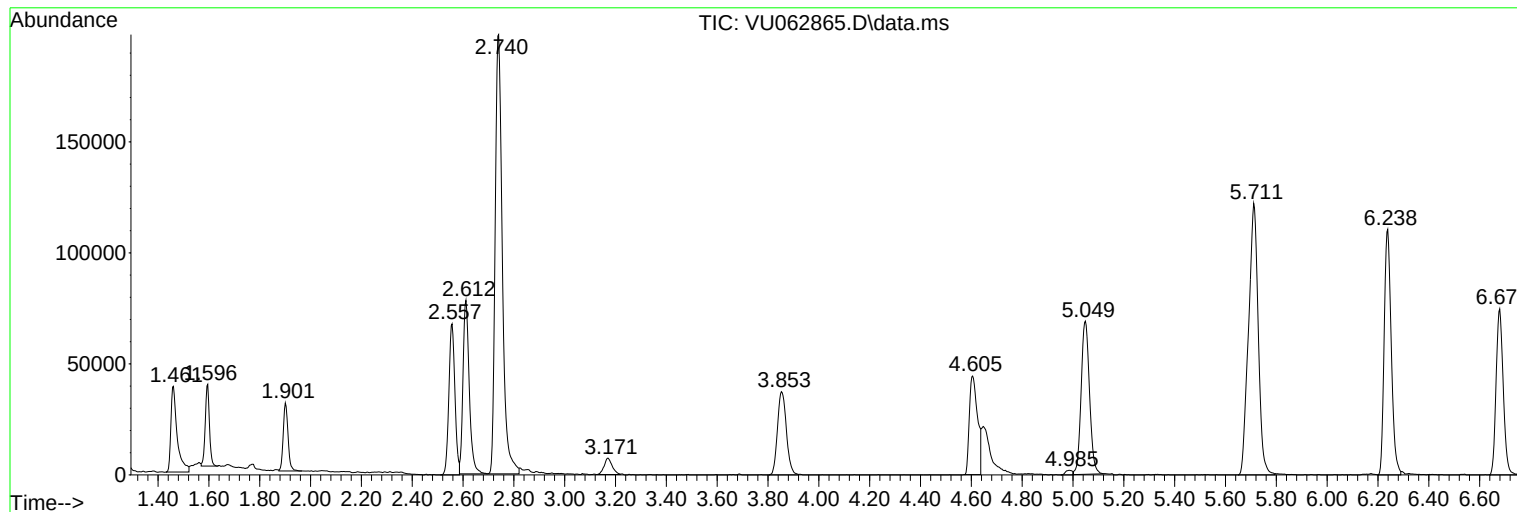
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ClientSampleId :  
GCQ95

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR010225WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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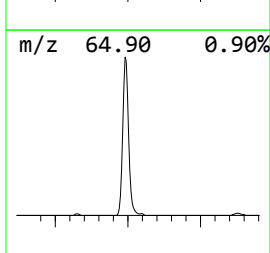
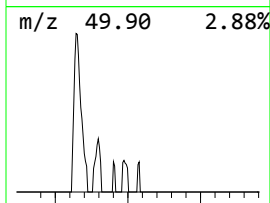
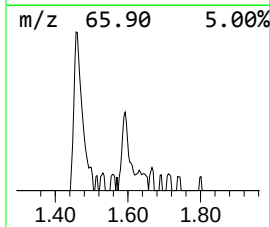
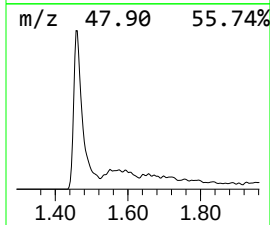
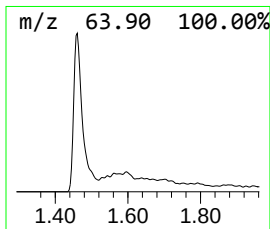
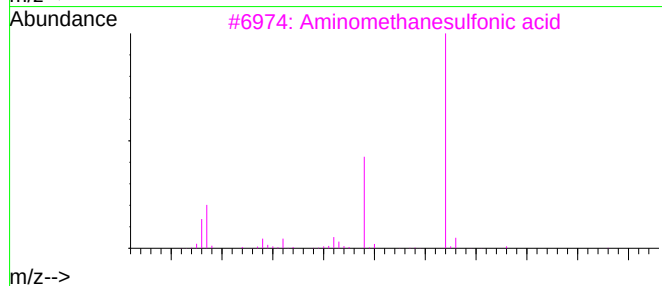
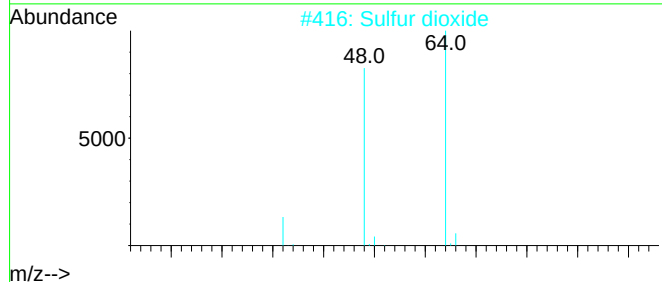
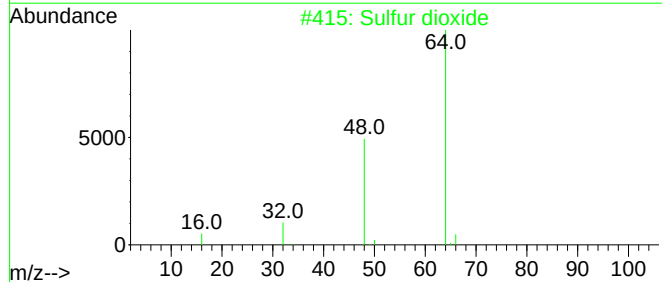
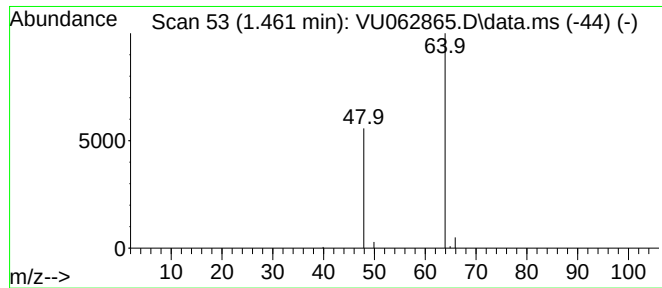
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR010225WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 Sulfur dioxide Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.461 | 1.55 ug/L | 66024 | 1,4-Difluorobenzene | 6.238 |

| Hit# of 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|-----------|---------------------------|-----|----------|-------------|------|
| 1         | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 90   |
| 2         | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 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 | # | RT    | Resp   | Conc |
|------------------|-------|---------|-------|----------|---|-------|--------|------|
| Sulfur dioxide   | 1.461 | 1.6     | ug/L  | 66024    | 1 | 6.238 | 213322 | 5.0  |