

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121222\  
 Data File : VU052362.D  
 Acq On : 12 Dec 2022 18:54  
 Operator : JC/MD  
 Sample : N5961-05  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F5N39

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: VU052362.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         | 1.478       | 33            | 43          | 74           | rBV      | 518214         | 1617288       | 100.00%         | 15.719%       |
| 2         | 1.600       | 75            | 81          | 96           | rVB      | 140689         | 208166        | 12.87%          | 2.023%        |
| 3         | 1.916       | 172           | 179         | 197          | rVB      | 105381         | 146681        | 9.07%           | 1.426%        |
| 4         | 2.568       | 370           | 382         | 396          | rBV      | 200342         | 324304        | 20.05%          | 3.152%        |
| 5         | 2.793       | 443           | 452         | 465          | rVB      | 19244          | 34008         | 2.10%           | 0.331%        |
| 6         | 4.655       | 1015          | 1031        | 1094         | rBV      | 92919          | 515477        | 31.87%          | 5.010%        |
| 7         | 5.063       | 1141          | 1158        | 1203         | rBV2     | 219035         | 612376        | 37.86%          | 5.952%        |
| 8         | 5.722       | 1342          | 1363        | 1383         | rBV2     | 372363         | 964012        | 59.61%          | 9.370%        |
| 9         | 6.247       | 1508          | 1526        | 1546         | rBV2     | 309598         | 597854        | 36.97%          | 5.811%        |
| 10        | 6.687       | 1647          | 1663        | 1692         | rBV      | 234059         | 464278        | 28.71%          | 4.513%        |
| 11        | 7.565       | 1924          | 1936        | 1952         | rBV      | 97098          | 176932        | 10.94%          | 1.720%        |
| 12        | 7.896       | 2024          | 2039        | 2062         | rBV      | 416370         | 726382        | 44.91%          | 7.060%        |
| 13        | 8.179       | 2115          | 2127        | 2143         | rBV      | 61687          | 108425        | 6.70%           | 1.054%        |
| 14        | 8.636       | 2252          | 2269        | 2307         | rBV      | 598725         | 1226795       | 75.86%          | 11.924%       |
| 15        | 9.414       | 2495          | 2511        | 2538         | rBV      | 450101         | 754122        | 46.63%          | 7.330%        |
| 16        | 10.751      | 2907          | 2927        | 2944         | rBV      | 213403         | 359073        | 22.20%          | 3.490%        |
| 17        | 11.809      | 3242          | 3256        | 3280         | rBV      | 416794         | 665153        | 41.13%          | 6.465%        |
| 18        | 12.188      | 3360          | 3374        | 3390         | rBV      | 424184         | 682437        | 42.20%          | 6.633%        |
| 19        | 16.764      | 4785          | 4797        | 4809         | rBV3     | 48165          | 82899         | 5.13%           | 0.806%        |
| 20        | 16.880      | 4826          | 4833        | 4844         | rVB3     | 14805          | 21850         | 1.35%           | 0.212%        |

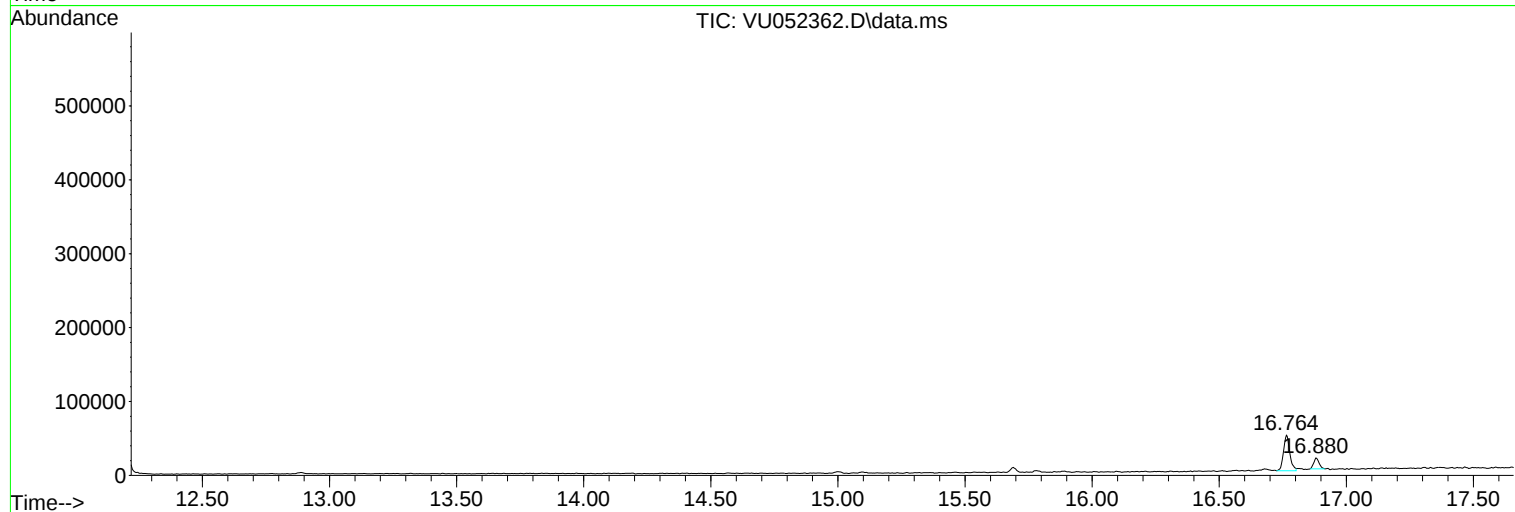
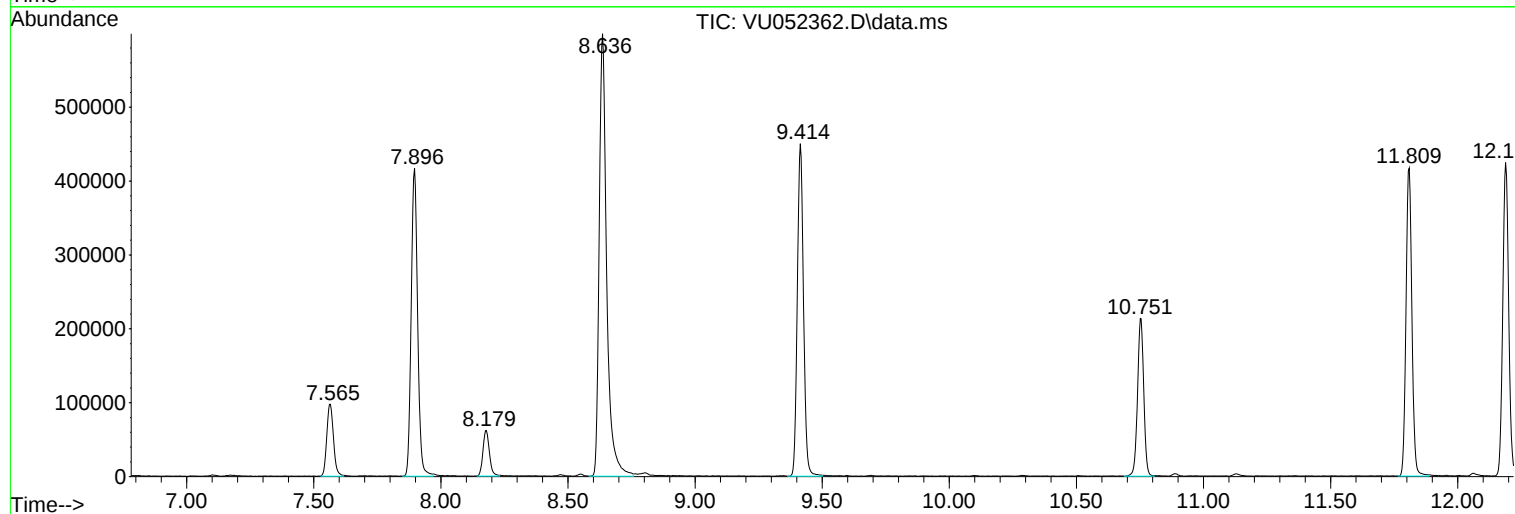
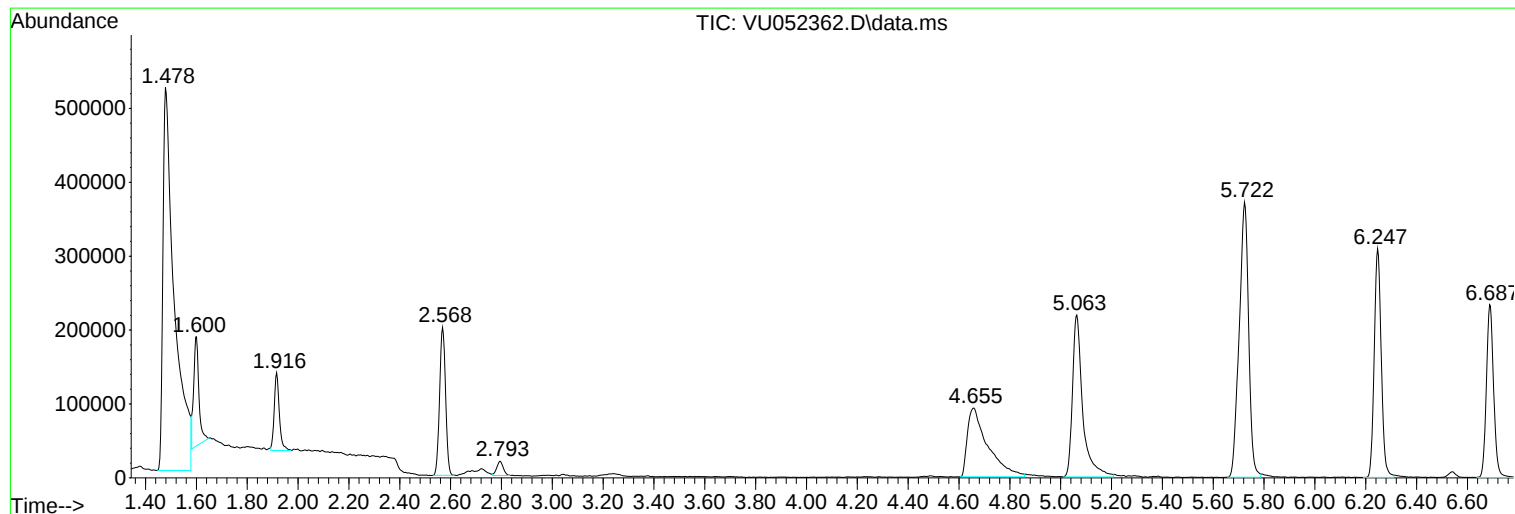
Sum of corrected areas: 10288512

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Instrument :  
MSVOA\_U  
ClientSampleId :  
F5N39

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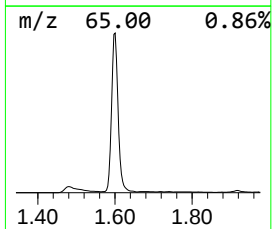
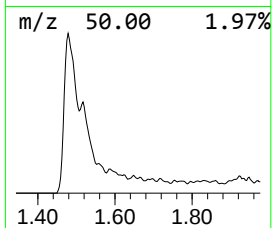
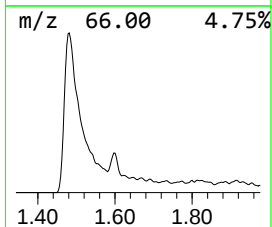
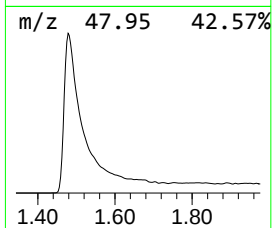
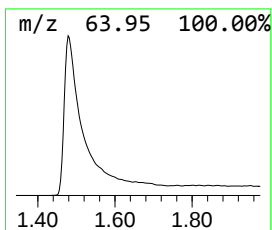
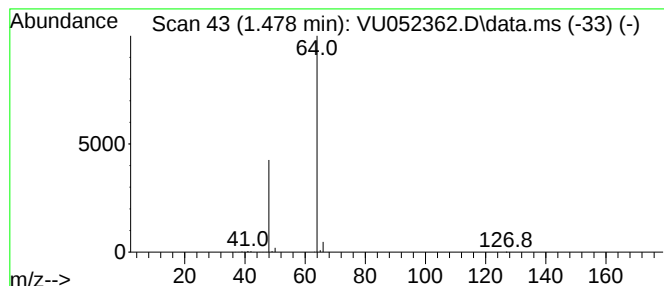
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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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.  |
|-------|------------|---------|---------------------|-------|
| 1.478 | 13.53 ug/L | 1617290 | 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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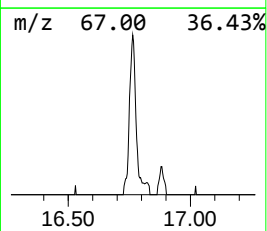
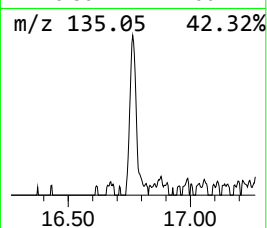
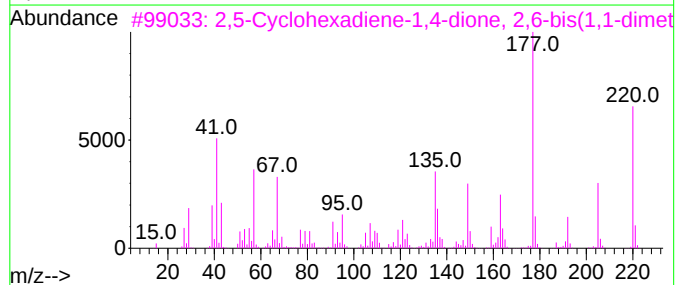
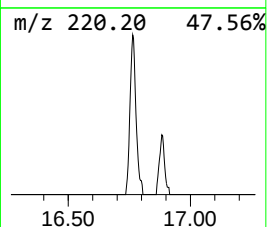
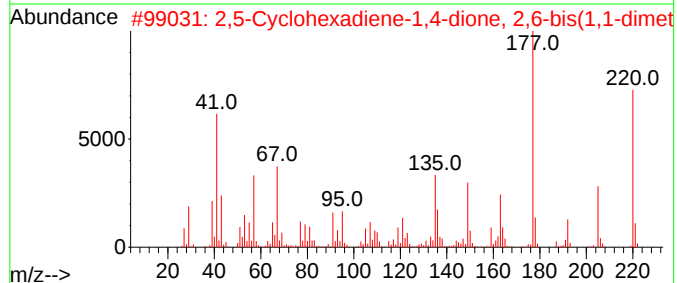
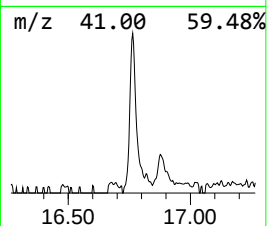
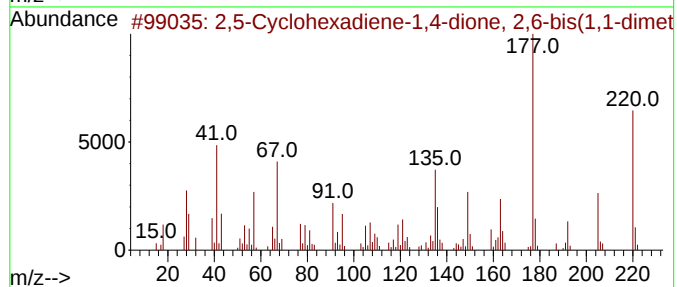
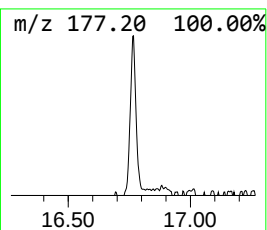
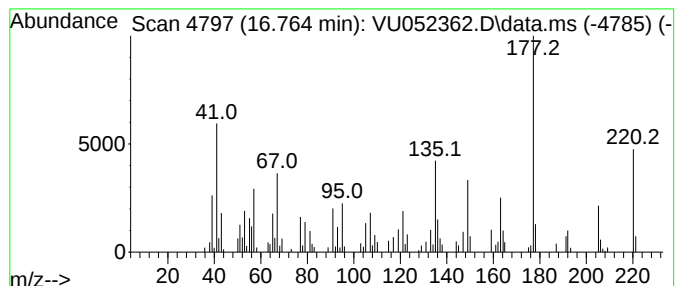
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Peak Number 3 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 16.764 | 0.62 ug/L | 82899 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2  | 96      |      |      |
| 2    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2  | 96      |      |      |
| 3    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2  | 96      |      |      |
| 4    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2  | 92      |      |      |
| 5    | 2H-1-benzopyran-6-ol, 3,4-dihydr... | 220 | C14H2002     | 1000396-25-4 | 53      |      |      |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Sulfur dioxide     | 1.478  | 13.5    | ug/L  | 1617290  | 1                     | 6.247  | 597854 | 5.0  |
| 2,5-Cyclohexadi... | 16.764 | 0.6     | ug/L  | 82899    | 3                     | 11.809 | 665153 | 5.0  |