

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051823\  
 Data File : VU054177.D  
 Acq On : 18 May 2023 20:05  
 Operator : JC/MD  
 Sample : 02844-11  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 GBX05

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: VU054177.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         | 1.359       | 3             | 6           | 17           | rVB2     | 41539          | 39606         | 3.55%           | 0.755%        |
| 2         | 1.485       | 37            | 45          | 56           | rBV      | 39764          | 98466         | 8.84%           | 1.877%        |
| 3         | 1.597       | 74            | 80          | 95           | rVB      | 62219          | 81921         | 7.35%           | 1.562%        |
| 4         | 1.912       | 171           | 178         | 191          | rVB      | 44253          | 63529         | 5.70%           | 1.211%        |
| 5         | 2.565       | 369           | 381         | 394          | rBV      | 98027          | 161314        | 14.48%          | 3.075%        |
| 6         | 2.642       | 394           | 405         | 434          | rVB2     | 18404          | 53687         | 4.82%           | 1.023%        |
| 7         | 2.871       | 437           | 476         | 553          | rBV2     | 115387         | 1114153       | 100.00%         | 21.238%       |
| 8         | 4.629       | 1011          | 1023        | 1041         | rBV      | 44554          | 124571        | 11.18%          | 2.375%        |
| 9         | 4.803       | 1067          | 1077        | 1106         | rVB3     | 32876          | 78975         | 7.09%           | 1.505%        |
| 10        | 5.057       | 1138          | 1156        | 1186         | rVB      | 83679          | 199281        | 17.89%          | 3.799%        |
| 11        | 5.719       | 1340          | 1362        | 1381         | rBV2     | 163874         | 418882        | 37.60%          | 7.985%        |
| 12        | 6.243       | 1512          | 1525        | 1552         | rBV      | 202644         | 389891        | 34.99%          | 7.432%        |
| 13        | 6.687       | 1649          | 1663        | 1680         | rBV      | 98205          | 192651        | 17.29%          | 3.672%        |
| 14        | 7.562       | 1920          | 1935        | 1950         | rBV2     | 49997          | 87166         | 7.82%           | 1.662%        |
| 15        | 7.893       | 2026          | 2038        | 2057         | rBV      | 205647         | 362661        | 32.55%          | 6.913%        |
| 16        | 8.176       | 2115          | 2126        | 2146         | rBV      | 29091          | 49953         | 4.48%           | 0.952%        |
| 17        | 8.629       | 2256          | 2267        | 2308         | rBV2     | 173027         | 339874        | 30.51%          | 6.479%        |
| 18        | 8.931       | 2347          | 2361        | 2382         | rVB2     | 11499          | 26522         | 2.38%           | 0.506%        |
| 19        | 9.414       | 2496          | 2511        | 2540         | rBV      | 281627         | 476796        | 42.79%          | 9.089%        |
| 20        | 10.751      | 2915          | 2927        | 2944         | rVB2     | 69967          | 111692        | 10.02%          | 2.129%        |
| 21        | 11.806      | 3241          | 3255        | 3274         | rBV      | 290137         | 466977        | 41.91%          | 8.902%        |
| 22        | 12.189      | 3362          | 3374        | 3391         | rBV      | 185991         | 307395        | 27.59%          | 5.860%        |

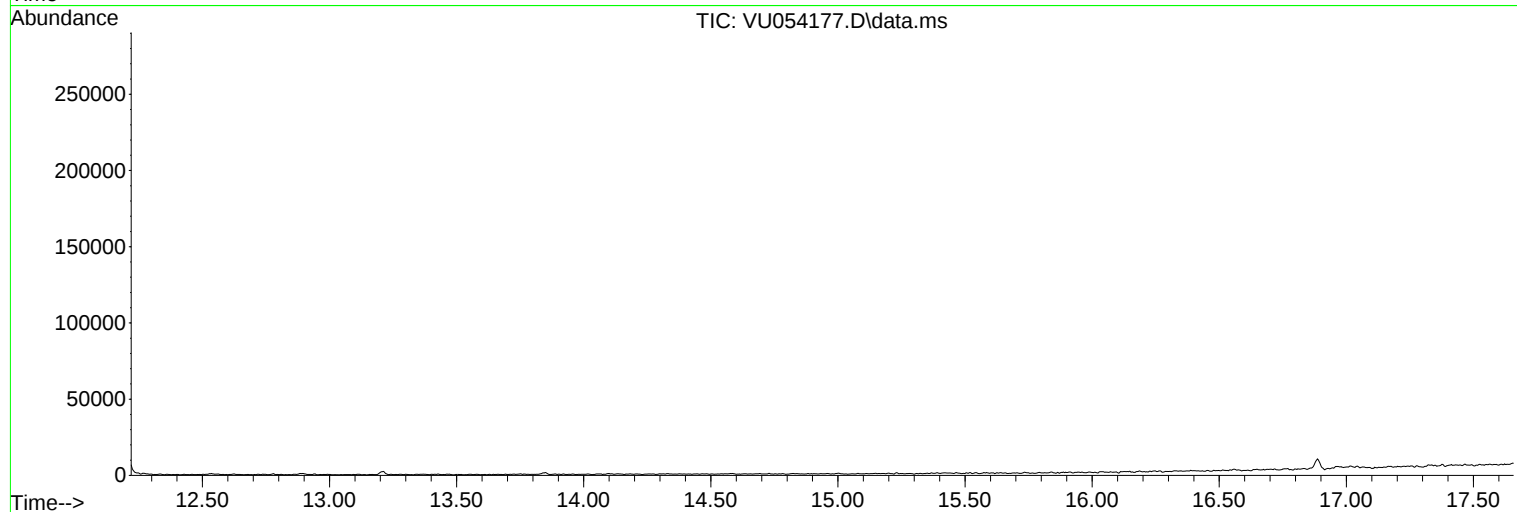
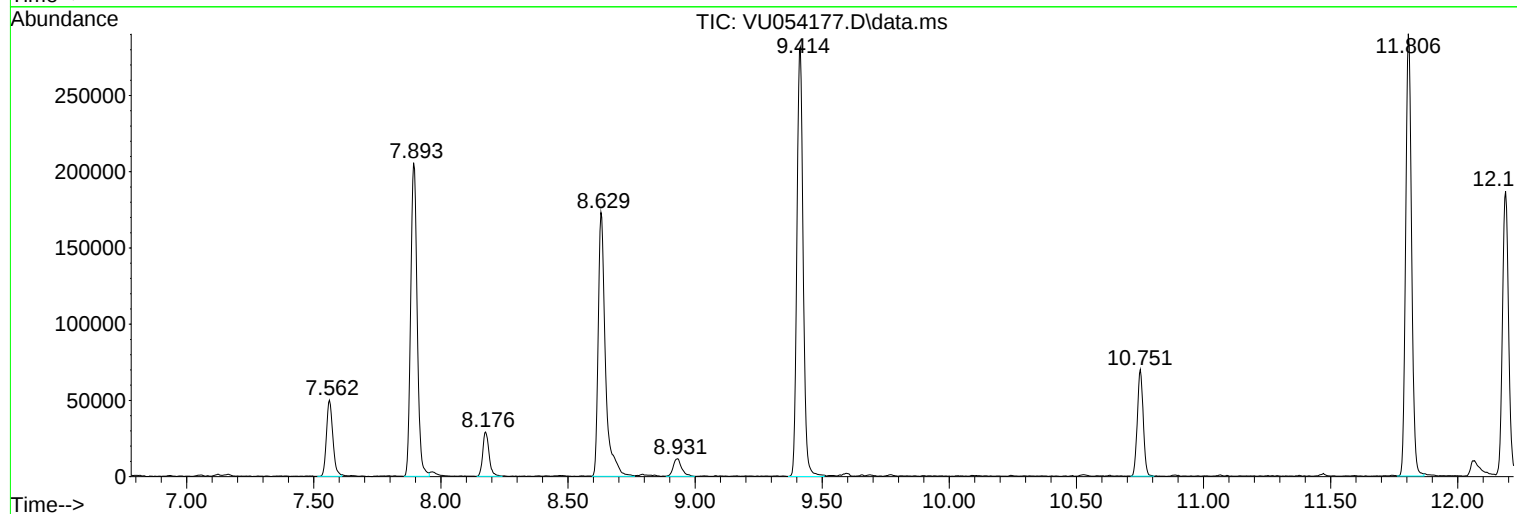
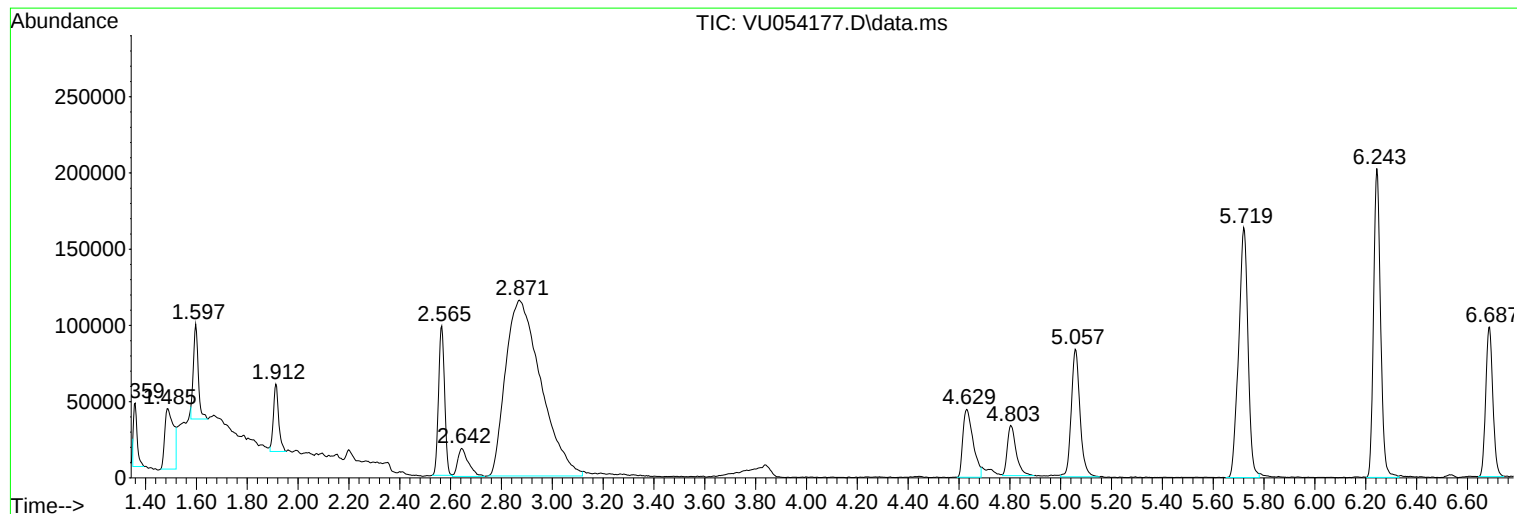
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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GBX05

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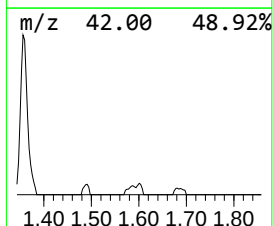
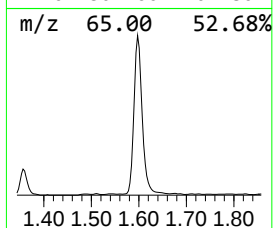
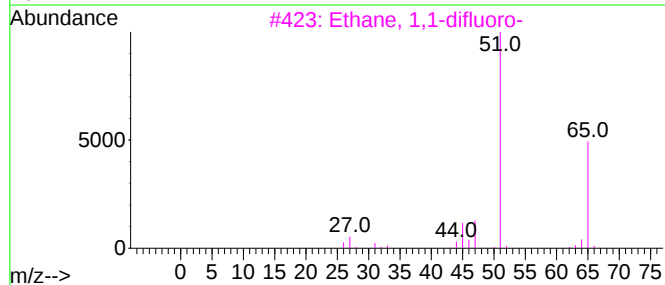
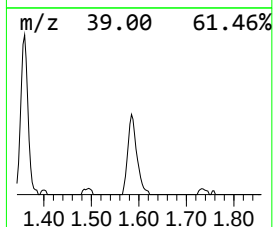
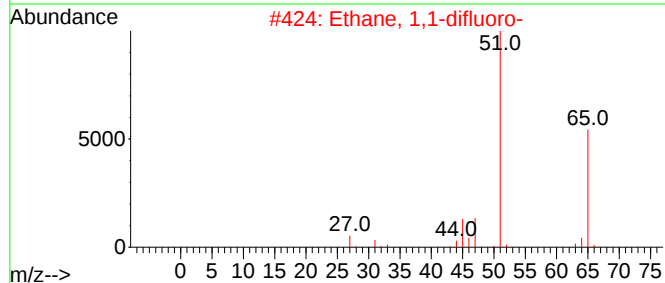
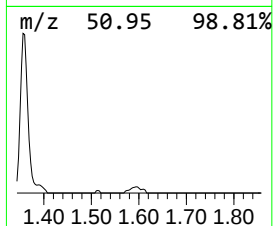
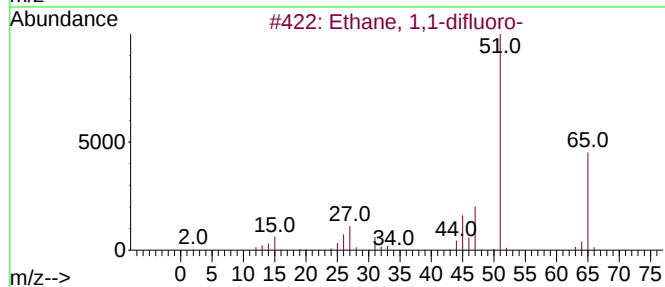
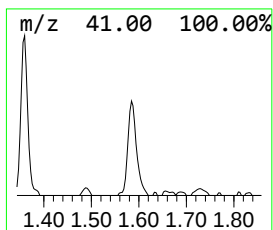
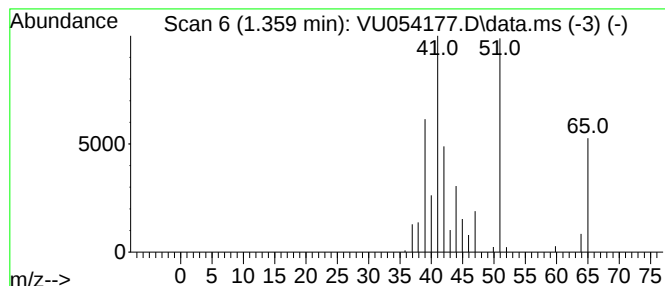
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR051823WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.359 | 0.51 ug/L | 39606 | 1,4-Difluorobenzene | 6.243 |

| Hit# | of | 5 | Tentative ID           | MW | MolForm | CAS#        | Qual |
|------|----|---|------------------------|----|---------|-------------|------|
| 1    |    |   | Ethane, 1,1-difluoro-  | 66 | C2H4F2  | 000075-37-6 | 64   |
| 2    |    |   | Ethane, 1,1-difluoro-  | 66 | C2H4F2  | 000075-37-6 | 59   |
| 3    |    |   | Ethane, 1,1-difluoro-  | 66 | C2H4F2  | 000075-37-6 | 45   |
| 4    |    |   | Propiolonitrile        | 51 | C3HN    | 001070-71-9 | 4    |
| 5    |    |   | Propane, 2,2-difluoro- | 80 | C3H6F2  | 000420-45-1 | 1    |



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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GBX05

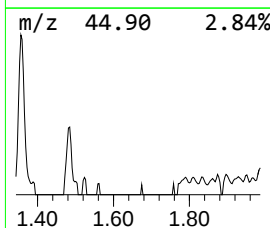
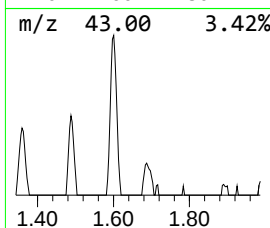
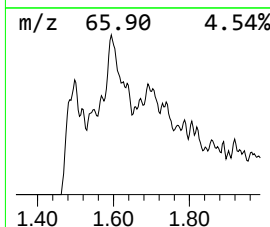
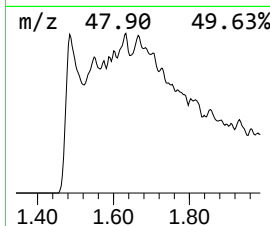
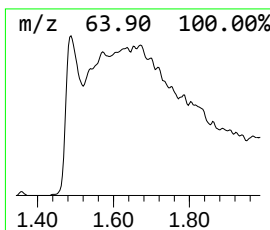
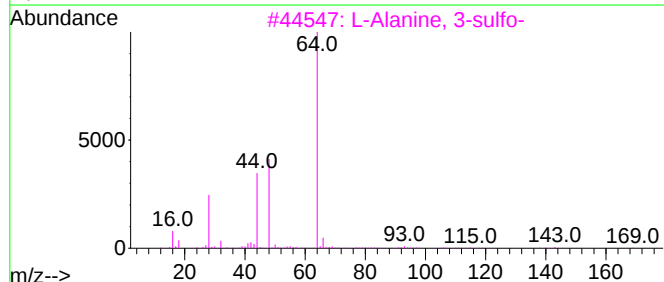
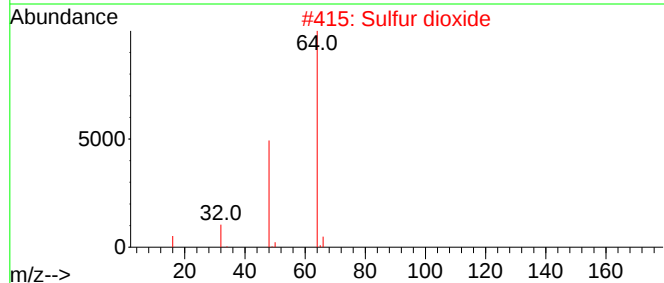
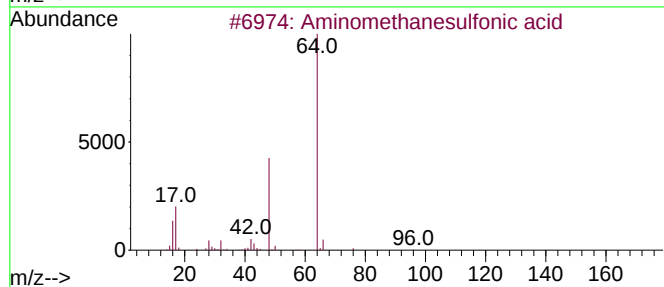
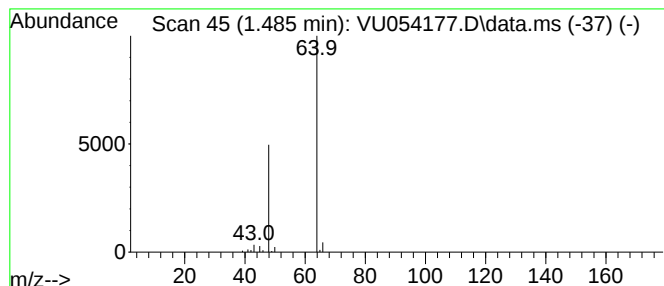
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR051823WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 Aminomethanesulfonic acid Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.485 | 1.26 ug/L | 98466 | 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    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |
| 5    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 4    |



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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GBX05

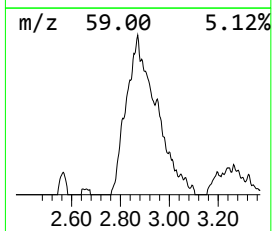
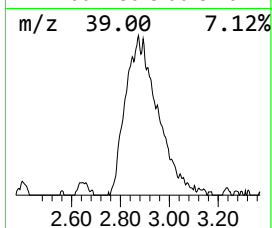
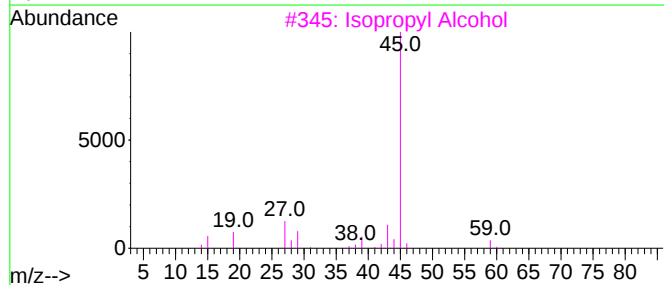
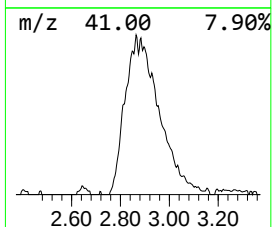
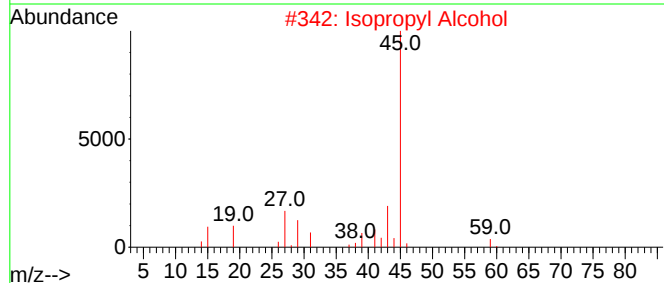
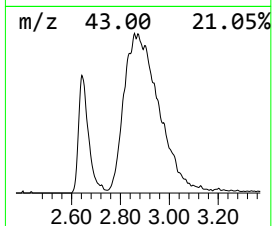
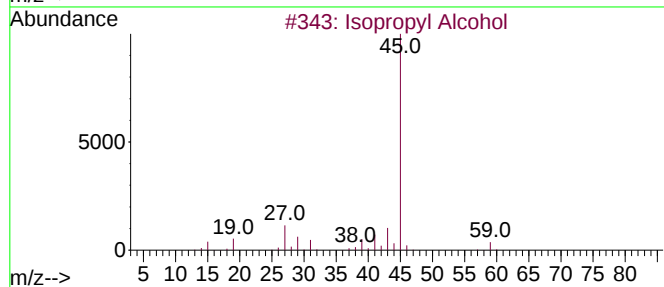
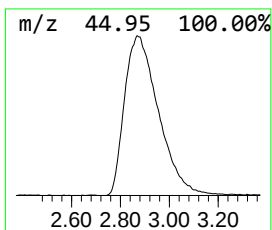
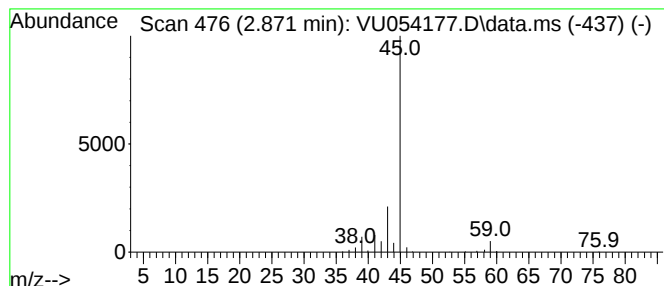
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR051823WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 3 Isopropyl Alcohol Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD    | R.T.  |
|-------|------------|---------|---------------------|-------|
| 2.871 | 14.29 ug/L | 1114150 | 1,4-Difluorobenzene | 6.243 |

| Hit# | of                | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|-------------------|---|--------------|----|---------|-------------|------|
| 1    | Isopropyl Alcohol |   |              | 60 | C3H8O   | 000067-63-0 | 86   |
| 2    | Isopropyl Alcohol |   |              | 60 | C3H8O   | 000067-63-0 | 78   |
| 3    | Isopropyl Alcohol |   |              | 60 | C3H8O   | 000067-63-0 | 64   |
| 4    | Isopropyl Alcohol |   |              | 60 | C3H8O   | 000067-63-0 | 56   |
| 5    | Isopropyl Alcohol |   |              | 60 | C3H8O   | 000067-63-0 | 56   |



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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GBX05

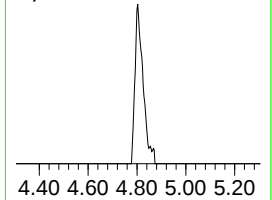
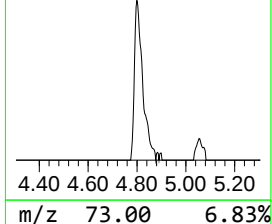
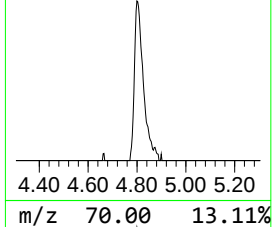
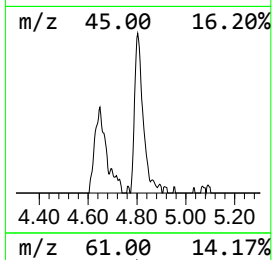
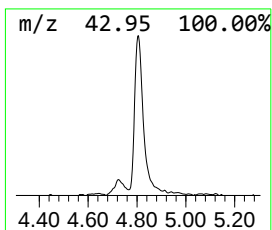
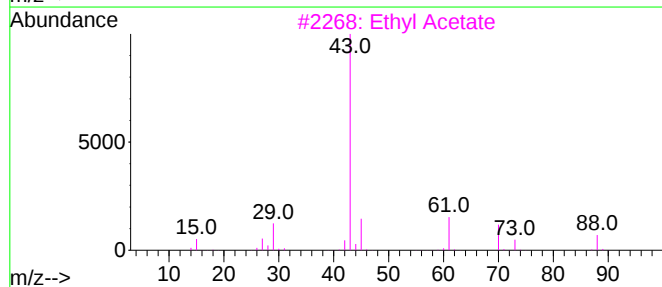
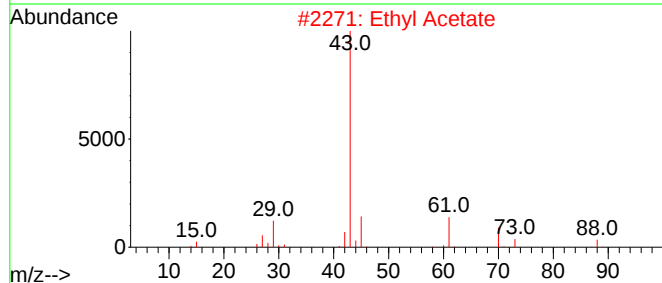
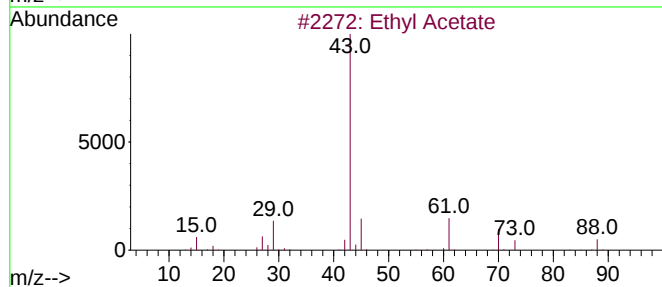
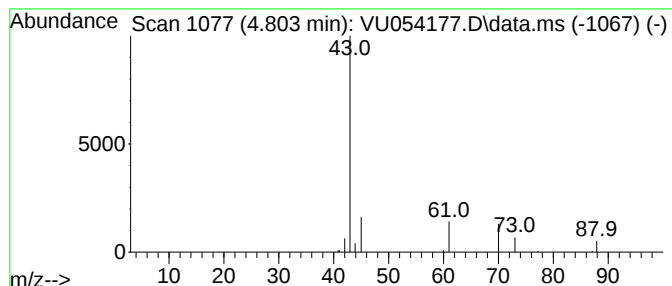
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR051823WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 Ethyl Acetate Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 4.803 | 1.01 ug/L | 78975 | 1,4-Difluorobenzene | 6.243 |

| Hit# | of | 5 | Tentative ID    | MW | MolForm | CAS#        | Qual |
|------|----|---|-----------------|----|---------|-------------|------|
| 1    |    |   | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 90   |
| 2    |    |   | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 90   |
| 3    |    |   | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 90   |
| 4    |    |   | CH3C(O)CH2CH2OH | 88 | C4H8O2  | 000590-90-9 | 72   |
| 5    |    |   | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 50   |



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Quant Title : TRACE VOA SFAM1.0

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

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Ethane, 1,1-dif... | 1.359 | 0.5     | ug/L  | 39606    | 1                     | 6.243 | 389891 | 5.0  |
| Aminomethanesul... | 1.485 | 1.3     | ug/L  | 98466    | 1                     | 6.243 | 389891 | 5.0  |
| Isopropyl Alcohol  | 2.871 | 14.3    | ug/L  | 1114150  | 1                     | 6.243 | 389891 | 5.0  |
| Ethyl Acetate      | 4.803 | 1.0     | ug/L  | 78975    | 1                     | 6.243 | 389891 | 5.0  |