

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU081021\  
 Data File : VU044409.D  
 Acq On : 10 Aug 2021 13:36  
 Operator : SY/MD  
 Sample : M3344-02  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AS5

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\SFAMUTR072321WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU044409.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         | 1.600       | 73            | 81          | 91           | rBV      | 68869          | 80553         | 11.63%          | 1.463%        |
| 2         | 1.912       | 170           | 178         | 193          | rVB      | 78901          | 102502        | 14.80%          | 1.862%        |
| 3         | 2.568       | 369           | 382         | 395          | rBV      | 122924         | 199404        | 28.78%          | 3.622%        |
| 4         | 2.629       | 395           | 401         | 412          | rVB      | 4732           | 7645          | 1.10%           | 0.139%        |
| 5         | 2.768       | 434           | 444         | 460          | rBV3     | 4218           | 8630          | 1.25%           | 0.157%        |
| 6         | 3.192       | 563           | 576         | 592          | rBV2     | 5781           | 12777         | 1.84%           | 0.232%        |
| 7         | 3.584       | 688           | 698         | 714          | rVB2     | 6438           | 14647         | 2.11%           | 0.266%        |
| 8         | 4.629       | 1007          | 1023        | 1056         | rBV      | 116019         | 290166        | 41.88%          | 5.271%        |
| 9         | 5.070       | 1143          | 1160        | 1180         | rBV      | 119867         | 268530        | 38.76%          | 4.878%        |
| 10        | 5.732       | 1339          | 1366        | 1387         | rBV2     | 249712         | 645463        | 93.17%          | 11.726%       |
| 11        | 6.157       | 1486          | 1498        | 1515         | rVB3     | 3540           | 8766          | 1.27%           | 0.159%        |
| 12        | 6.256       | 1515          | 1529        | 1549         | rBV      | 192454         | 366502        | 52.90%          | 6.658%        |
| 13        | 6.530       | 1603          | 1614        | 1627         | rVB7     | 7941           | 15582         | 2.25%           | 0.283%        |
| 14        | 6.697       | 1653          | 1666        | 1685         | rBV      | 157228         | 306622        | 44.26%          | 5.570%        |
| 15        | 7.169       | 1797          | 1813        | 1831         | rBV7     | 31210          | 69835         | 10.08%          | 1.269%        |
| 16        | 7.571       | 1926          | 1938        | 1954         | rBV2     | 65215          | 113855        | 16.43%          | 2.068%        |
| 17        | 7.719       | 1966          | 1984        | 2000         | rBV      | 43271          | 84267         | 12.16%          | 1.531%        |
| 18        | 7.902       | 2028          | 2041        | 2057         | rBV      | 312035         | 541790        | 78.21%          | 9.842%        |
| 19        | 8.185       | 2118          | 2129        | 2143         | rBV      | 38509          | 65222         | 9.41%           | 1.185%        |
| 20        | 8.639       | 2257          | 2270        | 2304         | rBV      | 367285         | 692773        | 100.00%         | 12.585%       |
| 21        | 9.423       | 2501          | 2514        | 2550         | rVB      | 278251         | 470413        | 67.90%          | 8.546%        |
| 22        | 9.687       | 2587          | 2596        | 2607         | rVB5     | 6405           | 10326         | 1.49%           | 0.188%        |
| 23        | 10.761      | 2918          | 2930        | 2953         | rBV      | 123653         | 200538        | 28.95%          | 3.643%        |
| 24        | 11.819      | 3243          | 3259        | 3277         | rBV      | 278606         | 446048        | 64.39%          | 8.103%        |
| 25        | 12.198      | 3363          | 3377        | 3397         | rBV      | 298153         | 481860        | 69.56%          | 8.754%        |

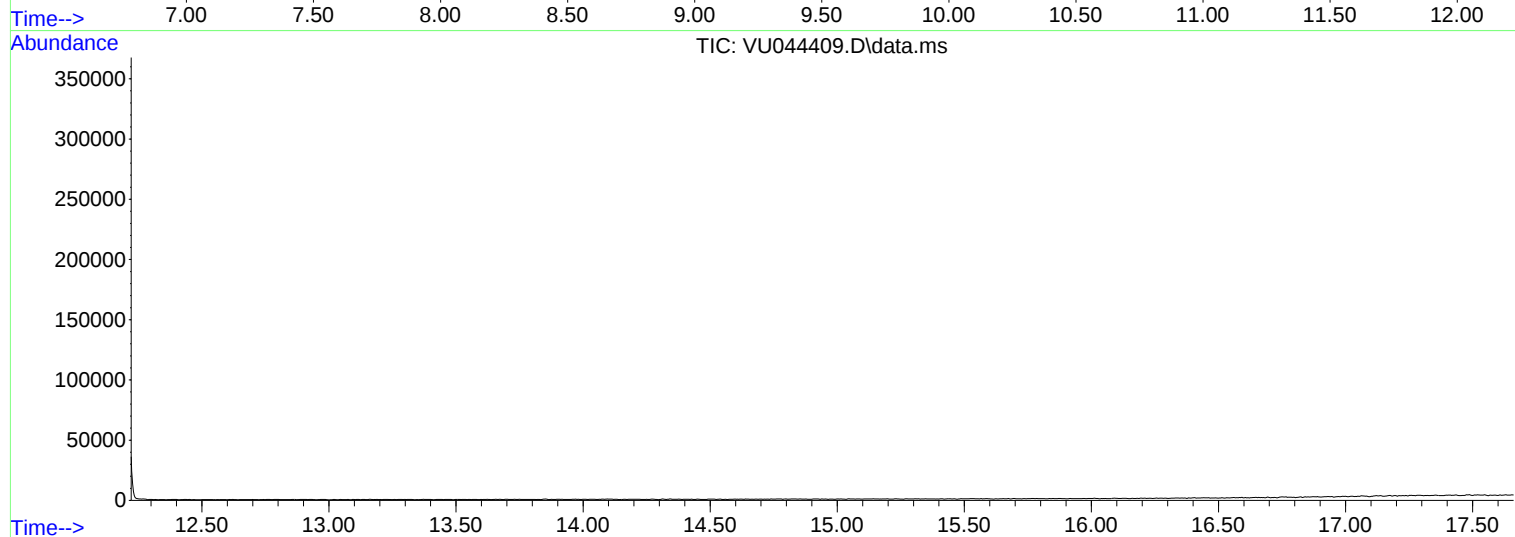
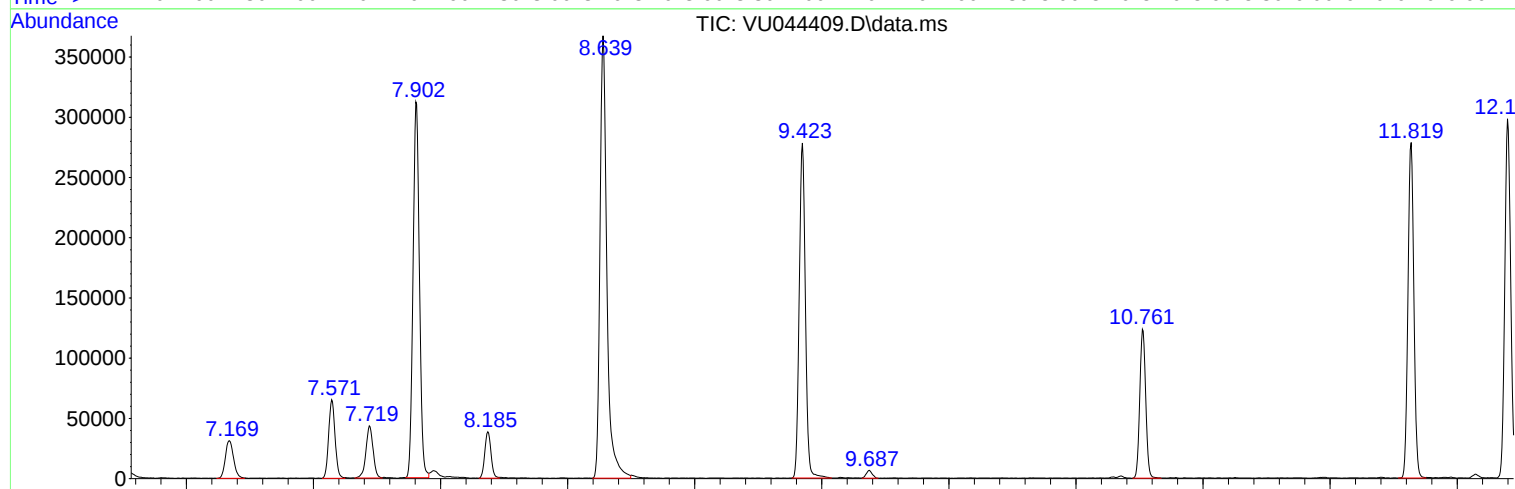
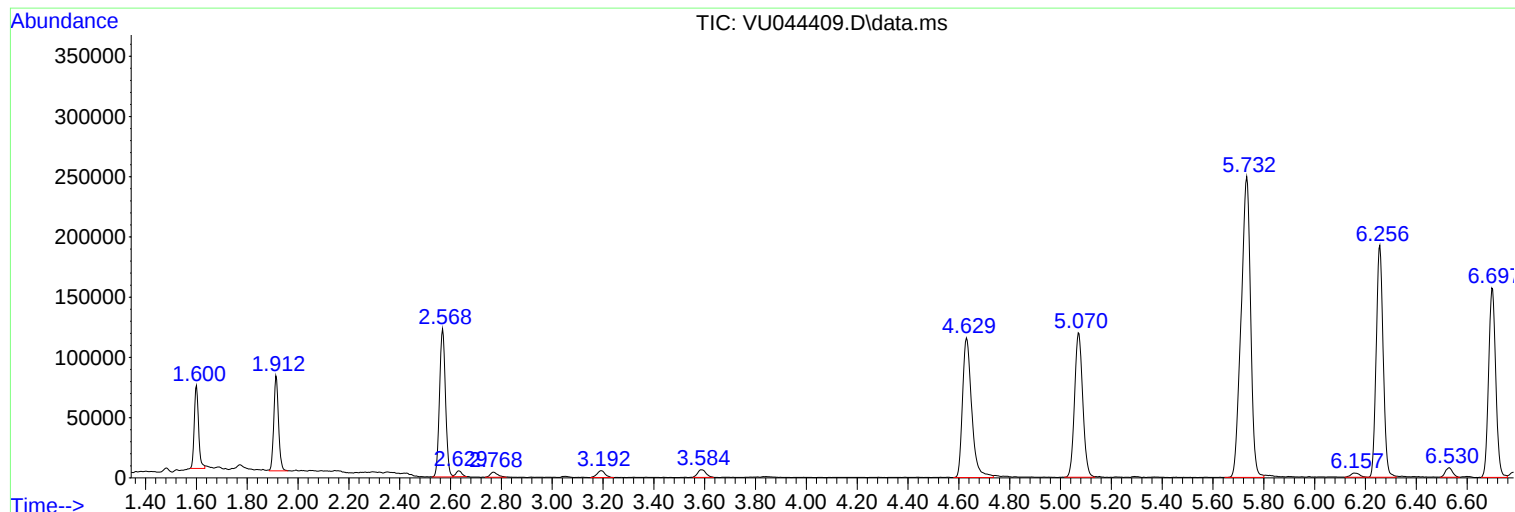
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MSVOA\_U  
ClientSampleId :  
C0AS5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR072321WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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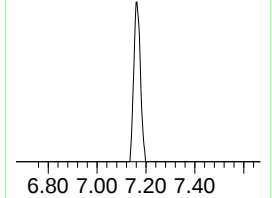
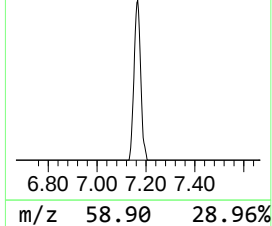
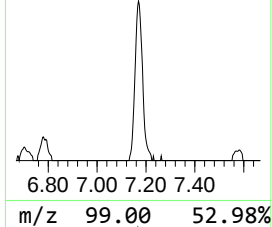
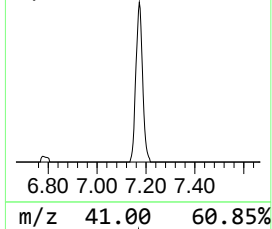
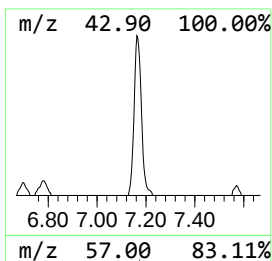
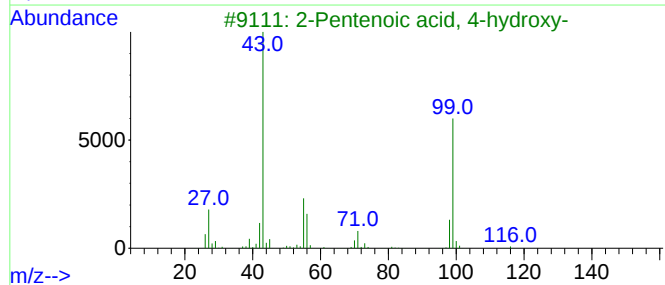
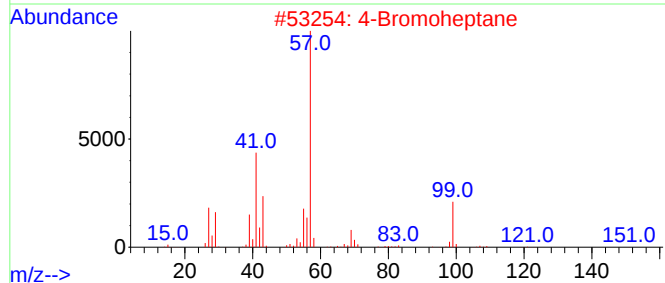
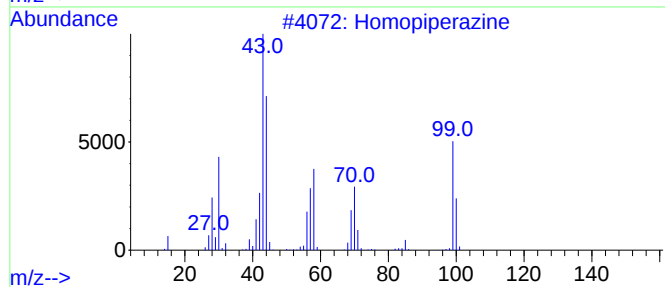
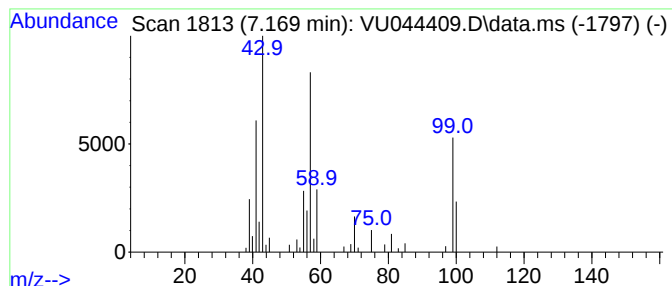
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR072321WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 unknown-01 Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 7.169 | 0.95 ug/L | 69835 | 1,4-Difluorobenzene | 6.256 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Homopiperazine                      | 100 | C5H12N2  | 000505-66-8  | 38   |
| 2    |    |   | 4-Bromoheptane                      | 178 | C7H15Br  | 000998-93-6  | 38   |
| 3    |    |   | 2-Pentenoic acid, 4-hydroxy-        | 116 | C5H8O3   | 028525-83-9  | 37   |
| 4    |    |   | Carbonic acid, decyl prop-1-en-2... | 242 | C14H26O3 | 1000382-90-5 | 37   |
| 5    |    |   | Carbonic acid, prop-1-en-2-yl un... | 256 | C15H28O3 | 1000382-90-6 | 37   |



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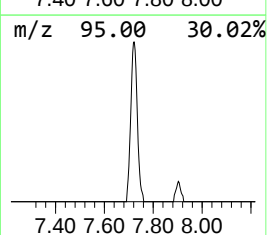
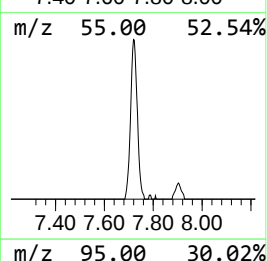
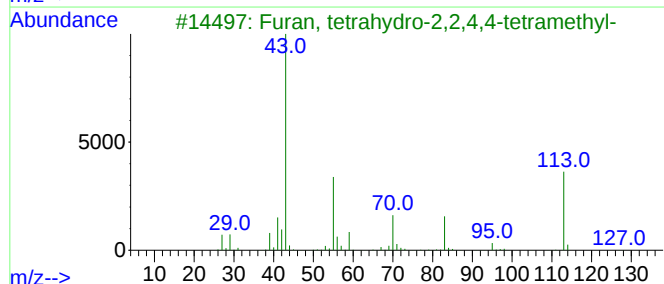
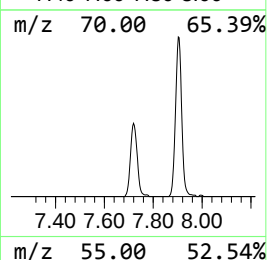
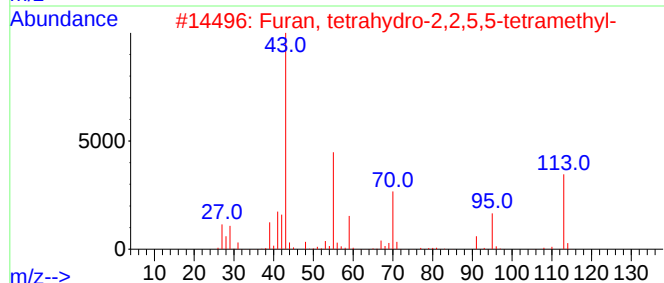
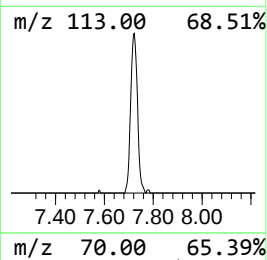
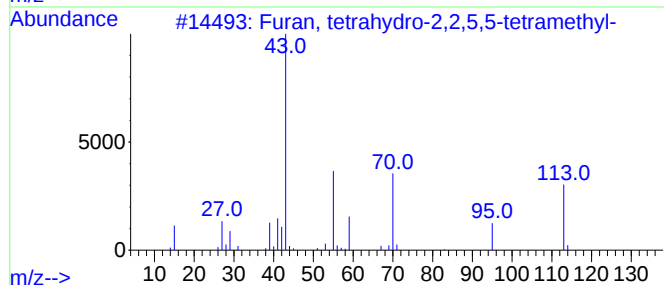
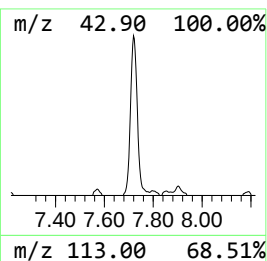
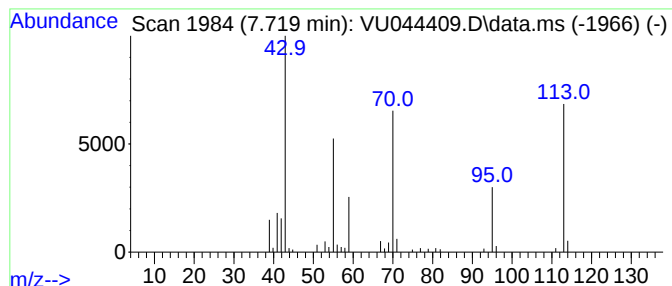
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 7.719 | 1.15 ug/L | 84267 | 1,4-Difluorobenzene | 6.256 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Furan, tetrahydro-2,2,5,5-tetram... | 128 | C8H16O  | 015045-43-9 | 83   |
| 2    |    |   | Furan, tetrahydro-2,2,5,5-tetram... | 128 | C8H16O  | 015045-43-9 | 72   |
| 3    |    |   | Furan, tetrahydro-2,2,4,4-tetram... | 128 | C8H16O  | 003358-28-9 | 53   |
| 4    |    |   | Furan, tetrahydro-2,2,4,4-tetram... | 128 | C8H16O  | 003358-28-9 | 53   |
| 5    |    |   | 4-Piperidinone, 1-methyl-           | 113 | C6H11NO | 001445-73-4 | 50   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown-01         | 7.169 | 0.9     | ug/L  | 69835    | 1                     | 6.256 | 366502 | 5.0  |
| Furan, tetrahyd... | 7.719 | 1.1     | ug/L  | 84267    | 1                     | 6.256 | 366502 | 5.0  |