

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU070324\  
 Data File : VU059779.D  
 Acq On : 03 Jul 2024 07:54  
 Operator : MD/SY  
 Sample : P3122-07  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 60 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0BP4

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\SFAMUTR061724WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU059779.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         | 1.358       | 14            | 21          | 35           | rBV      | 131493         | 137328        | 27.73%          | 2.903%        |
| 2         | 1.486       | 55            | 61          | 68           | rBV      | 16356          | 16878         | 3.41%           | 0.357%        |
| 3         | 1.593       | 83            | 94          | 112          | rVB2     | 82701          | 136123        | 27.49%          | 2.878%        |
| 4         | 1.686       | 115           | 123         | 132          | rBV      | 9420           | 12574         | 2.54%           | 0.266%        |
| 5         | 1.908       | 184           | 192         | 207          | rVB      | 59398          | 78605         | 15.87%          | 1.662%        |
| 6         | 2.329       | 313           | 323         | 329          | rBV2     | 3828           | 5787          | 1.17%           | 0.122%        |
| 7         | 2.560       | 382           | 395         | 408          | rBV      | 106269         | 173565        | 35.05%          | 3.669%        |
| 8         | 2.634       | 408           | 418         | 441          | rVB      | 36888          | 76986         | 15.55%          | 1.627%        |
| 9         | 3.197       | 576           | 593         | 617          | rBV2     | 20131          | 71731         | 14.49%          | 1.516%        |
| 10        | 4.425       | 961           | 975         | 1000         | rBV4     | 7606           | 24069         | 4.86%           | 0.509%        |
| 11        | 4.621       | 1024          | 1036        | 1064         | rBV      | 63170          | 176602        | 35.66%          | 3.733%        |
| 12        | 5.052       | 1153          | 1170        | 1190         | rBV2     | 96361          | 214008        | 43.22%          | 4.524%        |
| 13        | 5.718       | 1355          | 1377        | 1405         | rBV2     | 190280         | 495199        | 100.00%         | 10.468%       |
| 14        | 6.242       | 1527          | 1540        | 1565         | rBV      | 184141         | 356255        | 71.94%          | 7.531%        |
| 15        | 6.538       | 1624          | 1632        | 1633         | rBV3     | 4678           | 5423          | 1.10%           | 0.115%        |
| 16        | 6.682       | 1664          | 1677        | 1696         | rBV      | 119217         | 230404        | 46.53%          | 4.871%        |
| 17        | 7.158       | 1805          | 1825        | 1842         | rBV2     | 22821          | 47823         | 9.66%           | 1.011%        |
| 18        | 7.560       | 1939          | 1950        | 1970         | rBV      | 50724          | 93051         | 18.79%          | 1.967%        |
| 19        | 7.891       | 2041          | 2053        | 2070         | rBV      | 235542         | 408726        | 82.54%          | 8.640%        |
| 20        | 8.174       | 2132          | 2141        | 2155         | rBV      | 29619          | 51752         | 10.45%          | 1.094%        |
| 21        | 8.470       | 2223          | 2233        | 2245         | rBV8     | 3048           | 5665          | 1.14%           | 0.120%        |
| 22        | 8.547       | 2246          | 2257        | 2272         | rVB2     | 20532          | 34588         | 6.98%           | 0.731%        |
| 23        | 8.628       | 2272          | 2282        | 2317         | rBV      | 214334         | 437565        | 88.36%          | 9.250%        |
| 24        | 9.412       | 2512          | 2526        | 2551         | rBV      | 277450         | 472048        | 95.32%          | 9.979%        |
| 25        | 10.750      | 2930          | 2942        | 2964         | rBV      | 90271          | 148391        | 29.97%          | 3.137%        |
| 26        | 11.576      | 3192          | 3199        | 3207         | rBV5     | 4663           | 6530          | 1.32%           | 0.138%        |
| 27        | 11.808      | 3258          | 3271        | 3289         | rBV      | 247248         | 414271        | 83.66%          | 8.757%        |
| 28        | 11.888      | 3289          | 3296        | 3302         | rBV3     | 9001           | 13369         | 2.70%           | 0.283%        |
| 29        | 12.187      | 3376          | 3389        | 3409         | rBV      | 214522         | 358414        | 72.38%          | 7.577%        |
| 30        | 13.377      | 3750          | 3759        | 3775         | rBV5     | 10686          | 20197         | 4.08%           | 0.427%        |
| 31        | 14.714      | 4164          | 4175        | 4185         | rBV2     | 4146           | 6562          | 1.33%           | 0.139%        |

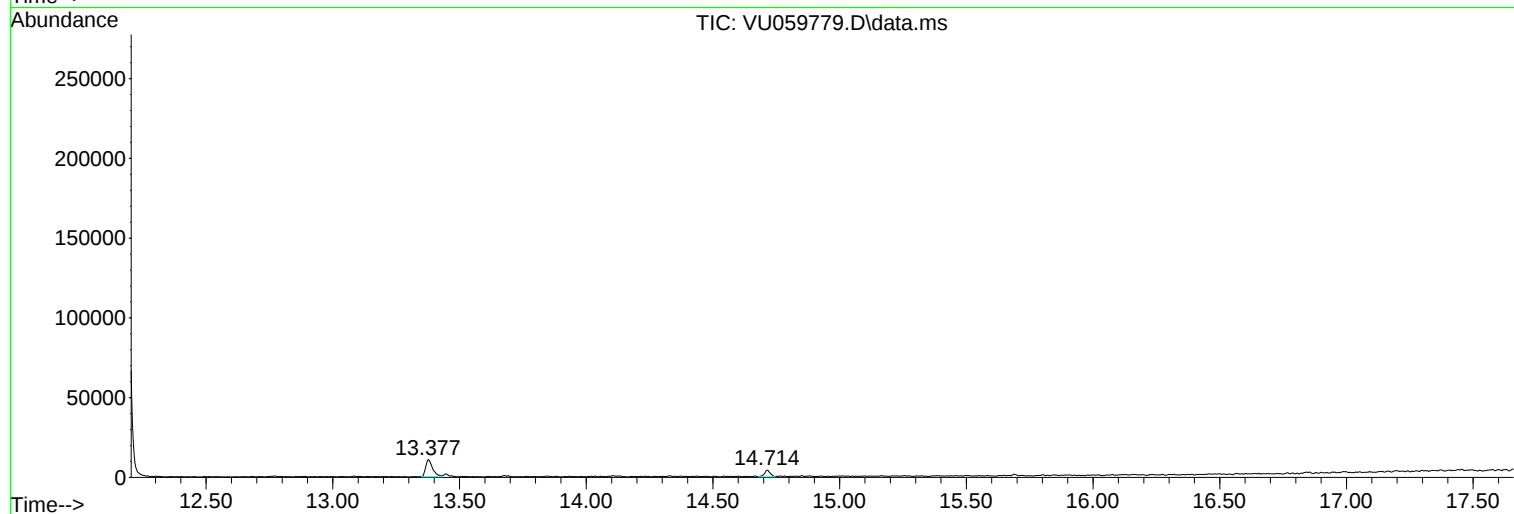
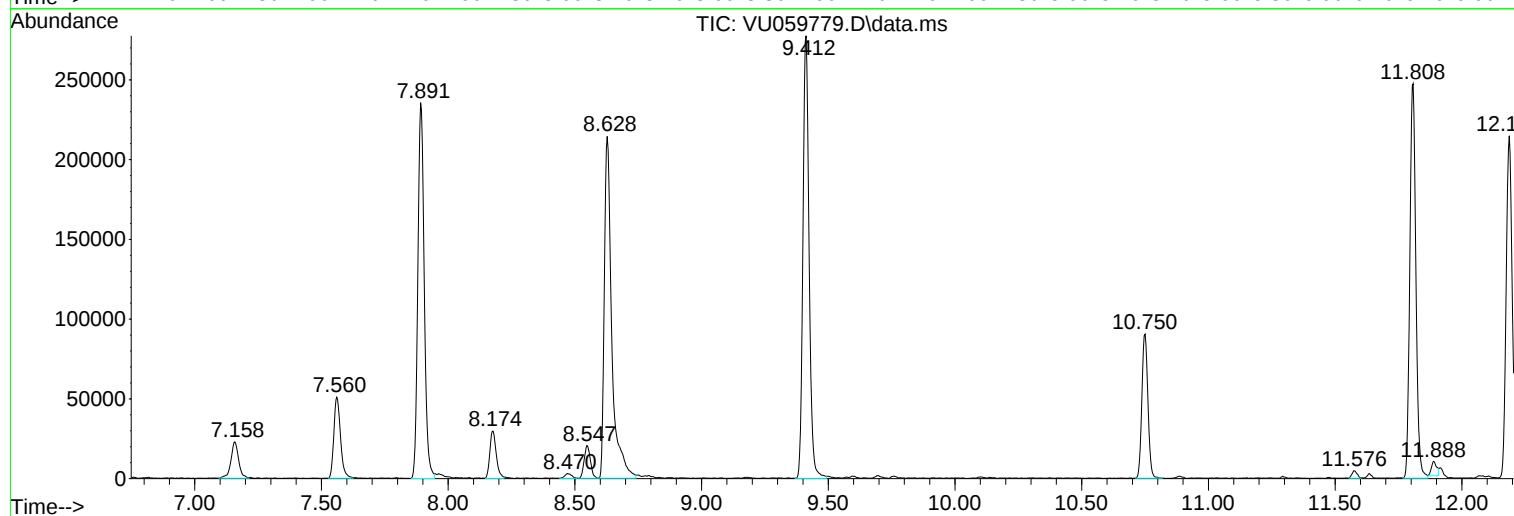
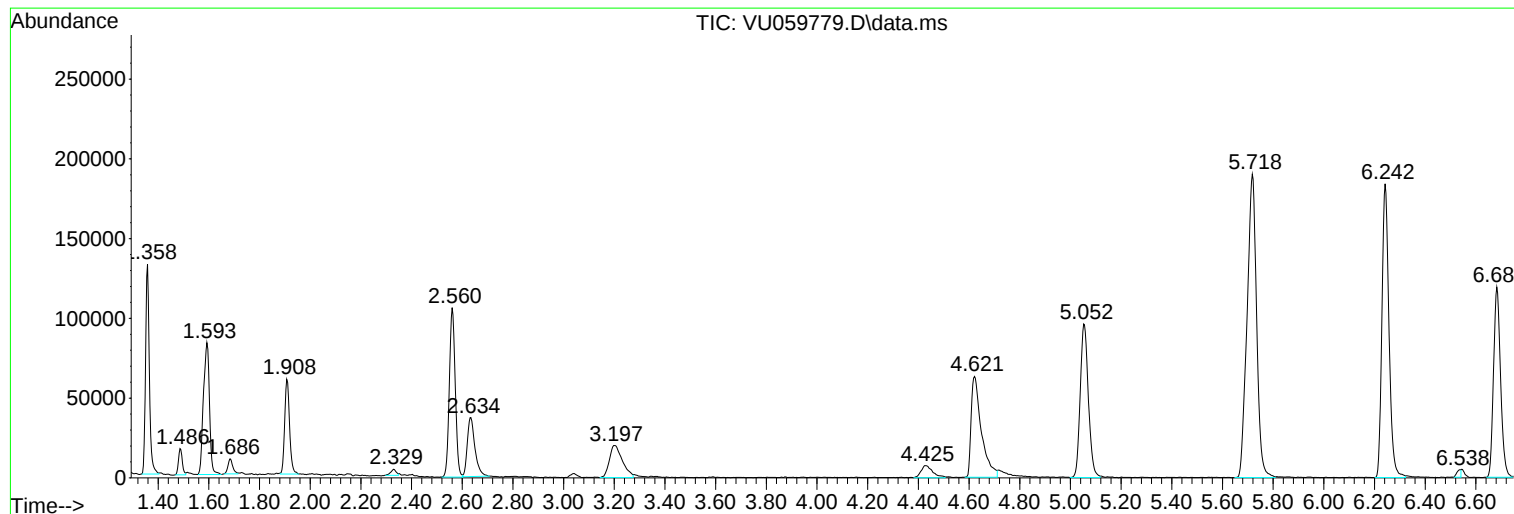
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ALS Vial : 60 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
C0BP4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR061724WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :  
MSVOA\_U  
ClientSampleId :  
C0BP4

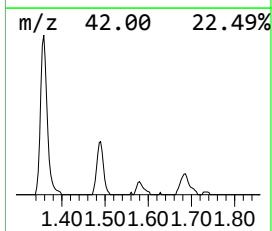
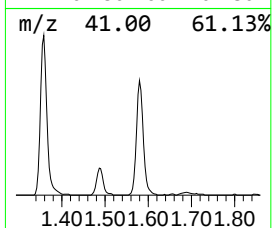
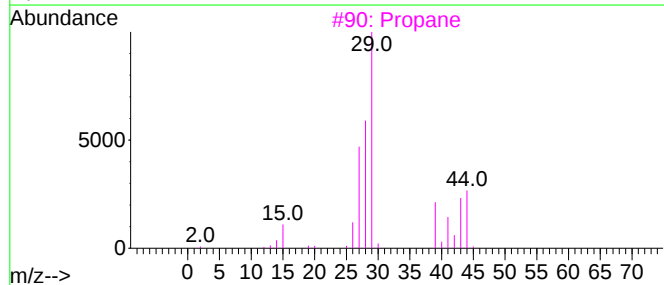
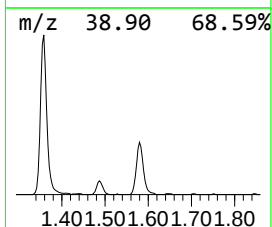
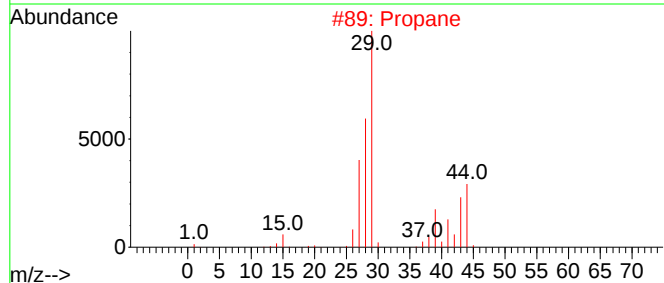
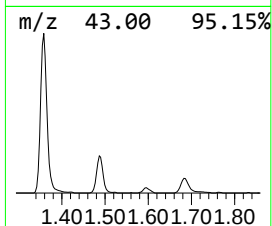
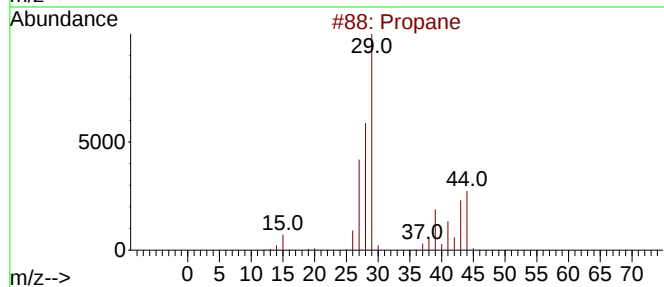
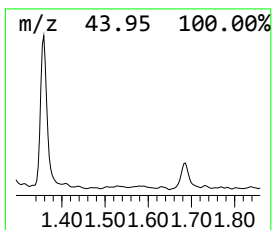
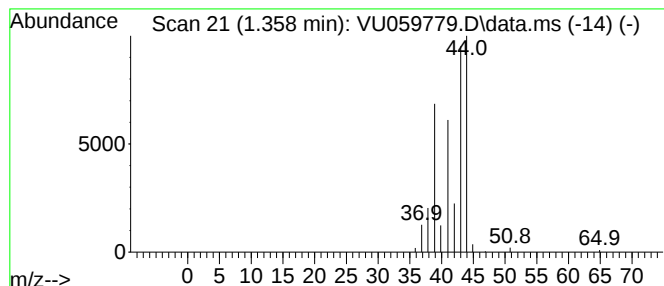
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR061724WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.358 | 1.93 ug/L | 137328 | 1,4-Difluorobenzene | 6.242 |

| Hit# | of | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------|----|---------|-------------|------|
| 1    |    |   | Propane      | 44 | C3H8    | 000074-98-6 | 90   |
| 2    |    |   | Propane      | 44 | C3H8    | 000074-98-6 | 83   |
| 3    |    |   | Propane      | 44 | C3H8    | 000074-98-6 | 9    |
| 4    |    |   | Propene      | 42 | C3H6    | 000115-07-1 | 9    |
| 5    |    |   | Acetaldehyde | 44 | C2H4O   | 000075-07-0 | 5    |



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ALS Vial : 60 Sample Multiplier: 1

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MSVOA\_U  
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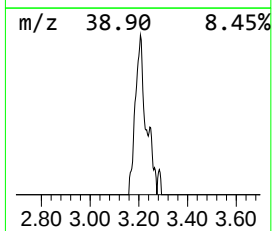
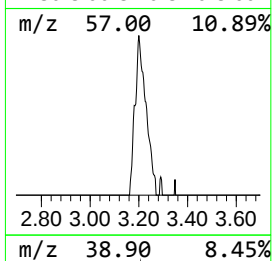
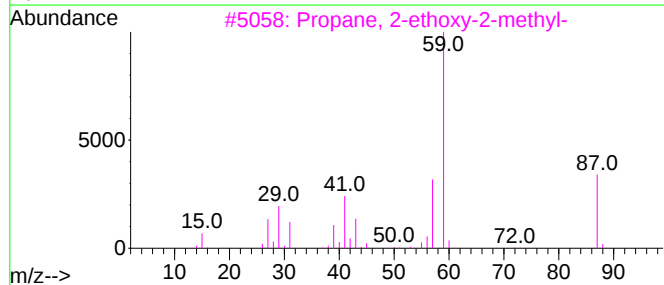
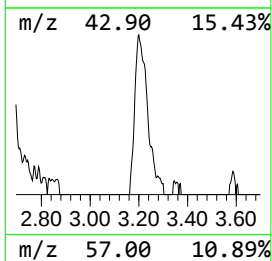
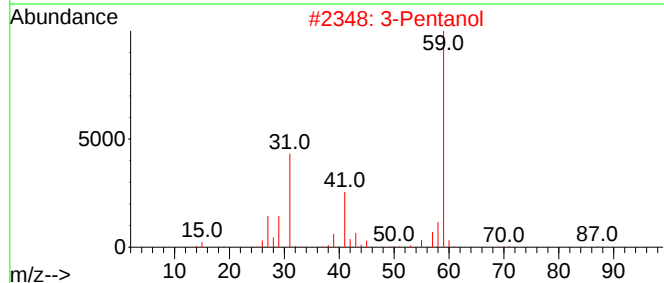
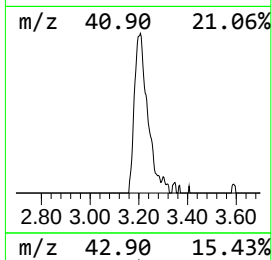
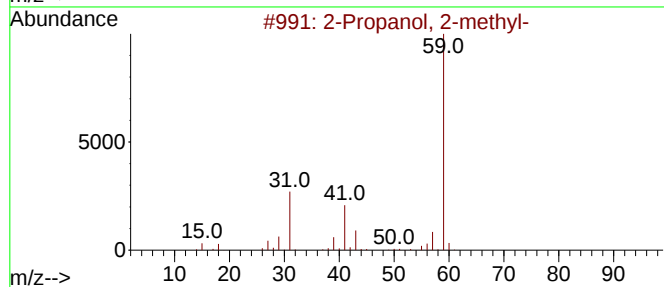
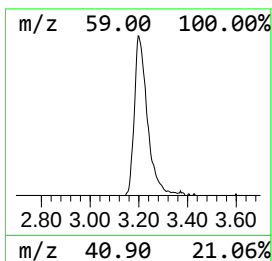
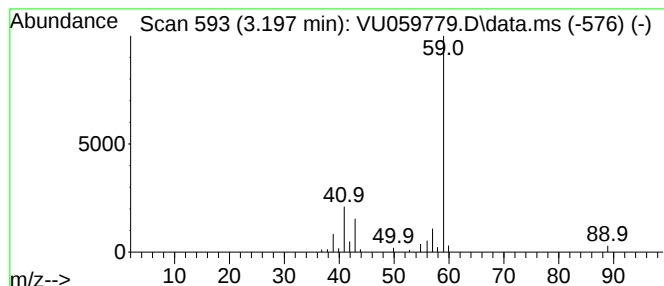
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR061724WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 2-Propanol, 2-methyl- Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 3.197 | 1.01 ug/L | 71731 | 1,4-Difluorobenzene | 6.242 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|---------|-------------|------|
| 1    | 2-Propanol, 2-methyl-               |   |              | 74  | C4H10O  | 000075-65-0 | 64   |
| 2    | 3-Pentanol                          |   |              | 88  | C5H12O  | 000584-02-1 | 40   |
| 3    | Propane, 2-ethoxy-2-methyl-         |   |              | 102 | C6H14O  | 000637-92-3 | 39   |
| 4    | Propanoic acid, 2-hydroxy-2-methyl- |   |              | 104 | C4H8O3  | 000594-61-6 | 38   |
| 5    | Propanoic acid, 2-hydroxy-2-methyl- |   |              | 104 | C4H8O3  | 000594-61-6 | 38   |



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ALS Vial : 60 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
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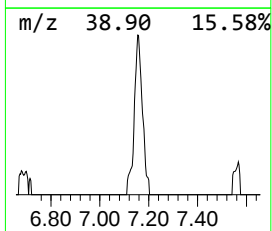
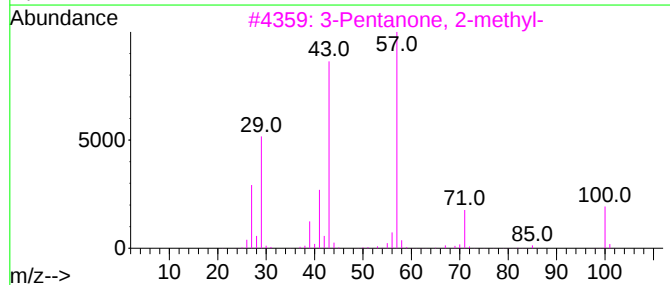
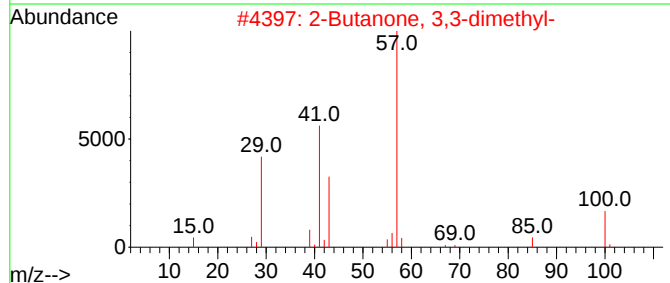
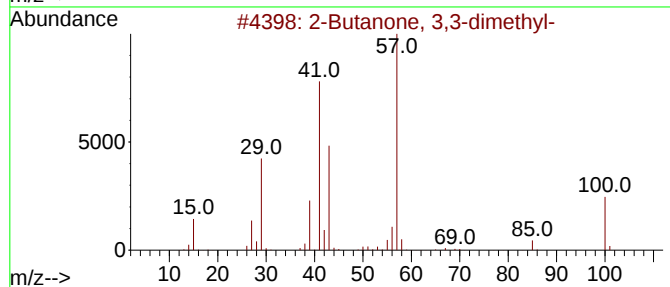
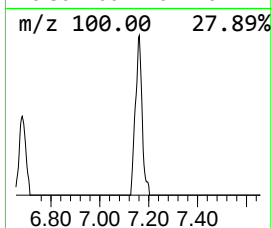
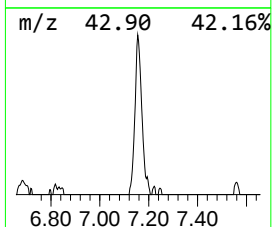
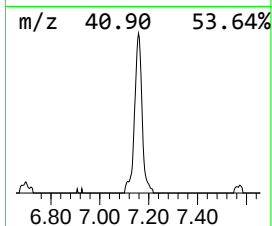
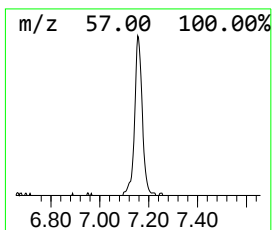
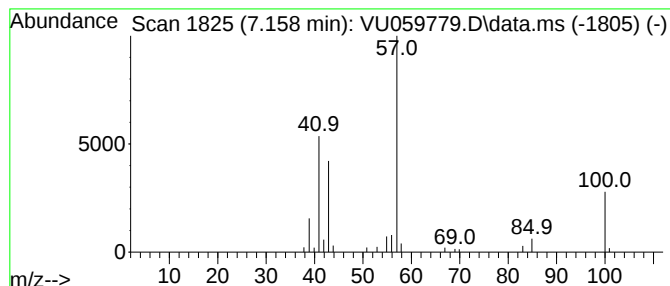
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR061724WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 7.158 | 0.67 ug/L | 47823 | 1,4-Difluorobenzene | 6.242 |

| Hit# | of                        | 5 | Tentative ID | MW     | MolForm      | CAS# | Qual |
|------|---------------------------|---|--------------|--------|--------------|------|------|
| 1    | 2-Butanone, 3,3-dimethyl- |   | 100          | C6H12O | 000075-97-8  | 83   |      |
| 2    | 2-Butanone, 3,3-dimethyl- |   | 100          | C6H12O | 000075-97-8  | 72   |      |
| 3    | 3-Pentanone, 2-methyl-    |   | 100          | C6H12O | 000565-69-5  | 50   |      |
| 4    | 2-Butanone, 3,3-dimethyl- |   | 100          | C6H12O | 000075-97-8  | 47   |      |
| 5    | cis-1-Ethoxy-1-butene     |   | 100          | C6H12O | 1000139-43-8 | 47   |      |



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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 |
| (DEL) Alkane: S... | 1.358 | 1.9     | ug/L  | 137328   | 1                     | 6.242 | 356255 | 5.0  |
| 2-Propanol, 2-m... | 3.197 | 1.0     | ug/L  | 71731    | 1                     | 6.242 | 356255 | 5.0  |
| 2-Butanone, 3,3... | 7.158 | 0.7     | ug/L  | 47823    | 1                     | 6.242 | 356255 | 5.0  |