

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011222\  
 Data File : VU046747.D  
 Acq On : 12 Jan 2022 17:07  
 Operator : SY/MD  
 Sample : N1101-06  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFXW8

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\SFAMUTR122121WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU046747.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       | 72            | 81          | 90           | rBV      | 26555          | 32777         | 2.07%           | 0.603%        |
| 2         | 1.919       | 171           | 180         | 197          | rVB      | 21596          | 29248         | 1.85%           | 0.538%        |
| 3         | 2.578       | 368           | 385         | 399          | rBV3     | 61133          | 122321        | 7.74%           | 2.249%        |
| 4         | 4.655       | 1012          | 1031        | 1079         | rBV2     | 35782          | 169257        | 10.71%          | 3.113%        |
| 5         | 5.067       | 1145          | 1159        | 1183         | rBV2     | 46225          | 108668        | 6.87%           | 1.998%        |
| 6         | 5.321       | 1221          | 1238        | 1253         | rBB2     | 28166          | 61271         | 3.88%           | 1.127%        |
| 7         | 5.729       | 1345          | 1365        | 1384         | rBV3     | 86440          | 230188        | 14.56%          | 4.233%        |
| 8         | 6.250       | 1514          | 1527        | 1544         | rBV      | 86307          | 163417        | 10.34%          | 3.005%        |
| 9         | 6.693       | 1652          | 1665        | 1683         | rBV      | 56787          | 109922        | 6.95%           | 2.021%        |
| 10        | 6.880       | 1714          | 1723        | 1752         | rVB      | 16647          | 35541         | 2.25%           | 0.654%        |
| 11        | 7.568       | 1924          | 1937        | 1954         | rBV2     | 29147          | 50502         | 3.19%           | 0.929%        |
| 12        | 7.899       | 2027          | 2040        | 2054         | rBV      | 103166         | 176989        | 11.19%          | 3.255%        |
| 13        | 8.182       | 2116          | 2128        | 2140         | rBV      | 18287          | 30191         | 1.91%           | 0.555%        |
| 14        | 8.555       | 2231          | 2244        | 2257         | rBV      | 216772         | 364029        | 23.02%          | 6.694%        |
| 15        | 8.635       | 2257          | 2269        | 2301         | rVV      | 199150         | 370309        | 23.42%          | 6.810%        |
| 16        | 8.787       | 2304          | 2316        | 2345         | rBV2     | 146692         | 255028        | 16.13%          | 4.690%        |
| 17        | 9.417       | 2498          | 2512        | 2532         | rBV      | 132442         | 219256        | 13.87%          | 4.032%        |
| 18        | 10.343      | 2788          | 2800        | 2821         | rBV2     | 72841          | 116602        | 7.37%           | 2.144%        |
| 19        | 10.758      | 2917          | 2929        | 2943         | rVB2     | 61993          | 98242         | 6.21%           | 1.807%        |
| 20        | 11.687      | 3206          | 3218        | 3233         | rBV      | 376563         | 551220        | 34.86%          | 10.137%       |
| 21        | 11.812      | 3244          | 3257        | 3275         | rVB      | 166121         | 262867        | 16.63%          | 4.834%        |
| 22        | 12.195      | 3362          | 3376        | 3387         | rBV      | 125297         | 197466        | 12.49%          | 3.631%        |
| 23        | 12.539      | 3471          | 3483        | 3501         | rBV4     | 24471          | 48663         | 3.08%           | 0.895%        |
| 24        | 12.886      | 3576          | 3591        | 3622         | rBV      | 1090172        | 1581045       | 100.00%         | 29.074%       |
| 25        | 14.732      | 4156          | 4165        | 4179         | rVB3     | 35487          | 52927         | 3.35%           | 0.973%        |

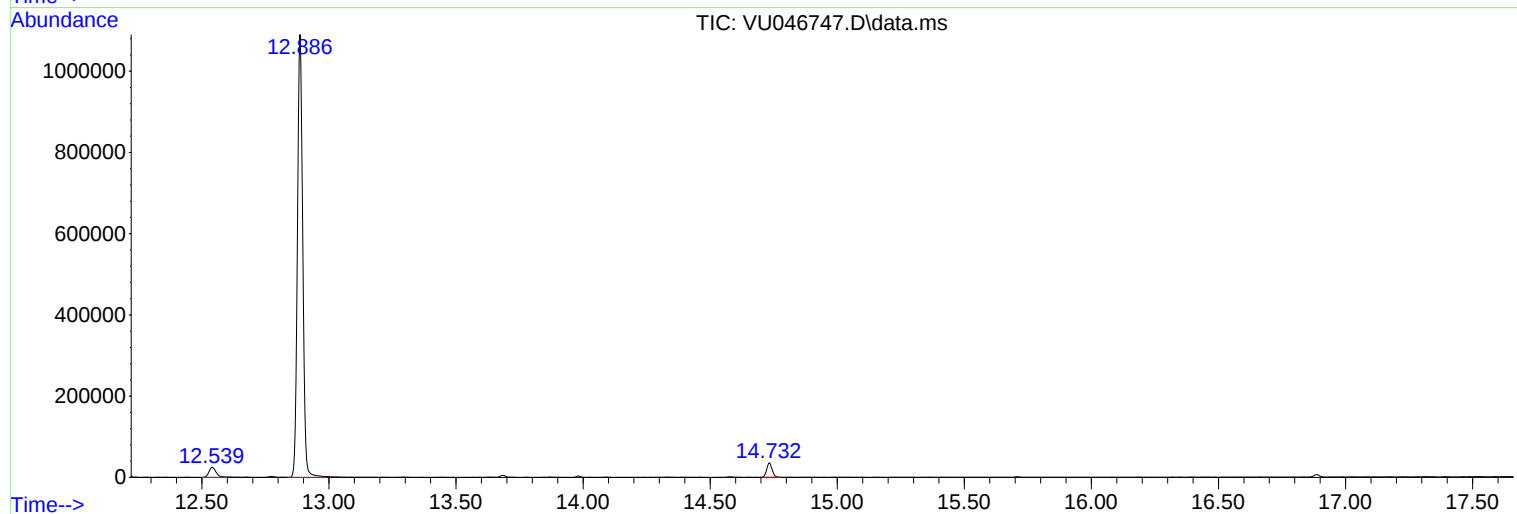
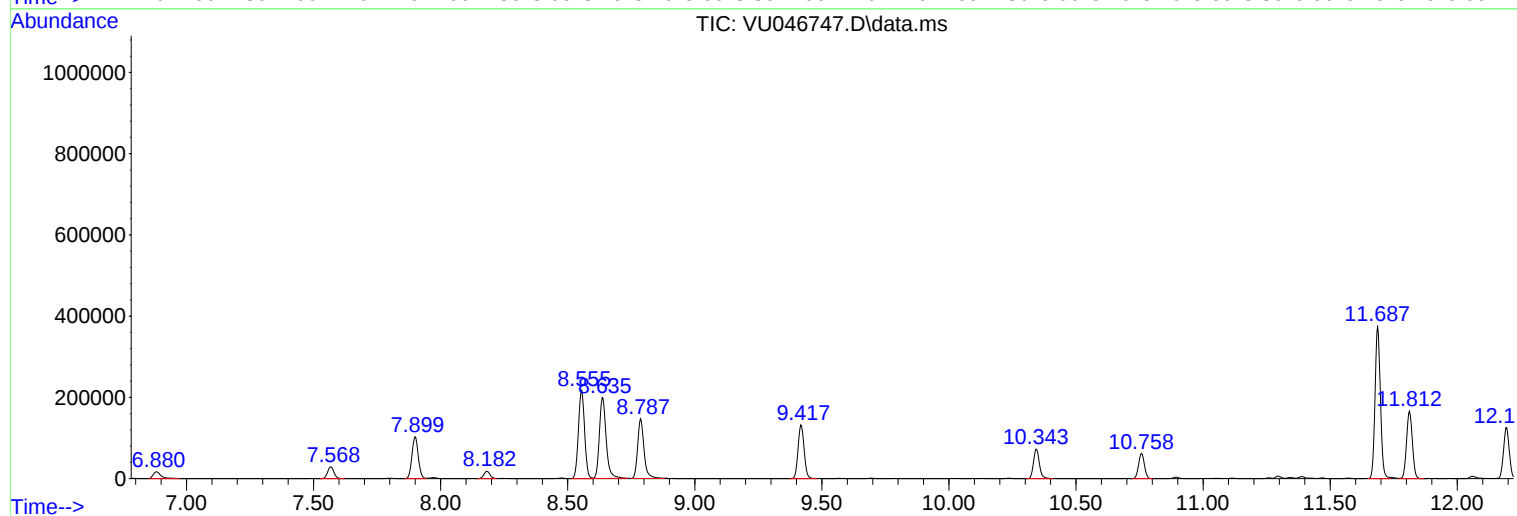
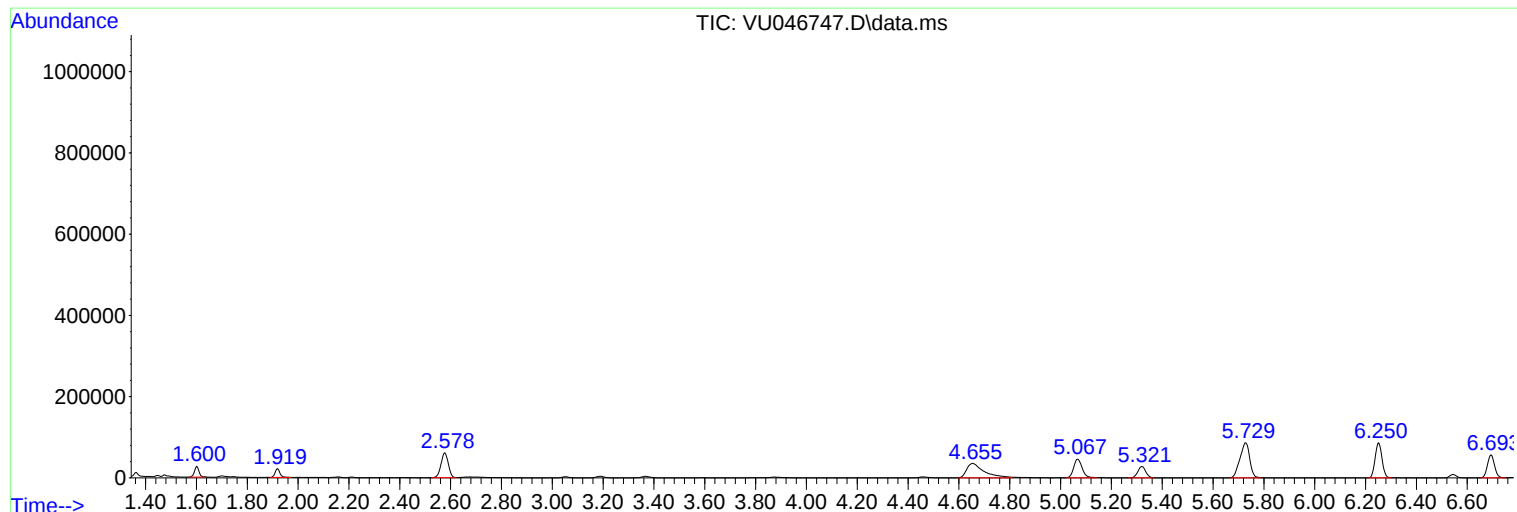
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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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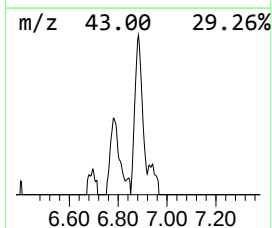
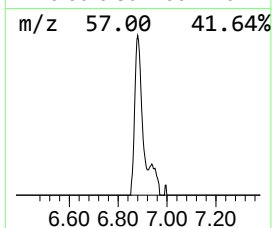
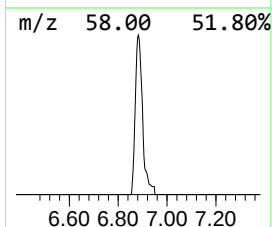
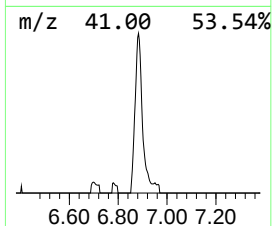
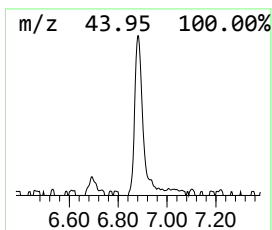
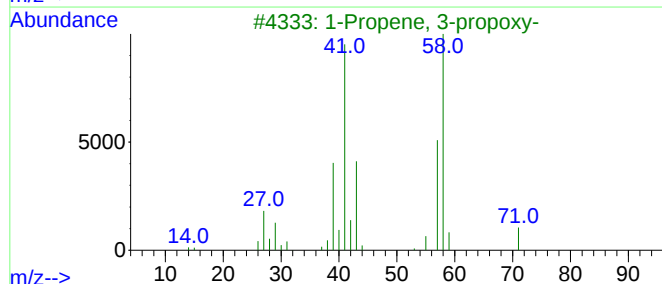
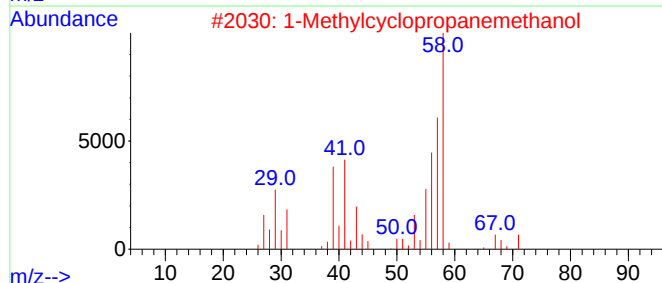
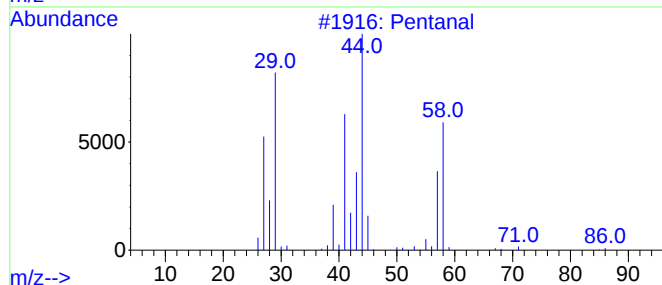
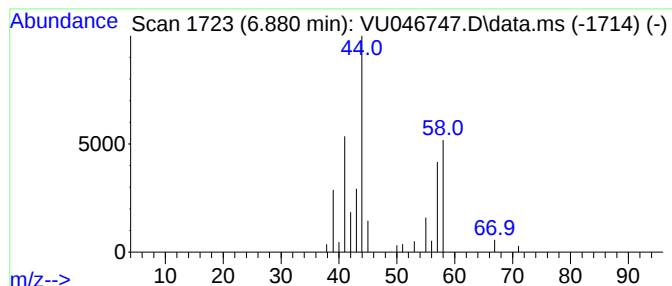
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 Pentanal Concentration Rank 6

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 6.880 | 1.09 ug/L | 35541 | 1,4-Difluorobenzene | 6.250 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentanal                     | 86  | C5H10O  | 000110-62-3 | 72   |
| 2    |    |   | 1-Methylcyclopropanemethanol | 86  | C5H10O  | 002746-14-7 | 10   |
| 3    |    |   | 1-Propene, 3-propoxy-        | 100 | C6H12O  | 001471-03-0 | 10   |
| 4    |    |   | Cyclopropyl carbinol         | 72  | C4H8O   | 002516-33-8 | 9    |
| 5    |    |   | Ethylene oxide               | 44  | C2H4O   | 000075-21-8 | 5    |



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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW8

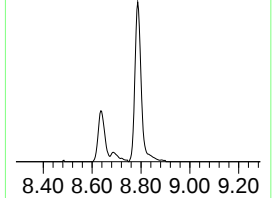
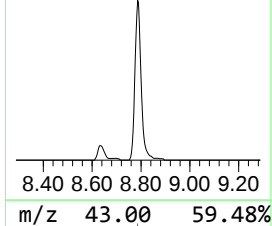
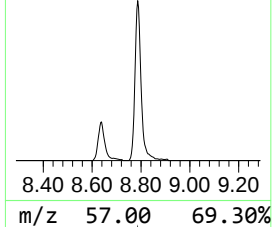
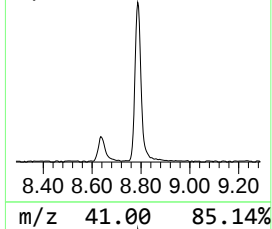
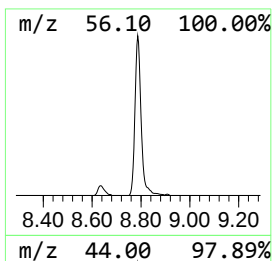
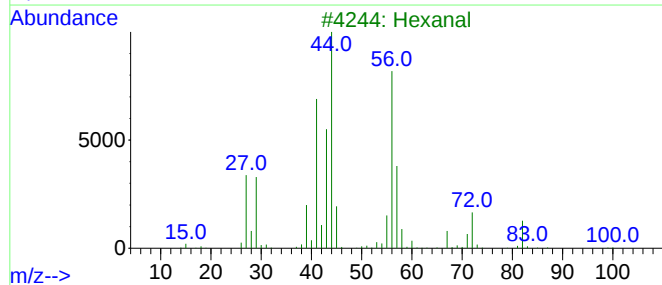
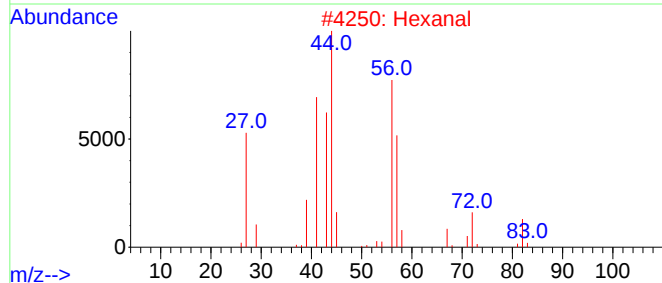
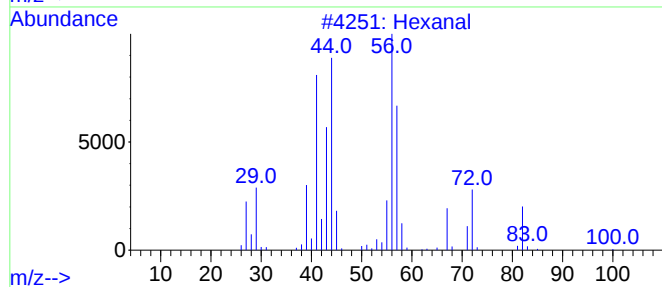
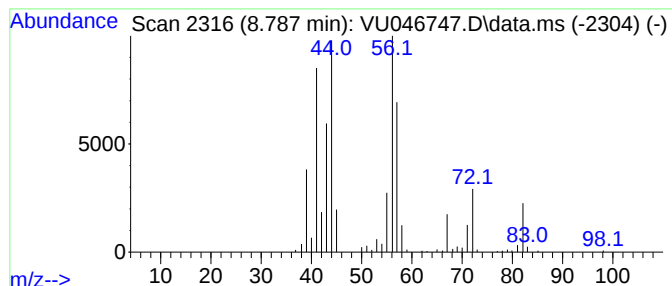
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 3 Hexanal Concentration Rank 3

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 8.787 | 5.82 ug/L | 255028 | Chlorobenzene-d5 | 9.417 |

| Hit# | of      | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------|---|--------------|-----|---------|-------------|------|
| 1    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 83   |
| 2    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 80   |
| 3    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 72   |
| 4    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 72   |
| 5    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 72   |



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Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW8

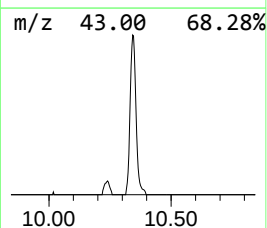
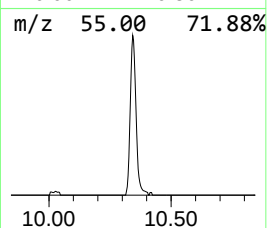
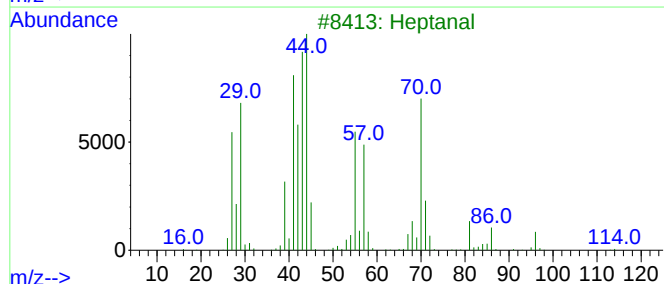
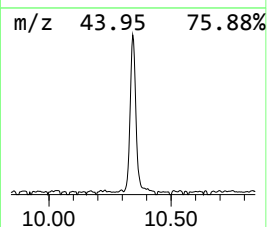
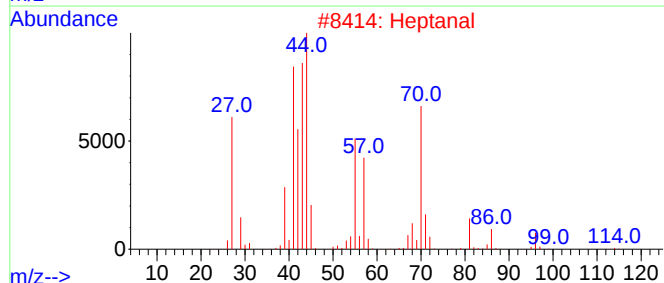
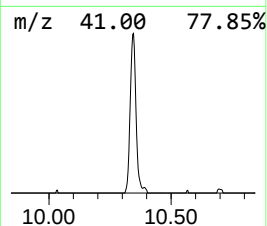
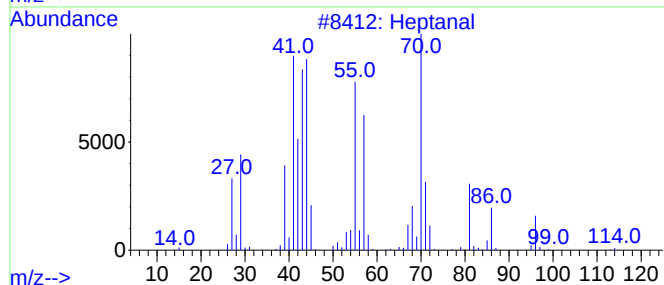
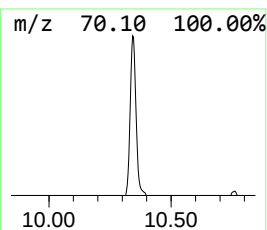
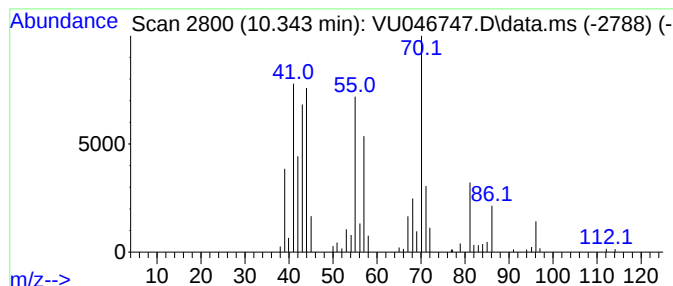
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 Heptanal Concentration Rank 4

| R.T.   | EstConc   | Area   | Relative to ISTD | R.T.  |
|--------|-----------|--------|------------------|-------|
| 10.343 | 2.66 ug/L | 116602 | Chlorobenzene-d5 | 9.417 |

| Hit# | of       | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----------|---|--------------|-----|---------|-------------|------|
| 1    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 96   |
| 2    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 94   |
| 3    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 93   |
| 4    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 76   |
| 5    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 72   |



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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW8

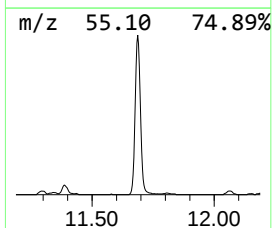
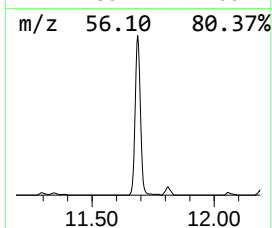
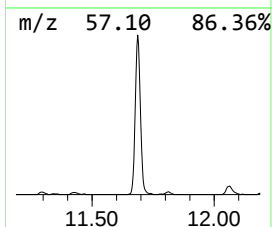
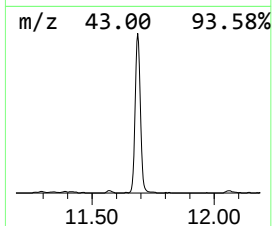
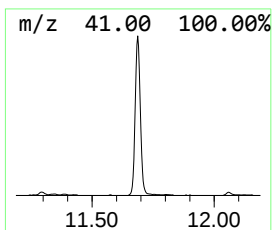
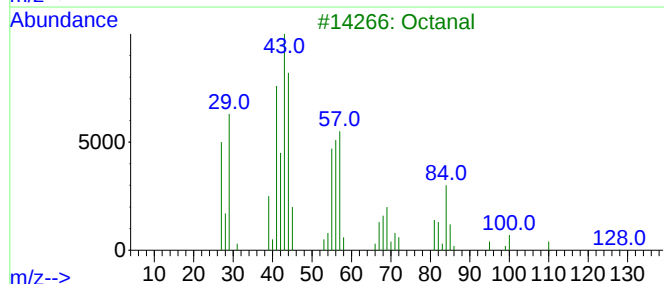
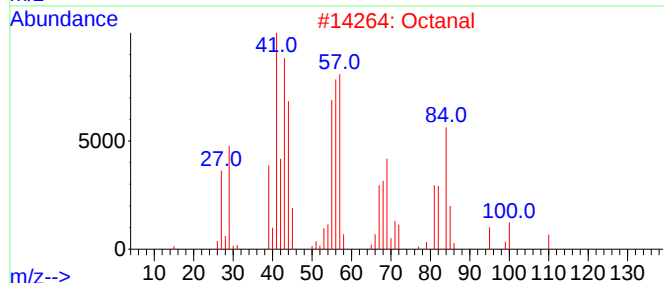
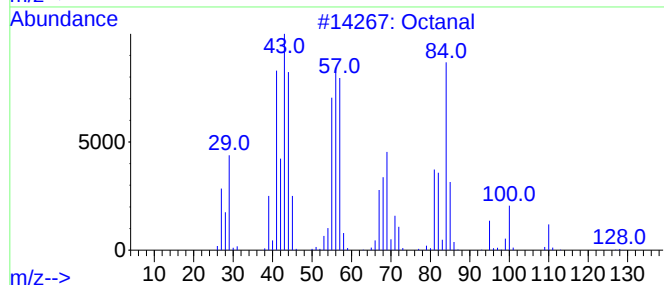
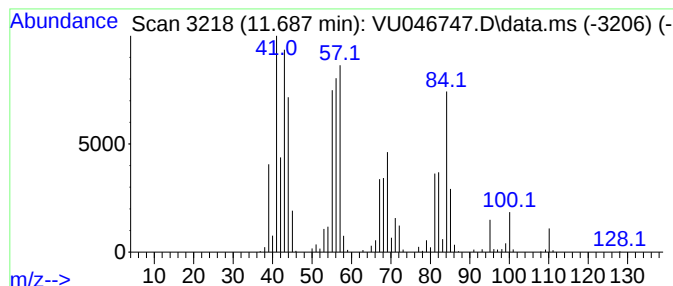
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Octanal Concentration Rank 2

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 11.687 | 10.48 ug/L | 551220 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# | of      | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------|---|--------------|-----|---------|-------------|------|
| 1    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 98   |
| 2    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 91   |
| 3    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 90   |
| 4    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 72   |
| 5    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 52   |



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Instrument :  
MSVOA\_U  
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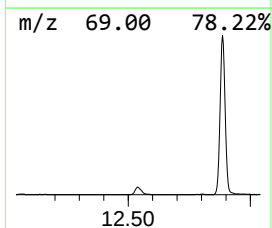
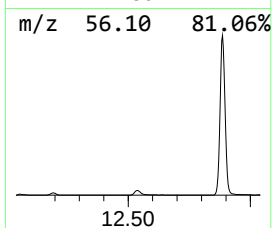
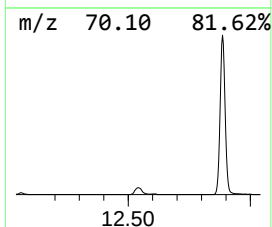
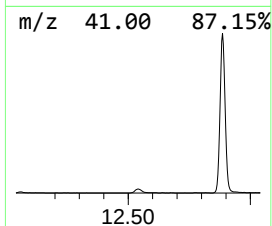
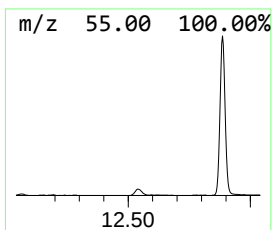
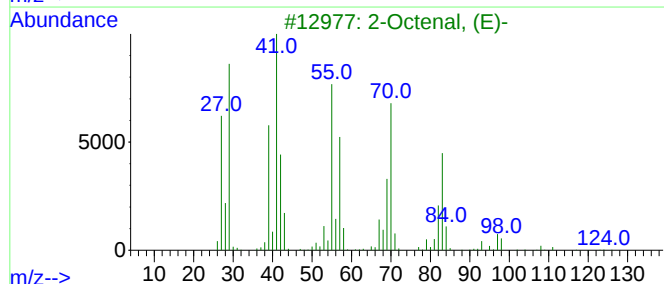
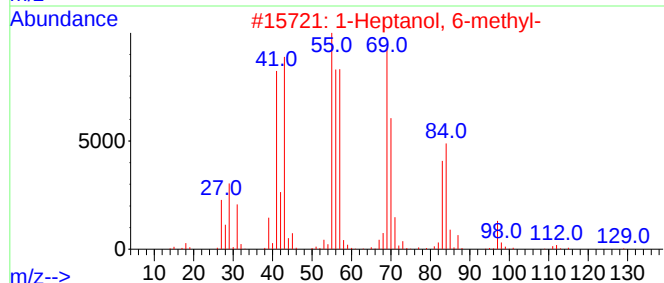
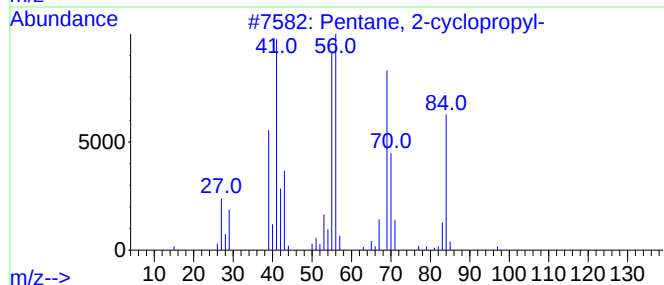
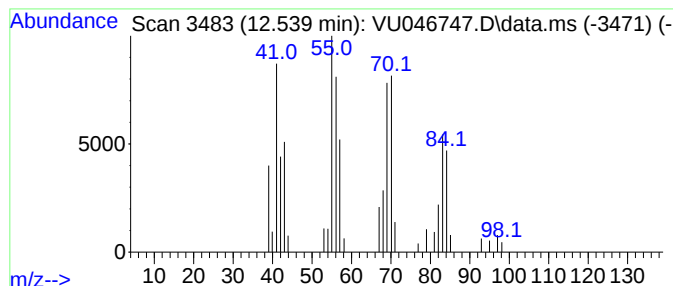
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 6 (DEL) Alkane: Cyclic12.539 Concentration Rank 8

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.539 | 0.93 ug/L | 48663 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Pentane, 2-cyclopropyl-             | 112 | C8H16    | 005458-16-2  | 43   |
| 2    |    |   | 1-Heptanol, 6-methyl-               | 130 | C8H18O   | 001653-40-3  | 43   |
| 3    |    |   | 2-Octenal, (E)-                     | 126 | C8H14O   | 002548-87-0  | 43   |
| 4    |    |   | Cyclopentane, 1,2-dimethyl-, cis-   | 98  | C7H14    | 001192-18-3  | 38   |
| 5    |    |   | cis-2,4-Dimethylthiane, S,S-dioxide | 162 | C7H14O2S | 1000215-67-5 | 38   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011222\  
Data File : VU046747.D  
Acq On : 12 Jan 2022 17:07  
Operator : SY/MD  
Sample : N1101-06  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW8

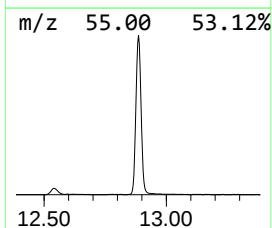
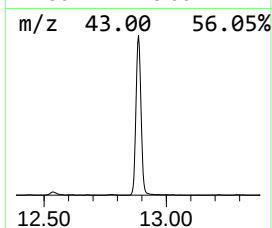
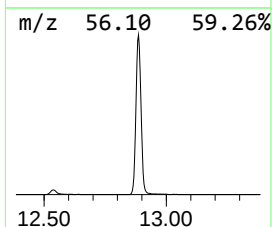
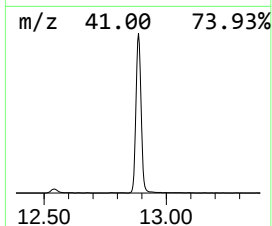
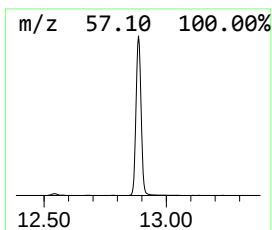
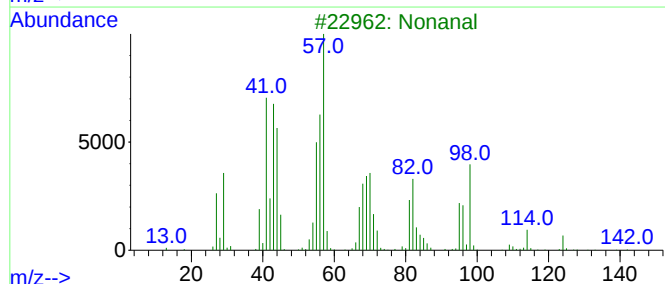
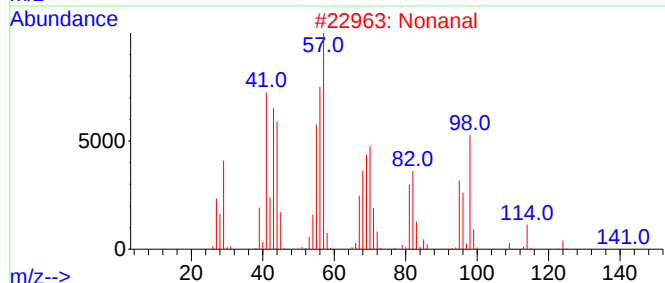
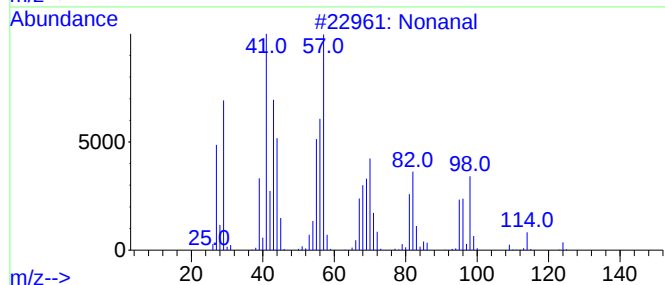
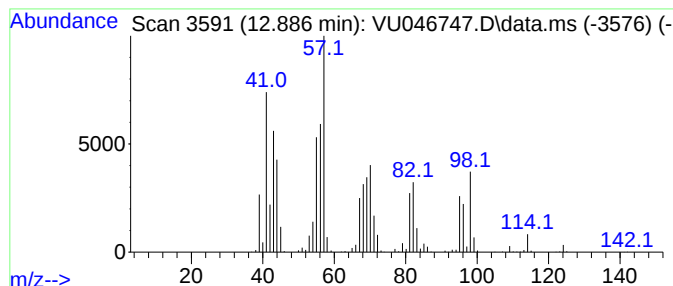
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Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 7 Nonanal Concentration Rank 1

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 12.886 | 30.07 ug/L | 1581050 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-----------------------------------|-----|----------|--------------|------|
| 1    |    |   | Nonanal                           | 142 | C9H18O   | 000124-19-6  | 91   |
| 2    |    |   | Nonanal                           | 142 | C9H18O   | 000124-19-6  | 91   |
| 3    |    |   | Nonanal                           | 142 | C9H18O   | 000124-19-6  | 86   |
| 4    |    |   | Nonanal                           | 142 | C9H18O   | 000124-19-6  | 83   |
| 5    |    |   | Carbonic acid, heptyl vinyl ester | 186 | C10H18O3 | 1010383-25-4 | 35   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011222\  
Data File : VU046747.D  
Acq On : 12 Jan 2022 17:07  
Operator : SY/MD  
Sample : N1101-06  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW8

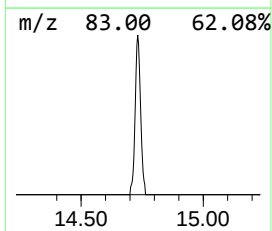
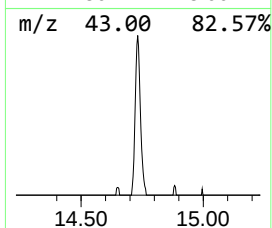
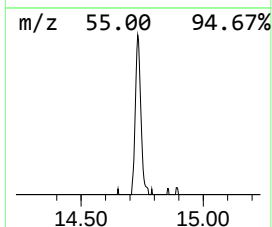
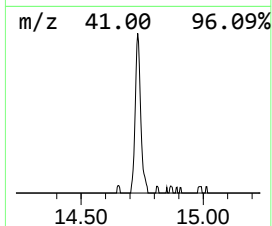
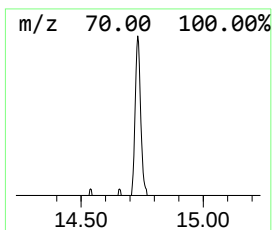
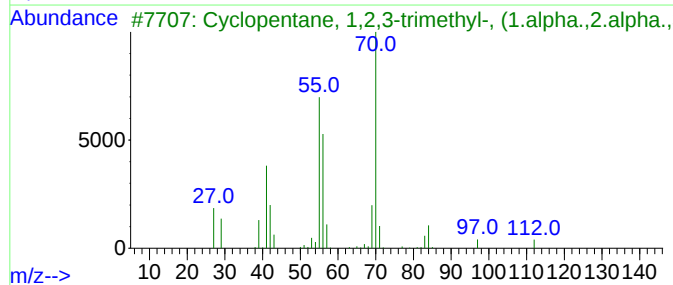
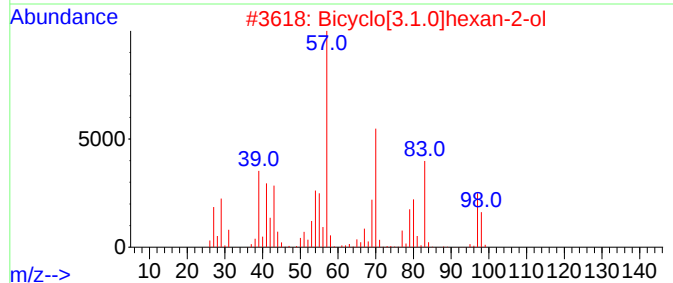
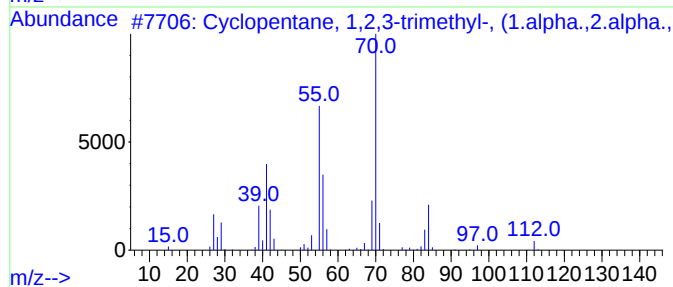
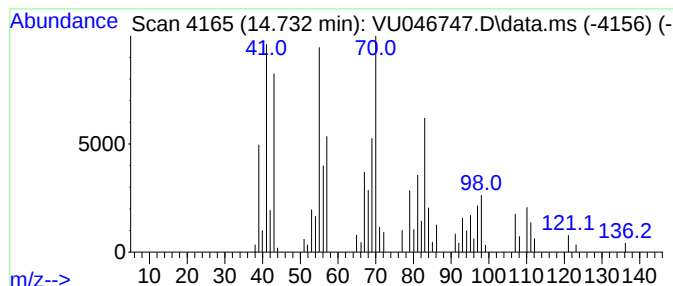
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Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 8 (DEL) Alkane: Cyclic14.732 Concentration Rank 7

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 14.732 | 1.01 ug/L | 52927 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Cyclopentane, 1,2,3-trimethyl-, ... | 112 | C8H16   | 002613-69-6  | 46   |
| 2    |    |   | Bicyclo[3.1.0]hexan-2-ol            | 98  | C6H10O  | 1000194-18-6 | 46   |
| 3    |    |   | Cyclopentane, 1,2,3-trimethyl-, ... | 112 | C8H16   | 002613-69-6  | 43   |
| 4    |    |   | 1-Undecanol                         | 172 | C11H24O | 000112-42-5  | 38   |
| 5    |    |   | 2-Heptenal, (Z)-                    | 112 | C7H12O  | 057266-86-1  | 38   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011222\  
Data File : VU046747.D  
Acq On : 12 Jan 2022 17:07  
Operator : SY/MD  
Sample : N1101-06  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Pentanal           | 6.880  | 1.1     | ug/L  | 35541    | 1                     | 6.250  | 163417 | 5.0  |
| Hexanal            | 8.787  | 5.8     | ug/L  | 255028   | 2                     | 9.417  | 219256 | 5.0  |
| Heptanal           | 10.343 | 2.7     | ug/L  | 116602   | 2                     | 9.417  | 219256 | 5.0  |
| Octanal            | 11.687 | 10.5    | ug/L  | 551220   | 3                     | 11.812 | 262867 | 5.0  |
| (DEL) Alkane: C... | 12.539 | 0.9     | ug/L  | 48663    | 3                     | 11.812 | 262867 | 5.0  |
| Nonanal            | 12.886 | 30.1    | ug/L  | 1581050  | 3                     | 11.812 | 262867 | 5.0  |
| (DEL) Alkane: C... | 14.732 | 1.0     | ug/L  | 52927    | 3                     | 11.812 | 262867 | 5.0  |