

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012022\  
 Data File : VU046804.D  
 Acq On : 20 Jan 2022 12:17  
 Operator : SY/MD  
 Sample : N1194-01DL 4X  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFX1DL

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\SFAMUTR011822WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU046804.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         | 1.472       | 34            | 41          | 56           | rVB      | 202303         | 200839        | 56.80%          | 5.860%        |
| 2         | 1.600       | 72            | 81          | 95           | rVB      | 36570          | 44838         | 12.68%          | 1.308%        |
| 3         | 1.919       | 171           | 180         | 198          | rBV      | 27196          | 39187         | 11.08%          | 1.143%        |
| 4         | 2.571       | 368           | 383         | 406          | rBV2     | 66338          | 118000        | 33.37%          | 3.443%        |
| 5         | 3.051       | 522           | 532         | 544          | rVB3     | 4634           | 8303          | 2.35%           | 0.242%        |
| 6         | 3.189       | 563           | 575         | 591          | rBV2     | 3819           | 9034          | 2.55%           | 0.264%        |
| 7         | 3.874       | 774           | 788         | 802          | rBV      | 17872          | 41866         | 11.84%          | 1.221%        |
| 8         | 4.645       | 1013          | 1028        | 1078         | rBV      | 39935          | 147343        | 41.67%          | 4.299%        |
| 9         | 5.067       | 1145          | 1159        | 1180         | rBV      | 53126          | 127412        | 36.03%          | 3.717%        |
| 10        | 5.729       | 1344          | 1365        | 1383         | rBV2     | 106765         | 279710        | 79.10%          | 8.161%        |
| 11        | 6.250       | 1513          | 1527        | 1551         | rBV      | 122644         | 231806        | 65.55%          | 6.763%        |
| 12        | 6.546       | 1606          | 1619        | 1633         | rBV3     | 41378          | 76895         | 21.75%          | 2.243%        |
| 13        | 6.693       | 1652          | 1665        | 1688         | rBV      | 67836          | 128188        | 36.25%          | 3.740%        |
| 14        | 7.568       | 1926          | 1937        | 1951         | rBV2     | 32467          | 56029         | 15.84%          | 1.635%        |
| 15        | 7.899       | 2028          | 2040        | 2055         | rBV      | 127627         | 220347        | 62.31%          | 6.429%        |
| 16        | 8.131       | 2105          | 2112        | 2118         | rBV3     | 3299           | 4523          | 1.28%           | 0.132%        |
| 17        | 8.182       | 2118          | 2128        | 2144         | rVB      | 20510          | 34680         | 9.81%           | 1.012%        |
| 18        | 8.555       | 2236          | 2244        | 2252         | rBV4     | 3377           | 5259          | 1.49%           | 0.153%        |
| 19        | 8.639       | 2258          | 2270        | 2306         | rBV      | 196996         | 353612        | 100.00%         | 10.317%       |
| 20        | 8.790       | 2306          | 2317        | 2339         | rVB2     | 33153          | 59477         | 16.82%          | 1.735%        |
| 21        | 9.420       | 2500          | 2513        | 2531         | rBV      | 194105         | 318112        | 89.96%          | 9.281%        |
| 22        | 10.346      | 2793          | 2801        | 2814         | rVB2     | 6590           | 9671          | 2.73%           | 0.282%        |
| 23        | 10.758      | 2917          | 2929        | 2943         | rVB2     | 60703          | 98524         | 27.86%          | 2.874%        |
| 24        | 11.690      | 3207          | 3219        | 3229         | rBV3     | 19231          | 28608         | 8.09%           | 0.835%        |
| 25        | 11.812      | 3245          | 3257        | 3273         | rBV      | 213265         | 339219        | 95.93%          | 9.897%        |
| 26        | 12.195      | 3361          | 3376        | 3393         | rBV      | 130960         | 209880        | 59.35%          | 6.123%        |
| 27        | 12.889      | 3582          | 3592        | 3613         | rBV      | 160165         | 236161        | 66.79%          | 6.890%        |

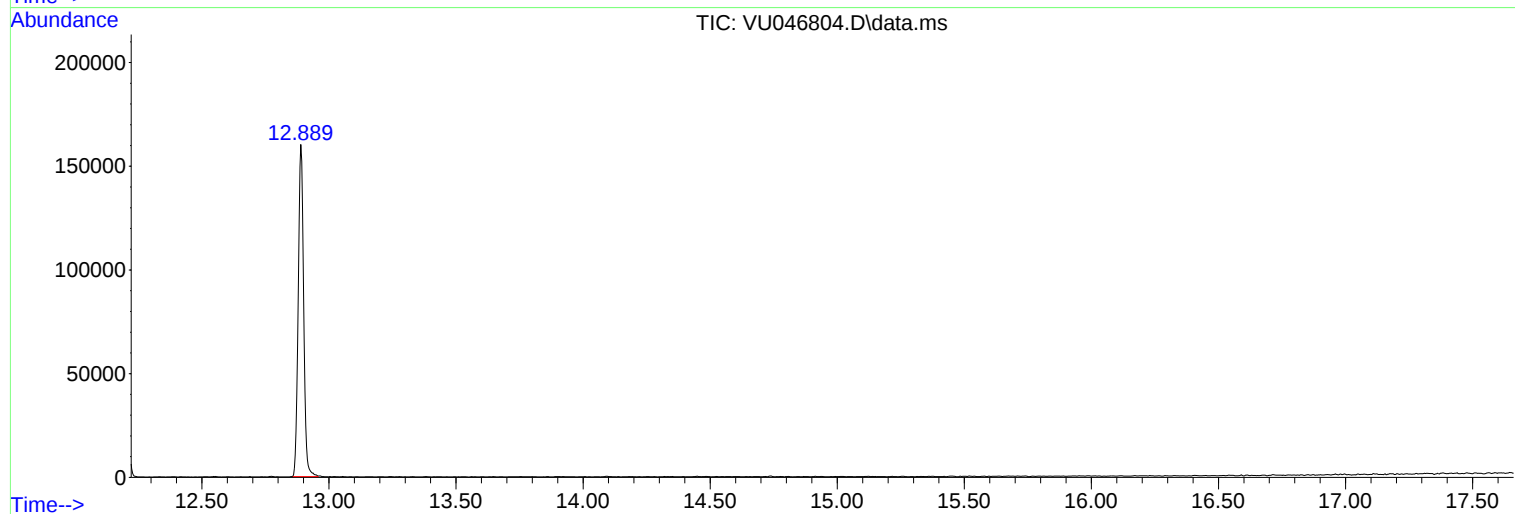
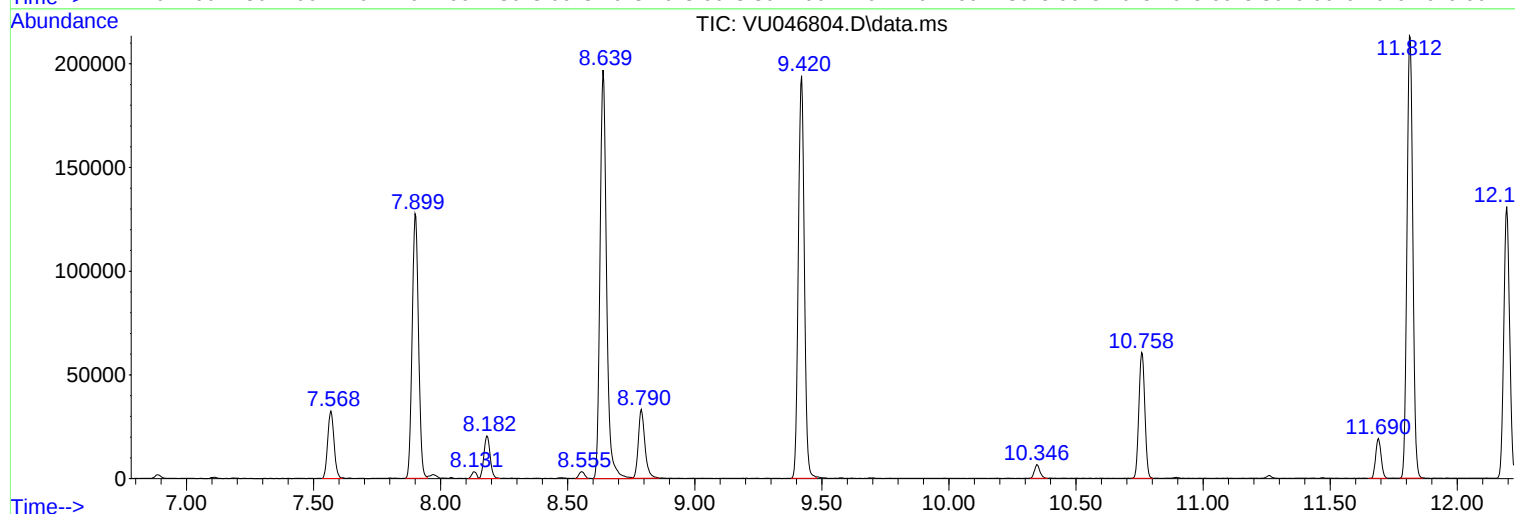
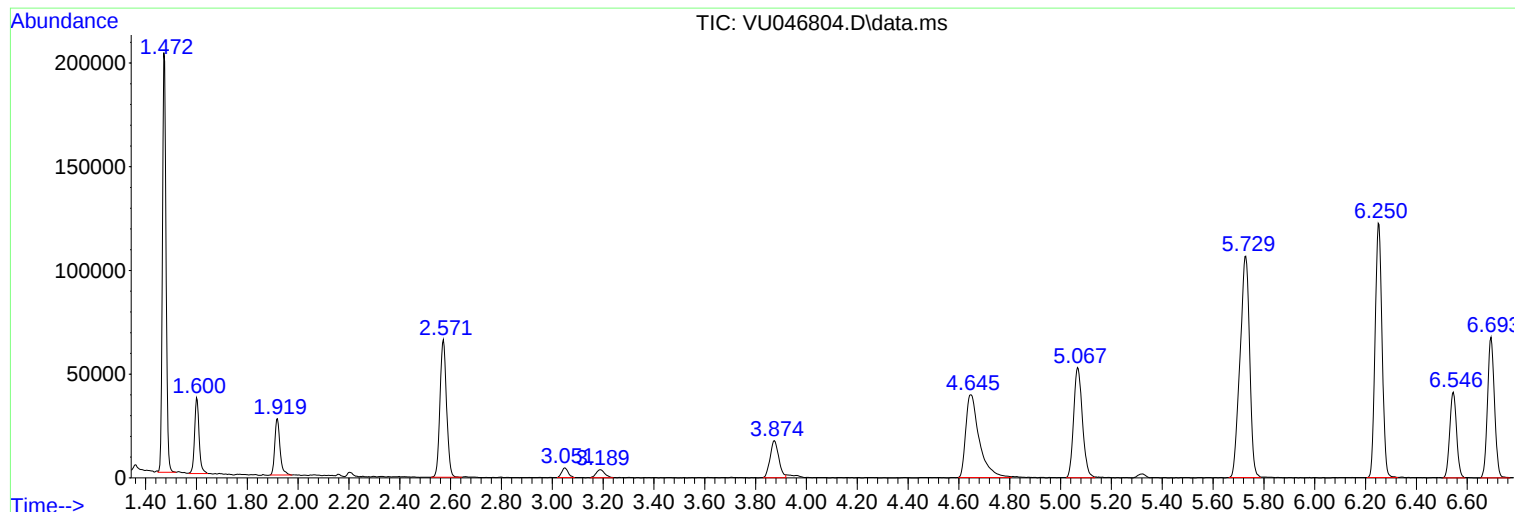
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Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXX1DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR011822WMA.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 :  
BFXX1DL

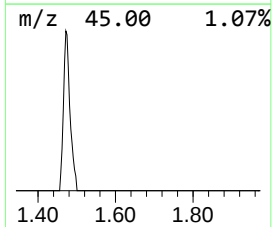
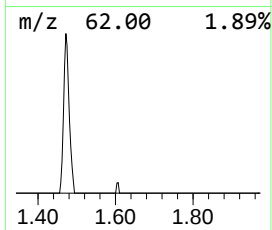
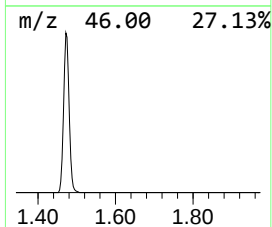
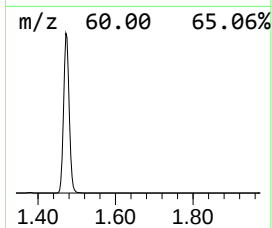
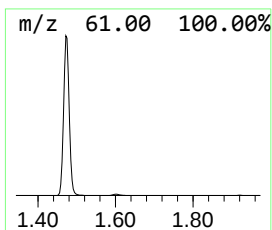
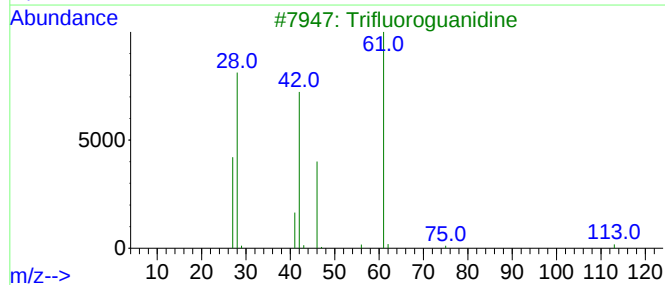
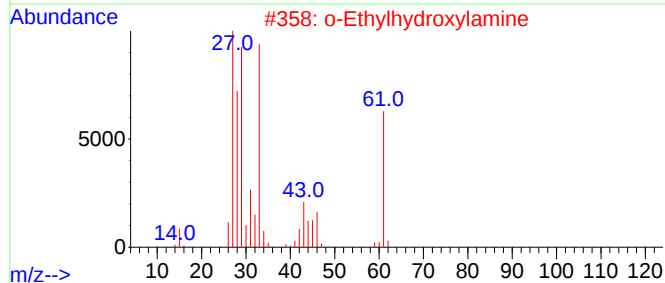
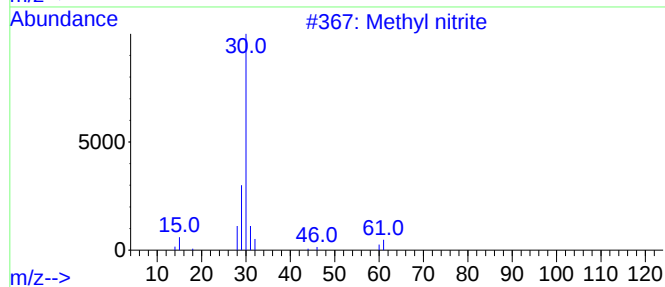
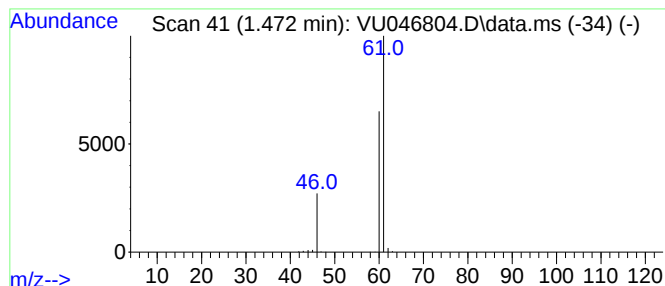
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR011822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 unknown-01 Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.472 | 4.33 ug/L | 200839 | 1,4-Difluorobenzene | 6.250 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Methyl nitrite       | 61  | CH3NO2  | 000624-91-9 | 5    |
| 2    |    |   | o-Ethylhydroxylamine | 61  | C2H7NO  | 000624-86-2 | 4    |
| 3    |    |   | Trifluoroguanidine   | 113 | CH2F3N3 | 037950-72-4 | 4    |
| 4    |    |   | Cyanogen chloride    | 61  | CClN    | 000506-77-4 | 4    |
| 5    |    |   | Cyanogen chloride    | 61  | CClN    | 000506-77-4 | 4    |



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Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFX1DL

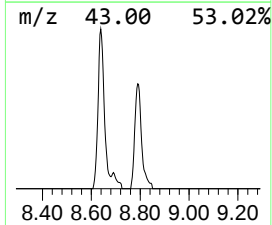
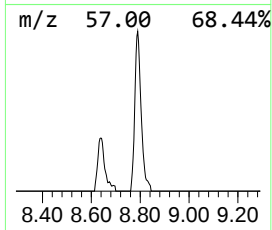
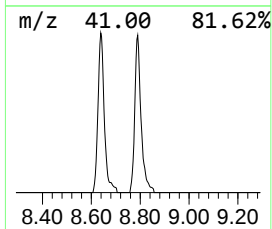
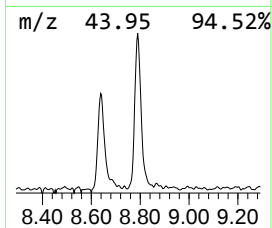
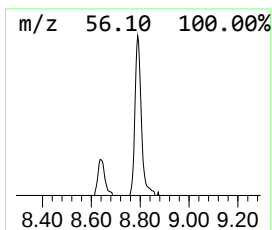
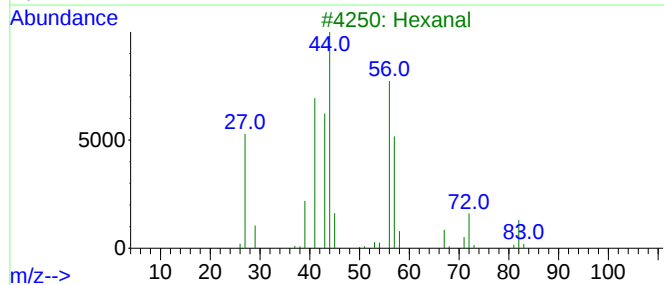
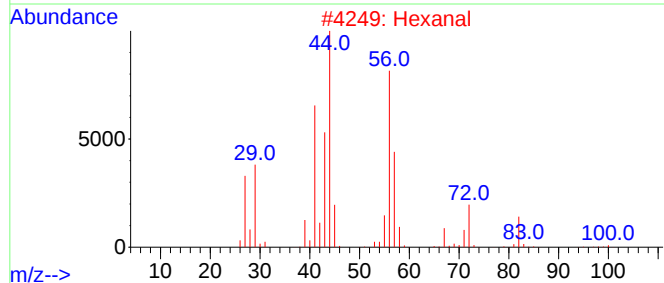
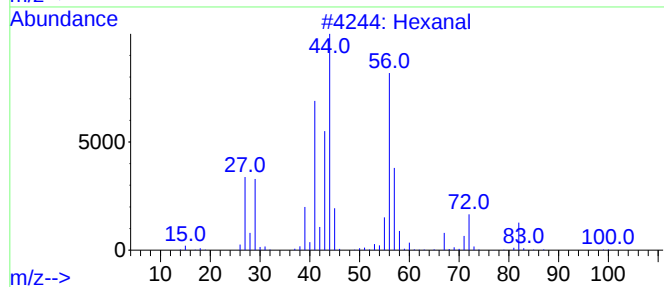
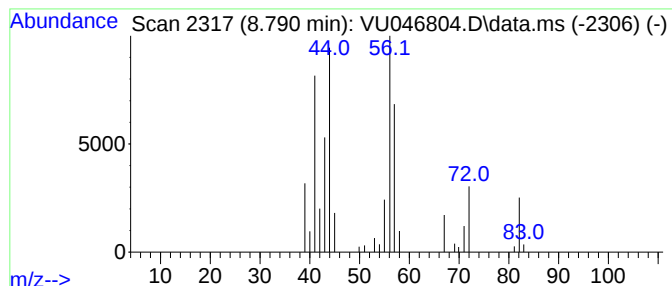
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR011822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 3 Hexanal Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 8.790 | 0.93 ug/L | 59477 | Chlorobenzene-d5 | 9.420 |

| Hit# | of             | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----------------|---|--------------|-----|---------|-------------|------|
| 1    | Hexanal        |   |              | 100 | C6H12O  | 000066-25-1 | 83   |
| 2    | Hexanal        |   |              | 100 | C6H12O  | 000066-25-1 | 78   |
| 3    | Hexanal        |   |              | 100 | C6H12O  | 000066-25-1 | 78   |
| 4    | Hexanal        |   |              | 100 | C6H12O  | 000066-25-1 | 78   |
| 5    | Glutaraldehyde |   |              | 100 | C5H8O2  | 000111-30-8 | 37   |



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MSVOA\_U  
ClientSampleId :  
BFX1DL

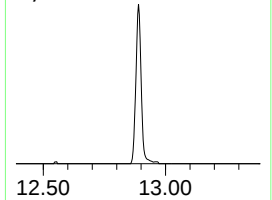
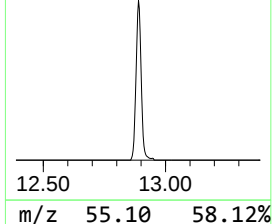
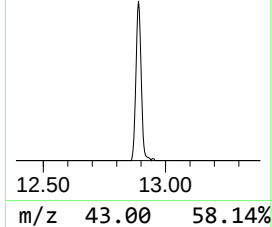
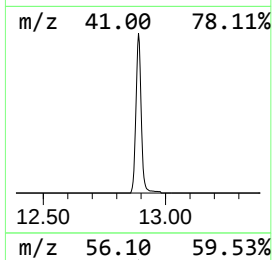
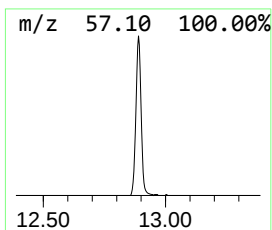
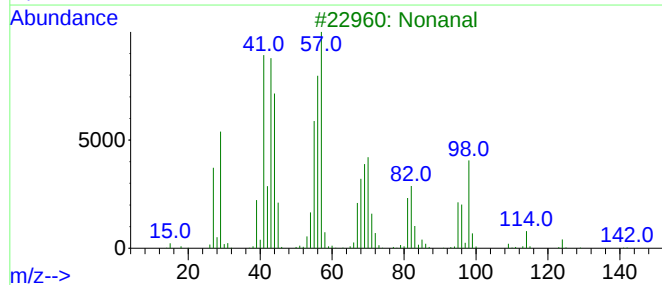
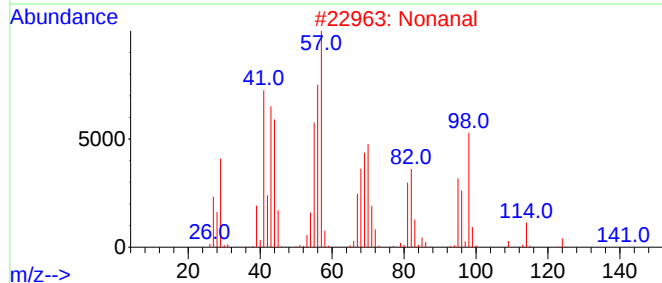
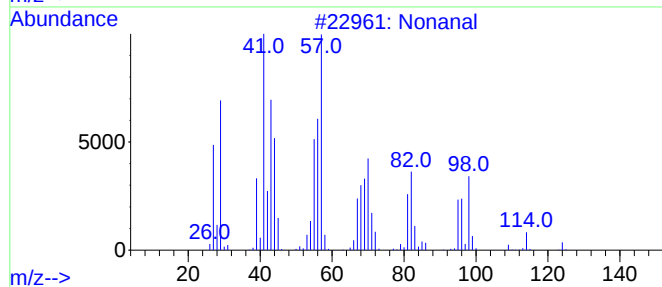
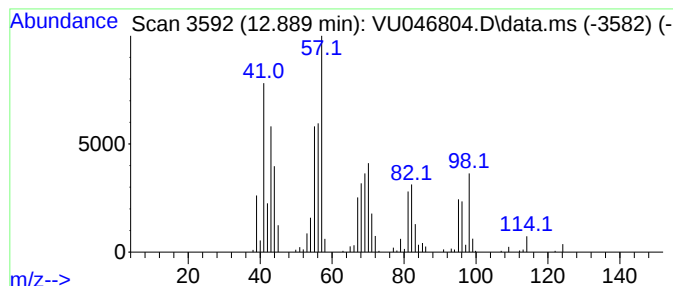
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR011822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 Nonanal Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.889 | 3.48 ug/L | 236161 | 1,4-Dichlorobenzene-d4 | 11.815 |

| 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 | 83   |
| 4    | Nonanal                         |   |              | 142 | C9H18O  | 000124-19-6 | 64   |
| 5    | Cyclohexanol, 2-methyl-, trans- |   |              | 114 | C7H14O  | 007443-52-9 | 42   |



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MSVOA\_U  
ClientSampleId :  
BFXX1DL

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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 |
| unknown-01       | 1.472  | 4.3     | ug/L  | 200839   | 1                     | 6.250  | 231806 | 5.0  |
| Hexanal          | 8.790  | 0.9     | ug/L  | 59477    | 2                     | 9.420  | 318112 | 5.0  |
| Nonanal          | 12.889 | 3.5     | ug/L  | 236161   | 3                     | 11.815 | 339219 | 5.0  |