

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011322\  
 Data File : VU046753.D  
 Acq On : 13 Jan 2022 13:35  
 Operator : SY/MD  
 Sample : N1101-07  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFXW9

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: VU046753.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         | 1.363       | 3             | 7           | 14           | rVB2     | 34144          | 31300         | 2.12%           | 0.641%        |
| 2         | 1.475       | 36            | 42          | 53           | rVB      | 34218          | 36425         | 2.46%           | 0.746%        |
| 3         | 1.600       | 71            | 81          | 94           | rVB2     | 35676          | 49951         | 3.38%           | 1.023%        |
| 4         | 1.919       | 172           | 180         | 195          | rBV      | 22952          | 31447         | 2.13%           | 0.644%        |
| 5         | 2.581       | 365           | 386         | 401          | rBV4     | 107982         | 209320        | 14.15%          | 4.285%        |
| 6         | 3.877       | 771           | 789         | 808          | rBV      | 157832         | 375565        | 25.40%          | 7.688%        |
| 7         | 4.645       | 1012          | 1028        | 1068         | rBV      | 44038          | 162871        | 11.01%          | 3.334%        |
| 8         | 5.070       | 1145          | 1160        | 1179         | rBV      | 48223          | 113428        | 7.67%           | 2.322%        |
| 9         | 5.324       | 1224          | 1239        | 1253         | rBB      | 21880          | 48175         | 3.26%           | 0.986%        |
| 10        | 5.729       | 1345          | 1365        | 1380         | rBV2     | 90991          | 240497        | 16.26%          | 4.923%        |
| 11        | 6.253       | 1514          | 1528        | 1544         | rBV      | 95755          | 177376        | 11.99%          | 3.631%        |
| 12        | 6.546       | 1604          | 1619        | 1653         | rBV      | 792898         | 1478858       | 100.00%         | 30.274%       |
| 13        | 6.693       | 1653          | 1665        | 1685         | rVB      | 60680          | 119579        | 8.09%           | 2.448%        |
| 14        | 7.568       | 1926          | 1937        | 1953         | rBV2     | 30578          | 52813         | 3.57%           | 1.081%        |
| 15        | 7.902       | 2028          | 2041        | 2055         | rBV      | 106071         | 181056        | 12.24%          | 3.706%        |
| 16        | 8.182       | 2116          | 2128        | 2141         | rBV3     | 19527          | 32505         | 2.20%           | 0.665%        |
| 17        | 8.555       | 2232          | 2244        | 2258         | rVB2     | 52194          | 84907         | 5.74%           | 1.738%        |
| 18        | 8.639       | 2258          | 2270        | 2299         | rBV      | 210739         | 376149        | 25.44%          | 7.700%        |
| 19        | 8.790       | 2307          | 2317        | 2340         | rBV      | 39974          | 71274         | 4.82%           | 1.459%        |
| 20        | 9.420       | 2501          | 2513        | 2536         | rBV      | 140836         | 233554        | 15.79%          | 4.781%        |
| 21        | 10.346      | 2792          | 2801        | 2812         | rBV4     | 9831           | 15223         | 1.03%           | 0.312%        |
| 22        | 10.761      | 2919          | 2930        | 2945         | rVB      | 63931          | 100819        | 6.82%           | 2.064%        |
| 23        | 11.690      | 3210          | 3219        | 3230         | rBV2     | 25724          | 39042         | 2.64%           | 0.799%        |
| 24        | 11.815      | 3245          | 3258        | 3275         | rBV      | 162595         | 260147        | 17.59%          | 5.326%        |
| 25        | 12.195      | 3364          | 3376        | 3393         | rVB      | 121931         | 194675        | 13.16%          | 3.985%        |
| 26        | 12.889      | 3580          | 3592        | 3607         | rBV2     | 113575         | 167907        | 11.35%          | 3.437%        |

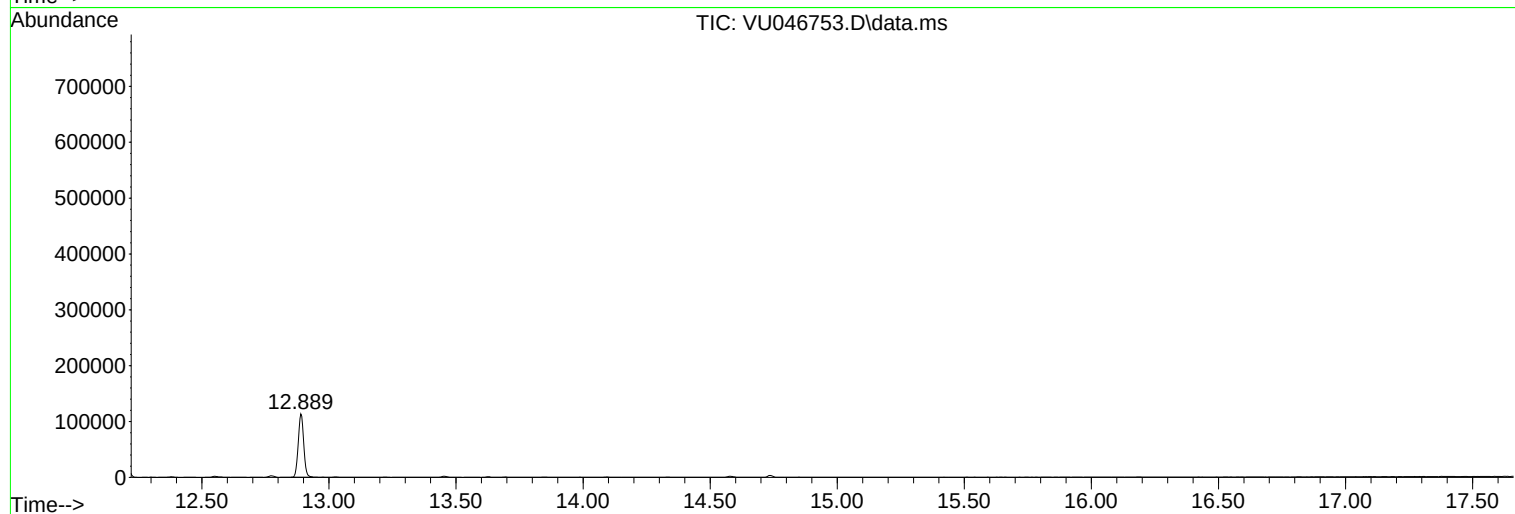
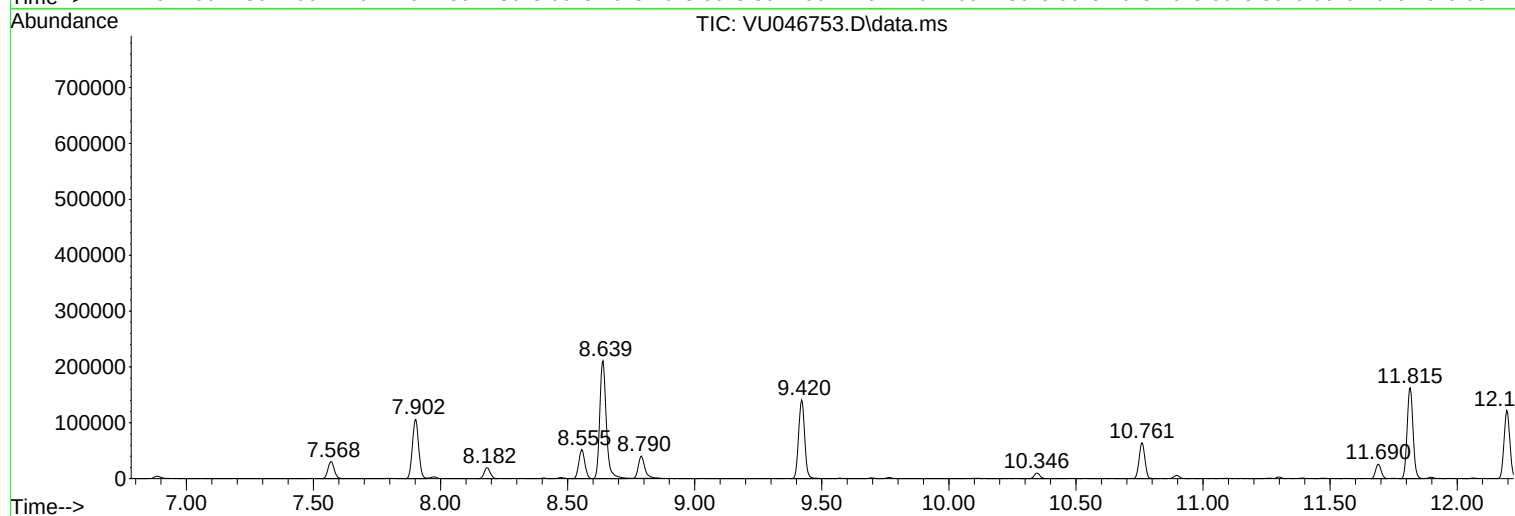
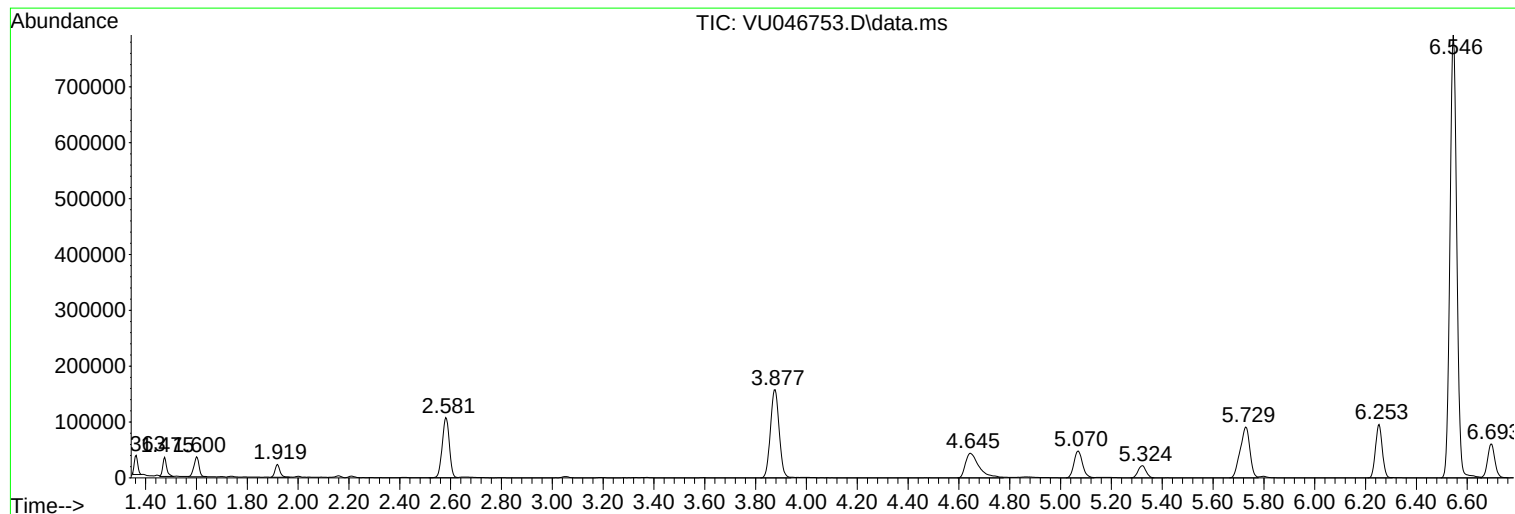
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Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW9

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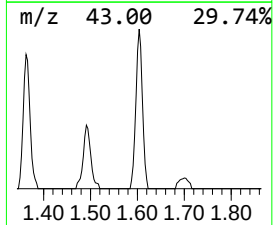
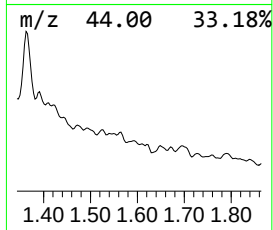
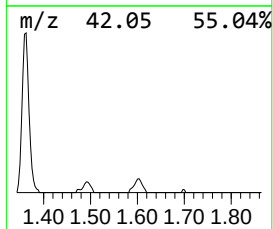
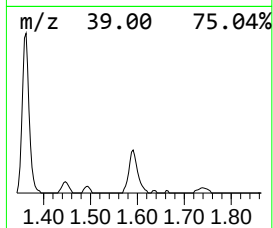
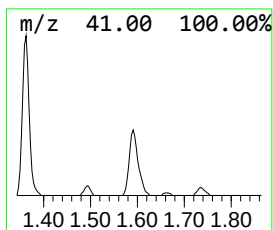
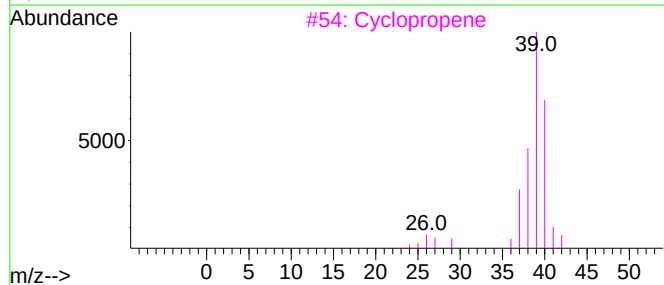
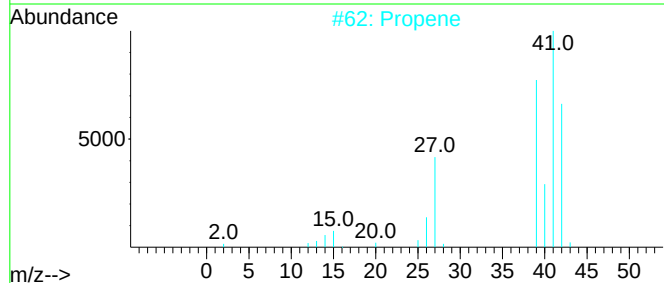
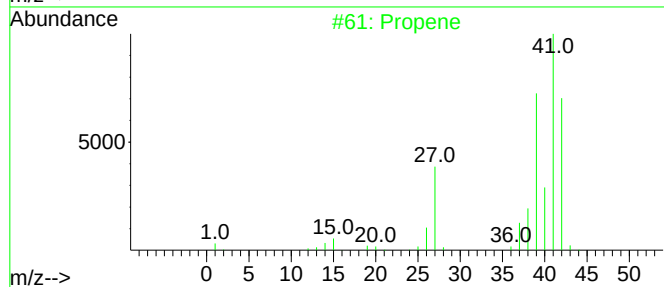
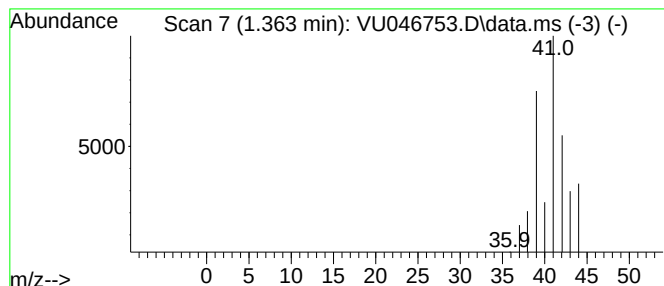
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.363 | 0.88 ug/L | 31300 | 1,4-Difluorobenzene | 6.253 |

| Hit# | of | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------|----|---------|-------------|------|
| 1    |    |   | Propene      | 42 | C3H6    | 000115-07-1 | 90   |
| 2    |    |   | Propene      | 42 | C3H6    | 000115-07-1 | 42   |
| 3    |    |   | Cyclopropene | 40 | C3H4    | 002781-85-3 | 9    |
| 4    |    |   | Cyclopropane | 42 | C3H6    | 000075-19-4 | 7    |
| 5    |    |   | Cyclopropane | 42 | C3H6    | 000075-19-4 | 7    |



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Sample : N1101-07  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW9

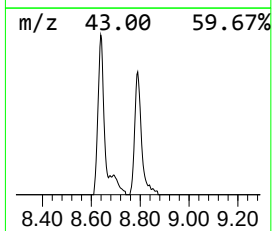
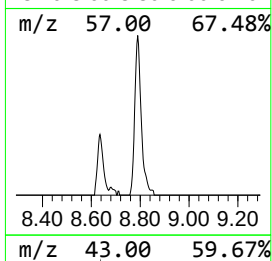
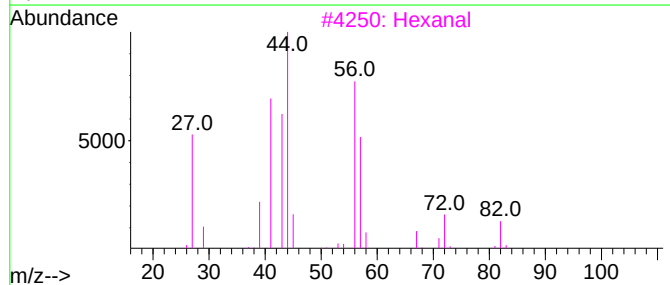
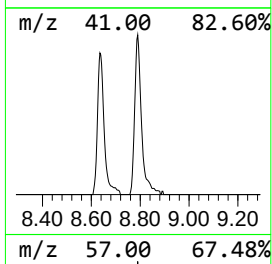
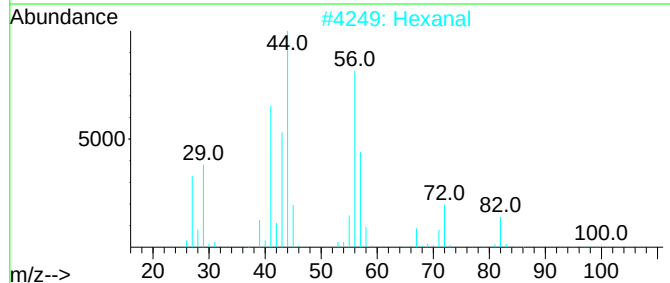
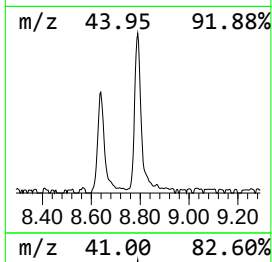
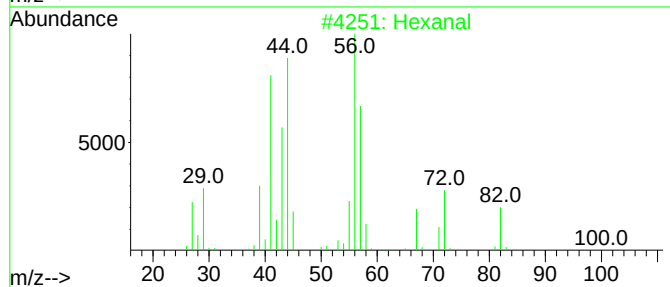
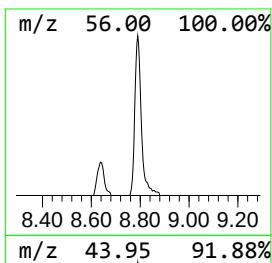
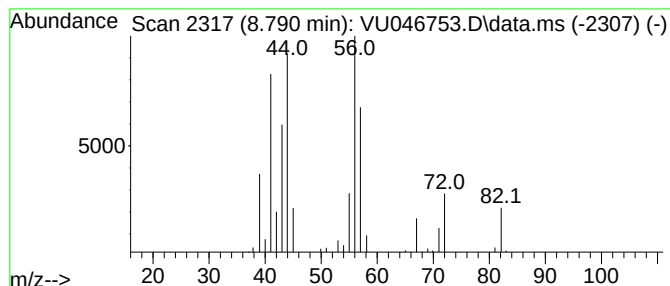
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 Hexanal Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 8.790 | 1.53 ug/L | 71274 | Chlorobenzene-d5 | 9.420 |

| Hit# | of      | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------|---|--------------|-----|---------|-------------|------|
| 1    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 78   |
| 2    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 78   |
| 3    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 78   |
| 4    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 72   |
| 5    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 64   |



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Sample : N1101-07  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW9

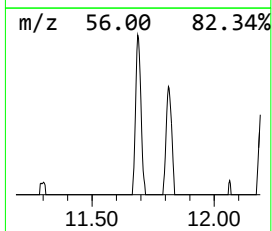
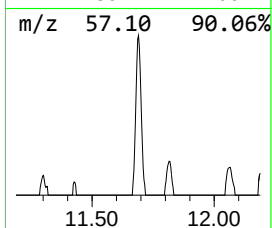
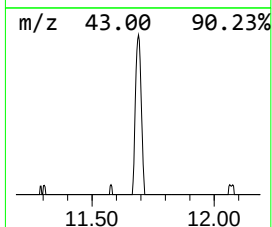
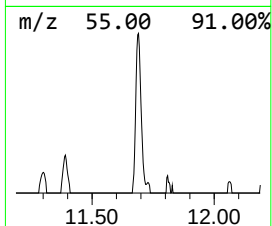
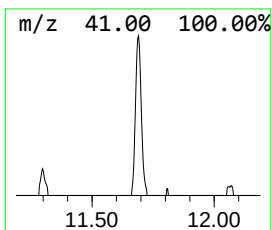
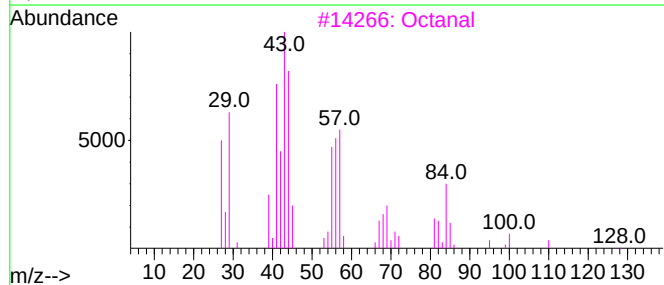
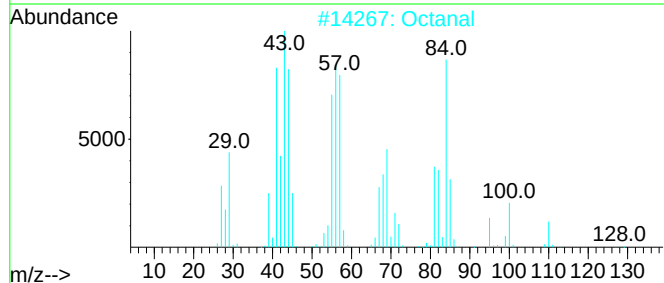
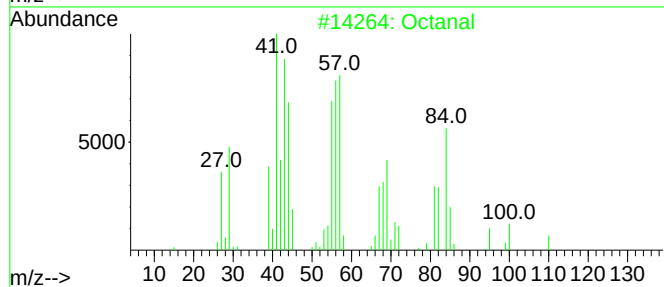
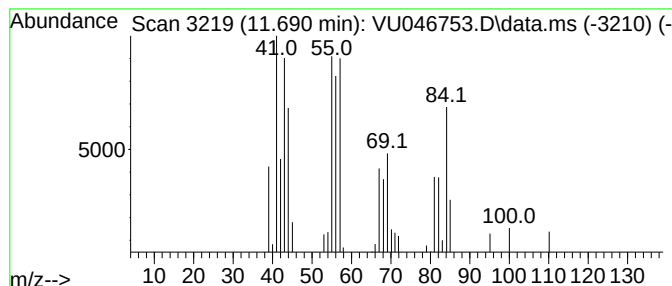
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 5 Octanal Concentration Rank 6

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 11.690 | 0.75 ug/L | 39042 | 1,4-Dichlorobenzene-d4 | 11.816 |

| Hit# | of      | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------|---|--------------|-----|---------|-------------|------|
| 1    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 91   |
| 2    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 87   |
| 3    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 72   |
| 4    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 72   |
| 5    | Octanal |   |              | 128 | C8H16O  | 000124-13-0 | 64   |



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

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFXW9

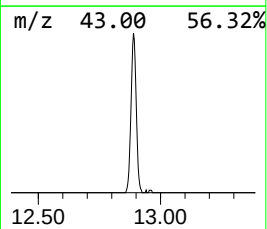
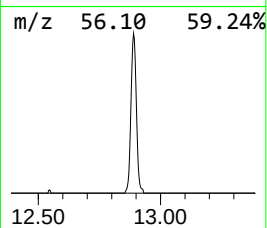
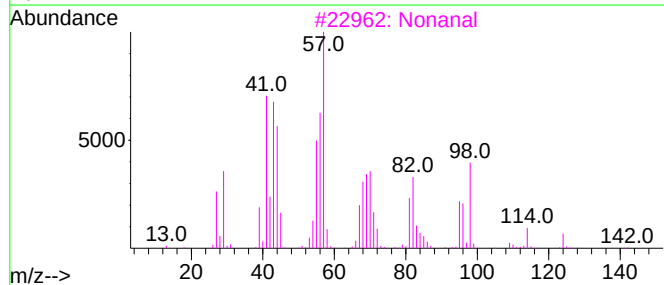
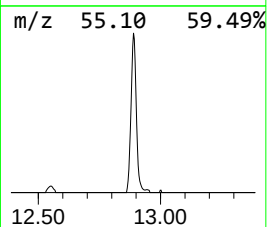
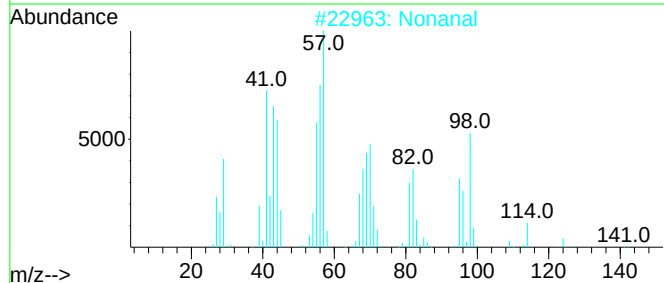
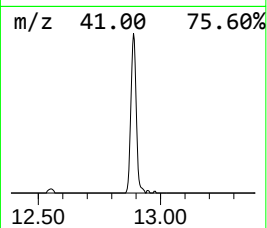
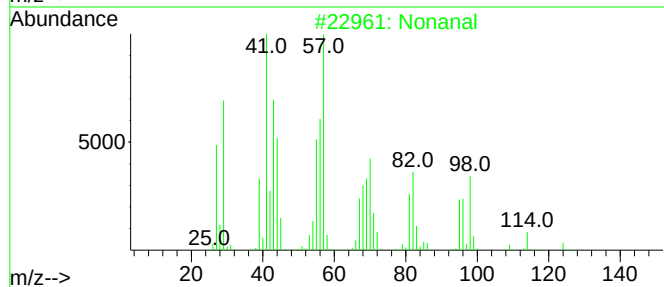
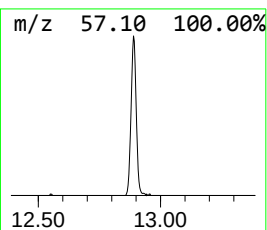
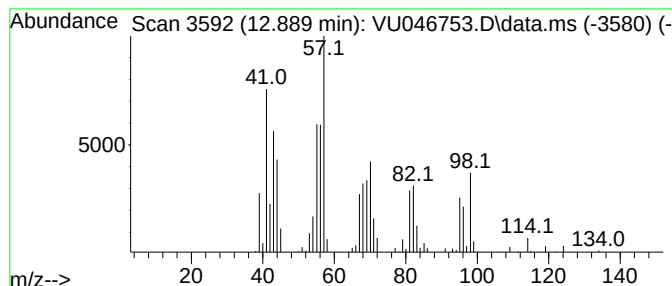
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 6 Nonanal Concentration Rank 1

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.889 | 3.23 ug/L | 167907 | 1,4-Dichlorobenzene-d4 | 11.816 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-----------------------------------|-----|----------|--------------|------|
| 1    |    |   | Nonanal                           | 142 | C9H18O   | 000124-19-6  | 91   |
| 2    |    |   | Nonanal                           | 142 | C9H18O   | 000124-19-6  | 90   |
| 3    |    |   | Nonanal                           | 142 | C9H18O   | 000124-19-6  | 72   |
| 4    |    |   | Aziridine, 2-ethyl-               | 71  | C4H9N    | 002549-67-9  | 22   |
| 5    |    |   | Carbonic acid, heptyl vinyl ester | 186 | C10H18O3 | 1010383-25-4 | 22   |



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BFXW9

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| (DEL) Alkane: S... | 1.363  | 0.9     | ug/L  | 31300    | 1                     | 6.253  | 177376 | 5.0  |
| Hexanal            | 8.790  | 1.5     | ug/L  | 71274    | 2                     | 9.420  | 233554 | 5.0  |
| Octanal            | 11.690 | 0.8     | ug/L  | 39042    | 3                     | 11.816 | 260147 | 5.0  |
| Nonanal            | 12.889 | 3.2     | ug/L  | 167907   | 3                     | 11.816 | 260147 | 5.0  |