

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101022\  
 Data File : VU051364.D  
 Acq On : 11 Oct 2022 07:02  
 Operator : JC/MD  
 Sample : N5071-20  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 53 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C1BD5

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\SFAMUTR100722WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051364.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         | 1.485       | 39            | 45          | 51           | rBV      | 8592           | 9362          | 1.26%           | 0.154%        |
| 2         | 1.597       | 71            | 80          | 90           | rBV      | 71283          | 81526         | 11.01%          | 1.344%        |
| 3         | 1.764       | 125           | 132         | 141          | rBV3     | 5169           | 8174          | 1.10%           | 0.135%        |
| 4         | 1.912       | 169           | 178         | 191          | rVB      | 76162          | 99539         | 13.44%          | 1.641%        |
| 5         | 2.565       | 367           | 381         | 392          | rBV      | 116400         | 187824        | 25.36%          | 3.097%        |
| 6         | 2.623       | 392           | 399         | 414          | rVB      | 16446          | 28481         | 3.85%           | 0.470%        |
| 7         | 3.835       | 758           | 776         | 788          | rVB      | 5948           | 17176         | 2.32%           | 0.283%        |
| 8         | 4.620       | 1008          | 1020        | 1046         | rBV2     | 118455         | 307288        | 41.49%          | 5.067%        |
| 9         | 4.813       | 1069          | 1080        | 1098         | rVB2     | 7710           | 16843         | 2.27%           | 0.278%        |
| 10        | 5.060       | 1142          | 1157        | 1177         | rBV      | 161809         | 361214        | 48.77%          | 5.957%        |
| 11        | 5.192       | 1180          | 1198        | 1215         | rVB      | 6084           | 21639         | 2.92%           | 0.357%        |
| 12        | 5.726       | 1341          | 1364        | 1389         | rBV2     | 255563         | 680198        | 91.84%          | 11.217%       |
| 13        | 6.247       | 1510          | 1526        | 1544         | rBV      | 229485         | 439677        | 59.36%          | 7.251%        |
| 14        | 6.690       | 1650          | 1664        | 1683         | rBV      | 180454         | 352979        | 47.66%          | 5.821%        |
| 15        | 7.565       | 1923          | 1936        | 1956         | rBV2     | 69212          | 122042        | 16.48%          | 2.013%        |
| 16        | 7.896       | 2025          | 2039        | 2054         | rBV      | 249909         | 441744        | 59.64%          | 7.285%        |
| 17        | 7.967       | 2055          | 2061        | 2072         | rVB2     | 8663           | 15446         | 2.09%           | 0.255%        |
| 18        | 8.179       | 2116          | 2127        | 2144         | rBV      | 42860          | 72844         | 9.83%           | 1.201%        |
| 19        | 8.632       | 2256          | 2268        | 2301         | rBV3     | 318089         | 740668        | 100.00%         | 12.214%       |
| 20        | 8.787       | 2306          | 2316        | 2328         | rVV3     | 60585          | 102872        | 13.89%          | 1.696%        |
| 21        | 9.417       | 2499          | 2512        | 2534         | rBV      | 370595         | 624822        | 84.36%          | 10.304%       |
| 22        | 10.082      | 2709          | 2719        | 2732         | rBV3     | 10282          | 19608         | 2.65%           | 0.323%        |
| 23        | 10.346      | 2793          | 2801        | 2813         | rVB8     | 5447           | 8869          | 1.20%           | 0.146%        |
| 24        | 10.754      | 2915          | 2928        | 2942         | rBV      | 150084         | 242155        | 32.69%          | 3.993%        |
| 25        | 11.690      | 3204          | 3219        | 3228         | rBV7     | 5339           | 8883          | 1.20%           | 0.146%        |
| 26        | 11.809      | 3244          | 3256        | 3278         | rBV      | 300311         | 489952        | 66.15%          | 8.080%        |
| 27        | 12.060      | 3323          | 3334        | 3356         | rBV2     | 42847          | 83978         | 11.34%          | 1.385%        |
| 28        | 12.192      | 3362          | 3375        | 3392         | rBV      | 270976         | 442752        | 59.78%          | 7.301%        |
| 29        | 12.889      | 3581          | 3592        | 3601         | rBV3     | 15574          | 24752         | 3.34%           | 0.408%        |
| 30        | 16.291      | 4643          | 4650        | 4659         | rBV6     | 6877           | 10695         | 1.44%           | 0.176%        |

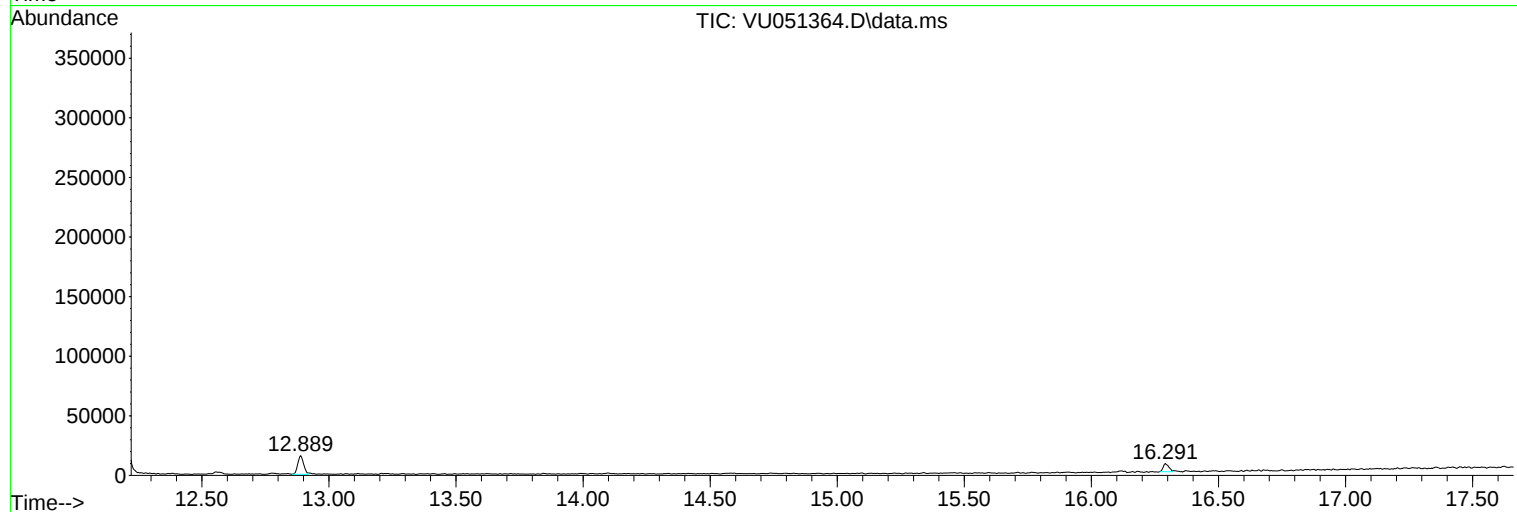
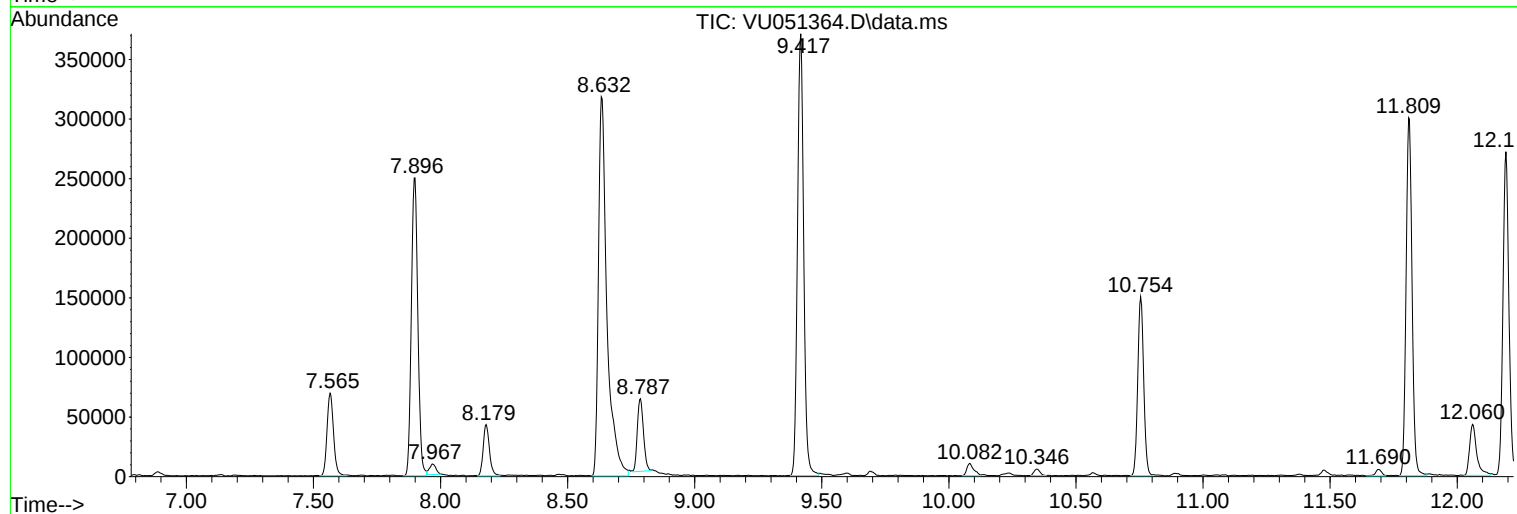
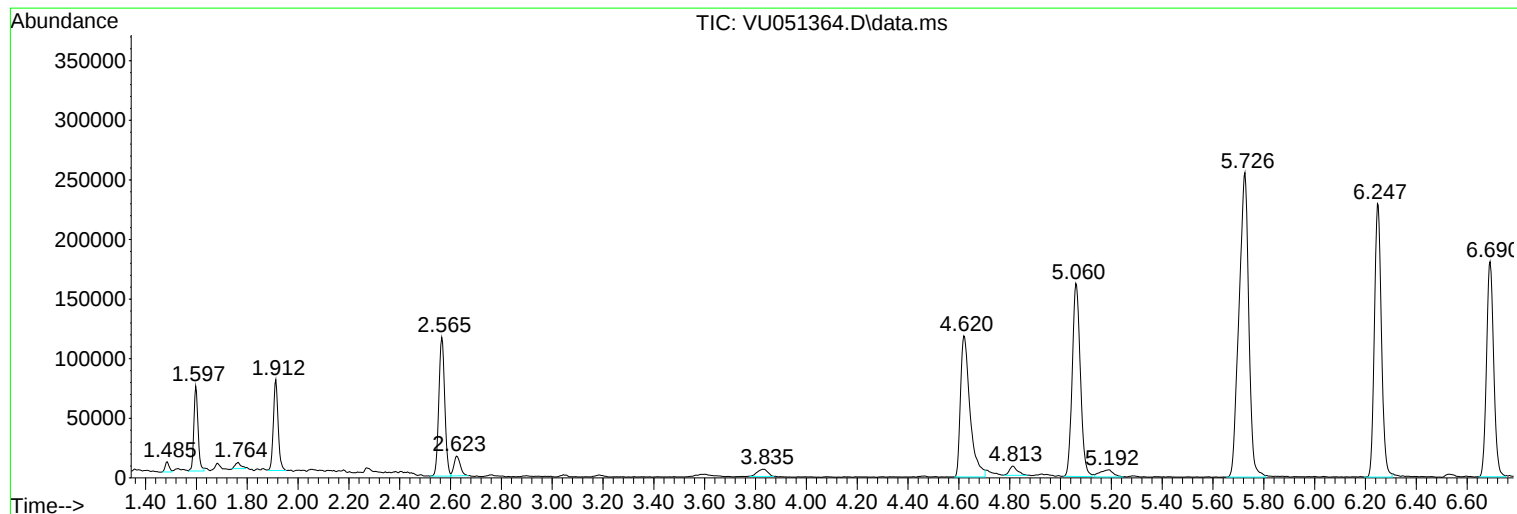
Sum of corrected areas: 6064002

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ALS Vial : 53 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
C1BD5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR100722WMA.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 :  
C1BD5

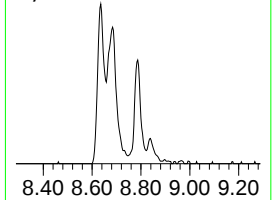
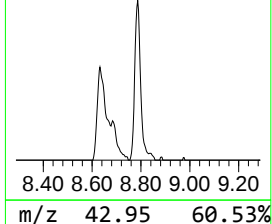
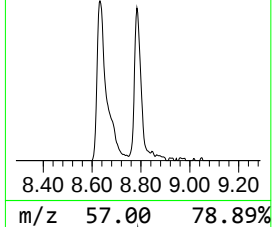
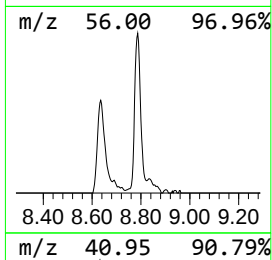
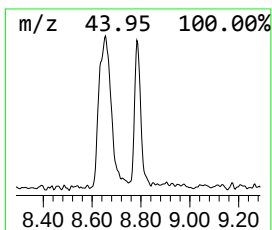
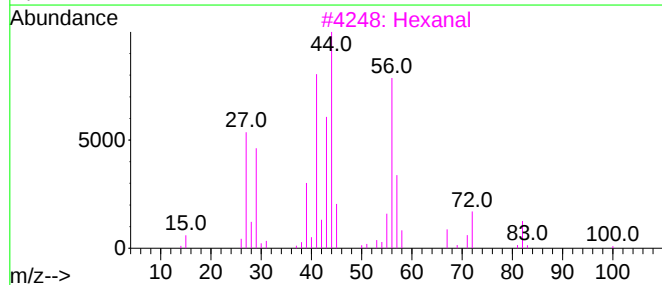
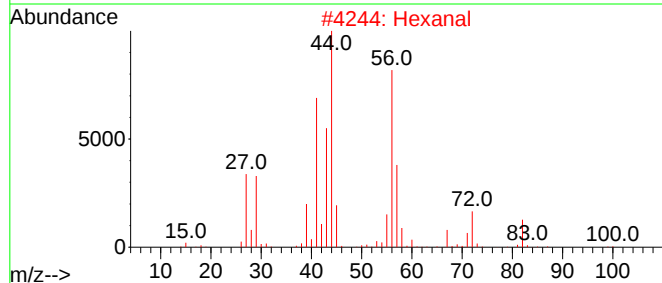
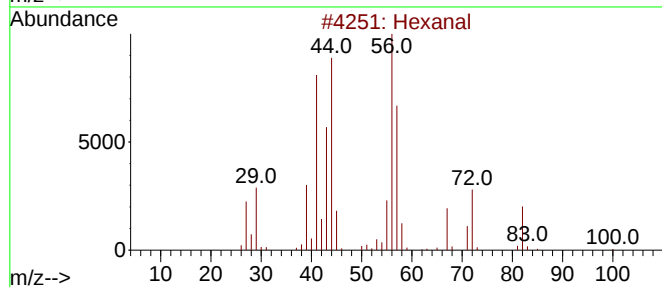
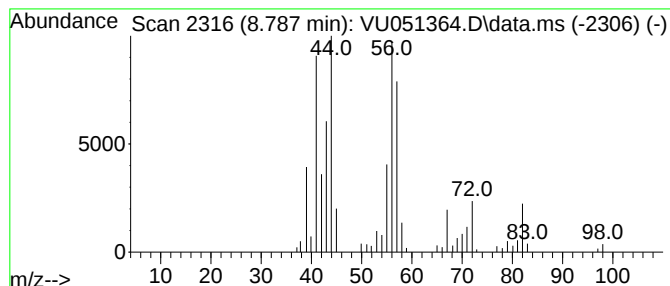
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR100722WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 Hexanal Concentration Rank 3

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 8.787 | 0.82 ug/L | 102872 | Chlorobenzene-d5 | 9.417 |

| Hit# | of      | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------|---|--------------|-----|---------|-------------|------|
| 1    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 72   |
| 2    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 59   |
| 3    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 53   |
| 4    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 53   |
| 5    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 53   |



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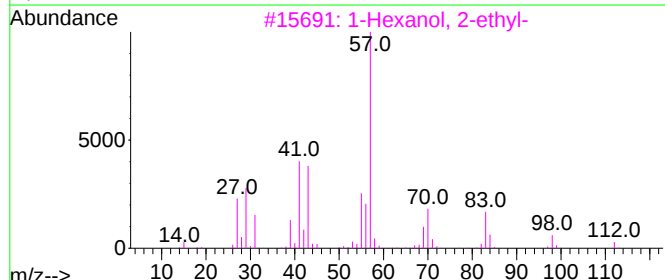
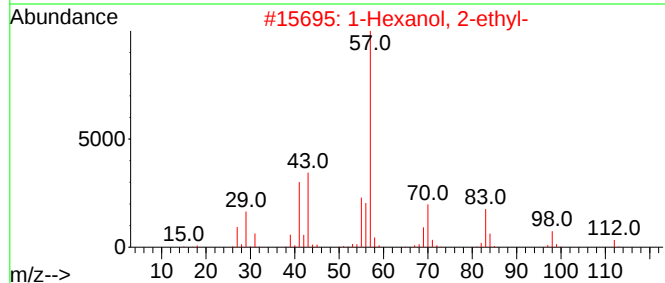
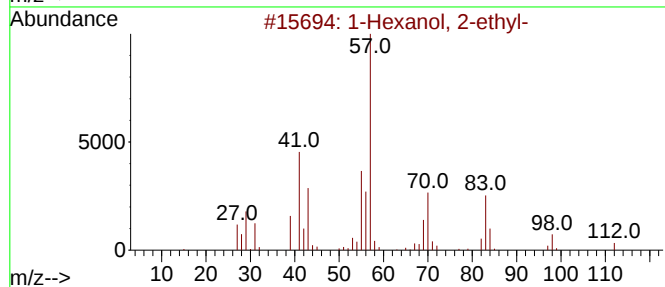
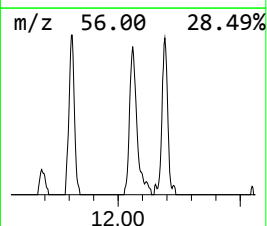
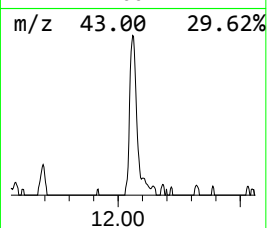
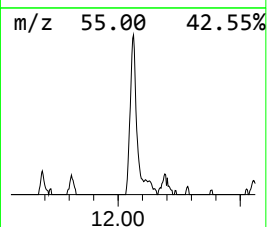
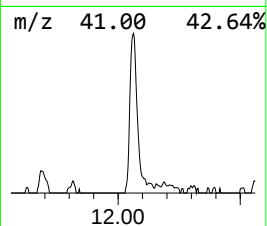
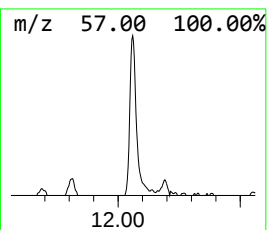
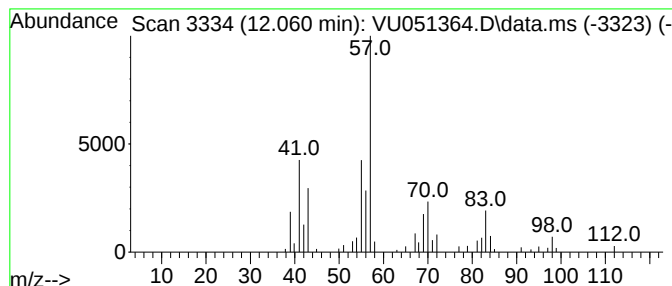
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.060 | 0.86 ug/L | 83978 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------|-----|---------|-------------|------|
| 1    |    |   | 1-Hexanol, 2-ethyl-           | 130 | C8H18O  | 000104-76-7 | 78   |
| 2    |    |   | 1-Hexanol, 2-ethyl-           | 130 | C8H18O  | 000104-76-7 | 72   |
| 3    |    |   | 1-Hexanol, 2-ethyl-           | 130 | C8H18O  | 000104-76-7 | 64   |
| 4    |    |   | 1-Pentanol, 2-ethyl-4-methyl- | 130 | C8H18O  | 000106-67-2 | 64   |
| 5    |    |   | 1-Hexanol, 2-ethyl-           | 130 | C8H18O  | 000104-76-7 | 59   |



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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 |
| Hexanal            | 8.787  | 0.8     | ug/L  | 102872   | 2                     | 9.417  | 624822 | 5.0  |
| 1-Hexanol, 2-et... | 12.060 | 0.9     | ug/L  | 83978    | 3                     | 11.812 | 489952 | 5.0  |