

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU122623\  
 Data File : VU057252.D  
 Acq On : 26 Dec 2023 22:25  
 Operator : MD/SY  
 Sample : 05976-11  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BH7X4

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\SFAMUTR122123WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU057252.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         | 1.686       | 115           | 123         | 135          | rVB2     | 108940         | 147820        | 22.06%          | 2.709%        |
| 2         | 1.776       | 145           | 151         | 152          | rBV      | 14210          | 12618         | 1.88%           | 0.231%        |
| 3         | 2.033       | 224           | 231         | 242          | rVB      | 73143          | 103185        | 15.40%          | 1.891%        |
| 4         | 2.721       | 435           | 445         | 464          | rVB      | 140097         | 262370        | 39.15%          | 4.809%        |
| 5         | 4.872       | 1089          | 1114        | 1115         | rBV4     | 26895          | 75255         | 11.23%          | 1.379%        |
| 6         | 5.197       | 1202          | 1215        | 1230         | rBV      | 118607         | 264881        | 39.52%          | 4.855%        |
| 7         | 5.888       | 1407          | 1430        | 1449         | rBV2     | 235350         | 670188        | 100.00%         | 12.284%       |
| 8         | 6.386       | 1572          | 1585        | 1609         | rBV      | 169208         | 344444        | 51.40%          | 6.313%        |
| 9         | 6.808       | 1699          | 1716        | 1743         | rBV2     | 151152         | 310429        | 46.32%          | 5.690%        |
| 10        | 7.644       | 1961          | 1976        | 1997         | rBV2     | 66314          | 129401        | 19.31%          | 2.372%        |
| 11        | 7.965       | 2062          | 2076        | 2089         | rBV      | 248193         | 458502        | 68.41%          | 8.404%        |
| 12        | 8.033       | 2090          | 2097        | 2113         | rVB2     | 51113          | 103590        | 15.46%          | 1.899%        |
| 13        | 8.235       | 2149          | 2160        | 2178         | rBV2     | 42103          | 75828         | 11.31%          | 1.390%        |
| 14        | 8.512       | 2235          | 2246        | 2258         | rBV2     | 18916          | 36837         | 5.50%           | 0.675%        |
| 15        | 8.685       | 2283          | 2300        | 2319         | rBV      | 242363         | 533653        | 79.63%          | 9.781%        |
| 16        | 9.447       | 2524          | 2537        | 2562         | rBV      | 242362         | 472980        | 70.57%          | 8.669%        |
| 17        | 9.717       | 2609          | 2621        | 2628         | rBV4     | 9643           | 17794         | 2.66%           | 0.326%        |
| 18        | 10.766      | 2934          | 2947        | 2965         | rVB      | 102110         | 180263        | 26.90%          | 3.304%        |
| 19        | 10.897      | 2977          | 2988        | 3001         | rBV3     | 39872          | 71261         | 10.63%          | 1.306%        |
| 20        | 11.817      | 3261          | 3274        | 3295         | rVB      | 247546         | 433768        | 64.72%          | 7.950%        |
| 21        | 12.071      | 3339          | 3353        | 3366         | rBV4     | 16940          | 46179         | 6.89%           | 0.846%        |
| 22        | 12.196      | 3379          | 3392        | 3410         | rVB      | 266415         | 459613        | 68.58%          | 8.424%        |
| 23        | 12.769      | 3560          | 3570        | 3579         | rVB      | 26819          | 44032         | 6.57%           | 0.807%        |
| 24        | 12.884      | 3597          | 3606        | 3617         | rVB      | 9339           | 16220         | 2.42%           | 0.297%        |
| 25        | 14.569      | 4118          | 4130        | 4142         | rBV2     | 10469          | 17603         | 2.63%           | 0.323%        |
| 26        | 16.180      | 4623          | 4631        | 4636         | rBV4     | 6627           | 9753          | 1.46%           | 0.179%        |
| 27        | 17.122      | 4918          | 4924        | 4938         | rVB4     | 3816           | 6979          | 1.04%           | 0.128%        |
| 28        | 17.457      | 5018          | 5028        | 5042         | rBV4     | 70824          | 150413        | 22.44%          | 2.757%        |

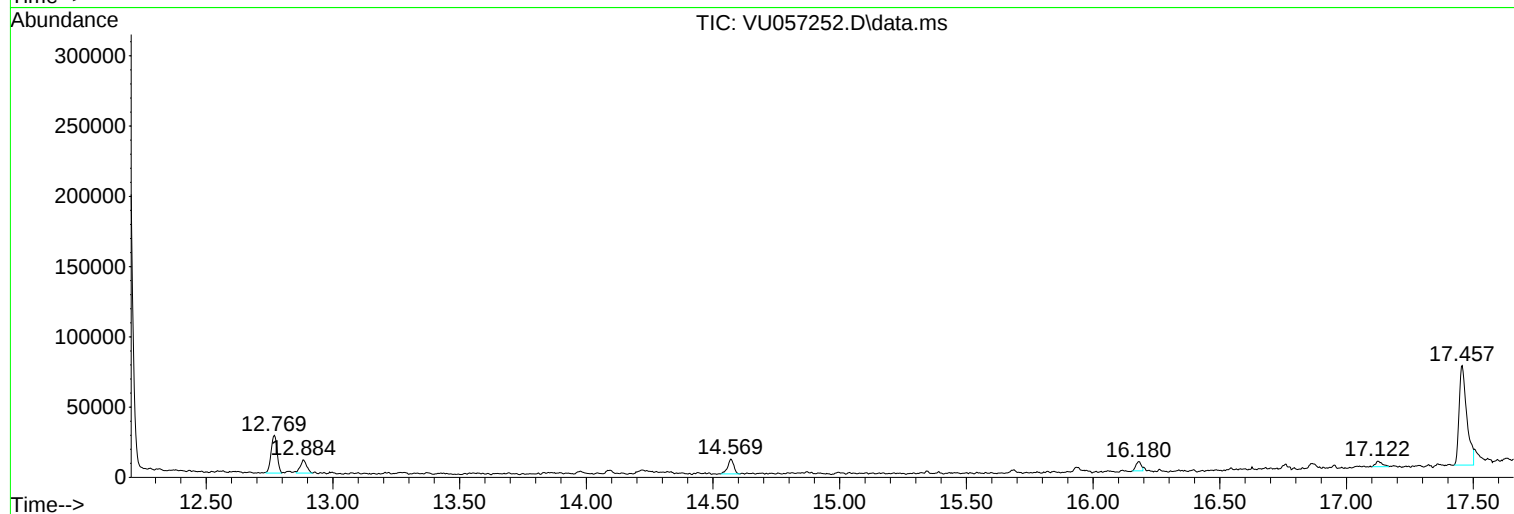
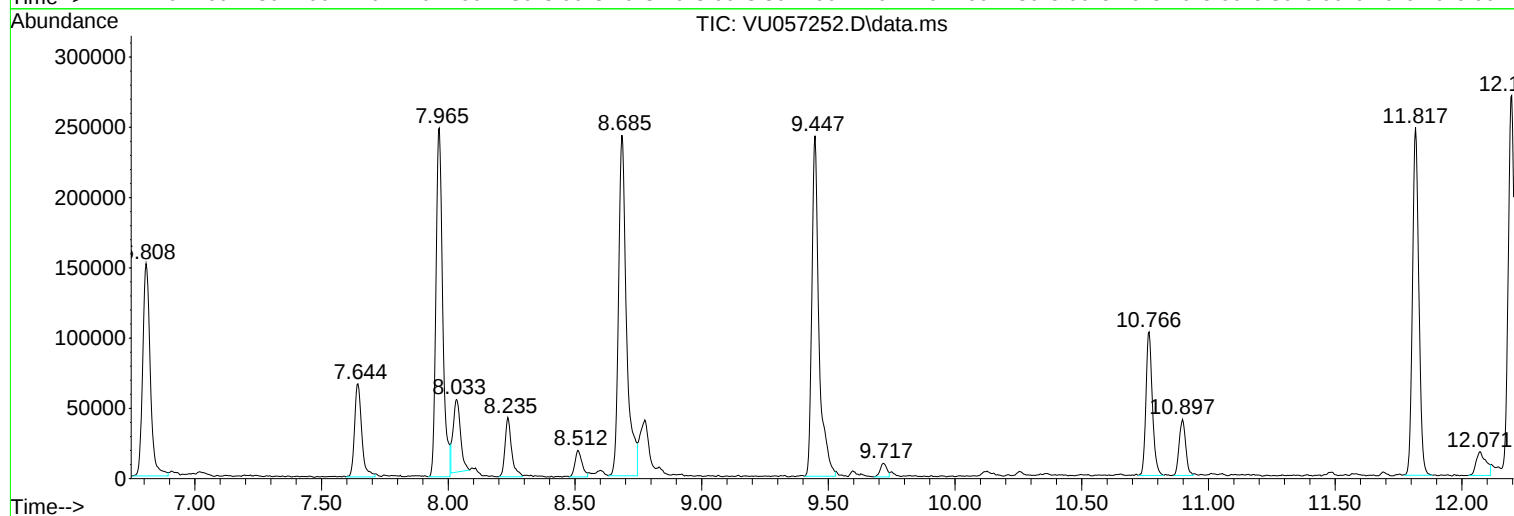
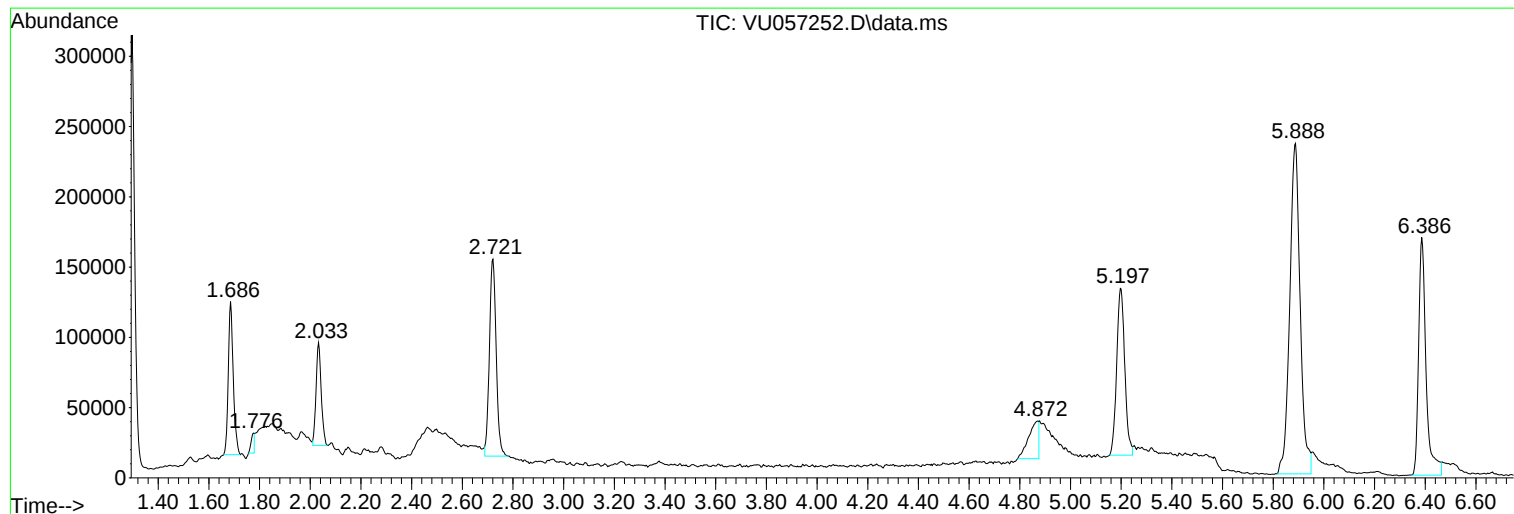
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ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BH7X4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122123WMA.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  
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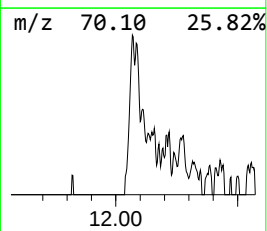
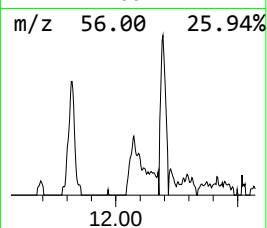
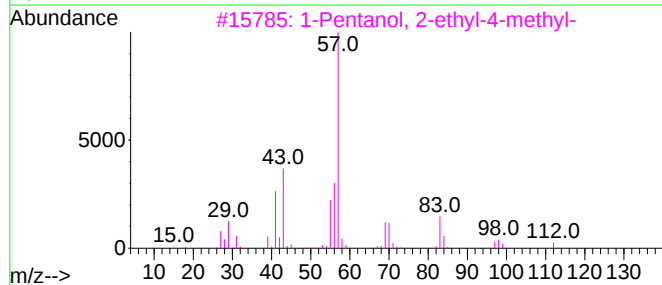
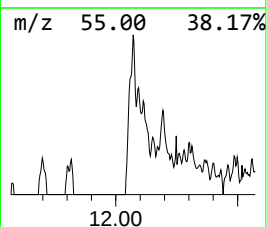
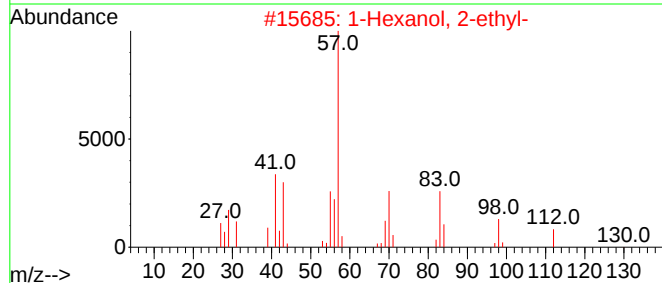
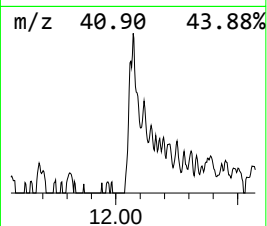
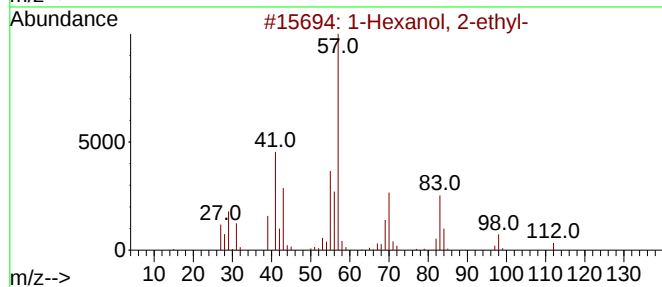
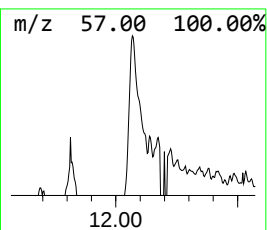
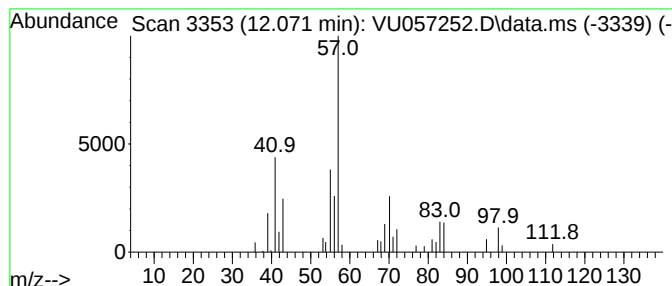
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122123WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.071 | 0.53 ug/L | 46179 | 1,4-Dichlorobenzene-d4 | 11.817 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm  | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|----------|-------------|------|
| 1    | 1-Hexanol, 2-ethyl-                 |   |              | 130 | C8H18O   | 000104-76-7 | 64   |
| 2    | 1-Hexanol, 2-ethyl-                 |   |              | 130 | C8H18O   | 000104-76-7 | 59   |
| 3    | 1-Pentanol, 2-ethyl-4-methyl-       |   |              | 130 | C8H18O   | 000106-67-2 | 53   |
| 4    | Octane, 2,3-dimethyl-               |   |              | 142 | C10H22   | 007146-60-3 | 50   |
| 5    | Oxirane, [[(2-ethylhexyl)oxy]met... |   |              | 186 | C11H22O2 | 002461-15-6 | 50   |



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122123WMA.M  
Quant Title : TRACE VOA SFAM1.0

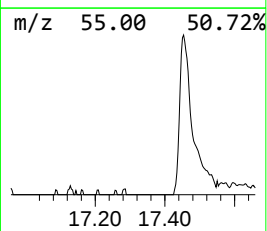
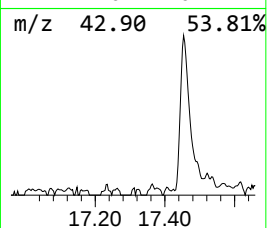
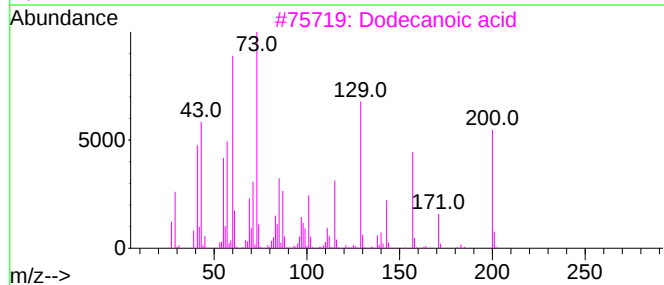
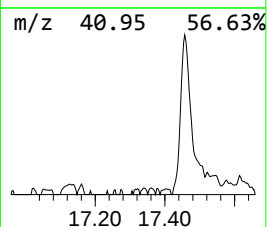
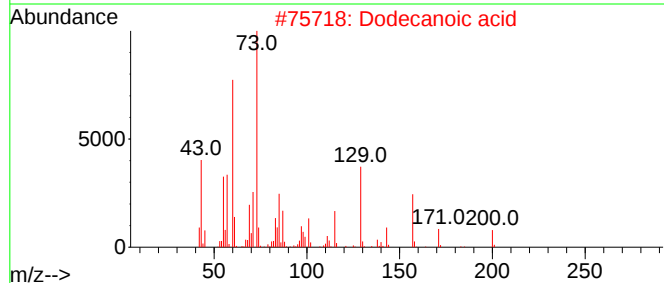
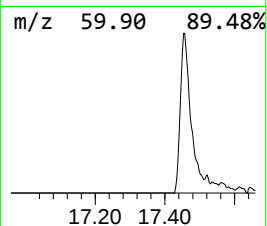
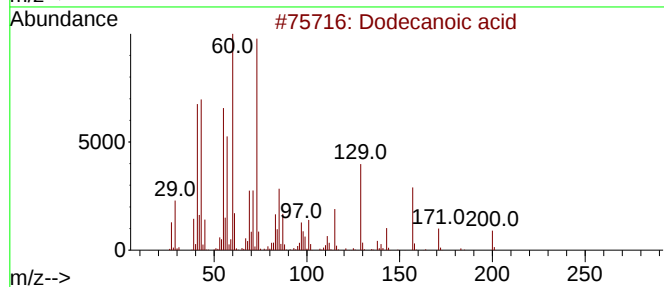
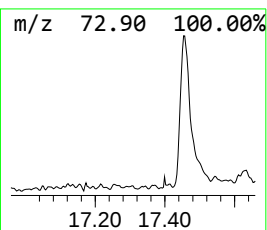
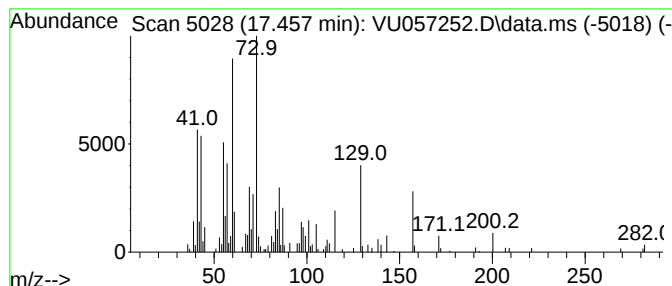
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Dodecanoic acid Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 17.457 | 1.73 ug/L | 150413 | 1,4-Dichlorobenzene-d4 | 11.817 |

| Hit# | of | 5 | Tentative ID    | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-----------------|-----|----------|-------------|------|
| 1    |    |   | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 99   |
| 2    |    |   | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 98   |
| 3    |    |   | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 95   |
| 4    |    |   | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 91   |
| 5    |    |   | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 87   |



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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 |
| 1-Hexanol, 2-et... | 12.071 | 0.5     | ug/L  | 46179    | 3                     | 11.817 | 433768 | 5.0  |
| Dodecanoic acid    | 17.457 | 1.7     | ug/L  | 150413   | 3                     | 11.817 | 433768 | 5.0  |