

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU060923\  
 Data File : VU054467.D  
 Acq On : 09 Jun 2023 16:59  
 Operator : MD/SY  
 Sample : 03118-05  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0FK9

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\SFAMUTR060723WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054467.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         | 1.599       | 88            | 96          | 108          | rVB      | 80732          | 97969         | 3.66%           | 0.889%        |
| 2         | 1.911       | 186           | 193         | 205          | rBV      | 84613          | 112824        | 4.22%           | 1.024%        |
| 3         | 2.566       | 385           | 397         | 412          | rBV      | 142762         | 235261        | 8.80%           | 2.135%        |
| 4         | 4.631       | 1025          | 1039        | 1080         | rBV      | 145088         | 452900        | 16.94%          | 4.111%        |
| 5         | 5.062       | 1156          | 1173        | 1200         | rBV      | 182775         | 438445        | 16.40%          | 3.980%        |
| 6         | 5.724       | 1358          | 1379        | 1403         | rBV2     | 331043         | 884083        | 33.07%          | 8.024%        |
| 7         | 6.245       | 1528          | 1541        | 1581         | rBV      | 360539         | 716996        | 26.82%          | 6.508%        |
| 8         | 6.689       | 1664          | 1679        | 1698         | rBV      | 222285         | 440980        | 16.49%          | 4.003%        |
| 9         | 7.563       | 1938          | 1951        | 1969         | rBV2     | 98508          | 183092        | 6.85%           | 1.662%        |
| 10        | 7.894       | 2039          | 2054        | 2076         | rBV      | 386187         | 688767        | 25.76%          | 6.252%        |
| 11        | 8.177       | 2131          | 2142        | 2164         | rBV2     | 60676          | 110042        | 4.12%           | 0.999%        |
| 12        | 8.631       | 2270          | 2283        | 2319         | rBV2     | 479249         | 1017362       | 38.05%          | 9.234%        |
| 13        | 9.415       | 2514          | 2527        | 2548         | rBV      | 493898         | 855276        | 31.99%          | 7.763%        |
| 14        | 10.753      | 2928          | 2943        | 2963         | rBV      | 170928         | 287998        | 10.77%          | 2.614%        |
| 15        | 11.042      | 3022          | 3033        | 3054         | rBV      | 149755         | 242621        | 9.07%           | 2.202%        |
| 16        | 11.807      | 3259          | 3271        | 3297         | rBV      | 515904         | 837379        | 31.32%          | 7.601%        |
| 17        | 12.055      | 3334          | 3348        | 3379         | rBV      | 1389275        | 2673709       | 100.00%         | 24.268%       |
| 18        | 12.190      | 3380          | 3390        | 3413         | rVB      | 426770         | 741698        | 27.74%          | 6.732%        |

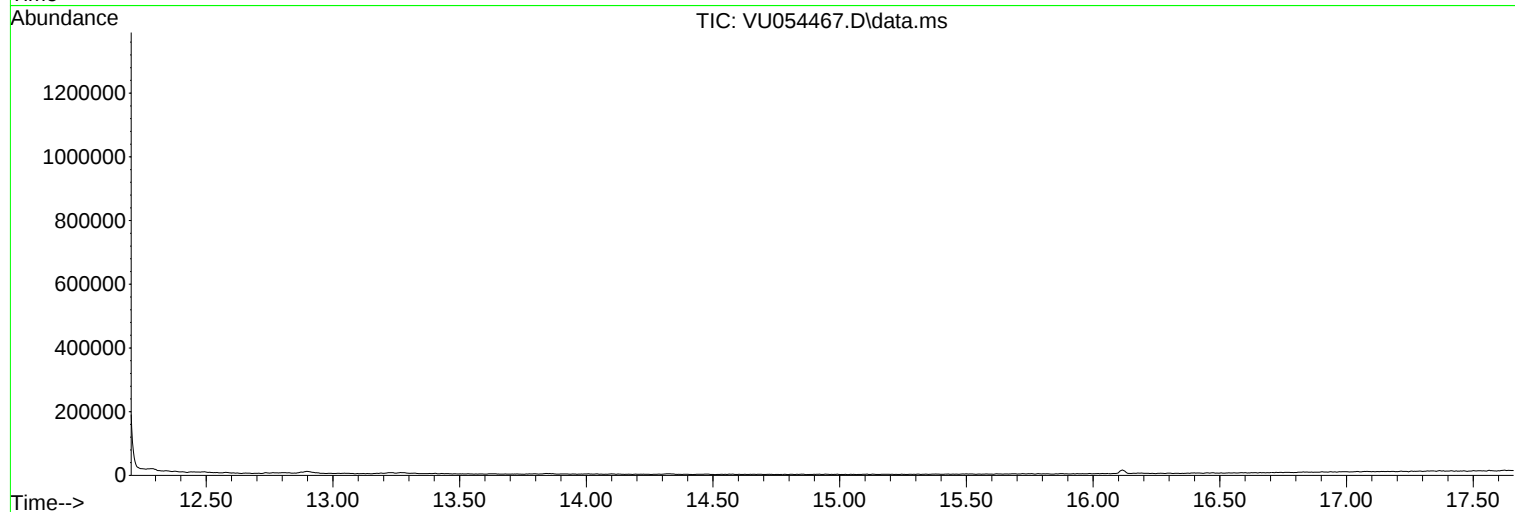
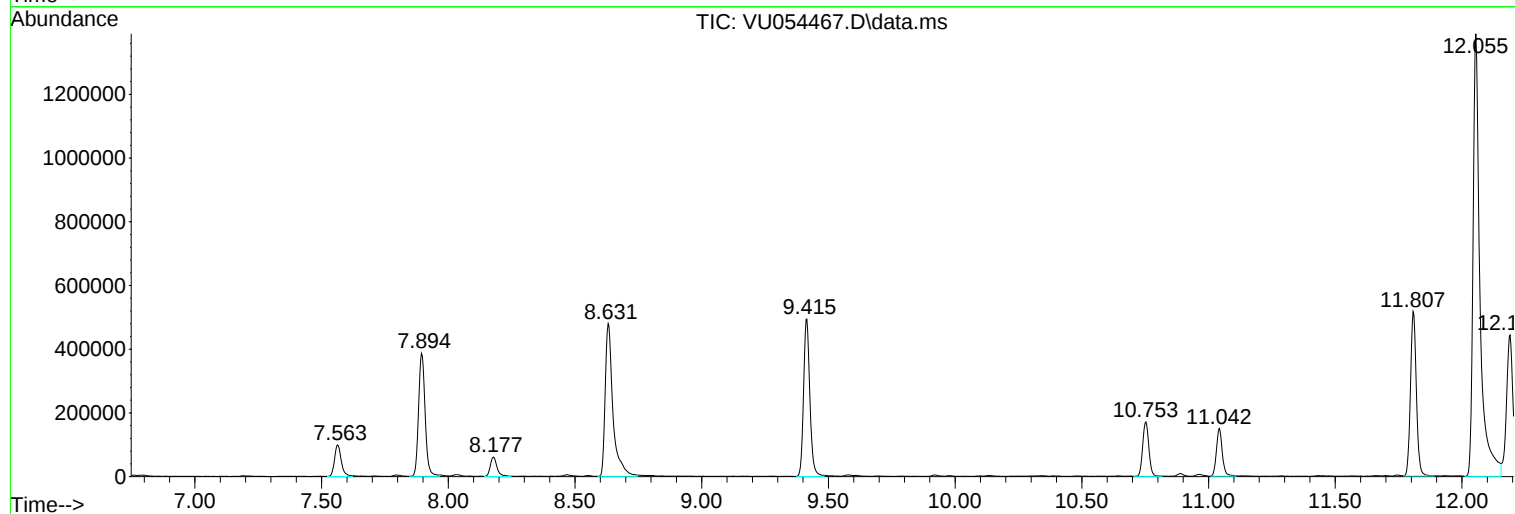
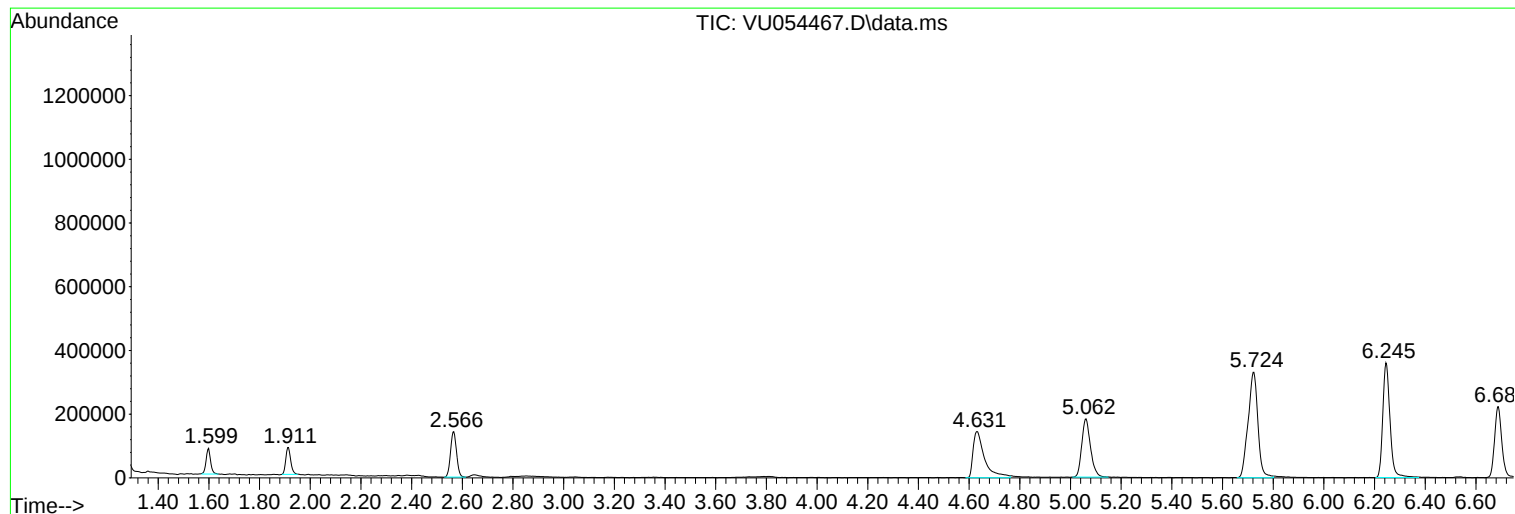
Sum of corrected areas: 11017402

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Instrument :  
MSVOA\_U  
ClientSampleId :  
C0FK9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :  
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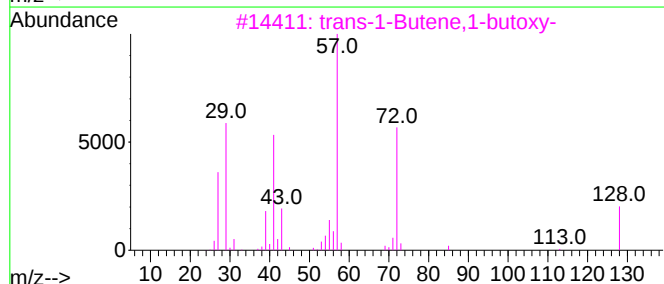
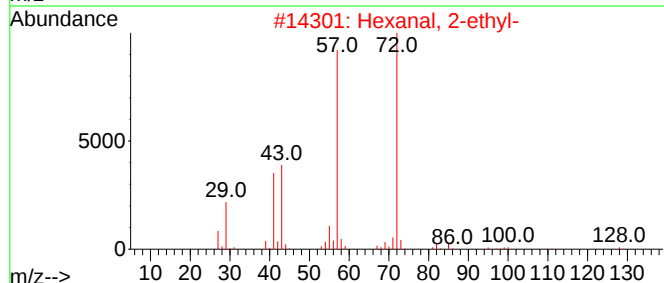
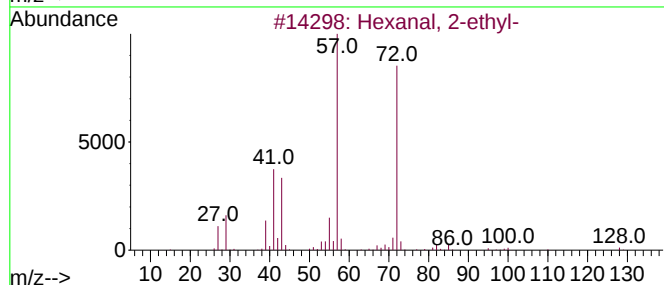
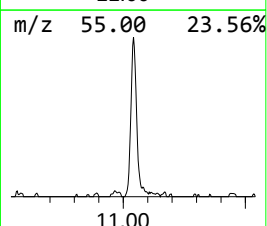
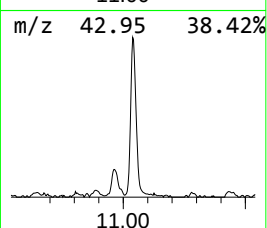
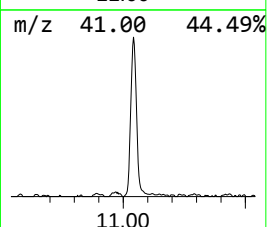
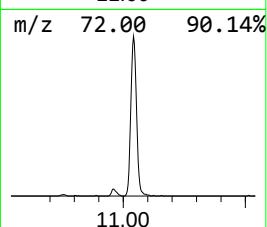
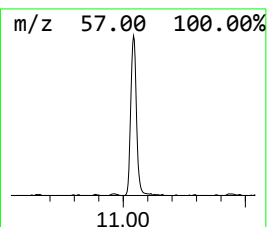
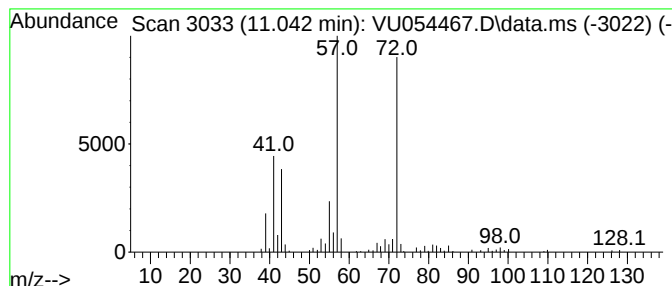
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 Hexanal, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 11.042 | 1.45 ug/L | 242621 | 1,4-Dichlorobenzene-d4 | 11.810 |

| Hit# | of | 5 | Tentative ID             | MW  | MolForm | CAS#         | Qual |
|------|----|---|--------------------------|-----|---------|--------------|------|
| 1    |    |   | Hexanal, 2-ethyl-        | 128 | C8H16O  | 000123-05-7  | 87   |
| 2    |    |   | Hexanal, 2-ethyl-        | 128 | C8H16O  | 000123-05-7  | 80   |
| 3    |    |   | trans-1-Butene,1-butoxy- | 128 | C8H16O  | 1000139-52-8 | 78   |
| 4    |    |   | Hexanal, 2-ethyl-        | 128 | C8H16O  | 000123-05-7  | 64   |
| 5    |    |   | 2-Propanone, hydrazone   | 72  | C3H8N2  | 005281-20-9  | 56   |



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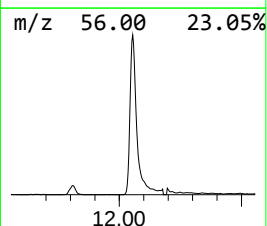
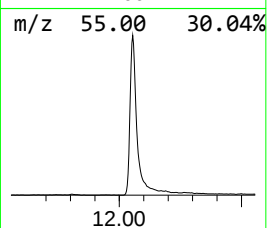
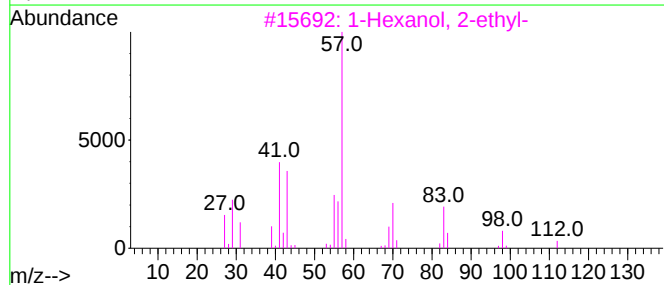
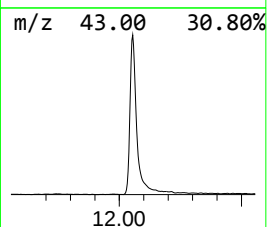
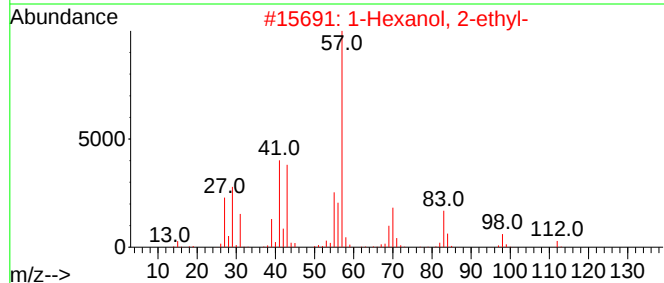
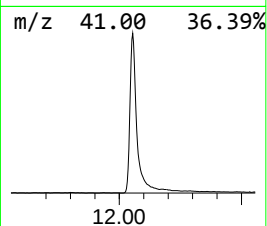
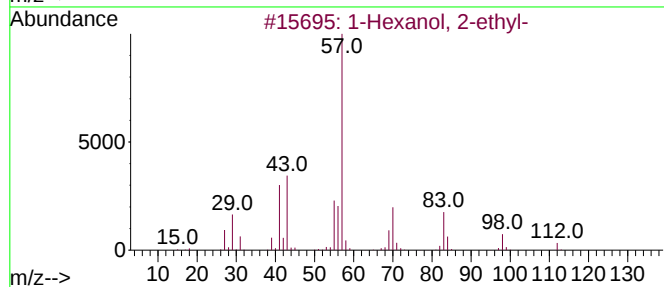
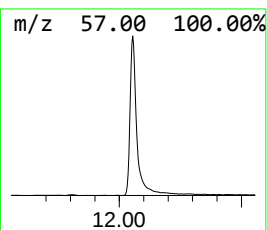
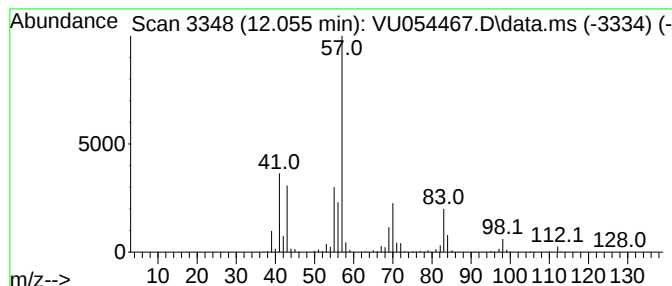
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TIC Integration Parameters: LSCINT.P

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

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 12.055 | 15.96 ug/L | 2673710 | 1,4-Dichlorobenzene-d4 | 11.810 |

| Hit# | of                  | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------------------|---|--------------|-----|---------|-------------|------|
| 1    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 2    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 3    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 83   |
| 4    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 72   |
| 5    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 64   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Hexanal, 2-ethyl-  | 11.042 | 1.5     | ug/L  | 242621   | 3                     | 11.810 | 837379 | 5.0  |
| 1-Hexanol, 2-et... | 12.055 | 16.0    | ug/L  | 2673710  | 3                     | 11.810 | 837379 | 5.0  |