

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082420\  
 Data File : VU039954.D  
 Acq On : 24 Aug 2020 18:11  
 Operator : SY/MD  
 Sample : L3789-02  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFSH0

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR081920WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

| 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         | 1.527       | 51            | 58          | 65           | rBV      | 9337           | 10634         | 3.34%           | 0.415%        |
| 2         | 1.604       | 74            | 82          | 94           | rVB      | 42103          | 43840         | 13.75%          | 1.710%        |
| 3         | 1.922       | 173           | 181         | 194          | rVB      | 33479          | 42770         | 13.42%          | 1.668%        |
| 4         | 2.466       | 339           | 350         | 361          | rVB      | 7117           | 11181         | 3.51%           | 0.436%        |
| 5         | 2.578       | 374           | 385         | 400          | rBV      | 66900          | 110537        | 34.68%          | 4.310%        |
| 6         | 2.658       | 400           | 410         | 421          | rBV2     | 6916           | 15749         | 4.94%           | 0.614%        |
| 7         | 2.829       | 453           | 463         | 464          | rBV3     | 2732           | 3638          | 1.14%           | 0.142%        |
| 8         | 4.655       | 1015          | 1031        | 1049         | rBV2     | 46106          | 125102        | 39.25%          | 4.878%        |
| 9         | 5.083       | 1149          | 1164        | 1185         | rVB      | 59866          | 130555        | 40.96%          | 5.091%        |
| 10        | 5.742       | 1347          | 1369        | 1389         | rBV2     | 117805         | 302838        | 95.00%          | 11.809%       |
| 11        | 6.173       | 1494          | 1503        | 1516         | rBV3     | 1709           | 3899          | 1.22%           | 0.152%        |
| 12        | 6.263       | 1517          | 1531        | 1545         | rBV      | 90029          | 165860        | 52.03%          | 6.468%        |
| 13        | 6.703       | 1654          | 1668        | 1683         | rBV      | 77310          | 146467        | 45.95%          | 5.712%        |
| 14        | 7.575       | 1928          | 1939        | 1953         | rBV      | 39294          | 66799         | 20.96%          | 2.605%        |
| 15        | 7.723       | 1977          | 1985        | 1997         | rVB4     | 2422           | 3846          | 1.21%           | 0.150%        |
| 16        | 7.906       | 2027          | 2042        | 2057         | rBV      | 140444         | 239000        | 74.98%          | 9.320%        |
| 17        | 8.186       | 2119          | 2129        | 2146         | rBV2     | 25169          | 42952         | 13.47%          | 1.675%        |
| 18        | 8.559       | 2236          | 2245        | 2256         | rBV2     | 13143          | 20166         | 6.33%           | 0.786%        |
| 19        | 8.639       | 2256          | 2270        | 2294         | rBV      | 183848         | 318765        | 100.00%         | 12.430%       |
| 20        | 8.790       | 2310          | 2317        | 2326         | rBV5     | 2840           | 5155          | 1.62%           | 0.201%        |
| 21        | 8.841       | 2326          | 2333        | 2343         | rVB4     | 2093           | 3219          | 1.01%           | 0.126%        |
| 22        | 9.420       | 2499          | 2513        | 2530         | rBV      | 130730         | 211007        | 66.20%          | 8.228%        |
| 23        | 10.237      | 2759          | 2767        | 2778         | rBV2     | 3328           | 4757          | 1.49%           | 0.186%        |
| 24        | 10.755      | 2917          | 2928        | 2942         | rVB      | 51837          | 83824         | 26.30%          | 3.269%        |
| 25        | 11.806      | 3243          | 3255        | 3272         | rBV      | 129029         | 201279        | 63.14%          | 7.849%        |
| 26        | 12.054      | 3323          | 3332        | 3344         | rBV2     | 15873          | 24684         | 7.74%           | 0.963%        |
| 27        | 12.189      | 3362          | 3374        | 3390         | rBV      | 141514         | 222192        | 69.70%          | 8.664%        |
| 28        | 12.877      | 3583          | 3588        | 3595         | rVB4     | 3239           | 3690          | 1.16%           | 0.144%        |

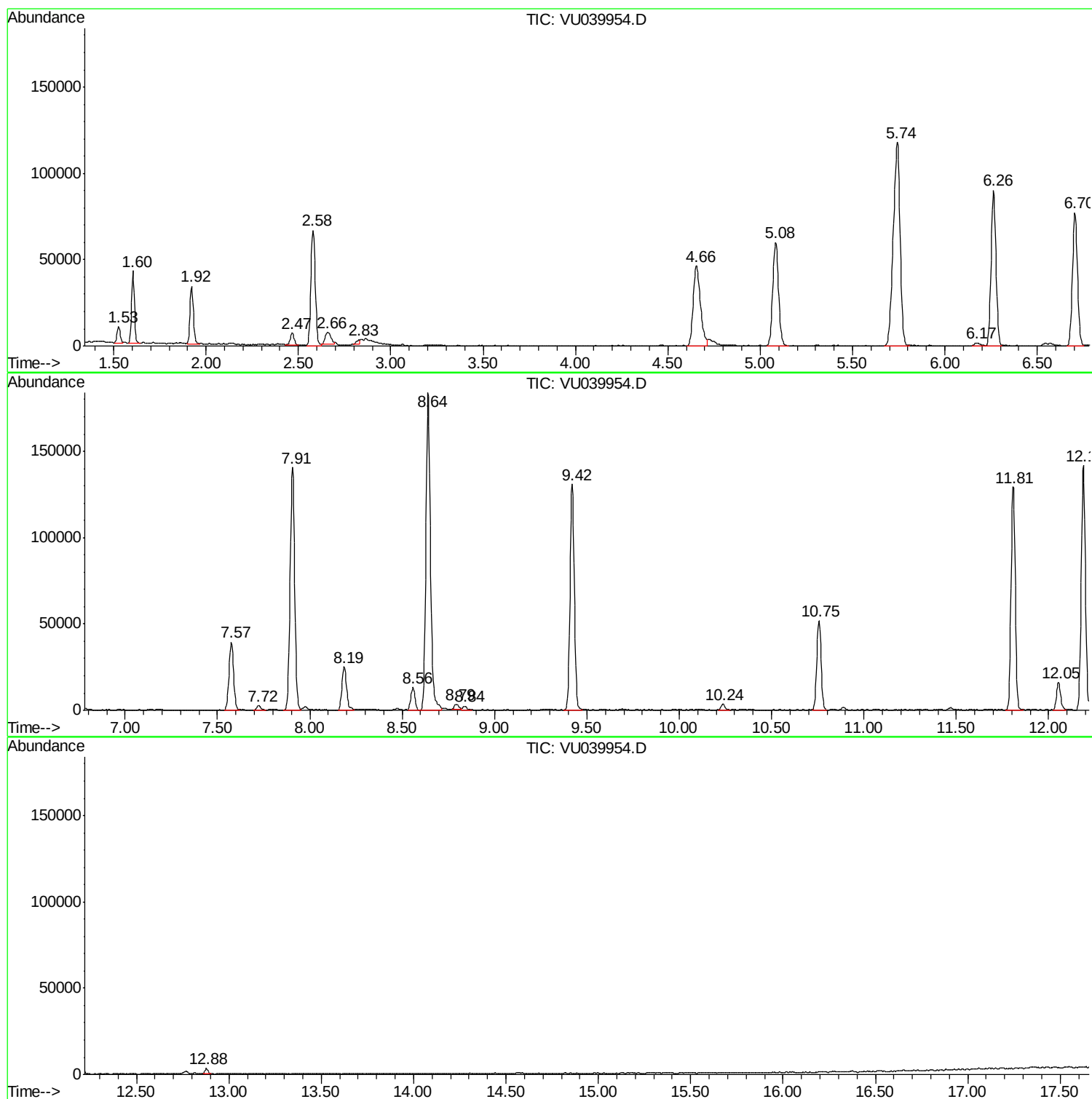
Sum of corrected areas: 2564405

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR081920WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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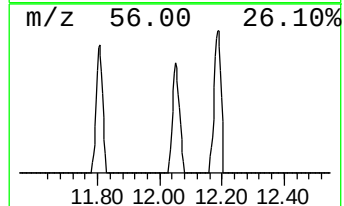
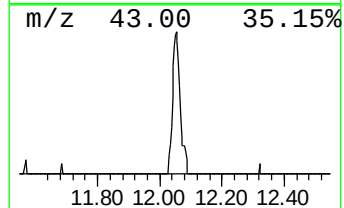
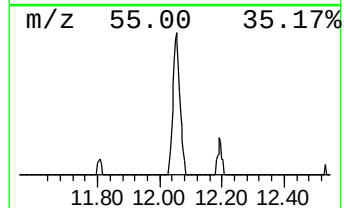
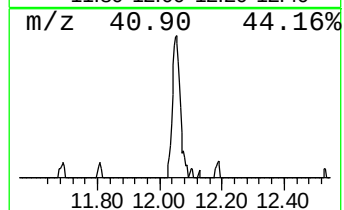
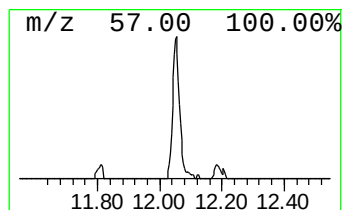
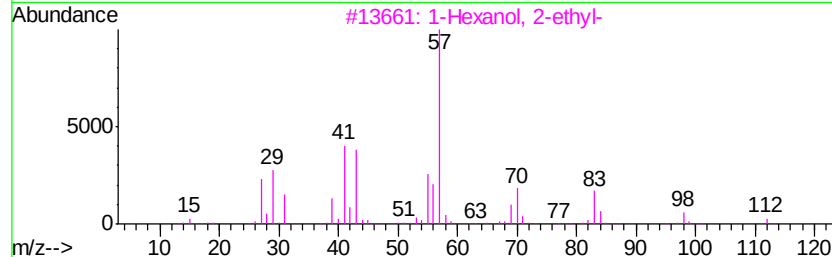
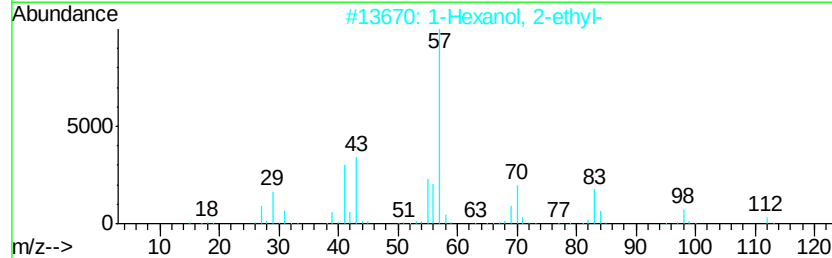
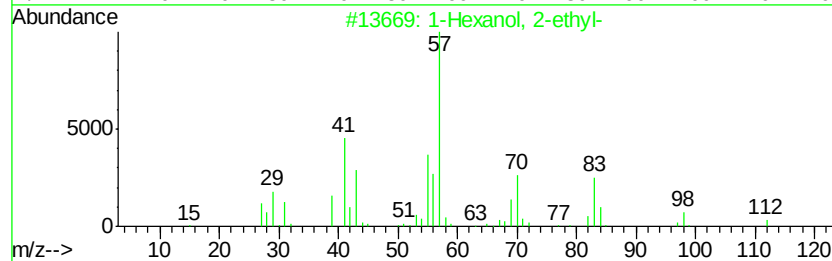
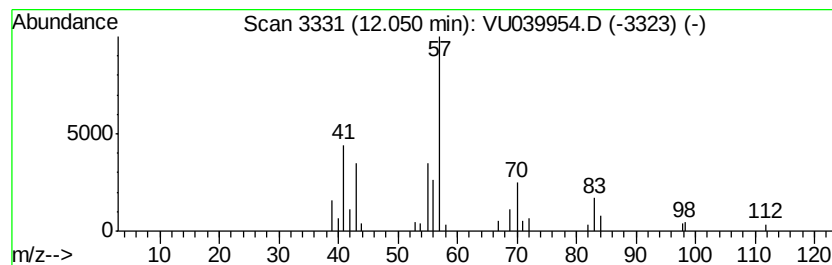
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TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc   | Area  | Relative to ISTD       | R.T.  |
|-------|-----------|-------|------------------------|-------|
| 12.05 | 0.61 ug/L | 24684 | 1,4-Dichlorobenzene-d4 | 11.81 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------|-----|----------|-------------|------|
| 1    |    |   | 1-Hexanol, 2-ethyl-           | 130 | C8H18O   | 000104-76-7 | 83   |
| 2    |    |   | 1-Hexanol, 2-ethyl-           | 130 | C8H18O   | 000104-76-7 | 72   |
| 3    |    |   | 1-Hexanol, 2-ethyl-           | 130 | C8H18O   | 000104-76-7 | 72   |
| 4    |    |   | Heptyl isobutyl carbonate     | 216 | C12H24O3 | 959068-08-7 | 53   |
| 5    |    |   | 1-Pentanol, 2-ethyl-4-methyl- | 130 | C8H18O   | 000106-67-2 | 50   |



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| TIC Top Hit name    | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|---------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                     |       |         |       |          | #                     | RT    | Resp   | Conc |
| 1-Hexanol, 2-ethyl- | 12.05 | 0.6     | ug/L  | 24684    | 3                     | 11.81 | 201279 | 5.0  |