

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU041123\  
 Data File : VU053648.D  
 Acq On : 11 Apr 2023 20:20  
 Operator : JC/MD  
 Sample : 02252-08 200X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 COME4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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\SFAMULM033123WMA.M

Title : VOC Analysis

Signal : TIC: VU053648.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         | 1.597       | 73            | 80          | 94           | rBV      | 88173          | 104739        | 2.38%           | 0.891%        |
| 2         | 1.909       | 169           | 177         | 194          | rVB      | 75755          | 108597        | 2.47%           | 0.924%        |
| 3         | 2.565       | 369           | 381         | 405          | rBV      | 141857         | 233600        | 5.31%           | 1.987%        |
| 4         | 3.044       | 520           | 530         | 536          | rBV5     | 1521           | 2709          | 0.06%           | 0.023%        |
| 5         | 3.292       | 605           | 607         | 608          | rBV      | 279            | 99            | 0.00%           | 0.001%        |
| 6         | 3.350       | 623           | 625         | 626          | rBV      | 185            | 63            | 0.00%           | 0.001%        |
| 7         | 3.401       | 638           | 641         | 643          | rBV2     | 229            | 146           | 0.00%           | 0.001%        |
| 8         | 3.526       | 678           | 680         | 683          | rBV      | 188            | 69            | 0.00%           | 0.001%        |
| 9         | 3.848       | 778           | 780         | 783          | rVB2     | 185            | 90            | 0.00%           | 0.001%        |
| 10        | 3.964       | 813           | 816         | 819          | rVB2     | 229            | 130           | 0.00%           | 0.001%        |
| 11        | 4.166       | 877           | 879         | 884          | rBV      | 167            | 182           | 0.00%           | 0.002%        |
| 12        | 4.202       | 888           | 890         | 894          | rVB      | 265            | 148           | 0.00%           | 0.001%        |
| 13        | 4.285       | 914           | 916         | 919          | rBV      | 173            | 67            | 0.00%           | 0.001%        |
| 14        | 4.372       | 941           | 943         | 945          | rBV      | 186            | 97            | 0.00%           | 0.001%        |
| 15        | 4.449       | 962           | 967         | 969          | rBV      | 381            | 390           | 0.01%           | 0.003%        |
| 16        | 4.613       | 1006          | 1018        | 1045         | rBV2     | 69267          | 164027        | 3.73%           | 1.395%        |
| 17        | 4.880       | 1099          | 1101        | 1103         | rBV      | 338            | 139           | 0.00%           | 0.001%        |
| 18        | 5.057       | 1140          | 1156        | 1181         | rBV      | 144590         | 316849        | 7.20%           | 2.695%        |
| 19        | 5.231       | 1208          | 1210        | 1212         | rBV2     | 265            | 152           | 0.00%           | 0.001%        |
| 20        | 5.272       | 1220          | 1223        | 1227         | rVB      | 422            | 308           | 0.01%           | 0.003%        |
| 21        | 5.292       | 1227          | 1229        | 1233         | rBV2     | 349            | 263           | 0.01%           | 0.002%        |
| 22        | 5.395       | 1258          | 1261        | 1262         | rBV      | 159            | 87            | 0.00%           | 0.001%        |
| 23        | 5.536       | 1300          | 1305        | 1307         | rBV2     | 316            | 340           | 0.01%           | 0.003%        |
| 24        | 5.562       | 1310          | 1313        | 1315         | rBV2     | 233            | 155           | 0.00%           | 0.001%        |
| 25        | 5.594       | 1321          | 1323        | 1326         | rVB      | 293            | 145           | 0.00%           | 0.001%        |
| 26        | 5.719       | 1341          | 1362        | 1367         | rBV2     | 271947         | 694060        | 15.76%          | 5.903%        |
| 27        | 6.243       | 1512          | 1525        | 1546         | rBV      | 258369         | 493513        | 11.21%          | 4.197%        |
| 28        | 6.523       | 1604          | 1612        | 1624         | rBV4     | 3693           | 6849          | 0.16%           | 0.058%        |
| 29        | 6.603       | 1634          | 1637        | 1640         | rVB      | 472            | 341           | 0.01%           | 0.003%        |
| 30        | 6.629       | 1640          | 1645        | 1648         | rBV2     | 291            | 325           | 0.01%           | 0.003%        |
| 31        | 6.684       | 1649          | 1662        | 1686         | rBV2     | 178336         | 344808        | 7.83%           | 2.933%        |
| 32        | 6.851       | 1711          | 1714        | 1715         | rBV      | 179            | 85            | 0.00%           | 0.001%        |
| 33        | 6.903       | 1728          | 1730        | 1733         | rBV      | 180            | 102           | 0.00%           | 0.001%        |
| 34        | 6.919       | 1733          | 1735        | 1737         | rBV      | 170            | 84            | 0.00%           | 0.001%        |
| 35        | 6.993       | 1755          | 1758        | 1759         | rBV      | 203            | 142           | 0.00%           | 0.001%        |
| 36        | 7.025       | 1766          | 1768        | 1772         | rBV      | 180            | 134           | 0.00%           | 0.001%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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\SFAMULM033123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |         |         |
|----|--------|------|------|------|------|---------|---------|---------|---------|
| 37 | 7.121  | 1796 | 1798 | 1800 | rVB  | 162     | 65      | 0.00%   | 0.001%  |
| 38 | 7.144  | 1802 | 1805 | 1807 | rBV  | 229     | 130     | 0.00%   | 0.001%  |
| 39 | 7.189  | 1811 | 1819 | 1825 | rBV3 | 1300    | 1855    | 0.04%   | 0.016%  |
| 40 | 7.317  | 1856 | 1859 | 1862 | rBV  | 297     | 167     | 0.00%   | 0.001%  |
| 41 | 7.369  | 1869 | 1875 | 1876 | rBV  | 381     | 327     | 0.01%   | 0.003%  |
| 42 | 7.388  | 1880 | 1881 | 1885 | rVV2 | 219     | 129     | 0.00%   | 0.001%  |
| 43 | 7.494  | 1912 | 1914 | 1919 | rBV2 | 194     | 107     | 0.00%   | 0.001%  |
| 44 | 7.562  | 1923 | 1935 | 1958 | rVV  | 97070   | 167069  | 3.79%   | 1.421%  |
| 45 | 7.893  | 2025 | 2038 | 2059 | rBV  | 352614  | 609203  | 13.84%  | 5.181%  |
| 46 | 8.176  | 2115 | 2126 | 2143 | rBV  | 66422   | 112420  | 2.55%   | 0.956%  |
| 47 | 8.295  | 2161 | 2163 | 2165 | rBV  | 177     | 58      | 0.00%   | 0.000%  |
| 48 | 8.337  | 2174 | 2176 | 2178 | rBV  | 186     | 89      | 0.00%   | 0.001%  |
| 49 | 8.388  | 2189 | 2192 | 2194 | rBV  | 235     | 129     | 0.00%   | 0.001%  |
| 50 | 8.414  | 2198 | 2200 | 2202 | rBV2 | 260     | 146     | 0.00%   | 0.001%  |
| 51 | 8.459  | 2211 | 2214 | 2215 | rBV  | 237     | 141     | 0.00%   | 0.001%  |
| 52 | 8.626  | 2255 | 2266 | 2296 | rBV  | 208630  | 375872  | 8.54%   | 3.197%  |
| 53 | 8.755  | 2304 | 2306 | 2309 | rBV  | 321     | 201     | 0.00%   | 0.002%  |
| 54 | 8.912  | 2352 | 2355 | 2362 | rVB2 | 469     | 502     | 0.01%   | 0.004%  |
| 55 | 8.947  | 2362 | 2366 | 2367 | rBV  | 305     | 232     | 0.01%   | 0.002%  |
| 56 | 9.021  | 2386 | 2389 | 2392 | rBV  | 319     | 152     | 0.00%   | 0.001%  |
| 57 | 9.153  | 2427 | 2430 | 2435 | rBV2 | 186     | 188     | 0.00%   | 0.002%  |
| 58 | 9.211  | 2446 | 2448 | 2449 | rBV2 | 231     | 117     | 0.00%   | 0.001%  |
| 59 | 9.304  | 2474 | 2477 | 2480 | rBV  | 247     | 184     | 0.00%   | 0.002%  |
| 60 | 9.443  | 2498 | 2520 | 2556 | rBV2 | 2320708 | 4402903 | 100.00% | 37.446% |
| 61 | 9.713  | 2602 | 2604 | 2607 | rVB2 | 303     | 165     | 0.00%   | 0.001%  |
| 62 | 9.774  | 2621 | 2623 | 2626 | rVB  | 199     | 88      | 0.00%   | 0.001%  |
| 63 | 9.877  | 2653 | 2655 | 2661 | rBV  | 299     | 219     | 0.00%   | 0.002%  |
| 64 | 10.108 | 2724 | 2727 | 2732 | rVB  | 321     | 319     | 0.01%   | 0.003%  |
| 65 | 10.137 | 2734 | 2736 | 2738 | rVV  | 145     | 45      | 0.00%   | 0.000%  |
| 66 | 10.169 | 2743 | 2746 | 2749 | rBV  | 261     | 235     | 0.01%   | 0.002%  |
| 67 | 10.639 | 2890 | 2892 | 2895 | rBV  | 201     | 92      | 0.00%   | 0.001%  |
| 68 | 10.751 | 2914 | 2927 | 2943 | rBV  | 261491  | 425767  | 9.67%   | 3.621%  |
| 69 | 10.854 | 2958 | 2959 | 2960 | rBV  | 163     | 35      | 0.00%   | 0.000%  |
| 70 | 11.008 | 3003 | 3007 | 3010 | rBV  | 247     | 197     | 0.00%   | 0.002%  |
| 71 | 11.108 | 3035 | 3038 | 3041 | rBV  | 222     | 132     | 0.00%   | 0.001%  |
| 72 | 11.160 | 3052 | 3054 | 3056 | rBV2 | 206     | 125     | 0.00%   | 0.001%  |
| 73 | 11.439 | 3140 | 3141 | 3143 | rBV  | 125     | 50      | 0.00%   | 0.000%  |
| 74 | 11.561 | 3176 | 3179 | 3181 | rBV2 | 320     | 202     | 0.00%   | 0.002%  |
| 75 | 11.690 | 3216 | 3219 | 3221 | rBV  | 163     | 95      | 0.00%   | 0.001%  |
| 76 | 11.742 | 3226 | 3235 | 3244 | rBV  | 28301   | 43860   | 1.00%   | 0.373%  |

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Min Area: 0 % of largest Peak

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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\SFAMULM033123WMA.M

Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 77 | 11.828 | 3244 | 3262 | 3282 | rVV2 | 768133 | 1797119 | 40.82% | 15.284% |
| 78 | 12.198 | 3361 | 3377 | 3399 | rBV2 | 544884 | 1300496 | 29.54% | 11.060% |
| 79 | 12.362 | 3426 | 3428 | 3434 | rVB  | 544    | 270     | 0.01%  | 0.002%  |
| 80 | 12.954 | 3610 | 3612 | 3615 | rBV  | 222    | 110     | 0.00%  | 0.001%  |
| 81 | 13.224 | 3694 | 3696 | 3698 | rVB2 | 491    | 199     | 0.00%  | 0.002%  |
| 82 | 13.288 | 3714 | 3716 | 3719 | rBV  | 261    | 124     | 0.00%  | 0.001%  |
| 83 | 13.838 | 3877 | 3887 | 3899 | rBV  | 24514  | 39727   | 0.90%  | 0.338%  |
| 84 | 14.089 | 3963 | 3965 | 3966 | rBV  | 626    | 241     | 0.01%  | 0.002%  |
| 85 | 14.163 | 3986 | 3988 | 3992 | rBV  | 375    | 217     | 0.00%  | 0.002%  |
| 86 | 14.330 | 4035 | 4040 | 4048 | rVB4 | 1363   | 1608    | 0.04%  | 0.014%  |

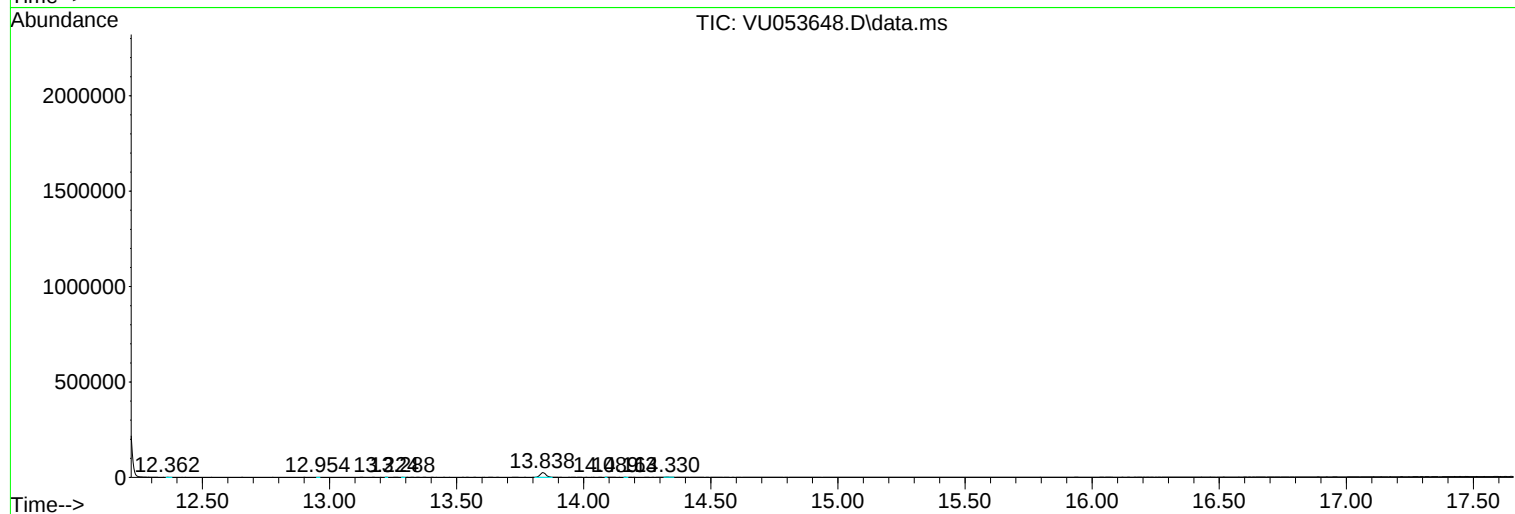
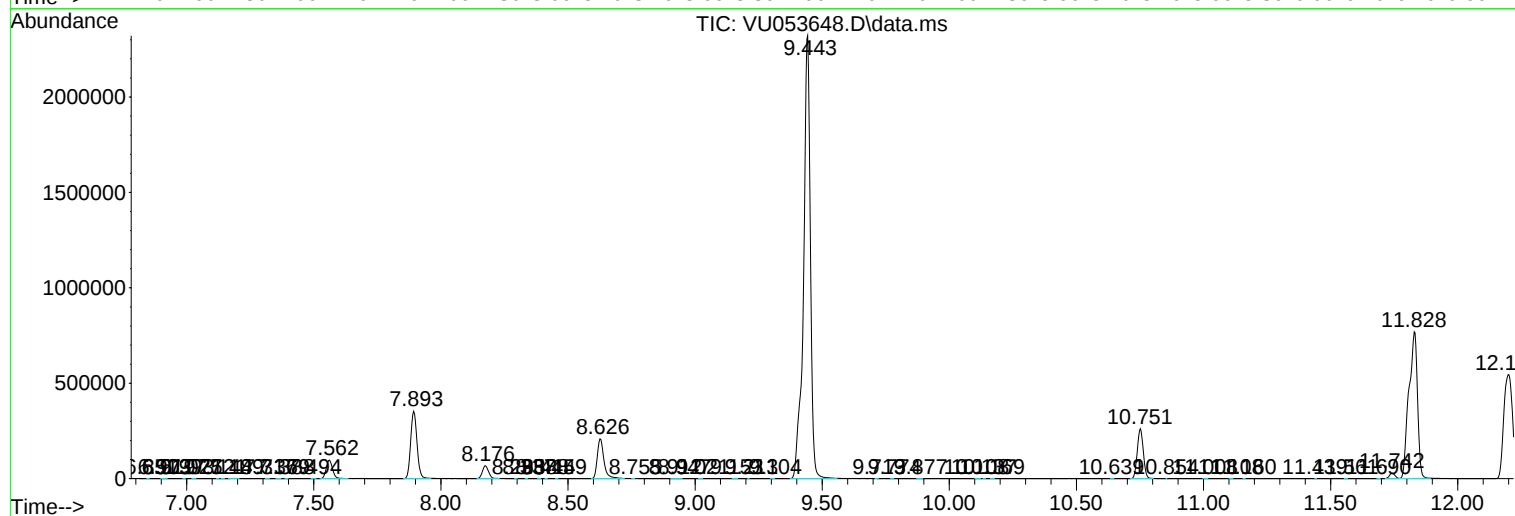
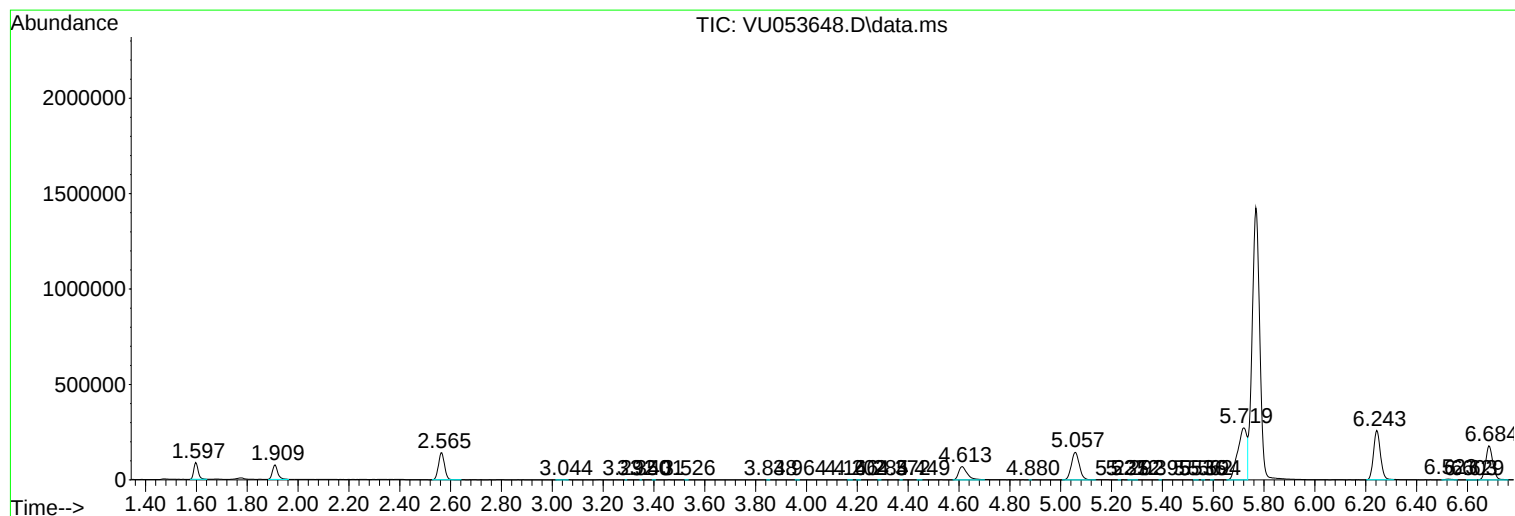
Sum of corrected areas: 11758157

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU041123\  
Data File : VU053648.D  
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Instrument :  
MSVOA\_U  
ClientSampleId :  
C0ME4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

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| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|