

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052718\  
 Data File : VU024206.D  
 Acq On : 27 May 2018 23:01  
 Operator : MD/SY  
 Sample : VU0527WBL02  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 27 Sample Multiplier: 1

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM052518WMA.M  
 Title : VOC Analysis

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         | 0.616       | 5             | 8           | 12           | rVB2     | 166            | 156           | 0.01%           | 0.002%        |
| 2         | 0.635       | 12            | 14          | 16           | rBV      | 178            | 84            | 0.01%           | 0.001%        |
| 3         | 0.648       | 16            | 18          | 21           | rVB2     | 174            | 101           | 0.01%           | 0.001%        |
| 4         | 0.671       | 21            | 25          | 28           | rBV2     | 173            | 119           | 0.01%           | 0.001%        |
| 5         | 0.690       | 29            | 31          | 34           | rVB2     | 130            | 71            | 0.00%           | 0.001%        |
| 6         | 0.722       | 39            | 41          | 43           | rVB      | 123            | 64            | 0.00%           | 0.001%        |
| 7         | 0.738       | 43            | 46          | 47           | rBV      | 120            | 68            | 0.00%           | 0.001%        |
| 8         | 0.790       | 56            | 62          | 65           | rBV2     | 193            | 193           | 0.01%           | 0.002%        |
| 9         | 0.838       | 73            | 77          | 78           | rBV      | 94             | 61            | 0.00%           | 0.001%        |
| 10        | 0.844       | 78            | 79          | 82           | rVB      | 195            | 93            | 0.01%           | 0.001%        |
| 11        | 0.867       | 82            | 86          | 89           | rBV2     | 201            | 167           | 0.01%           | 0.002%        |
| 12        | 0.941       | 105           | 109         | 111          | rBV      | 210            | 131           | 0.01%           | 0.001%        |
| 13        | 0.957       | 111           | 114         | 116          | rVB      | 136            | 94            | 0.01%           | 0.001%        |
| 14        | 0.989       | 121           | 124         | 125          | rBV      | 173            | 98            | 0.01%           | 0.001%        |
| 15        | 1.089       | 134           | 155         | 179          | rBV      | 1360388        | 1532855       | 100.00%         | 15.209%       |
| 16        | 1.400       | 245           | 252         | 262          | rBV      | 177551         | 186962        | 12.20%          | 1.855%        |
| 17        | 1.677       | 330           | 338         | 359          | rVB      | 130957         | 174707        | 11.40%          | 1.733%        |
| 18        | 2.272       | 512           | 523         | 537          | rBV      | 273886         | 419625        | 27.38%          | 4.163%        |
| 19        | 2.561       | 611           | 613         | 616          | rBV      | 190            | 118           | 0.01%           | 0.001%        |
| 20        | 2.600       | 623           | 625         | 626          | rBV      | 365            | 149           | 0.01%           | 0.001%        |
| 21        | 2.703       | 651           | 657         | 663          | rVV3     | 824            | 962           | 0.06%           | 0.010%        |
| 22        | 2.728       | 663           | 665         | 668          | rVB2     | 194            | 109           | 0.01%           | 0.001%        |
| 23        | 2.802       | 685           | 688         | 690          | rBV      | 200            | 153           | 0.01%           | 0.002%        |
| 24        | 2.912       | 719           | 722         | 725          | rBV2     | 210            | 195           | 0.01%           | 0.002%        |
| 25        | 2.947       | 729           | 733         | 735          | rBV      | 139            | 109           | 0.01%           | 0.001%        |
| 26        | 2.989       | 743           | 746         | 749          | rBV2     | 147            | 95            | 0.01%           | 0.001%        |
| 27        | 3.060       | 765           | 768         | 774          | rVB      | 237            | 158           | 0.01%           | 0.002%        |
| 28        | 3.162       | 796           | 800         | 803          | rBV2     | 190            | 192           | 0.01%           | 0.002%        |
| 29        | 3.233       | 820           | 822         | 825          | rBV      | 165            | 84            | 0.01%           | 0.001%        |
| 30        | 3.265       | 830           | 832         | 836          | rVB      | 150            | 76            | 0.00%           | 0.001%        |
| 31        | 3.301       | 840           | 843         | 844          | rBV      | 141            | 63            | 0.00%           | 0.001%        |
| 32        | 3.352       | 857           | 859         | 862          | rVB      | 238            | 129           | 0.01%           | 0.001%        |
| 33        | 3.378       | 862           | 867         | 868          | rBV      | 190            | 88            | 0.01%           | 0.001%        |
| 34        | 3.387       | 868           | 870         | 873          | rBV2     | 148            | 126           | 0.01%           | 0.001%        |

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 Sampling : 1  
 Start Thrs: 0.2  
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Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM052518WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |        |         |
|----|-------|------|------|------|------|--------|---------|--------|---------|
| 35 | 3.442 | 885  | 887  | 891  | rVB  | 179    | 74      | 0.00%  | 0.001%  |
| 36 | 3.474 | 894  | 897  | 899  | rVV  | 128    | 74      | 0.00%  | 0.001%  |
| 37 | 3.532 | 910  | 915  | 916  | rBV  | 190    | 133     | 0.01%  | 0.001%  |
| 38 | 3.558 | 920  | 923  | 925  | rBV  | 85     | 60      | 0.00%  | 0.001%  |
| 39 | 3.690 | 961  | 964  | 967  | rBV2 | 248    | 167     | 0.01%  | 0.002%  |
| 40 | 3.738 | 976  | 979  | 981  | rBV  | 144    | 77      | 0.01%  | 0.001%  |
| 41 | 3.764 | 985  | 987  | 989  | rBV  | 187    | 86      | 0.01%  | 0.001%  |
| 42 | 3.805 | 998  | 1000 | 1002 | rBV  | 127    | 81      | 0.01%  | 0.001%  |
| 43 | 3.844 | 1008 | 1012 | 1016 | rVB2 | 211    | 221     | 0.01%  | 0.002%  |
| 44 | 3.912 | 1031 | 1033 | 1034 | rBV  | 146    | 77      | 0.01%  | 0.001%  |
| 45 | 4.079 | 1083 | 1085 | 1088 | rVB  | 174    | 72      | 0.00%  | 0.001%  |
| 46 | 4.178 | 1099 | 1116 | 1153 | rBV2 | 107255 | 289858  | 18.91% | 2.876%  |
| 47 | 4.651 | 1245 | 1263 | 1288 | rBV  | 199634 | 467686  | 30.51% | 4.640%  |
| 48 | 4.899 | 1330 | 1340 | 1346 | rVB4 | 689    | 1356    | 0.09%  | 0.013%  |
| 49 | 4.931 | 1347 | 1350 | 1357 | rBV2 | 182    | 248     | 0.02%  | 0.002%  |
| 50 | 4.998 | 1361 | 1371 | 1372 | rBV  | 537    | 718     | 0.05%  | 0.007%  |
| 51 | 5.072 | 1392 | 1394 | 1397 | rVB  | 209    | 107     | 0.01%  | 0.001%  |
| 52 | 5.095 | 1400 | 1401 | 1403 | rBV  | 116    | 62      | 0.00%  | 0.001%  |
| 53 | 5.156 | 1417 | 1420 | 1421 | rBV  | 143    | 85      | 0.01%  | 0.001%  |
| 54 | 5.217 | 1437 | 1439 | 1443 | rVB  | 157    | 73      | 0.00%  | 0.001%  |
| 55 | 5.239 | 1443 | 1446 | 1449 | rBV2 | 212    | 194     | 0.01%  | 0.002%  |
| 56 | 5.346 | 1454 | 1479 | 1528 | rBV2 | 399065 | 1217107 | 79.40% | 12.076% |
| 57 | 5.731 | 1596 | 1599 | 1602 | rBV2 | 128    | 129     | 0.01%  | 0.001%  |
| 58 | 5.754 | 1602 | 1606 | 1611 | rVB2 | 335    | 376     | 0.02%  | 0.004%  |
| 59 | 5.780 | 1611 | 1614 | 1619 | rBV2 | 147    | 171     | 0.01%  | 0.002%  |
| 60 | 5.802 | 1619 | 1621 | 1623 | rBV  | 203    | 90      | 0.01%  | 0.001%  |
| 61 | 5.841 | 1628 | 1633 | 1634 | rBV  | 178    | 173     | 0.01%  | 0.002%  |
| 62 | 5.889 | 1634 | 1648 | 1675 | rBV  | 338531 | 686073  | 44.76% | 6.807%  |
| 63 | 6.188 | 1730 | 1741 | 1751 | rVB4 | 5073   | 10962   | 0.72%  | 0.109%  |
| 64 | 6.230 | 1751 | 1754 | 1758 | rBV2 | 274    | 245     | 0.02%  | 0.002%  |
| 65 | 6.336 | 1772 | 1787 | 1820 | rBV  | 268339 | 546547  | 35.66% | 5.423%  |
| 66 | 6.535 | 1847 | 1849 | 1855 | rBV3 | 175    | 171     | 0.01%  | 0.002%  |
| 67 | 6.580 | 1860 | 1863 | 1866 | rVB2 | 179    | 125     | 0.01%  | 0.001%  |
| 68 | 6.609 | 1866 | 1872 | 1877 | rVB2 | 239    | 329     | 0.02%  | 0.003%  |
| 69 | 6.638 | 1878 | 1881 | 1883 | rBV  | 156    | 119     | 0.01%  | 0.001%  |
| 70 | 6.731 | 1908 | 1910 | 1912 | rBV  | 202    | 141     | 0.01%  | 0.001%  |
| 71 | 6.863 | 1945 | 1951 | 1952 | rBV2 | 308    | 300     | 0.02%  | 0.003%  |

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ALS Vial : 27 Sample Multiplier: 1

## Integration Parameters: LSCINT.P

Integrator: RTE  
Smoothing : OFF  
Sampling : 1  
Start Thrs: 0.2  
Stop Thrs : 0

Filtering: 5  
Min Area: 0 % of largest Peak  
Max Peaks: 100  
Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
Peak separation: 5

Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM052518WMA.M  
Title : VOC Analysis

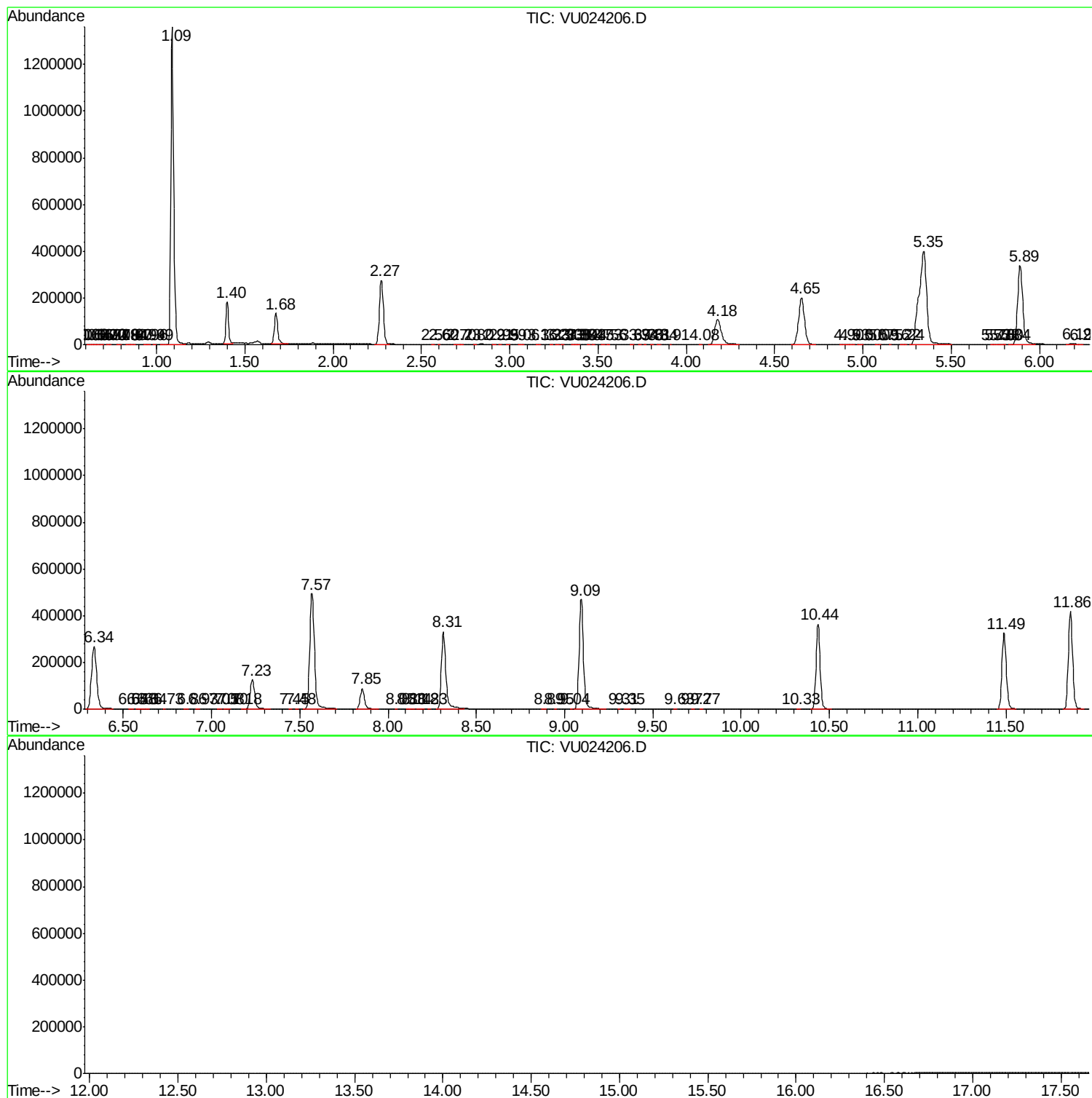
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 6.928  | 1966 | 1971 | 1973 | rBV  | 156    | 169    | 0.01%  | 0.002% |
| 73  | 7.047  | 2003 | 2008 | 2012 | rVB2 | 229    | 246    | 0.02%  | 0.002% |
| 74  | 7.075  | 2015 | 2017 | 2020 | rVB2 | 175    | 100    | 0.01%  | 0.001% |
| 75  | 7.098  | 2021 | 2024 | 2027 | rBV  | 151    | 124    | 0.01%  | 0.001% |
| 76  | 7.175  | 2046 | 2048 | 2052 | rVB2 | 167    | 103    | 0.01%  | 0.001% |
| 77  | 7.230  | 2053 | 2065 | 2097 | rBV  | 126127 | 228988 | 14.94% | 2.272% |
| 78  | 7.448  | 2130 | 2133 | 2134 | rBV  | 222    | 132    | 0.01%  | 0.001% |
| 79  | 7.484  | 2141 | 2144 | 2147 | rBV2 | 170    | 112    | 0.01%  | 0.001% |
| 80  | 7.567  | 2155 | 2170 | 2214 | rBV  | 493933 | 917030 | 59.82% | 9.099% |
| 81  | 7.854  | 2248 | 2259 | 2288 | rBV  | 87884  | 148732 | 9.70%  | 1.476% |
| 82  | 8.046  | 2317 | 2319 | 2320 | rBV  | 161    | 68     | 0.00%  | 0.001% |
| 83  | 8.111  | 2336 | 2339 | 2342 | rVB2 | 188    | 120    | 0.01%  | 0.001% |
| 84  | 8.140  | 2342 | 2348 | 2351 | rBV2 | 262    | 288    | 0.02%  | 0.003% |
| 85  | 8.181  | 2354 | 2361 | 2367 | rBV2 | 348    | 527    | 0.03%  | 0.005% |
| 86  | 8.230  | 2374 | 2376 | 2379 | rBV2 | 221    | 117    | 0.01%  | 0.001% |
| 87  | 8.313  | 2389 | 2402 | 2438 | rBV  | 331620 | 589924 | 38.49% | 5.853% |
| 88  | 8.886  | 2575 | 2580 | 2583 | rBV2 | 232    | 228    | 0.01%  | 0.002% |
| 89  | 8.947  | 2597 | 2599 | 2601 | rVB  | 191    | 60     | 0.00%  | 0.001% |
| 90  | 9.037  | 2625 | 2627 | 2629 | rBV  | 197    | 128    | 0.01%  | 0.001% |
| 91  | 9.095  | 2632 | 2645 | 2687 | rVV  | 469573 | 809195 | 52.79% | 8.029% |
| 92  | 9.307  | 2709 | 2711 | 2712 | rBV  | 154    | 67     | 0.00%  | 0.001% |
| 93  | 9.345  | 2720 | 2723 | 2730 | rBV2 | 218    | 241    | 0.02%  | 0.002% |
| 94  | 9.625  | 2807 | 2810 | 2813 | rBV  | 250    | 238    | 0.02%  | 0.002% |
| 95  | 9.722  | 2838 | 2840 | 2843 | rBV  | 173    | 120    | 0.01%  | 0.001% |
| 96  | 9.773  | 2853 | 2856 | 2858 | rBV2 | 217    | 148    | 0.01%  | 0.001% |
| 97  | 10.326 | 3025 | 3028 | 3031 | rVB2 | 575    | 345    | 0.02%  | 0.003% |
| 98  | 10.435 | 3049 | 3062 | 3085 | rBV  | 363906 | 585660 | 38.21% | 5.811% |
| 99  | 11.487 | 3377 | 3389 | 3410 | rBV  | 324875 | 556504 | 36.31% | 5.522% |
| 100 | 11.863 | 3494 | 3506 | 3530 | rBV  | 417246 | 696110 | 45.41% | 6.907% |

Sum of corrected areas: 10078846

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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM052518WMA.M  
Quant Title : VOC Analysis

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



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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM052518WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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

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