

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052118\  
 Data File : VU023966.D  
 Acq On : 21 May 2018 12:24  
 Operator : MD/SY  
 Sample : J3032-09  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 5 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\SOMULM051218WMA.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         | 0.612       | 3             | 7           | 10           | rBV      | 203            | 211           | 0.002%          | 0.0002%       |
| 2         | 0.645       | 14            | 17          | 24           | rBV      | 152            | 168           | 0.001%          | 0.0002%       |
| 3         | 0.683       | 26            | 29          | 31           | rBV      | 147            | 92            | 0.001%          | 0.0001%       |
| 4         | 0.757       | 47            | 52          | 56           | rVV2     | 135            | 150           | 0.001%          | 0.0002%       |
| 5         | 0.841       | 76            | 78          | 83           | rVB      | 188            | 145           | 0.001%          | 0.0002%       |
| 6         | 0.873       | 83            | 88          | 92           | rBV2     | 173            | 217           | 0.002%          | 0.0002%       |
| 7         | 0.928       | 103           | 105         | 109          | rBV2     | 141            | 136           | 0.001%          | 0.0001%       |
| 8         | 1.088       | 136           | 155         | 176          | rBV      | 336762         | 401769        | 34.04%          | 4.208%        |
| 9         | 1.185       | 180           | 185         | 190          | rVV3     | 5758           | 5934          | 0.50%           | 0.0062%       |
| 10        | 1.397       | 244           | 251         | 266          | rBV      | 147017         | 156509        | 13.26%          | 1.639%        |
| 11        | 1.680       | 331           | 339         | 357          | rVB      | 124945         | 155774        | 13.20%          | 1.631%        |
| 12        | 2.272       | 512           | 523         | 534          | rBV      | 258332         | 386638        | 32.76%          | 4.049%        |
| 13        | 2.448       | 572           | 578         | 582          | rBV4     | 960            | 1355          | 0.11%           | 0.0014%       |
| 14        | 2.545       | 606           | 608         | 610          | rBV      | 231            | 158           | 0.001%          | 0.0002%       |
| 15        | 2.616       | 626           | 630         | 631          | rBV2     | 296            | 233           | 0.002%          | 0.0002%       |
| 16        | 2.699       | 651           | 656         | 664          | rBV3     | 1051           | 1398          | 0.12%           | 0.0015%       |
| 17        | 2.834       | 686           | 698         | 712          | rVB3     | 5097           | 10650         | 0.90%           | 0.112%        |
| 18        | 2.908       | 718           | 721         | 724          | rBV2     | 164            | 110           | 0.001%          | 0.0001%       |
| 19        | 2.953       | 730           | 735         | 740          | rBV2     | 173            | 218           | 0.002%          | 0.0002%       |
| 20        | 3.317       | 845           | 848         | 851          | rBV      | 101            | 81            | 0.001%          | 0.0001%       |
| 21        | 3.342       | 853           | 856         | 858          | rVV2     | 122            | 83            | 0.001%          | 0.0001%       |
| 22        | 3.390       | 867           | 871         | 874          | rBV2     | 150            | 177           | 0.001%          | 0.0002%       |
| 23        | 3.506       | 904           | 907         | 910          | rBV      | 113            | 76            | 0.001%          | 0.0001%       |
| 24        | 3.535       | 914           | 916         | 920          | rVB      | 190            | 124           | 0.001%          | 0.0001%       |
| 25        | 3.561       | 920           | 924         | 929          | rBV2     | 200            | 226           | 0.002%          | 0.0002%       |
| 26        | 3.606       | 934           | 938         | 941          | rBV2     | 189            | 163           | 0.001%          | 0.0002%       |
| 27        | 3.667       | 950           | 957         | 959          | rBV2     | 179            | 218           | 0.002%          | 0.0002%       |
| 28        | 3.728       | 972           | 976         | 977          | rBV      | 184            | 146           | 0.001%          | 0.0002%       |
| 29        | 3.805       | 997           | 1000        | 1003         | rBV2     | 269            | 223           | 0.002%          | 0.0002%       |
| 30        | 3.828       | 1003          | 1007        | 1009         | rBV      | 173            | 156           | 0.001%          | 0.0002%       |
| 31        | 3.886       | 1021          | 1025        | 1026         | rBV      | 122            | 81            | 0.001%          | 0.0001%       |
| 32        | 3.985       | 1045          | 1056        | 1073         | rVB4     | 2616           | 7037          | 0.60%           | 0.074%        |
| 33        | 4.178       | 1101          | 1116        | 1142         | rBV      | 111073         | 295754        | 25.06%          | 3.097%        |
| 34        | 4.513       | 1217          | 1220        | 1224         | rBV2     | 312            | 312           | 0.003%          | 0.0003%       |

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM051218WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |         |         |
|----|-------|------|------|------|------|--------|---------|---------|---------|
| 35 | 4.558 | 1232 | 1234 | 1237 | rVB2 | 222    | 131     | 0.01%   | 0.001%  |
| 36 | 4.651 | 1246 | 1263 | 1290 | rBV  | 194695 | 463435  | 39.26%  | 4.853%  |
| 37 | 4.886 | 1330 | 1336 | 1346 | rVB3 | 746    | 1163    | 0.10%   | 0.012%  |
| 38 | 4.944 | 1350 | 1354 | 1360 | rVB2 | 186    | 273     | 0.02%   | 0.003%  |
| 39 | 4.976 | 1360 | 1364 | 1368 | rBV2 | 340    | 332     | 0.03%   | 0.003%  |
| 40 | 4.995 | 1368 | 1370 | 1373 | rBV  | 210    | 130     | 0.01%   | 0.001%  |
| 41 | 5.037 | 1380 | 1383 | 1388 | rVB2 | 193    | 186     | 0.02%   | 0.002%  |
| 42 | 5.066 | 1388 | 1392 | 1395 | rBV2 | 152    | 138     | 0.01%   | 0.001%  |
| 43 | 5.107 | 1402 | 1405 | 1409 | rVB  | 233    | 191     | 0.02%   | 0.002%  |
| 44 | 5.165 | 1420 | 1423 | 1425 | rBV  | 168    | 91      | 0.01%   | 0.001%  |
| 45 | 5.194 | 1429 | 1432 | 1434 | rBV  | 202    | 138     | 0.01%   | 0.001%  |
| 46 | 5.243 | 1444 | 1447 | 1451 | rBV  | 215    | 195     | 0.02%   | 0.002%  |
| 47 | 5.342 | 1451 | 1478 | 1511 | rBV2 | 384994 | 1180321 | 100.00% | 12.361% |
| 48 | 5.680 | 1579 | 1583 | 1587 | rVB2 | 334    | 331     | 0.03%   | 0.003%  |
| 49 | 5.699 | 1587 | 1589 | 1592 | rBV  | 149    | 70      | 0.01%   | 0.001%  |
| 50 | 5.760 | 1604 | 1608 | 1610 | rBV2 | 223    | 124     | 0.01%   | 0.001%  |
| 51 | 5.789 | 1613 | 1617 | 1619 | rBV  | 164    | 166     | 0.01%   | 0.002%  |
| 52 | 5.799 | 1619 | 1620 | 1624 | rVB  | 203    | 102     | 0.01%   | 0.001%  |
| 53 | 5.831 | 1627 | 1630 | 1633 | rVB  | 143    | 91      | 0.01%   | 0.001%  |
| 54 | 5.889 | 1633 | 1648 | 1672 | rBV  | 337973 | 689980  | 58.46%  | 7.226%  |
| 55 | 6.175 | 1732 | 1737 | 1738 | rBV2 | 1204   | 938     | 0.08%   | 0.010%  |
| 56 | 6.223 | 1750 | 1752 | 1757 | rVB  | 188    | 102     | 0.01%   | 0.001%  |
| 57 | 6.246 | 1757 | 1759 | 1763 | rVB  | 214    | 134     | 0.01%   | 0.001%  |
| 58 | 6.336 | 1769 | 1787 | 1820 | rBV  | 262497 | 544005  | 46.09%  | 5.697%  |
| 59 | 6.551 | 1852 | 1854 | 1857 | rVV  | 168    | 108     | 0.01%   | 0.001%  |
| 60 | 6.609 | 1870 | 1872 | 1874 | rVB  | 136    | 73      | 0.01%   | 0.001%  |
| 61 | 6.641 | 1878 | 1882 | 1883 | rBV  | 114    | 88      | 0.01%   | 0.001%  |
| 62 | 6.657 | 1883 | 1887 | 1888 | rBV2 | 177    | 137     | 0.01%   | 0.001%  |
| 63 | 6.747 | 1912 | 1915 | 1918 | rBV2 | 199    | 187     | 0.02%   | 0.002%  |
| 64 | 6.786 | 1918 | 1927 | 1932 | rBV4 | 995    | 1453    | 0.12%   | 0.015%  |
| 65 | 6.824 | 1932 | 1939 | 1940 | rBV3 | 836    | 734     | 0.06%   | 0.008%  |
| 66 | 6.918 | 1966 | 1968 | 1972 | rVB2 | 128    | 78      | 0.01%   | 0.001%  |
| 67 | 6.960 | 1977 | 1981 | 1982 | rBV  | 172    | 114     | 0.01%   | 0.001%  |
| 68 | 7.021 | 1998 | 2000 | 2004 | rVB2 | 349    | 272     | 0.02%   | 0.003%  |
| 69 | 7.053 | 2004 | 2010 | 2012 | rBV2 | 232    | 272     | 0.02%   | 0.003%  |
| 70 | 7.078 | 2016 | 2018 | 2022 | rBV2 | 120    | 94      | 0.01%   | 0.001%  |
| 71 | 7.101 | 2022 | 2025 | 2029 | rVB  | 208    | 170     | 0.01%   | 0.002%  |

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM051218WMA.M  
 Title : VOC Analysis

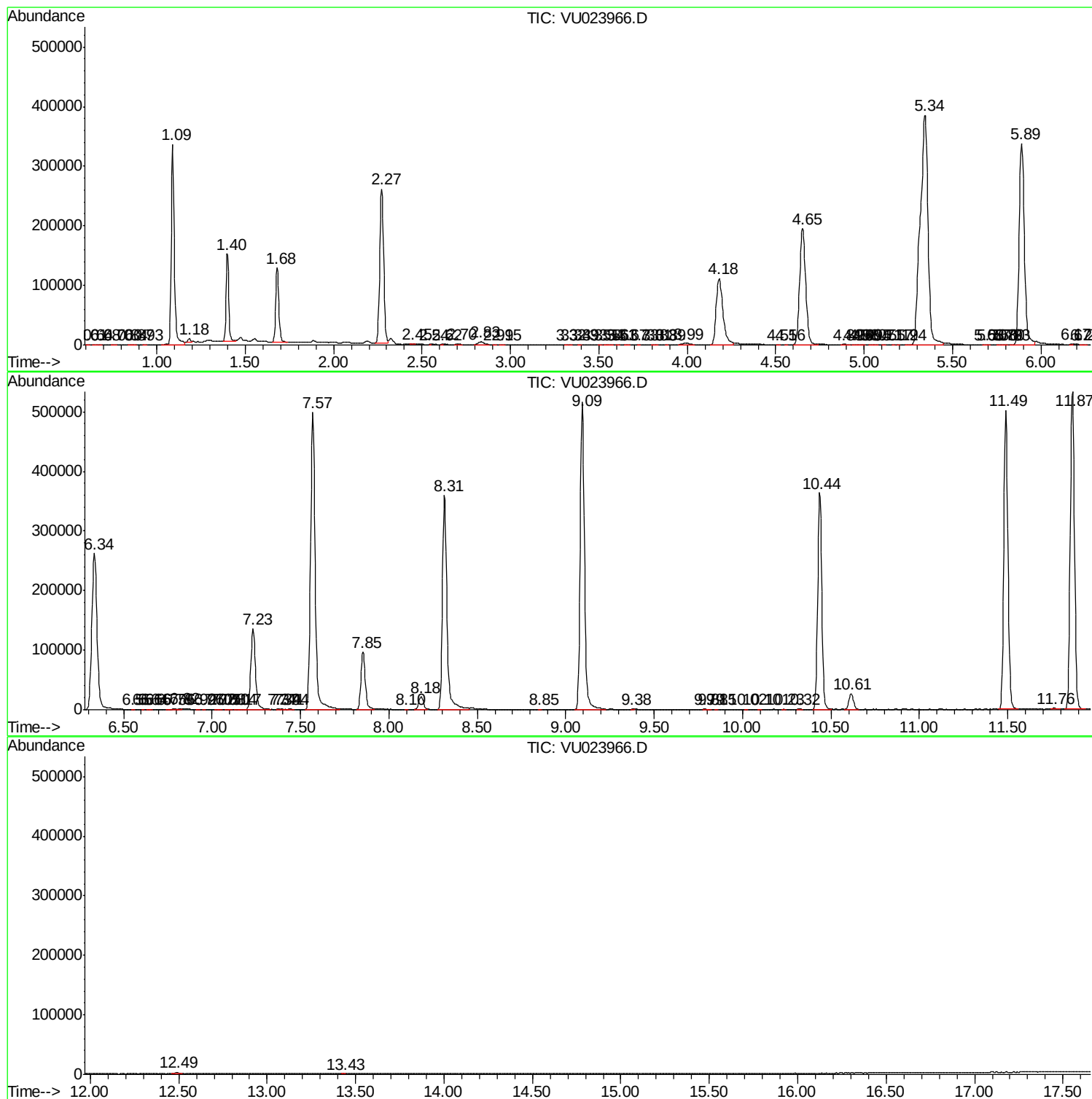
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 7.143  | 2033 | 2038 | 2041 | rVB  | 223    | 224    | 0.02%  | 0.002% |
| 73  | 7.168  | 2041 | 2046 | 2052 | rBV2 | 221    | 306    | 0.03%  | 0.003% |
| 74  | 7.233  | 2052 | 2066 | 2096 | rBV  | 135269 | 250164 | 21.19% | 2.620% |
| 75  | 7.374  | 2106 | 2110 | 2113 | rBV3 | 265    | 291    | 0.02%  | 0.003% |
| 76  | 7.394  | 2113 | 2116 | 2120 | rVV4 | 411    | 372    | 0.03%  | 0.004% |
| 77  | 7.413  | 2120 | 2122 | 2126 | rVB  | 255    | 138    | 0.01%  | 0.001% |
| 78  | 7.442  | 2126 | 2131 | 2137 | rBV2 | 582    | 642    | 0.05%  | 0.007% |
| 79  | 7.570  | 2157 | 2171 | 2218 | rBV  | 498230 | 908168 | 76.94% | 9.511% |
| 80  | 7.853  | 2247 | 2259 | 2279 | rBV  | 96045  | 166237 | 14.08% | 1.741% |
| 81  | 8.098  | 2332 | 2335 | 2338 | rBV  | 189    | 137    | 0.01%  | 0.001% |
| 82  | 8.185  | 2350 | 2362 | 2373 | rBV2 | 20723  | 39189  | 3.32%  | 0.410% |
| 83  | 8.313  | 2390 | 2402 | 2446 | rBV  | 359189 | 649451 | 55.02% | 6.801% |
| 84  | 8.853  | 2567 | 2570 | 2573 | rVV  | 174    | 146    | 0.01%  | 0.002% |
| 85  | 9.094  | 2631 | 2645 | 2686 | rBV  | 516376 | 876868 | 74.29% | 9.183% |
| 86  | 9.377  | 2730 | 2733 | 2736 | rBV3 | 278    | 262    | 0.02%  | 0.003% |
| 87  | 9.789  | 2856 | 2861 | 2865 | rBV2 | 500    | 541    | 0.05%  | 0.006% |
| 88  | 9.808  | 2865 | 2867 | 2871 | rBV  | 175    | 135    | 0.01%  | 0.001% |
| 89  | 9.853  | 2878 | 2881 | 2883 | rBV2 | 256    | 184    | 0.02%  | 0.002% |
| 90  | 10.017 | 2930 | 2932 | 2935 | rBV2 | 179    | 140    | 0.01%  | 0.001% |
| 91  | 10.101 | 2953 | 2958 | 2960 | rBV  | 282    | 267    | 0.02%  | 0.003% |
| 92  | 10.233 | 2996 | 2999 | 3003 | rVB  | 266    | 174    | 0.01%  | 0.002% |
| 93  | 10.319 | 3022 | 3026 | 3032 | rVB3 | 520    | 618    | 0.05%  | 0.006% |
| 94  | 10.435 | 3050 | 3062 | 3082 | rBV  | 363480 | 594507 | 50.37% | 6.226% |
| 95  | 10.612 | 3106 | 3117 | 3131 | rBV  | 26536  | 45853  | 3.88%  | 0.480% |
| 96  | 11.490 | 3377 | 3390 | 3411 | rBV  | 502227 | 815989 | 69.13% | 8.546% |
| 97  | 11.763 | 3468 | 3475 | 3484 | rBV3 | 1677   | 2566   | 0.22%  | 0.027% |
| 98  | 11.866 | 3493 | 3507 | 3529 | rBV  | 532939 | 877275 | 74.33% | 9.187% |
| 99  | 12.487 | 3691 | 3700 | 3710 | rBV2 | 2567   | 4165   | 0.35%  | 0.044% |
| 100 | 13.432 | 3991 | 3994 | 3997 | rBV  | 438    | 392    | 0.03%  | 0.004% |

Sum of corrected areas: 9548670

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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM051218WMA.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\SOMULM051218WMA.M  
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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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