

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052118\  
 Data File : VU023995.D  
 Acq On : 22 May 2018 02:46  
 Operator : MD/SY  
 Sample : J3031-13  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 35 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         | 0.619       | 6             | 9           | 12           | rBV2     | 184            | 166           | 0.001%          | 0.0002%       |
| 2         | 0.806       | 60            | 67          | 70           | rBV      | 268            | 360           | 0.002%          | 0.0004%       |
| 3         | 0.844       | 76            | 79          | 83           | rVB2     | 117            | 87            | 0.000%          | 0.0001%       |
| 4         | 0.867       | 83            | 86          | 88           | rBV2     | 116            | 79            | 0.000%          | 0.0001%       |
| 5         | 0.899       | 94            | 96          | 101          | rVB      | 106            | 64            | 0.000%          | 0.0001%       |
| 6         | 0.944       | 107           | 110         | 111          | rBV      | 136            | 100           | 0.001%          | 0.0001%       |
| 7         | 0.970       | 115           | 118         | 121          | rBV      | 291            | 240           | 0.001%          | 0.0002%       |
| 8         | 1.089       | 137           | 155         | 178          | rBV      | 1566723        | 1787044       | 100.000%        | 18.112%       |
| 9         | 1.182       | 179           | 184         | 193          | rVB      | 18249          | 19483         | 1.009%          | 0.197%        |
| 10        | 1.397       | 244           | 251         | 263          | rBV      | 141107         | 144993        | 8.111%          | 1.470%        |
| 11        | 1.471       | 270           | 274         | 285          | rVB      | 15502          | 16734         | 0.944%          | 0.170%        |
| 12        | 1.680       | 331           | 339         | 353          | rVB      | 104141         | 131340        | 7.355%          | 1.331%        |
| 13        | 2.272       | 512           | 523         | 534          | rBV      | 211178         | 324124        | 18.144%         | 3.285%        |
| 14        | 2.449       | 571           | 578         | 581          | rBV2     | 1262           | 1699          | 0.100%          | 0.017%        |
| 15        | 2.622       | 623           | 632         | 640          | rBV2     | 2654           | 4274          | 0.244%          | 0.043%        |
| 16        | 2.677       | 646           | 649         | 651          | rVB      | 245            | 133           | 0.001%          | 0.0001%       |
| 17        | 2.700       | 651           | 656         | 663          | rBV2     | 862            | 1182          | 0.007%          | 0.0012%       |
| 18        | 2.841       | 689           | 700         | 710          | rVB4     | 1724           | 4112          | 0.233%          | 0.042%        |
| 19        | 2.886       | 710           | 714         | 716          | rBV2     | 151            | 138           | 0.001%          | 0.0001%       |
| 20        | 2.950       | 732           | 734         | 740          | rVB2     | 369            | 353           | 0.002%          | 0.0004%       |
| 21        | 2.992       | 740           | 747         | 752          | rBV3     | 473            | 618           | 0.003%          | 0.0006%       |
| 22        | 3.044       | 759           | 763         | 764          | rBV2     | 243            | 187           | 0.001%          | 0.0002%       |
| 23        | 3.072       | 770           | 772         | 775          | rBV      | 195            | 137           | 0.001%          | 0.0001%       |
| 24        | 3.130       | 787           | 790         | 792          | rBV2     | 173            | 120           | 0.001%          | 0.0001%       |
| 25        | 3.188       | 804           | 808         | 817          | rVB3     | 554            | 738           | 0.004%          | 0.0007%       |
| 26        | 3.391       | 867           | 871         | 876          | rBV2     | 301            | 306           | 0.002%          | 0.0003%       |
| 27        | 3.458       | 888           | 892         | 893          | rBV2     | 162            | 102           | 0.001%          | 0.0001%       |
| 28        | 3.468       | 893           | 895         | 899          | rVV2     | 158            | 100           | 0.001%          | 0.0001%       |
| 29        | 3.555       | 919           | 922         | 924          | rVB2     | 187            | 100           | 0.001%          | 0.0001%       |
| 30        | 3.587       | 927           | 932         | 937          | rBV2     | 248            | 291           | 0.002%          | 0.0003%       |
| 31        | 3.609       | 937           | 939         | 942          | rVB      | 166            | 72            | 0.000%          | 0.0001%       |
| 32        | 3.651       | 948           | 952         | 954          | rVB2     | 175            | 127           | 0.001%          | 0.0001%       |
| 33        | 3.674       | 954           | 959         | 965          | rBV2     | 227            | 289           | 0.002%          | 0.0003%       |
| 34        | 3.799       | 993           | 998         | 999          | rBV2     | 168            | 161           | 0.001%          | 0.0002%       |

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Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM051218WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |        |         |
|----|-------|------|------|------|------|--------|---------|--------|---------|
| 35 | 3.876 | 1019 | 1022 | 1026 | rBV2 | 90     | 72      | 0.00%  | 0.001%  |
| 36 | 3.918 | 1032 | 1035 | 1037 | rBV  | 307    | 236     | 0.01%  | 0.002%  |
| 37 | 4.005 | 1050 | 1062 | 1072 | rBV5 | 1493   | 3393    | 0.19%  | 0.034%  |
| 38 | 4.066 | 1078 | 1081 | 1084 | rBV  | 124    | 107     | 0.01%  | 0.001%  |
| 39 | 4.085 | 1084 | 1087 | 1089 | rVB2 | 212    | 133     | 0.01%  | 0.001%  |
| 40 | 4.182 | 1102 | 1117 | 1154 | rBV  | 104097 | 285447  | 15.97% | 2.893%  |
| 41 | 4.503 | 1214 | 1217 | 1219 | rBV2 | 154    | 110     | 0.01%  | 0.001%  |
| 42 | 4.523 | 1219 | 1223 | 1227 | rVB2 | 307    | 239     | 0.01%  | 0.002%  |
| 43 | 4.651 | 1245 | 1263 | 1290 | rBV  | 172075 | 407260  | 22.79% | 4.128%  |
| 44 | 4.831 | 1316 | 1319 | 1322 | rVB2 | 270    | 128     | 0.01%  | 0.001%  |
| 45 | 4.879 | 1331 | 1334 | 1336 | rBV2 | 455    | 381     | 0.02%  | 0.004%  |
| 46 | 4.986 | 1366 | 1367 | 1368 | rBV2 | 202    | 57      | 0.00%  | 0.001%  |
| 47 | 4.998 | 1369 | 1371 | 1373 | rVV2 | 311    | 152     | 0.01%  | 0.002%  |
| 48 | 5.008 | 1373 | 1374 | 1377 | rVB2 | 191    | 71      | 0.00%  | 0.001%  |
| 49 | 5.085 | 1392 | 1398 | 1401 | rBV2 | 199    | 207     | 0.01%  | 0.002%  |
| 50 | 5.124 | 1408 | 1410 | 1415 | rVB2 | 167    | 103     | 0.01%  | 0.001%  |
| 51 | 5.259 | 1450 | 1452 | 1454 | rBV  | 133    | 73      | 0.00%  | 0.001%  |
| 52 | 5.342 | 1454 | 1478 | 1518 | rBV2 | 334663 | 1020213 | 57.09% | 10.340% |
| 53 | 5.751 | 1602 | 1605 | 1608 | rBV  | 212    | 160     | 0.01%  | 0.002%  |
| 54 | 5.783 | 1613 | 1615 | 1618 | rBV  | 210    | 110     | 0.01%  | 0.001%  |
| 55 | 5.831 | 1628 | 1630 | 1633 | rBV  | 113    | 55      | 0.00%  | 0.001%  |
| 56 | 5.892 | 1633 | 1649 | 1679 | rBV  | 314881 | 639878  | 35.81% | 6.485%  |
| 57 | 6.169 | 1733 | 1735 | 1736 | rBV  | 374    | 210     | 0.01%  | 0.002%  |
| 58 | 6.217 | 1748 | 1750 | 1752 | rVB2 | 245    | 76      | 0.00%  | 0.001%  |
| 59 | 6.336 | 1772 | 1787 | 1810 | rBV  | 237917 | 485520  | 27.17% | 4.921%  |
| 60 | 6.532 | 1846 | 1848 | 1851 | rBV2 | 146    | 117     | 0.01%  | 0.001%  |
| 61 | 6.632 | 1877 | 1879 | 1882 | rVB2 | 142    | 65      | 0.00%  | 0.001%  |
| 62 | 6.654 | 1882 | 1886 | 1891 | rBV2 | 169    | 174     | 0.01%  | 0.002%  |
| 63 | 6.677 | 1891 | 1893 | 1895 | rVV  | 107    | 52      | 0.00%  | 0.001%  |
| 64 | 6.690 | 1895 | 1897 | 1900 | rVB2 | 123    | 76      | 0.00%  | 0.001%  |
| 65 | 6.738 | 1908 | 1912 | 1914 | rBV2 | 200    | 164     | 0.01%  | 0.002%  |
| 66 | 6.799 | 1928 | 1931 | 1933 | rBV  | 139    | 97      | 0.01%  | 0.001%  |
| 67 | 6.876 | 1948 | 1955 | 1957 | rBV2 | 246    | 246     | 0.01%  | 0.002%  |
| 68 | 7.008 | 1988 | 1996 | 2001 | rBV2 | 197    | 384     | 0.02%  | 0.004%  |
| 69 | 7.101 | 2022 | 2025 | 2031 | rVB2 | 215    | 266     | 0.01%  | 0.003%  |
| 70 | 7.146 | 2036 | 2039 | 2041 | rBV2 | 116    | 76      | 0.00%  | 0.001%  |
| 71 | 7.233 | 2053 | 2066 | 2088 | rBV  | 109641 | 199468  | 11.16% | 2.022%  |

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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

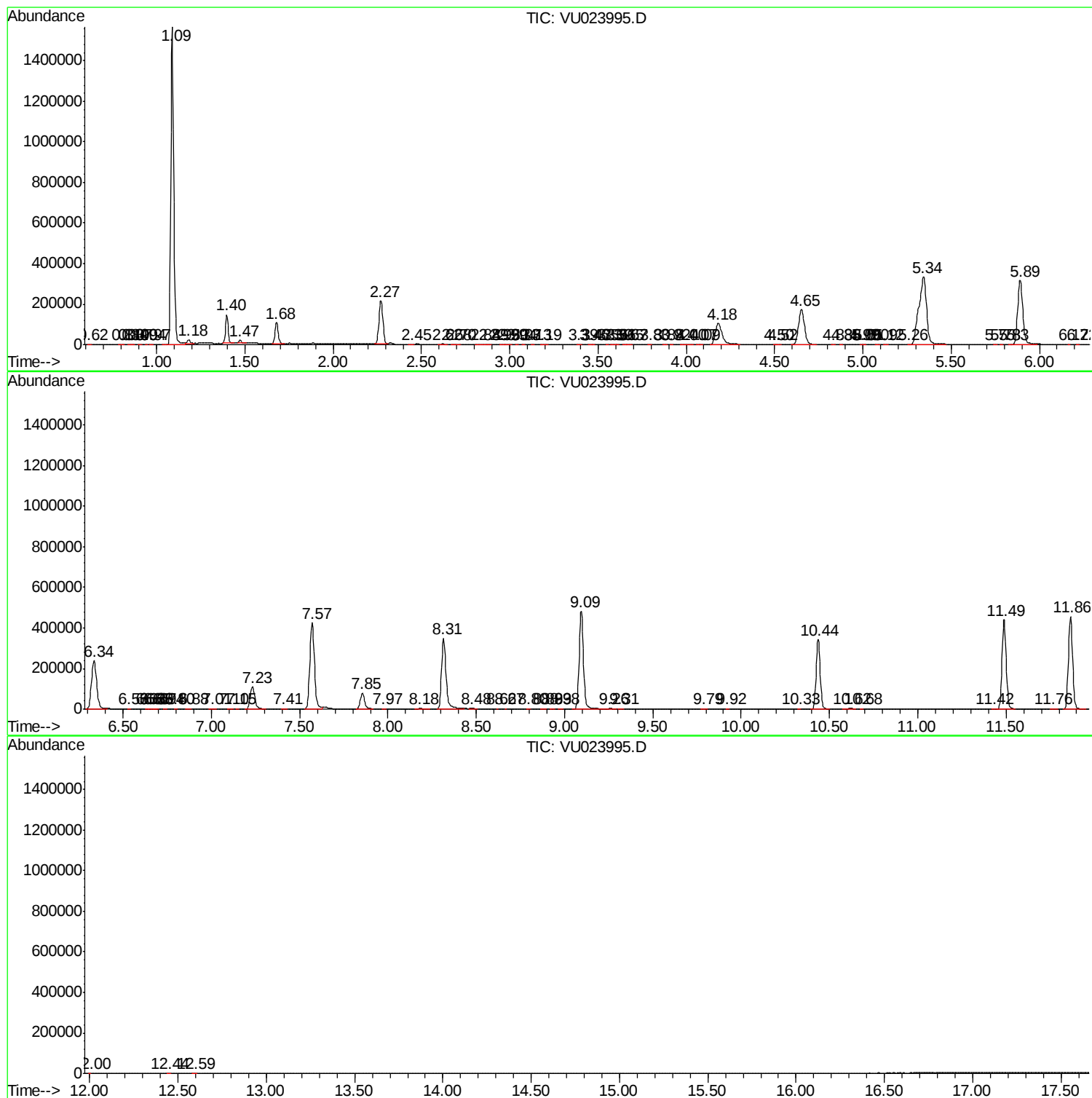
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 7.410  | 2117 | 2121 | 2127 | rBV2 | 266    | 299    | 0.02%  | 0.003% |
| 73  | 7.571  | 2157 | 2171 | 2189 | rBV  | 426283 | 764969 | 42.81% | 7.753% |
| 74  | 7.854  | 2248 | 2259 | 2278 | rBV  | 78610  | 135333 | 7.57%  | 1.372% |
| 75  | 7.973  | 2294 | 2296 | 2300 | rVB3 | 230    | 162    | 0.01%  | 0.002% |
| 76  | 8.182  | 2351 | 2361 | 2377 | rBV3 | 2832   | 4772   | 0.27%  | 0.048% |
| 77  | 8.313  | 2390 | 2402 | 2439 | rBV  | 346900 | 622750 | 34.85% | 6.312% |
| 78  | 8.477  | 2446 | 2453 | 2462 | rVB7 | 2385   | 4570   | 0.26%  | 0.046% |
| 79  | 8.619  | 2495 | 2497 | 2498 | rBV7 | 346    | 146    | 0.01%  | 0.001% |
| 80  | 8.667  | 2510 | 2512 | 2513 | rBV  | 141    | 78     | 0.00%  | 0.001% |
| 81  | 8.799  | 2548 | 2553 | 2555 | rBV2 | 313    | 296    | 0.02%  | 0.003% |
| 82  | 8.879  | 2573 | 2578 | 2583 | rBV2 | 195    | 298    | 0.02%  | 0.003% |
| 83  | 8.931  | 2589 | 2594 | 2597 | rBV  | 291    | 283    | 0.02%  | 0.003% |
| 84  | 8.976  | 2604 | 2608 | 2613 | rBV2 | 246    | 323    | 0.02%  | 0.003% |
| 85  | 9.095  | 2629 | 2645 | 2687 | rBV  | 480807 | 821934 | 45.99% | 8.331% |
| 86  | 9.256  | 2690 | 2695 | 2706 | rVB4 | 2516   | 3777   | 0.21%  | 0.038% |
| 87  | 9.313  | 2709 | 2713 | 2719 | rBV2 | 451    | 592    | 0.03%  | 0.006% |
| 88  | 9.789  | 2855 | 2861 | 2867 | rBB2 | 608    | 790    | 0.04%  | 0.008% |
| 89  | 9.921  | 2899 | 2902 | 2904 | rBV  | 181    | 135    | 0.01%  | 0.001% |
| 90  | 10.326 | 3026 | 3028 | 3031 | rVB  | 335    | 132    | 0.01%  | 0.001% |
| 91  | 10.436 | 3049 | 3062 | 3082 | rBV  | 343311 | 551753 | 30.88% | 5.592% |
| 92  | 10.616 | 3104 | 3118 | 3128 | rBV4 | 3200   | 6132   | 0.34%  | 0.062% |
| 93  | 10.683 | 3136 | 3139 | 3141 | rBV2 | 328    | 211    | 0.01%  | 0.002% |
| 94  | 11.423 | 3367 | 3369 | 3377 | rBV  | 280    | 280    | 0.02%  | 0.003% |
| 95  | 11.487 | 3377 | 3389 | 3409 | rBV  | 439367 | 714772 | 40.00% | 7.244% |
| 96  | 11.760 | 3470 | 3474 | 3483 | rVB6 | 1189   | 1607   | 0.09%  | 0.016% |
| 97  | 11.863 | 3493 | 3506 | 3533 | rBV  | 454435 | 743948 | 41.63% | 7.540% |
| 98  | 11.998 | 3546 | 3548 | 3550 | rVB  | 306    | 85     | 0.00%  | 0.001% |
| 99  | 12.442 | 3684 | 3686 | 3690 | rBV2 | 279    | 209    | 0.01%  | 0.002% |
| 100 | 12.590 | 3729 | 3732 | 3737 | rBV2 | 221    | 256    | 0.01%  | 0.003% |

Sum of corrected areas: 9866521

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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  
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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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