

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052218\  
 Data File : VU024025.D  
 Acq On : 22 May 2018 19:27  
 Operator : MD/SY  
 Sample : J3043-12  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 23 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         | 0.883       | 88            | 91          | 96           | rBV      | 276            | 327           | 0.01%           | 0.002%        |
| 2         | 1.089       | 136           | 155         | 179          | rBV      | 4212360        | 4973098       | 100.00%         | 36.643%       |
| 3         | 1.182       | 180           | 184         | 193          | rVB      | 15197          | 17434         | 0.35%           | 0.128%        |
| 4         | 1.397       | 244           | 251         | 263          | rBV      | 135213         | 141130        | 2.84%           | 1.040%        |
| 5         | 1.680       | 331           | 339         | 353          | rVB      | 105276         | 133497        | 2.68%           | 0.984%        |
| 6         | 2.272       | 512           | 523         | 533          | rBV      | 220232         | 331675        | 6.67%           | 2.444%        |
| 7         | 2.323       | 534           | 539         | 552          | rVB      | 16611          | 25896         | 0.52%           | 0.191%        |
| 8         | 2.449       | 568           | 578         | 594          | rBV2     | 7106           | 13995         | 0.28%           | 0.103%        |
| 9         | 2.532       | 601           | 604         | 606          | rBV      | 198            | 122           | 0.00%           | 0.001%        |
| 10        | 2.709       | 650           | 659         | 665          | rBV4     | 1207           | 1827          | 0.04%           | 0.013%        |
| 11        | 2.741       | 665           | 669         | 677          | rVB4     | 868            | 1019          | 0.02%           | 0.008%        |
| 12        | 2.838       | 691           | 699         | 703          | rBV3     | 912            | 1303          | 0.03%           | 0.010%        |
| 13        | 2.998       | 739           | 749         | 763          | rBV3     | 2702           | 5859          | 0.12%           | 0.043%        |
| 14        | 3.188       | 799           | 808         | 816          | rBV4     | 1089           | 1870          | 0.04%           | 0.014%        |
| 15        | 3.304       | 842           | 844         | 847          | rBV      | 335            | 238           | 0.00%           | 0.002%        |
| 16        | 3.384       | 866           | 869         | 873          | rBV2     | 280            | 242           | 0.00%           | 0.002%        |
| 17        | 3.436       | 879           | 885         | 889          | rBV2     | 140            | 190           | 0.00%           | 0.001%        |
| 18        | 3.474       | 895           | 897         | 903          | rVB2     | 192            | 133           | 0.00%           | 0.001%        |
| 19        | 3.558       | 919           | 923         | 927          | rBV2     | 150            | 143           | 0.00%           | 0.001%        |
| 20        | 3.609       | 936           | 939         | 941          | rVB2     | 250            | 157           | 0.00%           | 0.001%        |
| 21        | 3.635       | 943           | 947         | 952          | rBV2     | 203            | 230           | 0.00%           | 0.002%        |
| 22        | 3.661       | 952           | 955         | 961          | rVB      | 216            | 192           | 0.00%           | 0.001%        |
| 23        | 3.722       | 971           | 974         | 979          | rVB      | 228            | 176           | 0.00%           | 0.001%        |
| 24        | 3.764       | 983           | 987         | 993          | rVB      | 183            | 197           | 0.00%           | 0.001%        |
| 25        | 3.850       | 1009          | 1014        | 1018         | rBV2     | 243            | 345           | 0.01%           | 0.003%        |
| 26        | 3.892       | 1022          | 1027        | 1028         | rBV      | 204            | 187           | 0.00%           | 0.001%        |
| 27        | 3.944       | 1038          | 1043        | 1046         | rVB2     | 297            | 254           | 0.01%           | 0.002%        |
| 28        | 3.966       | 1046          | 1050        | 1051         | rBV      | 200            | 140           | 0.00%           | 0.001%        |
| 29        | 4.005       | 1059          | 1062        | 1070         | rBV2     | 181            | 304           | 0.01%           | 0.002%        |
| 30        | 4.085       | 1082          | 1087        | 1088         | rBV2     | 453            | 410           | 0.01%           | 0.003%        |
| 31        | 4.182       | 1101          | 1117        | 1142         | rBV      | 115353         | 306580        | 6.16%           | 2.259%        |
| 32        | 4.561       | 1231          | 1235        | 1238         | rBV2     | 305            | 189           | 0.00%           | 0.001%        |
| 33        | 4.587       | 1240          | 1243        | 1245         | rBV2     | 302            | 206           | 0.00%           | 0.002%        |
| 34        | 4.651       | 1245          | 1263        | 1292         | rVV      | 170822         | 426727        | 8.58%           | 3.144%        |

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

|    |       |      |      |      |      |        |         |        |        |
|----|-------|------|------|------|------|--------|---------|--------|--------|
| 35 | 4.838 | 1318 | 1321 | 1324 | rBV2 | 329    | 262     | 0.01%  | 0.002% |
| 36 | 4.854 | 1324 | 1326 | 1330 | rVV  | 191    | 161     | 0.00%  | 0.001% |
| 37 | 4.892 | 1333 | 1338 | 1345 | rVB4 | 639    | 947     | 0.02%  | 0.007% |
| 38 | 4.985 | 1364 | 1367 | 1369 | rBV  | 489    | 388     | 0.01%  | 0.003% |
| 39 | 5.002 | 1369 | 1372 | 1375 | rVB4 | 516    | 465     | 0.01%  | 0.003% |
| 40 | 5.111 | 1402 | 1406 | 1413 | rBV2 | 246    | 332     | 0.01%  | 0.002% |
| 41 | 5.143 | 1413 | 1416 | 1421 | rVB  | 224    | 205     | 0.00%  | 0.002% |
| 42 | 5.169 | 1421 | 1424 | 1426 | rBV2 | 181    | 151     | 0.00%  | 0.001% |
| 43 | 5.236 | 1439 | 1445 | 1449 | rBV2 | 287    | 349     | 0.01%  | 0.003% |
| 44 | 5.342 | 1454 | 1478 | 1518 | rBV2 | 344836 | 1063524 | 21.39% | 7.836% |
| 45 | 5.683 | 1582 | 1584 | 1588 | rBV  | 176    | 118     | 0.00%  | 0.001% |
| 46 | 5.754 | 1602 | 1606 | 1611 | rBV2 | 316    | 311     | 0.01%  | 0.002% |
| 47 | 5.799 | 1611 | 1620 | 1628 | rBV3 | 1107   | 2106    | 0.04%  | 0.016% |
| 48 | 5.892 | 1633 | 1649 | 1674 | rBV  | 332172 | 668777  | 13.45% | 4.928% |
| 49 | 6.188 | 1731 | 1741 | 1748 | rBV8 | 1935   | 3195    | 0.06%  | 0.024% |
| 50 | 6.336 | 1771 | 1787 | 1807 | rBV  | 251185 | 506995  | 10.19% | 3.736% |
| 51 | 6.645 | 1880 | 1883 | 1890 | rVB2 | 174    | 176     | 0.00%  | 0.001% |
| 52 | 6.677 | 1890 | 1893 | 1900 | rBV2 | 148    | 188     | 0.00%  | 0.001% |
| 53 | 6.860 | 1947 | 1950 | 1951 | rBV2 | 293    | 134     | 0.00%  | 0.001% |
| 54 | 7.233 | 2052 | 2066 | 2090 | rBV  | 124240 | 226244  | 4.55%  | 1.667% |
| 55 | 7.387 | 2112 | 2114 | 2118 | rBV  | 249    | 173     | 0.00%  | 0.001% |
| 56 | 7.571 | 2157 | 2171 | 2187 | rBV  | 446023 | 793623  | 15.96% | 5.848% |
| 57 | 7.854 | 2248 | 2259 | 2282 | rBV  | 89033  | 153984  | 3.10%  | 1.135% |
| 58 | 8.001 | 2303 | 2305 | 2308 | rVB  | 334    | 184     | 0.00%  | 0.001% |
| 59 | 8.024 | 2310 | 2312 | 2317 | rVB  | 433    | 242     | 0.00%  | 0.002% |
| 60 | 8.053 | 2317 | 2321 | 2322 | rBV2 | 215    | 180     | 0.00%  | 0.001% |
| 61 | 8.114 | 2337 | 2340 | 2345 | rVB3 | 221    | 153     | 0.00%  | 0.001% |
| 62 | 8.162 | 2352 | 2355 | 2357 | rBV2 | 217    | 138     | 0.00%  | 0.001% |
| 63 | 8.185 | 2357 | 2362 | 2370 | rVB2 | 348    | 530     | 0.01%  | 0.004% |
| 64 | 8.313 | 2389 | 2402 | 2448 | rBV  | 390960 | 695854  | 13.99% | 5.127% |
| 65 | 8.599 | 2488 | 2491 | 2493 | rBV  | 303    | 174     | 0.00%  | 0.001% |
| 66 | 8.866 | 2571 | 2574 | 2579 | rBV  | 220    | 166     | 0.00%  | 0.001% |
| 67 | 9.095 | 2632 | 2645 | 2675 | rBV  | 511430 | 857780  | 17.25% | 6.320% |
| 68 | 9.255 | 2688 | 2695 | 2707 | rVB3 | 1880   | 2905    | 0.06%  | 0.021% |
| 69 | 9.333 | 2716 | 2719 | 2722 | rBV2 | 153    | 112     | 0.00%  | 0.001% |
| 70 | 9.384 | 2727 | 2735 | 2747 | rVB3 | 1483   | 2712    | 0.05%  | 0.020% |
| 71 | 9.435 | 2747 | 2751 | 2755 | rBV2 | 207    | 177     | 0.00%  | 0.001% |

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Filtering: 5  
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 Peak separation: 5

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

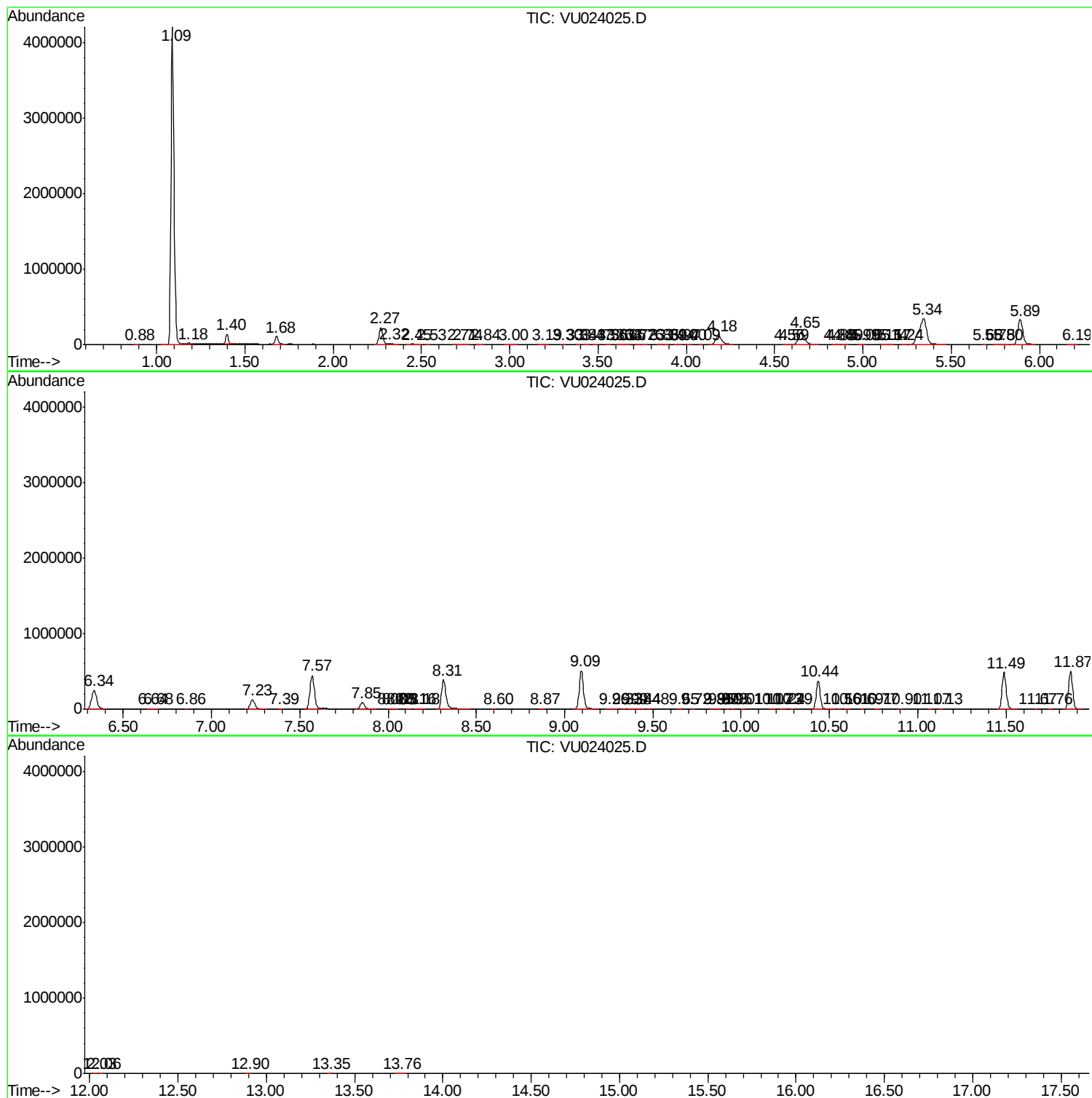
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 9.484  | 2761 | 2766 | 2769 | rBV  | 178    | 203    | 0.00%  | 0.001% |
| 73  | 9.651  | 2814 | 2818 | 2821 | rBV  | 198    | 213    | 0.00%  | 0.002% |
| 74  | 9.722  | 2838 | 2840 | 2843 | rBV2 | 308    | 126    | 0.00%  | 0.001% |
| 75  | 9.847  | 2872 | 2879 | 2883 | rBV  | 199    | 305    | 0.01%  | 0.002% |
| 76  | 9.873  | 2883 | 2887 | 2890 | rBV  | 174    | 140    | 0.00%  | 0.001% |
| 77  | 9.927  | 2900 | 2904 | 2905 | rBV  | 310    | 164    | 0.00%  | 0.001% |
| 78  | 9.953  | 2910 | 2912 | 2914 | rBV2 | 193    | 114    | 0.00%  | 0.001% |
| 79  | 10.008 | 2925 | 2929 | 2932 | rBV2 | 215    | 218    | 0.00%  | 0.002% |
| 80  | 10.169 | 2975 | 2979 | 2986 | rVB3 | 380    | 449    | 0.01%  | 0.003% |
| 81  | 10.230 | 2994 | 2998 | 2999 | rBV2 | 194    | 154    | 0.00%  | 0.001% |
| 82  | 10.242 | 3000 | 3002 | 3004 | rVV2 | 233    | 125    | 0.00%  | 0.001% |
| 83  | 10.287 | 3012 | 3016 | 3019 | rBV2 | 228    | 205    | 0.00%  | 0.002% |
| 84  | 10.435 | 3050 | 3062 | 3091 | rBV  | 373039 | 595856 | 11.98% | 4.390% |
| 85  | 10.561 | 3097 | 3101 | 3102 | rBV  | 261    | 228    | 0.00%  | 0.002% |
| 86  | 10.606 | 3109 | 3115 | 3116 | rBV  | 976    | 785    | 0.02%  | 0.006% |
| 87  | 10.686 | 3137 | 3140 | 3143 | rBV2 | 312    | 216    | 0.00%  | 0.002% |
| 88  | 10.773 | 3162 | 3167 | 3170 | rBV2 | 374    | 266    | 0.01%  | 0.002% |
| 89  | 10.905 | 3204 | 3208 | 3209 | rBV  | 269    | 194    | 0.00%  | 0.001% |
| 90  | 11.069 | 3256 | 3259 | 3262 | rBV2 | 267    | 168    | 0.00%  | 0.001% |
| 91  | 11.133 | 3276 | 3279 | 3280 | rBV  | 235    | 139    | 0.00%  | 0.001% |
| 92  | 11.490 | 3377 | 3390 | 3413 | rBV  | 488941 | 784828 | 15.78% | 5.783% |
| 93  | 11.670 | 3444 | 3446 | 3448 | rBV  | 283    | 134    | 0.00%  | 0.001% |
| 94  | 11.757 | 3467 | 3473 | 3474 | rBV3 | 1011   | 744    | 0.01%  | 0.005% |
| 95  | 11.866 | 3494 | 3507 | 3527 | rBV  | 503568 | 810719 | 16.30% | 5.974% |
| 96  | 12.030 | 3554 | 3558 | 3560 | rBV  | 249    | 215    | 0.00%  | 0.002% |
| 97  | 12.059 | 3564 | 3567 | 3571 | rBV2 | 388    | 395    | 0.01%  | 0.003% |
| 98  | 12.895 | 3824 | 3827 | 3832 | rVB3 | 482    | 502    | 0.01%  | 0.004% |
| 99  | 13.355 | 3967 | 3970 | 3973 | rBV2 | 483    | 382    | 0.01%  | 0.003% |
| 100 | 13.757 | 4087 | 4095 | 4104 | rBV3 | 1783   | 3217   | 0.06%  | 0.024% |

Sum of corrected areas: 13571811

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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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