

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052118\  
 Data File : VU024002.D  
 Acq On : 22 May 2018 05:45  
 Operator : MD/SY  
 Sample : J3031-20  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 42 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         | 0.831       | 72            | 75          | 82           | rBV      | 154            | 208           | 0.002%          | 0.002%        |
| 2         | 0.892       | 91            | 94          | 99           | rBV2     | 298            | 300           | 0.003%          | 0.003%        |
| 3         | 1.088       | 137           | 155         | 178          | rBV      | 874544         | 1017347       | 100.00%         | 11.732%       |
| 4         | 1.182       | 179           | 184         | 194          | rVB      | 29415          | 30257         | 2.97%           | 0.349%        |
| 5         | 1.285       | 212           | 216         | 228          | rVB4     | 8109           | 11222         | 1.10%           | 0.129%        |
| 6         | 1.397       | 244           | 251         | 264          | rBV      | 118613         | 125399        | 12.33%          | 1.446%        |
| 7         | 1.680       | 331           | 339         | 355          | rVB      | 98567          | 122907        | 12.08%          | 1.417%        |
| 8         | 2.272       | 512           | 523         | 535          | rBV      | 190783         | 288193        | 28.33%          | 3.323%        |
| 9         | 2.413       | 565           | 567         | 571          | rBV2     | 269            | 217           | 0.002%          | 0.003%        |
| 10        | 2.436       | 572           | 574         | 577          | rBV      | 327            | 253           | 0.002%          | 0.003%        |
| 11        | 2.516       | 595           | 599         | 605          | rBV2     | 194            | 277           | 0.003%          | 0.003%        |
| 12        | 2.699       | 651           | 656         | 660          | rBV3     | 538            | 611           | 0.006%          | 0.007%        |
| 13        | 2.744       | 668           | 670         | 674          | rVB2     | 385            | 221           | 0.002%          | 0.003%        |
| 14        | 2.809       | 685           | 690         | 691          | rBV2     | 311            | 247           | 0.002%          | 0.003%        |
| 15        | 2.834       | 691           | 698         | 711          | rVB2     | 933            | 2094          | 0.21%           | 0.024%        |
| 16        | 2.895       | 714           | 717         | 721          | rBV2     | 207            | 219           | 0.002%          | 0.003%        |
| 17        | 2.947       | 728           | 733         | 739          | rVB      | 427            | 513           | 0.005%          | 0.006%        |
| 18        | 2.995       | 746           | 748         | 751          | rVB      | 282            | 134           | 0.001%          | 0.002%        |
| 19        | 3.014       | 751           | 754         | 757          | rBV2     | 158            | 126           | 0.001%          | 0.001%        |
| 20        | 3.188       | 805           | 808         | 809          | rBV2     | 218            | 141           | 0.001%          | 0.002%        |
| 21        | 3.352       | 855           | 859         | 865          | rBV2     | 133            | 170           | 0.002%          | 0.002%        |
| 22        | 3.394       | 869           | 872         | 877          | rVB2     | 277            | 290           | 0.003%          | 0.003%        |
| 23        | 3.448       | 886           | 889         | 893          | rVB      | 196            | 121           | 0.001%          | 0.001%        |
| 24        | 3.500       | 902           | 905         | 912          | rVB2     | 142            | 169           | 0.002%          | 0.002%        |
| 25        | 3.719       | 969           | 973         | 978          | rVB2     | 275            | 263           | 0.003%          | 0.003%        |
| 26        | 3.751       | 978           | 983         | 986          | rBV2     | 298            | 349           | 0.003%          | 0.004%        |
| 27        | 3.789       | 990           | 995         | 997          | rBV      | 233            | 227           | 0.002%          | 0.003%        |
| 28        | 3.844       | 1009          | 1012        | 1015         | rVB2     | 239            | 169           | 0.002%          | 0.002%        |
| 29        | 3.883       | 1021          | 1024        | 1025         | rBV2     | 220            | 142           | 0.001%          | 0.002%        |
| 30        | 3.973       | 1049          | 1052        | 1057         | rVB2     | 130            | 111           | 0.001%          | 0.001%        |
| 31        | 3.998       | 1057          | 1060        | 1061         | rBV2     | 245            | 142           | 0.001%          | 0.002%        |
| 32        | 4.043       | 1069          | 1074        | 1079         | rBV2     | 184            | 242           | 0.002%          | 0.003%        |
| 33        | 4.104       | 1090          | 1093        | 1097         | rVB2     | 229            | 186           | 0.002%          | 0.002%        |
| 34        | 4.182       | 1101          | 1117        | 1153         | rBV      | 107127         | 287463        | 28.26%          | 3.315%        |

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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 | 4.651 | 1244 | 1263 | 1288 | rBV  | 164680 | 389969 | 38.33% | 4.497%  |
| 36 | 4.809 | 1308 | 1312 | 1313 | rBV2 | 211    | 159    | 0.02%  | 0.002%  |
| 37 | 4.883 | 1327 | 1335 | 1337 | rBV3 | 670    | 723    | 0.07%  | 0.008%  |
| 38 | 4.982 | 1364 | 1366 | 1369 | rVB2 | 174    | 116    | 0.01%  | 0.001%  |
| 39 | 5.005 | 1370 | 1373 | 1377 | rVB2 | 228    | 148    | 0.01%  | 0.002%  |
| 40 | 5.075 | 1389 | 1395 | 1397 | rBV2 | 249    | 230    | 0.02%  | 0.003%  |
| 41 | 5.091 | 1397 | 1400 | 1403 | rVV2 | 166    | 107    | 0.01%  | 0.001%  |
| 42 | 5.175 | 1423 | 1426 | 1430 | rBV2 | 176    | 209    | 0.02%  | 0.002%  |
| 43 | 5.342 | 1452 | 1478 | 1504 | rBV2 | 309062 | 951236 | 93.50% | 10.970% |
| 44 | 5.587 | 1551 | 1554 | 1559 | rVB2 | 272    | 281    | 0.03%  | 0.003%  |
| 45 | 5.619 | 1562 | 1564 | 1569 | rVB2 | 330    | 272    | 0.03%  | 0.003%  |
| 46 | 5.648 | 1569 | 1573 | 1575 | rBV3 | 342    | 316    | 0.03%  | 0.004%  |
| 47 | 5.702 | 1585 | 1590 | 1591 | rBV2 | 142    | 130    | 0.01%  | 0.001%  |
| 48 | 5.757 | 1603 | 1607 | 1612 | rVB2 | 359    | 344    | 0.03%  | 0.004%  |
| 49 | 5.783 | 1612 | 1615 | 1619 | rVB2 | 216    | 151    | 0.01%  | 0.002%  |
| 50 | 5.821 | 1622 | 1627 | 1629 | rBV2 | 206    | 225    | 0.02%  | 0.003%  |
| 51 | 5.889 | 1633 | 1648 | 1699 | rBV  | 308027 | 635188 | 62.44% | 7.325%  |
| 52 | 6.188 | 1734 | 1741 | 1746 | rBV5 | 985    | 1111   | 0.11%  | 0.013%  |
| 53 | 6.336 | 1772 | 1787 | 1808 | rBV  | 224935 | 459988 | 45.21% | 5.305%  |
| 54 | 6.538 | 1847 | 1850 | 1852 | rBV2 | 191    | 130    | 0.01%  | 0.001%  |
| 55 | 6.638 | 1877 | 1881 | 1883 | rBV2 | 225    | 156    | 0.02%  | 0.002%  |
| 56 | 6.651 | 1883 | 1885 | 1888 | rBV  | 151    | 114    | 0.01%  | 0.001%  |
| 57 | 6.712 | 1901 | 1904 | 1908 | rBV  | 176    | 164    | 0.02%  | 0.002%  |
| 58 | 6.763 | 1916 | 1920 | 1924 | rBV2 | 255    | 322    | 0.03%  | 0.004%  |
| 59 | 6.847 | 1938 | 1946 | 1948 | rBV2 | 401    | 531    | 0.05%  | 0.006%  |
| 60 | 6.944 | 1974 | 1976 | 1986 | rVB  | 203    | 269    | 0.03%  | 0.003%  |
| 61 | 7.037 | 2001 | 2005 | 2009 | rBV  | 216    | 224    | 0.02%  | 0.003%  |
| 62 | 7.233 | 2054 | 2066 | 2092 | rBV  | 98021  | 178882 | 17.58% | 2.063%  |
| 63 | 7.387 | 2110 | 2114 | 2116 | rBV3 | 248    | 215    | 0.02%  | 0.002%  |
| 64 | 7.426 | 2123 | 2126 | 2130 | rBV2 | 211    | 169    | 0.02%  | 0.002%  |
| 65 | 7.480 | 2141 | 2143 | 2147 | rVB  | 354    | 226    | 0.02%  | 0.003%  |
| 66 | 7.571 | 2155 | 2171 | 2199 | rBV  | 383474 | 692715 | 68.09% | 7.988%  |
| 67 | 7.853 | 2248 | 2259 | 2284 | rBV  | 68745  | 119847 | 11.78% | 1.382%  |
| 68 | 8.181 | 2348 | 2361 | 2374 | rBV2 | 1882   | 3417   | 0.34%  | 0.039%  |
| 69 | 8.313 | 2390 | 2402 | 2437 | rBV  | 346796 | 621165 | 61.06% | 7.163%  |
| 70 | 8.632 | 2498 | 2501 | 2504 | rBV3 | 175    | 110    | 0.01%  | 0.001%  |
| 71 | 9.021 | 2619 | 2622 | 2625 | rBV2 | 193    | 122    | 0.01%  | 0.001%  |

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 Peak separation: 5

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

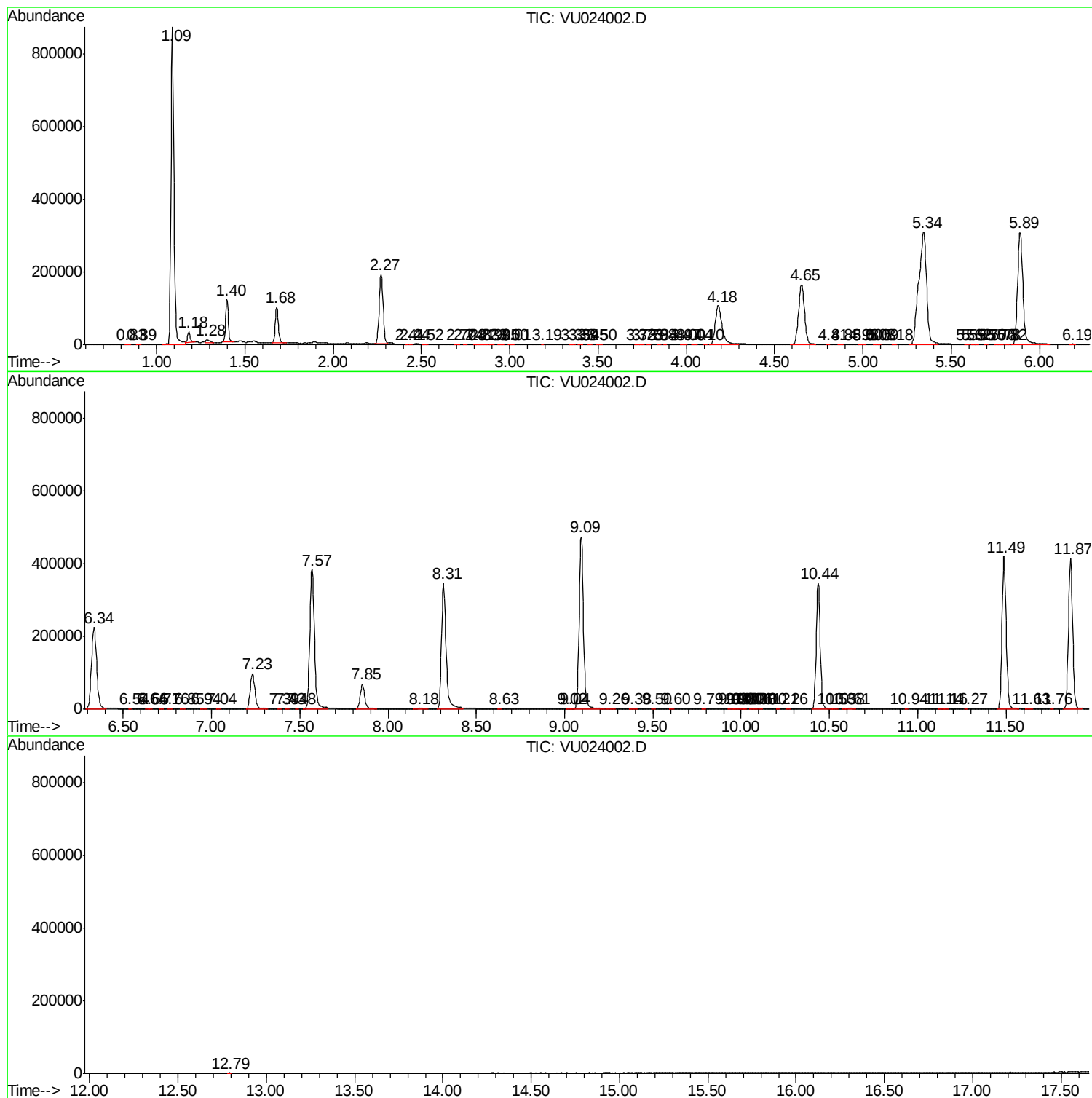
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 9.037  | 2625 | 2627 | 2632 | rVV  | 237    | 180    | 0.02%  | 0.002% |
| 73  | 9.095  | 2632 | 2645 | 2686 | rVV  | 474900 | 803709 | 79.00% | 9.268% |
| 74  | 9.255  | 2690 | 2695 | 2704 | rVB4 | 508    | 804    | 0.08%  | 0.009% |
| 75  | 9.384  | 2728 | 2735 | 2744 | rVB2 | 498    | 709    | 0.07%  | 0.008% |
| 76  | 9.500  | 2768 | 2771 | 2774 | rBV  | 227    | 209    | 0.02%  | 0.002% |
| 77  | 9.603  | 2799 | 2803 | 2808 | rBV  | 168    | 194    | 0.02%  | 0.002% |
| 78  | 9.789  | 2857 | 2861 | 2864 | rBV2 | 418    | 370    | 0.04%  | 0.004% |
| 79  | 9.934  | 2903 | 2906 | 2913 | rVB2 | 267    | 338    | 0.03%  | 0.004% |
| 80  | 9.976  | 2913 | 2919 | 2924 | rBV2 | 340    | 419    | 0.04%  | 0.005% |
| 81  | 9.998  | 2924 | 2926 | 2930 | rVB2 | 228    | 172    | 0.02%  | 0.002% |
| 82  | 10.021 | 2930 | 2933 | 2936 | rBV  | 264    | 236    | 0.02%  | 0.003% |
| 83  | 10.056 | 2940 | 2944 | 2947 | rBV  | 283    | 202    | 0.02%  | 0.002% |
| 84  | 10.082 | 2947 | 2952 | 2956 | rBV2 | 267    | 325    | 0.03%  | 0.004% |
| 85  | 10.107 | 2957 | 2960 | 2963 | rBV  | 162    | 110    | 0.01%  | 0.001% |
| 86  | 10.207 | 2988 | 2991 | 2993 | rBV2 | 143    | 128    | 0.01%  | 0.001% |
| 87  | 10.259 | 3004 | 3007 | 3012 | rBV2 | 178    | 184    | 0.02%  | 0.002% |
| 88  | 10.435 | 3050 | 3062 | 3087 | rVB  | 346670 | 551249 | 54.18% | 6.357% |
| 89  | 10.529 | 3087 | 3091 | 3097 | rBV3 | 411    | 446    | 0.04%  | 0.005% |
| 90  | 10.583 | 3105 | 3108 | 3109 | rBV  | 211    | 125    | 0.01%  | 0.001% |
| 91  | 10.612 | 3109 | 3117 | 3128 | rVV2 | 1414   | 2720   | 0.27%  | 0.031% |
| 92  | 10.937 | 3214 | 3218 | 3220 | rBV2 | 221    | 188    | 0.02%  | 0.002% |
| 93  | 11.136 | 3273 | 3280 | 3283 | rBV  | 326    | 466    | 0.05%  | 0.005% |
| 94  | 11.159 | 3283 | 3287 | 3291 | rVB2 | 229    | 214    | 0.02%  | 0.002% |
| 95  | 11.275 | 3320 | 3323 | 3324 | rBV2 | 197    | 136    | 0.01%  | 0.002% |
| 96  | 11.487 | 3377 | 3389 | 3415 | rVV  | 419026 | 680876 | 66.93% | 7.852% |
| 97  | 11.628 | 3426 | 3433 | 3439 | rBV4 | 459    | 723    | 0.07%  | 0.008% |
| 98  | 11.757 | 3471 | 3473 | 3475 | rBV2 | 272    | 136    | 0.01%  | 0.002% |
| 99  | 11.866 | 3493 | 3507 | 3527 | rBV  | 413875 | 674880 | 66.34% | 7.783% |
| 100 | 12.789 | 3791 | 3794 | 3798 | rBV  | 523    | 451    | 0.04%  | 0.005% |

Sum of corrected areas: 8671510

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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        |