

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050218\  
 Data File : VU023587.D  
 Acq On : 02 May 2018 19:12  
 Operator : MD/SY  
 Sample : J2627-14  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 21 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\SOMULM050118WMA.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         | 0.609       | 3             | 6           | 9            | rBV      | 141            | 113           | 0.01%           | 0.001%        |
| 2         | 0.786       | 59            | 61          | 66           | rVB2     | 184            | 146           | 0.01%           | 0.002%        |
| 3         | 0.857       | 79            | 83          | 85           | rBV      | 200            | 138           | 0.01%           | 0.001%        |
| 4         | 0.989       | 116           | 124         | 131          | rBV2     | 152            | 240           | 0.02%           | 0.003%        |
| 5         | 1.089       | 135           | 155         | 176          | rBV      | 743719         | 860705        | 80.11%          | 9.235%        |
| 6         | 1.182       | 180           | 184         | 193          | rVV      | 12216          | 12788         | 1.19%           | 0.137%        |
| 7         | 1.397       | 245           | 251         | 265          | rVB      | 134163         | 135243        | 12.59%          | 1.451%        |
| 8         | 1.680       | 331           | 339         | 354          | rVB      | 99330          | 124972        | 11.63%          | 1.341%        |
| 9         | 2.272       | 511           | 523         | 536          | rBV      | 215380         | 328288        | 30.56%          | 3.522%        |
| 10        | 2.449       | 570           | 578         | 596          | rVB3     | 3244           | 6109          | 0.57%           | 0.066%        |
| 11        | 2.622       | 628           | 632         | 640          | rVB3     | 573            | 636           | 0.06%           | 0.007%        |
| 12        | 2.677       | 646           | 649         | 652          | rBV      | 235            | 171           | 0.02%           | 0.002%        |
| 13        | 2.706       | 652           | 658         | 664          | rVB4     | 489            | 573           | 0.05%           | 0.006%        |
| 14        | 2.744       | 664           | 670         | 678          | rBV2     | 198            | 319           | 0.03%           | 0.003%        |
| 15        | 2.844       | 689           | 701         | 712          | rVB2     | 1467           | 3222          | 0.30%           | 0.035%        |
| 16        | 2.941       | 728           | 731         | 734          | rVB2     | 212            | 114           | 0.01%           | 0.001%        |
| 17        | 2.966       | 734           | 739         | 742          | rBV2     | 228            | 207           | 0.02%           | 0.002%        |
| 18        | 2.992       | 744           | 747         | 751          | rBV2     | 144            | 124           | 0.01%           | 0.001%        |
| 19        | 3.027       | 756           | 758         | 764          | rVB2     | 199            | 170           | 0.02%           | 0.002%        |
| 20        | 3.133       | 783           | 791         | 793          | rBV      | 224            | 234           | 0.02%           | 0.003%        |
| 21        | 3.313       | 844           | 847         | 853          | rBV2     | 196            | 174           | 0.02%           | 0.002%        |
| 22        | 3.349       | 853           | 858         | 861          | rBV2     | 312            | 221           | 0.02%           | 0.002%        |
| 23        | 3.387       | 866           | 870         | 875          | rVB3     | 211            | 202           | 0.02%           | 0.002%        |
| 24        | 3.445       | 886           | 888         | 895          | rVB2     | 184            | 159           | 0.01%           | 0.002%        |
| 25        | 3.484       | 895           | 900         | 902          | rBV      | 158            | 134           | 0.01%           | 0.001%        |
| 26        | 3.551       | 915           | 921         | 925          | rBV2     | 268            | 315           | 0.03%           | 0.003%        |
| 27        | 3.667       | 953           | 957         | 963          | rBV2     | 429            | 566           | 0.05%           | 0.006%        |
| 28        | 3.796       | 994           | 997         | 1002         | rVB2     | 161            | 122           | 0.01%           | 0.001%        |
| 29        | 3.879       | 1020          | 1023        | 1025         | rBV2     | 190            | 131           | 0.01%           | 0.001%        |
| 30        | 3.895       | 1025          | 1028        | 1035         | rVB2     | 199            | 232           | 0.02%           | 0.002%        |
| 31        | 3.957       | 1044          | 1047        | 1052         | rBV2     | 112            | 113           | 0.01%           | 0.001%        |
| 32        | 3.982       | 1052          | 1055        | 1059         | rBV2     | 124            | 138           | 0.01%           | 0.001%        |
| 33        | 4.005       | 1060          | 1062        | 1068         | rVB2     | 132            | 131           | 0.01%           | 0.001%        |
| 34        | 4.053       | 1075          | 1077        | 1082         | rVB2     | 163            | 111           | 0.01%           | 0.001%        |

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 Max Peaks: 100  
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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\SOMULM050118WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |         |         |
|----|-------|------|------|------|------|--------|---------|---------|---------|
| 35 | 4.085 | 1082 | 1087 | 1090 | rBV2 | 158    | 163     | 0.02%   | 0.002%  |
| 36 | 4.182 | 1101 | 1117 | 1155 | rBV  | 117031 | 312748  | 29.11%  | 3.356%  |
| 37 | 4.452 | 1198 | 1201 | 1204 | rVB2 | 211    | 131     | 0.01%   | 0.001%  |
| 38 | 4.651 | 1243 | 1263 | 1295 | rBV  | 179941 | 420809  | 39.17%  | 4.515%  |
| 39 | 4.834 | 1318 | 1320 | 1323 | rVB  | 291    | 131     | 0.01%   | 0.001%  |
| 40 | 4.883 | 1329 | 1335 | 1336 | rBV2 | 717    | 729     | 0.07%   | 0.008%  |
| 41 | 4.966 | 1355 | 1361 | 1362 | rBV  | 114    | 113     | 0.01%   | 0.001%  |
| 42 | 4.985 | 1364 | 1367 | 1371 | rVV2 | 289    | 276     | 0.03%   | 0.003%  |
| 43 | 5.024 | 1375 | 1379 | 1384 | rVB2 | 140    | 147     | 0.01%   | 0.002%  |
| 44 | 5.063 | 1384 | 1391 | 1394 | rBV  | 166    | 153     | 0.01%   | 0.002%  |
| 45 | 5.214 | 1432 | 1438 | 1444 | rBV2 | 188    | 269     | 0.03%   | 0.003%  |
| 46 | 5.342 | 1454 | 1478 | 1512 | rBV2 | 355638 | 1074405 | 100.00% | 11.528% |
| 47 | 5.648 | 1570 | 1573 | 1576 | rBV  | 177    | 161     | 0.01%   | 0.002%  |
| 48 | 5.661 | 1576 | 1577 | 1582 | rVB  | 229    | 144     | 0.01%   | 0.002%  |
| 49 | 5.747 | 1600 | 1604 | 1608 | rBV  | 332    | 321     | 0.03%   | 0.003%  |
| 50 | 5.889 | 1636 | 1648 | 1680 | rBV  | 321440 | 655356  | 61.00%  | 7.032%  |
| 51 | 6.336 | 1772 | 1787 | 1816 | rBV  | 248830 | 507175  | 47.21%  | 5.442%  |
| 52 | 6.522 | 1841 | 1845 | 1846 | rBV2 | 285    | 186     | 0.02%   | 0.002%  |
| 53 | 6.641 | 1880 | 1882 | 1883 | rBV  | 228    | 111     | 0.01%   | 0.001%  |
| 54 | 6.690 | 1894 | 1897 | 1898 | rBV  | 307    | 168     | 0.02%   | 0.002%  |
| 55 | 6.751 | 1913 | 1916 | 1917 | rBV  | 241    | 166     | 0.02%   | 0.002%  |
| 56 | 6.780 | 1923 | 1925 | 1929 | rVB2 | 381    | 252     | 0.02%   | 0.003%  |
| 57 | 6.857 | 1939 | 1949 | 1951 | rBV4 | 672    | 801     | 0.07%   | 0.009%  |
| 58 | 6.973 | 1982 | 1985 | 1990 | rBV2 | 221    | 168     | 0.02%   | 0.002%  |
| 59 | 6.998 | 1990 | 1993 | 2002 | rVB2 | 361    | 471     | 0.04%   | 0.005%  |
| 60 | 7.040 | 2002 | 2006 | 2009 | rBV3 | 207    | 173     | 0.02%   | 0.002%  |
| 61 | 7.104 | 2023 | 2026 | 2029 | rBV  | 259    | 163     | 0.02%   | 0.002%  |
| 62 | 7.233 | 2053 | 2066 | 2094 | rVV  | 130346 | 237871  | 22.14%  | 2.552%  |
| 63 | 7.381 | 2110 | 2112 | 2115 | rVV2 | 231    | 187     | 0.02%   | 0.002%  |
| 64 | 7.432 | 2126 | 2128 | 2132 | rVB2 | 254    | 139     | 0.01%   | 0.001%  |
| 65 | 7.571 | 2156 | 2171 | 2198 | rBV  | 476107 | 840462  | 78.23%  | 9.018%  |
| 66 | 7.854 | 2248 | 2259 | 2282 | rBV  | 91677  | 159889  | 14.88%  | 1.716%  |
| 67 | 7.969 | 2292 | 2295 | 2299 | rVV2 | 337    | 222     | 0.02%   | 0.002%  |
| 68 | 7.989 | 2299 | 2301 | 2305 | rVB2 | 357    | 217     | 0.02%   | 0.002%  |
| 69 | 8.017 | 2305 | 2310 | 2315 | rVB3 | 434    | 496     | 0.05%   | 0.005%  |
| 70 | 8.040 | 2315 | 2317 | 2321 | rVB  | 330    | 204     | 0.02%   | 0.002%  |
| 71 | 8.181 | 2349 | 2361 | 2373 | rBV  | 2595   | 5055    | 0.47%   | 0.054%  |

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Filtering: 5  
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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\SOMULM050118WMA.M  
 Title : VOC Analysis

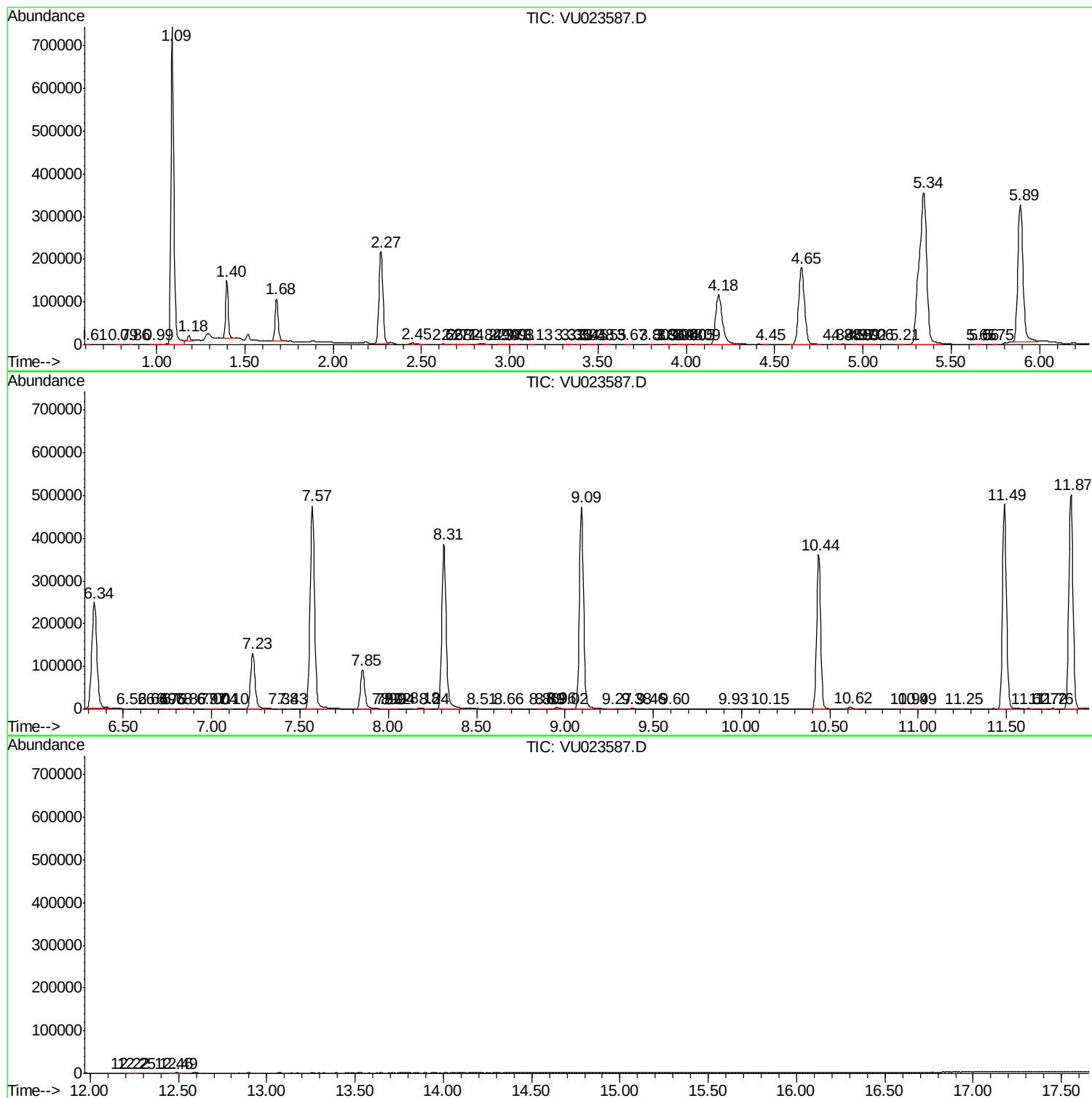
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 8.236  | 2373 | 2378 | 2379 | rBV2 | 232    | 162    | 0.02%  | 0.002% |
| 73  | 8.313  | 2390 | 2402 | 2437 | rBV  | 386291 | 666798 | 62.06% | 7.155% |
| 74  | 8.506  | 2460 | 2462 | 2466 | rBV3 | 374    | 276    | 0.03%  | 0.003% |
| 75  | 8.657  | 2506 | 2509 | 2517 | rVB  | 282    | 252    | 0.02%  | 0.003% |
| 76  | 8.860  | 2568 | 2572 | 2575 | rBV2 | 201    | 177    | 0.02%  | 0.002% |
| 77  | 8.889  | 2578 | 2581 | 2587 | rVB2 | 283    | 259    | 0.02%  | 0.003% |
| 78  | 8.956  | 2592 | 2602 | 2614 | rVB  | 2821   | 4912   | 0.46%  | 0.053% |
| 79  | 9.024  | 2619 | 2623 | 2626 | rBV  | 148    | 146    | 0.01%  | 0.002% |
| 80  | 9.095  | 2631 | 2645 | 2672 | rBV  | 473439 | 795407 | 74.03% | 8.535% |
| 81  | 9.268  | 2690 | 2699 | 2703 | rBV2 | 289    | 446    | 0.04%  | 0.005% |
| 82  | 9.381  | 2728 | 2734 | 2738 | rBV3 | 783    | 1005   | 0.09%  | 0.011% |
| 83  | 9.464  | 2756 | 2760 | 2763 | rBV  | 130    | 122    | 0.01%  | 0.001% |
| 84  | 9.599  | 2799 | 2802 | 2808 | rVB2 | 170    | 145    | 0.01%  | 0.002% |
| 85  | 9.927  | 2901 | 2904 | 2908 | rBV2 | 183    | 137    | 0.01%  | 0.001% |
| 86  | 10.152 | 2971 | 2974 | 2977 | rVB2 | 166    | 112    | 0.01%  | 0.001% |
| 87  | 10.435 | 3050 | 3062 | 3085 | rBV  | 360774 | 573582 | 53.39% | 6.154% |
| 88  | 10.619 | 3110 | 3119 | 3130 | rVB2 | 3021   | 4955   | 0.46%  | 0.053% |
| 89  | 10.937 | 3214 | 3218 | 3223 | rBV2 | 261    | 272    | 0.03%  | 0.003% |
| 90  | 10.985 | 3231 | 3233 | 3240 | rVB  | 256    | 202    | 0.02%  | 0.002% |
| 91  | 11.249 | 3313 | 3315 | 3318 | rVB  | 231    | 125    | 0.01%  | 0.001% |
| 92  | 11.490 | 3377 | 3390 | 3411 | rBV  | 479280 | 760149 | 70.75% | 8.156% |
| 93  | 11.622 | 3428 | 3431 | 3440 | rBV3 | 460    | 743    | 0.07%  | 0.008% |
| 94  | 11.722 | 3456 | 3462 | 3464 | rBV  | 272    | 316    | 0.03%  | 0.003% |
| 95  | 11.760 | 3471 | 3474 | 3480 | rVB3 | 540    | 467    | 0.04%  | 0.005% |
| 96  | 11.866 | 3494 | 3507 | 3527 | rBV  | 501878 | 809387 | 75.33% | 8.685% |
| 97  | 12.217 | 3614 | 3616 | 3619 | rBV  | 290    | 150    | 0.01%  | 0.002% |
| 98  | 12.252 | 3625 | 3627 | 3631 | rBV2 | 249    | 186    | 0.02%  | 0.002% |
| 99  | 12.461 | 3689 | 3692 | 3694 | rBV3 | 267    | 178    | 0.02%  | 0.002% |
| 100 | 12.487 | 3696 | 3700 | 3710 | rVB2 | 648    | 804    | 0.07%  | 0.009% |

Sum of corrected areas: 9319765

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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050118WMA.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\SOMULM050118WMA.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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