

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052318\  
 Data File : VU024031.D  
 Acq On : 23 May 2018 12:25  
 Operator : MD/SY  
 Sample : VU0523WBL01  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 4 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         | 0.629       | 9             | 12          | 15           | rVB      | 209            | 143           | 0.01%           | 0.001%        |
| 2         | 0.648       | 15            | 18          | 22           | rBV      | 274            | 246           | 0.02%           | 0.002%        |
| 3         | 0.696       | 31            | 33          | 37           | rVB2     | 202            | 149           | 0.01%           | 0.001%        |
| 4         | 0.725       | 37            | 42          | 46           | rBV      | 245            | 293           | 0.02%           | 0.003%        |
| 5         | 0.748       | 46            | 49          | 52           | rBV      | 142            | 85            | 0.01%           | 0.001%        |
| 6         | 0.770       | 53            | 56          | 60           | rVB2     | 125            | 104           | 0.01%           | 0.001%        |
| 7         | 0.857       | 80            | 83          | 85           | rBV      | 152            | 103           | 0.01%           | 0.001%        |
| 8         | 0.899       | 93            | 96          | 97           | rBV      | 146            | 81            | 0.01%           | 0.001%        |
| 9         | 0.931       | 104           | 106         | 112          | rVB2     | 134            | 120           | 0.01%           | 0.001%        |
| 10        | 0.989       | 117           | 124         | 126          | rBV2     | 183            | 201           | 0.01%           | 0.002%        |
| 11        | 1.088       | 137           | 155         | 179          | rBV      | 1316447        | 1550872       | 100.00%         | 13.773%       |
| 12        | 1.182       | 181           | 184         | 194          | rVB2     | 5269           | 6135          | 0.40%           | 0.054%        |
| 13        | 1.397       | 244           | 251         | 263          | rBV      | 185171         | 193535        | 12.48%          | 1.719%        |
| 14        | 1.680       | 331           | 339         | 355          | rVB      | 135998         | 171142        | 11.04%          | 1.520%        |
| 15        | 2.272       | 512           | 523         | 536          | rVB      | 292173         | 435735        | 28.10%          | 3.870%        |
| 16        | 2.365       | 550           | 552         | 559          | rVB3     | 503            | 320           | 0.02%           | 0.003%        |
| 17        | 2.564       | 611           | 614         | 615          | rBV3     | 182            | 92            | 0.01%           | 0.001%        |
| 18        | 2.616       | 624           | 630         | 634          | rBV4     | 581            | 717           | 0.05%           | 0.006%        |
| 19        | 2.703       | 650           | 657         | 664          | rBV3     | 1092           | 1598          | 0.10%           | 0.014%        |
| 20        | 2.844       | 690           | 701         | 711          | rVB2     | 1636           | 3330          | 0.21%           | 0.030%        |
| 21        | 3.031       | 757           | 759         | 766          | rBV      | 235            | 165           | 0.01%           | 0.001%        |
| 22        | 3.149       | 793           | 796         | 799          | rBV2     | 147            | 100           | 0.01%           | 0.001%        |
| 23        | 3.198       | 808           | 811         | 814          | rBV2     | 169            | 138           | 0.01%           | 0.001%        |
| 24        | 3.352       | 856           | 859         | 861          | rBV2     | 106            | 73            | 0.00%           | 0.001%        |
| 25        | 3.387       | 867           | 870         | 873          | rVB2     | 363            | 260           | 0.02%           | 0.002%        |
| 26        | 3.410       | 873           | 877         | 882          | rBV2     | 304            | 396           | 0.03%           | 0.004%        |
| 27        | 3.481       | 896           | 899         | 902          | rBV2     | 174            | 146           | 0.01%           | 0.001%        |
| 28        | 3.612       | 937           | 940         | 945          | rBV2     | 159            | 148           | 0.01%           | 0.001%        |
| 29        | 3.693       | 960           | 965         | 967          | rBV2     | 225            | 213           | 0.01%           | 0.002%        |
| 30        | 3.760       | 982           | 986         | 990          | rBV2     | 245            | 268           | 0.02%           | 0.002%        |
| 31        | 3.805       | 997           | 1000        | 1003         | rVB      | 213            | 168           | 0.01%           | 0.001%        |
| 32        | 3.825       | 1003          | 1006        | 1008         | rBV2     | 241            | 169           | 0.01%           | 0.002%        |
| 33        | 3.841       | 1008          | 1011        | 1013         | rBV2     | 107            | 73            | 0.00%           | 0.001%        |
| 34        | 3.918       | 1031          | 1035        | 1036         | rBV2     | 183            | 135           | 0.01%           | 0.001%        |

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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 | 3.966 | 1046 | 1050 | 1052 | rVV2 | 142    | 123     | 0.01%  | 0.001%  |
| 36 | 3.979 | 1052 | 1054 | 1059 | rVB2 | 182    | 146     | 0.01%  | 0.001%  |
| 37 | 4.008 | 1059 | 1063 | 1065 | rBV2 | 150    | 132     | 0.01%  | 0.001%  |
| 38 | 4.047 | 1073 | 1075 | 1080 | rVB2 | 179    | 161     | 0.01%  | 0.001%  |
| 39 | 4.072 | 1080 | 1083 | 1087 | rBV2 | 271    | 309     | 0.02%  | 0.003%  |
| 40 | 4.117 | 1095 | 1097 | 1102 | rVB  | 192    | 149     | 0.01%  | 0.001%  |
| 41 | 4.182 | 1102 | 1117 | 1147 | rBV  | 125970 | 334582  | 21.57% | 2.971%  |
| 42 | 4.474 | 1205 | 1208 | 1211 | rBV3 | 207    | 157     | 0.01%  | 0.001%  |
| 43 | 4.503 | 1215 | 1217 | 1222 | rVV2 | 123    | 94      | 0.01%  | 0.001%  |
| 44 | 4.651 | 1244 | 1263 | 1295 | rBV  | 208471 | 504410  | 32.52% | 4.479%  |
| 45 | 4.796 | 1305 | 1308 | 1314 | rVB4 | 360    | 258     | 0.02%  | 0.002%  |
| 46 | 4.850 | 1321 | 1325 | 1330 | rBV2 | 341    | 421     | 0.03%  | 0.004%  |
| 47 | 4.873 | 1330 | 1332 | 1333 | rBV  | 439    | 182     | 0.01%  | 0.002%  |
| 48 | 4.934 | 1344 | 1351 | 1355 | rVB2 | 164    | 215     | 0.01%  | 0.002%  |
| 49 | 4.966 | 1359 | 1361 | 1363 | rBV  | 146    | 91      | 0.01%  | 0.001%  |
| 50 | 4.985 | 1363 | 1367 | 1370 | rVV2 | 323    | 315     | 0.02%  | 0.003%  |
| 51 | 5.021 | 1374 | 1378 | 1381 | rVV  | 162    | 139     | 0.01%  | 0.001%  |
| 52 | 5.053 | 1385 | 1388 | 1393 | rVV2 | 148    | 110     | 0.01%  | 0.001%  |
| 53 | 5.108 | 1402 | 1405 | 1407 | rBV2 | 143    | 129     | 0.01%  | 0.001%  |
| 54 | 5.153 | 1415 | 1419 | 1423 | rBV  | 280    | 251     | 0.02%  | 0.002%  |
| 55 | 5.175 | 1423 | 1426 | 1428 | rBV2 | 144    | 112     | 0.01%  | 0.001%  |
| 56 | 5.207 | 1433 | 1436 | 1441 | rVB2 | 216    | 182     | 0.01%  | 0.002%  |
| 57 | 5.236 | 1442 | 1445 | 1448 | rBV  | 239    | 194     | 0.01%  | 0.002%  |
| 58 | 5.346 | 1454 | 1479 | 1505 | rBV2 | 420850 | 1263828 | 81.49% | 11.224% |
| 59 | 5.622 | 1562 | 1565 | 1567 | rBV  | 207    | 147     | 0.01%  | 0.001%  |
| 60 | 5.670 | 1578 | 1580 | 1581 | rBV  | 264    | 116     | 0.01%  | 0.001%  |
| 61 | 5.680 | 1581 | 1583 | 1586 | rVB2 | 304    | 185     | 0.01%  | 0.002%  |
| 62 | 5.731 | 1597 | 1599 | 1603 | rVB  | 259    | 145     | 0.01%  | 0.001%  |
| 63 | 5.757 | 1605 | 1607 | 1609 | rVB  | 181    | 92      | 0.01%  | 0.001%  |
| 64 | 5.773 | 1609 | 1612 | 1617 | rBV2 | 134    | 123     | 0.01%  | 0.001%  |
| 65 | 5.805 | 1619 | 1622 | 1625 | rVV2 | 147    | 76      | 0.00%  | 0.001%  |
| 66 | 5.892 | 1633 | 1649 | 1680 | rBV  | 347014 | 699439  | 45.10% | 6.211%  |
| 67 | 6.120 | 1718 | 1720 | 1721 | rVB2 | 274    | 73      | 0.00%  | 0.001%  |
| 68 | 6.178 | 1732 | 1738 | 1739 | rBV2 | 1446   | 1437    | 0.09%  | 0.013%  |
| 69 | 6.214 | 1747 | 1749 | 1751 | rBV  | 398    | 192     | 0.01%  | 0.002%  |
| 70 | 6.239 | 1755 | 1757 | 1761 | rVB2 | 362    | 220     | 0.01%  | 0.002%  |
| 71 | 6.275 | 1765 | 1768 | 1772 | rVB2 | 245    | 234     | 0.02%  | 0.002%  |

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 Peak separation: 5

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

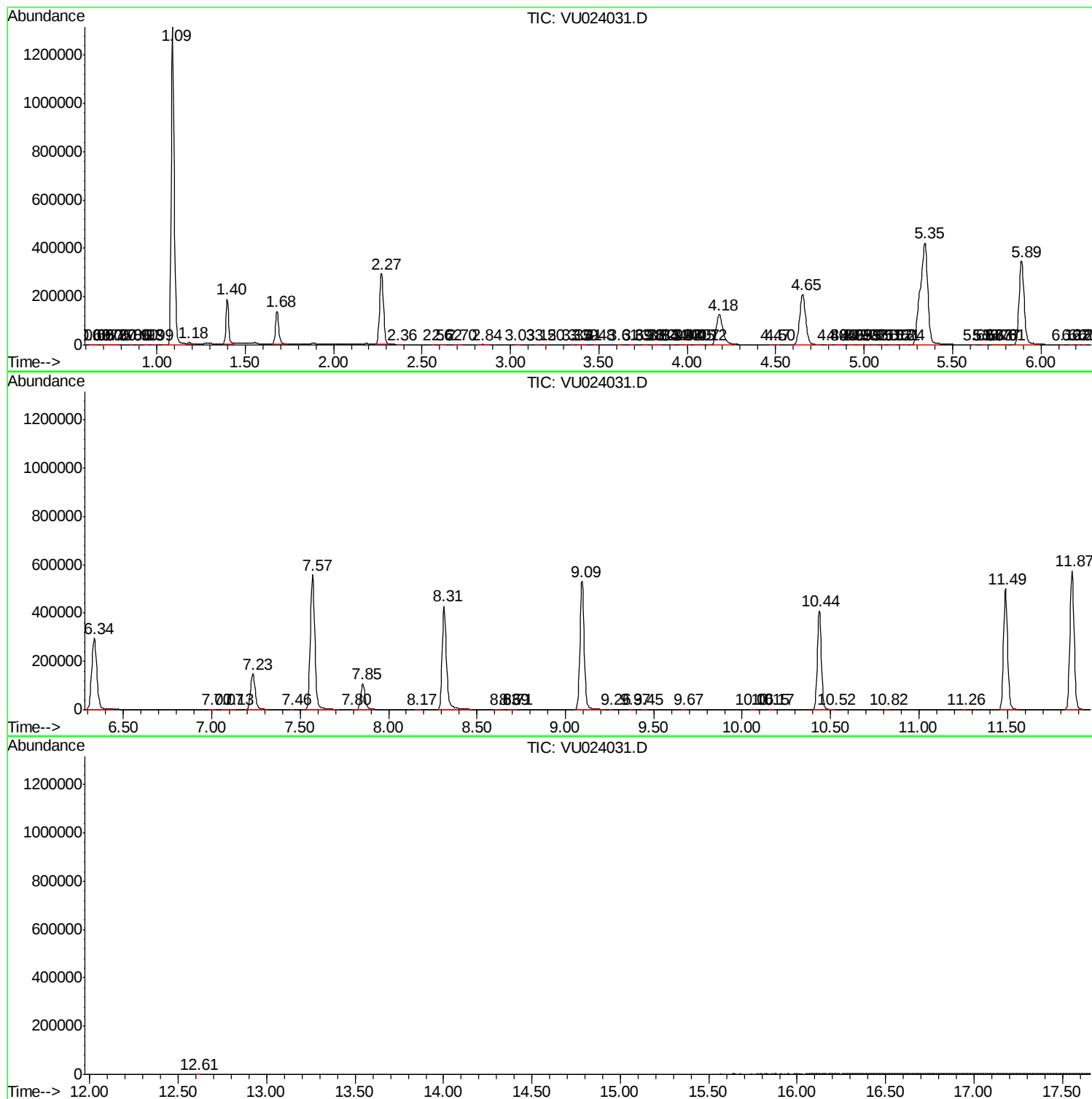
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 6.336  | 1772 | 1787 | 1820 | rBV  | 297087 | 604107 | 38.95% | 5.365% |
| 73  | 7.001  | 1988 | 1994 | 2000 | rBV2 | 222    | 321    | 0.02%  | 0.003% |
| 74  | 7.072  | 2012 | 2016 | 2025 | rVB2 | 180    | 279    | 0.02%  | 0.002% |
| 75  | 7.127  | 2025 | 2033 | 2035 | rBV2 | 242    | 337    | 0.02%  | 0.003% |
| 76  | 7.233  | 2053 | 2066 | 2091 | rBV  | 149705 | 273874 | 17.66% | 2.432% |
| 77  | 7.458  | 2131 | 2136 | 2137 | rBV  | 341    | 313    | 0.02%  | 0.003% |
| 78  | 7.571  | 2152 | 2171 | 2215 | rBV  | 558338 | 996437 | 64.25% | 8.849% |
| 79  | 7.796  | 2239 | 2241 | 2247 | rVB2 | 361    | 291    | 0.02%  | 0.003% |
| 80  | 7.853  | 2247 | 2259 | 2277 | rBV  | 108071 | 184080 | 11.87% | 1.635% |
| 81  | 8.165  | 2352 | 2356 | 2360 | rBV2 | 166    | 162    | 0.01%  | 0.001% |
| 82  | 8.313  | 2390 | 2402 | 2450 | rBV  | 428020 | 739389 | 47.68% | 6.566% |
| 83  | 8.632  | 2490 | 2501 | 2505 | rBV3 | 1200   | 2023   | 0.13%  | 0.018% |
| 84  | 8.686  | 2516 | 2518 | 2522 | rVB  | 215    | 117    | 0.01%  | 0.001% |
| 85  | 8.709  | 2522 | 2525 | 2528 | rBV  | 165    | 148    | 0.01%  | 0.001% |
| 86  | 9.095  | 2631 | 2645 | 2683 | rBV  | 531513 | 888024 | 57.26% | 7.886% |
| 87  | 9.262  | 2693 | 2697 | 2698 | rBV2 | 334    | 233    | 0.02%  | 0.002% |
| 88  | 9.374  | 2727 | 2732 | 2733 | rBV2 | 244    | 249    | 0.02%  | 0.002% |
| 89  | 9.445  | 2750 | 2754 | 2759 | rBV2 | 210    | 275    | 0.02%  | 0.002% |
| 90  | 9.673  | 2819 | 2825 | 2827 | rBV2 | 249    | 281    | 0.02%  | 0.002% |
| 91  | 10.059 | 2941 | 2945 | 2948 | rBV2 | 305    | 280    | 0.02%  | 0.002% |
| 92  | 10.146 | 2971 | 2972 | 2975 | rVB  | 165    | 84     | 0.01%  | 0.001% |
| 93  | 10.172 | 2975 | 2980 | 2981 | rBV  | 199    | 183    | 0.01%  | 0.002% |
| 94  | 10.435 | 3050 | 3062 | 3086 | rVB  | 408865 | 654578 | 42.21% | 5.813% |
| 95  | 10.522 | 3086 | 3089 | 3090 | rBV  | 231    | 147    | 0.01%  | 0.001% |
| 96  | 10.818 | 3178 | 3181 | 3184 | rBV2 | 230    | 146    | 0.01%  | 0.001% |
| 97  | 11.258 | 3315 | 3318 | 3320 | rVB2 | 171    | 95     | 0.01%  | 0.001% |
| 98  | 11.490 | 3378 | 3390 | 3410 | rBV  | 500480 | 797408 | 51.42% | 7.081% |
| 99  | 11.866 | 3493 | 3507 | 3525 | rBV  | 575082 | 939776 | 60.60% | 8.346% |
| 100 | 12.606 | 3735 | 3737 | 3742 | rBV2 | 257    | 231    | 0.01%  | 0.002% |

Sum of corrected areas: 11260490

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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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