

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU013123\  
 Data File : VU052886.D  
 Acq On : 31 Jan 2023 18:03  
 Operator : JC/MD  
 Sample : 01381-01  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A44K6

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
 Title : VOC Analysis

Signal : TIC: VU052886.D\data.ms

| 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         | 1.597       | 73            | 80          | 101          | rVB      | 77317          | 93255         | 11.01%          | 1.475%        |
| 2         | 1.909       | 170           | 177         | 198          | rVB      | 81617          | 114348        | 13.50%          | 1.809%        |
| 3         | 2.565       | 368           | 381         | 396          | rBV      | 157678         | 258339        | 30.51%          | 4.087%        |
| 4         | 2.706       | 423           | 425         | 430          | rVB2     | 261            | 127           | 0.01%           | 0.002%        |
| 5         | 2.864       | 472           | 474         | 476          | rBV      | 299            | 184           | 0.02%           | 0.003%        |
| 6         | 2.932       | 491           | 495         | 497          | rBV      | 310            | 257           | 0.03%           | 0.004%        |
| 7         | 3.121       | 550           | 554         | 556          | rBV      | 337            | 238           | 0.03%           | 0.004%        |
| 8         | 3.186       | 566           | 574         | 578          | rBV2     | 698            | 1100          | 0.13%           | 0.017%        |
| 9         | 3.295       | 603           | 608         | 610          | rBV2     | 221            | 227           | 0.03%           | 0.004%        |
| 10        | 3.395       | 637           | 639         | 641          | rBV2     | 252            | 149           | 0.02%           | 0.002%        |
| 11        | 3.546       | 683           | 686         | 688          | rBV      | 187            | 161           | 0.02%           | 0.003%        |
| 12        | 3.558       | 688           | 690         | 695          | rVB      | 206            | 134           | 0.02%           | 0.002%        |
| 13        | 3.610       | 701           | 706         | 710          | rBV2     | 286            | 359           | 0.04%           | 0.006%        |
| 14        | 3.748       | 745           | 749         | 752          | rBV      | 154            | 153           | 0.02%           | 0.002%        |
| 15        | 3.845       | 774           | 779         | 781          | rBV      | 183            | 198           | 0.02%           | 0.003%        |
| 16        | 3.941       | 805           | 809         | 814          | rBV      | 242            | 312           | 0.04%           | 0.005%        |
| 17        | 4.060       | 842           | 846         | 850          | rBB      | 212            | 205           | 0.02%           | 0.003%        |
| 18        | 4.189       | 884           | 886         | 890          | rBV      | 207            | 210           | 0.02%           | 0.003%        |
| 19        | 4.256       | 905           | 907         | 911          | rBB      | 208            | 160           | 0.02%           | 0.003%        |
| 20        | 4.359       | 936           | 939         | 943          | rBV      | 287            | 262           | 0.03%           | 0.004%        |
| 21        | 4.411       | 952           | 955         | 961          | rBV      | 281            | 285           | 0.03%           | 0.005%        |
| 22        | 4.472       | 971           | 974         | 976          | rBV      | 344            | 255           | 0.03%           | 0.004%        |
| 23        | 4.526       | 988           | 991         | 993          | rVB      | 330            | 192           | 0.02%           | 0.003%        |
| 24        | 4.552       | 994           | 999         | 1001         | rBB      | 155            | 152           | 0.02%           | 0.002%        |
| 25        | 4.568       | 1002          | 1004        | 1007         | rBB2     | 263            | 163           | 0.02%           | 0.003%        |
| 26        | 4.623       | 1008          | 1021        | 1053         | rBV      | 74475          | 193343        | 22.83%          | 3.059%        |
| 27        | 4.883       | 1099          | 1102        | 1104         | rBV      | 295            | 246           | 0.03%           | 0.004%        |
| 28        | 4.993       | 1132          | 1136        | 1140         | rBV2     | 251            | 200           | 0.02%           | 0.003%        |
| 29        | 5.057       | 1140          | 1156        | 1182         | rBV      | 169532         | 372794        | 44.03%          | 5.898%        |
| 30        | 5.221       | 1204          | 1207        | 1210         | rVB      | 238            | 145           | 0.02%           | 0.002%        |
| 31        | 5.266       | 1217          | 1221        | 1223         | rBV      | 279            | 214           | 0.03%           | 0.003%        |
| 32        | 5.282       | 1224          | 1226        | 1232         | rVV2     | 351            | 278           | 0.03%           | 0.004%        |
| 33        | 5.308       | 1232          | 1234        | 1238         | rVV2     | 178            | 158           | 0.02%           | 0.002%        |
| 34        | 5.430       | 1269          | 1272        | 1276         | rBV2     | 269            | 240           | 0.03%           | 0.004%        |
| 35        | 5.549       | 1306          | 1309        | 1313         | rVB2     | 187            | 128           | 0.02%           | 0.002%        |
| 36        | 5.587       | 1318          | 1321        | 1323         | rBV      | 171            | 147           | 0.02%           | 0.002%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |        |         |         |
|----|-------|------|------|------|------|--------|--------|---------|---------|
| 37 | 5.719 | 1337 | 1362 | 1387 | rBV2 | 305097 | 846752 | 100.00% | 13.397% |
| 38 | 5.999 | 1446 | 1449 | 1450 | rBV  | 247    | 160    | 0.02%   | 0.003%  |
| 39 | 6.041 | 1460 | 1462 | 1465 | rBB  | 284    | 175    | 0.02%   | 0.003%  |
| 40 | 6.150 | 1493 | 1496 | 1499 | rVB2 | 323    | 212    | 0.03%   | 0.003%  |
| 41 | 6.179 | 1502 | 1505 | 1507 | rBV  | 229    | 157    | 0.02%   | 0.002%  |
| 42 | 6.243 | 1512 | 1525 | 1547 | rBV  | 269127 | 509103 | 60.12%  | 8.055%  |
| 43 | 6.391 | 1568 | 1571 | 1572 | rBV  | 446    | 291    | 0.03%   | 0.005%  |
| 44 | 6.494 | 1598 | 1603 | 1604 | rBV  | 290    | 218    | 0.03%   | 0.003%  |
| 45 | 6.536 | 1607 | 1616 | 1628 | rVV9 | 1859   | 3969   | 0.47%   | 0.063%  |
| 46 | 6.594 | 1632 | 1634 | 1637 | rBV  | 244    | 163    | 0.02%   | 0.003%  |
| 47 | 6.687 | 1646 | 1663 | 1684 | rBV  | 204366 | 395121 | 46.66%  | 6.251%  |
| 48 | 6.809 | 1695 | 1701 | 1707 | rVB3 | 587    | 814    | 0.10%   | 0.013%  |
| 49 | 6.838 | 1707 | 1710 | 1713 | rBV  | 281    | 213    | 0.03%   | 0.003%  |
| 50 | 6.989 | 1753 | 1757 | 1765 | rBB  | 201    | 296    | 0.03%   | 0.005%  |
| 51 | 7.044 | 1771 | 1774 | 1776 | rBV  | 163    | 136    | 0.02%   | 0.002%  |
| 52 | 7.137 | 1800 | 1803 | 1806 | rVB  | 327    | 232    | 0.03%   | 0.004%  |
| 53 | 7.156 | 1806 | 1809 | 1811 | rBV2 | 315    | 230    | 0.03%   | 0.004%  |
| 54 | 7.185 | 1812 | 1818 | 1826 | rVB5 | 1541   | 2395   | 0.28%   | 0.038%  |
| 55 | 7.298 | 1851 | 1853 | 1855 | rBV  | 179    | 124    | 0.01%   | 0.002%  |
| 56 | 7.330 | 1860 | 1863 | 1866 | rBV  | 181    | 165    | 0.02%   | 0.003%  |
| 57 | 7.398 | 1882 | 1884 | 1886 | rVB  | 254    | 124    | 0.01%   | 0.002%  |
| 58 | 7.562 | 1922 | 1935 | 1952 | rBV  | 99661  | 175181 | 20.69%  | 2.772%  |
| 59 | 7.687 | 1968 | 1974 | 1981 | rBV5 | 1042   | 1576   | 0.19%   | 0.025%  |
| 60 | 7.893 | 2025 | 2038 | 2057 | rBV  | 356081 | 608836 | 71.90%  | 9.633%  |
| 61 | 8.034 | 2080 | 2082 | 2086 | rVB2 | 312    | 196    | 0.02%   | 0.003%  |
| 62 | 8.131 | 2108 | 2112 | 2114 | rBV  | 223    | 206    | 0.02%   | 0.003%  |
| 63 | 8.176 | 2114 | 2126 | 2145 | rVV  | 71051  | 121418 | 14.34%  | 1.921%  |
| 64 | 8.295 | 2160 | 2163 | 2165 | rBV2 | 301    | 166    | 0.02%   | 0.003%  |
| 65 | 8.359 | 2179 | 2183 | 2184 | rBV2 | 266    | 154    | 0.02%   | 0.002%  |
| 66 | 8.516 | 2226 | 2232 | 2235 | rBV  | 251    | 289    | 0.03%   | 0.005%  |
| 67 | 8.565 | 2244 | 2247 | 2251 | rVB  | 289    | 223    | 0.03%   | 0.004%  |
| 68 | 8.632 | 2251 | 2268 | 2299 | rBV2 | 219348 | 430090 | 50.79%  | 6.805%  |
| 69 | 8.857 | 2336 | 2338 | 2343 | rVB  | 312    | 240    | 0.03%   | 0.004%  |
| 70 | 8.883 | 2343 | 2346 | 2350 | rBV  | 342    | 334    | 0.04%   | 0.005%  |
| 71 | 9.018 | 2386 | 2388 | 2394 | rVB2 | 248    | 188    | 0.02%   | 0.003%  |
| 72 | 9.198 | 2441 | 2444 | 2447 | rBB2 | 244    | 199    | 0.02%   | 0.003%  |
| 73 | 9.217 | 2447 | 2450 | 2454 | rBV  | 171    | 193    | 0.02%   | 0.003%  |
| 74 | 9.256 | 2458 | 2462 | 2472 | rVB3 | 418    | 556    | 0.07%   | 0.009%  |
| 75 | 9.369 | 2491 | 2497 | 2498 | rBV  | 362    | 305    | 0.04%   | 0.005%  |
| 76 | 9.414 | 2498 | 2511 | 2527 | rVV  | 376700 | 612499 | 72.34%  | 9.691%  |

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Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 9.539  | 2547 | 2550 | 2555 | rVB2 | 477    | 360    | 0.04%  | 0.006% |
| 78  | 9.565  | 2555 | 2558 | 2561 | rBV2 | 391    | 288    | 0.03%  | 0.005% |
| 79  | 9.693  | 2594 | 2598 | 2600 | rBV  | 270    | 213    | 0.03%  | 0.003% |
| 80  | 9.883  | 2653 | 2657 | 2658 | rBV  | 259    | 174    | 0.02%  | 0.003% |
| 81  | 10.369 | 2805 | 2808 | 2814 | rVB2 | 222    | 188    | 0.02%  | 0.003% |
| 82  | 10.539 | 2859 | 2861 | 2867 | rVB2 | 191    | 155    | 0.02%  | 0.002% |
| 83  | 10.668 | 2898 | 2901 | 2904 | rBV  | 336    | 248    | 0.03%  | 0.004% |
| 84  | 10.751 | 2915 | 2927 | 2942 | rBV  | 298530 | 481264 | 56.84% | 7.614% |
| 85  | 10.873 | 2963 | 2965 | 2966 | rBV  | 276    | 148    | 0.02%  | 0.002% |
| 86  | 11.385 | 3122 | 3124 | 3129 | rVB  | 292    | 135    | 0.02%  | 0.002% |
| 87  | 11.410 | 3130 | 3132 | 3134 | rBV  | 270    | 125    | 0.01%  | 0.002% |
| 88  | 11.558 | 3175 | 3178 | 3183 | rBV  | 237    | 209    | 0.02%  | 0.003% |
| 89  | 11.806 | 3244 | 3255 | 3270 | rBV  | 329174 | 516506 | 61.00% | 8.172% |
| 90  | 12.063 | 3331 | 3335 | 3343 | rVB6 | 981    | 1155   | 0.14%  | 0.018% |
| 91  | 12.188 | 3361 | 3374 | 3393 | rBV  | 338306 | 550323 | 64.99% | 8.707% |
| 92  | 12.346 | 3421 | 3423 | 3425 | rBV2 | 326    | 148    | 0.02%  | 0.002% |
| 93  | 12.423 | 3444 | 3447 | 3449 | rBV  | 232    | 174    | 0.02%  | 0.003% |
| 94  | 13.227 | 3694 | 3697 | 3700 | rBV  | 263    | 204    | 0.02%  | 0.003% |
| 95  | 13.664 | 3830 | 3833 | 3835 | rBV2 | 279    | 152    | 0.02%  | 0.002% |
| 96  | 13.712 | 3846 | 3848 | 3852 | rBV  | 261    | 196    | 0.02%  | 0.003% |
| 97  | 13.838 | 3878 | 3887 | 3902 | rBV3 | 8756   | 14249  | 1.68%  | 0.225% |
| 98  | 13.909 | 3906 | 3909 | 3911 | rBV  | 357    | 234    | 0.03%  | 0.004% |
| 99  | 14.237 | 4007 | 4011 | 4013 | rBV2 | 337    | 260    | 0.03%  | 0.004% |
| 100 | 15.124 | 4284 | 4287 | 4289 | rBV3 | 373    | 246    | 0.03%  | 0.004% |

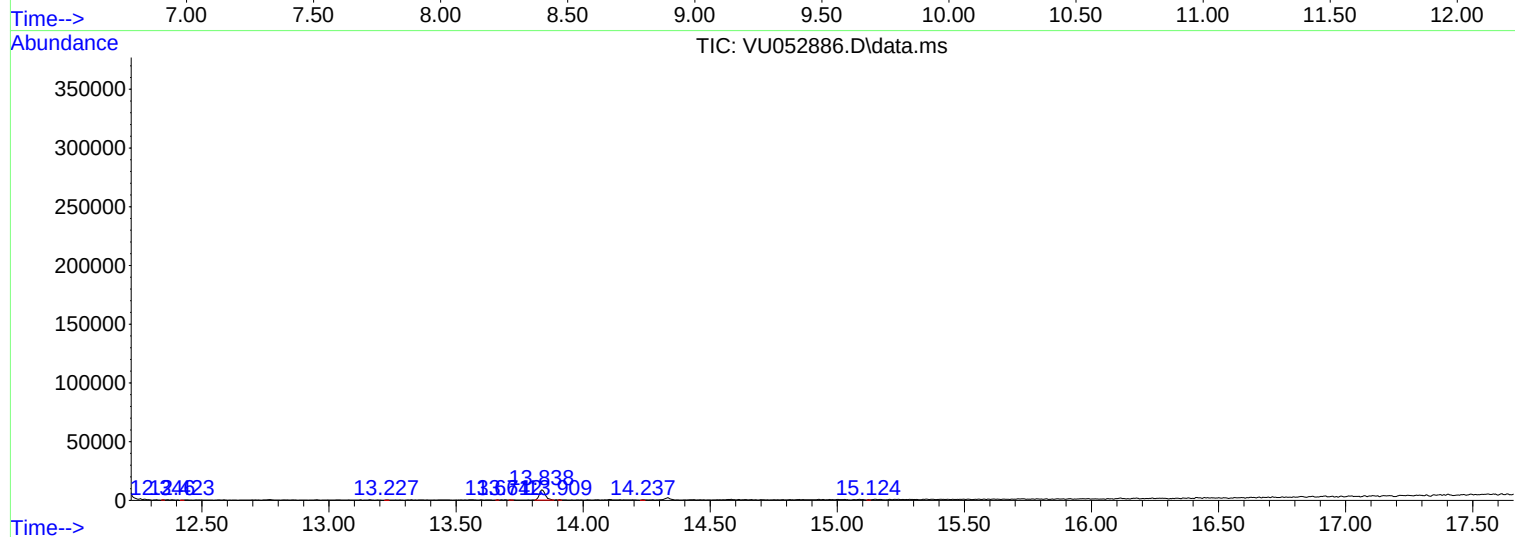
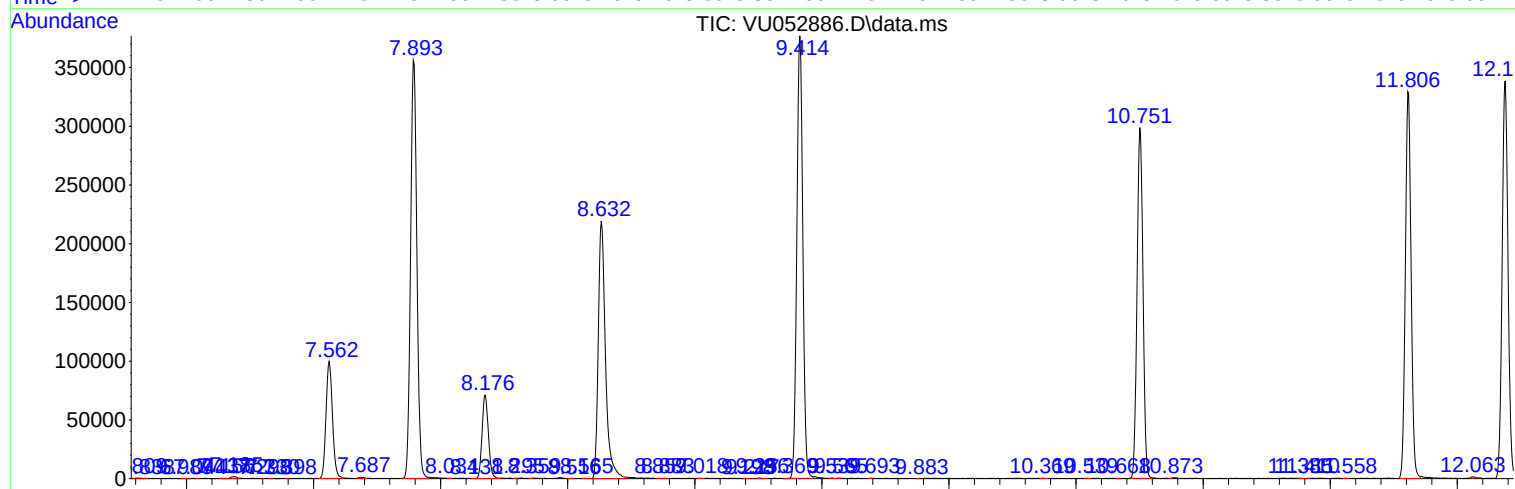
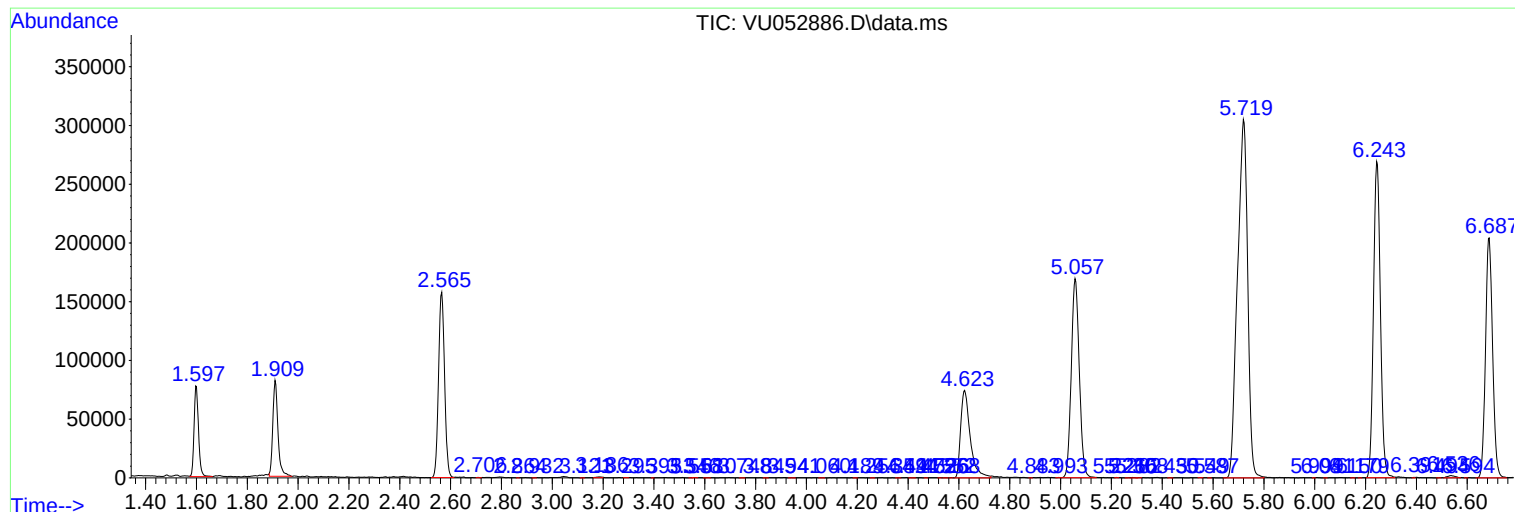
Sum of corrected areas: 6320571

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU013123\  
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No Library Search Compounds Detected

\*\*\*\*\*

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TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT | EstConc | Units | Response | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |