

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU013123\  
 Data File : VU052887.D  
 Acq On : 31 Jan 2023 18:27  
 Operator : JC/MD  
 Sample : 01381-02  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A44M6

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: VU052887.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         | 1.491       | 43            | 47          | 54           | rBV2     | 6142           | 5835          | 0.05%           | 0.016%        |
| 2         | 1.601       | 73            | 81          | 93           | rVB      | 86710          | 100960        | 0.85%           | 0.272%        |
| 3         | 1.909       | 169           | 177         | 192          | rVB      | 79158          | 107490        | 0.91%           | 0.289%        |
| 4         | 2.208       | 268           | 270         | 275          | rBV3     | 587            | 378           | 0.00%           | 0.001%        |
| 5         | 2.565       | 369           | 381         | 399          | rVB      | 163644         | 273409        | 2.31%           | 0.736%        |
| 6         | 2.832       | 461           | 464         | 467          | rVB      | 231            | 154           | 0.00%           | 0.000%        |
| 7         | 3.041       | 523           | 529         | 531          | rBV2     | 1263           | 1153          | 0.01%           | 0.003%        |
| 8         | 3.186       | 572           | 574         | 577          | rVB2     | 352            | 214           | 0.00%           | 0.001%        |
| 9         | 3.240       | 587           | 591         | 597          | rBV      | 269            | 437           | 0.00%           | 0.001%        |
| 10        | 3.353       | 614           | 626         | 640          | rVV4     | 11711          | 24091         | 0.20%           | 0.065%        |
| 11        | 3.459       | 655           | 659         | 662          | rBV2     | 305            | 328           | 0.00%           | 0.001%        |
| 12        | 3.629       | 708           | 712         | 714          | rBV      | 179            | 172           | 0.00%           | 0.000%        |
| 13        | 3.642       | 714           | 716         | 719          | rVB      | 273            | 152           | 0.00%           | 0.000%        |
| 14        | 3.668       | 720           | 724         | 726          | rBV      | 197            | 161           | 0.00%           | 0.000%        |
| 15        | 3.736       | 741           | 745         | 747          | rBV      | 288            | 212           | 0.00%           | 0.001%        |
| 16        | 3.977       | 818           | 820         | 821          | rBV      | 352            | 169           | 0.00%           | 0.000%        |
| 17        | 4.031       | 833           | 837         | 842          | rVB2     | 347            | 344           | 0.00%           | 0.001%        |
| 18        | 4.218       | 890           | 895         | 897          | rBB2     | 383            | 303           | 0.00%           | 0.001%        |
| 19        | 4.266       | 907           | 910         | 913          | rBB      | 272            | 155           | 0.00%           | 0.000%        |
| 20        | 4.305       | 917           | 922         | 923          | rBB      | 237            | 168           | 0.00%           | 0.000%        |
| 21        | 4.520       | 986           | 989         | 991          | rBV      | 219            | 164           | 0.00%           | 0.000%        |
| 22        | 4.562       | 1000          | 1002        | 1005         | rVB      | 360            | 209           | 0.00%           | 0.001%        |
| 23        | 4.662       | 1008          | 1033        | 1063         | rBV2     | 1062953        | 2542421       | 21.48%          | 6.844%        |
| 24        | 4.887       | 1100          | 1103        | 1106         | rBV3     | 296            | 172           | 0.00%           | 0.000%        |
| 25        | 4.935       | 1114          | 1118        | 1121         | rBV      | 351            | 314           | 0.00%           | 0.001%        |
| 26        | 4.967       | 1126          | 1128        | 1132         | rVB3     | 279            | 182           | 0.00%           | 0.000%        |
| 27        | 4.993       | 1133          | 1136        | 1137         | rBV2     | 406            | 192           | 0.00%           | 0.001%        |
| 28        | 5.057       | 1142          | 1156        | 1178         | rVB      | 172734         | 387777        | 3.28%           | 1.044%        |
| 29        | 5.221       | 1205          | 1207        | 1211         | rBB      | 510            | 320           | 0.00%           | 0.001%        |
| 30        | 5.263       | 1218          | 1220        | 1223         | rVV      | 246            | 193           | 0.00%           | 0.001%        |
| 31        | 5.285       | 1223          | 1227        | 1234         | rVB3     | 441            | 487           | 0.00%           | 0.001%        |
| 32        | 5.321       | 1234          | 1238        | 1242         | rBB      | 249            | 231           | 0.00%           | 0.001%        |
| 33        | 5.385       | 1250          | 1258        | 1263         | rBV3     | 703            | 1130          | 0.01%           | 0.003%        |
| 34        | 5.433       | 1270          | 1273        | 1276         | rBV      | 314            | 235           | 0.00%           | 0.001%        |
| 35        | 5.507       | 1293          | 1296        | 1298         | rBV      | 305            | 174           | 0.00%           | 0.000%        |
| 36        | 5.719       | 1339          | 1362        | 1373         | rBV2     | 307149         | 879203        | 7.43%           | 2.367%        |

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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 | 5.874  | 1408 | 1410 | 1414 | rBV2 | 288     | 183      | 0.00%  | 0.000%  |
| 38 | 5.938  | 1421 | 1430 | 1435 | rBV5 | 1706    | 2167     | 0.02%  | 0.006%  |
| 39 | 6.141  | 1491 | 1493 | 1498 | rBB  | 266     | 225      | 0.00%  | 0.001%  |
| 40 | 6.189  | 1502 | 1508 | 1510 | rBV  | 338     | 285      | 0.00%  | 0.001%  |
| 41 | 6.243  | 1510 | 1525 | 1549 | rVV  | 255966  | 487969   | 4.12%  | 1.314%  |
| 42 | 6.372  | 1561 | 1565 | 1573 | rVB2 | 470     | 633      | 0.01%  | 0.002%  |
| 43 | 6.407  | 1573 | 1576 | 1579 | rBV  | 323     | 242      | 0.00%  | 0.001%  |
| 44 | 6.446  | 1585 | 1588 | 1594 | rVB2 | 254     | 294      | 0.00%  | 0.001%  |
| 45 | 6.536  | 1595 | 1616 | 1638 | rBV  | 1103152 | 2043400  | 17.26% | 5.501%  |
| 46 | 6.687  | 1649 | 1663 | 1679 | rBV  | 204716  | 400145   | 3.38%  | 1.077%  |
| 47 | 6.835  | 1707 | 1709 | 1714 | rBV2 | 477     | 389      | 0.00%  | 0.001%  |
| 48 | 6.986  | 1751 | 1756 | 1759 | rBV  | 329     | 342      | 0.00%  | 0.001%  |
| 49 | 7.025  | 1765 | 1768 | 1772 | rBB  | 341     | 238      | 0.00%  | 0.001%  |
| 50 | 7.099  | 1784 | 1791 | 1801 | rVB4 | 1267    | 2069     | 0.02%  | 0.006%  |
| 51 | 7.141  | 1801 | 1804 | 1806 | rBV2 | 262     | 179      | 0.00%  | 0.000%  |
| 52 | 7.186  | 1809 | 1818 | 1819 | rBV3 | 1421    | 1484     | 0.01%  | 0.004%  |
| 53 | 7.263  | 1839 | 1842 | 1845 | rBB2 | 231     | 162      | 0.00%  | 0.000%  |
| 54 | 7.330  | 1858 | 1863 | 1864 | rBV  | 148     | 153      | 0.00%  | 0.000%  |
| 55 | 7.562  | 1923 | 1935 | 1957 | rBV  | 107272  | 186899   | 1.58%  | 0.503%  |
| 56 | 7.687  | 1968 | 1974 | 1980 | rBV4 | 988     | 1084     | 0.01%  | 0.003%  |
| 57 | 7.822  | 2013 | 2016 | 2020 | rBV  | 149     | 176      | 0.00%  | 0.000%  |
| 58 | 7.893  | 2025 | 2038 | 2056 | rBV  | 375973  | 644363   | 5.44%  | 1.735%  |
| 59 | 8.018  | 2074 | 2077 | 2084 | rVB3 | 507     | 587      | 0.00%  | 0.002%  |
| 60 | 8.050  | 2084 | 2087 | 2089 | rBV  | 240     | 172      | 0.00%  | 0.000%  |
| 61 | 8.128  | 2108 | 2111 | 2114 | rBV  | 367     | 268      | 0.00%  | 0.001%  |
| 62 | 8.176  | 2114 | 2126 | 2143 | rVV  | 74336   | 127642   | 1.08%  | 0.344%  |
| 63 | 8.401  | 2193 | 2196 | 2199 | rVB2 | 495     | 341      | 0.00%  | 0.001%  |
| 64 | 8.427  | 2200 | 2204 | 2209 | rBV2 | 412     | 524      | 0.00%  | 0.001%  |
| 65 | 8.465  | 2209 | 2216 | 2227 | rVV4 | 1717    | 2728     | 0.02%  | 0.007%  |
| 66 | 8.549  | 2238 | 2242 | 2246 | rBV2 | 379     | 340      | 0.00%  | 0.001%  |
| 67 | 8.591  | 2251 | 2255 | 2256 | rBV  | 296     | 184      | 0.00%  | 0.000%  |
| 68 | 8.629  | 2256 | 2267 | 2296 | rBV3 | 216481  | 421768   | 3.56%  | 1.135%  |
| 69 | 8.784  | 2312 | 2315 | 2317 | rBV2 | 347     | 246      | 0.00%  | 0.001%  |
| 70 | 8.983  | 2374 | 2377 | 2384 | rVB  | 358     | 379      | 0.00%  | 0.001%  |
| 71 | 9.089  | 2406 | 2410 | 2414 | rBB  | 207     | 216      | 0.00%  | 0.001%  |
| 72 | 9.321  | 2479 | 2482 | 2488 | rVB2 | 213     | 177      | 0.00%  | 0.000%  |
| 73 | 9.443  | 2497 | 2520 | 2549 | rBV  | 6085491 | 10334609 | 87.31% | 27.821% |
| 74 | 9.780  | 2624 | 2625 | 2629 | rBV2 | 446     | 277      | 0.00%  | 0.001%  |
| 75 | 10.478 | 2837 | 2842 | 2851 | rVB3 | 1456    | 1811     | 0.02%  | 0.005%  |
| 76 | 10.562 | 2861 | 2868 | 2876 | rBV3 | 976     | 1563     | 0.01%  | 0.004%  |

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Integration Parameters: LSCINT.P

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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

|     |        |      |      |      |      |         |          |         |         |
|-----|--------|------|------|------|------|---------|----------|---------|---------|
| 77  | 10.661 | 2896 | 2899 | 2903 | rBV  | 195     | 183      | 0.00%   | 0.000%  |
| 78  | 10.751 | 2914 | 2927 | 2941 | rBV  | 307332  | 485194   | 4.10%   | 1.306%  |
| 79  | 11.279 | 3086 | 3091 | 3101 | rVB2 | 765     | 1084     | 0.01%   | 0.003%  |
| 80  | 11.510 | 3156 | 3163 | 3166 | rBV3 | 647     | 757      | 0.01%   | 0.002%  |
| 81  | 11.742 | 3222 | 3235 | 3245 | rBV  | 135862  | 214923   | 1.82%   | 0.579%  |
| 82  | 11.832 | 3245 | 3263 | 3278 | rVV2 | 1288485 | 2550874  | 21.55%  | 6.867%  |
| 83  | 12.057 | 3322 | 3333 | 3338 | rBV3 | 9165    | 14763    | 0.12%   | 0.040%  |
| 84  | 12.208 | 3360 | 3380 | 3417 | rBV  | 7166428 | 11836917 | 100.00% | 31.866% |
| 85  | 12.558 | 3488 | 3489 | 3494 | rVB2 | 275     | 174      | 0.00%   | 0.000%  |
| 86  | 12.658 | 3518 | 3520 | 3523 | rBV2 | 279     | 154      | 0.00%   | 0.000%  |
| 87  | 12.719 | 3536 | 3539 | 3540 | rBV2 | 493     | 273      | 0.00%   | 0.001%  |
| 88  | 12.761 | 3547 | 3552 | 3559 | rBV4 | 990     | 1692     | 0.01%   | 0.005%  |
| 89  | 12.806 | 3559 | 3566 | 3578 | rVB6 | 4686    | 6521     | 0.06%   | 0.018%  |
| 90  | 12.857 | 3580 | 3582 | 3588 | rVB2 | 431     | 335      | 0.00%   | 0.001%  |
| 91  | 12.883 | 3588 | 3590 | 3593 | rBV2 | 268     | 185      | 0.00%   | 0.000%  |
| 92  | 13.028 | 3632 | 3635 | 3637 | rBV  | 327     | 167      | 0.00%   | 0.000%  |
| 93  | 13.140 | 3667 | 3670 | 3671 | rBV  | 643     | 355      | 0.00%   | 0.001%  |
| 94  | 13.221 | 3689 | 3695 | 3704 | rVB6 | 2316    | 2772     | 0.02%   | 0.007%  |
| 95  | 13.449 | 3763 | 3766 | 3768 | rVB  | 375     | 204      | 0.00%   | 0.001%  |
| 96  | 13.481 | 3768 | 3776 | 3779 | rBV2 | 260     | 407      | 0.00%   | 0.001%  |
| 97  | 13.835 | 3873 | 3886 | 3910 | rBV  | 1617387 | 2469348  | 20.86%  | 6.648%  |
| 98  | 14.246 | 4010 | 4014 | 4016 | rBV2 | 450     | 354      | 0.00%   | 0.001%  |
| 99  | 14.324 | 4025 | 4038 | 4059 | rBV  | 351178  | 561167   | 4.74%   | 1.511%  |
| 100 | 14.629 | 4130 | 4133 | 4140 | rBV3 | 800     | 806      | 0.01%   | 0.002%  |

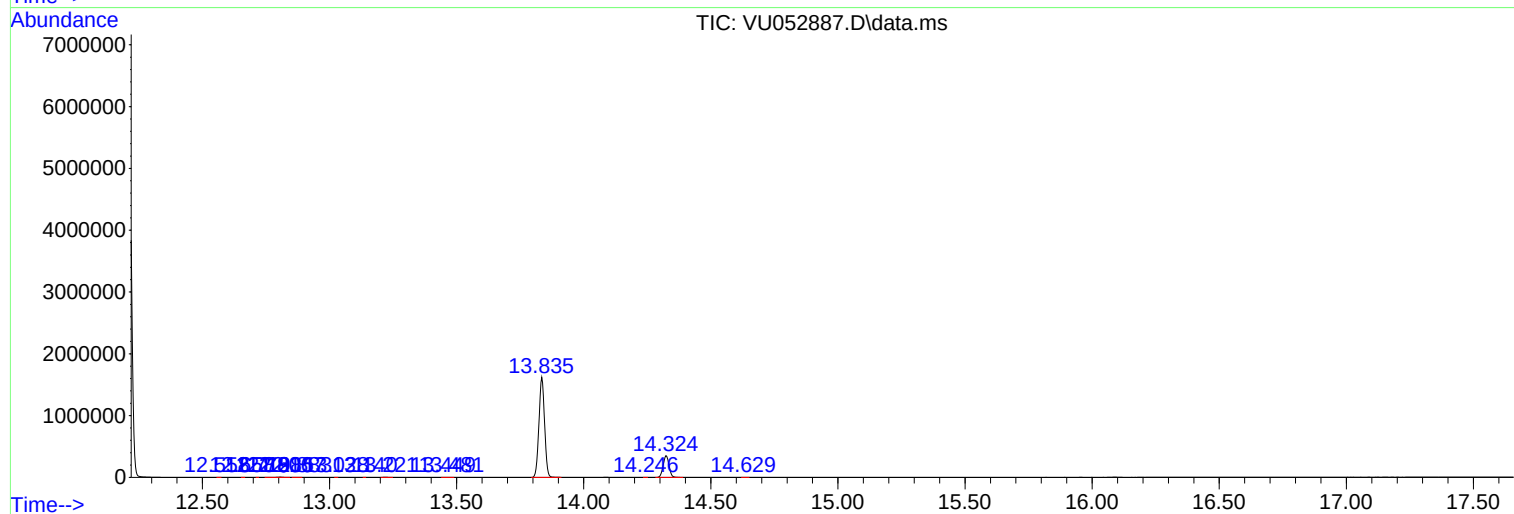
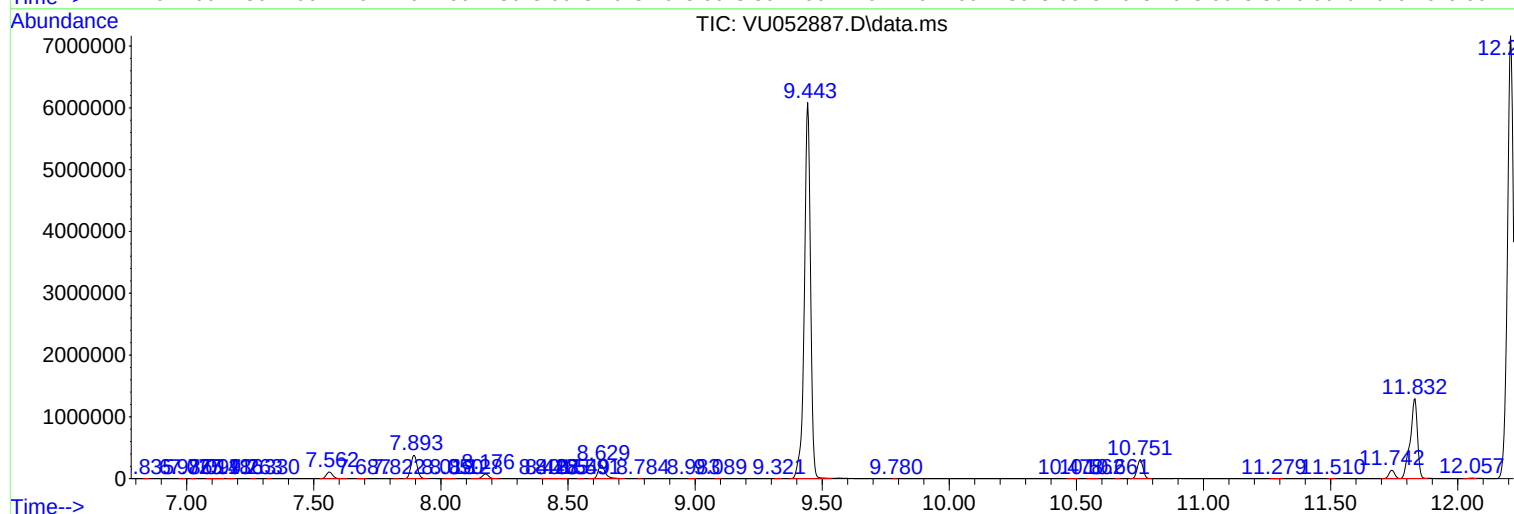
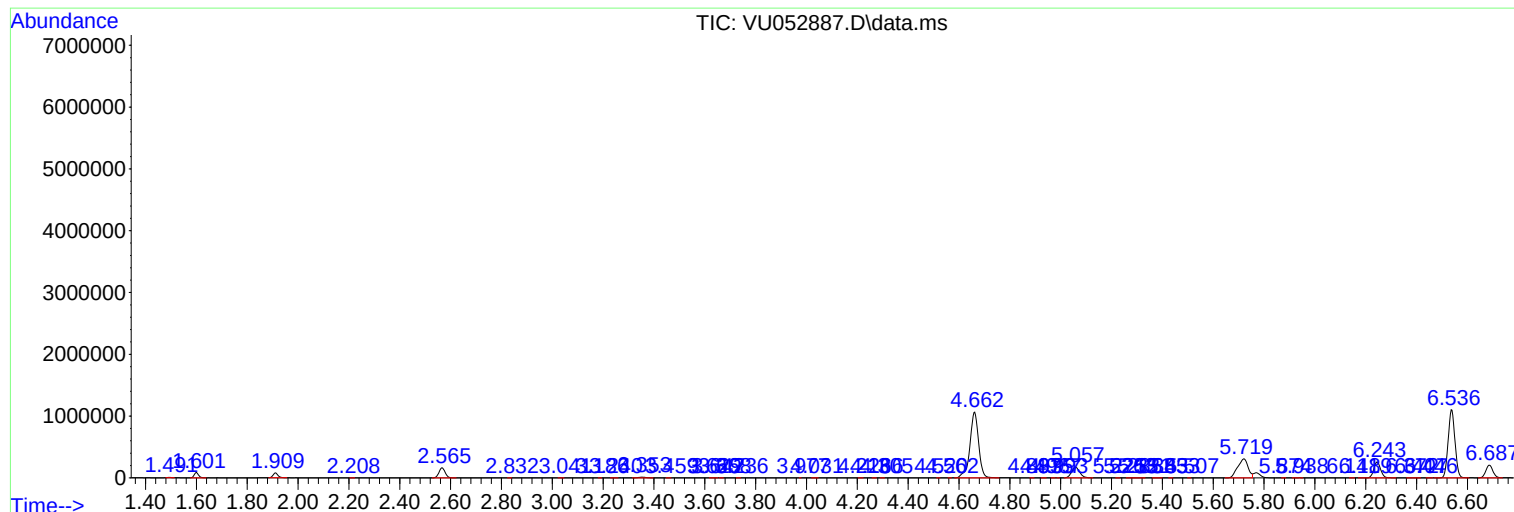
Sum of corrected areas: 37146211

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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



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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 | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|