

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU010623\  
 Data File : VU052630.D  
 Acq On : 06 Jan 2023 16:03  
 Operator : JC/MD  
 Sample : 01036-01  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 COLD5

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\SFAMULM010623WMA.M  
 Title : VOC Analysis

Signal : TIC: VU052630.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         | 1.520       | 51            | 56          | 64           | rBV      | 9979           | 10749         | 0.29%           | 0.061%        |
| 2         | 1.601       | 73            | 81          | 99           | rVB      | 225801         | 265174        | 7.03%           | 1.493%        |
| 3         | 1.906       | 169           | 176         | 199          | rVB      | 179631         | 254425        | 6.75%           | 1.433%        |
| 4         | 2.565       | 368           | 381         | 395          | rBV      | 346448         | 559121        | 14.83%          | 3.148%        |
| 5         | 2.636       | 396           | 403         | 419          | rVB2     | 5240           | 10858         | 0.29%           | 0.061%        |
| 6         | 2.797       | 442           | 453         | 456          | rBV3     | 767            | 1255          | 0.03%           | 0.007%        |
| 7         | 2.861       | 470           | 473         | 476          | rVB4     | 396            | 305           | 0.01%           | 0.002%        |
| 8         | 2.961       | 500           | 504         | 506          | rVB2     | 478            | 278           | 0.01%           | 0.002%        |
| 9         | 3.044       | 521           | 530         | 541          | rVB5     | 2229           | 5002          | 0.13%           | 0.028%        |
| 10        | 3.183       | 555           | 573         | 586          | rBV2     | 28886          | 64872         | 1.72%           | 0.365%        |
| 11        | 3.359       | 625           | 628         | 632          | rBV4     | 397            | 284           | 0.01%           | 0.002%        |
| 12        | 3.379       | 632           | 634         | 640          | rVB2     | 264            | 258           | 0.01%           | 0.001%        |
| 13        | 3.552       | 684           | 688         | 693          | rBV3     | 440            | 419           | 0.01%           | 0.002%        |
| 14        | 3.829       | 771           | 774         | 778          | rBV3     | 255            | 289           | 0.01%           | 0.002%        |
| 15        | 3.925       | 801           | 804         | 811          | rVV3     | 391            | 485           | 0.01%           | 0.003%        |
| 16        | 4.144       | 867           | 872         | 880          | rBV2     | 484            | 524           | 0.01%           | 0.003%        |
| 17        | 4.202       | 886           | 890         | 892          | rBV      | 287            | 274           | 0.01%           | 0.002%        |
| 18        | 4.501       | 977           | 983         | 986          | rVB2     | 284            | 260           | 0.01%           | 0.001%        |
| 19        | 4.568       | 999           | 1004        | 1005         | rBV2     | 583            | 391           | 0.01%           | 0.002%        |
| 20        | 4.620       | 1005          | 1020        | 1059         | rBV      | 155234         | 420290        | 11.15%          | 2.367%        |
| 21        | 4.877       | 1097          | 1100        | 1104         | rVB3     | 354            | 295           | 0.01%           | 0.002%        |
| 22        | 4.919       | 1111          | 1113        | 1118         | rVB3     | 553            | 423           | 0.01%           | 0.002%        |
| 23        | 5.057       | 1140          | 1156        | 1179         | rVV      | 287085         | 628069        | 16.66%          | 3.537%        |
| 24        | 5.276       | 1221          | 1224        | 1226         | rBV2     | 466            | 294           | 0.01%           | 0.002%        |
| 25        | 5.346       | 1242          | 1246        | 1250         | rBV2     | 382            | 394           | 0.01%           | 0.002%        |
| 26        | 5.372       | 1250          | 1254        | 1255         | rBV4     | 573            | 444           | 0.01%           | 0.003%        |
| 27        | 5.398       | 1260          | 1262        | 1270         | rVB3     | 309            | 359           | 0.01%           | 0.002%        |
| 28        | 5.559       | 1309          | 1312        | 1318         | rVB3     | 287            | 257           | 0.01%           | 0.001%        |
| 29        | 5.719       | 1339          | 1362        | 1397         | rBV2     | 607764         | 1680771       | 44.57%          | 9.464%        |
| 30        | 5.986       | 1439          | 1445        | 1449         | rVB3     | 342            | 358           | 0.01%           | 0.002%        |
| 31        | 6.031       | 1455          | 1459        | 1461         | rBV3     | 413            | 295           | 0.01%           | 0.002%        |
| 32        | 6.105       | 1474          | 1482        | 1485         | rBV3     | 387            | 460           | 0.01%           | 0.003%        |
| 33        | 6.166       | 1496          | 1501        | 1504         | rBV3     | 343            | 320           | 0.01%           | 0.002%        |
| 34        | 6.243       | 1511          | 1525        | 1552         | rBV      | 444534         | 840483        | 22.29%          | 4.733%        |
| 35        | 6.411       | 1575          | 1577        | 1582         | rVB3     | 365            | 289           | 0.01%           | 0.002%        |
| 36        | 6.481       | 1594          | 1599        | 1603         | rBV3     | 412            | 414           | 0.01%           | 0.002%        |

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Integrator: RTE

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Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM010623WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 6.504  | 1603 | 1606 | 1608 | rBV  | 405    | 296     | 0.01%  | 0.002% |
| 38 | 6.526  | 1608 | 1613 | 1618 | rVB6 | 1063   | 1404    | 0.04%  | 0.008% |
| 39 | 6.575  | 1622 | 1628 | 1630 | rBV3 | 312    | 311     | 0.01%  | 0.002% |
| 40 | 6.594  | 1630 | 1634 | 1638 | rVB4 | 550    | 550     | 0.01%  | 0.003% |
| 41 | 6.684  | 1646 | 1662 | 1683 | rBV  | 393664 | 771395  | 20.46% | 4.344% |
| 42 | 6.803  | 1695 | 1699 | 1712 | rVB4 | 1062   | 1775    | 0.05%  | 0.010% |
| 43 | 6.957  | 1742 | 1747 | 1749 | rBV2 | 338    | 348     | 0.01%  | 0.002% |
| 44 | 7.006  | 1758 | 1762 | 1765 | rBV3 | 342    | 298     | 0.01%  | 0.002% |
| 45 | 7.076  | 1779 | 1784 | 1787 | rBV2 | 322    | 317     | 0.01%  | 0.002% |
| 46 | 7.189  | 1809 | 1819 | 1830 | rBV8 | 1475   | 3052    | 0.08%  | 0.017% |
| 47 | 7.266  | 1839 | 1843 | 1848 | rVB2 | 433    | 418     | 0.01%  | 0.002% |
| 48 | 7.343  | 1861 | 1867 | 1870 | rBV3 | 400    | 321     | 0.01%  | 0.002% |
| 49 | 7.510  | 1911 | 1919 | 1922 | rBV3 | 270    | 344     | 0.01%  | 0.002% |
| 50 | 7.562  | 1922 | 1935 | 1955 | rBV  | 197454 | 347921  | 9.23%  | 1.959% |
| 51 | 7.687  | 1968 | 1974 | 1980 | rVB4 | 1152   | 1518    | 0.04%  | 0.009% |
| 52 | 7.893  | 2024 | 2038 | 2060 | rBV  | 699607 | 1189057 | 31.53% | 6.696% |
| 53 | 8.092  | 2098 | 2100 | 2104 | rBV3 | 406    | 359     | 0.01%  | 0.002% |
| 54 | 8.118  | 2106 | 2108 | 2113 | rVB3 | 658    | 415     | 0.01%  | 0.002% |
| 55 | 8.176  | 2113 | 2126 | 2140 | rBV  | 141349 | 238845  | 6.33%  | 1.345% |
| 56 | 8.440  | 2204 | 2208 | 2212 | rBV3 | 463    | 526     | 0.01%  | 0.003% |
| 57 | 8.468  | 2212 | 2217 | 2221 | rVV2 | 859    | 971     | 0.03%  | 0.005% |
| 58 | 8.632  | 2255 | 2268 | 2300 | rBV2 | 427657 | 834564  | 22.13% | 4.699% |
| 59 | 8.848  | 2333 | 2335 | 2341 | rVB4 | 470    | 399     | 0.01%  | 0.002% |
| 60 | 8.970  | 2370 | 2373 | 2377 | rBV4 | 327    | 318     | 0.01%  | 0.002% |
| 61 | 9.044  | 2393 | 2396 | 2399 | rVB3 | 430    | 331     | 0.01%  | 0.002% |
| 62 | 9.063  | 2399 | 2402 | 2406 | rBV2 | 453    | 358     | 0.01%  | 0.002% |
| 63 | 9.333  | 2476 | 2486 | 2490 | rVB2 | 507    | 719     | 0.02%  | 0.004% |
| 64 | 9.414  | 2490 | 2511 | 2539 | rBV2 | 629396 | 1449672 | 38.44% | 8.163% |
| 65 | 9.562  | 2553 | 2557 | 2563 | rVB4 | 690    | 741     | 0.02%  | 0.004% |
| 66 | 9.597  | 2563 | 2568 | 2571 | rBV  | 459    | 374     | 0.01%  | 0.002% |
| 67 | 9.649  | 2580 | 2584 | 2586 | rBV3 | 375    | 293     | 0.01%  | 0.002% |
| 68 | 9.748  | 2611 | 2615 | 2620 | rVB3 | 471    | 477     | 0.01%  | 0.003% |
| 69 | 9.925  | 2668 | 2670 | 2675 | rVB2 | 429    | 337     | 0.01%  | 0.002% |
| 70 | 9.960  | 2675 | 2681 | 2684 | rBV  | 425    | 496     | 0.01%  | 0.003% |
| 71 | 10.108 | 2720 | 2727 | 2732 | rBV2 | 435    | 631     | 0.02%  | 0.004% |
| 72 | 10.218 | 2758 | 2761 | 2766 | rVV2 | 364    | 395     | 0.01%  | 0.002% |
| 73 | 10.292 | 2779 | 2784 | 2785 | rBV2 | 478    | 325     | 0.01%  | 0.002% |
| 74 | 10.394 | 2813 | 2816 | 2821 | rBV2 | 326    | 354     | 0.01%  | 0.002% |
| 75 | 10.449 | 2827 | 2833 | 2840 | rBV3 | 522    | 706     | 0.02%  | 0.004% |
| 76 | 10.497 | 2846 | 2848 | 2852 | rVB2 | 528    | 295     | 0.01%  | 0.002% |

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Integration Parameters: LSCINT.P

Integrator: RTE

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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\SFAMULM010623WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |         |         |         |         |
|-----|--------|------|------|------|------|---------|---------|---------|---------|
| 77  | 10.594 | 2874 | 2878 | 2880 | rBV2 | 316     | 275     | 0.01%   | 0.002%  |
| 78  | 10.697 | 2903 | 2910 | 2914 | rBV2 | 354     | 582     | 0.02%   | 0.003%  |
| 79  | 10.751 | 2914 | 2927 | 2944 | rBV  | 495511  | 799641  | 21.21%  | 4.503%  |
| 80  | 10.890 | 2965 | 2970 | 2977 | rVB2 | 1449    | 1621    | 0.04%   | 0.009%  |
| 81  | 11.083 | 3027 | 3030 | 3033 | rBV2 | 391     | 282     | 0.01%   | 0.002%  |
| 82  | 11.189 | 3059 | 3063 | 3066 | rBV2 | 429     | 427     | 0.01%   | 0.002%  |
| 83  | 11.256 | 3081 | 3084 | 3090 | rBV2 | 479     | 444     | 0.01%   | 0.003%  |
| 84  | 11.304 | 3094 | 3099 | 3102 | rVB  | 361     | 422     | 0.01%   | 0.002%  |
| 85  | 11.456 | 3141 | 3146 | 3147 | rBV2 | 317     | 266     | 0.01%   | 0.001%  |
| 86  | 11.468 | 3147 | 3150 | 3156 | rVB2 | 458     | 427     | 0.01%   | 0.002%  |
| 87  | 11.684 | 3210 | 3217 | 3218 | rBV2 | 439     | 431     | 0.01%   | 0.002%  |
| 88  | 11.742 | 3223 | 3235 | 3244 | rBV  | 139814  | 221076  | 5.86%   | 1.245%  |
| 89  | 11.806 | 3244 | 3255 | 3283 | rVB2 | 651555  | 1236593 | 32.79%  | 6.963%  |
| 90  | 12.060 | 3318 | 3334 | 3354 | rVB5 | 8608    | 18582   | 0.49%   | 0.105%  |
| 91  | 12.205 | 3360 | 3379 | 3403 | rBV2 | 1871509 | 3770980 | 100.00% | 21.235% |
| 92  | 12.362 | 3424 | 3428 | 3432 | rVB3 | 583     | 480     | 0.01%   | 0.003%  |
| 93  | 13.201 | 3679 | 3689 | 3709 | rBV  | 30813   | 54830   | 1.45%   | 0.309%  |
| 94  | 13.327 | 3719 | 3728 | 3735 | rVB7 | 2263    | 3390    | 0.09%   | 0.019%  |
| 95  | 13.835 | 3873 | 3886 | 3903 | rBV  | 784493  | 1230376 | 32.63%  | 6.928%  |
| 96  | 14.324 | 4026 | 4038 | 4054 | rBV  | 435428  | 710191  | 18.83%  | 3.999%  |
| 97  | 14.725 | 4155 | 4163 | 4178 | rVB2 | 10250   | 17027   | 0.45%   | 0.096%  |
| 98  | 14.812 | 4187 | 4190 | 4194 | rBV3 | 871     | 878     | 0.02%   | 0.005%  |
| 99  | 15.407 | 4371 | 4375 | 4388 | rVB5 | 9618    | 13495   | 0.36%   | 0.076%  |
| 100 | 15.992 | 4548 | 4557 | 4570 | rBV  | 47977   | 74356   | 1.97%   | 0.419%  |

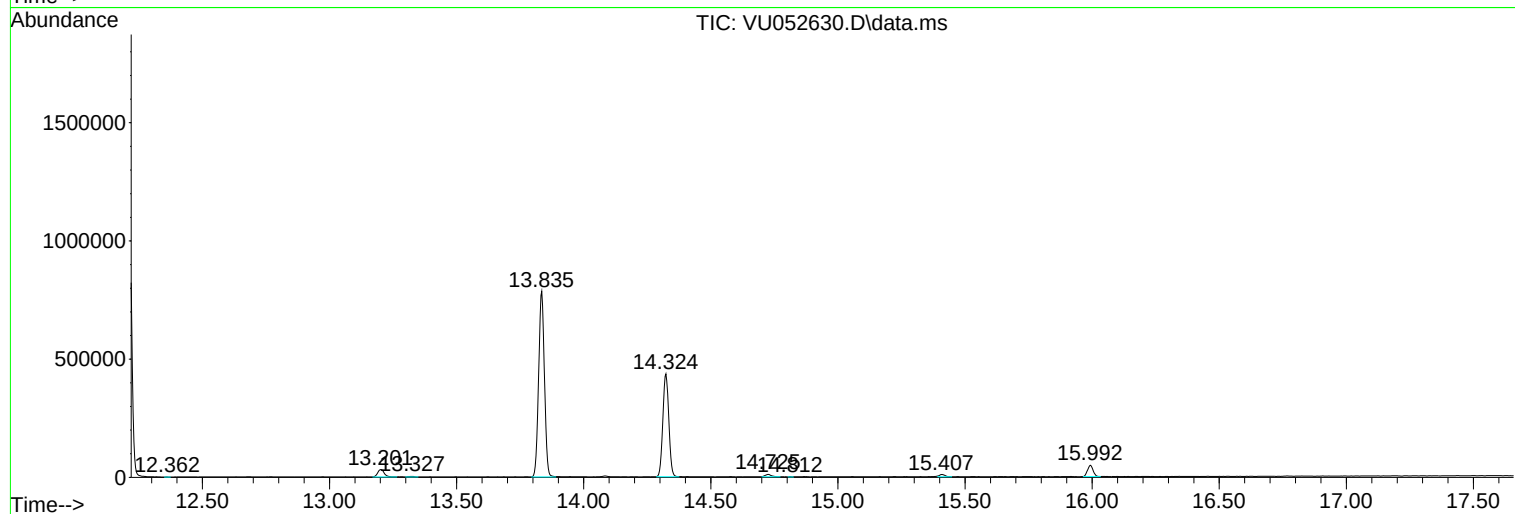
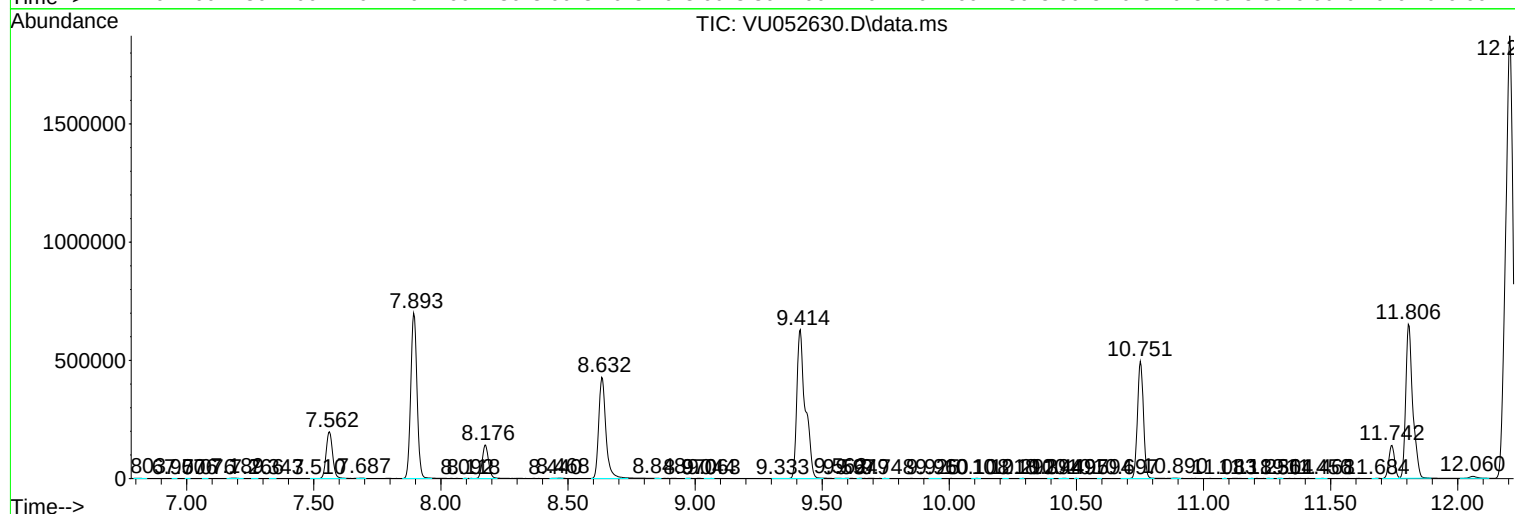
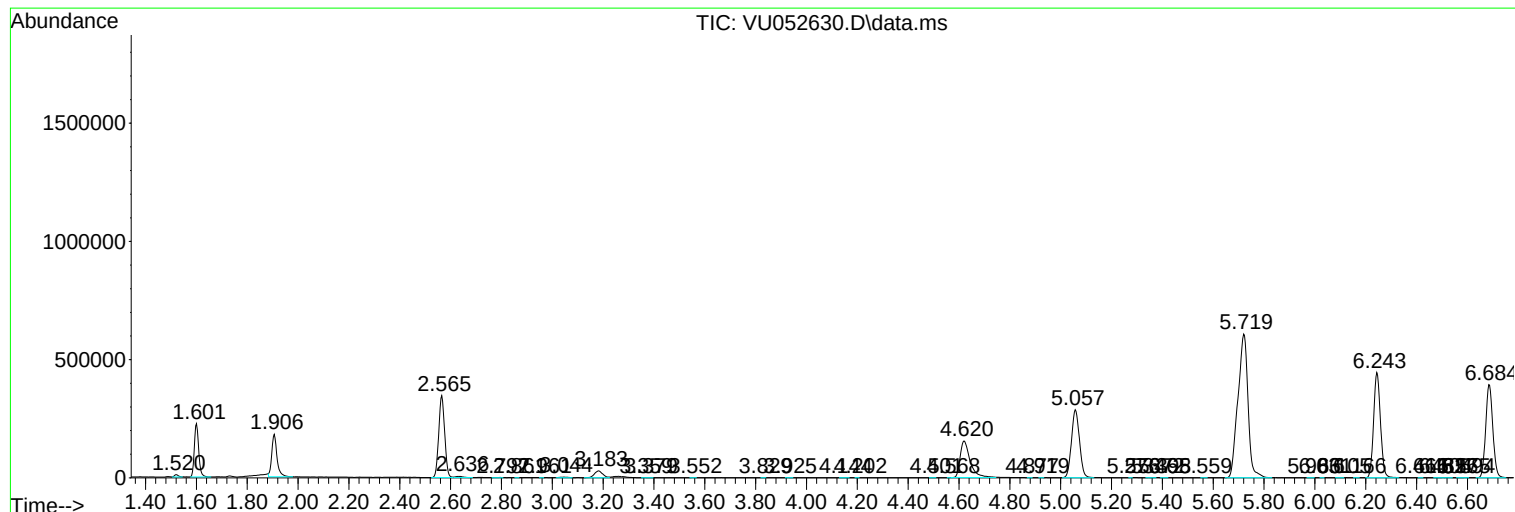
Sum of corrected areas: 17758736

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM010623WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU010623\  
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No Library Search Compounds Detected

\*\*\*\*\*

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