

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050823\  
 Data File : VU054104.D  
 Acq On : 09 May 2023 01:02  
 Operator : JC/MD  
 Sample : 02663-14  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 34 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 JREK3

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\SFAMULM042923WMA.M

Title : VOC Analysis

Signal : TIC: VU054104.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          | 100          | rVB      | 76921          | 92634         | 11.78%          | 1.501%        |
| 2         | 1.903       | 167           | 175         | 193          | rVB      | 65188          | 91920         | 11.69%          | 1.489%        |
| 3         | 2.562       | 368           | 380         | 393          | rBV      | 151591         | 243623        | 30.98%          | 3.948%        |
| 4         | 2.781       | 433           | 448         | 449          | rBV3     | 3826           | 6729          | 0.86%           | 0.109%        |
| 5         | 3.041       | 523           | 529         | 537          | rVB5     | 1154           | 1648          | 0.21%           | 0.027%        |
| 6         | 3.179       | 560           | 572         | 588          | rBV2     | 7497           | 19746         | 2.51%           | 0.320%        |
| 7         | 3.359       | 625           | 628         | 630          | rBV2     | 165            | 120           | 0.02%           | 0.002%        |
| 8         | 3.565       | 689           | 692         | 701          | rVB2     | 315            | 414           | 0.05%           | 0.007%        |
| 9         | 3.700       | 732           | 734         | 737          | rBV      | 119            | 99            | 0.01%           | 0.002%        |
| 10        | 3.736       | 742           | 745         | 746          | rBV2     | 208            | 107           | 0.01%           | 0.002%        |
| 11        | 3.816       | 768           | 770         | 772          | rBV2     | 298            | 144           | 0.02%           | 0.002%        |
| 12        | 3.903       | 795           | 797         | 799          | rBV2     | 179            | 95            | 0.01%           | 0.002%        |
| 13        | 4.070       | 847           | 849         | 851          | rBV      | 122            | 28            | 0.00%           | 0.000%        |
| 14        | 4.086       | 851           | 854         | 856          | rBV2     | 177            | 112           | 0.01%           | 0.002%        |
| 15        | 4.276       | 911           | 913         | 916          | rBV2     | 137            | 91            | 0.01%           | 0.001%        |
| 16        | 4.617       | 1007          | 1019        | 1041         | rBV      | 64438          | 161641        | 20.56%          | 2.619%        |
| 17        | 4.822       | 1080          | 1083        | 1084         | rBV2     | 288            | 129           | 0.02%           | 0.002%        |
| 18        | 4.912       | 1109          | 1111        | 1112         | rBV      | 205            | 94            | 0.01%           | 0.002%        |
| 19        | 4.977       | 1125          | 1131        | 1132         | rBV      | 307            | 266           | 0.03%           | 0.004%        |
| 20        | 5.057       | 1140          | 1156        | 1179         | rBV      | 144259         | 322782        | 41.05%          | 5.230%        |
| 21        | 5.253       | 1213          | 1217        | 1219         | rBV      | 208            | 176           | 0.02%           | 0.003%        |
| 22        | 5.292       | 1225          | 1229        | 1230         | rBV      | 324            | 201           | 0.03%           | 0.003%        |
| 23        | 5.414       | 1264          | 1267        | 1269         | rBV      | 176            | 140           | 0.02%           | 0.002%        |
| 24        | 5.440       | 1272          | 1275        | 1277         | rBV      | 201            | 130           | 0.02%           | 0.002%        |
| 25        | 5.498       | 1292          | 1293        | 1295         | rBV      | 96             | 51            | 0.01%           | 0.001%        |
| 26        | 5.520       | 1299          | 1300        | 1301         | rVB      | 97             | 19            | 0.00%           | 0.000%        |
| 27        | 5.533       | 1302          | 1304        | 1306         | rBV2     | 123            | 67            | 0.01%           | 0.001%        |
| 28        | 5.594       | 1321          | 1323        | 1325         | rBV      | 170            | 91            | 0.01%           | 0.001%        |
| 29        | 5.610       | 1325          | 1328        | 1331         | rVV      | 248            | 203           | 0.03%           | 0.003%        |
| 30        | 5.719       | 1340          | 1362        | 1384         | rBV2     | 285141         | 786308        | 100.00%         | 12.741%       |
| 31        | 5.967       | 1437          | 1439        | 1442         | rBV      | 139            | 110           | 0.01%           | 0.002%        |
| 32        | 6.006       | 1448          | 1451        | 1458         | rVB2     | 267            | 274           | 0.03%           | 0.004%        |
| 33        | 6.047       | 1458          | 1464        | 1468         | rBV2     | 213            | 344           | 0.04%           | 0.006%        |
| 34        | 6.067       | 1468          | 1470        | 1472         | rVV2     | 143            | 47            | 0.01%           | 0.001%        |
| 35        | 6.243       | 1510          | 1525        | 1548         | rBV      | 272908         | 521434        | 66.31%          | 8.449%        |
| 36        | 6.469       | 1593          | 1595        | 1598         | rBV2     | 292            | 220           | 0.03%           | 0.004%        |

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Integrator: RTE

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Filtering: 5

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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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.488  | 1598 | 1601 | 1603 | rVV  | 257    | 176    | 0.02%  | 0.003%  |
| 38 | 6.520  | 1605 | 1611 | 1621 | rVV6 | 1895   | 3370   | 0.43%  | 0.055%  |
| 39 | 6.684  | 1647 | 1662 | 1681 | rBV  | 185299 | 363407 | 46.22% | 5.889%  |
| 40 | 6.858  | 1711 | 1716 | 1719 | rBV2 | 208    | 273    | 0.03%  | 0.004%  |
| 41 | 7.009  | 1759 | 1763 | 1766 | rBV  | 160    | 164    | 0.02%  | 0.003%  |
| 42 | 7.050  | 1775 | 1776 | 1777 | rBV  | 81     | 17     | 0.00%  | 0.000%  |
| 43 | 7.073  | 1778 | 1783 | 1786 | rBV2 | 187    | 197    | 0.03%  | 0.003%  |
| 44 | 7.163  | 1809 | 1811 | 1812 | rBV2 | 256    | 109    | 0.01%  | 0.002%  |
| 45 | 7.182  | 1812 | 1817 | 1820 | rBV4 | 863    | 948    | 0.12%  | 0.015%  |
| 46 | 7.269  | 1841 | 1844 | 1848 | rVB2 | 251    | 218    | 0.03%  | 0.004%  |
| 47 | 7.298  | 1848 | 1853 | 1859 | rBV2 | 325    | 459    | 0.06%  | 0.007%  |
| 48 | 7.359  | 1869 | 1872 | 1874 | rBV2 | 246    | 205    | 0.03%  | 0.003%  |
| 49 | 7.468  | 1902 | 1906 | 1909 | rBV  | 315    | 294    | 0.04%  | 0.005%  |
| 50 | 7.559  | 1923 | 1934 | 1956 | rBV  | 97071  | 170980 | 21.74% | 2.771%  |
| 51 | 7.787  | 2002 | 2005 | 2013 | rBV3 | 791    | 1010   | 0.13%  | 0.016%  |
| 52 | 7.893  | 2025 | 2038 | 2057 | rBV  | 354194 | 621220 | 79.00% | 10.066% |
| 53 | 8.173  | 2114 | 2125 | 2145 | rBV  | 70677  | 118838 | 15.11% | 1.926%  |
| 54 | 8.343  | 2172 | 2178 | 2182 | rBV  | 328    | 368    | 0.05%  | 0.006%  |
| 55 | 8.462  | 2207 | 2215 | 2219 | rBV3 | 540    | 859    | 0.11%  | 0.014%  |
| 56 | 8.517  | 2227 | 2232 | 2235 | rBV  | 281    | 295    | 0.04%  | 0.005%  |
| 57 | 8.546  | 2239 | 2241 | 2244 | rVV2 | 466    | 209    | 0.03%  | 0.003%  |
| 58 | 8.629  | 2255 | 2267 | 2299 | rBV2 | 183355 | 355571 | 45.22% | 5.762%  |
| 59 | 9.086  | 2406 | 2409 | 2411 | rBV  | 253    | 139    | 0.02%  | 0.002%  |
| 60 | 9.131  | 2420 | 2423 | 2425 | rBV2 | 159    | 110    | 0.01%  | 0.002%  |
| 61 | 9.189  | 2438 | 2441 | 2444 | rBV2 | 234    | 205    | 0.03%  | 0.003%  |
| 62 | 9.314  | 2474 | 2480 | 2485 | rBV2 | 225    | 313    | 0.04%  | 0.005%  |
| 63 | 9.349  | 2488 | 2491 | 2494 | rBV  | 206    | 191    | 0.02%  | 0.003%  |
| 64 | 9.411  | 2498 | 2510 | 2536 | rBV  | 373026 | 623079 | 79.24% | 10.096% |
| 65 | 9.565  | 2555 | 2558 | 2561 | rBV2 | 620    | 557    | 0.07%  | 0.009%  |
| 66 | 9.613  | 2570 | 2573 | 2577 | rBV  | 233    | 138    | 0.02%  | 0.002%  |
| 67 | 9.777  | 2623 | 2624 | 2625 | rBV  | 232    | 75     | 0.01%  | 0.001%  |
| 68 | 9.803  | 2629 | 2632 | 2635 | rVV  | 220    | 163    | 0.02%  | 0.003%  |
| 69 | 9.925  | 2668 | 2670 | 2673 | rBV2 | 359    | 187    | 0.02%  | 0.003%  |
| 70 | 10.018 | 2697 | 2699 | 2700 | rBV  | 154    | 65     | 0.01%  | 0.001%  |
| 71 | 10.083 | 2717 | 2719 | 2721 | rBV  | 205    | 85     | 0.01%  | 0.001%  |
| 72 | 10.105 | 2721 | 2726 | 2728 | rBV4 | 600    | 591    | 0.08%  | 0.010%  |
| 73 | 10.173 | 2744 | 2747 | 2749 | rBV  | 219    | 100    | 0.01%  | 0.002%  |
| 74 | 10.189 | 2749 | 2752 | 2754 | rBV2 | 189    | 155    | 0.02%  | 0.003%  |
| 75 | 10.259 | 2771 | 2774 | 2775 | rBV  | 131    | 77     | 0.01%  | 0.001%  |
| 76 | 10.517 | 2851 | 2854 | 2857 | rBV2 | 233    | 180    | 0.02%  | 0.003%  |

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Min Area: 0 % of largest Peak

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Max Peaks: 100

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 77 | 10.597 | 2876 | 2879 | 2884 | rVB2 | 229    | 205    | 0.03%  | 0.003%  |
| 78 | 10.687 | 2904 | 2907 | 2910 | rBV2 | 231    | 210    | 0.03%  | 0.003%  |
| 79 | 10.751 | 2915 | 2927 | 2945 | rVV  | 252253 | 416057 | 52.91% | 6.742%  |
| 80 | 10.919 | 2976 | 2979 | 2981 | rBV  | 280    | 217    | 0.03%  | 0.004%  |
| 81 | 11.015 | 3004 | 3009 | 3013 | rVB2 | 329    | 353    | 0.04%  | 0.006%  |
| 82 | 11.037 | 3013 | 3016 | 3020 | rBV2 | 317    | 253    | 0.03%  | 0.004%  |
| 83 | 11.060 | 3020 | 3023 | 3026 | rBV  | 317    | 238    | 0.03%  | 0.004%  |
| 84 | 11.201 | 3065 | 3067 | 3070 | rVB2 | 287    | 159    | 0.02%  | 0.003%  |
| 85 | 11.263 | 3082 | 3086 | 3089 | rBV  | 413    | 296    | 0.04%  | 0.005%  |
| 86 | 11.324 | 3102 | 3105 | 3107 | rBV  | 291    | 185    | 0.02%  | 0.003%  |
| 87 | 11.745 | 3231 | 3236 | 3238 | rBV2 | 546    | 448    | 0.06%  | 0.007%  |
| 88 | 11.806 | 3243 | 3255 | 3280 | rVV  | 392483 | 624944 | 79.48% | 10.126% |
| 89 | 12.189 | 3361 | 3374 | 3398 | rBV  | 374949 | 609011 | 77.45% | 9.868%  |
| 90 | 12.767 | 3548 | 3554 | 3558 | rVB  | 409    | 463    | 0.06%  | 0.008%  |
| 91 | 12.790 | 3558 | 3561 | 3562 | rBV2 | 296    | 160    | 0.02%  | 0.003%  |
| 92 | 13.475 | 3771 | 3774 | 3777 | rBV2 | 494    | 349    | 0.04%  | 0.006%  |

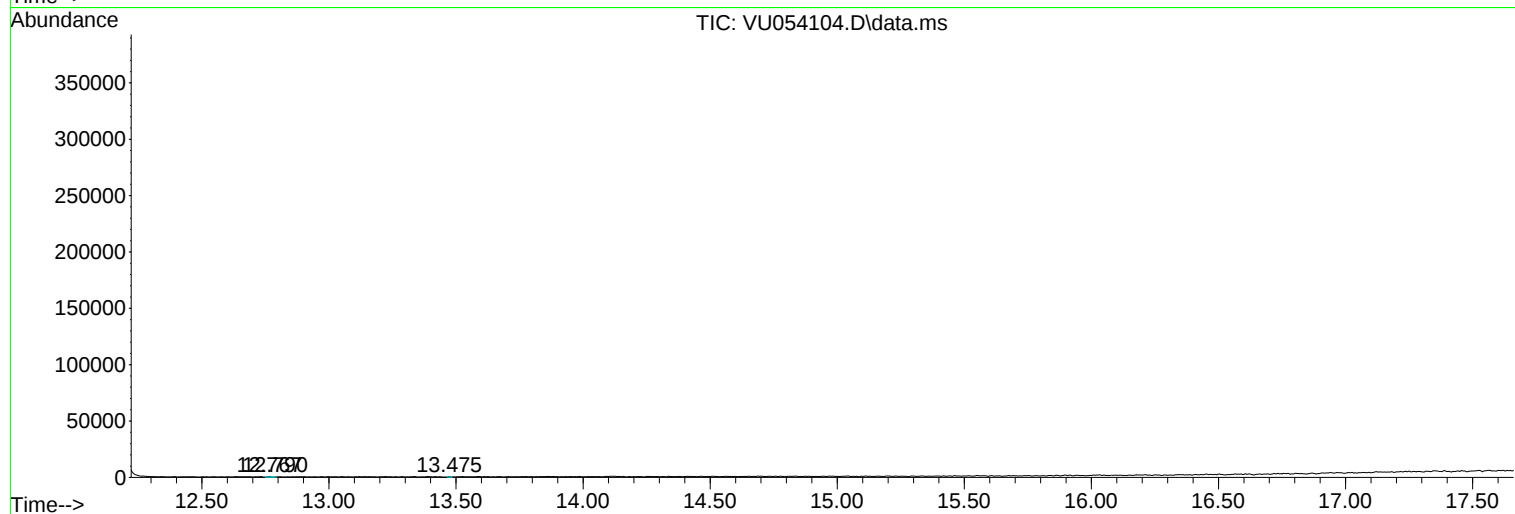
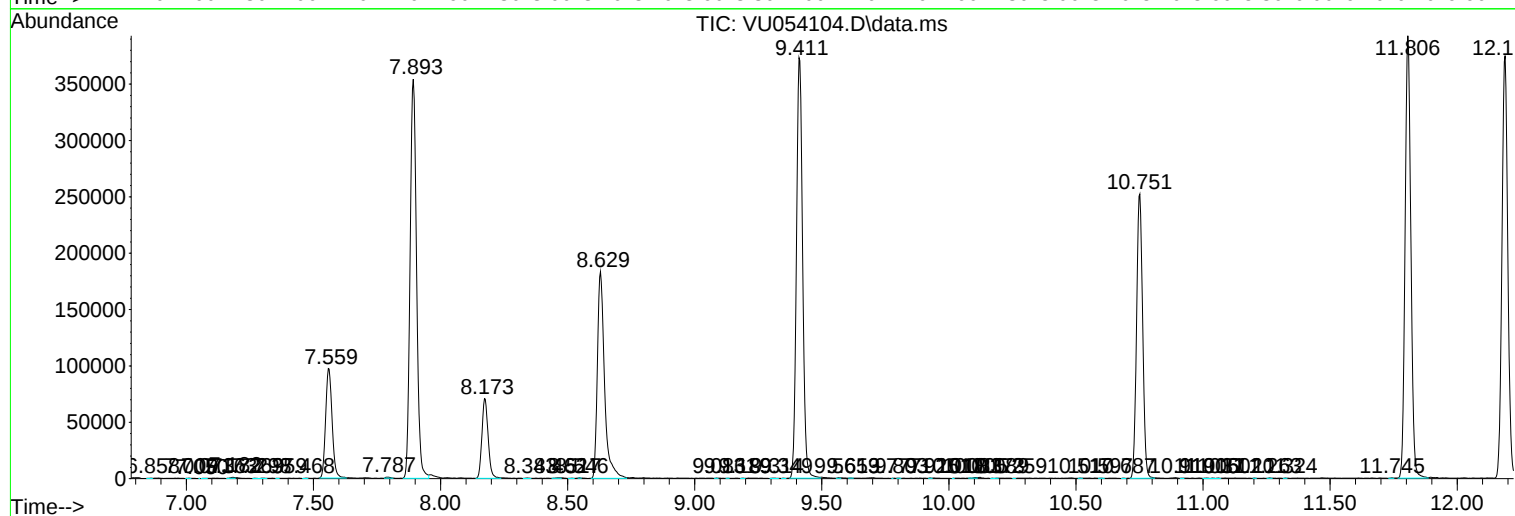
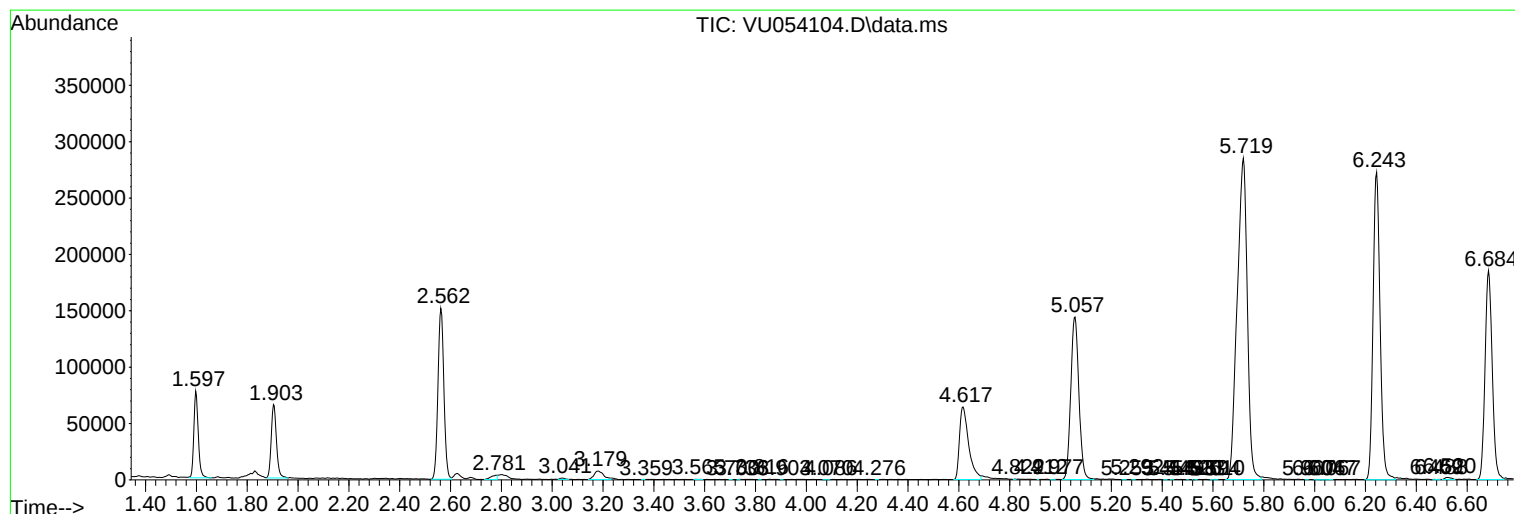
Sum of corrected areas: 6171382

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050823\  
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No Library Search Compounds Detected

\*\*\*\*\*

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