

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU040323\  
 Data File : VU053511.D  
 Acq On : 03 Apr 2023 11:43  
 Operator : JC/MD  
 Sample : VU0403MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK063

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\SFAMULM033123WMA.M  
 Title : VOC Analysis

Signal : TIC: VU053511.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          | 91           | rBV      | 145751         | 161301        | 16.79%          | 2.097%        |
| 2         | 1.909       | 170           | 177         | 195          | rVB      | 111010         | 151662        | 15.78%          | 1.972%        |
| 3         | 2.565       | 369           | 381         | 396          | rBV      | 217509         | 349749        | 36.40%          | 4.548%        |
| 4         | 2.787       | 444           | 450         | 459          | rBV3     | 1629           | 2322          | 0.24%           | 0.030%        |
| 5         | 2.861       | 470           | 473         | 475          | rBV      | 307            | 150           | 0.02%           | 0.002%        |
| 6         | 3.118       | 551           | 553         | 555          | rBV      | 246            | 94            | 0.01%           | 0.001%        |
| 7         | 3.446       | 653           | 655         | 661          | rBV2     | 208            | 164           | 0.02%           | 0.002%        |
| 8         | 3.710       | 735           | 737         | 740          | rVB2     | 356            | 184           | 0.02%           | 0.002%        |
| 9         | 3.729       | 740           | 743         | 746          | rBV2     | 208            | 130           | 0.01%           | 0.002%        |
| 10        | 3.890       | 790           | 793         | 795          | rBV      | 202            | 100           | 0.01%           | 0.001%        |
| 11        | 4.083       | 852           | 853         | 854          | rBV      | 186            | 50            | 0.01%           | 0.001%        |
| 12        | 4.108       | 858           | 861         | 864          | rBV      | 229            | 168           | 0.02%           | 0.002%        |
| 13        | 4.176       | 880           | 882         | 884          | rBV      | 153            | 82            | 0.01%           | 0.001%        |
| 14        | 4.208       | 890           | 892         | 893          | rBV      | 156            | 66            | 0.01%           | 0.001%        |
| 15        | 4.327       | 921           | 929         | 930          | rBV      | 231            | 334           | 0.03%           | 0.004%        |
| 16        | 4.378       | 942           | 945         | 949          | rBB      | 289            | 148           | 0.02%           | 0.002%        |
| 17        | 4.533       | 991           | 993         | 996          | rVB      | 221            | 99            | 0.01%           | 0.001%        |
| 18        | 4.549       | 996           | 998         | 1004         | rVB2     | 180            | 127           | 0.01%           | 0.002%        |
| 19        | 4.610       | 1006          | 1017        | 1049         | rBV      | 74078          | 183063        | 19.05%          | 2.380%        |
| 20        | 4.887       | 1099          | 1103        | 1104         | rBV      | 408            | 299           | 0.03%           | 0.004%        |
| 21        | 4.922       | 1112          | 1114        | 1116         | rBV      | 200            | 120           | 0.01%           | 0.002%        |
| 22        | 4.980       | 1129          | 1132        | 1136         | rVB2     | 359            | 252           | 0.03%           | 0.003%        |
| 23        | 5.057       | 1139          | 1156        | 1180         | rBV      | 182779         | 396514        | 41.27%          | 5.156%        |
| 24        | 5.359       | 1248          | 1250        | 1254         | rBV      | 183            | 152           | 0.02%           | 0.002%        |
| 25        | 5.398       | 1260          | 1262        | 1264         | rVB      | 300            | 114           | 0.01%           | 0.001%        |
| 26        | 5.433       | 1271          | 1273        | 1276         | rVB      | 178            | 82            | 0.01%           | 0.001%        |
| 27        | 5.562       | 1308          | 1313        | 1315         | rBV2     | 190            | 180           | 0.02%           | 0.002%        |
| 28        | 5.600       | 1322          | 1325        | 1327         | rBV      | 204            | 164           | 0.02%           | 0.002%        |
| 29        | 5.719       | 1341          | 1362        | 1394         | rBV3     | 350255         | 960889        | 100.00%         | 12.494%       |
| 30        | 5.957       | 1434          | 1436        | 1439         | rBV      | 365            | 231           | 0.02%           | 0.003%        |
| 31        | 6.015       | 1451          | 1454        | 1458         | rBV      | 331            | 204           | 0.02%           | 0.003%        |
| 32        | 6.050       | 1460          | 1465        | 1468         | rVB3     | 642            | 450           | 0.05%           | 0.006%        |
| 33        | 6.163       | 1498          | 1500        | 1502         | rBV      | 169            | 57            | 0.01%           | 0.001%        |
| 34        | 6.189       | 1505          | 1508        | 1509         | rBV      | 171            | 83            | 0.01%           | 0.001%        |
| 35        | 6.243       | 1511          | 1525        | 1546         | rBV      | 314787         | 601047        | 62.55%          | 7.815%        |
| 36        | 6.526       | 1602          | 1613        | 1627         | rVB7     | 5876           | 11513         | 1.20%           | 0.150%        |

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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\SFAMULM033123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.581  | 1627 | 1630 | 1632 | rBV2 | 257    | 157    | 0.02%  | 0.002%  |
| 38 | 6.684  | 1647 | 1662 | 1694 | rBV  | 217670 | 430310 | 44.78% | 5.595%  |
| 39 | 6.880  | 1721 | 1723 | 1724 | rBV  | 149    | 60     | 0.01%  | 0.001%  |
| 40 | 6.890  | 1724 | 1726 | 1730 | rVV  | 151    | 116    | 0.01%  | 0.002%  |
| 41 | 6.941  | 1741 | 1742 | 1745 | rVB  | 147    | 57     | 0.01%  | 0.001%  |
| 42 | 7.124  | 1797 | 1799 | 1800 | rBV  | 250    | 100    | 0.01%  | 0.001%  |
| 43 | 7.150  | 1805 | 1807 | 1809 | rBB  | 141    | 74     | 0.01%  | 0.001%  |
| 44 | 7.176  | 1811 | 1815 | 1816 | rBV  | 352    | 238    | 0.02%  | 0.003%  |
| 45 | 7.224  | 1827 | 1830 | 1833 | rVB2 | 233    | 163    | 0.02%  | 0.002%  |
| 46 | 7.266  | 1841 | 1843 | 1845 | rBV  | 125    | 69     | 0.01%  | 0.001%  |
| 47 | 7.308  | 1854 | 1856 | 1861 | rVB  | 185    | 79     | 0.01%  | 0.001%  |
| 48 | 7.333  | 1861 | 1864 | 1865 | rBV  | 132    | 72     | 0.01%  | 0.001%  |
| 49 | 7.375  | 1874 | 1877 | 1880 | rBV  | 174    | 76     | 0.01%  | 0.001%  |
| 50 | 7.398  | 1880 | 1884 | 1886 | rBV  | 180    | 158    | 0.02%  | 0.002%  |
| 51 | 7.558  | 1922 | 1934 | 1957 | rBV  | 129492 | 229776 | 23.91% | 2.988%  |
| 52 | 7.687  | 1972 | 1974 | 1977 | rBV3 | 296    | 159    | 0.02%  | 0.002%  |
| 53 | 7.829  | 2015 | 2018 | 2020 | rBV  | 173    | 111    | 0.01%  | 0.001%  |
| 54 | 7.893  | 2025 | 2038 | 2056 | rBV  | 461265 | 800263 | 83.28% | 10.406% |
| 55 | 8.176  | 2114 | 2126 | 2150 | rBV  | 90336  | 154917 | 16.12% | 2.014%  |
| 56 | 8.443  | 2203 | 2209 | 2210 | rBV  | 219    | 212    | 0.02%  | 0.003%  |
| 57 | 8.549  | 2238 | 2242 | 2248 | rVB3 | 923    | 1026   | 0.11%  | 0.013%  |
| 58 | 8.626  | 2254 | 2266 | 2301 | rBV  | 230207 | 421568 | 43.87% | 5.482%  |
| 59 | 8.832  | 2326 | 2330 | 2333 | rBV2 | 236    | 177    | 0.02%  | 0.002%  |
| 60 | 8.918  | 2355 | 2357 | 2362 | rBV2 | 507    | 449    | 0.05%  | 0.006%  |
| 61 | 9.031  | 2390 | 2392 | 2394 | rBV  | 192    | 92     | 0.01%  | 0.001%  |
| 62 | 9.317  | 2479 | 2481 | 2483 | rBV  | 338    | 128    | 0.01%  | 0.002%  |
| 63 | 9.365  | 2493 | 2496 | 2498 | rBV  | 265    | 145    | 0.02%  | 0.002%  |
| 64 | 9.410  | 2498 | 2510 | 2536 | rBV  | 433653 | 717939 | 74.72% | 9.335%  |
| 65 | 9.565  | 2552 | 2558 | 2570 | rVB4 | 977    | 1726   | 0.18%  | 0.022%  |
| 66 | 9.619  | 2572 | 2575 | 2580 | rVB  | 245    | 141    | 0.01%  | 0.002%  |
| 67 | 9.693  | 2593 | 2598 | 2605 | rBV4 | 877    | 1172   | 0.12%  | 0.015%  |
| 68 | 9.758  | 2617 | 2618 | 2622 | rBV2 | 255    | 125    | 0.01%  | 0.002%  |
| 69 | 9.806  | 2631 | 2633 | 2636 | rBV  | 241    | 146    | 0.02%  | 0.002%  |
| 70 | 9.893  | 2657 | 2660 | 2661 | rBV  | 190    | 85     | 0.01%  | 0.001%  |
| 71 | 9.970  | 2682 | 2684 | 2687 | rVB  | 156    | 49     | 0.01%  | 0.001%  |
| 72 | 10.343 | 2796 | 2800 | 2802 | rBV2 | 275    | 212    | 0.02%  | 0.003%  |
| 73 | 10.488 | 2837 | 2845 | 2851 | rBV3 | 648    | 1027   | 0.11%  | 0.013%  |
| 74 | 10.635 | 2885 | 2891 | 2901 | rBV3 | 1373   | 2040   | 0.21%  | 0.027%  |
| 75 | 10.693 | 2907 | 2909 | 2914 | rVB  | 178    | 117    | 0.01%  | 0.002%  |
| 76 | 10.751 | 2914 | 2927 | 2943 | rBV  | 313391 | 497611 | 51.79% | 6.470%  |

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Instrument :  
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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\SFAMULM033123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 77 | 10.864 | 2961 | 2962 | 2966 | rBV  | 317    | 113    | 0.01%  | 0.001%  |
| 78 | 10.886 | 2967 | 2969 | 2972 | rVB  | 362    | 187    | 0.02%  | 0.002%  |
| 79 | 11.089 | 3026 | 3032 | 3033 | rBV2 | 704    | 563    | 0.06%  | 0.007%  |
| 80 | 11.259 | 3081 | 3085 | 3091 | rBV2 | 287    | 298    | 0.03%  | 0.004%  |
| 81 | 11.516 | 3163 | 3165 | 3169 | rVB  | 246    | 139    | 0.01%  | 0.002%  |
| 82 | 11.578 | 3182 | 3184 | 3187 | rBV  | 168    | 101    | 0.01%  | 0.001%  |
| 83 | 11.806 | 3243 | 3255 | 3274 | rBV  | 485978 | 779837 | 81.16% | 10.140% |
| 84 | 11.986 | 3308 | 3311 | 3313 | rBV  | 264    | 172    | 0.02%  | 0.002%  |
| 85 | 12.188 | 3361 | 3374 | 3395 | rBV  | 491105 | 791057 | 82.33% | 10.286% |
| 86 | 12.391 | 3435 | 3437 | 3439 | rBV2 | 259    | 151    | 0.02%  | 0.002%  |
| 87 | 12.886 | 3584 | 3591 | 3595 | rBV3 | 490    | 736    | 0.08%  | 0.010%  |
| 88 | 12.996 | 3621 | 3625 | 3627 | rBV2 | 475    | 360    | 0.04%  | 0.005%  |
| 89 | 13.041 | 3636 | 3639 | 3641 | rBV  | 303    | 159    | 0.02%  | 0.002%  |
| 90 | 13.176 | 3678 | 3681 | 3684 | rBV  | 351    | 219    | 0.02%  | 0.003%  |
| 91 | 13.217 | 3687 | 3694 | 3695 | rBV3 | 1903   | 1766   | 0.18%  | 0.023%  |
| 92 | 13.841 | 3880 | 3888 | 3900 | rVB6 | 4586   | 7441   | 0.77%  | 0.097%  |
| 93 | 13.983 | 3929 | 3932 | 3933 | rBV2 | 406    | 239    | 0.02%  | 0.003%  |
| 94 | 14.012 | 3939 | 3941 | 3943 | rBV2 | 276    | 99     | 0.01%  | 0.001%  |
| 95 | 14.089 | 3957 | 3965 | 3977 | rBV  | 8508   | 14089  | 1.47%  | 0.183%  |
| 96 | 14.330 | 4033 | 4040 | 4050 | rVB3 | 5222   | 7438   | 0.77%  | 0.097%  |

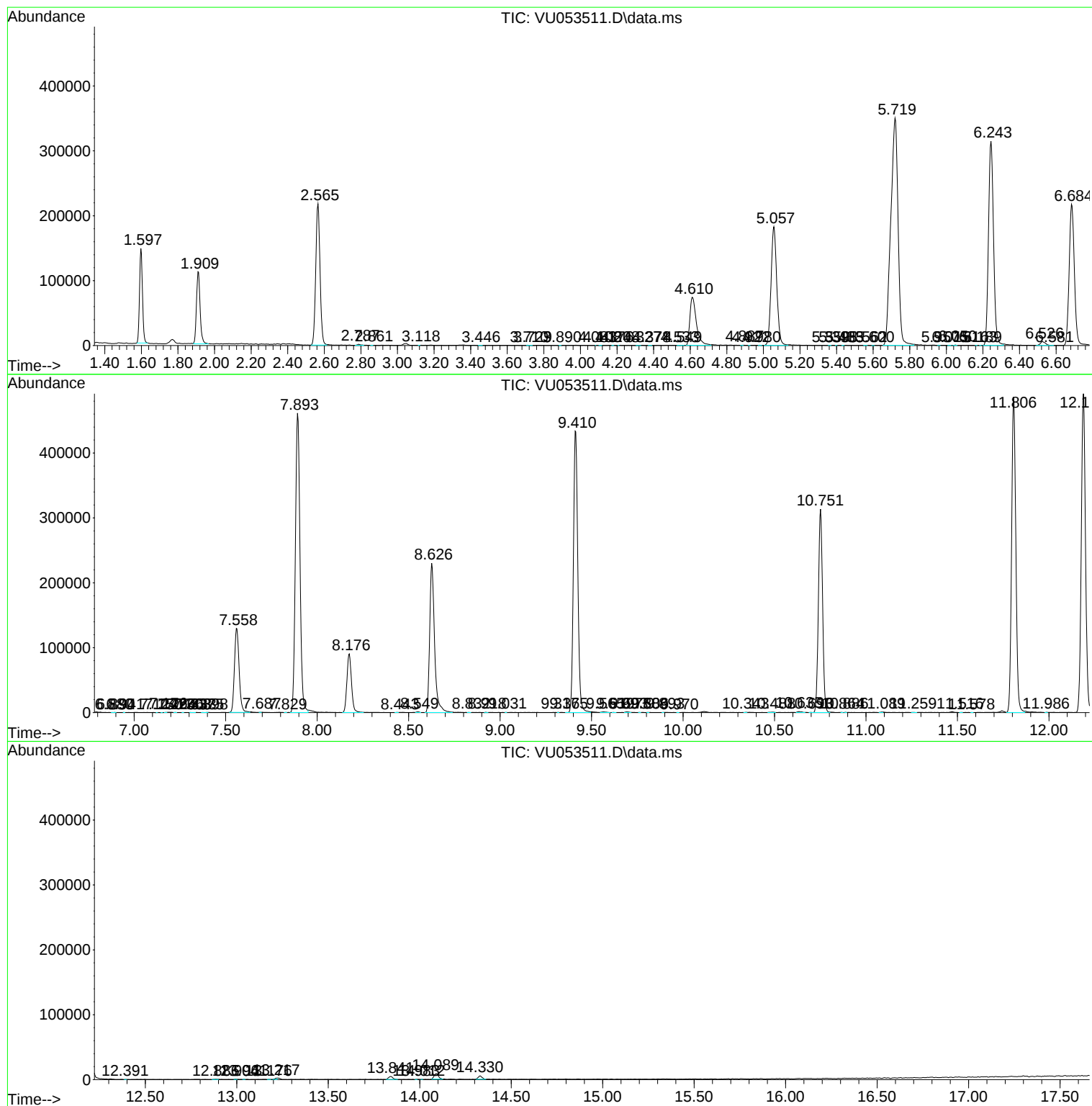
Sum of corrected areas: 7690650

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU040323\  
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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 |