

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050123\  
 Data File : VU054026.D  
 Acq On : 01 May 2023 15:19  
 Operator : JC/MD  
 Sample : 02525-08ME  
 Misc : 5.68g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DCCK5ME

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: VU054026.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          | 96           | rVB      | 101005         | 120563        | 12.65%          | 1.687%        |
| 2         | 1.906       | 169           | 176         | 194          | rVB      | 73655          | 101144        | 10.62%          | 1.415%        |
| 3         | 2.514       | 363           | 365         | 368          | rBV2     | 391            | 339           | 0.04%           | 0.005%        |
| 4         | 2.562       | 369           | 380         | 397          | rVB      | 181467         | 293797        | 30.84%          | 4.111%        |
| 5         | 2.784       | 446           | 449         | 450          | rBV      | 314            | 176           | 0.02%           | 0.002%        |
| 6         | 2.999       | 514           | 516         | 518          | rBV      | 196            | 121           | 0.01%           | 0.002%        |
| 7         | 3.041       | 521           | 529         | 542          | rVB3     | 3722           | 6450          | 0.68%           | 0.090%        |
| 8         | 3.289       | 604           | 606         | 609          | rVB      | 265            | 124           | 0.01%           | 0.002%        |
| 9         | 3.305       | 609           | 611         | 612          | rBV      | 143            | 59            | 0.01%           | 0.001%        |
| 10        | 3.408       | 641           | 643         | 645          | rBV      | 192            | 84            | 0.01%           | 0.001%        |
| 11        | 3.424       | 645           | 648         | 649          | rBV      | 196            | 98            | 0.01%           | 0.001%        |
| 12        | 3.546       | 683           | 686         | 687          | rBV2     | 145            | 79            | 0.01%           | 0.001%        |
| 13        | 3.736       | 742           | 745         | 746          | rBV      | 170            | 89            | 0.01%           | 0.001%        |
| 14        | 3.764       | 752           | 754         | 756          | rBV      | 149            | 91            | 0.01%           | 0.001%        |
| 15        | 3.813       | 767           | 769         | 773          | rVB2     | 156            | 87            | 0.01%           | 0.001%        |
| 16        | 3.925       | 802           | 804         | 805          | rBV      | 181            | 81            | 0.01%           | 0.001%        |
| 17        | 4.060       | 843           | 846         | 847          | rBV      | 205            | 123           | 0.01%           | 0.002%        |
| 18        | 4.105       | 857           | 860         | 861          | rBV      | 194            | 121           | 0.01%           | 0.002%        |
| 19        | 4.208       | 890           | 892         | 896          | rVB      | 209            | 104           | 0.01%           | 0.001%        |
| 20        | 4.231       | 896           | 899         | 900          | rBV      | 208            | 124           | 0.01%           | 0.002%        |
| 21        | 4.266       | 908           | 910         | 912          | rBV2     | 217            | 133           | 0.01%           | 0.002%        |
| 22        | 4.346       | 934           | 935         | 936          | rBV2     | 112            | 30            | 0.00%           | 0.000%        |
| 23        | 4.359       | 936           | 939         | 943          | rVV      | 175            | 180           | 0.02%           | 0.003%        |
| 24        | 4.456       | 965           | 969         | 971          | rBV2     | 174            | 124           | 0.01%           | 0.002%        |
| 25        | 4.501       | 980           | 983         | 985          | rBV2     | 160            | 105           | 0.01%           | 0.001%        |
| 26        | 4.539       | 993           | 995         | 998          | rBV2     | 199            | 135           | 0.01%           | 0.002%        |
| 27        | 4.623       | 1009          | 1021        | 1056         | rBV      | 74583          | 196199        | 20.59%          | 2.745%        |
| 28        | 5.057       | 1140          | 1156        | 1177         | rBV2     | 167503         | 375428        | 39.40%          | 5.253%        |
| 29        | 5.465       | 1280          | 1283        | 1284         | rBV      | 292            | 160           | 0.02%           | 0.002%        |
| 30        | 5.600       | 1320          | 1325        | 1327         | rBV2     | 194            | 152           | 0.02%           | 0.002%        |
| 31        | 5.613       | 1327          | 1329        | 1332         | rBV      | 152            | 71            | 0.01%           | 0.001%        |
| 32        | 5.716       | 1339          | 1361        | 1383         | rBV2     | 343315         | 952778        | 100.00%         | 13.332%       |
| 33        | 5.932       | 1426          | 1428        | 1432         | rBV2     | 279            | 201           | 0.02%           | 0.003%        |
| 34        | 6.102       | 1476          | 1481        | 1482         | rBV2     | 291            | 217           | 0.02%           | 0.003%        |
| 35        | 6.170       | 1500          | 1502        | 1505         | rVB      | 296            | 148           | 0.02%           | 0.002%        |
| 36        | 6.189       | 1505          | 1508        | 1511         | rBV      | 188            | 178           | 0.02%           | 0.002%        |

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Integrator: RTE

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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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.243  | 1511 | 1525 | 1551 | rBV  | 295397 | 567850 | 59.60% | 7.946%  |
| 38 | 6.530  | 1606 | 1614 | 1615 | rBV3 | 2282   | 2690   | 0.28%  | 0.038%  |
| 39 | 6.623  | 1640 | 1643 | 1646 | rBV2 | 293    | 222    | 0.02%  | 0.003%  |
| 40 | 6.684  | 1648 | 1662 | 1688 | rVV  | 226475 | 438994 | 46.08% | 6.143%  |
| 41 | 6.800  | 1695 | 1698 | 1701 | rBV  | 520    | 416    | 0.04%  | 0.006%  |
| 42 | 6.912  | 1731 | 1733 | 1735 | rVB  | 300    | 143    | 0.02%  | 0.002%  |
| 43 | 6.932  | 1735 | 1739 | 1741 | rBV  | 258    | 241    | 0.03%  | 0.003%  |
| 44 | 7.028  | 1766 | 1769 | 1773 | rVB2 | 238    | 211    | 0.02%  | 0.003%  |
| 45 | 7.128  | 1798 | 1800 | 1803 | rVB2 | 190    | 108    | 0.01%  | 0.002%  |
| 46 | 7.195  | 1813 | 1821 | 1824 | rBV3 | 703    | 795    | 0.08%  | 0.011%  |
| 47 | 7.305  | 1853 | 1855 | 1856 | rBV  | 168    | 50     | 0.01%  | 0.001%  |
| 48 | 7.559  | 1923 | 1934 | 1961 | rBV  | 124151 | 219590 | 23.05% | 3.073%  |
| 49 | 7.706  | 1979 | 1980 | 1984 | rVB  | 246    | 175    | 0.02%  | 0.002%  |
| 50 | 7.732  | 1984 | 1988 | 1992 | rBV2 | 148    | 141    | 0.01%  | 0.002%  |
| 51 | 7.893  | 2024 | 2038 | 2063 | rBV  | 431631 | 751021 | 78.82% | 10.509% |
| 52 | 8.112  | 2104 | 2106 | 2108 | rVB  | 275    | 97     | 0.01%  | 0.001%  |
| 53 | 8.173  | 2113 | 2125 | 2147 | rBV  | 89310  | 151505 | 15.90% | 2.120%  |
| 54 | 8.337  | 2174 | 2176 | 2177 | rBV  | 134    | 34     | 0.00%  | 0.000%  |
| 55 | 8.375  | 2185 | 2188 | 2191 | rVB  | 219    | 121    | 0.01%  | 0.002%  |
| 56 | 8.398  | 2193 | 2195 | 2198 | rVV  | 186    | 70     | 0.01%  | 0.001%  |
| 57 | 8.417  | 2198 | 2201 | 2204 | rVV  | 243    | 181    | 0.02%  | 0.003%  |
| 58 | 8.465  | 2208 | 2216 | 2229 | rVV2 | 1468   | 2572   | 0.27%  | 0.036%  |
| 59 | 8.549  | 2239 | 2242 | 2247 | rVB4 | 1291   | 1291   | 0.14%  | 0.018%  |
| 60 | 8.629  | 2255 | 2267 | 2303 | rBV2 | 221964 | 430787 | 45.21% | 6.028%  |
| 61 | 9.253  | 2458 | 2461 | 2464 | rBB2 | 196    | 121    | 0.01%  | 0.002%  |
| 62 | 9.411  | 2498 | 2510 | 2544 | rBV  | 405211 | 681247 | 71.50% | 9.533%  |
| 63 | 9.620  | 2573 | 2575 | 2580 | rBV3 | 321    | 218    | 0.02%  | 0.003%  |
| 64 | 9.732  | 2608 | 2610 | 2615 | rBV2 | 225    | 214    | 0.02%  | 0.003%  |
| 65 | 10.115 | 2726 | 2729 | 2731 | rBV2 | 194    | 129    | 0.01%  | 0.002%  |
| 66 | 10.259 | 2767 | 2774 | 2776 | rBV  | 288    | 387    | 0.04%  | 0.005%  |
| 67 | 10.523 | 2853 | 2856 | 2859 | rBV2 | 226    | 187    | 0.02%  | 0.003%  |
| 68 | 10.751 | 2915 | 2927 | 2947 | rBV  | 300798 | 484419 | 50.84% | 6.778%  |
| 69 | 11.121 | 3039 | 3042 | 3045 | rBV  | 258    | 187    | 0.02%  | 0.003%  |
| 70 | 11.369 | 3117 | 3119 | 3123 | rBV  | 353    | 215    | 0.02%  | 0.003%  |
| 71 | 11.806 | 3243 | 3255 | 3277 | rBV  | 414639 | 659110 | 69.18% | 9.223%  |
| 72 | 12.102 | 3345 | 3347 | 3349 | rBV2 | 502    | 227    | 0.02%  | 0.003%  |
| 73 | 12.189 | 3361 | 3374 | 3394 | rBV  | 434852 | 699620 | 73.43% | 9.790%  |
| 74 | 13.854 | 3887 | 3892 | 3896 | rBV2 | 663    | 758    | 0.08%  | 0.011%  |

Sum of corrected areas: 7146437

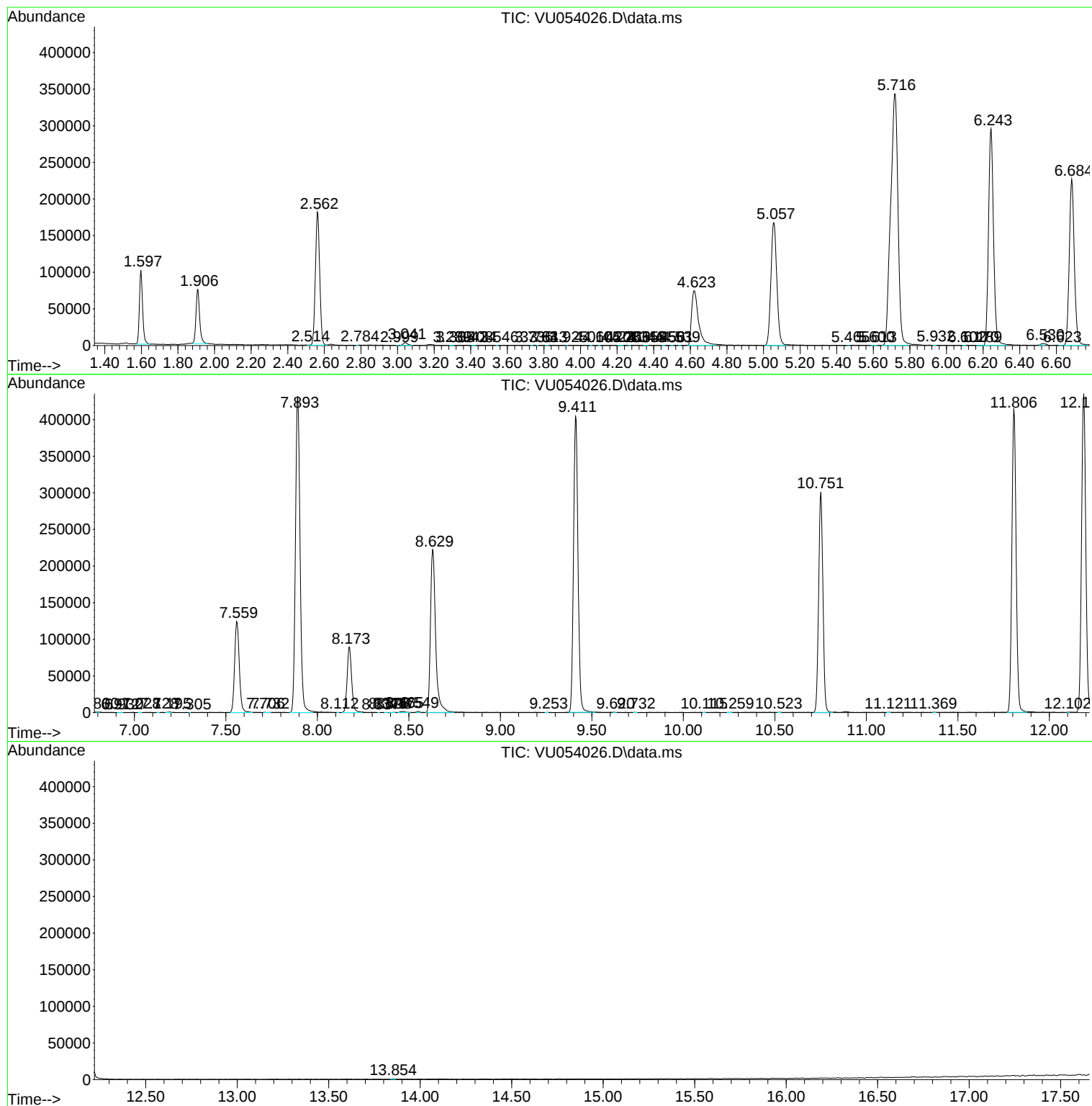
**Instrument :**  
MSVOA\_U  
**ClientSampleId :**  
DCCK5ME

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

TIC Library :  
TIC Integration Parameters: LSCINT.P



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No Library Search Compounds Detected

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