

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU090122\  
 Data File : VU050584.D  
 Acq On : 01 Sep 2022 16:34  
 Operator : SY/MD  
 Sample : N4363-17ME  
 Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DBVX1ME

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\SFAMULM083022WMA.M  
 Title : VOC Analysis

Signal : TIC: VU050584.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         | 1.594       | 72            | 79          | 90           | rBV      | 56572          | 81720         | 6.55%           | 0.893%        |
| 2         | 2.526       | 357           | 369         | 384          | rBV      | 219300         | 352055        | 28.20%          | 3.846%        |
| 3         | 2.652       | 402           | 408         | 417          | rBV3     | 1512           | 2651          | 0.21%           | 0.029%        |
| 4         | 2.977       | 505           | 509         | 511          | rBV2     | 242            | 163           | 0.01%           | 0.002%        |
| 5         | 3.035       | 516           | 527         | 540          | rVB6     | 1814           | 4089          | 0.33%           | 0.045%        |
| 6         | 3.176       | 562           | 571         | 584          | rBV2     | 7216           | 16981         | 1.36%           | 0.185%        |
| 7         | 3.330       | 616           | 619         | 624          | rBV3     | 371            | 356           | 0.03%           | 0.004%        |
| 8         | 3.485       | 665           | 667         | 671          | rVB      | 205            | 83            | 0.01%           | 0.001%        |
| 9         | 3.526       | 676           | 680         | 681          | rBV      | 225            | 125           | 0.01%           | 0.001%        |
| 10        | 3.575       | 692           | 695         | 699          | rVB2     | 277            | 183           | 0.01%           | 0.002%        |
| 11        | 3.610       | 699           | 706         | 715          | rVB2     | 314            | 435           | 0.03%           | 0.005%        |
| 12        | 3.649       | 715           | 718         | 720          | rBV      | 220            | 143           | 0.01%           | 0.002%        |
| 13        | 3.671       | 720           | 725         | 731          | rBV2     | 259            | 366           | 0.03%           | 0.004%        |
| 14        | 3.768       | 747           | 755         | 760          | rBV2     | 295            | 373           | 0.03%           | 0.004%        |
| 15        | 3.787       | 760           | 761         | 763          | rVB2     | 154            | 54            | 0.00%           | 0.001%        |
| 16        | 3.803       | 763           | 766         | 767          | rBV      | 214            | 133           | 0.01%           | 0.001%        |
| 17        | 3.835       | 772           | 776         | 778          | rBV2     | 335            | 168           | 0.01%           | 0.002%        |
| 18        | 3.851       | 778           | 781         | 784          | rVB2     | 259            | 163           | 0.01%           | 0.002%        |
| 19        | 3.877       | 786           | 789         | 791          | rBV      | 280            | 188           | 0.02%           | 0.002%        |
| 20        | 3.993       | 822           | 825         | 829          | rVB2     | 194            | 146           | 0.01%           | 0.002%        |
| 21        | 4.034       | 835           | 838         | 841          | rVB      | 206            | 138           | 0.01%           | 0.002%        |
| 22        | 4.054       | 841           | 844         | 845          | rBV      | 196            | 113           | 0.01%           | 0.001%        |
| 23        | 4.070       | 845           | 849         | 854          | rBV2     | 325            | 401           | 0.03%           | 0.004%        |
| 24        | 4.115       | 860           | 863         | 865          | rBV      | 211            | 149           | 0.01%           | 0.002%        |
| 25        | 4.144       | 869           | 872         | 875          | rBV3     | 281            | 193           | 0.02%           | 0.002%        |
| 26        | 4.179       | 880           | 883         | 885          | rBV2     | 213            | 137           | 0.01%           | 0.001%        |
| 27        | 4.260       | 904           | 908         | 912          | rBV2     | 194            | 226           | 0.02%           | 0.002%        |
| 28        | 4.292       | 915           | 918         | 922          | rVB3     | 277            | 192           | 0.02%           | 0.002%        |
| 29        | 4.311       | 922           | 924         | 926          | rBV3     | 127            | 56            | 0.00%           | 0.001%        |
| 30        | 4.330       | 929           | 930         | 933          | rVB      | 144            | 46            | 0.00%           | 0.001%        |
| 31        | 4.366       | 936           | 941         | 947          | rBV2     | 252            | 357           | 0.03%           | 0.004%        |
| 32        | 4.485       | 975           | 978         | 979          | rBV      | 173            | 99            | 0.01%           | 0.001%        |
| 33        | 4.533       | 988           | 993         | 996          | rBV2     | 354            | 309           | 0.02%           | 0.003%        |
| 34        | 4.581       | 1005          | 1008        | 1012         | rBV      | 128            | 93            | 0.01%           | 0.001%        |
| 35        | 4.649       | 1013          | 1029        | 1047         | rBV      | 82066          | 267654        | 21.44%          | 2.924%        |
| 36        | 5.060       | 1139          | 1157        | 1185         | rBV      | 205971         | 492493        | 39.44%          | 5.380%        |

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 DBVX1ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

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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\SFAMULM083022WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |         |         |
|----|-------|------|------|------|------|--------|---------|---------|---------|
| 37 | 5.288 | 1221 | 1228 | 1236 | rBV3 | 1096   | 1750    | 0.14%   | 0.019%  |
| 38 | 5.359 | 1246 | 1250 | 1251 | rBV2 | 625    | 400     | 0.03%   | 0.004%  |
| 39 | 5.446 | 1273 | 1277 | 1282 | rBV  | 224    | 250     | 0.02%   | 0.003%  |
| 40 | 5.472 | 1282 | 1285 | 1287 | rVV2 | 233    | 160     | 0.01%   | 0.002%  |
| 41 | 5.497 | 1291 | 1293 | 1295 | rBV  | 163    | 93      | 0.01%   | 0.001%  |
| 42 | 5.591 | 1319 | 1322 | 1324 | rBV2 | 188    | 127     | 0.01%   | 0.001%  |
| 43 | 5.629 | 1331 | 1334 | 1336 | rBV2 | 170    | 121     | 0.01%   | 0.001%  |
| 44 | 5.716 | 1342 | 1361 | 1388 | rBV2 | 490866 | 1248578 | 100.00% | 13.639% |
| 45 | 5.980 | 1433 | 1443 | 1464 | rBV4 | 9335   | 23002   | 1.84%   | 0.251%  |
| 46 | 6.108 | 1478 | 1483 | 1486 | rBV2 | 360    | 445     | 0.04%   | 0.005%  |
| 47 | 6.150 | 1493 | 1496 | 1498 | rBV  | 321    | 198     | 0.02%   | 0.002%  |
| 48 | 6.247 | 1513 | 1526 | 1546 | rBV  | 394566 | 797782  | 63.90%  | 8.714%  |
| 49 | 6.462 | 1591 | 1593 | 1600 | rVB  | 575    | 416     | 0.03%   | 0.005%  |
| 50 | 6.494 | 1600 | 1603 | 1605 | rBV  | 338    | 239     | 0.02%   | 0.003%  |
| 51 | 6.530 | 1605 | 1614 | 1622 | rBV7 | 3688   | 6906    | 0.55%   | 0.075%  |
| 52 | 6.597 | 1630 | 1635 | 1637 | rBV3 | 3540   | 3260    | 0.26%   | 0.036%  |
| 53 | 6.690 | 1650 | 1664 | 1691 | rVB  | 275301 | 573808  | 45.96%  | 6.268%  |
| 54 | 6.796 | 1694 | 1697 | 1699 | rBV  | 815    | 671     | 0.05%   | 0.007%  |
| 55 | 7.034 | 1767 | 1771 | 1778 | rBV2 | 288    | 326     | 0.03%   | 0.004%  |
| 56 | 7.070 | 1778 | 1782 | 1784 | rBV  | 219    | 183     | 0.01%   | 0.002%  |
| 57 | 7.140 | 1802 | 1804 | 1806 | rBV  | 116    | 59      | 0.00%   | 0.001%  |
| 58 | 7.224 | 1819 | 1830 | 1846 | rBV6 | 4317   | 10328   | 0.83%   | 0.113%  |
| 59 | 7.430 | 1891 | 1894 | 1897 | rBV2 | 261    | 201     | 0.02%   | 0.002%  |
| 60 | 7.468 | 1901 | 1906 | 1911 | rBV2 | 340    | 447     | 0.04%   | 0.005%  |
| 61 | 7.565 | 1923 | 1936 | 1955 | rBV  | 130359 | 254034  | 20.35%  | 2.775%  |
| 62 | 7.713 | 1980 | 1982 | 1984 | rBV2 | 299    | 152     | 0.01%   | 0.002%  |
| 63 | 7.806 | 2008 | 2011 | 2015 | rVB2 | 287    | 185     | 0.01%   | 0.002%  |
| 64 | 7.896 | 2026 | 2039 | 2060 | rBV  | 528251 | 964720  | 77.27%  | 10.538% |
| 65 | 8.182 | 2116 | 2128 | 2147 | rBV2 | 83511  | 168631  | 13.51%  | 1.842%  |
| 66 | 8.356 | 2176 | 2182 | 2190 | rBV3 | 932    | 1646    | 0.13%   | 0.018%  |
| 67 | 8.478 | 2217 | 2220 | 2224 | rBV2 | 353    | 244     | 0.02%   | 0.003%  |
| 68 | 8.552 | 2232 | 2243 | 2255 | rVB3 | 27001  | 46973   | 3.76%   | 0.513%  |
| 69 | 8.597 | 2255 | 2257 | 2259 | rVB  | 182    | 53      | 0.00%   | 0.001%  |
| 70 | 8.664 | 2259 | 2278 | 2311 | rBV4 | 208740 | 672158  | 53.83%  | 7.342%  |
| 71 | 8.980 | 2375 | 2376 | 2379 | rBV  | 291    | 129     | 0.01%   | 0.001%  |
| 72 | 9.054 | 2395 | 2399 | 2402 | rBV2 | 201    | 167     | 0.01%   | 0.002%  |
| 73 | 9.420 | 2500 | 2513 | 2533 | rBV  | 502333 | 958137  | 76.74%  | 10.466% |
| 74 | 9.613 | 2570 | 2573 | 2577 | rBV2 | 341    | 304     | 0.02%   | 0.003%  |
| 75 | 9.767 | 2618 | 2621 | 2622 | rBV2 | 376    | 173     | 0.01%   | 0.002%  |
| 76 | 9.812 | 2633 | 2635 | 2638 | rBV  | 225    | 140     | 0.01%   | 0.002%  |

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 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
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 DBVX1ME

Integration Parameters: LSCINT.P

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Min Area: 0 % of largest Peak

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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\SFAMULM083022WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 9.835  | 2639 | 2642 | 2645 | rVB  | 427    | 246    | 0.02%  | 0.003% |
| 78  | 9.848  | 2645 | 2646 | 2649 | rBV  | 272    | 106    | 0.01%  | 0.001% |
| 79  | 9.867  | 2649 | 2652 | 2655 | rBV2 | 246    | 159    | 0.01%  | 0.002% |
| 80  | 9.980  | 2683 | 2687 | 2692 | rBV2 | 298    | 330    | 0.03%  | 0.004% |
| 81  | 10.012 | 2694 | 2697 | 2700 | rBV  | 200    | 159    | 0.01%  | 0.002% |
| 82  | 10.472 | 2837 | 2840 | 2841 | rBV  | 149    | 99     | 0.01%  | 0.001% |
| 83  | 10.523 | 2851 | 2856 | 2860 | rBV2 | 320    | 368    | 0.03%  | 0.004% |
| 84  | 10.610 | 2881 | 2883 | 2885 | rVB  | 141    | 52     | 0.00%  | 0.001% |
| 85  | 10.764 | 2918 | 2931 | 2950 | rBV  | 399023 | 680708 | 54.52% | 7.436% |
| 86  | 10.883 | 2964 | 2968 | 2977 | rVB3 | 542    | 637    | 0.05%  | 0.007% |
| 87  | 10.918 | 2977 | 2979 | 2982 | rBV  | 238    | 148    | 0.01%  | 0.002% |
| 88  | 10.951 | 2987 | 2989 | 2992 | rVB  | 198    | 100    | 0.01%  | 0.001% |
| 89  | 11.092 | 3030 | 3033 | 3034 | rBV  | 315    | 181    | 0.01%  | 0.002% |
| 90  | 11.118 | 3034 | 3041 | 3047 | rVV6 | 2414   | 3183   | 0.25%  | 0.035% |
| 91  | 11.336 | 3106 | 3109 | 3115 | rBV2 | 353    | 352    | 0.03%  | 0.004% |
| 92  | 11.385 | 3121 | 3124 | 3127 | rBV  | 258    | 191    | 0.02%  | 0.002% |
| 93  | 11.623 | 3194 | 3198 | 3199 | rBV  | 252    | 181    | 0.01%  | 0.002% |
| 94  | 11.815 | 3245 | 3258 | 3277 | rBV  | 462587 | 736424 | 58.98% | 8.044% |
| 95  | 12.198 | 3364 | 3377 | 3397 | rBV  | 464656 | 768981 | 61.59% | 8.400% |
| 96  | 12.529 | 3478 | 3480 | 3486 | rBV3 | 411    | 280    | 0.02%  | 0.003% |
| 97  | 13.012 | 3627 | 3630 | 3633 | rBV  | 337    | 273    | 0.02%  | 0.003% |
| 98  | 13.111 | 3657 | 3661 | 3662 | rBV2 | 324    | 216    | 0.02%  | 0.002% |
| 99  | 13.330 | 3726 | 3729 | 3731 | rBV2 | 416    | 351    | 0.03%  | 0.004% |
| 100 | 13.658 | 3829 | 3831 | 3834 | rBV2 | 347    | 249    | 0.02%  | 0.003% |

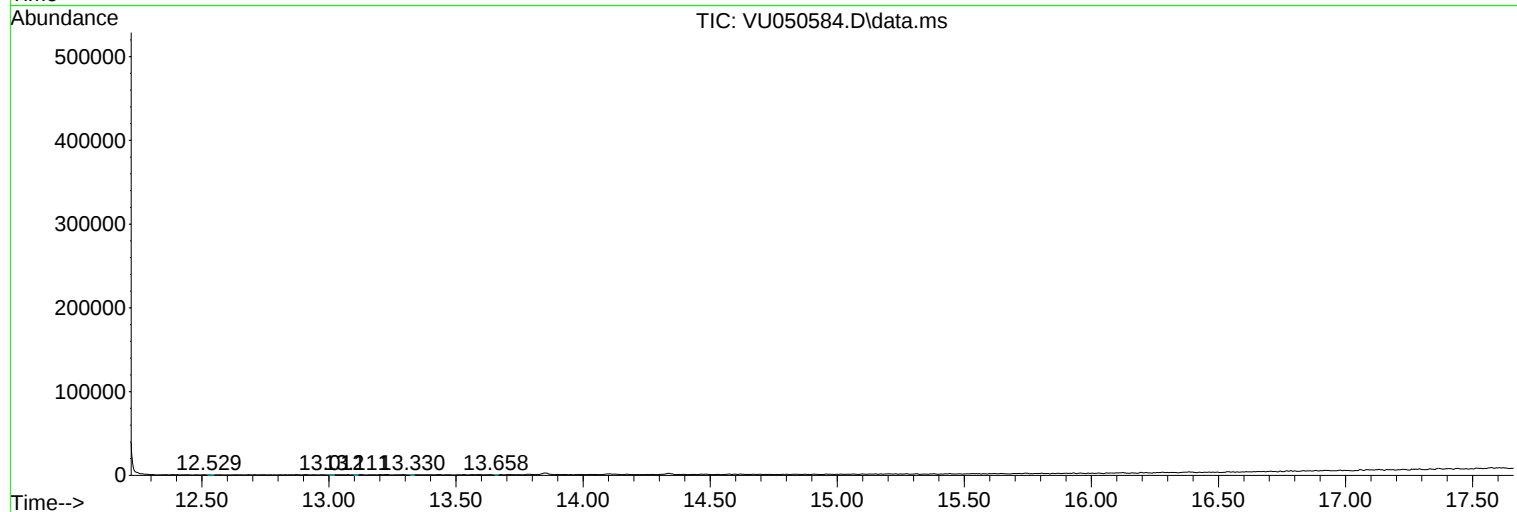
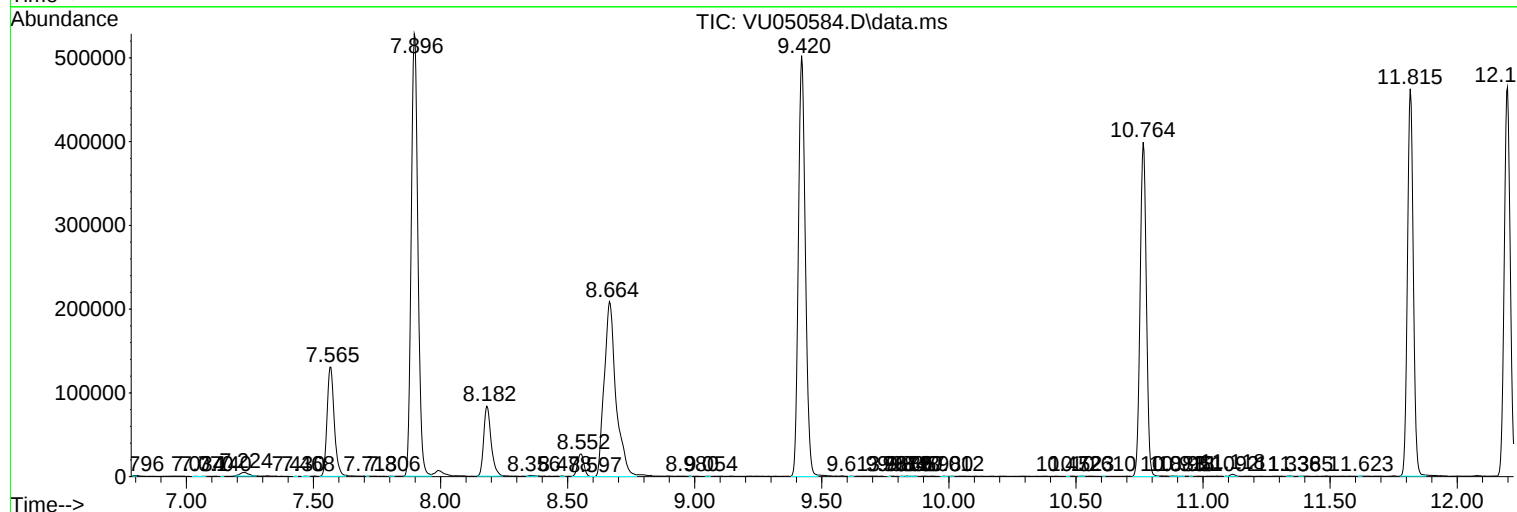
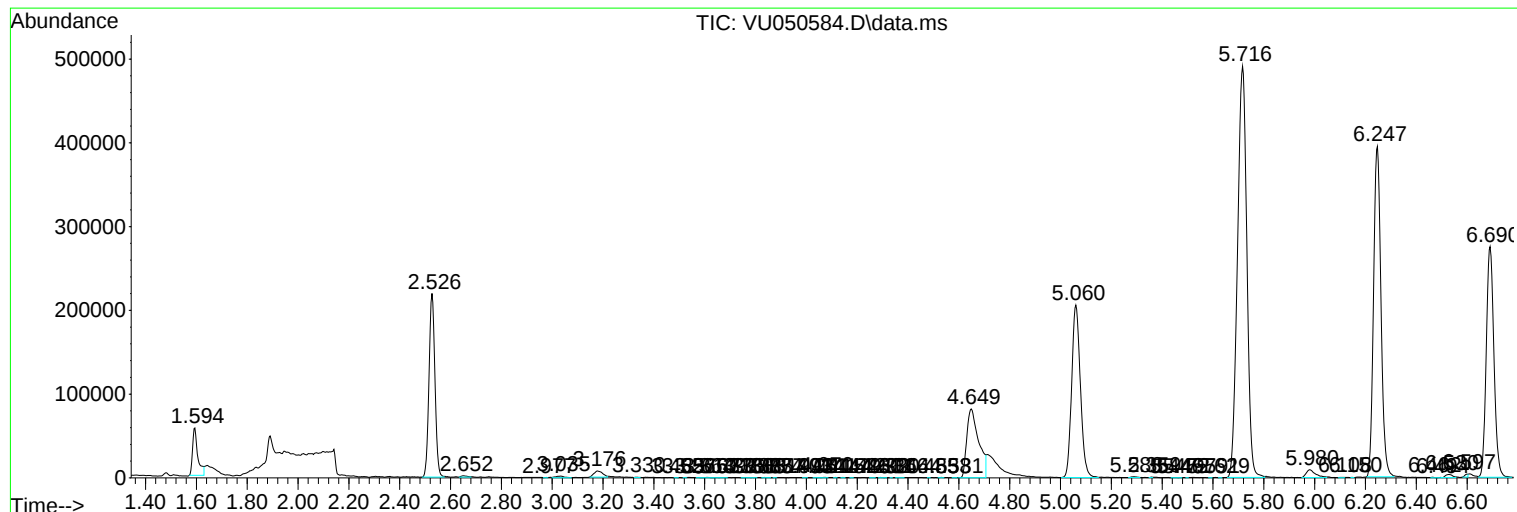
Sum of corrected areas: 9154801

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Instrument :  
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DBVX1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM083022WMA.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 Top Hit name | RT | EstConc | Units | Response | --Internal Standard-- |
|------------------|----|---------|-------|----------|-----------------------|
|                  |    |         |       | #        | RT Resp Conc          |