

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091818\  
 Data File : VU026872.D  
 Acq On : 18 Sep 2018 19:07  
 Operator : MD/SY  
 Sample : VU0918MBL02  
 Misc : 5.00g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 30 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK44

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM091718WMA.M  
 Title : VOC Analysis

Signal : TIC

| 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         | 1.395       | 63            | 69          | 84           | rVB      | 133716         | 138039        | 14.14%          | 1.939%        |
| 2         | 1.678       | 149           | 157         | 172          | rVB      | 106746         | 136680        | 14.00%          | 1.920%        |
| 3         | 2.270       | 331           | 341         | 355          | rBV      | 221765         | 334765        | 34.29%          | 4.703%        |
| 4         | 2.701       | 468           | 475         | 486          | rVB2     | 2274           | 4151          | 0.43%           | 0.058%        |
| 5         | 2.839       | 511           | 518         | 523          | rBV2     | 500            | 846           | 0.09%           | 0.012%        |
| 6         | 2.906       | 535           | 539         | 542          | rBV      | 222            | 181           | 0.02%           | 0.003%        |
| 7         | 2.929       | 542           | 546         | 547          | rBV      | 165            | 137           | 0.01%           | 0.002%        |
| 8         | 2.990       | 562           | 565         | 568          | rVB2     | 457            | 270           | 0.03%           | 0.004%        |
| 9         | 3.096       | 596           | 598         | 600          | rVV      | 176            | 79            | 0.01%           | 0.001%        |
| 10        | 3.112       | 600           | 603         | 607          | rVB      | 159            | 112           | 0.01%           | 0.002%        |
| 11        | 3.180       | 622           | 624         | 625          | rBV      | 150            | 46            | 0.00%           | 0.001%        |
| 12        | 3.292       | 657           | 659         | 661          | rBV      | 138            | 74            | 0.01%           | 0.001%        |
| 13        | 3.520       | 727           | 730         | 735          | rBV      | 83             | 89            | 0.01%           | 0.001%        |
| 14        | 3.562       | 741           | 743         | 746          | rVB2     | 226            | 128           | 0.01%           | 0.002%        |
| 15        | 3.749       | 799           | 801         | 803          | rBV      | 75             | 43            | 0.00%           | 0.001%        |
| 16        | 3.848       | 829           | 832         | 835          | rBV      | 111            | 97            | 0.01%           | 0.001%        |
| 17        | 3.909       | 848           | 851         | 857          | rVB      | 109            | 99            | 0.01%           | 0.001%        |
| 18        | 3.951       | 861           | 864         | 869          | rVB      | 86             | 80            | 0.01%           | 0.001%        |
| 19        | 4.115       | 911           | 915         | 917          | rBV      | 98             | 78            | 0.01%           | 0.001%        |
| 20        | 4.180       | 920           | 935         | 975          | rVV      | 83893          | 220380        | 22.57%          | 3.096%        |
| 21        | 4.450       | 1016          | 1019        | 1023         | rBV2     | 167            | 127           | 0.01%           | 0.002%        |
| 22        | 4.498       | 1030          | 1034        | 1038         | rBV      | 139            | 175           | 0.02%           | 0.002%        |
| 23        | 4.527       | 1041          | 1043        | 1050         | rBV      | 95             | 121           | 0.01%           | 0.002%        |
| 24        | 4.591       | 1057          | 1063        | 1064         | rBV      | 445            | 415           | 0.04%           | 0.006%        |
| 25        | 4.649       | 1066          | 1081        | 1109         | rVB      | 159524         | 382826        | 39.21%          | 5.378%        |
| 26        | 4.945       | 1171          | 1173        | 1176         | rVB      | 161            | 69            | 0.01%           | 0.001%        |
| 27        | 4.987       | 1182          | 1186        | 1187         | rBV      | 228            | 181           | 0.02%           | 0.003%        |
| 28        | 5.009       | 1191          | 1193        | 1196         | rVB      | 142            | 59            | 0.01%           | 0.001%        |
| 29        | 5.035       | 1197          | 1201        | 1205         | rVB2     | 227            | 174           | 0.02%           | 0.002%        |
| 30        | 5.077       | 1211          | 1214        | 1217         | rBV      | 175            | 109           | 0.01%           | 0.002%        |
| 31        | 5.122       | 1225          | 1228        | 1230         | rBV2     | 152            | 90            | 0.01%           | 0.001%        |
| 32        | 5.186       | 1245          | 1248        | 1250         | rBV      | 124            | 80            | 0.01%           | 0.001%        |
| 33        | 5.228       | 1257          | 1261        | 1265         | rBV      | 107            | 91            | 0.01%           | 0.001%        |
| 34        | 5.340       | 1271          | 1296        | 1324         | rBV2     | 332853         | 976402        | 100.00%         | 13.716%       |

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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\SOMULM091718WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |        |        |         |
|----|-------|------|------|------|------|--------|--------|--------|---------|
| 35 | 5.588 | 1371 | 1373 | 1376 | rBV  | 141    | 73     | 0.01%  | 0.001%  |
| 36 | 5.604 | 1376 | 1378 | 1381 | rVV2 | 193    | 114    | 0.01%  | 0.002%  |
| 37 | 5.626 | 1383 | 1385 | 1387 | rVB  | 156    | 46     | 0.00%  | 0.001%  |
| 38 | 5.643 | 1387 | 1390 | 1391 | rBV  | 109    | 62     | 0.01%  | 0.001%  |
| 39 | 5.707 | 1407 | 1410 | 1414 | rVB  | 218    | 137    | 0.01%  | 0.002%  |
| 40 | 5.758 | 1424 | 1426 | 1430 | rVB  | 196    | 103    | 0.01%  | 0.001%  |
| 41 | 5.781 | 1430 | 1433 | 1435 | rBV  | 78     | 50     | 0.01%  | 0.001%  |
| 42 | 5.807 | 1440 | 1441 | 1444 | rBV  | 201    | 93     | 0.01%  | 0.001%  |
| 43 | 5.887 | 1451 | 1466 | 1487 | rBV  | 292174 | 565652 | 57.93% | 7.946%  |
| 44 | 6.173 | 1549 | 1555 | 1563 | rBV4 | 1004   | 1513   | 0.15%  | 0.021%  |
| 45 | 6.247 | 1573 | 1578 | 1580 | rBV2 | 193    | 160    | 0.02%  | 0.002%  |
| 46 | 6.266 | 1583 | 1584 | 1586 | rVB2 | 140    | 49     | 0.01%  | 0.001%  |
| 47 | 6.282 | 1586 | 1589 | 1590 | rBV  | 117    | 63     | 0.01%  | 0.001%  |
| 48 | 6.334 | 1590 | 1605 | 1627 | rVV  | 223203 | 446539 | 45.73% | 6.273%  |
| 49 | 6.430 | 1633 | 1635 | 1640 | rVB2 | 240    | 120    | 0.01%  | 0.002%  |
| 50 | 6.459 | 1640 | 1644 | 1649 | rBV3 | 577    | 595    | 0.06%  | 0.008%  |
| 51 | 6.504 | 1655 | 1658 | 1661 | rBV  | 145    | 107    | 0.01%  | 0.002%  |
| 52 | 6.540 | 1665 | 1669 | 1672 | rVB  | 278    | 225    | 0.02%  | 0.003%  |
| 53 | 6.575 | 1677 | 1680 | 1684 | rVV  | 102    | 80     | 0.01%  | 0.001%  |
| 54 | 6.610 | 1685 | 1691 | 1696 | rVB2 | 214    | 241    | 0.02%  | 0.003%  |
| 55 | 6.662 | 1703 | 1707 | 1709 | rBV  | 63     | 53     | 0.01%  | 0.001%  |
| 56 | 6.697 | 1713 | 1718 | 1722 | rBV  | 174    | 135    | 0.01%  | 0.002%  |
| 57 | 6.720 | 1722 | 1725 | 1727 | rBV  | 82     | 62     | 0.01%  | 0.001%  |
| 58 | 6.813 | 1752 | 1754 | 1756 | rBV  | 168    | 62     | 0.01%  | 0.001%  |
| 59 | 7.067 | 1830 | 1833 | 1834 | rBV  | 116    | 65     | 0.01%  | 0.001%  |
| 60 | 7.112 | 1843 | 1847 | 1853 | rBV  | 226    | 176    | 0.02%  | 0.002%  |
| 61 | 7.186 | 1869 | 1870 | 1871 | rBV  | 117    | 40     | 0.00%  | 0.001%  |
| 62 | 7.231 | 1871 | 1884 | 1901 | rVV  | 106677 | 187101 | 19.16% | 2.628%  |
| 63 | 7.382 | 1926 | 1931 | 1932 | rBV2 | 360    | 330    | 0.03%  | 0.005%  |
| 64 | 7.440 | 1946 | 1949 | 1950 | rBV2 | 156    | 89     | 0.01%  | 0.001%  |
| 65 | 7.488 | 1958 | 1964 | 1969 | rBV2 | 181    | 195    | 0.02%  | 0.003%  |
| 66 | 7.569 | 1975 | 1989 | 2014 | rBV  | 433713 | 743454 | 76.14% | 10.443% |
| 67 | 7.765 | 2047 | 2050 | 2053 | rBV2 | 376    | 323    | 0.03%  | 0.005%  |
| 68 | 7.851 | 2066 | 2077 | 2098 | rBV  | 74296  | 127854 | 13.09% | 1.796%  |
| 69 | 7.983 | 2116 | 2118 | 2121 | rBV2 | 243    | 134    | 0.01%  | 0.002%  |
| 70 | 8.054 | 2138 | 2140 | 2143 | rVB  | 161    | 55     | 0.01%  | 0.001%  |
| 71 | 8.067 | 2143 | 2144 | 2145 | rBV  | 200    | 60     | 0.01%  | 0.001%  |

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## Integration Parameters: LSCINT.P

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 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM091718WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 8.144  | 2166 | 2168 | 2169 | rBV  | 128    | 61     | 0.01%  | 0.001% |
| 73  | 8.186  | 2172 | 2181 | 2184 | rVV3 | 818    | 1278   | 0.13%  | 0.018% |
| 74  | 8.311  | 2209 | 2220 | 2249 | rBV  | 267444 | 465767 | 47.70% | 6.543% |
| 75  | 8.585  | 2303 | 2305 | 2308 | rBV2 | 140    | 68     | 0.01%  | 0.001% |
| 76  | 8.607  | 2308 | 2312 | 2313 | rBV  | 312    | 211    | 0.02%  | 0.003% |
| 77  | 8.736  | 2349 | 2352 | 2356 | rVB2 | 219    | 192    | 0.02%  | 0.003% |
| 78  | 8.758  | 2357 | 2359 | 2361 | rBV  | 160    | 90     | 0.01%  | 0.001% |
| 79  | 8.851  | 2386 | 2388 | 2389 | rVB  | 113    | 43     | 0.00%  | 0.001% |
| 80  | 8.877  | 2393 | 2396 | 2400 | rVB  | 165    | 102    | 0.01%  | 0.001% |
| 81  | 8.916  | 2405 | 2408 | 2412 | rBV  | 187    | 126    | 0.01%  | 0.002% |
| 82  | 8.935  | 2412 | 2414 | 2417 | rBV  | 189    | 111    | 0.01%  | 0.002% |
| 83  | 9.041  | 2444 | 2447 | 2449 | rBV  | 181    | 97     | 0.01%  | 0.001% |
| 84  | 9.089  | 2449 | 2462 | 2482 | rBV  | 417066 | 693503 | 71.03% | 9.742% |
| 85  | 9.353  | 2542 | 2544 | 2547 | rVB  | 235    | 97     | 0.01%  | 0.001% |
| 86  | 9.437  | 2568 | 2570 | 2572 | rBV  | 168    | 75     | 0.01%  | 0.001% |
| 87  | 9.478  | 2581 | 2583 | 2587 | rVB2 | 177    | 106    | 0.01%  | 0.001% |
| 88  | 9.658  | 2638 | 2639 | 2646 | rVB  | 306    | 167    | 0.02%  | 0.002% |
| 89  | 9.851  | 2696 | 2699 | 2700 | rBV  | 185    | 96     | 0.01%  | 0.001% |
| 90  | 10.038 | 2754 | 2757 | 2759 | rBV  | 197    | 113    | 0.01%  | 0.002% |
| 91  | 10.163 | 2795 | 2796 | 2798 | rBV  | 209    | 103    | 0.01%  | 0.001% |
| 92  | 10.363 | 2856 | 2858 | 2861 | rBV  | 212    | 92     | 0.01%  | 0.001% |
| 93  | 10.433 | 2867 | 2880 | 2894 | rBV  | 303909 | 474102 | 48.56% | 6.660% |
| 94  | 10.652 | 2946 | 2948 | 2955 | rBV  | 227    | 142    | 0.01%  | 0.002% |
| 95  | 10.822 | 2998 | 3001 | 3004 | rBV  | 183    | 117    | 0.01%  | 0.002% |
| 96  | 11.420 | 3180 | 3187 | 3195 | rVB3 | 2115   | 2942   | 0.30%  | 0.041% |
| 97  | 11.485 | 3195 | 3207 | 3226 | rBV  | 355046 | 565774 | 57.94% | 7.948% |
| 98  | 11.861 | 3311 | 3324 | 3346 | rBV  | 398863 | 638383 | 65.38% | 8.968% |
| 99  | 12.154 | 3412 | 3415 | 3423 | rVB2 | 478    | 431    | 0.04%  | 0.006% |
| 100 | 12.893 | 3640 | 3645 | 3648 | rBV2 | 897    | 935    | 0.10%  | 0.013% |

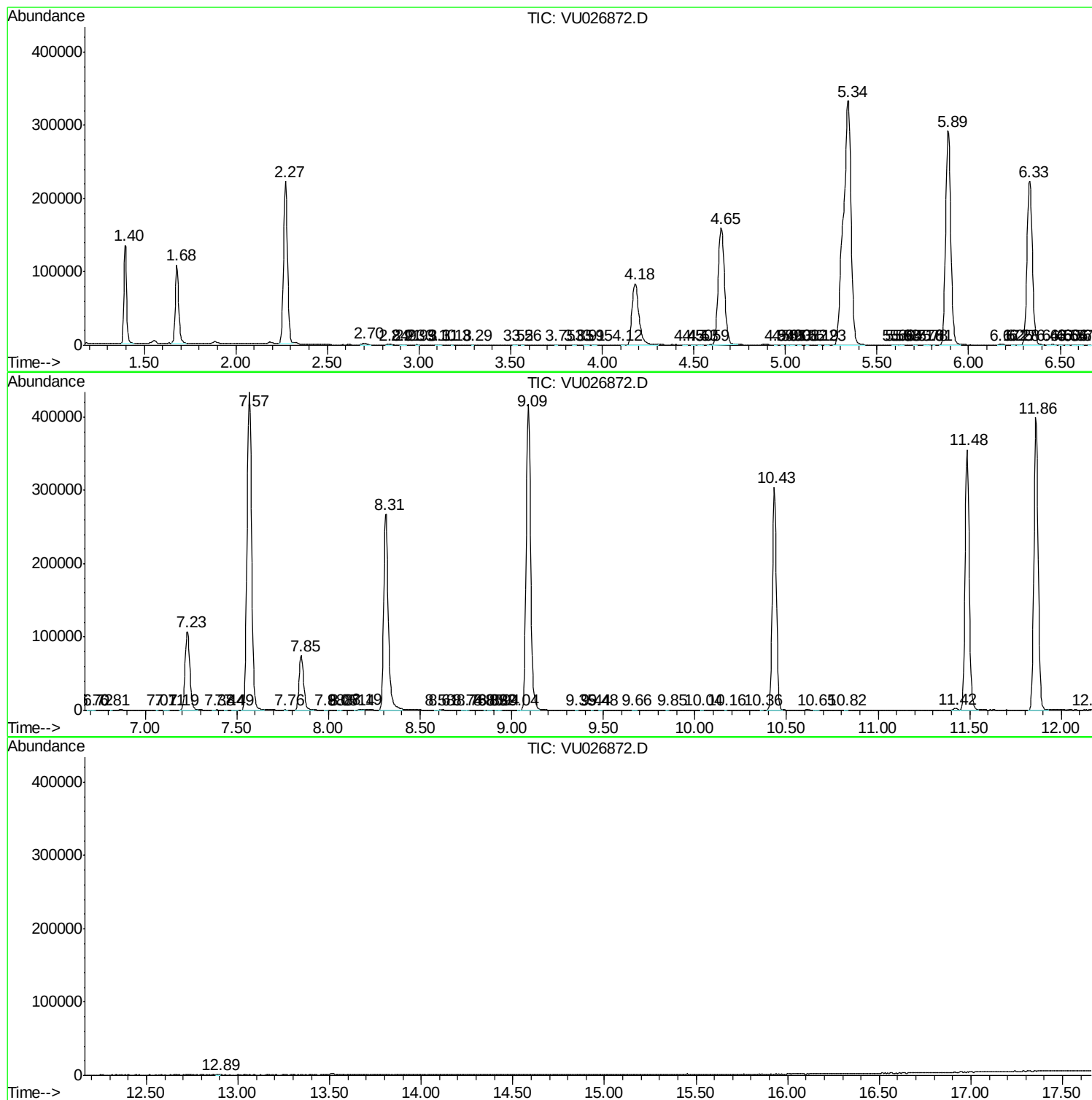
Sum of corrected areas: 7118827

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Instrument :  
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ClientSampled :  
VBLK44

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM091718WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU091818\  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM091718WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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