

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU120721\  
 Data File : VU046159.D  
 Acq On : 07 Dec 2021 22:55  
 Operator : SY/MD  
 Sample : M4960-05 10X  
 Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 43 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGKS0

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\SFAMULM112921WMA.M  
 Title : VOC Analysis

Signal : TIC: VU046169.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         | 1.604       | 74            | 82          | 95           | rVB      | 119483         | 132295        | 15.11%          | 1.843%        |
| 2         | 1.919       | 171           | 180         | 193          | rBV      | 81478          | 104209        | 11.90%          | 1.451%        |
| 3         | 2.571       | 371           | 383         | 425          | rVB      | 192222         | 321832        | 36.77%          | 4.483%        |
| 4         | 2.800       | 449           | 454         | 462          | rVB2     | 261            | 337           | 0.04%           | 0.005%        |
| 5         | 3.051       | 525           | 532         | 540          | rVB3     | 1229           | 1976          | 0.23%           | 0.028%        |
| 6         | 3.189       | 560           | 575         | 595          | rVB      | 11159          | 26212         | 2.99%           | 0.365%        |
| 7         | 3.436       | 649           | 652         | 656          | rBV      | 177            | 189           | 0.02%           | 0.003%        |
| 8         | 3.520       | 675           | 678         | 681          | rBV      | 154            | 158           | 0.02%           | 0.002%        |
| 9         | 3.571       | 691           | 694         | 697          | rBV      | 187            | 157           | 0.02%           | 0.002%        |
| 10        | 3.661       | 720           | 722         | 726          | rBV      | 144            | 139           | 0.02%           | 0.002%        |
| 11        | 3.915       | 795           | 801         | 805          | rBB      | 139            | 213           | 0.02%           | 0.003%        |
| 12        | 3.989       | 820           | 824         | 828          | rBV      | 124            | 155           | 0.02%           | 0.002%        |
| 13        | 4.231       | 890           | 899         | 901          | rBV      | 165            | 299           | 0.03%           | 0.004%        |
| 14        | 4.269       | 909           | 911         | 915          | rBV      | 129            | 135           | 0.02%           | 0.002%        |
| 15        | 4.327       | 926           | 929         | 935          | rBB      | 185            | 213           | 0.02%           | 0.003%        |
| 16        | 4.362       | 937           | 940         | 944          | rBB      | 150            | 146           | 0.02%           | 0.002%        |
| 17        | 4.639       | 1009          | 1026        | 1068         | rBV      | 76144          | 230782        | 26.36%          | 3.214%        |
| 18        | 4.931       | 1112          | 1117        | 1120         | rBB2     | 318            | 351           | 0.04%           | 0.005%        |
| 19        | 4.957       | 1121          | 1125        | 1128         | rBV      | 135            | 135           | 0.02%           | 0.002%        |
| 20        | 5.067       | 1143          | 1159        | 1184         | rVB      | 146224         | 333355        | 38.08%          | 4.643%        |
| 21        | 5.295       | 1227          | 1230        | 1232         | rBV      | 242            | 153           | 0.02%           | 0.002%        |
| 22        | 5.359       | 1248          | 1250        | 1254         | rBV2     | 362            | 237           | 0.03%           | 0.003%        |
| 23        | 5.375       | 1254          | 1255        | 1263         | rVB      | 227            | 211           | 0.02%           | 0.003%        |
| 24        | 5.423       | 1268          | 1270        | 1274         | rBV      | 134            | 144           | 0.02%           | 0.002%        |
| 25        | 5.494       | 1289          | 1292        | 1296         | rBV      | 133            | 163           | 0.02%           | 0.002%        |
| 26        | 5.578       | 1314          | 1318        | 1320         | rBV      | 142            | 149           | 0.02%           | 0.002%        |
| 27        | 5.594       | 1320          | 1323        | 1328         | rVB      | 510            | 333           | 0.04%           | 0.005%        |
| 28        | 5.729       | 1343          | 1365        | 1391         | rBV2     | 324332         | 875348        | 100.00%         | 12.192%       |
| 29        | 5.967       | 1435          | 1439        | 1440         | rBV2     | 484            | 295           | 0.03%           | 0.004%        |
| 30        | 6.038       | 1458          | 1461        | 1462         | rBV      | 265            | 153           | 0.02%           | 0.002%        |
| 31        | 6.111       | 1481          | 1484        | 1487         | rBV2     | 265            | 217           | 0.02%           | 0.003%        |
| 32        | 6.250       | 1513          | 1527        | 1550         | rBV      | 291306         | 550902        | 62.94%          | 7.673%        |
| 33        | 6.533       | 1605          | 1615        | 1629         | rBV3     | 4352           | 8976          | 1.03%           | 0.125%        |
| 34        | 6.693       | 1649          | 1665        | 1683         | rBV      | 195873         | 377214        | 43.09%          | 5.254%        |
| 35        | 6.928       | 1735          | 1738        | 1740         | rBV      | 163            | 131           | 0.01%           | 0.002%        |
| 36        | 7.041       | 1767          | 1773        | 1781         | rBB2     | 414            | 707           | 0.08%           | 0.010%        |

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Integration Parameters: LSCINT.P

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\SFAMULM112921WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.083  | 1782 | 1786 | 1789 | rBV  | 167    | 196    | 0.02%  | 0.003%  |
| 38 | 7.144  | 1802 | 1805 | 1808 | rBB  | 161    | 127    | 0.01%  | 0.002%  |
| 39 | 7.484  | 1908 | 1911 | 1914 | rBV  | 181    | 178    | 0.02%  | 0.002%  |
| 40 | 7.568  | 1924 | 1937 | 1951 | rBV  | 110198 | 191567 | 21.88% | 2.668%  |
| 41 | 7.732  | 1984 | 1988 | 1997 | rBV  | 206    | 340    | 0.04%  | 0.005%  |
| 42 | 7.783  | 1998 | 2004 | 2011 | rBV3 | 731    | 1249   | 0.14%  | 0.017%  |
| 43 | 7.899  | 2025 | 2040 | 2056 | rBV  | 428518 | 735982 | 84.08% | 10.251% |
| 44 | 8.179  | 2116 | 2127 | 2147 | rBV  | 75813  | 126779 | 14.48% | 1.766%  |
| 45 | 8.436  | 2205 | 2207 | 2211 | rBV  | 166    | 159    | 0.02%  | 0.002%  |
| 46 | 8.478  | 2217 | 2220 | 2224 | rVB2 | 169    | 146    | 0.02%  | 0.002%  |
| 47 | 8.545  | 2236 | 2241 | 2244 | rBV  | 142    | 191    | 0.02%  | 0.003%  |
| 48 | 8.636  | 2256 | 2269 | 2295 | rBV  | 256354 | 456956 | 52.20% | 6.365%  |
| 49 | 8.861  | 2334 | 2339 | 2345 | rBV2 | 496    | 726    | 0.08%  | 0.010%  |
| 50 | 8.915  | 2349 | 2356 | 2359 | rBV2 | 1948   | 2445   | 0.28%  | 0.034%  |
| 51 | 8.970  | 2370 | 2373 | 2376 | rBV  | 292    | 143    | 0.02%  | 0.002%  |
| 52 | 9.115  | 2415 | 2418 | 2420 | rBV  | 178    | 134    | 0.02%  | 0.002%  |
| 53 | 9.163  | 2429 | 2433 | 2436 | rBV4 | 759    | 651    | 0.07%  | 0.009%  |
| 54 | 9.208  | 2445 | 2447 | 2449 | rBV2 | 252    | 130    | 0.01%  | 0.002%  |
| 55 | 9.333  | 2482 | 2486 | 2488 | rBV  | 628    | 559    | 0.06%  | 0.008%  |
| 56 | 9.417  | 2499 | 2512 | 2536 | rBV  | 412567 | 685818 | 78.35% | 9.552%  |
| 57 | 9.571  | 2553 | 2560 | 2567 | rBV  | 579    | 807    | 0.09%  | 0.011%  |
| 58 | 9.697  | 2592 | 2599 | 2600 | rBV3 | 810    | 928    | 0.11%  | 0.013%  |
| 59 | 10.025 | 2693 | 2701 | 2713 | rBV5 | 1292   | 2848   | 0.33%  | 0.040%  |
| 60 | 10.076 | 2713 | 2717 | 2720 | rVV2 | 232    | 190    | 0.02%  | 0.003%  |
| 61 | 10.115 | 2725 | 2729 | 2736 | rVB3 | 751    | 960    | 0.11%  | 0.013%  |
| 62 | 10.243 | 2763 | 2769 | 2782 | rVB7 | 1452   | 3323   | 0.38%  | 0.046%  |
| 63 | 10.359 | 2796 | 2805 | 2810 | rBV4 | 2687   | 4227   | 0.48%  | 0.059%  |
| 64 | 10.481 | 2840 | 2843 | 2845 | rBV2 | 228    | 177    | 0.02%  | 0.002%  |
| 65 | 10.558 | 2861 | 2867 | 2868 | rBV  | 964    | 852    | 0.10%  | 0.012%  |
| 66 | 10.623 | 2882 | 2887 | 2895 | rBV5 | 1368   | 1581   | 0.18%  | 0.022%  |
| 67 | 10.671 | 2895 | 2902 | 2914 | rVB4 | 3530   | 5071   | 0.58%  | 0.071%  |
| 68 | 10.758 | 2916 | 2929 | 2941 | rBV  | 284877 | 454779 | 51.95% | 6.334%  |
| 69 | 10.889 | 2959 | 2970 | 2971 | rBV5 | 823    | 1289   | 0.15%  | 0.018%  |
| 70 | 10.954 | 2984 | 2990 | 2993 | rBV3 | 441    | 467    | 0.05%  | 0.007%  |
| 71 | 11.005 | 3003 | 3006 | 3008 | rBV3 | 731    | 450    | 0.05%  | 0.006%  |
| 72 | 11.063 | 3017 | 3024 | 3031 | rBV3 | 999    | 1592   | 0.18%  | 0.022%  |
| 73 | 11.208 | 3064 | 3069 | 3074 | rVB3 | 689    | 716    | 0.08%  | 0.010%  |
| 74 | 11.282 | 3087 | 3092 | 3096 | rBV3 | 392    | 489    | 0.06%  | 0.007%  |
| 75 | 11.311 | 3096 | 3101 | 3109 | rVV5 | 1761   | 2496   | 0.29%  | 0.035%  |
| 76 | 11.375 | 3114 | 3121 | 3125 | rBV4 | 1840   | 2465   | 0.28%  | 0.034%  |

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Integration Parameters: LSCINT.P

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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\SFAMULM112921WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.417 | 3129 | 3134 | 3140 | rVB4 | 3683   | 4335   | 0.50%  | 0.060%  |
| 78  | 11.578 | 3176 | 3184 | 3191 | rBV5 | 1942   | 3335   | 0.38%  | 0.046%  |
| 79  | 11.696 | 3213 | 3221 | 3230 | rBV8 | 3999   | 6628   | 0.76%  | 0.092%  |
| 80  | 11.812 | 3245 | 3257 | 3271 | rBV  | 491130 | 753657 | 86.10% | 10.497% |
| 81  | 11.896 | 3281 | 3283 | 3285 | rVB  | 291    | 139    | 0.02%  | 0.002%  |
| 82  | 11.944 | 3287 | 3298 | 3301 | rBV4 | 3019   | 4666   | 0.53%  | 0.065%  |
| 83  | 12.037 | 3323 | 3327 | 3332 | rVB3 | 511    | 430    | 0.05%  | 0.006%  |
| 84  | 12.076 | 3332 | 3339 | 3344 | rBV5 | 592    | 795    | 0.09%  | 0.011%  |
| 85  | 12.195 | 3360 | 3376 | 3390 | rBV  | 443119 | 715015 | 81.68% | 9.959%  |
| 86  | 12.323 | 3409 | 3416 | 3418 | rBV4 | 2179   | 2445   | 0.28%  | 0.034%  |
| 87  | 12.388 | 3428 | 3436 | 3438 | rBV3 | 1578   | 2045   | 0.23%  | 0.028%  |
| 88  | 12.725 | 3538 | 3541 | 3543 | rBV2 | 684    | 495    | 0.06%  | 0.007%  |
| 89  | 13.024 | 3628 | 3634 | 3639 | rBV4 | 649    | 867    | 0.10%  | 0.012%  |
| 90  | 13.060 | 3641 | 3645 | 3647 | rVV2 | 451    | 299    | 0.03%  | 0.004%  |
| 91  | 13.587 | 3803 | 3809 | 3818 | rVB5 | 2285   | 3017   | 0.34%  | 0.042%  |
| 92  | 14.085 | 3957 | 3964 | 3973 | rVB2 | 7702   | 10728  | 1.23%  | 0.149%  |
| 93  | 14.192 | 3989 | 3997 | 4008 | rBV4 | 2395   | 3680   | 0.42%  | 0.051%  |
| 94  | 14.272 | 4017 | 4022 | 4031 | rBV4 | 566    | 744    | 0.08%  | 0.010%  |
| 95  | 14.520 | 4097 | 4099 | 4100 | rBV4 | 429    | 185    | 0.02%  | 0.003%  |
| 96  | 14.574 | 4109 | 4116 | 4124 | rBV4 | 1658   | 2860   | 0.33%  | 0.040%  |
| 97  | 14.745 | 4167 | 4169 | 4175 | rBV2 | 321    | 308    | 0.04%  | 0.004%  |
| 98  | 14.799 | 4183 | 4186 | 4187 | rBV3 | 396    | 245    | 0.03%  | 0.003%  |
| 99  | 14.973 | 4237 | 4240 | 4242 | rBV2 | 420    | 290    | 0.03%  | 0.004%  |
| 100 | 15.214 | 4307 | 4315 | 4321 | rBV9 | 2260   | 3638   | 0.42%  | 0.051%  |

Sum of corrected areas: 7179650



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ALS Vial : 43 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU120721\  
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Quant Title : VOC Analysis

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

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