

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121621\  
 Data File : VU046448.D  
 Acq On : 17 Dec 2021 02:18  
 Operator : SY/MD  
 Sample : M5121-02 20X  
 Misc : 7.20g/5.0mL/100ul/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 41 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGL51

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: VU046448.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       | 75            | 82          | 103          | rVB      | 60283          | 74479         | 14.64%          | 1.827%        |
| 2         | 1.919       | 172           | 180         | 202          | rBV      | 42924          | 61926         | 12.18%          | 1.519%        |
| 3         | 2.571       | 371           | 383         | 406          | rBV      | 106577         | 177701        | 34.94%          | 4.359%        |
| 4         | 2.748       | 433           | 438         | 441          | rBV      | 130            | 163           | 0.03%           | 0.004%        |
| 5         | 2.964       | 502           | 505         | 508          | rBB      | 147            | 122           | 0.02%           | 0.003%        |
| 6         | 3.015       | 518           | 521         | 525          | rBV      | 158            | 189           | 0.04%           | 0.005%        |
| 7         | 3.047       | 525           | 531         | 534          | rBV2     | 701            | 835           | 0.16%           | 0.020%        |
| 8         | 3.189       | 563           | 575         | 591          | rVB      | 5910           | 12890         | 2.53%           | 0.316%        |
| 9         | 3.404       | 639           | 642         | 645          | rBB      | 124            | 108           | 0.02%           | 0.003%        |
| 10        | 3.497       | 667           | 671         | 673          | rBB      | 152            | 123           | 0.02%           | 0.003%        |
| 11        | 3.594       | 697           | 701         | 703          | rBV      | 137            | 142           | 0.03%           | 0.003%        |
| 12        | 3.732       | 739           | 744         | 749          | rBV      | 145            | 252           | 0.05%           | 0.006%        |
| 13        | 4.005       | 826           | 829         | 833          | rBB      | 148            | 151           | 0.03%           | 0.004%        |
| 14        | 4.250       | 901           | 905         | 908          | rBB      | 152            | 144           | 0.03%           | 0.004%        |
| 15        | 4.632       | 1011          | 1024        | 1051         | rBV      | 45225          | 122963        | 24.18%          | 3.016%        |
| 16        | 4.841       | 1086          | 1089        | 1091         | rBB2     | 226            | 127           | 0.02%           | 0.003%        |
| 17        | 5.066       | 1144          | 1159        | 1176         | rBV      | 92935          | 202471        | 39.81%          | 4.966%        |
| 18        | 5.230       | 1206          | 1210        | 1212         | rBV      | 165            | 164           | 0.03%           | 0.004%        |
| 19        | 5.250       | 1213          | 1216        | 1220         | rVB      | 189            | 152           | 0.03%           | 0.004%        |
| 20        | 5.353       | 1247          | 1248        | 1251         | rVB      | 249            | 115           | 0.02%           | 0.003%        |
| 21        | 5.729       | 1344          | 1365        | 1388         | rBV2     | 189054         | 508606        | 100.00%         | 12.476%       |
| 22        | 5.835       | 1396          | 1398        | 1401         | rVB      | 275            | 158           | 0.03%           | 0.004%        |
| 23        | 6.002       | 1445          | 1450        | 1453         | rBB      | 138            | 139           | 0.03%           | 0.003%        |
| 24        | 6.060       | 1466          | 1468        | 1471         | rBB      | 154            | 104           | 0.02%           | 0.003%        |
| 25        | 6.108       | 1480          | 1483        | 1485         | rBV      | 124            | 108           | 0.02%           | 0.003%        |
| 26        | 6.169       | 1499          | 1502        | 1505         | rBB      | 151            | 123           | 0.02%           | 0.003%        |
| 27        | 6.195       | 1508          | 1510        | 1513         | rBB      | 143            | 98            | 0.02%           | 0.002%        |
| 28        | 6.250       | 1514          | 1527        | 1554         | rBV      | 173450         | 329701        | 64.82%          | 8.087%        |
| 29        | 6.346       | 1555          | 1557        | 1559         | rVV      | 334            | 184           | 0.04%           | 0.005%        |
| 30        | 6.372       | 1563          | 1565        | 1567         | rBB      | 248            | 115           | 0.02%           | 0.003%        |
| 31        | 6.449       | 1586          | 1589        | 1591         | rBB      | 148            | 97            | 0.02%           | 0.002%        |
| 32        | 6.529       | 1610          | 1614        | 1617         | rBB2     | 424            | 384           | 0.08%           | 0.009%        |
| 33        | 6.693       | 1652          | 1665        | 1684         | rBV      | 118763         | 227647        | 44.76%          | 5.584%        |
| 34        | 6.812       | 1698          | 1702        | 1706         | rBV2     | 252            | 267           | 0.05%           | 0.007%        |
| 35        | 6.867       | 1716          | 1719        | 1722         | rBB      | 142            | 121           | 0.02%           | 0.003%        |
| 36        | 7.054       | 1773          | 1777        | 1782         | rBB      | 254            | 240           | 0.05%           | 0.006%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Sampling : 1

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.189  | 1818 | 1819 | 1822 | rVB  | 233    | 93     | 0.02%  | 0.002%  |
| 38 | 7.224  | 1827 | 1830 | 1833 | rBB  | 161    | 134    | 0.03%  | 0.003%  |
| 39 | 7.568  | 1925 | 1937 | 1951 | rBV  | 61245  | 103697 | 20.39% | 2.544%  |
| 40 | 7.687  | 1971 | 1974 | 1978 | rBB  | 153    | 147    | 0.03%  | 0.004%  |
| 41 | 7.787  | 2000 | 2005 | 2010 | rBB3 | 546    | 611    | 0.12%  | 0.015%  |
| 42 | 7.819  | 2011 | 2015 | 2017 | rBV  | 147    | 121    | 0.02%  | 0.003%  |
| 43 | 7.899  | 2028 | 2040 | 2055 | rBV  | 229876 | 389671 | 76.62% | 9.558%  |
| 44 | 8.073  | 2091 | 2094 | 2097 | rBB  | 138    | 94     | 0.02%  | 0.002%  |
| 45 | 8.182  | 2116 | 2128 | 2142 | rBV  | 43163  | 69472  | 13.66% | 1.704%  |
| 46 | 8.250  | 2147 | 2149 | 2153 | rBB  | 125    | 111    | 0.02%  | 0.003%  |
| 47 | 8.459  | 2212 | 2214 | 2215 | rBV  | 230    | 115    | 0.02%  | 0.003%  |
| 48 | 8.562  | 2245 | 2246 | 2253 | rVB2 | 340    | 290    | 0.06%  | 0.007%  |
| 49 | 8.635  | 2257 | 2269 | 2294 | rBV  | 153524 | 250846 | 49.32% | 6.153%  |
| 50 | 8.774  | 2309 | 2312 | 2314 | rBV  | 190    | 129    | 0.03%  | 0.003%  |
| 51 | 8.873  | 2340 | 2343 | 2345 | rBV  | 131    | 118    | 0.02%  | 0.003%  |
| 52 | 8.918  | 2349 | 2357 | 2363 | rVB3 | 1078   | 1585   | 0.31%  | 0.039%  |
| 53 | 9.021  | 2387 | 2389 | 2391 | rBV  | 132    | 96     | 0.02%  | 0.002%  |
| 54 | 9.092  | 2407 | 2411 | 2414 | rBV  | 150    | 167    | 0.03%  | 0.004%  |
| 55 | 9.250  | 2456 | 2460 | 2462 | rBV  | 153    | 155    | 0.03%  | 0.004%  |
| 56 | 9.301  | 2472 | 2476 | 2479 | rBV  | 163    | 174    | 0.03%  | 0.004%  |
| 57 | 9.356  | 2490 | 2493 | 2495 | rBV  | 135    | 122    | 0.02%  | 0.003%  |
| 58 | 9.420  | 2500 | 2513 | 2540 | rVV  | 263464 | 427831 | 84.12% | 10.494% |
| 59 | 9.513  | 2540 | 2542 | 2547 | rVB  | 239    | 189    | 0.04%  | 0.005%  |
| 60 | 9.545  | 2548 | 2552 | 2558 | rBV  | 156    | 256    | 0.05%  | 0.006%  |
| 61 | 9.668  | 2587 | 2590 | 2593 | rBB  | 127    | 109    | 0.02%  | 0.003%  |
| 62 | 9.722  | 2606 | 2607 | 2611 | rVB  | 354    | 183    | 0.04%  | 0.004%  |
| 63 | 9.761  | 2616 | 2619 | 2622 | rBV  | 133    | 137    | 0.03%  | 0.003%  |
| 64 | 9.832  | 2639 | 2641 | 2643 | rBV  | 136    | 97     | 0.02%  | 0.002%  |
| 65 | 9.880  | 2653 | 2656 | 2658 | rBV  | 124    | 110    | 0.02%  | 0.003%  |
| 66 | 9.970  | 2682 | 2684 | 2687 | rBB  | 143    | 97     | 0.02%  | 0.002%  |
| 67 | 10.063 | 2709 | 2713 | 2715 | rBV  | 151    | 126    | 0.02%  | 0.003%  |
| 68 | 10.137 | 2733 | 2736 | 2739 | rBV  | 175    | 164    | 0.03%  | 0.004%  |
| 69 | 10.330 | 2793 | 2796 | 2799 | rBB  | 149    | 122    | 0.02%  | 0.003%  |
| 70 | 10.352 | 2800 | 2803 | 2806 | rBB  | 166    | 135    | 0.03%  | 0.003%  |
| 71 | 10.375 | 2807 | 2810 | 2811 | rBV  | 129    | 94     | 0.02%  | 0.002%  |
| 72 | 10.674 | 2896 | 2903 | 2910 | rVB3 | 1275   | 1560   | 0.31%  | 0.038%  |
| 73 | 10.758 | 2917 | 2929 | 2942 | rBV  | 167626 | 268040 | 52.70% | 6.575%  |
| 74 | 10.867 | 2960 | 2963 | 2967 | rBV2 | 201    | 204    | 0.04%  | 0.005%  |
| 75 | 11.069 | 3023 | 3026 | 3029 | rBV2 | 405    | 382    | 0.08%  | 0.009%  |
| 76 | 11.118 | 3039 | 3041 | 3043 | rBV2 | 227    | 146    | 0.03%  | 0.004%  |

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Instrument :  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMULM112921WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.249 | 3078 | 3082 | 3084 | rBV  | 152    | 125    | 0.02%  | 0.003%  |
| 78  | 11.314 | 3101 | 3102 | 3110 | rVB  | 273    | 126    | 0.02%  | 0.003%  |
| 79  | 11.362 | 3113 | 3117 | 3118 | rBV  | 176    | 144    | 0.03%  | 0.004%  |
| 80  | 11.417 | 3128 | 3134 | 3140 | rBV4 | 1115   | 1280   | 0.25%  | 0.031%  |
| 81  | 11.458 | 3141 | 3147 | 3155 | rVB5 | 1223   | 1837   | 0.36%  | 0.045%  |
| 82  | 11.497 | 3156 | 3159 | 3162 | rBV  | 205    | 149    | 0.03%  | 0.004%  |
| 83  | 11.577 | 3179 | 3184 | 3192 | rVB2 | 812    | 733    | 0.14%  | 0.018%  |
| 84  | 11.700 | 3215 | 3222 | 3227 | rVB4 | 1131   | 1263   | 0.25%  | 0.031%  |
| 85  | 11.748 | 3235 | 3237 | 3241 | rVB  | 273    | 176    | 0.03%  | 0.004%  |
| 86  | 11.812 | 3241 | 3257 | 3273 | rBV  | 285446 | 441692 | 86.84% | 10.834% |
| 87  | 11.944 | 3293 | 3298 | 3301 | rBV5 | 869    | 954    | 0.19%  | 0.023%  |
| 88  | 12.118 | 3348 | 3352 | 3356 | rBV2 | 255    | 237    | 0.05%  | 0.006%  |
| 89  | 12.195 | 3361 | 3376 | 3393 | rBV  | 237495 | 378533 | 74.43% | 9.285%  |
| 90  | 12.330 | 3414 | 3418 | 3420 | rBV2 | 446    | 354    | 0.07%  | 0.009%  |
| 91  | 12.410 | 3435 | 3443 | 3449 | rVB6 | 693    | 919    | 0.18%  | 0.023%  |
| 92  | 12.526 | 3476 | 3479 | 3482 | rBV2 | 343    | 306    | 0.06%  | 0.008%  |
| 93  | 12.738 | 3542 | 3545 | 3549 | rVB  | 209    | 112    | 0.02%  | 0.003%  |
| 94  | 12.770 | 3549 | 3555 | 3563 | rBV  | 847    | 1295   | 0.25%  | 0.032%  |
| 95  | 12.831 | 3570 | 3574 | 3575 | rBV  | 261    | 146    | 0.03%  | 0.004%  |
| 96  | 13.590 | 3804 | 3810 | 3816 | rBV4 | 853    | 1065   | 0.21%  | 0.026%  |
| 97  | 14.195 | 3992 | 3998 | 4003 | rBV3 | 1630   | 1866   | 0.37%  | 0.046%  |
| 98  | 15.211 | 4308 | 4314 | 4322 | rVB5 | 1439   | 1805   | 0.35%  | 0.044%  |
| 99  | 15.413 | 4375 | 4377 | 4380 | rBV2 | 326    | 188    | 0.04%  | 0.005%  |
| 100 | 15.452 | 4386 | 4389 | 4391 | rBV3 | 302    | 209    | 0.04%  | 0.005%  |

Sum of corrected areas: 4076753



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ALS Vial : 41 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

\*\*\*\*\*

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

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