

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU052424\  
 Data File : VU058965.D  
 Acq On : 24 May 2024 12:18  
 Operator : MD/SY  
 Sample : VU0524MBL02  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK051

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\SFAMULM052324WMA.M

Title : VOC Analysis

Signal : TIC: VU058965.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         | 1.595       | 88            | 95          | 116          | rVB      | 119009         | 143293        | 15.37%          | 2.214%        |
| 2         | 1.856       | 173           | 176         | 177          | rBV      | 1371           | 921           | 0.10%           | 0.014%        |
| 3         | 1.911       | 184           | 193         | 205          | rBV      | 111351         | 149940        | 16.08%          | 2.317%        |
| 4         | 2.367       | 331           | 335         | 338          | rBV2     | 629            | 542           | 0.06%           | 0.008%        |
| 5         | 2.560       | 383           | 395         | 414          | rBV      | 179562         | 295034        | 31.64%          | 4.559%        |
| 6         | 2.775       | 459           | 462         | 463          | rBV      | 424            | 244           | 0.03%           | 0.004%        |
| 7         | 2.788       | 463           | 466         | 474          | rVB2     | 869            | 1117          | 0.12%           | 0.017%        |
| 8         | 3.042       | 536           | 545         | 557          | rVB2     | 3059           | 5352          | 0.57%           | 0.083%        |
| 9         | 3.168       | 580           | 584         | 585          | rBV      | 469            | 326           | 0.03%           | 0.005%        |
| 10        | 3.679       | 736           | 743         | 744          | rBV2     | 203            | 213           | 0.02%           | 0.003%        |
| 11        | 3.730       | 756           | 759         | 763          | rVB      | 276            | 192           | 0.02%           | 0.003%        |
| 12        | 3.827       | 786           | 789         | 793          | rVV2     | 229            | 183           | 0.02%           | 0.003%        |
| 13        | 3.997       | 839           | 842         | 851          | rVB2     | 317            | 432           | 0.05%           | 0.007%        |
| 14        | 4.136       | 879           | 885         | 888          | rBV2     | 336            | 296           | 0.03%           | 0.005%        |
| 15        | 4.242       | 914           | 918         | 920          | rBV2     | 240            | 208           | 0.02%           | 0.003%        |
| 16        | 4.364       | 952           | 956         | 959          | rBV      | 265            | 260           | 0.03%           | 0.004%        |
| 17        | 4.435       | 973           | 978         | 982          | rVB2     | 243            | 253           | 0.03%           | 0.004%        |
| 18        | 4.499       | 994           | 998         | 1001         | rVB2     | 220            | 203           | 0.02%           | 0.003%        |
| 19        | 4.531       | 1005          | 1008        | 1013         | rBV2     | 211            | 204           | 0.02%           | 0.003%        |
| 20        | 4.624       | 1027          | 1037        | 1070         | rBV      | 80347          | 225171        | 24.14%          | 3.479%        |
| 21        | 4.955       | 1137          | 1140        | 1144         | rBV3     | 238            | 203           | 0.02%           | 0.003%        |
| 22        | 5.055       | 1152          | 1171        | 1200         | rBV      | 162886         | 364766        | 39.11%          | 5.636%        |
| 23        | 5.193       | 1212          | 1214        | 1219         | rVB3     | 481            | 306           | 0.03%           | 0.005%        |
| 24        | 5.226       | 1222          | 1224        | 1232         | rVB2     | 348            | 378           | 0.04%           | 0.006%        |
| 25        | 5.489       | 1304          | 1306        | 1310         | rVB2     | 271            | 172           | 0.02%           | 0.003%        |
| 26        | 5.541       | 1316          | 1322        | 1326         | rBV2     | 234            | 242           | 0.03%           | 0.004%        |
| 27        | 5.717       | 1356          | 1377        | 1410         | rBV2     | 340482         | 932590        | 100.00%         | 14.410%       |
| 28        | 6.036       | 1473          | 1476        | 1480         | rVB3     | 235            | 185           | 0.02%           | 0.003%        |
| 29        | 6.116       | 1497          | 1501        | 1503         | rBV2     | 250            | 189           | 0.02%           | 0.003%        |
| 30        | 6.245       | 1526          | 1541        | 1561         | rBV      | 225783         | 436841        | 46.84%          | 6.750%        |
| 31        | 6.447       | 1601          | 1604        | 1609         | rVB3     | 280            | 232           | 0.02%           | 0.004%        |
| 32        | 6.537       | 1622          | 1632        | 1644         | rVB5     | 7082           | 14454         | 1.55%           | 0.223%        |
| 33        | 6.582       | 1644          | 1646        | 1649         | rBV      | 415            | 185           | 0.02%           | 0.003%        |
| 34        | 6.608       | 1650          | 1654        | 1657         | rVB2     | 467            | 279           | 0.03%           | 0.004%        |
| 35        | 6.685       | 1664          | 1678        | 1702         | rBV      | 212545         | 421810        | 45.23%          | 6.518%        |
| 36        | 6.801       | 1712          | 1714        | 1716         | rBV      | 354            | 194           | 0.02%           | 0.003%        |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK051

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\SFAMULM052324WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.856  | 1729 | 1731 | 1734 | rVB  | 365    | 196    | 0.02%  | 0.003%  |
| 38 | 7.264  | 1857 | 1858 | 1862 | rVB  | 351    | 201    | 0.02%  | 0.003%  |
| 39 | 7.505  | 1925 | 1933 | 1938 | rBV  | 308    | 391    | 0.04%  | 0.006%  |
| 40 | 7.560  | 1938 | 1950 | 1976 | rBV  | 104509 | 192452 | 20.64% | 2.974%  |
| 41 | 7.894  | 2036 | 2054 | 2078 | rBV  | 381353 | 678329 | 72.74% | 10.481% |
| 42 | 8.078  | 2107 | 2111 | 2114 | rVB3 | 371    | 310    | 0.03%  | 0.005%  |
| 43 | 8.094  | 2114 | 2116 | 2126 | rVB3 | 544    | 594    | 0.06%  | 0.009%  |
| 44 | 8.139  | 2126 | 2130 | 2131 | rBV2 | 282    | 176    | 0.02%  | 0.003%  |
| 45 | 8.177  | 2131 | 2142 | 2165 | rBV  | 69750  | 126256 | 13.54% | 1.951%  |
| 46 | 8.283  | 2171 | 2175 | 2180 | rVB3 | 521    | 508    | 0.05%  | 0.008%  |
| 47 | 8.322  | 2185 | 2187 | 2192 | rVB2 | 278    | 193    | 0.02%  | 0.003%  |
| 48 | 8.354  | 2192 | 2197 | 2203 | rBV2 | 214    | 261    | 0.03%  | 0.004%  |
| 49 | 8.467  | 2227 | 2232 | 2237 | rBV2 | 466    | 444    | 0.05%  | 0.007%  |
| 50 | 8.566  | 2259 | 2263 | 2270 | rBV2 | 244    | 299    | 0.03%  | 0.005%  |
| 51 | 8.631  | 2271 | 2283 | 2318 | rBV  | 222537 | 460609 | 49.39% | 7.117%  |
| 52 | 8.823  | 2341 | 2343 | 2346 | rVB3 | 388    | 173    | 0.02%  | 0.003%  |
| 53 | 8.885  | 2359 | 2362 | 2364 | rBV2 | 331    | 203    | 0.02%  | 0.003%  |
| 54 | 8.959  | 2383 | 2385 | 2388 | rVB  | 346    | 212    | 0.02%  | 0.003%  |
| 55 | 9.007  | 2397 | 2400 | 2404 | rVV3 | 288    | 256    | 0.03%  | 0.004%  |
| 56 | 9.074  | 2417 | 2421 | 2425 | rBV  | 303    | 298    | 0.03%  | 0.005%  |
| 57 | 9.232  | 2467 | 2470 | 2473 | rVB  | 360    | 225    | 0.02%  | 0.003%  |
| 58 | 9.270  | 2473 | 2482 | 2485 | rBV2 | 177    | 271    | 0.03%  | 0.004%  |
| 59 | 9.412  | 2514 | 2526 | 2545 | rBV  | 316565 | 542887 | 58.21% | 8.388%  |
| 60 | 9.630  | 2590 | 2594 | 2597 | rVB2 | 290    | 191    | 0.02%  | 0.003%  |
| 61 | 9.666  | 2599 | 2605 | 2608 | rBV2 | 276    | 240    | 0.03%  | 0.004%  |
| 62 | 9.698  | 2608 | 2615 | 2629 | rBV4 | 925    | 1838   | 0.20%  | 0.028%  |
| 63 | 9.862  | 2663 | 2666 | 2674 | rVB2 | 192    | 173    | 0.02%  | 0.003%  |
| 64 | 9.987  | 2702 | 2705 | 2709 | rBV2 | 184    | 189    | 0.02%  | 0.003%  |
| 65 | 10.103 | 2736 | 2741 | 2747 | rVB3 | 687    | 707    | 0.08%  | 0.011%  |
| 66 | 10.241 | 2780 | 2784 | 2788 | rVB  | 372    | 305    | 0.03%  | 0.005%  |
| 67 | 10.270 | 2788 | 2793 | 2796 | rBV2 | 227    | 221    | 0.02%  | 0.003%  |
| 68 | 10.412 | 2833 | 2837 | 2839 | rBV2 | 311    | 245    | 0.03%  | 0.004%  |
| 69 | 10.486 | 2852 | 2860 | 2864 | rBV3 | 359    | 459    | 0.05%  | 0.007%  |
| 70 | 10.611 | 2893 | 2899 | 2906 | rVV2 | 264    | 420    | 0.05%  | 0.006%  |
| 71 | 10.647 | 2907 | 2910 | 2917 | rVB2 | 206    | 187    | 0.02%  | 0.003%  |
| 72 | 10.749 | 2927 | 2942 | 2964 | rBV  | 294492 | 476631 | 51.11% | 7.365%  |
| 73 | 10.888 | 2982 | 2985 | 2990 | rVV2 | 417    | 356    | 0.04%  | 0.006%  |
| 74 | 11.003 | 3016 | 3021 | 3025 | rBV2 | 246    | 248    | 0.03%  | 0.004%  |
| 75 | 11.473 | 3164 | 3167 | 3171 | rVB2 | 372    | 249    | 0.03%  | 0.004%  |
| 76 | 11.499 | 3171 | 3175 | 3177 | rBV  | 241    | 181    | 0.02%  | 0.003%  |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
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 ClientSampleId :  
 VBLK051

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\SFAMULM052324WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.611 | 3205 | 3210 | 3213 | rBV2 | 265    | 288    | 0.03%  | 0.004% |
| 78  | 11.708 | 3238 | 3240 | 3246 | rVB2 | 293    | 218    | 0.02%  | 0.003% |
| 79  | 11.749 | 3249 | 3253 | 3256 | rBV2 | 310    | 240    | 0.03%  | 0.004% |
| 80  | 11.807 | 3259 | 3271 | 3298 | rBV  | 266739 | 447484 | 47.98% | 6.914% |
| 81  | 11.955 | 3314 | 3317 | 3322 | rVB5 | 541    | 380    | 0.04%  | 0.006% |
| 82  | 12.036 | 3339 | 3342 | 3344 | rBV  | 318    | 176    | 0.02%  | 0.003% |
| 83  | 12.109 | 3361 | 3365 | 3368 | rBV  | 269    | 256    | 0.03%  | 0.004% |
| 84  | 12.190 | 3377 | 3390 | 3421 | rBV  | 318261 | 531123 | 56.95% | 8.207% |
| 85  | 12.331 | 3432 | 3434 | 3438 | rVB2 | 456    | 236    | 0.03%  | 0.004% |
| 86  | 12.373 | 3443 | 3447 | 3449 | rVB2 | 337    | 234    | 0.03%  | 0.004% |
| 87  | 12.444 | 3466 | 3469 | 3473 | rBV2 | 449    | 385    | 0.04%  | 0.006% |
| 88  | 12.650 | 3530 | 3533 | 3539 | rVB2 | 412    | 376    | 0.04%  | 0.006% |
| 89  | 13.627 | 3833 | 3837 | 3838 | rBV  | 279    | 188    | 0.02%  | 0.003% |
| 90  | 13.740 | 3869 | 3872 | 3878 | rVB2 | 381    | 379    | 0.04%  | 0.006% |
| 91  | 13.926 | 3927 | 3930 | 3935 | rBV2 | 358    | 354    | 0.04%  | 0.005% |
| 92  | 13.990 | 3947 | 3950 | 3953 | rBV  | 327    | 229    | 0.02%  | 0.004% |
| 93  | 14.087 | 3977 | 3980 | 3982 | rBV  | 361    | 263    | 0.03%  | 0.004% |
| 94  | 14.521 | 4112 | 4115 | 4118 | rBV2 | 288    | 206    | 0.02%  | 0.003% |
| 95  | 14.675 | 4160 | 4163 | 4166 | rBV  | 360    | 298    | 0.03%  | 0.005% |
| 96  | 14.759 | 4186 | 4189 | 4192 | rBV2 | 364    | 226    | 0.02%  | 0.003% |
| 97  | 15.039 | 4270 | 4276 | 4280 | rBV3 | 552    | 795    | 0.09%  | 0.012% |
| 98  | 15.338 | 4367 | 4369 | 4372 | rBV2 | 565    | 395    | 0.04%  | 0.006% |
| 99  | 15.402 | 4383 | 4389 | 4392 | rBV3 | 575    | 706    | 0.08%  | 0.011% |
| 100 | 15.817 | 4516 | 4518 | 4524 | rVB4 | 569    | 486    | 0.05%  | 0.008% |

Sum of corrected areas: 6471915



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Instrument :  
MSVOA\_U  
ClientSampleId :  
VBLK051

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052324WMA.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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Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU052424\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052324WMA.M  
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 |