

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100521\  
 Data File : VU045152.D  
 Acq On : 05 Oct 2021 18:07  
 Operator : SY/MD  
 Sample : M4025-04  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AM4

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\SFAMULM092321WMA.M  
 Title : VOC Analysis

Signal : TIC: VU045152.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         | 1.601       | 74            | 81          | 96           | rBV      | 163789         | 189851        | 13.93%          | 1.832%        |
| 2         | 1.909       | 169           | 177         | 192          | rVB      | 138671         | 191129        | 14.03%          | 1.845%        |
| 3         | 2.572       | 370           | 383         | 403          | rBV      | 275958         | 463942        | 34.05%          | 4.478%        |
| 4         | 2.691       | 416           | 420         | 422          | rBV      | 290            | 249           | 0.02%           | 0.002%        |
| 5         | 2.771       | 440           | 445         | 448          | rBV2     | 282            | 278           | 0.02%           | 0.003%        |
| 6         | 2.793       | 448           | 452         | 453          | rBV      | 476            | 345           | 0.03%           | 0.003%        |
| 7         | 2.864       | 470           | 474         | 476          | rBV      | 159            | 125           | 0.01%           | 0.001%        |
| 8         | 2.896       | 482           | 484         | 490          | rVB2     | 206            | 166           | 0.01%           | 0.002%        |
| 9         | 2.928       | 490           | 494         | 497          | rBV2     | 230            | 254           | 0.02%           | 0.002%        |
| 10        | 2.954       | 497           | 502         | 506          | rBV2     | 347            | 423           | 0.03%           | 0.004%        |
| 11        | 3.006       | 512           | 518         | 520          | rBV2     | 173            | 194           | 0.01%           | 0.002%        |
| 12        | 3.044       | 528           | 530         | 534          | rBV2     | 220            | 187           | 0.01%           | 0.002%        |
| 13        | 3.099       | 543           | 547         | 554          | rBV      | 250            | 212           | 0.02%           | 0.002%        |
| 14        | 3.163       | 561           | 567         | 570          | rBV2     | 202            | 229           | 0.02%           | 0.002%        |
| 15        | 3.182       | 570           | 573         | 575          | rBV      | 422            | 331           | 0.02%           | 0.003%        |
| 16        | 3.237       | 587           | 590         | 597          | rVB      | 234            | 187           | 0.01%           | 0.002%        |
| 17        | 3.395       | 636           | 639         | 641          | rBV2     | 183            | 126           | 0.01%           | 0.001%        |
| 18        | 3.623       | 707           | 710         | 711          | rBV      | 176            | 125           | 0.01%           | 0.001%        |
| 19        | 3.668       | 723           | 724         | 729          | rVB2     | 175            | 135           | 0.01%           | 0.001%        |
| 20        | 3.713       | 735           | 738         | 742          | rVB      | 219            | 148           | 0.01%           | 0.001%        |
| 21        | 3.819       | 767           | 771         | 776          | rBV2     | 204            | 173           | 0.01%           | 0.002%        |
| 22        | 3.864       | 782           | 785         | 789          | rVB      | 156            | 160           | 0.01%           | 0.002%        |
| 23        | 4.285       | 913           | 916         | 918          | rVB      | 189            | 128           | 0.01%           | 0.001%        |
| 24        | 4.311       | 918           | 924         | 926          | rBV2     | 204            | 258           | 0.02%           | 0.002%        |
| 25        | 4.369       | 937           | 942         | 945          | rBV2     | 199            | 238           | 0.02%           | 0.002%        |
| 26        | 4.462       | 966           | 971         | 974          | rBV      | 276            | 248           | 0.02%           | 0.002%        |
| 27        | 4.633       | 1006          | 1024        | 1052         | rBV      | 151625         | 386469        | 28.36%          | 3.730%        |
| 28        | 4.996       | 1135          | 1137        | 1141         | rVB3     | 177            | 132           | 0.01%           | 0.001%        |
| 29        | 5.070       | 1141          | 1160        | 1187         | rBV      | 243149         | 529140        | 38.83%          | 5.107%        |
| 30        | 5.215       | 1202          | 1205        | 1211         | rVB3     | 303            | 326           | 0.02%           | 0.003%        |
| 31        | 5.269       | 1217          | 1222        | 1223         | rBV      | 564            | 384           | 0.03%           | 0.004%        |
| 32        | 5.379       | 1251          | 1256        | 1263         | rVB3     | 359            | 393           | 0.03%           | 0.004%        |
| 33        | 5.520       | 1296          | 1300        | 1303         | rBV2     | 170            | 182           | 0.01%           | 0.002%        |
| 34        | 5.552       | 1303          | 1310        | 1312         | rBV      | 222            | 280           | 0.02%           | 0.003%        |
| 35        | 5.729       | 1343          | 1365        | 1393         | rVV2     | 501874         | 1362570       | 100.00%         | 13.150%       |
| 36        | 5.867       | 1406          | 1408        | 1411         | rBV2     | 306            | 214           | 0.02%           | 0.002%        |

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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\SFAMULM092321WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 6.076  | 1469 | 1473 | 1477 | rBV3 | 190    | 223     | 0.02%  | 0.002%  |
| 38 | 6.108  | 1479 | 1483 | 1485 | rBV2 | 331    | 240     | 0.02%  | 0.002%  |
| 39 | 6.157  | 1496 | 1498 | 1504 | rVB3 | 217    | 220     | 0.02%  | 0.002%  |
| 40 | 6.253  | 1512 | 1528 | 1546 | rBV  | 407752 | 761672  | 55.90% | 7.351%  |
| 41 | 6.536  | 1607 | 1616 | 1626 | rBV8 | 4319   | 7987    | 0.59%  | 0.077%  |
| 42 | 6.697  | 1650 | 1666 | 1685 | rBV  | 317705 | 619980  | 45.50% | 5.984%  |
| 43 | 6.793  | 1693 | 1696 | 1697 | rBV2 | 328    | 171     | 0.01%  | 0.002%  |
| 44 | 6.851  | 1711 | 1714 | 1716 | rBV2 | 201    | 132     | 0.01%  | 0.001%  |
| 45 | 6.890  | 1723 | 1726 | 1730 | rBV2 | 176    | 129     | 0.01%  | 0.001%  |
| 46 | 7.047  | 1768 | 1775 | 1787 | rVB3 | 633    | 1209    | 0.09%  | 0.012%  |
| 47 | 7.099  | 1787 | 1791 | 1794 | rBV2 | 199    | 205     | 0.02%  | 0.002%  |
| 48 | 7.186  | 1810 | 1818 | 1831 | rVB3 | 2145   | 3610    | 0.26%  | 0.035%  |
| 49 | 7.568  | 1923 | 1937 | 1957 | rBV  | 176960 | 310993  | 22.82% | 3.001%  |
| 50 | 7.694  | 1968 | 1976 | 1984 | rVB4 | 1289   | 2107    | 0.15%  | 0.020%  |
| 51 | 7.903  | 2027 | 2041 | 2056 | rBV  | 619716 | 1061947 | 77.94% | 10.249% |
| 52 | 7.973  | 2058 | 2063 | 2077 | rVB  | 9557   | 15389   | 1.13%  | 0.149%  |
| 53 | 8.112  | 2104 | 2106 | 2112 | rVB2 | 297    | 241     | 0.02%  | 0.002%  |
| 54 | 8.182  | 2116 | 2128 | 2148 | rVV2 | 125052 | 208155  | 15.28% | 2.009%  |
| 55 | 8.382  | 2186 | 2190 | 2191 | rBV2 | 188    | 164     | 0.01%  | 0.002%  |
| 56 | 8.475  | 2214 | 2219 | 2223 | rBV2 | 272    | 345     | 0.03%  | 0.003%  |
| 57 | 8.555  | 2238 | 2244 | 2255 | rBV4 | 1266   | 1861    | 0.14%  | 0.018%  |
| 58 | 8.639  | 2255 | 2270 | 2302 | rBV  | 465207 | 818637  | 60.08% | 7.901%  |
| 59 | 8.989  | 2374 | 2379 | 2382 | rBV2 | 127    | 146     | 0.01%  | 0.001%  |
| 60 | 9.050  | 2394 | 2398 | 2403 | rBV2 | 255    | 342     | 0.03%  | 0.003%  |
| 61 | 9.105  | 2412 | 2415 | 2422 | rBV2 | 188    | 300     | 0.02%  | 0.003%  |
| 62 | 9.147  | 2426 | 2428 | 2434 | rBV  | 171    | 215     | 0.02%  | 0.002%  |
| 63 | 9.366  | 2491 | 2496 | 2499 | rBV2 | 224    | 215     | 0.02%  | 0.002%  |
| 64 | 9.420  | 2499 | 2513 | 2554 | rBV  | 567509 | 932065  | 68.40% | 8.996%  |
| 65 | 9.693  | 2593 | 2598 | 2606 | rVB4 | 1062   | 1450    | 0.11%  | 0.014%  |
| 66 | 9.796  | 2626 | 2630 | 2636 | rVB2 | 247    | 287     | 0.02%  | 0.003%  |
| 67 | 9.890  | 2654 | 2659 | 2663 | rBV2 | 186    | 258     | 0.02%  | 0.002%  |
| 68 | 10.021 | 2697 | 2700 | 2705 | rBV2 | 170    | 161     | 0.01%  | 0.002%  |
| 69 | 10.099 | 2722 | 2724 | 2725 | rBV  | 316    | 155     | 0.01%  | 0.001%  |
| 70 | 10.218 | 2757 | 2761 | 2765 | rBV2 | 206    | 199     | 0.01%  | 0.002%  |
| 71 | 10.356 | 2801 | 2804 | 2806 | rBV  | 198    | 126     | 0.01%  | 0.001%  |
| 72 | 10.439 | 2828 | 2830 | 2834 | rVB  | 298    | 220     | 0.02%  | 0.002%  |
| 73 | 10.674 | 2894 | 2903 | 2911 | rBV3 | 3093   | 4665    | 0.34%  | 0.045%  |
| 74 | 10.761 | 2917 | 2930 | 2950 | rVB  | 439559 | 701377  | 51.47% | 6.769%  |
| 75 | 10.838 | 2950 | 2954 | 2958 | rBV3 | 256    | 251     | 0.02%  | 0.002%  |
| 76 | 10.867 | 2958 | 2963 | 2968 | rBV3 | 604    | 787     | 0.06%  | 0.008%  |

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Instrument :  
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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\SFAMULM092321WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 10.922 | 2978 | 2980 | 2987 | rVB3 | 334    | 331    | 0.02%  | 0.003% |
| 78  | 11.124 | 3036 | 3043 | 3046 | rBV3 | 540    | 702    | 0.05%  | 0.007% |
| 79  | 11.144 | 3047 | 3049 | 3053 | rVB3 | 612    | 371    | 0.03%  | 0.004% |
| 80  | 11.253 | 3080 | 3083 | 3085 | rBV  | 220    | 174    | 0.01%  | 0.002% |
| 81  | 11.295 | 3093 | 3096 | 3102 | rVB3 | 368    | 307    | 0.02%  | 0.003% |
| 82  | 11.430 | 3134 | 3138 | 3139 | rBV  | 276    | 167    | 0.01%  | 0.002% |
| 83  | 11.459 | 3141 | 3147 | 3159 | rVB6 | 1978   | 3537   | 0.26%  | 0.034% |
| 84  | 11.581 | 3182 | 3185 | 3189 | rVB2 | 522    | 377    | 0.03%  | 0.004% |
| 85  | 11.636 | 3200 | 3202 | 3206 | rVB  | 297    | 207    | 0.02%  | 0.002% |
| 86  | 11.697 | 3215 | 3221 | 3222 | rBV2 | 1065   | 972    | 0.07%  | 0.009% |
| 87  | 11.751 | 3234 | 3238 | 3242 | rBV  | 199    | 179    | 0.01%  | 0.002% |
| 88  | 11.816 | 3245 | 3258 | 3276 | rBV  | 540866 | 848489 | 62.27% | 8.189% |
| 89  | 11.976 | 3304 | 3308 | 3315 | rVB3 | 2112   | 2436   | 0.18%  | 0.024% |
| 90  | 12.195 | 3361 | 3376 | 3398 | rVV  | 565642 | 912033 | 66.93% | 8.802% |
| 91  | 12.333 | 3417 | 3419 | 3424 | rVB3 | 640    | 446    | 0.03%  | 0.004% |
| 92  | 12.517 | 3473 | 3476 | 3481 | rBV2 | 257    | 301    | 0.02%  | 0.003% |
| 93  | 12.635 | 3510 | 3513 | 3517 | rBV3 | 242    | 205    | 0.02%  | 0.002% |
| 94  | 13.005 | 3624 | 3628 | 3632 | rBV2 | 295    | 352    | 0.03%  | 0.003% |
| 95  | 13.153 | 3671 | 3674 | 3676 | rBV  | 199    | 143    | 0.01%  | 0.001% |
| 96  | 13.989 | 3931 | 3934 | 3939 | rBV2 | 187    | 181    | 0.01%  | 0.002% |
| 97  | 14.060 | 3954 | 3956 | 3960 | rBV2 | 159    | 136    | 0.01%  | 0.001% |
| 98  | 14.259 | 4015 | 4018 | 4021 | rBV2 | 211    | 191    | 0.01%  | 0.002% |
| 99  | 14.719 | 4160 | 4161 | 4166 | rBV2 | 250    | 236    | 0.02%  | 0.002% |
| 100 | 14.806 | 4186 | 4188 | 4191 | rBV  | 315    | 213    | 0.02%  | 0.002% |

Sum of corrected areas: 10361453



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MSVOA\_U  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.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 |

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