

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU032422\  
 Data File : VU047658.D  
 Acq On : 25 Mar 2022 01:17  
 Operator : SY/MD  
 Sample : N2081-17  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 29 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 EW5Y4

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\SFAMULM032422WMA.M  
 Title : VOC Analysis

Signal : TIC: VU047658.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          | 97           | rVB      | 134900         | 155159        | 13.72%          | 1.552%        |
| 2         | 1.919       | 172           | 180         | 200          | rVB      | 102585         | 139400        | 12.33%          | 1.394%        |
| 3         | 2.571       | 371           | 383         | 405          | rBV      | 243904         | 408231        | 36.11%          | 4.083%        |
| 4         | 2.790       | 446           | 451         | 452          | rBV2     | 694            | 503           | 0.04%           | 0.005%        |
| 5         | 2.861       | 470           | 473         | 476          | rBV5     | 381            | 277           | 0.02%           | 0.003%        |
| 6         | 3.362       | 623           | 629         | 633          | rBV4     | 665            | 683           | 0.06%           | 0.007%        |
| 7         | 3.443       | 649           | 654         | 657          | rBV3     | 299            | 254           | 0.02%           | 0.003%        |
| 8         | 3.880       | 780           | 790         | 800          | rVB      | 1384           | 2890          | 0.26%           | 0.029%        |
| 9         | 4.054       | 841           | 844         | 848          | rBV      | 343            | 309           | 0.03%           | 0.003%        |
| 10        | 4.250       | 902           | 905         | 909          | rVB3     | 283            | 245           | 0.02%           | 0.002%        |
| 11        | 4.288       | 909           | 917         | 921          | rBV3     | 326            | 493           | 0.04%           | 0.005%        |
| 12        | 4.382       | 943           | 946         | 955          | rBV2     | 247            | 328           | 0.03%           | 0.003%        |
| 13        | 4.645       | 1012          | 1028        | 1065         | rBV      | 101798         | 369502        | 32.68%          | 3.696%        |
| 14        | 5.067       | 1142          | 1159        | 1180         | rBV      | 205719         | 450560        | 39.85%          | 4.506%        |
| 15        | 5.218       | 1203          | 1206        | 1209         | rVB2     | 509            | 291           | 0.03%           | 0.003%        |
| 16        | 5.321       | 1225          | 1238        | 1248         | rBV7     | 2317           | 5518          | 0.49%           | 0.055%        |
| 17        | 5.401       | 1261          | 1263        | 1270         | rVB2     | 249            | 239           | 0.02%           | 0.002%        |
| 18        | 5.729       | 1343          | 1365        | 1392         | rBV2     | 424166         | 1130674       | 100.00%         | 11.308%       |
| 19        | 6.112       | 1481          | 1484        | 1486         | rBV2     | 407            | 279           | 0.02%           | 0.003%        |
| 20        | 6.163       | 1493          | 1500        | 1501         | rBV2     | 580            | 614           | 0.05%           | 0.006%        |
| 21        | 6.250       | 1511          | 1527        | 1555         | rBV      | 407072         | 774055        | 68.46%          | 7.742%        |
| 22        | 6.462       | 1589          | 1593        | 1595         | rBV2     | 319            | 277           | 0.02%           | 0.003%        |
| 23        | 6.536       | 1607          | 1616        | 1618         | rBV5     | 1595           | 1858          | 0.16%           | 0.019%        |
| 24        | 6.613       | 1638          | 1640        | 1645         | rBV2     | 399            | 256           | 0.02%           | 0.003%        |
| 25        | 6.694       | 1651          | 1665        | 1685         | rBV      | 256036         | 503184        | 44.50%          | 5.033%        |
| 26        | 6.767       | 1686          | 1688        | 1691         | rVB5     | 697            | 485           | 0.04%           | 0.005%        |
| 27        | 6.806       | 1698          | 1700        | 1703         | rVB3     | 509            | 291           | 0.03%           | 0.003%        |
| 28        | 7.118       | 1794          | 1797        | 1803         | rVB3     | 313            | 243           | 0.02%           | 0.002%        |
| 29        | 7.192       | 1811          | 1820        | 1830         | rVB5     | 1057           | 1708          | 0.15%           | 0.017%        |
| 30        | 7.343       | 1862          | 1867        | 1872         | rVB3     | 293            | 320           | 0.03%           | 0.003%        |
| 31        | 7.385       | 1877          | 1880        | 1882         | rBV2     | 313            | 261           | 0.02%           | 0.003%        |
| 32        | 7.568       | 1923          | 1937        | 1957         | rBV      | 143647         | 256760        | 22.71%          | 2.568%        |
| 33        | 7.803       | 2002          | 2010        | 2021         | rVB2     | 2771           | 4894          | 0.43%           | 0.049%        |
| 34        | 7.899       | 2026          | 2040        | 2056         | rBV      | 533870         | 937714        | 82.93%          | 9.378%        |
| 35        | 8.179       | 2113          | 2127        | 2144         | rBV      | 108047         | 198320        | 17.54%          | 1.983%        |
| 36        | 8.465       | 2210          | 2216        | 2217         | rBV3     | 1592           | 1183          | 0.10%           | 0.012%        |

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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\SFAMULM032422WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 8.555  | 2236 | 2244 | 2252 | rBV5 | 3189   | 4243    | 0.38%  | 0.042%  |
| 38 | 8.639  | 2256 | 2270 | 2301 | rBV  | 410355 | 774548  | 68.50% | 7.746%  |
| 39 | 9.079  | 2404 | 2407 | 2410 | rBV  | 341    | 304     | 0.03%  | 0.003%  |
| 40 | 9.108  | 2414 | 2416 | 2421 | rVB2 | 377    | 271     | 0.02%  | 0.003%  |
| 41 | 9.221  | 2448 | 2451 | 2457 | rVB2 | 295    | 256     | 0.02%  | 0.003%  |
| 42 | 9.279  | 2462 | 2469 | 2476 | rBV4 | 596    | 1021    | 0.09%  | 0.010%  |
| 43 | 9.356  | 2488 | 2493 | 2496 | rBV2 | 352    | 284     | 0.03%  | 0.003%  |
| 44 | 9.417  | 2496 | 2512 | 2543 | rBV  | 597584 | 1015451 | 89.81% | 10.156% |
| 45 | 9.574  | 2554 | 2561 | 2574 | rVB4 | 1369   | 2340    | 0.21%  | 0.023%  |
| 46 | 9.693  | 2588 | 2598 | 2607 | rVB4 | 2299   | 3938    | 0.35%  | 0.039%  |
| 47 | 9.774  | 2617 | 2623 | 2626 | rBV4 | 332    | 392     | 0.03%  | 0.004%  |
| 48 | 9.832  | 2636 | 2641 | 2649 | rVB3 | 287    | 431     | 0.04%  | 0.004%  |
| 49 | 9.925  | 2663 | 2670 | 2680 | rVB3 | 1245   | 1872    | 0.17%  | 0.019%  |
| 50 | 9.976  | 2680 | 2686 | 2691 | rBV2 | 322    | 514     | 0.05%  | 0.005%  |
| 51 | 10.057 | 2706 | 2711 | 2717 | rBV  | 370    | 470     | 0.04%  | 0.005%  |
| 52 | 10.102 | 2717 | 2725 | 2730 | rBV3 | 1774   | 2316    | 0.20%  | 0.023%  |
| 53 | 10.156 | 2737 | 2742 | 2746 | rBV2 | 331    | 439     | 0.04%  | 0.004%  |
| 54 | 10.243 | 2765 | 2769 | 2770 | rBV3 | 334    | 273     | 0.02%  | 0.003%  |
| 55 | 10.282 | 2778 | 2781 | 2784 | rBV2 | 263    | 237     | 0.02%  | 0.002%  |
| 56 | 10.317 | 2788 | 2792 | 2798 | rVB2 | 367    | 483     | 0.04%  | 0.005%  |
| 57 | 10.394 | 2812 | 2816 | 2823 | rVB4 | 417    | 590     | 0.05%  | 0.006%  |
| 58 | 10.533 | 2854 | 2859 | 2865 | rVB2 | 234    | 299     | 0.03%  | 0.003%  |
| 59 | 10.574 | 2865 | 2872 | 2876 | rBV5 | 1189   | 1426    | 0.13%  | 0.014%  |
| 60 | 10.671 | 2893 | 2902 | 2912 | rVV4 | 4196   | 6437    | 0.57%  | 0.064%  |
| 61 | 10.758 | 2916 | 2929 | 2946 | rBV  | 406411 | 654965  | 57.93% | 6.551%  |
| 62 | 10.893 | 2959 | 2971 | 2987 | rVB5 | 5605   | 11305   | 1.00%  | 0.113%  |
| 63 | 10.996 | 2997 | 3003 | 3007 | rBV2 | 1668   | 2021    | 0.18%  | 0.020%  |
| 64 | 11.089 | 3026 | 3032 | 3041 | rBV2 | 3997   | 5811    | 0.51%  | 0.058%  |
| 65 | 11.147 | 3048 | 3050 | 3053 | rBV4 | 756    | 579     | 0.05%  | 0.006%  |
| 66 | 11.198 | 3064 | 3066 | 3072 | rVB2 | 621    | 498     | 0.04%  | 0.005%  |
| 67 | 11.243 | 3075 | 3080 | 3081 | rBV2 | 1071   | 898     | 0.08%  | 0.009%  |
| 68 | 11.295 | 3088 | 3096 | 3106 | rVB2 | 4217   | 6217    | 0.55%  | 0.062%  |
| 69 | 11.433 | 3136 | 3139 | 3140 | rBV  | 573    | 295     | 0.03%  | 0.003%  |
| 70 | 11.468 | 3140 | 3150 | 3164 | rVB3 | 23351  | 38455   | 3.40%  | 0.385%  |
| 71 | 11.558 | 3175 | 3178 | 3180 | rBV  | 372    | 266     | 0.02%  | 0.003%  |
| 72 | 11.578 | 3180 | 3184 | 3190 | rVV3 | 727    | 1028    | 0.09%  | 0.010%  |
| 73 | 11.693 | 3214 | 3220 | 3230 | rVB5 | 2183   | 3407    | 0.30%  | 0.034%  |
| 74 | 11.745 | 3231 | 3236 | 3237 | rBV4 | 1159   | 844     | 0.07%  | 0.008%  |
| 75 | 11.812 | 3244 | 3257 | 3275 | rBV  | 688878 | 1083581 | 95.83% | 10.837% |
| 76 | 11.896 | 3277 | 3283 | 3291 | rVB  | 6546   | 10093   | 0.89%  | 0.101%  |

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Start Thrs: 0.2

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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\SFAMULM032422WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |       |        |        |        |        |
|-----|--------|------|------|------|-------|--------|--------|--------|--------|
| 77  | 12.031 | 3323 | 3325 | 3328 | rVB2  | 797    | 337    | 0.03%  | 0.003% |
| 78  | 12.066 | 3328 | 3336 | 3337 | rBV4  | 1865   | 2025   | 0.18%  | 0.020% |
| 79  | 12.192 | 3362 | 3375 | 3392 | rVB   | 583436 | 938076 | 82.97% | 9.382% |
| 80  | 12.301 | 3407 | 3409 | 3412 | rBV2  | 395    | 329    | 0.03%  | 0.003% |
| 81  | 12.336 | 3412 | 3420 | 3426 | rVV5  | 2015   | 3505   | 0.31%  | 0.035% |
| 82  | 12.378 | 3428 | 3433 | 3448 | rVB10 | 2238   | 4620   | 0.41%  | 0.046% |
| 83  | 12.487 | 3454 | 3467 | 3478 | rBV5  | 6346   | 13402  | 1.19%  | 0.134% |
| 84  | 12.574 | 3489 | 3494 | 3502 | rVB2  | 2146   | 2816   | 0.25%  | 0.028% |
| 85  | 12.777 | 3551 | 3557 | 3566 | rVB3  | 909    | 1419   | 0.13%  | 0.014% |
| 86  | 12.880 | 3583 | 3589 | 3593 | rBV6  | 659    | 843    | 0.07%  | 0.008% |
| 87  | 12.934 | 3603 | 3606 | 3607 | rBV   | 679    | 359    | 0.03%  | 0.004% |
| 88  | 12.970 | 3608 | 3617 | 3626 | rVB6  | 1923   | 3625   | 0.32%  | 0.036% |
| 89  | 13.028 | 3630 | 3635 | 3642 | rVB3  | 1808   | 2497   | 0.22%  | 0.025% |
| 90  | 13.217 | 3691 | 3694 | 3696 | rBV3  | 414    | 296    | 0.03%  | 0.003% |
| 91  | 13.298 | 3712 | 3719 | 3723 | rBV2  | 723    | 913    | 0.08%  | 0.009% |
| 92  | 13.455 | 3758 | 3768 | 3777 | rVB6  | 2795   | 4653   | 0.41%  | 0.047% |
| 93  | 13.622 | 3817 | 3820 | 3826 | rVB4  | 768    | 635    | 0.06%  | 0.006% |
| 94  | 13.835 | 3883 | 3886 | 3887 | rBV   | 610    | 384    | 0.03%  | 0.004% |
| 95  | 14.089 | 3956 | 3965 | 3980 | rVB   | 13103  | 21543  | 1.91%  | 0.215% |
| 96  | 14.259 | 4015 | 4018 | 4022 | rVB2  | 753    | 468    | 0.04%  | 0.005% |
| 97  | 14.282 | 4022 | 4025 | 4027 | rBV   | 336    | 278    | 0.02%  | 0.003% |
| 98  | 14.452 | 4075 | 4078 | 4083 | rVB3  | 1089   | 832    | 0.07%  | 0.008% |
| 99  | 15.227 | 4313 | 4319 | 4326 | rBV5  | 2694   | 4097   | 0.36%  | 0.041% |
| 100 | 15.413 | 4369 | 4377 | 4381 | rBV6  | 2178   | 3380   | 0.30%  | 0.034% |

Sum of corrected areas: 9998688



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM032422WMA.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 Integration Parameters: LSCINT.P

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