

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121621\  
 Data File : VU046417.D  
 Acq On : 16 Dec 2021 13:45  
 Operator : SY/MD  
 Sample : PB141457TB  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VLEB457

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: VU046417.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          | 103          | rVB      | 75855          | 93836         | 16.35%          | 2.118%        |
| 2         | 1.919       | 171           | 180         | 203          | rBV      | 51333          | 73934         | 12.88%          | 1.669%        |
| 3         | 2.269       | 287           | 289         | 296          | rVB2     | 291            | 266           | 0.05%           | 0.006%        |
| 4         | 2.311       | 300           | 302         | 305          | rBV      | 186            | 110           | 0.02%           | 0.002%        |
| 5         | 2.572       | 371           | 383         | 398          | rBV      | 124801         | 206798        | 36.03%          | 4.668%        |
| 6         | 2.842       | 465           | 467         | 472          | rBB      | 139            | 142           | 0.02%           | 0.003%        |
| 7         | 3.057       | 522           | 534         | 547          | rBV2     | 4640           | 9942          | 1.73%           | 0.224%        |
| 8         | 3.147       | 560           | 562         | 566          | rBV      | 116            | 128           | 0.02%           | 0.003%        |
| 9         | 3.192       | 566           | 576         | 584          | rVB      | 1007           | 1919          | 0.33%           | 0.043%        |
| 10        | 3.311       | 610           | 613         | 617          | rVB      | 146            | 147           | 0.03%           | 0.003%        |
| 11        | 3.584       | 696           | 698         | 702          | rBB      | 172            | 140           | 0.02%           | 0.003%        |
| 12        | 3.697       | 729           | 733         | 735          | rBB      | 138            | 118           | 0.02%           | 0.003%        |
| 13        | 3.761       | 750           | 753         | 756          | rBB      | 143            | 121           | 0.02%           | 0.003%        |
| 14        | 4.083       | 850           | 853         | 855          | rBB      | 162            | 110           | 0.02%           | 0.002%        |
| 15        | 4.382       | 944           | 946         | 950          | rBV      | 130            | 137           | 0.02%           | 0.003%        |
| 16        | 4.636       | 1011          | 1025        | 1061         | rBV2     | 49307          | 132127        | 23.02%          | 2.982%        |
| 17        | 4.816       | 1076          | 1081        | 1085         | rVB2     | 196            | 209           | 0.04%           | 0.005%        |
| 18        | 4.851       | 1086          | 1092        | 1095         | rBV2     | 192            | 216           | 0.04%           | 0.005%        |
| 19        | 4.938       | 1117          | 1119        | 1122         | rBV      | 135            | 115           | 0.02%           | 0.003%        |
| 20        | 5.067       | 1142          | 1159        | 1179         | rBV      | 105259         | 229586        | 40.00%          | 5.182%        |
| 21        | 5.186       | 1194          | 1196        | 1199         | rVB2     | 237            | 115           | 0.02%           | 0.003%        |
| 22        | 5.218       | 1204          | 1206        | 1209         | rVB      | 205            | 103           | 0.02%           | 0.002%        |
| 23        | 5.243       | 1210          | 1214        | 1216         | rBV      | 246            | 189           | 0.03%           | 0.004%        |
| 24        | 5.295       | 1227          | 1230        | 1232         | rBV      | 240            | 140           | 0.02%           | 0.003%        |
| 25        | 5.308       | 1232          | 1234        | 1236         | rVB      | 253            | 120           | 0.02%           | 0.003%        |
| 26        | 5.549       | 1306          | 1309        | 1312         | rBV      | 151            | 153           | 0.03%           | 0.003%        |
| 27        | 5.729       | 1344          | 1365        | 1396         | rBV2     | 215522         | 574001        | 100.00%         | 12.957%       |
| 28        | 5.935       | 1426          | 1429        | 1432         | rBV      | 146            | 145           | 0.03%           | 0.003%        |
| 29        | 6.015       | 1451          | 1454        | 1457         | rBB      | 135            | 116           | 0.02%           | 0.003%        |
| 30        | 6.160       | 1496          | 1499        | 1501         | rBV      | 228            | 176           | 0.03%           | 0.004%        |
| 31        | 6.253       | 1514          | 1528        | 1559         | rBV      | 176900         | 337745        | 58.84%          | 7.624%        |
| 32        | 6.356       | 1559          | 1560        | 1562         | rVV      | 305            | 130           | 0.02%           | 0.003%        |
| 33        | 6.533       | 1611          | 1615        | 1618         | rBV3     | 228            | 229           | 0.04%           | 0.005%        |
| 34        | 6.694       | 1651          | 1665        | 1686         | rBV      | 131061         | 254097        | 44.27%          | 5.736%        |
| 35        | 6.809       | 1698          | 1701        | 1704         | rVB2     | 258            | 208           | 0.04%           | 0.005%        |
| 36        | 6.874       | 1718          | 1721        | 1723         | rBV      | 130            | 111           | 0.02%           | 0.003%        |

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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 | 6.886  | 1723 | 1725 | 1730 | rVV  | 157    | 169    | 0.03%  | 0.004%  |
| 38 | 7.038  | 1769 | 1772 | 1776 | rBB2 | 287    | 228    | 0.04%  | 0.005%  |
| 39 | 7.189  | 1813 | 1819 | 1825 | rBB2 | 298    | 459    | 0.08%  | 0.010%  |
| 40 | 7.234  | 1831 | 1833 | 1837 | rBV  | 130    | 132    | 0.02%  | 0.003%  |
| 41 | 7.288  | 1847 | 1850 | 1854 | rBV  | 147    | 172    | 0.03%  | 0.004%  |
| 42 | 7.394  | 1880 | 1883 | 1887 | rVB  | 176    | 162    | 0.03%  | 0.004%  |
| 43 | 7.520  | 1919 | 1922 | 1924 | rBV  | 132    | 117    | 0.02%  | 0.003%  |
| 44 | 7.568  | 1924 | 1937 | 1958 | rVB  | 69533  | 121049 | 21.09% | 2.732%  |
| 45 | 7.681  | 1969 | 1972 | 1974 | rVV2 | 200    | 134    | 0.02%  | 0.003%  |
| 46 | 7.745  | 1986 | 1992 | 1995 | rBV  | 159    | 244    | 0.04%  | 0.006%  |
| 47 | 7.796  | 2004 | 2008 | 2012 | rBV  | 393    | 383    | 0.07%  | 0.009%  |
| 48 | 7.854  | 2022 | 2026 | 2027 | rBV  | 169    | 152    | 0.03%  | 0.003%  |
| 49 | 7.899  | 2027 | 2040 | 2057 | rBV  | 264643 | 450177 | 78.43% | 10.162% |
| 50 | 8.182  | 2115 | 2128 | 2147 | rBV  | 50049  | 83377  | 14.53% | 1.882%  |
| 51 | 8.256  | 2147 | 2151 | 2154 | rVB  | 288    | 302    | 0.05%  | 0.007%  |
| 52 | 8.285  | 2155 | 2160 | 2164 | rBV2 | 283    | 394    | 0.07%  | 0.009%  |
| 53 | 8.304  | 2164 | 2166 | 2169 | rVV  | 156    | 119    | 0.02%  | 0.003%  |
| 54 | 8.430  | 2203 | 2205 | 2208 | rBV  | 163    | 126    | 0.02%  | 0.003%  |
| 55 | 8.475  | 2211 | 2219 | 2223 | rBV2 | 619    | 905    | 0.16%  | 0.020%  |
| 56 | 8.529  | 2229 | 2236 | 2240 | rBV2 | 348    | 505    | 0.09%  | 0.011%  |
| 57 | 8.549  | 2240 | 2242 | 2245 | rVV  | 257    | 165    | 0.03%  | 0.004%  |
| 58 | 8.636  | 2257 | 2269 | 2294 | rBV  | 161432 | 273601 | 47.67% | 6.176%  |
| 59 | 8.745  | 2301 | 2303 | 2309 | rVB  | 269    | 169    | 0.03%  | 0.004%  |
| 60 | 8.915  | 2350 | 2356 | 2362 | rBB2 | 676    | 1053   | 0.18%  | 0.024%  |
| 61 | 9.182  | 2436 | 2439 | 2442 | rBB  | 197    | 146    | 0.03%  | 0.003%  |
| 62 | 9.282  | 2465 | 2470 | 2475 | rBV  | 151    | 216    | 0.04%  | 0.005%  |
| 63 | 9.343  | 2485 | 2489 | 2494 | rBV  | 153    | 232    | 0.04%  | 0.005%  |
| 64 | 9.420  | 2499 | 2513 | 2537 | rVV  | 270203 | 440214 | 76.69% | 9.937%  |
| 65 | 9.568  | 2555 | 2559 | 2560 | rBV  | 235    | 161    | 0.03%  | 0.004%  |
| 66 | 9.697  | 2593 | 2599 | 2603 | rVB2 | 315    | 326    | 0.06%  | 0.007%  |
| 67 | 9.870  | 2650 | 2653 | 2656 | rBV  | 158    | 155    | 0.03%  | 0.003%  |
| 68 | 9.896  | 2658 | 2661 | 2665 | rVB  | 207    | 192    | 0.03%  | 0.004%  |
| 69 | 9.973  | 2678 | 2685 | 2690 | rBV  | 179    | 352    | 0.06%  | 0.008%  |
| 70 | 10.076 | 2710 | 2717 | 2720 | rBV  | 165    | 245    | 0.04%  | 0.006%  |
| 71 | 10.111 | 2725 | 2728 | 2731 | rVB  | 261    | 181    | 0.03%  | 0.004%  |
| 72 | 10.134 | 2732 | 2735 | 2739 | rBB  | 138    | 139    | 0.02%  | 0.003%  |
| 73 | 10.169 | 2742 | 2746 | 2750 | rBV  | 170    | 208    | 0.04%  | 0.005%  |
| 74 | 10.362 | 2802 | 2806 | 2811 | rBB  | 154    | 180    | 0.03%  | 0.004%  |
| 75 | 10.565 | 2867 | 2869 | 2871 | rBV  | 147    | 104    | 0.02%  | 0.002%  |
| 76 | 10.674 | 2896 | 2903 | 2909 | rBV3 | 1372   | 1816   | 0.32%  | 0.041%  |

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 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 10.758 | 2916 | 2929 | 2948 | rBV  | 184678 | 292922 | 51.03% | 6.612% |
| 78  | 10.902 | 2967 | 2974 | 2979 | rBV3 | 500    | 606    | 0.11%  | 0.014% |
| 79  | 10.989 | 2997 | 3001 | 3007 | rBV  | 120    | 137    | 0.02%  | 0.003% |
| 80  | 11.217 | 3069 | 3072 | 3074 | rBV  | 185    | 154    | 0.03%  | 0.003% |
| 81  | 11.459 | 3140 | 3147 | 3155 | rVB3 | 736    | 1012   | 0.18%  | 0.023% |
| 82  | 11.574 | 3181 | 3183 | 3187 | rBV  | 141    | 112    | 0.02%  | 0.003% |
| 83  | 11.697 | 3216 | 3221 | 3226 | rBV2 | 230    | 300    | 0.05%  | 0.007% |
| 84  | 11.812 | 3245 | 3257 | 3277 | rVB  | 275103 | 430370 | 74.98% | 9.715% |
| 85  | 11.889 | 3277 | 3281 | 3284 | rBV2 | 255    | 218    | 0.04%  | 0.005% |
| 86  | 11.941 | 3294 | 3297 | 3302 | rBV3 | 408    | 405    | 0.07%  | 0.009% |
| 87  | 11.973 | 3304 | 3307 | 3312 | rVB2 | 654    | 655    | 0.11%  | 0.015% |
| 88  | 12.012 | 3312 | 3319 | 3323 | rBV  | 127    | 151    | 0.03%  | 0.003% |
| 89  | 12.195 | 3364 | 3376 | 3402 | rVB  | 253235 | 402487 | 70.12% | 9.085% |
| 90  | 12.298 | 3403 | 3408 | 3412 | rBV  | 181    | 191    | 0.03%  | 0.004% |
| 91  | 12.642 | 3512 | 3515 | 3518 | rBV2 | 179    | 140    | 0.02%  | 0.003% |
| 92  | 12.777 | 3548 | 3557 | 3562 | rVB  | 565    | 788    | 0.14%  | 0.018% |
| 93  | 13.298 | 3716 | 3719 | 3727 | rVB  | 155    | 185    | 0.03%  | 0.004% |
| 94  | 13.793 | 3870 | 3873 | 3876 | rBV  | 163    | 101    | 0.02%  | 0.002% |
| 95  | 14.581 | 4110 | 4118 | 4124 | rVB2 | 445    | 697    | 0.12%  | 0.016% |
| 96  | 15.899 | 4526 | 4528 | 4532 | rBV  | 189    | 190    | 0.03%  | 0.004% |
| 97  | 16.407 | 4683 | 4686 | 4689 | rBV2 | 267    | 179    | 0.03%  | 0.004% |
| 98  | 16.912 | 4841 | 4843 | 4849 | rBV4 | 341    | 367    | 0.06%  | 0.008% |
| 99  | 17.298 | 4960 | 4963 | 4965 | rBV3 | 444    | 287    | 0.05%  | 0.006% |
| 100 | 17.420 | 4998 | 5001 | 5004 | rBV2 | 599    | 468    | 0.08%  | 0.011% |

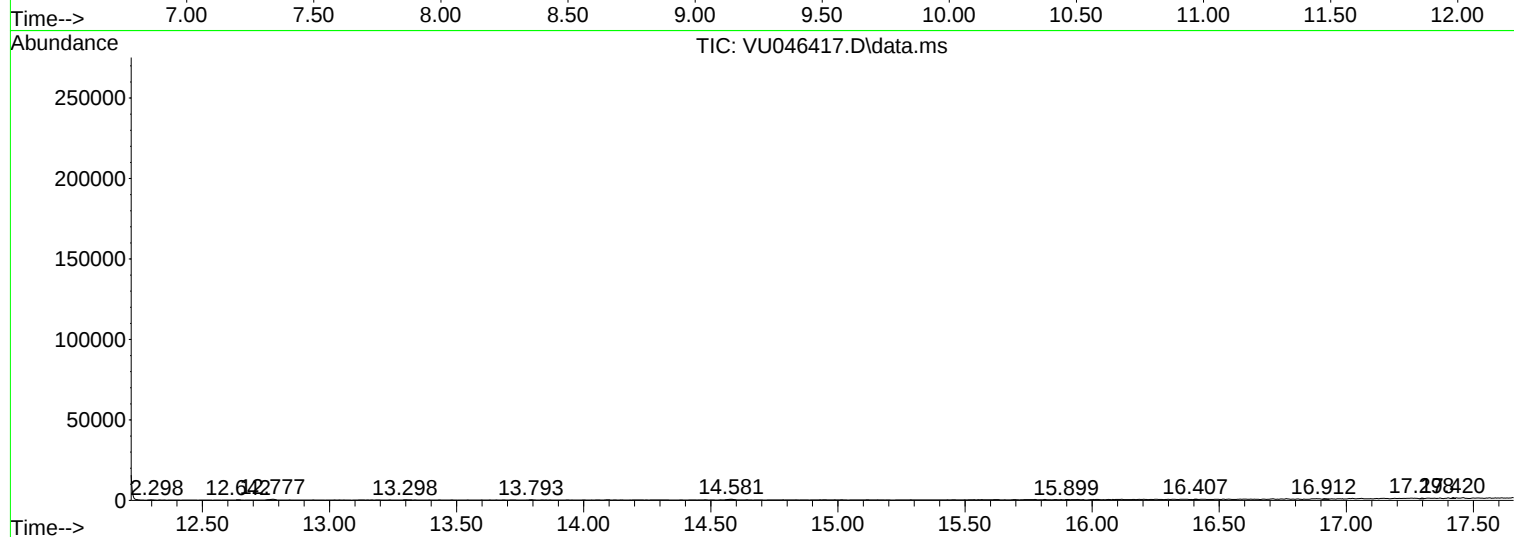
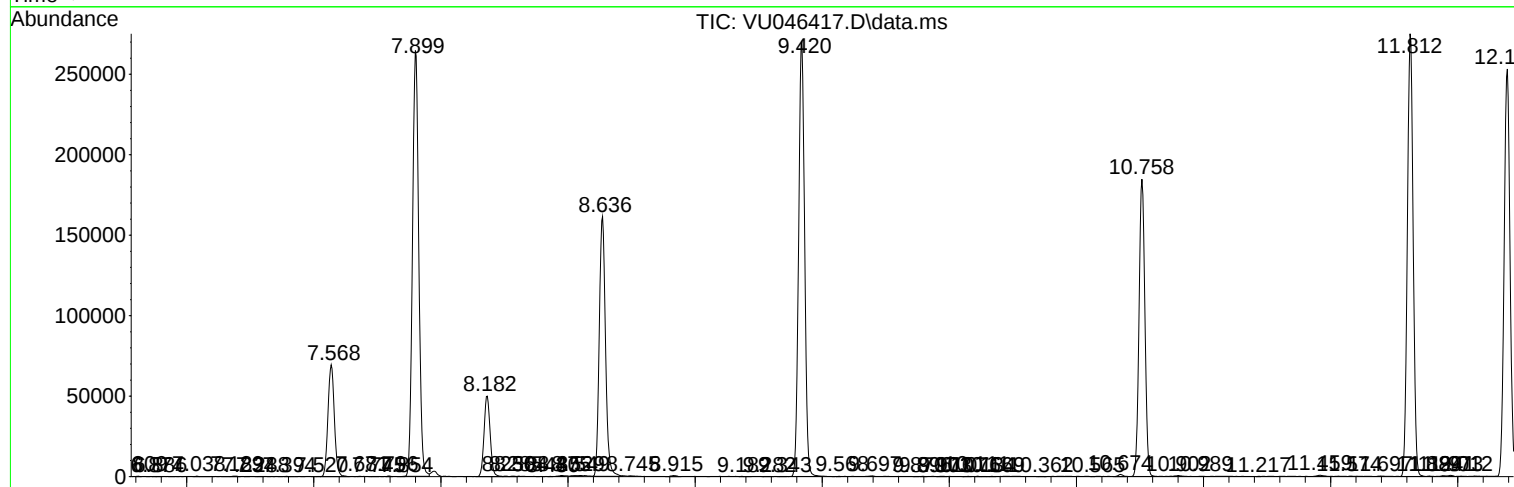
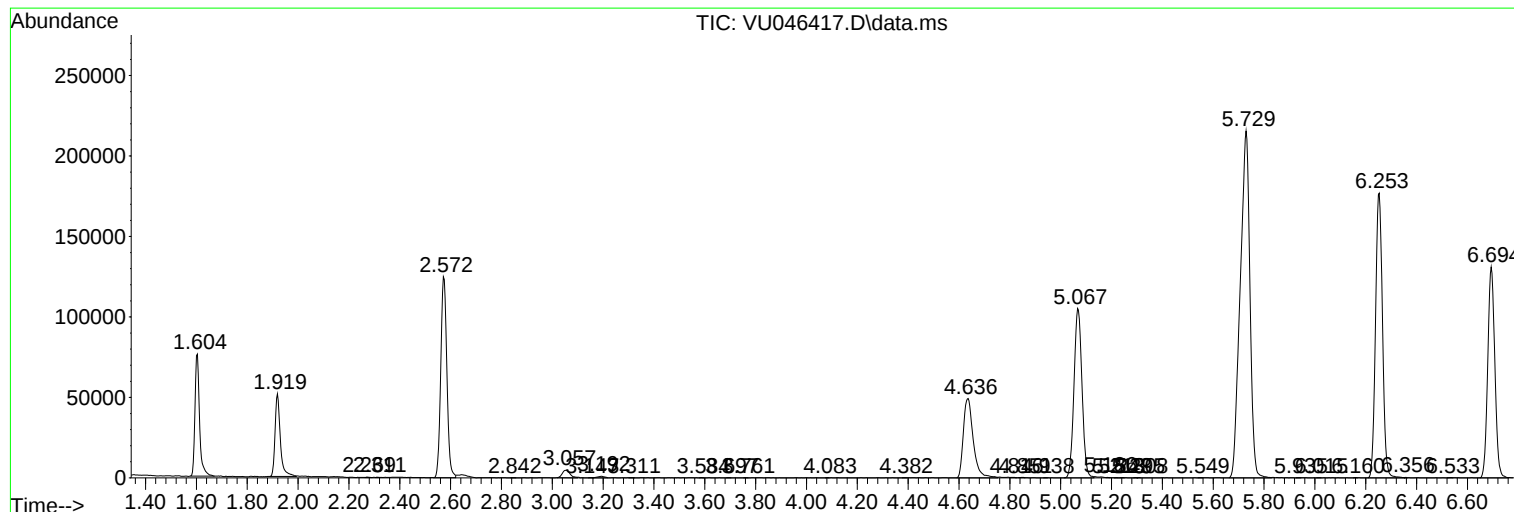
Sum of corrected areas: 4430162

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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



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No Library Search Compounds Detected

\*\*\*\*\*

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