

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU071923\  
 Data File : VU054822.D  
 Acq On : 19 Jul 2023 16:09  
 Operator : MD/SY  
 Sample : 03656-12  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VHBLK001

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\SFAMULM071723WMA.M  
 Title : VOC Analysis

Signal : TIC: VU054822.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         | 1.596       | 89            | 95          | 112          | rBV      | 47769          | 71831         | 15.55%          | 1.820%        |
| 2         | 2.551       | 380           | 392         | 406          | rBV      | 84069          | 133907        | 28.99%          | 3.393%        |
| 3         | 2.772       | 456           | 461         | 462          | rBV      | 517            | 389           | 0.08%           | 0.010%        |
| 4         | 2.846       | 481           | 484         | 485          | rBV2     | 584            | 296           | 0.06%           | 0.007%        |
| 5         | 3.152       | 574           | 579         | 581          | rBV2     | 603            | 420           | 0.09%           | 0.011%        |
| 6         | 3.168       | 581           | 584         | 585          | rVV2     | 476            | 270           | 0.06%           | 0.007%        |
| 7         | 3.177       | 585           | 587         | 591          | rVB3     | 564            | 334           | 0.07%           | 0.008%        |
| 8         | 3.370       | 644           | 647         | 649          | rVB      | 596            | 242           | 0.05%           | 0.006%        |
| 9         | 3.390       | 649           | 653         | 654          | rBV2     | 517            | 267           | 0.06%           | 0.007%        |
| 10        | 3.438       | 665           | 668         | 673          | rBV2     | 550            | 464           | 0.10%           | 0.012%        |
| 11        | 3.483       | 680           | 682         | 685          | rVB3     | 550            | 243           | 0.05%           | 0.006%        |
| 12        | 3.505       | 686           | 689         | 693          | rVV3     | 338            | 299           | 0.06%           | 0.008%        |
| 13        | 3.779       | 771           | 774         | 776          | rBV      | 448            | 269           | 0.06%           | 0.007%        |
| 14        | 3.811       | 780           | 784         | 789          | rBV2     | 426            | 407           | 0.09%           | 0.010%        |
| 15        | 3.988       | 836           | 839         | 842          | rBV      | 504            | 338           | 0.07%           | 0.009%        |
| 16        | 4.068       | 861           | 864         | 868          | rVB2     | 520            | 378           | 0.08%           | 0.010%        |
| 17        | 4.145       | 886           | 888         | 896          | rVB3     | 385            | 412           | 0.09%           | 0.010%        |
| 18        | 4.280       | 927           | 930         | 936          | rBV2     | 552            | 708           | 0.15%           | 0.018%        |
| 19        | 4.338       | 944           | 948         | 954          | rBV2     | 372            | 366           | 0.08%           | 0.009%        |
| 20        | 4.448       | 977           | 982         | 984          | rBV      | 355            | 295           | 0.06%           | 0.007%        |
| 21        | 4.557       | 1012          | 1016        | 1019         | rBV3     | 377            | 316           | 0.07%           | 0.008%        |
| 22        | 4.618       | 1023          | 1035        | 1055         | rBV      | 47583          | 115161        | 24.93%          | 2.918%        |
| 23        | 4.785       | 1084          | 1087        | 1091         | rBV3     | 837            | 893           | 0.19%           | 0.023%        |
| 24        | 4.853       | 1104          | 1108        | 1111         | rBV2     | 468            | 351           | 0.08%           | 0.009%        |
| 25        | 4.885       | 1116          | 1118        | 1122         | rVV3     | 550            | 487           | 0.11%           | 0.012%        |
| 26        | 4.917       | 1126          | 1128        | 1130         | rVV2     | 530            | 275           | 0.06%           | 0.007%        |
| 27        | 4.936       | 1130          | 1134        | 1136         | rVB3     | 516            | 349           | 0.08%           | 0.009%        |
| 28        | 4.975       | 1144          | 1146        | 1150         | rBV3     | 562            | 325           | 0.07%           | 0.008%        |
| 29        | 5.055       | 1157          | 1171        | 1195         | rBV      | 86497          | 189006        | 40.92%          | 4.789%        |
| 30        | 5.261       | 1232          | 1235        | 1240         | rVB3     | 506            | 457           | 0.10%           | 0.012%        |
| 31        | 5.287       | 1240          | 1243        | 1245         | rBV      | 485            | 245           | 0.05%           | 0.006%        |
| 32        | 5.325       | 1252          | 1255        | 1260         | rBV2     | 540            | 363           | 0.08%           | 0.009%        |
| 33        | 5.554       | 1319          | 1326        | 1328         | rBV      | 477            | 355           | 0.08%           | 0.009%        |
| 34        | 5.718       | 1358          | 1377        | 1399         | rBV3     | 168335         | 461846        | 100.00%         | 11.702%       |
| 35        | 5.956       | 1447          | 1451        | 1455         | rBV3     | 587            | 675           | 0.15%           | 0.017%        |
| 36        | 6.078       | 1486          | 1489        | 1491         | rBV2     | 462            | 312           | 0.07%           | 0.008%        |

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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\SFAMULM071723WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 6.129  | 1502 | 1505 | 1507 | rBV2 | 458    | 290    | 0.06%  | 0.007% |
| 38 | 6.242  | 1527 | 1540 | 1560 | rBV  | 155350 | 295815 | 64.05% | 7.495% |
| 39 | 6.521  | 1623 | 1627 | 1629 | rBV3 | 701    | 565    | 0.12%  | 0.014% |
| 40 | 6.685  | 1664 | 1678 | 1696 | rBV  | 112661 | 220177 | 47.67% | 5.579% |
| 41 | 7.017  | 1775 | 1781 | 1785 | rBV3 | 527    | 621    | 0.13%  | 0.016% |
| 42 | 7.113  | 1804 | 1811 | 1818 | rBV2 | 441    | 726    | 0.16%  | 0.018% |
| 43 | 7.345  | 1877 | 1883 | 1885 | rBV2 | 516    | 441    | 0.10%  | 0.011% |
| 44 | 7.380  | 1892 | 1894 | 1897 | rVB2 | 540    | 247    | 0.05%  | 0.006% |
| 45 | 7.406  | 1898 | 1902 | 1905 | rBV2 | 509    | 368    | 0.08%  | 0.009% |
| 46 | 7.454  | 1913 | 1917 | 1919 | rBV  | 462    | 326    | 0.07%  | 0.008% |
| 47 | 7.560  | 1933 | 1950 | 1967 | rBV3 | 65285  | 116909 | 25.31% | 2.962% |
| 48 | 7.695  | 1987 | 1992 | 1998 | rVB5 | 1150   | 1151   | 0.25%  | 0.029% |
| 49 | 7.894  | 2040 | 2054 | 2073 | rBV  | 214305 | 370924 | 80.31% | 9.398% |
| 50 | 8.174  | 2129 | 2141 | 2162 | rBV2 | 45136  | 77144  | 16.70% | 1.955% |
| 51 | 8.296  | 2176 | 2179 | 2184 | rVB2 | 466    | 304    | 0.07%  | 0.008% |
| 52 | 8.338  | 2190 | 2192 | 2195 | rVB  | 583    | 258    | 0.06%  | 0.007% |
| 53 | 8.406  | 2209 | 2213 | 2214 | rBV  | 535    | 325    | 0.07%  | 0.008% |
| 54 | 8.492  | 2237 | 2240 | 2243 | rVV2 | 376    | 246    | 0.05%  | 0.006% |
| 55 | 8.631  | 2271 | 2283 | 2299 | rBV  | 151385 | 282816 | 61.24% | 7.166% |
| 56 | 8.782  | 2328 | 2330 | 2332 | rVB2 | 726    | 335    | 0.07%  | 0.008% |
| 57 | 8.801  | 2332 | 2336 | 2340 | rBV2 | 686    | 648    | 0.14%  | 0.016% |
| 58 | 8.875  | 2355 | 2359 | 2362 | rBV2 | 226    | 249    | 0.05%  | 0.006% |
| 59 | 9.415  | 2514 | 2527 | 2549 | rVV  | 228831 | 386220 | 83.63% | 9.786% |
| 60 | 9.566  | 2568 | 2574 | 2577 | rVB4 | 576    | 491    | 0.11%  | 0.012% |
| 61 | 9.692  | 2609 | 2613 | 2614 | rBV4 | 582    | 355    | 0.08%  | 0.009% |
| 62 | 9.811  | 2648 | 2650 | 2653 | rBV2 | 477    | 277    | 0.06%  | 0.007% |
| 63 | 9.946  | 2688 | 2692 | 2693 | rBV2 | 373    | 291    | 0.06%  | 0.007% |
| 64 | 9.984  | 2700 | 2704 | 2710 | rVB3 | 425    | 446    | 0.10%  | 0.011% |
| 65 | 10.132 | 2746 | 2750 | 2752 | rVB3 | 701    | 480    | 0.10%  | 0.012% |
| 66 | 10.171 | 2759 | 2762 | 2764 | rBV2 | 436    | 249    | 0.05%  | 0.006% |
| 67 | 10.264 | 2787 | 2791 | 2795 | rBV2 | 366    | 346    | 0.07%  | 0.009% |
| 68 | 10.380 | 2824 | 2827 | 2833 | rVB2 | 439    | 445    | 0.10%  | 0.011% |
| 69 | 10.409 | 2833 | 2836 | 2839 | rBV2 | 468    | 287    | 0.06%  | 0.007% |
| 70 | 10.753 | 2931 | 2943 | 2957 | rBV  | 215460 | 346291 | 74.98% | 8.774% |
| 71 | 11.065 | 3037 | 3040 | 3043 | rBV  | 317    | 259    | 0.06%  | 0.007% |
| 72 | 11.103 | 3048 | 3052 | 3056 | rBV2 | 352    | 248    | 0.05%  | 0.006% |
| 73 | 11.325 | 3118 | 3121 | 3124 | rBV3 | 448    | 264    | 0.06%  | 0.007% |
| 74 | 11.476 | 3166 | 3168 | 3170 | rBV2 | 524    | 288    | 0.06%  | 0.007% |
| 75 | 11.531 | 3181 | 3185 | 3187 | rBV2 | 404    | 268    | 0.06%  | 0.007% |
| 76 | 11.618 | 3210 | 3212 | 3215 | rBV2 | 415    | 293    | 0.06%  | 0.007% |

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM071723WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.807 | 3260 | 3271 | 3284 | rBV  | 276097 | 430688 | 93.25% | 10.912% |
| 78  | 11.936 | 3308 | 3311 | 3313 | rBV2 | 396    | 277    | 0.06%  | 0.007%  |
| 79  | 12.039 | 3337 | 3343 | 3346 | rBV2 | 333    | 303    | 0.07%  | 0.008%  |
| 80  | 12.100 | 3360 | 3362 | 3365 | rVB2 | 757    | 302    | 0.07%  | 0.008%  |
| 81  | 12.190 | 3375 | 3390 | 3409 | rBV  | 257683 | 413279 | 89.48% | 10.471% |
| 82  | 12.528 | 3492 | 3495 | 3497 | rBV2 | 858    | 636    | 0.14%  | 0.016%  |
| 83  | 12.598 | 3512 | 3517 | 3519 | rBV3 | 593    | 401    | 0.09%  | 0.010%  |
| 84  | 12.685 | 3541 | 3544 | 3548 | rVB  | 547    | 426    | 0.09%  | 0.011%  |
| 85  | 12.830 | 3583 | 3589 | 3593 | rBV2 | 442    | 515    | 0.11%  | 0.013%  |
| 86  | 12.859 | 3593 | 3598 | 3599 | rBV2 | 321    | 245    | 0.05%  | 0.006%  |
| 87  | 12.997 | 3639 | 3641 | 3646 | rVB  | 442    | 307    | 0.07%  | 0.008%  |
| 88  | 13.132 | 3679 | 3683 | 3688 | rBV2 | 363    | 357    | 0.08%  | 0.009%  |
| 89  | 13.196 | 3698 | 3703 | 3705 | rBV3 | 651    | 579    | 0.13%  | 0.015%  |
| 90  | 13.309 | 3736 | 3738 | 3742 | rBV2 | 321    | 289    | 0.06%  | 0.007%  |
| 91  | 13.470 | 3786 | 3788 | 3793 | rBV2 | 454    | 380    | 0.08%  | 0.010%  |
| 92  | 13.540 | 3808 | 3810 | 3813 | rBV2 | 356    | 270    | 0.06%  | 0.007%  |
| 93  | 13.663 | 3846 | 3848 | 3852 | rBV2 | 611    | 379    | 0.08%  | 0.010%  |
| 94  | 13.820 | 3894 | 3897 | 3901 | rBV2 | 471    | 414    | 0.09%  | 0.010%  |
| 95  | 13.952 | 3936 | 3938 | 3940 | rBV2 | 459    | 255    | 0.06%  | 0.006%  |
| 96  | 14.081 | 3975 | 3978 | 3980 | rBV  | 594    | 405    | 0.09%  | 0.010%  |
| 97  | 14.257 | 4030 | 4033 | 4038 | rBV  | 396    | 336    | 0.07%  | 0.009%  |
| 98  | 14.322 | 4051 | 4053 | 4060 | rVB3 | 775    | 638    | 0.14%  | 0.016%  |
| 99  | 14.476 | 4097 | 4101 | 4103 | rBV4 | 2914   | 2569   | 0.56%  | 0.065%  |
| 100 | 14.708 | 4170 | 4173 | 4177 | rVB  | 313    | 289    | 0.06%  | 0.007%  |

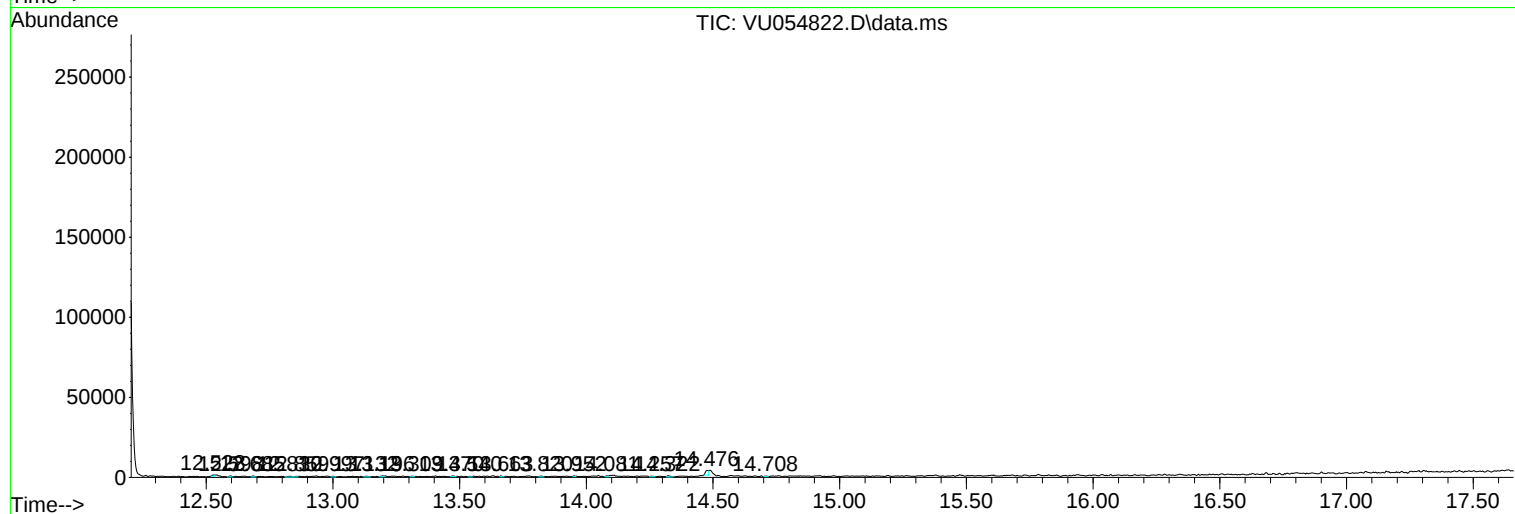
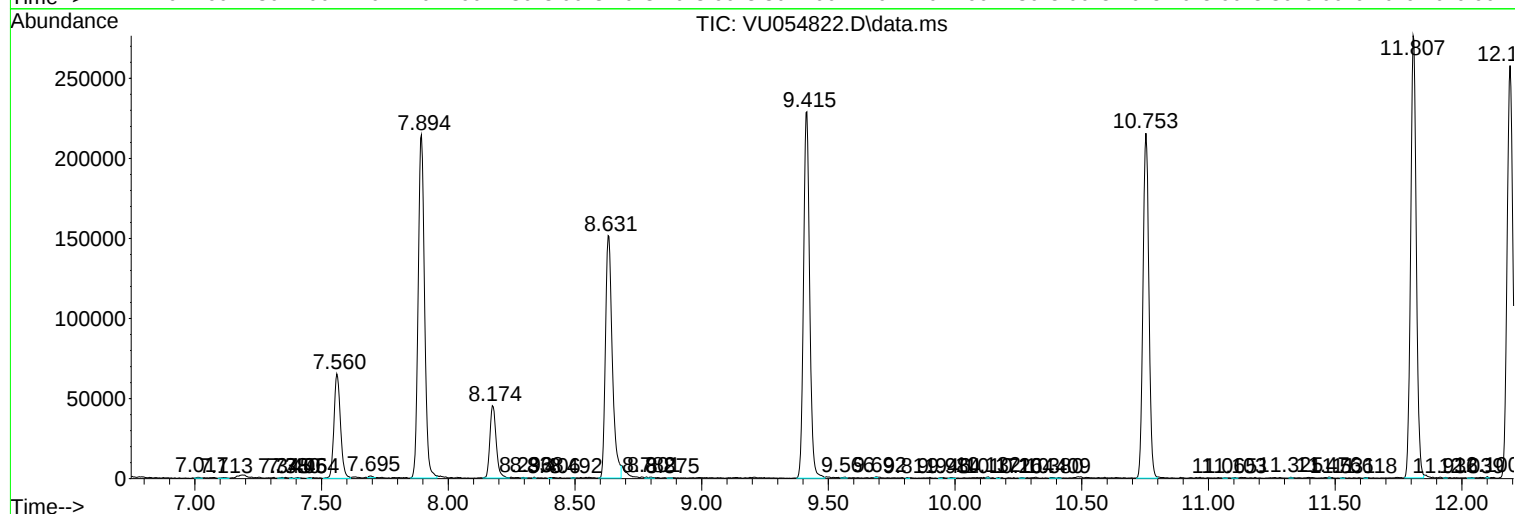
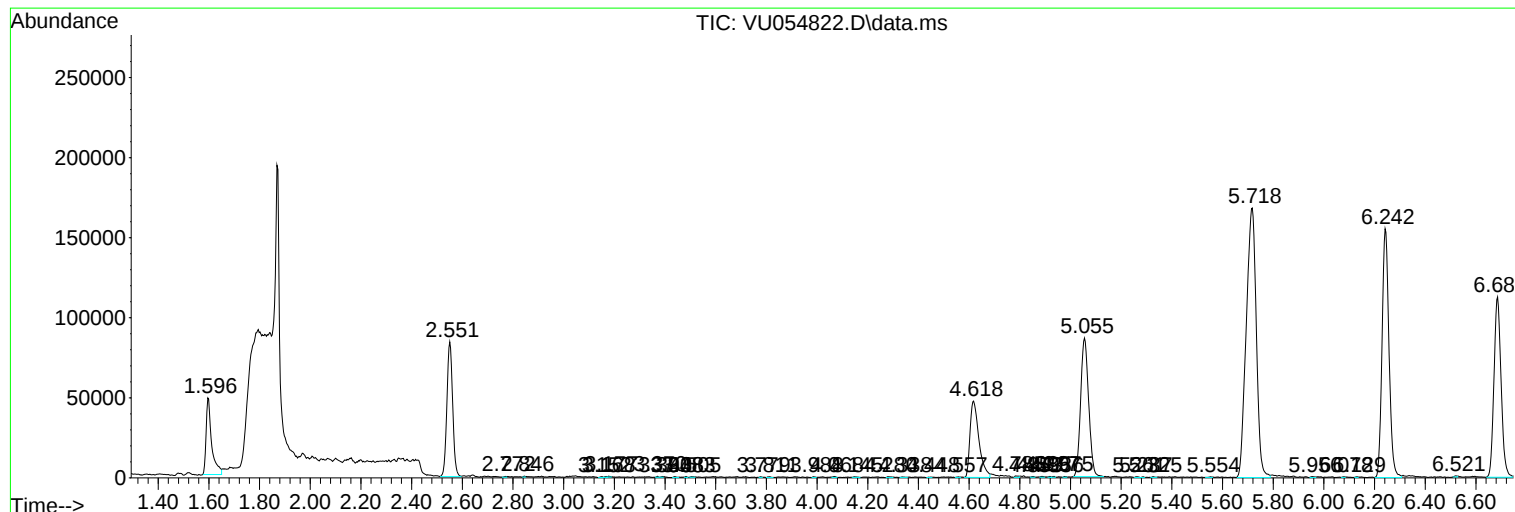
Sum of corrected areas: 3946773

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM071723WMA.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 |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|