

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101723\  
 Data File : VU055787.D  
 Acq On : 17 Oct 2023 12:02  
 Operator : MD/SY  
 Sample : VU1017WBL01  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK110

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\SFAMULM101023WMA.M  
 Title : VOC Analysis

Signal : TIC: VU055787.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         | 1.599       | 88            | 96          | 112          | rBV      | 220391         | 261971        | 12.59%          | 1.640%        |
| 2         | 1.891       | 179           | 187         | 207          | rVB      | 178179         | 258943        | 12.44%          | 1.621%        |
| 3         | 2.560       | 382           | 395         | 413          | rBV      | 390679         | 643160        | 30.90%          | 4.027%        |
| 4         | 2.695       | 435           | 437         | 439          | rBV3     | 621            | 287           | 0.01%           | 0.002%        |
| 5         | 2.718       | 440           | 444         | 449          | rVB4     | 1300           | 978           | 0.05%           | 0.006%        |
| 6         | 2.821       | 473           | 476         | 481          | rVB3     | 360            | 360           | 0.02%           | 0.002%        |
| 7         | 2.895       | 496           | 499         | 508          | rVB3     | 528            | 596           | 0.03%           | 0.004%        |
| 8         | 2.956       | 516           | 518         | 524          | rVB2     | 624            | 498           | 0.02%           | 0.003%        |
| 9         | 2.985       | 524           | 527         | 533          | rBV      | 417            | 404           | 0.02%           | 0.003%        |
| 10        | 3.039       | 534           | 544         | 554          | rVB4     | 3429           | 6100          | 0.29%           | 0.038%        |
| 11        | 3.168       | 581           | 584         | 585          | rBV2     | 661            | 451           | 0.02%           | 0.003%        |
| 12        | 3.431       | 662           | 666         | 670          | rVB      | 353            | 283           | 0.01%           | 0.002%        |
| 13        | 3.570       | 706           | 709         | 711          | rVV      | 489            | 345           | 0.02%           | 0.002%        |
| 14        | 3.608       | 715           | 721         | 724          | rBV2     | 386            | 404           | 0.02%           | 0.003%        |
| 15        | 3.631       | 724           | 728         | 734          | rVB2     | 557            | 571           | 0.03%           | 0.004%        |
| 16        | 3.731       | 755           | 759         | 766          | rVB2     | 414            | 455           | 0.02%           | 0.003%        |
| 17        | 3.763       | 766           | 769         | 774          | rBV2     | 356            | 364           | 0.02%           | 0.002%        |
| 18        | 3.824       | 783           | 788         | 791          | rBV      | 299            | 323           | 0.02%           | 0.002%        |
| 19        | 3.859       | 795           | 799         | 803          | rVV2     | 686            | 538           | 0.03%           | 0.003%        |
| 20        | 3.907       | 809           | 814         | 818          | rVB2     | 519            | 447           | 0.02%           | 0.003%        |
| 21        | 3.952       | 825           | 828         | 832          | rVV2     | 528            | 448           | 0.02%           | 0.003%        |
| 22        | 3.985       | 835           | 838         | 840          | rVV2     | 402            | 290           | 0.01%           | 0.002%        |
| 23        | 3.997       | 840           | 842         | 846          | rVV2     | 439            | 282           | 0.01%           | 0.002%        |
| 24        | 4.049       | 855           | 858         | 864          | rVB      | 471            | 322           | 0.02%           | 0.002%        |
| 25        | 4.110       | 874           | 877         | 882          | rVV2     | 394            | 341           | 0.02%           | 0.002%        |
| 26        | 4.264       | 921           | 925         | 930          | rVB2     | 340            | 310           | 0.01%           | 0.002%        |
| 27        | 4.296       | 930           | 935         | 939          | rBV      | 473            | 459           | 0.02%           | 0.003%        |
| 28        | 4.338       | 946           | 948         | 954          | rVB3     | 368            | 324           | 0.02%           | 0.002%        |
| 29        | 4.493       | 992           | 996         | 1002         | rBV2     | 353            | 296           | 0.01%           | 0.002%        |
| 30        | 4.615       | 1019          | 1034        | 1061         | rBV      | 178493         | 471980        | 22.68%          | 2.955%        |
| 31        | 4.840       | 1101          | 1104        | 1111         | rVV3     | 842            | 869           | 0.04%           | 0.005%        |
| 32        | 4.894       | 1115          | 1121        | 1126         | rVV4     | 718            | 971           | 0.05%           | 0.006%        |
| 33        | 4.930       | 1130          | 1132        | 1137         | rVB3     | 723            | 485           | 0.02%           | 0.003%        |
| 34        | 5.055       | 1154          | 1171        | 1198         | rBV      | 381678         | 851214        | 40.90%          | 5.329%        |
| 35        | 5.255       | 1231          | 1233        | 1239         | rVB3     | 608            | 420           | 0.02%           | 0.003%        |
| 36        | 5.332       | 1252          | 1257        | 1264         | rVB3     | 998            | 1520          | 0.07%           | 0.010%        |

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Integrator: RTE

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Start Thrs: 0.2

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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\SFAMULM101023WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |         |         |
|----|-------|------|------|------|------|--------|---------|---------|---------|
| 37 | 5.390 | 1272 | 1275 | 1279 | rBV2 | 569    | 387     | 0.02%   | 0.002%  |
| 38 | 5.473 | 1298 | 1301 | 1306 | rVB2 | 332    | 311     | 0.01%   | 0.002%  |
| 39 | 5.525 | 1313 | 1317 | 1321 | rVB3 | 612    | 452     | 0.02%   | 0.003%  |
| 40 | 5.599 | 1335 | 1340 | 1342 | rVB2 | 416    | 343     | 0.02%   | 0.002%  |
| 41 | 5.631 | 1342 | 1350 | 1354 | rBV2 | 284    | 329     | 0.02%   | 0.002%  |
| 42 | 5.718 | 1356 | 1377 | 1404 | rBV2 | 758069 | 2081106 | 100.00% | 13.030% |
| 43 | 5.972 | 1452 | 1456 | 1458 | rBV3 | 877    | 733     | 0.04%   | 0.005%  |
| 44 | 5.994 | 1461 | 1463 | 1466 | rBV3 | 703    | 368     | 0.02%   | 0.002%  |
| 45 | 6.042 | 1475 | 1478 | 1480 | rBV3 | 450    | 323     | 0.02%   | 0.002%  |
| 46 | 6.123 | 1501 | 1503 | 1509 | rVB2 | 423    | 333     | 0.02%   | 0.002%  |
| 47 | 6.148 | 1509 | 1511 | 1516 | rVB2 | 497    | 311     | 0.01%   | 0.002%  |
| 48 | 6.245 | 1526 | 1541 | 1573 | rBV  | 577310 | 1127444 | 54.18%  | 7.059%  |
| 49 | 6.447 | 1601 | 1604 | 1608 | rBV3 | 430    | 373     | 0.02%   | 0.002%  |
| 50 | 6.528 | 1618 | 1629 | 1644 | rVV  | 24647  | 48052   | 2.31%   | 0.301%  |
| 51 | 6.582 | 1644 | 1646 | 1647 | rVV  | 565    | 290     | 0.01%   | 0.002%  |
| 52 | 6.595 | 1648 | 1650 | 1657 | rVB6 | 1213   | 1173    | 0.06%   | 0.007%  |
| 53 | 6.685 | 1664 | 1678 | 1702 | rBV  | 478726 | 946124  | 45.46%  | 5.924%  |
| 54 | 6.859 | 1731 | 1732 | 1740 | rVB4 | 741    | 668     | 0.03%   | 0.004%  |
| 55 | 6.914 | 1743 | 1749 | 1752 | rBV3 | 448    | 424     | 0.02%   | 0.003%  |
| 56 | 7.023 | 1780 | 1783 | 1790 | rVB3 | 535    | 565     | 0.03%   | 0.004%  |
| 57 | 7.084 | 1800 | 1802 | 1807 | rBV  | 324    | 361     | 0.02%   | 0.002%  |
| 58 | 7.139 | 1814 | 1819 | 1822 | rVB3 | 472    | 424     | 0.02%   | 0.003%  |
| 59 | 7.190 | 1822 | 1835 | 1845 | rBV6 | 3622   | 8752    | 0.42%   | 0.055%  |
| 60 | 7.303 | 1866 | 1870 | 1872 | rBV2 | 460    | 363     | 0.02%   | 0.002%  |
| 61 | 7.454 | 1915 | 1917 | 1920 | rVB  | 508    | 277     | 0.01%   | 0.002%  |
| 62 | 7.515 | 1932 | 1936 | 1938 | rBV2 | 358    | 318     | 0.02%   | 0.002%  |
| 63 | 7.563 | 1938 | 1951 | 1985 | rVV  | 252722 | 463722  | 22.28%  | 2.903%  |
| 64 | 7.685 | 1986 | 1989 | 1990 | rVV2 | 1083   | 662     | 0.03%   | 0.004%  |
| 65 | 7.701 | 1991 | 1994 | 2003 | rVB6 | 2226   | 3262    | 0.16%   | 0.020%  |
| 66 | 7.894 | 2040 | 2054 | 2084 | rBV  | 898720 | 1597825 | 76.78%  | 10.004% |
| 67 | 8.132 | 2125 | 2128 | 2131 | rBV3 | 487    | 512     | 0.02%   | 0.003%  |
| 68 | 8.174 | 2131 | 2141 | 2165 | rVV  | 175701 | 309100  | 14.85%  | 1.935%  |
| 69 | 8.634 | 2272 | 2284 | 2317 | rBV3 | 488434 | 1223530 | 58.79%  | 7.661%  |
| 70 | 8.936 | 2372 | 2378 | 2380 | rBV3 | 537    | 584     | 0.03%   | 0.004%  |
| 71 | 8.965 | 2384 | 2387 | 2391 | rVV3 | 474    | 276     | 0.01%   | 0.002%  |
| 72 | 9.049 | 2411 | 2413 | 2417 | rBV3 | 435    | 336     | 0.02%   | 0.002%  |
| 73 | 9.090 | 2424 | 2426 | 2430 | rVB2 | 446    | 288     | 0.01%   | 0.002%  |
| 74 | 9.296 | 2486 | 2490 | 2497 | rVB4 | 373    | 339     | 0.02%   | 0.002%  |
| 75 | 9.348 | 2504 | 2506 | 2511 | rVB2 | 511    | 356     | 0.02%   | 0.002%  |
| 76 | 9.415 | 2511 | 2527 | 2564 | rBV  | 859443 | 1453751 | 69.85%  | 9.102%  |

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 MSVOA\_U  
 ClientSampleId :  
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Integration Parameters: LSCINT.P

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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\SFAMULM101023WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 9.695  | 2609 | 2614 | 2615 | rBV  | 545    | 405     | 0.02%  | 0.003% |
| 78  | 9.843  | 2656 | 2660 | 2666 | rVB3 | 428    | 378     | 0.02%  | 0.002% |
| 79  | 10.004 | 2707 | 2710 | 2716 | rVB2 | 750    | 506     | 0.02%  | 0.003% |
| 80  | 10.084 | 2731 | 2735 | 2737 | rBV2 | 371    | 300     | 0.01%  | 0.002% |
| 81  | 10.197 | 2765 | 2770 | 2774 | rBV2 | 418    | 538     | 0.03%  | 0.003% |
| 82  | 10.637 | 2901 | 2907 | 2910 | rBV  | 476    | 538     | 0.03%  | 0.003% |
| 83  | 10.753 | 2928 | 2943 | 2964 | rBV  | 736612 | 1222771 | 58.76% | 7.656% |
| 84  | 10.904 | 2984 | 2990 | 2993 | rVB3 | 721    | 812     | 0.04%  | 0.005% |
| 85  | 11.190 | 3076 | 3079 | 3083 | rVB3 | 481    | 308     | 0.01%  | 0.002% |
| 86  | 11.409 | 3143 | 3147 | 3154 | rVB3 | 773    | 907     | 0.04%  | 0.006% |
| 87  | 11.640 | 3217 | 3219 | 3226 | rVB  | 483    | 428     | 0.02%  | 0.003% |
| 88  | 11.811 | 3259 | 3272 | 3306 | rBV  | 849116 | 1402388 | 67.39% | 8.780% |
| 89  | 12.032 | 3339 | 3341 | 3345 | rBV4 | 376    | 302     | 0.01%  | 0.002% |
| 90  | 12.084 | 3355 | 3357 | 3361 | rBV3 | 416    | 363     | 0.02%  | 0.002% |
| 91  | 12.190 | 3376 | 3390 | 3418 | rBV  | 925027 | 1552228 | 74.59% | 9.719% |
| 92  | 12.415 | 3457 | 3460 | 3465 | rBV5 | 826    | 675     | 0.03%  | 0.004% |
| 93  | 12.560 | 3499 | 3505 | 3509 | rBV2 | 574    | 739     | 0.04%  | 0.005% |
| 94  | 12.582 | 3509 | 3512 | 3518 | rVV4 | 614    | 548     | 0.03%  | 0.003% |
| 95  | 13.306 | 3731 | 3737 | 3740 | rBV2 | 822    | 997     | 0.05%  | 0.006% |
| 96  | 13.489 | 3792 | 3794 | 3798 | rBV3 | 592    | 347     | 0.02%  | 0.002% |
| 97  | 13.534 | 3805 | 3808 | 3812 | rVB3 | 678    | 504     | 0.02%  | 0.003% |
| 98  | 13.865 | 3909 | 3911 | 3916 | rBV5 | 909    | 833     | 0.04%  | 0.005% |
| 99  | 14.319 | 4049 | 4052 | 4054 | rBV  | 714    | 486     | 0.02%  | 0.003% |
| 100 | 14.740 | 4181 | 4183 | 4188 | rBV3 | 617    | 396     | 0.02%  | 0.002% |

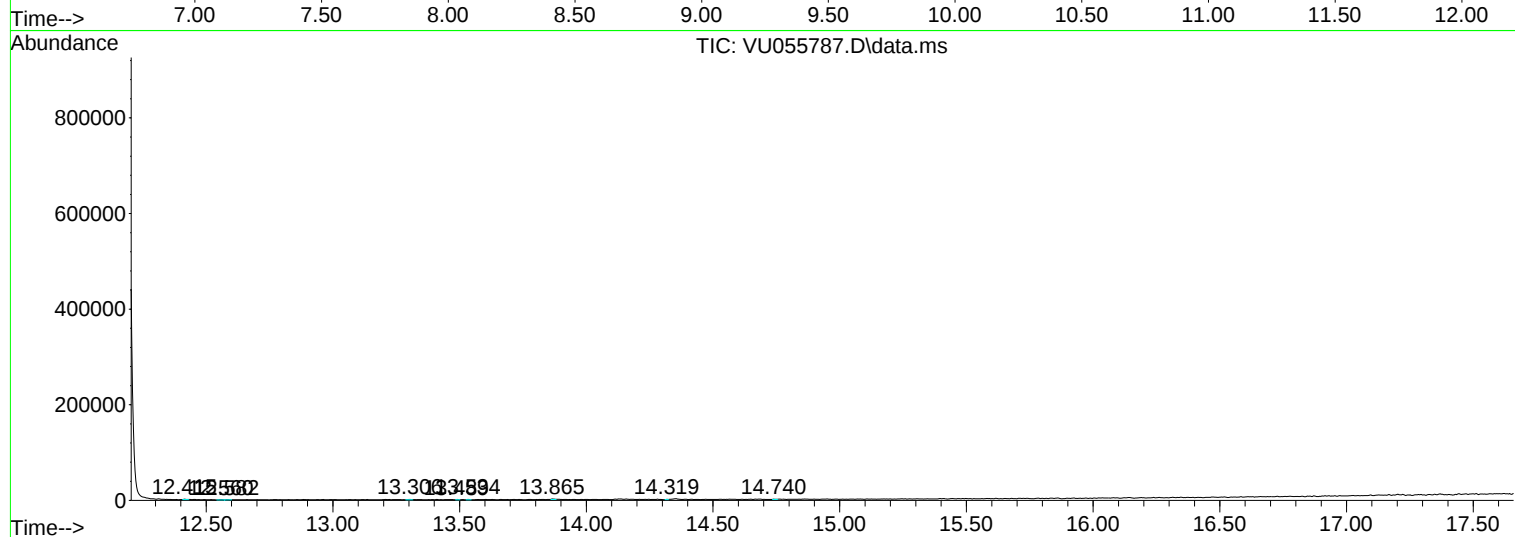
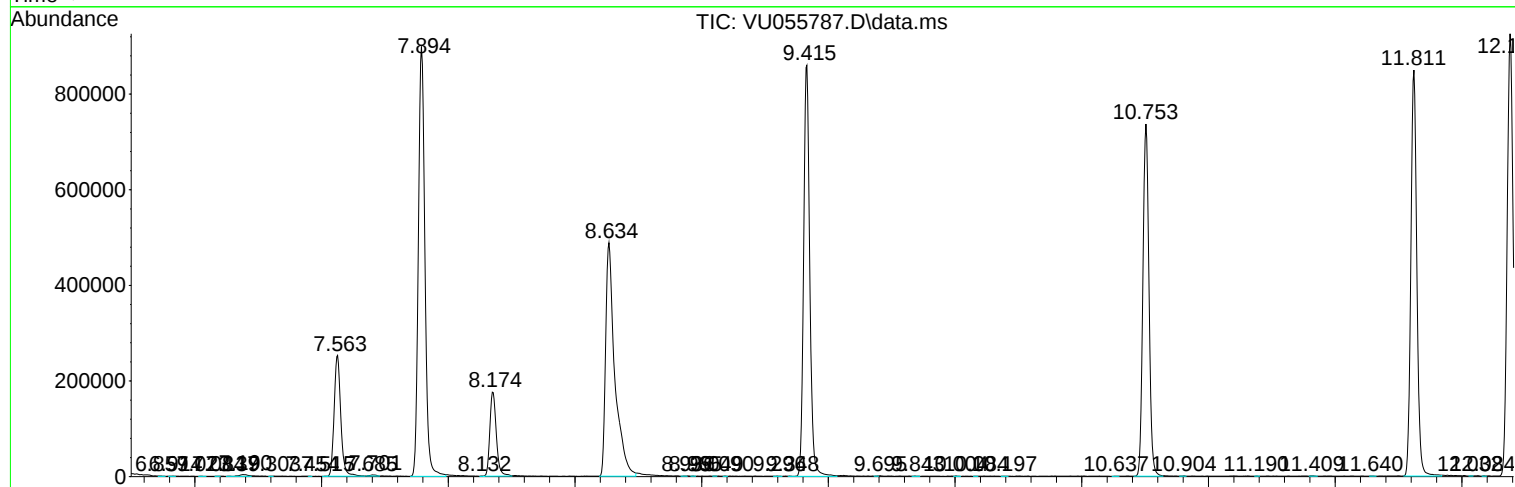
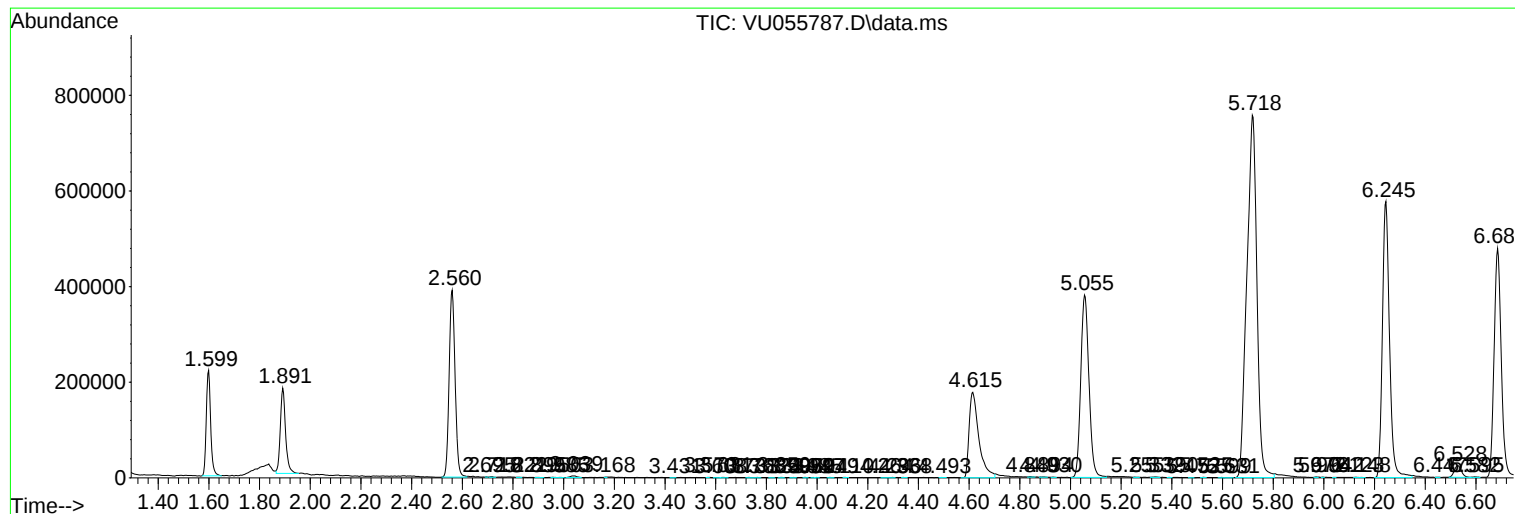
Sum of corrected areas: 15971853

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM101023WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101723\  
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No Library Search Compounds Detected

\*\*\*\*\*

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