

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU010824\  
 Data File : VU057385.D  
 Acq On : 08 Jan 2024 16:19  
 Operator : MD/SY  
 Sample : 05787-04  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DCME1

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\SFAMULM010824WMA.M  
 Title : VOC Analysis

Signal : TIC: VU057385.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         | 1.357       | 15            | 21          | 30           | rBV      | 24672          | 25738         | 2.53%           | 0.315%        |
| 2         | 1.599       | 87            | 96          | 110          | rVB      | 121347         | 151336        | 14.86%          | 1.852%        |
| 3         | 1.914       | 185           | 194         | 211          | rBV      | 84603          | 124590        | 12.23%          | 1.525%        |
| 4         | 2.399       | 340           | 345         | 348          | rBV2     | 1041           | 1044          | 0.10%           | 0.013%        |
| 5         | 2.464       | 363           | 365         | 371          | rVB      | 370            | 221           | 0.02%           | 0.003%        |
| 6         | 2.560       | 383           | 395         | 411          | rBV      | 223790         | 359385        | 35.29%          | 4.398%        |
| 7         | 2.644       | 415           | 421         | 423          | rBV5     | 3288           | 3564          | 0.35%           | 0.044%        |
| 8         | 2.737       | 448           | 450         | 453          | rBV2     | 369            | 264           | 0.03%           | 0.003%        |
| 9         | 2.830       | 476           | 479         | 481          | rBV      | 418            | 316           | 0.03%           | 0.004%        |
| 10        | 3.267       | 611           | 615         | 619          | rBV      | 204            | 228           | 0.02%           | 0.003%        |
| 11        | 3.351       | 635           | 641         | 643          | rBV2     | 751            | 644           | 0.06%           | 0.008%        |
| 12        | 3.386       | 649           | 652         | 654          | rVB      | 301            | 177           | 0.02%           | 0.002%        |
| 13        | 3.489       | 681           | 684         | 688          | rBB      | 218            | 178           | 0.02%           | 0.002%        |
| 14        | 3.550       | 702           | 703         | 707          | rVV      | 282            | 194           | 0.02%           | 0.002%        |
| 15        | 3.698       | 745           | 749         | 753          | rBB2     | 265            | 249           | 0.02%           | 0.003%        |
| 16        | 3.853       | 784           | 797         | 810          | rVV4     | 3566           | 8587          | 0.84%           | 0.105%        |
| 17        | 4.026       | 849           | 851         | 855          | rVB      | 285            | 173           | 0.02%           | 0.002%        |
| 18        | 4.518       | 1001          | 1004        | 1008         | rBB      | 261            | 190           | 0.02%           | 0.002%        |
| 19        | 4.637       | 1029          | 1041        | 1073         | rBV2     | 49110          | 159482        | 15.66%          | 1.952%        |
| 20        | 4.949       | 1136          | 1138        | 1141         | rVB2     | 399            | 193           | 0.02%           | 0.002%        |
| 21        | 4.965       | 1141          | 1143        | 1145         | rBV      | 324            | 206           | 0.02%           | 0.003%        |
| 22        | 5.055       | 1154          | 1171        | 1193         | rBV      | 198547         | 444394        | 43.64%          | 5.439%        |
| 23        | 5.209       | 1217          | 1219        | 1222         | rVB2     | 578            | 316           | 0.03%           | 0.004%        |
| 24        | 5.229       | 1222          | 1225        | 1228         | rBV2     | 374            | 210           | 0.02%           | 0.003%        |
| 25        | 5.283       | 1238          | 1242        | 1247         | rVB3     | 526            | 455           | 0.04%           | 0.006%        |
| 26        | 5.525       | 1314          | 1317        | 1320         | rBV2     | 406            | 316           | 0.03%           | 0.004%        |
| 27        | 5.717       | 1357          | 1377        | 1401         | rBV2     | 366552         | 1018311       | 100.00%         | 12.463%       |
| 28        | 5.971       | 1454          | 1456        | 1459         | rVB2     | 465            | 268           | 0.03%           | 0.003%        |
| 29        | 6.026       | 1471          | 1473        | 1476         | rBV      | 261            | 220           | 0.02%           | 0.003%        |
| 30        | 6.042       | 1476          | 1478        | 1482         | rVV      | 384            | 200           | 0.02%           | 0.002%        |
| 31        | 6.094       | 1491          | 1494        | 1498         | rBV2     | 340            | 347           | 0.03%           | 0.004%        |
| 32        | 6.242       | 1527          | 1540        | 1564         | rBV      | 337101         | 651296        | 63.96%          | 7.971%        |
| 33        | 6.479       | 1611          | 1614        | 1617         | rVB2     | 324            | 204           | 0.02%           | 0.002%        |
| 34        | 6.502       | 1618          | 1621        | 1624         | rBV      | 252            | 200           | 0.02%           | 0.002%        |
| 35        | 6.537       | 1624          | 1632        | 1642         | rBV7     | 5831           | 10620         | 1.04%           | 0.130%        |
| 36        | 6.598       | 1649          | 1651        | 1656         | rVB      | 355            | 179           | 0.02%           | 0.002%        |

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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\SFAMULM010824WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 6.631  | 1659 | 1661 | 1663 | rBV  | 279    | 186    | 0.02%  | 0.002% |
| 38 | 6.682  | 1663 | 1677 | 1701 | rBV  | 222154 | 434487 | 42.67% | 5.318% |
| 39 | 6.798  | 1711 | 1713 | 1714 | rBV3 | 359    | 178    | 0.02%  | 0.002% |
| 40 | 7.029  | 1777 | 1785 | 1787 | rBV  | 184    | 277    | 0.03%  | 0.003% |
| 41 | 7.113  | 1810 | 1811 | 1816 | rBV  | 243    | 176    | 0.02%  | 0.002% |
| 42 | 7.193  | 1834 | 1836 | 1838 | rBV2 | 353    | 203    | 0.02%  | 0.002% |
| 43 | 7.261  | 1852 | 1857 | 1861 | rBV2 | 348    | 389    | 0.04%  | 0.005% |
| 44 | 7.377  | 1890 | 1893 | 1896 | rVB2 | 377    | 262    | 0.03%  | 0.003% |
| 45 | 7.560  | 1937 | 1950 | 1973 | rBV  | 126645 | 232373 | 22.82% | 2.844% |
| 46 | 7.701  | 1988 | 1994 | 1997 | rBV3 | 807    | 966    | 0.09%  | 0.012% |
| 47 | 7.798  | 2019 | 2024 | 2028 | rBV2 | 627    | 592    | 0.06%  | 0.007% |
| 48 | 7.891  | 2039 | 2053 | 2071 | rBV  | 447645 | 791179 | 77.70% | 9.683% |
| 49 | 8.174  | 2130 | 2141 | 2161 | rVV  | 93025  | 162151 | 15.92% | 1.985% |
| 50 | 8.283  | 2173 | 2175 | 2177 | rVB  | 502    | 184    | 0.02%  | 0.002% |
| 51 | 8.428  | 2218 | 2220 | 2224 | rVB  | 390    | 224    | 0.02%  | 0.003% |
| 52 | 8.460  | 2227 | 2230 | 2232 | rBV  | 411    | 281    | 0.03%  | 0.003% |
| 53 | 8.547  | 2244 | 2257 | 2274 | rBV2 | 290737 | 502040 | 49.30% | 6.144% |
| 54 | 8.643  | 2275 | 2287 | 2317 | rVB3 | 178575 | 393690 | 38.66% | 4.818% |
| 55 | 8.843  | 2347 | 2349 | 2357 | rVB  | 430    | 401    | 0.04%  | 0.005% |
| 56 | 9.151  | 2441 | 2445 | 2447 | rBV  | 349    | 250    | 0.02%  | 0.003% |
| 57 | 9.232  | 2466 | 2470 | 2474 | rBB  | 154    | 178    | 0.02%  | 0.002% |
| 58 | 9.360  | 2507 | 2510 | 2512 | rBB2 | 458    | 247    | 0.02%  | 0.003% |
| 59 | 9.412  | 2513 | 2526 | 2553 | rBV  | 454140 | 791667 | 77.74% | 9.689% |
| 60 | 9.557  | 2568 | 2571 | 2573 | rBV2 | 538    | 395    | 0.04%  | 0.005% |
| 61 | 9.598  | 2582 | 2584 | 2586 | rBV  | 387    | 212    | 0.02%  | 0.003% |
| 62 | 9.688  | 2609 | 2612 | 2614 | rBV2 | 335    | 227    | 0.02%  | 0.003% |
| 63 | 9.701  | 2614 | 2616 | 2621 | rVB2 | 401    | 340    | 0.03%  | 0.004% |
| 64 | 9.791  | 2641 | 2644 | 2646 | rBV  | 240    | 197    | 0.02%  | 0.002% |
| 65 | 9.862  | 2662 | 2666 | 2668 | rBV  | 280    | 239    | 0.02%  | 0.003% |
| 66 | 9.891  | 2672 | 2675 | 2678 | rVV2 | 286    | 228    | 0.02%  | 0.003% |
| 67 | 9.975  | 2695 | 2701 | 2705 | rBB  | 230    | 262    | 0.03%  | 0.003% |
| 68 | 10.000 | 2705 | 2709 | 2711 | rBV  | 299    | 260    | 0.03%  | 0.003% |
| 69 | 10.016 | 2712 | 2714 | 2718 | rVV  | 327    | 189    | 0.02%  | 0.002% |
| 70 | 10.100 | 2738 | 2740 | 2742 | rVV  | 383    | 272    | 0.03%  | 0.003% |
| 71 | 10.126 | 2745 | 2748 | 2751 | rVB2 | 426    | 211    | 0.02%  | 0.003% |
| 72 | 10.225 | 2775 | 2779 | 2784 | rBB  | 267    | 313    | 0.03%  | 0.004% |
| 73 | 10.264 | 2784 | 2791 | 2794 | rBV  | 213    | 327    | 0.03%  | 0.004% |
| 74 | 10.483 | 2855 | 2859 | 2864 | rBV2 | 613    | 670    | 0.07%  | 0.008% |
| 75 | 10.534 | 2872 | 2875 | 2880 | rVB  | 336    | 291    | 0.03%  | 0.004% |
| 76 | 10.576 | 2886 | 2888 | 2891 | rVB  | 393    | 226    | 0.02%  | 0.003% |

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Integration Parameters: LSCINT.P

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Smoothing : OFF

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Max Peaks: 100

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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\SFAMULM010824WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 10.598 | 2891 | 2895 | 2898 | rBV2 | 337    | 256    | 0.03%  | 0.003% |
| 78  | 10.753 | 2929 | 2943 | 2958 | rBV  | 302160 | 491659 | 48.28% | 6.017% |
| 79  | 10.884 | 2978 | 2984 | 2985 | rBV2 | 1166   | 846    | 0.08%  | 0.010% |
| 80  | 11.093 | 3044 | 3049 | 3057 | rVB  | 606    | 754    | 0.07%  | 0.009% |
| 81  | 11.126 | 3057 | 3059 | 3063 | rVB  | 270    | 191    | 0.02%  | 0.002% |
| 82  | 11.743 | 3247 | 3251 | 3258 | rBV3 | 1356   | 1626   | 0.16%  | 0.020% |
| 83  | 11.807 | 3258 | 3271 | 3293 | rBV  | 419903 | 677456 | 66.53% | 8.291% |
| 84  | 12.042 | 3339 | 3344 | 3345 | rBV  | 467    | 303    | 0.03%  | 0.004% |
| 85  | 12.087 | 3352 | 3358 | 3364 | rBV3 | 491    | 637    | 0.06%  | 0.008% |
| 86  | 12.187 | 3377 | 3389 | 3407 | rBV  | 423555 | 691657 | 67.92% | 8.465% |
| 87  | 12.331 | 3431 | 3434 | 3436 | rVB  | 414    | 196    | 0.02%  | 0.002% |
| 88  | 12.392 | 3450 | 3453 | 3456 | rVB  | 321    | 209    | 0.02%  | 0.003% |
| 89  | 12.421 | 3459 | 3462 | 3466 | rVB  | 471    | 346    | 0.03%  | 0.004% |
| 90  | 12.454 | 3467 | 3472 | 3477 | rBV2 | 267    | 288    | 0.03%  | 0.004% |
| 91  | 12.589 | 3507 | 3514 | 3518 | rBV  | 321    | 462    | 0.05%  | 0.006% |
| 92  | 12.672 | 3538 | 3540 | 3542 | rBV  | 473    | 281    | 0.03%  | 0.003% |
| 93  | 12.765 | 3564 | 3569 | 3578 | rVB4 | 1198   | 1759   | 0.17%  | 0.022% |
| 94  | 12.907 | 3610 | 3613 | 3618 | rVB  | 291    | 223    | 0.02%  | 0.003% |
| 95  | 13.225 | 3705 | 3712 | 3718 | rVV4 | 2181   | 2806   | 0.28%  | 0.034% |
| 96  | 13.714 | 3862 | 3864 | 3867 | rBV2 | 325    | 172    | 0.02%  | 0.002% |
| 97  | 13.846 | 3899 | 3905 | 3915 | rVB6 | 3317   | 5072   | 0.50%  | 0.062% |
| 98  | 14.093 | 3974 | 3982 | 3989 | rBV2 | 3463   | 5732   | 0.56%  | 0.070% |
| 99  | 14.187 | 4009 | 4011 | 4015 | rBV2 | 499    | 353    | 0.03%  | 0.004% |
| 100 | 14.328 | 4049 | 4055 | 4063 | rBV5 | 3966   | 5411   | 0.53%  | 0.066% |

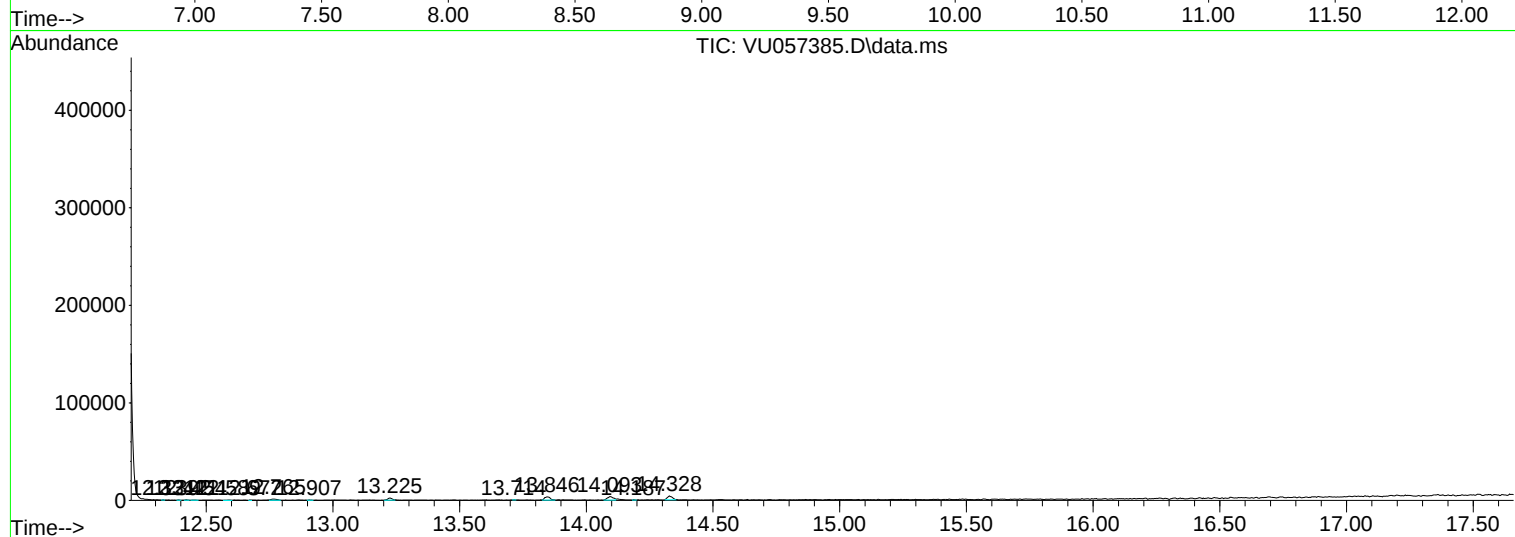
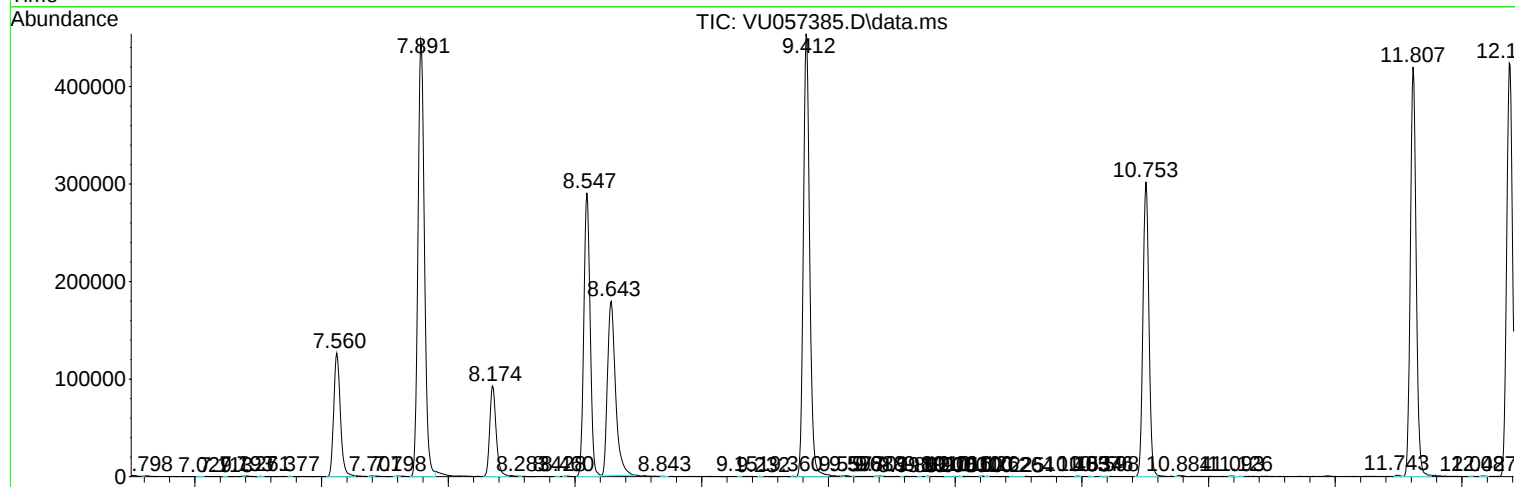
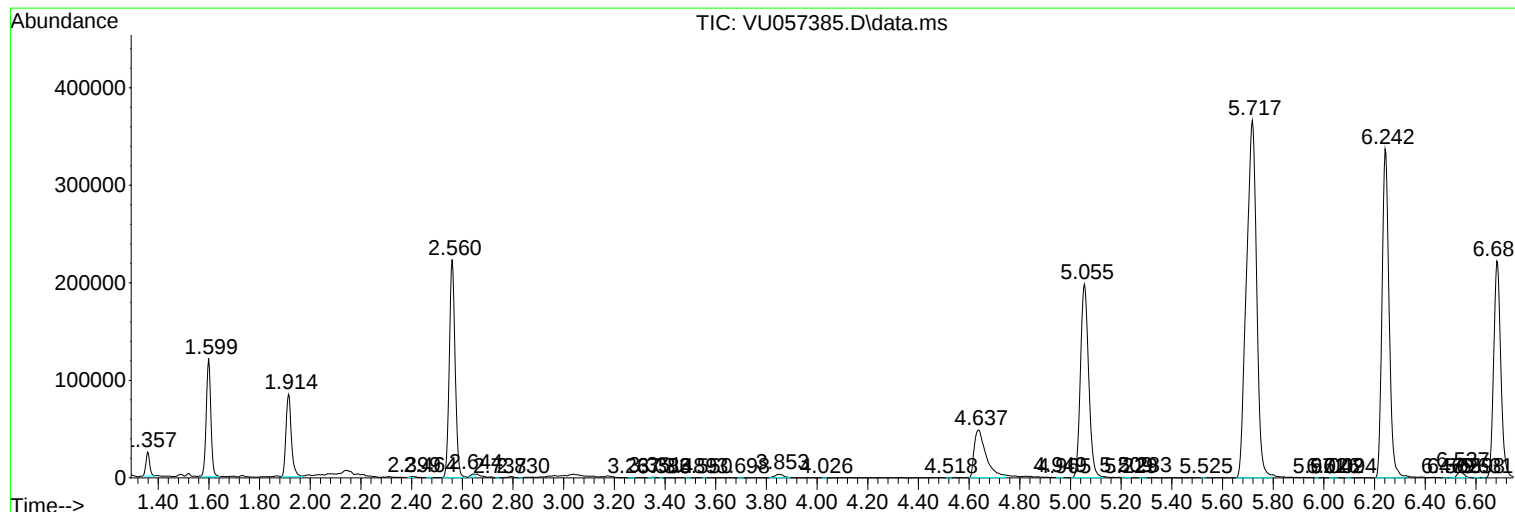
Sum of corrected areas: 8170630

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM010824WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU010824\  
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No Library Search Compounds Detected

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