

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051022\  
 Data File : VU048484.D  
 Acq On : 10 May 2022 12:30  
 Operator : SY/MD  
 Sample : N2736-05  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 EXEW0

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\SFAMULM050622WMA.M  
 Title : VOC Analysis

Signal : TIC: VU048484.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         | 1.597       | 74            | 80          | 95           | rVB      | 121248         | 138461        | 12.72%          | 1.637%        |
| 2         | 1.912       | 172           | 178         | 200          | rVB      | 98964          | 128974        | 11.84%          | 1.525%        |
| 3         | 2.568       | 369           | 382         | 396          | rBV      | 229548         | 374477        | 34.39%          | 4.428%        |
| 4         | 2.755       | 437           | 440         | 445          | rBV2     | 319            | 332           | 0.03%           | 0.004%        |
| 5         | 2.832       | 462           | 464         | 469          | rVB2     | 381            | 262           | 0.02%           | 0.003%        |
| 6         | 2.855       | 469           | 471         | 476          | rVB      | 315            | 231           | 0.02%           | 0.003%        |
| 7         | 2.896       | 481           | 484         | 486          | rBV2     | 213            | 145           | 0.01%           | 0.002%        |
| 8         | 2.974       | 505           | 508         | 512          | rVB      | 250            | 134           | 0.01%           | 0.002%        |
| 9         | 2.996       | 512           | 515         | 518          | rBV2     | 318            | 224           | 0.02%           | 0.003%        |
| 10        | 3.038       | 525           | 528         | 530          | rBV2     | 438            | 301           | 0.03%           | 0.004%        |
| 11        | 3.134       | 556           | 558         | 561          | rVB      | 291            | 151           | 0.01%           | 0.002%        |
| 12        | 3.173       | 567           | 570         | 571          | rBV2     | 624            | 369           | 0.03%           | 0.004%        |
| 13        | 3.301       | 606           | 610         | 612          | rBV2     | 263            | 187           | 0.02%           | 0.002%        |
| 14        | 3.353       | 622           | 626         | 630          | rVB2     | 473            | 406           | 0.04%           | 0.005%        |
| 15        | 3.385       | 630           | 636         | 637          | rBV      | 354            | 305           | 0.03%           | 0.004%        |
| 16        | 3.507       | 672           | 674         | 677          | rBV      | 300            | 206           | 0.02%           | 0.002%        |
| 17        | 3.533       | 680           | 682         | 686          | rVV2     | 292            | 208           | 0.02%           | 0.002%        |
| 18        | 3.565       | 687           | 692         | 695          | rVB2     | 216            | 211           | 0.02%           | 0.002%        |
| 19        | 3.584       | 695           | 698         | 699          | rBV      | 262            | 128           | 0.01%           | 0.002%        |
| 20        | 3.723       | 739           | 741         | 748          | rVB3     | 259            | 249           | 0.02%           | 0.003%        |
| 21        | 3.784       | 757           | 760         | 764          | rVB3     | 358            | 253           | 0.02%           | 0.003%        |
| 22        | 3.880       | 786           | 790         | 793          | rVB2     | 303            | 223           | 0.02%           | 0.003%        |
| 23        | 3.980       | 818           | 821         | 824          | rBB      | 254            | 187           | 0.02%           | 0.002%        |
| 24        | 4.002       | 824           | 828         | 830          | rBV2     | 302            | 265           | 0.02%           | 0.003%        |
| 25        | 4.031       | 834           | 837         | 839          | rBV      | 223            | 130           | 0.01%           | 0.002%        |
| 26        | 4.121       | 863           | 865         | 869          | rVB      | 324            | 263           | 0.02%           | 0.003%        |
| 27        | 4.147       | 869           | 873         | 876          | rBV2     | 308            | 253           | 0.02%           | 0.003%        |
| 28        | 4.273       | 909           | 912         | 918          | rVB2     | 310            | 223           | 0.02%           | 0.003%        |
| 29        | 4.305       | 918           | 922         | 925          | rBV      | 151            | 118           | 0.01%           | 0.001%        |
| 30        | 4.372       | 940           | 943         | 945          | rBV      | 205            | 120           | 0.01%           | 0.001%        |
| 31        | 4.440       | 962           | 964         | 966          | rBV2     | 201            | 111           | 0.01%           | 0.001%        |
| 32        | 4.498       | 979           | 982         | 985          | rBV2     | 297            | 257           | 0.02%           | 0.003%        |
| 33        | 4.620       | 1007          | 1020        | 1046         | rBV      | 111877         | 274159        | 25.18%          | 3.242%        |
| 34        | 5.063       | 1142          | 1158        | 1181         | rBV2     | 200112         | 443577        | 40.74%          | 5.245%        |
| 35        | 5.269       | 1219          | 1222        | 1225         | rBV      | 232            | 159           | 0.01%           | 0.002%        |
| 36        | 5.292       | 1226          | 1229        | 1238         | rVB4     | 461            | 466           | 0.04%           | 0.006%        |

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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\SFAMULM050622WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |         |         |
|----|-------|------|------|------|------|--------|---------|---------|---------|
| 37 | 5.330 | 1238 | 1241 | 1245 | rBV  | 262    | 219     | 0.02%   | 0.003%  |
| 38 | 5.388 | 1255 | 1259 | 1261 | rBV2 | 319    | 220     | 0.02%   | 0.003%  |
| 39 | 5.433 | 1270 | 1273 | 1276 | rBV2 | 360    | 301     | 0.03%   | 0.004%  |
| 40 | 5.526 | 1299 | 1302 | 1304 | rBV  | 130    | 117     | 0.01%   | 0.001%  |
| 41 | 5.546 | 1305 | 1308 | 1309 | rBV  | 259    | 128     | 0.01%   | 0.002%  |
| 42 | 5.604 | 1322 | 1326 | 1328 | rBV2 | 249    | 196     | 0.02%   | 0.002%  |
| 43 | 5.636 | 1333 | 1336 | 1338 | rVB2 | 247    | 161     | 0.01%   | 0.002%  |
| 44 | 5.726 | 1343 | 1364 | 1389 | rBV2 | 400605 | 1088891 | 100.00% | 12.875% |
| 45 | 5.973 | 1439 | 1441 | 1446 | rVB  | 286    | 229     | 0.02%   | 0.003%  |
| 46 | 5.999 | 1446 | 1449 | 1452 | rBV  | 300    | 283     | 0.03%   | 0.003%  |
| 47 | 6.073 | 1468 | 1472 | 1476 | rBV  | 372    | 324     | 0.03%   | 0.004%  |
| 48 | 6.092 | 1476 | 1478 | 1481 | rBV2 | 210    | 143     | 0.01%   | 0.002%  |
| 49 | 6.160 | 1496 | 1499 | 1502 | rBV2 | 326    | 255     | 0.02%   | 0.003%  |
| 50 | 6.250 | 1512 | 1527 | 1547 | rBV  | 344869 | 656409  | 60.28%  | 7.761%  |
| 51 | 6.382 | 1565 | 1568 | 1574 | rBV2 | 402    | 521     | 0.05%   | 0.006%  |
| 52 | 6.430 | 1580 | 1583 | 1586 | rBV2 | 339    | 225     | 0.02%   | 0.003%  |
| 53 | 6.475 | 1589 | 1597 | 1605 | rBV5 | 2615   | 4313    | 0.40%   | 0.051%  |
| 54 | 6.690 | 1650 | 1664 | 1685 | rBV  | 248668 | 483764  | 44.43%  | 5.720%  |
| 55 | 6.797 | 1693 | 1697 | 1698 | rBV2 | 437    | 327     | 0.03%   | 0.004%  |
| 56 | 6.954 | 1743 | 1746 | 1750 | rVB  | 330    | 247     | 0.02%   | 0.003%  |
| 57 | 6.983 | 1752 | 1755 | 1760 | rBV  | 288    | 194     | 0.02%   | 0.002%  |
| 58 | 7.112 | 1791 | 1795 | 1802 | rVB2 | 345    | 432     | 0.04%   | 0.005%  |
| 59 | 7.147 | 1802 | 1806 | 1808 | rBV2 | 275    | 234     | 0.02%   | 0.003%  |
| 60 | 7.186 | 1811 | 1818 | 1829 | rVB6 | 1564   | 2718    | 0.25%   | 0.032%  |
| 61 | 7.314 | 1855 | 1858 | 1863 | rVB  | 225    | 155     | 0.01%   | 0.002%  |
| 62 | 7.456 | 1897 | 1902 | 1905 | rBV2 | 310    | 341     | 0.03%   | 0.004%  |
| 63 | 7.565 | 1924 | 1936 | 1960 | rBV  | 99927  | 177940  | 16.34%  | 2.104%  |
| 64 | 7.690 | 1969 | 1975 | 1978 | rBV3 | 1344   | 1531    | 0.14%   | 0.018%  |
| 65 | 7.758 | 1993 | 1996 | 1999 | rBV  | 270    | 233     | 0.02%   | 0.003%  |
| 66 | 7.896 | 2026 | 2039 | 2055 | rBV  | 490564 | 845826  | 77.68%  | 10.001% |
| 67 | 8.179 | 2115 | 2127 | 2143 | rBV  | 74825  | 126907  | 11.65%  | 1.501%  |
| 68 | 8.472 | 2206 | 2218 | 2228 | rBV2 | 3681   | 6708    | 0.62%   | 0.079%  |
| 69 | 8.575 | 2247 | 2250 | 2253 | rVB2 | 398    | 255     | 0.02%   | 0.003%  |
| 70 | 8.632 | 2256 | 2268 | 2298 | rBV  | 349112 | 632892  | 58.12%  | 7.483%  |
| 71 | 8.822 | 2324 | 2327 | 2329 | rBV2 | 430    | 197     | 0.02%   | 0.002%  |
| 72 | 8.867 | 2339 | 2341 | 2342 | rBV  | 265    | 135     | 0.01%   | 0.002%  |
| 73 | 8.996 | 2377 | 2381 | 2384 | rBV3 | 357    | 346     | 0.03%   | 0.004%  |
| 74 | 9.070 | 2401 | 2404 | 2410 | rBV  | 319    | 262     | 0.02%   | 0.003%  |
| 75 | 9.243 | 2456 | 2458 | 2462 | rVB  | 387    | 226     | 0.02%   | 0.003%  |
| 76 | 9.417 | 2499 | 2512 | 2536 | rBV  | 503113 | 828823  | 76.12%  | 9.800%  |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMULM050622WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 9.616  | 2572 | 2574 | 2576 | rBV2 | 211    | 112    | 0.01%  | 0.001% |
| 78  | 9.661  | 2585 | 2588 | 2590 | rBV  | 251    | 118    | 0.01%  | 0.001% |
| 79  | 9.687  | 2592 | 2596 | 2605 | rVB3 | 757    | 1004   | 0.09%  | 0.012% |
| 80  | 10.044 | 2704 | 2707 | 2710 | rBV  | 263    | 169    | 0.02%  | 0.002% |
| 81  | 10.144 | 2735 | 2738 | 2742 | rBV2 | 479    | 349    | 0.03%  | 0.004% |
| 82  | 10.179 | 2747 | 2749 | 2754 | rVB  | 192    | 143    | 0.01%  | 0.002% |
| 83  | 10.324 | 2792 | 2794 | 2797 | rVB  | 279    | 133    | 0.01%  | 0.002% |
| 84  | 10.346 | 2797 | 2801 | 2805 | rBV2 | 339    | 340    | 0.03%  | 0.004% |
| 85  | 10.481 | 2838 | 2843 | 2849 | rBV  | 485    | 642    | 0.06%  | 0.008% |
| 86  | 10.755 | 2916 | 2928 | 2948 | rBV  | 352598 | 573860 | 52.70% | 6.785% |
| 87  | 10.896 | 2963 | 2972 | 2979 | rBV3 | 3846   | 6143   | 0.56%  | 0.073% |
| 88  | 11.623 | 3195 | 3198 | 3202 | rBV  | 298    | 273    | 0.03%  | 0.003% |
| 89  | 11.742 | 3231 | 3235 | 3243 | rVB5 | 881    | 1024   | 0.09%  | 0.012% |
| 90  | 11.812 | 3244 | 3257 | 3278 | rBV  | 524262 | 826341 | 75.89% | 9.771% |
| 91  | 11.964 | 3302 | 3304 | 3308 | rBV2 | 588    | 452    | 0.04%  | 0.005% |
| 92  | 12.034 | 3322 | 3326 | 3327 | rBV2 | 366    | 243    | 0.02%  | 0.003% |
| 93  | 12.066 | 3328 | 3336 | 3345 | rVV5 | 5553   | 9445   | 0.87%  | 0.112% |
| 94  | 12.192 | 3362 | 3375 | 3394 | rBV  | 490496 | 802301 | 73.68% | 9.486% |
| 95  | 12.308 | 3409 | 3411 | 3413 | rBV2 | 435    | 194    | 0.02%  | 0.002% |
| 96  | 12.542 | 3482 | 3484 | 3485 | rBV  | 388    | 167    | 0.02%  | 0.002% |
| 97  | 12.703 | 3530 | 3534 | 3536 | rBV2 | 360    | 328    | 0.03%  | 0.004% |
| 98  | 13.748 | 3855 | 3859 | 3862 | rBV3 | 551    | 507    | 0.05%  | 0.006% |
| 99  | 13.844 | 3884 | 3889 | 3896 | rVB4 | 2035   | 2668   | 0.25%  | 0.032% |
| 100 | 14.317 | 4035 | 4036 | 4037 | rBV  | 572    | 158    | 0.01%  | 0.002% |

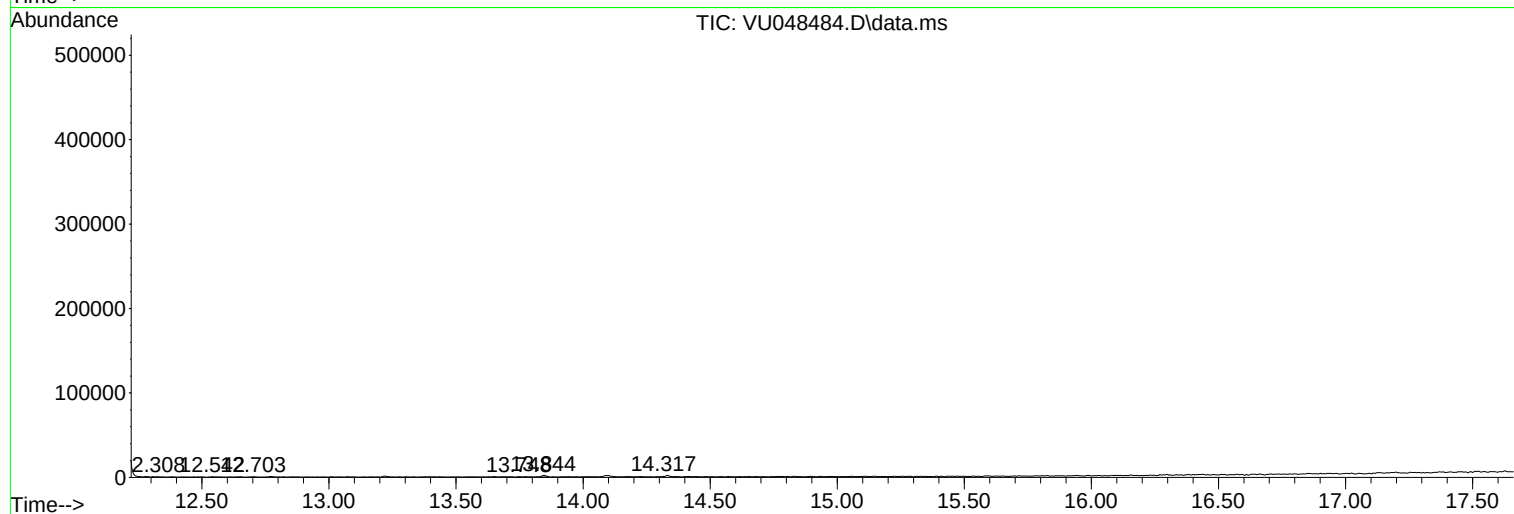
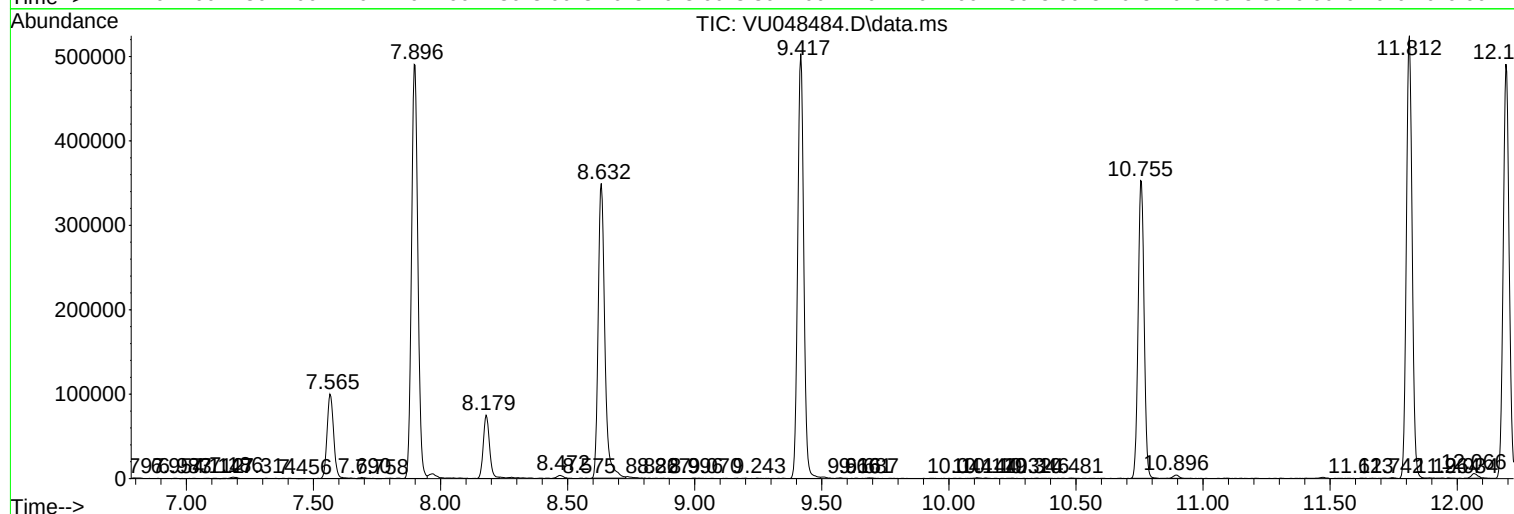
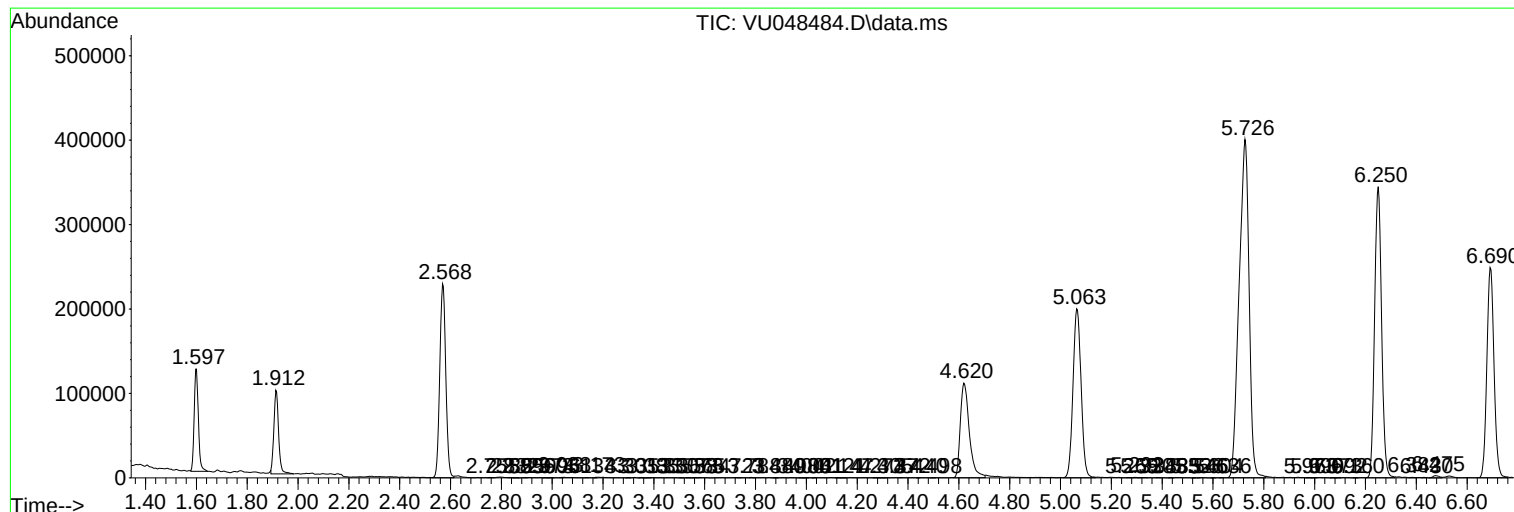
Sum of corrected areas: 8457467

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM050622WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051022\  
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No Library Search Compounds Detected

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