

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU043023\  
 Data File : VU053996.D  
 Acq On : 29 Apr 2023 19:13  
 Operator : JC/MD  
 Sample : 02565-06  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AX9

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\SFAMULM042923WMA.M  
 Title : VOC Analysis

Signal : TIC: VU053996.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         | 1.517       | 53            | 55          | 58           | rBV2     | 877            | 619           | 0.06%           | 0.008%        |
| 2         | 1.601       | 73            | 81          | 97           | rVB      | 125821         | 152632        | 14.69%          | 1.970%        |
| 3         | 1.822       | 148           | 150         | 155          | rBV2     | 678            | 567           | 0.05%           | 0.007%        |
| 4         | 1.912       | 169           | 178         | 191          | rBV      | 88015          | 119585        | 11.51%          | 1.543%        |
| 5         | 2.228       | 274           | 276         | 278          | rBV2     | 482            | 240           | 0.02%           | 0.003%        |
| 6         | 2.318       | 302           | 304         | 307          | rBV2     | 552            | 407           | 0.04%           | 0.005%        |
| 7         | 2.565       | 368           | 381         | 397          | rBV      | 223079         | 362909        | 34.92%          | 4.684%        |
| 8         | 2.787       | 445           | 450         | 457          | rBV2     | 751            | 887           | 0.09%           | 0.011%        |
| 9         | 2.851       | 465           | 470         | 475          | rBV3     | 351            | 452           | 0.04%           | 0.006%        |
| 10        | 2.945       | 493           | 499         | 500          | rBV2     | 218            | 231           | 0.02%           | 0.003%        |
| 11        | 3.038       | 522           | 528         | 531          | rBV4     | 1136           | 1245          | 0.12%           | 0.016%        |
| 12        | 3.186       | 570           | 574         | 577          | rVB3     | 294            | 282           | 0.03%           | 0.004%        |
| 13        | 3.318       | 612           | 615         | 619          | rVB2     | 259            | 212           | 0.02%           | 0.003%        |
| 14        | 3.353       | 619           | 626         | 632          | rBV3     | 430            | 499           | 0.05%           | 0.006%        |
| 15        | 3.414       | 643           | 645         | 651          | rVB2     | 190            | 199           | 0.02%           | 0.003%        |
| 16        | 3.504       | 670           | 673         | 676          | rBV2     | 255            | 231           | 0.02%           | 0.003%        |
| 17        | 3.565       | 686           | 692         | 694          | rVV      | 224            | 226           | 0.02%           | 0.003%        |
| 18        | 3.610       | 699           | 706         | 710          | rVB2     | 224            | 352           | 0.03%           | 0.005%        |
| 19        | 4.250       | 902           | 905         | 908          | rBV      | 292            | 199           | 0.02%           | 0.003%        |
| 20        | 4.527       | 987           | 991         | 996          | rBV      | 211            | 265           | 0.03%           | 0.003%        |
| 21        | 4.626       | 1007          | 1022        | 1056         | rBV      | 71657          | 194103        | 18.68%          | 2.505%        |
| 22        | 4.848       | 1087          | 1091        | 1094         | rBV2     | 348            | 302           | 0.03%           | 0.004%        |
| 23        | 4.909       | 1106          | 1110        | 1115         | rBV2     | 298            | 313           | 0.03%           | 0.004%        |
| 24        | 4.961       | 1122          | 1126        | 1127         | rVB      | 321            | 208           | 0.02%           | 0.003%        |
| 25        | 5.057       | 1141          | 1156        | 1180         | rBV      | 183581         | 405467        | 39.01%          | 5.233%        |
| 26        | 5.314       | 1230          | 1236        | 1240         | rVB4     | 674            | 734           | 0.07%           | 0.009%        |
| 27        | 5.337       | 1240          | 1243        | 1246         | rBV2     | 270            | 200           | 0.02%           | 0.003%        |
| 28        | 5.446       | 1273          | 1277        | 1280         | rBV2     | 431            | 379           | 0.04%           | 0.005%        |
| 29        | 5.488       | 1285          | 1290        | 1293         | rVB2     | 295            | 288           | 0.03%           | 0.004%        |
| 30        | 5.504       | 1293          | 1295        | 1301         | rVB      | 245            | 241           | 0.02%           | 0.003%        |
| 31        | 5.536       | 1301          | 1305        | 1307         | rBV2     | 340            | 342           | 0.03%           | 0.004%        |
| 32        | 5.719       | 1341          | 1362        | 1382         | rBV2     | 384352         | 1039358       | 100.00%         | 13.415%       |
| 33        | 5.858       | 1403          | 1405        | 1413         | rVB3     | 983            | 854           | 0.08%           | 0.011%        |
| 34        | 6.006       | 1446          | 1451        | 1452         | rBV      | 249            | 203           | 0.02%           | 0.003%        |
| 35        | 6.108       | 1479          | 1483        | 1485         | rBV2     | 397            | 327           | 0.03%           | 0.004%        |
| 36        | 6.243       | 1509          | 1525        | 1548         | rBV      | 338315         | 644440        | 62.00%          | 8.318%        |

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Integrator: RTE

Smoothing : OFF

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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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.530  | 1604 | 1614 | 1626 | rVB7 | 2874   | 6134   | 0.59%  | 0.079%  |
| 38 | 6.578  | 1626 | 1629 | 1634 | rBV2 | 206    | 246    | 0.02%  | 0.003%  |
| 39 | 6.684  | 1648 | 1662 | 1684 | rBV  | 236922 | 465284 | 44.77% | 6.005%  |
| 40 | 6.797  | 1694 | 1697 | 1699 | rBV2 | 570    | 359    | 0.03%  | 0.005%  |
| 41 | 6.809  | 1699 | 1701 | 1706 | rVB4 | 641    | 450    | 0.04%  | 0.006%  |
| 42 | 7.025  | 1765 | 1768 | 1774 | rBV2 | 347    | 456    | 0.04%  | 0.006%  |
| 43 | 7.173  | 1808 | 1814 | 1815 | rBV  | 258    | 244    | 0.02%  | 0.003%  |
| 44 | 7.359  | 1869 | 1872 | 1877 | rVB2 | 279    | 278    | 0.03%  | 0.004%  |
| 45 | 7.404  | 1879 | 1886 | 1890 | rVV2 | 195    | 236    | 0.02%  | 0.003%  |
| 46 | 7.559  | 1922 | 1934 | 1957 | rBV  | 131237 | 234911 | 22.60% | 3.032%  |
| 47 | 7.751  | 1991 | 1994 | 1998 | rBV2 | 274    | 271    | 0.03%  | 0.003%  |
| 48 | 7.822  | 2013 | 2016 | 2019 | rBV2 | 282    | 193    | 0.02%  | 0.002%  |
| 49 | 7.848  | 2019 | 2024 | 2025 | rBV  | 220    | 208    | 0.02%  | 0.003%  |
| 50 | 7.893  | 2025 | 2038 | 2074 | rVV  | 477735 | 830609 | 79.92% | 10.721% |
| 51 | 8.073  | 2092 | 2094 | 2097 | rVB2 | 531    | 273    | 0.03%  | 0.004%  |
| 52 | 8.176  | 2114 | 2126 | 2145 | rBV  | 90486  | 155401 | 14.95% | 2.006%  |
| 53 | 8.507  | 2226 | 2229 | 2234 | rVB  | 298    | 191    | 0.02%  | 0.002%  |
| 54 | 8.549  | 2234 | 2242 | 2251 | rBV5 | 2400   | 3497   | 0.34%  | 0.045%  |
| 55 | 8.629  | 2255 | 2267 | 2296 | rBV  | 228699 | 433304 | 41.69% | 5.593%  |
| 56 | 8.896  | 2346 | 2350 | 2354 | rBV2 | 232    | 206    | 0.02%  | 0.003%  |
| 57 | 8.928  | 2355 | 2360 | 2362 | rBV  | 342    | 299    | 0.03%  | 0.004%  |
| 58 | 9.076  | 2402 | 2406 | 2407 | rBV2 | 294    | 223    | 0.02%  | 0.003%  |
| 59 | 9.208  | 2443 | 2447 | 2451 | rBV2 | 346    | 347    | 0.03%  | 0.004%  |
| 60 | 9.411  | 2497 | 2510 | 2537 | rBV  | 444950 | 749153 | 72.08% | 9.669%  |
| 61 | 9.819  | 2631 | 2637 | 2640 | rBV  | 152    | 198    | 0.02%  | 0.003%  |
| 62 | 9.912  | 2661 | 2666 | 2672 | rVB2 | 333    | 390    | 0.04%  | 0.005%  |
| 63 | 10.005 | 2692 | 2695 | 2699 | rVV2 | 369    | 276    | 0.03%  | 0.004%  |
| 64 | 10.028 | 2699 | 2702 | 2706 | rVV  | 296    | 234    | 0.02%  | 0.003%  |
| 65 | 10.105 | 2721 | 2726 | 2727 | rBV2 | 356    | 293    | 0.03%  | 0.004%  |
| 66 | 10.443 | 2826 | 2831 | 2834 | rBV2 | 218    | 218    | 0.02%  | 0.003%  |
| 67 | 10.484 | 2840 | 2844 | 2848 | rVB  | 374    | 352    | 0.03%  | 0.005%  |
| 68 | 10.751 | 2913 | 2927 | 2945 | rBV  | 291410 | 481180 | 46.30% | 6.211%  |
| 69 | 10.845 | 2955 | 2956 | 2962 | rVB  | 244    | 192    | 0.02%  | 0.002%  |
| 70 | 10.980 | 2994 | 2998 | 3004 | rBV2 | 273    | 389    | 0.04%  | 0.005%  |
| 71 | 11.253 | 3079 | 3083 | 3087 | rBV2 | 286    | 274    | 0.03%  | 0.004%  |
| 72 | 11.462 | 3144 | 3148 | 3154 | rBV3 | 519    | 501    | 0.05%  | 0.006%  |
| 73 | 11.513 | 3159 | 3164 | 3169 | rBV2 | 300    | 343    | 0.03%  | 0.004%  |
| 74 | 11.552 | 3173 | 3176 | 3183 | rVB2 | 330    | 359    | 0.03%  | 0.005%  |
| 75 | 11.806 | 3243 | 3255 | 3286 | rBV  | 449108 | 713660 | 68.66% | 9.211%  |
| 76 | 11.999 | 3312 | 3315 | 3319 | rVB  | 394    | 313    | 0.03%  | 0.004%  |

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Integration Parameters: LSCINT.P

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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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.066 | 3333 | 3336 | 3340 | rVB2 | 289    | 265    | 0.03%  | 0.003% |
| 78  | 12.105 | 3345 | 3348 | 3353 | rVB2 | 295    | 272    | 0.03%  | 0.004% |
| 79  | 12.131 | 3353 | 3356 | 3358 | rBV  | 288    | 213    | 0.02%  | 0.003% |
| 80  | 12.189 | 3361 | 3374 | 3389 | rBV  | 445157 | 723876 | 69.65% | 9.343% |
|     |        |      |      |      |      |        |        |        |        |
| 81  | 12.333 | 3417 | 3419 | 3423 | rVB  | 448    | 256    | 0.02%  | 0.003% |
| 82  | 12.475 | 3460 | 3463 | 3466 | rVV2 | 241    | 188    | 0.02%  | 0.002% |
| 83  | 12.671 | 3520 | 3524 | 3526 | rBV  | 237    | 215    | 0.02%  | 0.003% |
| 84  | 12.754 | 3546 | 3550 | 3553 | rVB2 | 214    | 197    | 0.02%  | 0.003% |
| 85  | 12.799 | 3561 | 3564 | 3569 | rVB2 | 317    | 305    | 0.03%  | 0.004% |
|     |        |      |      |      |      |        |        |        |        |
| 86  | 12.838 | 3573 | 3576 | 3580 | rBV3 | 350    | 325    | 0.03%  | 0.004% |
| 87  | 13.201 | 3686 | 3689 | 3691 | rBV  | 319    | 254    | 0.02%  | 0.003% |
| 88  | 13.221 | 3691 | 3695 | 3700 | rVV2 | 474    | 506    | 0.05%  | 0.007% |
| 89  | 13.266 | 3707 | 3709 | 3711 | rBV  | 386    | 204    | 0.02%  | 0.003% |
| 90  | 13.301 | 3716 | 3720 | 3722 | rBV2 | 351    | 317    | 0.03%  | 0.004% |
|     |        |      |      |      |      |        |        |        |        |
| 91  | 13.848 | 3884 | 3890 | 3894 | rVB5 | 911    | 974    | 0.09%  | 0.013% |
| 92  | 14.082 | 3960 | 3963 | 3964 | rBV  | 757    | 493    | 0.05%  | 0.006% |
| 93  | 14.098 | 3964 | 3968 | 3979 | rVB3 | 1582   | 1968   | 0.19%  | 0.025% |
| 94  | 14.330 | 4035 | 4040 | 4048 | rVB5 | 1926   | 2618   | 0.25%  | 0.034% |
| 95  | 14.375 | 4048 | 4054 | 4059 | rBV3 | 518    | 677    | 0.07%  | 0.009% |
|     |        |      |      |      |      |        |        |        |        |
| 96  | 14.401 | 4059 | 4062 | 4066 | rVB2 | 483    | 390    | 0.04%  | 0.005% |
| 97  | 15.327 | 4347 | 4350 | 4351 | rBV  | 544    | 286    | 0.03%  | 0.004% |
| 98  | 15.841 | 4508 | 4510 | 4514 | rBV3 | 644    | 377    | 0.04%  | 0.005% |
| 99  | 16.021 | 4564 | 4566 | 4567 | rBV2 | 651    | 280    | 0.03%  | 0.004% |
| 100 | 16.156 | 4606 | 4608 | 4610 | rBV3 | 718    | 421    | 0.04%  | 0.005% |

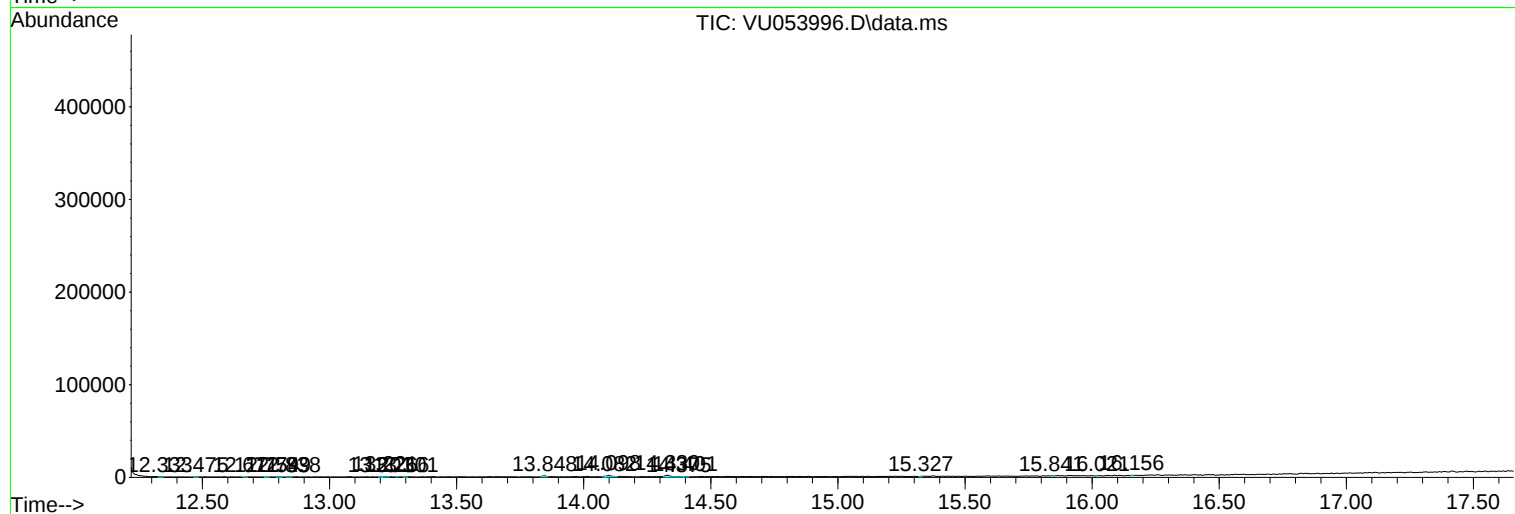
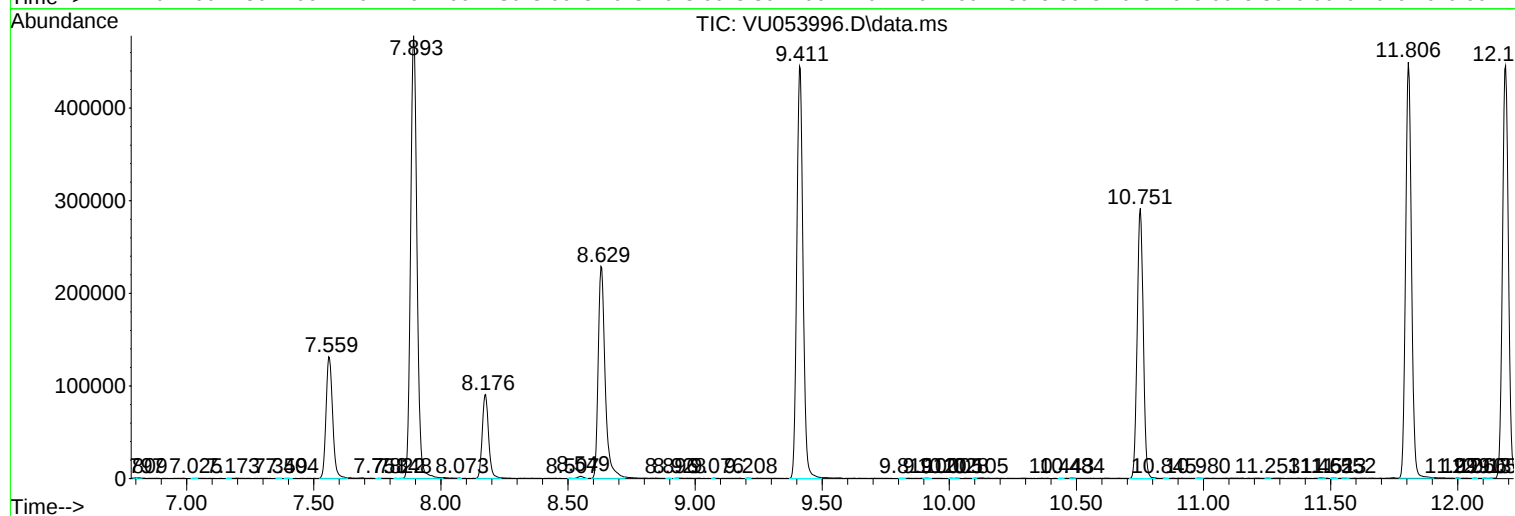
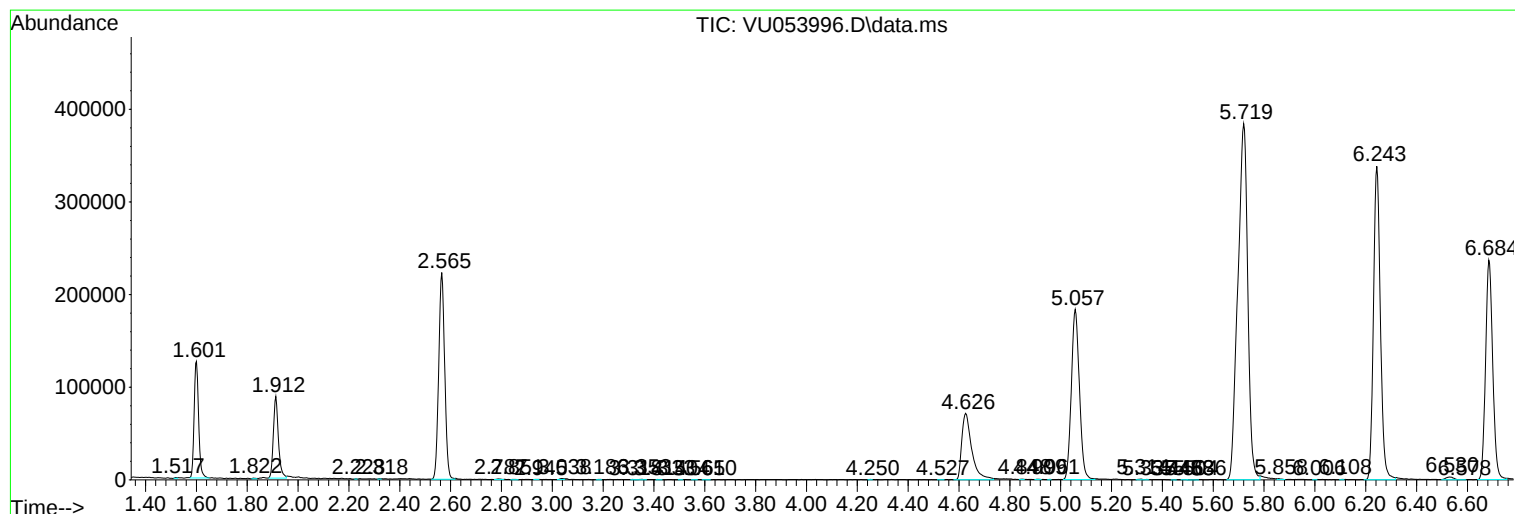
Sum of corrected areas: 7747820

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.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 |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|