

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050823\  
 Data File : VU054083.D  
 Acq On : 08 May 2023 16:20  
 Operator : JC/MD  
 Sample : 02662-06  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AZ5

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: VU054083.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         | 1.488       | 41            | 46          | 52           | rBV3     | 1834           | 2444          | 0.29%           | 0.037%        |
| 2         | 1.597       | 72            | 80          | 98           | rBV      | 84659          | 102698        | 12.01%          | 1.553%        |
| 3         | 1.906       | 167           | 176         | 197          | rVB      | 71508          | 102167        | 11.95%          | 1.545%        |
| 4         | 2.257       | 283           | 285         | 290          | rVB2     | 643            | 336           | 0.04%           | 0.005%        |
| 5         | 2.376       | 319           | 322         | 327          | rVB4     | 622            | 354           | 0.04%           | 0.005%        |
| 6         | 2.427       | 336           | 338         | 342          | rBV3     | 566            | 498           | 0.06%           | 0.008%        |
| 7         | 2.562       | 368           | 380         | 397          | rBV      | 167362         | 269174        | 31.49%          | 4.070%        |
| 8         | 2.626       | 397           | 400         | 404          | rBV      | 518            | 441           | 0.05%           | 0.007%        |
| 9         | 2.668       | 411           | 413         | 418          | rVB3     | 642            | 405           | 0.05%           | 0.006%        |
| 10        | 2.768       | 440           | 444         | 446          | rBV2     | 565            | 503           | 0.06%           | 0.008%        |
| 11        | 3.041       | 521           | 529         | 535          | rBV6     | 1025           | 1597          | 0.19%           | 0.024%        |
| 12        | 3.179       | 561           | 572         | 586          | rVV2     | 1610           | 3901          | 0.46%           | 0.059%        |
| 13        | 3.231       | 586           | 588         | 596          | rVV2     | 187            | 193           | 0.02%           | 0.003%        |
| 14        | 3.276       | 599           | 602         | 608          | rVB      | 313            | 335           | 0.04%           | 0.005%        |
| 15        | 3.314       | 608           | 614         | 617          | rBV2     | 186            | 213           | 0.02%           | 0.003%        |
| 16        | 3.668       | 722           | 724         | 728          | rBV2     | 255            | 240           | 0.03%           | 0.004%        |
| 17        | 3.880       | 785           | 790         | 794          | rBV2     | 189            | 234           | 0.03%           | 0.004%        |
| 18        | 3.974       | 816           | 819         | 823          | rBV      | 281            | 190           | 0.02%           | 0.003%        |
| 19        | 4.002       | 823           | 828         | 833          | rBV2     | 232            | 340           | 0.04%           | 0.005%        |
| 20        | 4.115       | 860           | 863         | 870          | rVB2     | 239            | 252           | 0.03%           | 0.004%        |
| 21        | 4.170       | 874           | 880         | 883          | rBV      | 371            | 344           | 0.04%           | 0.005%        |
| 22        | 4.437       | 958           | 963         | 968          | rBV      | 193            | 300           | 0.04%           | 0.005%        |
| 23        | 4.617       | 1007          | 1019        | 1056         | rBV      | 73365          | 182561        | 21.36%          | 2.760%        |
| 24        | 4.909       | 1107          | 1110        | 1114         | rBV3     | 232            | 219           | 0.03%           | 0.003%        |
| 25        | 5.057       | 1140          | 1156        | 1179         | rBV      | 157395         | 346142        | 40.49%          | 5.233%        |
| 26        | 5.298       | 1225          | 1231        | 1232         | rBV      | 643            | 563           | 0.07%           | 0.009%        |
| 27        | 5.411       | 1263          | 1266        | 1272         | rVB2     | 204            | 282           | 0.03%           | 0.004%        |
| 28        | 5.440       | 1272          | 1275        | 1279         | rBV      | 282            | 286           | 0.03%           | 0.004%        |
| 29        | 5.462       | 1280          | 1282        | 1287         | rVB2     | 328            | 287           | 0.03%           | 0.004%        |
| 30        | 5.491       | 1287          | 1291        | 1294         | rBV      | 382            | 339           | 0.04%           | 0.005%        |
| 31        | 5.623       | 1329          | 1332        | 1338         | rVB2     | 199            | 248           | 0.03%           | 0.004%        |
| 32        | 5.719       | 1338          | 1362        | 1391         | rBV2     | 313506         | 854863        | 100.00%         | 12.925%       |
| 33        | 5.983       | 1442          | 1444        | 1448         | rVB2     | 358            | 227           | 0.03%           | 0.003%        |
| 34        | 6.002       | 1448          | 1450        | 1452         | rBV2     | 304            | 186           | 0.02%           | 0.003%        |
| 35        | 6.244       | 1511          | 1525        | 1550         | rBV      | 276768         | 531879        | 62.22%          | 8.041%        |
| 36        | 6.533       | 1602          | 1615        | 1627         | rVB7     | 3958           | 8815          | 1.03%           | 0.133%        |

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Smoothing : OFF

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Min Area: 0 % of largest Peak

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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.684  | 1648 | 1662 | 1681 | rBV  | 199943 | 390466 | 45.68% | 5.903%  |
| 38 | 6.809  | 1698 | 1701 | 1706 | rVB3 | 692    | 585    | 0.07%  | 0.009%  |
| 39 | 6.835  | 1706 | 1709 | 1717 | rVB  | 260    | 202    | 0.02%  | 0.003%  |
| 40 | 6.932  | 1735 | 1739 | 1742 | rBV  | 281    | 253    | 0.03%  | 0.004%  |
| 41 | 7.047  | 1770 | 1775 | 1781 | rBV2 | 319    | 411    | 0.05%  | 0.006%  |
| 42 | 7.189  | 1814 | 1819 | 1829 | rVB5 | 1169   | 1985   | 0.23%  | 0.030%  |
| 43 | 7.234  | 1829 | 1833 | 1838 | rVB  | 298    | 329    | 0.04%  | 0.005%  |
| 44 | 7.427  | 1890 | 1893 | 1898 | rBV2 | 252    | 268    | 0.03%  | 0.004%  |
| 45 | 7.562  | 1923 | 1935 | 1952 | rBV  | 108875 | 195077 | 22.82% | 2.949%  |
| 46 | 7.684  | 1967 | 1973 | 1974 | rBV2 | 260    | 254    | 0.03%  | 0.004%  |
| 47 | 7.803  | 2004 | 2010 | 2014 | rBV2 | 398    | 370    | 0.04%  | 0.006%  |
| 48 | 7.893  | 2024 | 2038 | 2071 | rBV  | 387693 | 678466 | 79.37% | 10.258% |
| 49 | 8.173  | 2115 | 2125 | 2143 | rBV  | 77314  | 132531 | 15.50% | 2.004%  |
| 50 | 8.391  | 2190 | 2193 | 2197 | rVB2 | 349    | 280    | 0.03%  | 0.004%  |
| 51 | 8.424  | 2197 | 2203 | 2206 | rBV2 | 266    | 319    | 0.04%  | 0.005%  |
| 52 | 8.469  | 2208 | 2217 | 2227 | rBV2 | 2636   | 4683   | 0.55%  | 0.071%  |
| 53 | 8.629  | 2255 | 2267 | 2295 | rBV2 | 214504 | 401933 | 47.02% | 6.077%  |
| 54 | 8.784  | 2310 | 2315 | 2317 | rBV4 | 691    | 631    | 0.07%  | 0.010%  |
| 55 | 8.845  | 2330 | 2334 | 2338 | rVB3 | 235    | 217    | 0.03%  | 0.003%  |
| 56 | 8.941  | 2359 | 2364 | 2367 | rBV2 | 183    | 205    | 0.02%  | 0.003%  |
| 57 | 9.031  | 2388 | 2392 | 2395 | rBV  | 279    | 244    | 0.03%  | 0.004%  |
| 58 | 9.147  | 2424 | 2428 | 2431 | rBV  | 297    | 299    | 0.03%  | 0.005%  |
| 59 | 9.414  | 2497 | 2511 | 2535 | rBV  | 382423 | 639631 | 74.82% | 9.670%  |
| 60 | 9.559  | 2551 | 2556 | 2558 | rBV3 | 494    | 438    | 0.05%  | 0.007%  |
| 61 | 9.687  | 2592 | 2596 | 2599 | rBV  | 335    | 308    | 0.04%  | 0.005%  |
| 62 | 9.816  | 2633 | 2636 | 2640 | rBV2 | 222    | 237    | 0.03%  | 0.004%  |
| 63 | 9.883  | 2653 | 2657 | 2660 | rBV2 | 203    | 209    | 0.02%  | 0.003%  |
| 64 | 10.189 | 2749 | 2752 | 2755 | rBV  | 340    | 260    | 0.03%  | 0.004%  |
| 65 | 10.218 | 2759 | 2761 | 2769 | rVB2 | 327    | 337    | 0.04%  | 0.005%  |
| 66 | 10.253 | 2769 | 2772 | 2774 | rBV  | 240    | 189    | 0.02%  | 0.003%  |
| 67 | 10.369 | 2802 | 2808 | 2811 | rBV2 | 267    | 408    | 0.05%  | 0.006%  |
| 68 | 10.407 | 2817 | 2820 | 2823 | rBV2 | 244    | 185    | 0.02%  | 0.003%  |
| 69 | 10.751 | 2914 | 2927 | 2947 | rBV  | 276327 | 447840 | 52.39% | 6.771%  |
| 70 | 10.890 | 2962 | 2970 | 2978 | rBV3 | 2880   | 4149   | 0.49%  | 0.063%  |
| 71 | 11.054 | 3018 | 3021 | 3024 | rBV  | 303    | 277    | 0.03%  | 0.004%  |
| 72 | 11.140 | 3042 | 3048 | 3049 | rBV2 | 285    | 280    | 0.03%  | 0.004%  |
| 73 | 11.423 | 3130 | 3136 | 3141 | rBV2 | 227    | 418    | 0.05%  | 0.006%  |
| 74 | 11.481 | 3146 | 3154 | 3157 | rBV2 | 514    | 781    | 0.09%  | 0.012%  |
| 75 | 11.565 | 3171 | 3180 | 3182 | rBV2 | 167    | 234    | 0.03%  | 0.004%  |
| 76 | 11.620 | 3192 | 3197 | 3200 | rBV2 | 296    | 324    | 0.04%  | 0.005%  |

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Min Area: 0 % of largest Peak

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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.687 | 3215 | 3218 | 3223 | rBV2 | 248    | 228    | 0.03%  | 0.003% |
| 78  | 11.742 | 3233 | 3235 | 3241 | rBV2 | 513    | 586    | 0.07%  | 0.009% |
| 79  | 11.806 | 3243 | 3255 | 3277 | rBV  | 397648 | 632241 | 73.96% | 9.559% |
| 80  | 12.137 | 3353 | 3358 | 3361 | rBV2 | 221    | 209    | 0.02%  | 0.003% |
| 81  | 12.189 | 3361 | 3374 | 3409 | rVV  | 400924 | 654576 | 76.57% | 9.896% |
| 82  | 12.308 | 3409 | 3411 | 3416 | rVB2 | 309    | 246    | 0.03%  | 0.004% |
| 83  | 12.880 | 3585 | 3589 | 3592 | rBV2 | 237    | 246    | 0.03%  | 0.004% |
| 84  | 12.902 | 3592 | 3596 | 3598 | rVV2 | 374    | 278    | 0.03%  | 0.004% |
| 85  | 12.983 | 3617 | 3621 | 3623 | rBV2 | 322    | 245    | 0.03%  | 0.004% |
| 86  | 13.057 | 3640 | 3644 | 3648 | rBV  | 191    | 216    | 0.03%  | 0.003% |
| 87  | 13.111 | 3658 | 3661 | 3663 | rBV2 | 329    | 217    | 0.03%  | 0.003% |
| 88  | 13.224 | 3694 | 3696 | 3699 | rVB  | 305    | 197    | 0.02%  | 0.003% |
| 89  | 13.333 | 3727 | 3730 | 3733 | rBV  | 343    | 293    | 0.03%  | 0.004% |
| 90  | 13.517 | 3784 | 3787 | 3791 | rVB3 | 313    | 256    | 0.03%  | 0.004% |
| 91  | 13.636 | 3821 | 3824 | 3827 | rBV3 | 433    | 326    | 0.04%  | 0.005% |
| 92  | 13.751 | 3857 | 3860 | 3863 | rBV2 | 271    | 227    | 0.03%  | 0.003% |
| 93  | 13.812 | 3876 | 3879 | 3882 | rBV2 | 321    | 235    | 0.03%  | 0.004% |
| 94  | 13.848 | 3886 | 3890 | 3891 | rBV2 | 497    | 376    | 0.04%  | 0.006% |
| 95  | 13.992 | 3930 | 3935 | 3938 | rBV3 | 305    | 339    | 0.04%  | 0.005% |
| 96  | 14.253 | 4013 | 4016 | 4018 | rBV  | 315    | 223    | 0.03%  | 0.003% |
| 97  | 15.243 | 4322 | 4324 | 4327 | rBV  | 370    | 229    | 0.03%  | 0.003% |
| 98  | 15.545 | 4415 | 4418 | 4420 | rBV2 | 538    | 368    | 0.04%  | 0.006% |
| 99  | 15.661 | 4451 | 4454 | 4462 | rVB4 | 752    | 669    | 0.08%  | 0.010% |
| 100 | 15.963 | 4546 | 4548 | 4555 | rVB5 | 663    | 664    | 0.08%  | 0.010% |

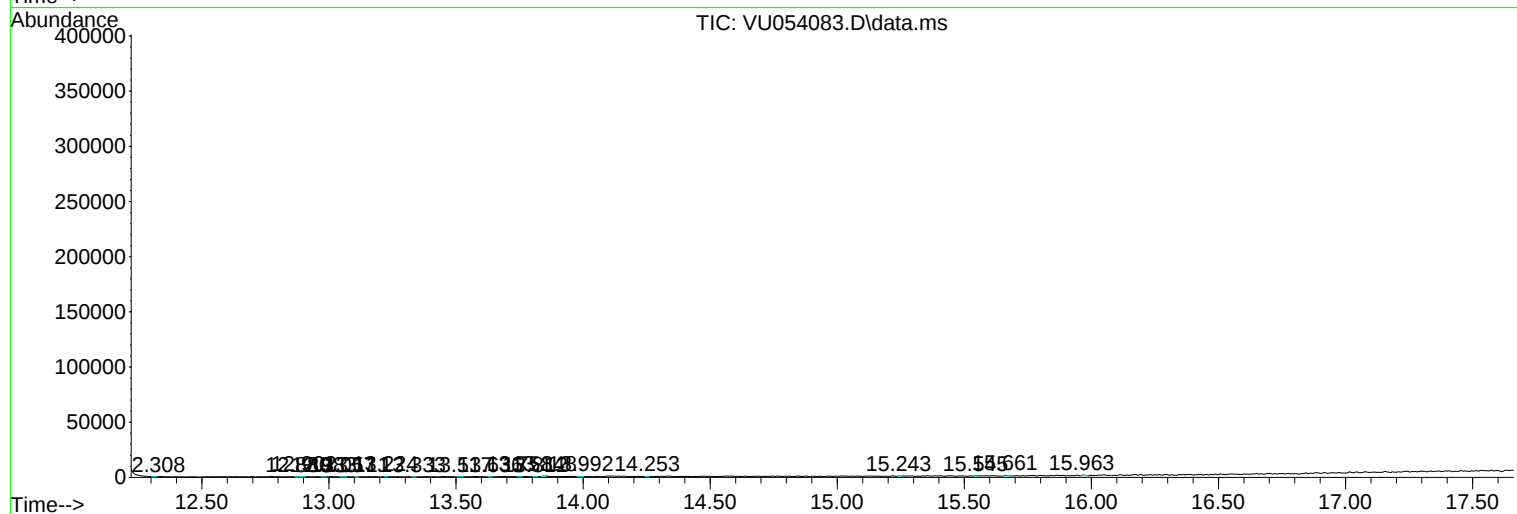
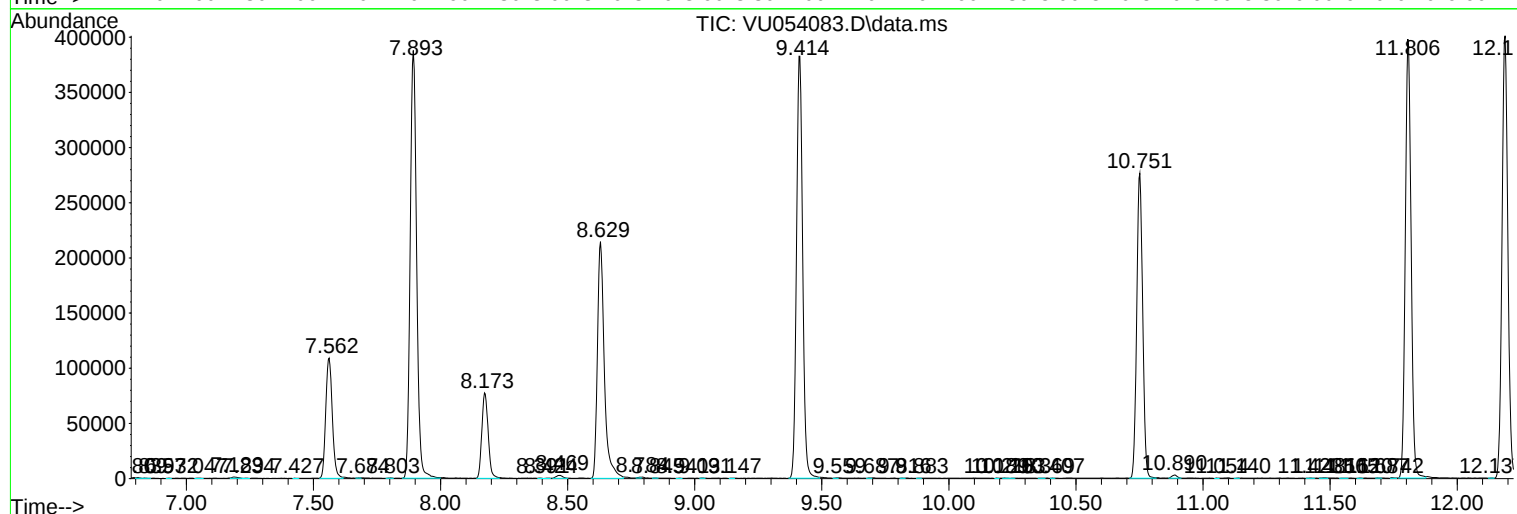
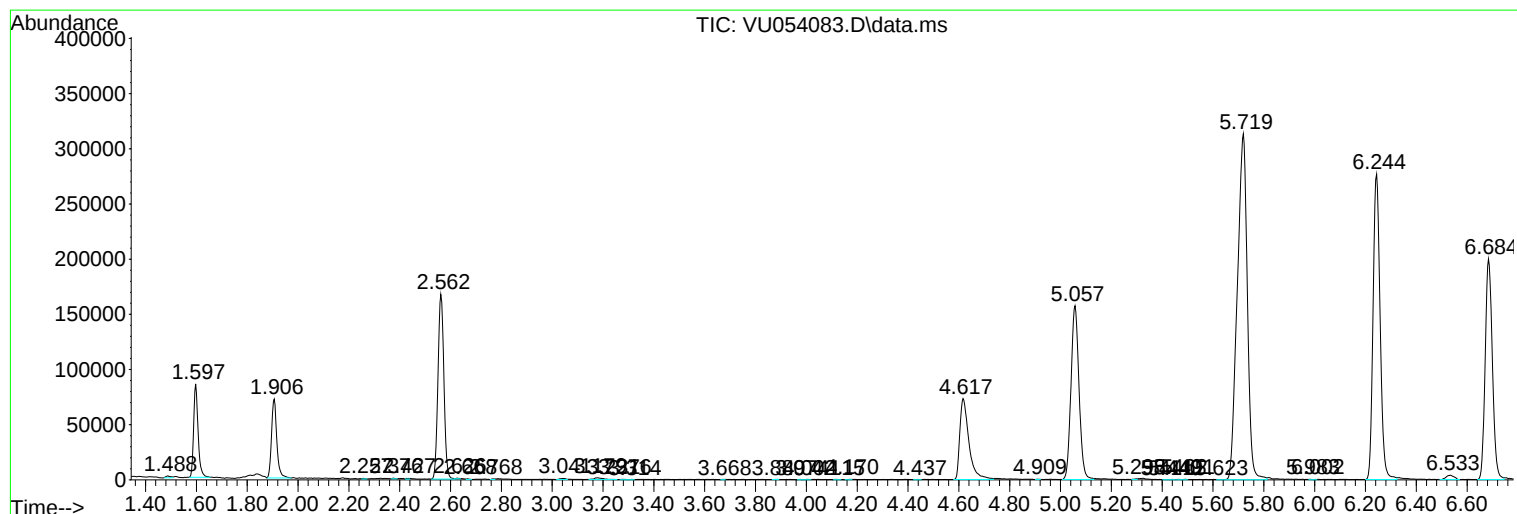
Sum of corrected areas: 6614259

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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050823\  
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No Library Search Compounds Detected

\*\*\*\*\*

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