

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU040323\  
 Data File : VU053540.D  
 Acq On : 03 Apr 2023 23:57  
 Operator : JC/MD  
 Sample : 02158-12  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 35 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 PMW-9S(20230330)

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\SFAMULM033123WMA.M

Title : VOC Analysis

Signal : TIC: VU053540.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       | 73            | 80          | 96           | rVB2     | 144726         | 167211        | 0.48%           | 0.251%        |
| 2         | 1.909       | 169           | 177         | 198          | rVB      | 101270         | 138457        | 0.40%           | 0.208%        |
| 3         | 2.565       | 369           | 381         | 399          | rBV      | 193234         | 317721        | 0.91%           | 0.477%        |
| 4         | 2.661       | 408           | 411         | 412          | rBV2     | 593            | 339           | 0.00%           | 0.001%        |
| 5         | 3.031       | 523           | 526         | 528          | rBV2     | 838            | 646           | 0.00%           | 0.001%        |
| 6         | 3.179       | 560           | 572         | 588          | rVB4     | 3926           | 8937          | 0.03%           | 0.013%        |
| 7         | 3.350       | 614           | 625         | 637          | rVB3     | 9522           | 18362         | 0.05%           | 0.028%        |
| 8         | 3.710       | 735           | 737         | 739          | rBV      | 229            | 137           | 0.00%           | 0.000%        |
| 9         | 3.986       | 816           | 823         | 825          | rBV3     | 614            | 788           | 0.00%           | 0.001%        |
| 10        | 4.083       | 851           | 853         | 856          | rBV2     | 244            | 186           | 0.00%           | 0.000%        |
| 11        | 4.263       | 906           | 909         | 910          | rBV2     | 202            | 85            | 0.00%           | 0.000%        |
| 12        | 4.481       | 975           | 977         | 980          | rBV      | 182            | 80            | 0.00%           | 0.000%        |
| 13        | 4.549       | 996           | 998         | 999          | rBV      | 223            | 69            | 0.00%           | 0.000%        |
| 14        | 4.613       | 1005          | 1018        | 1052         | rBV      | 81845          | 238558        | 0.69%           | 0.358%        |
| 15        | 4.941       | 1117          | 1120        | 1123         | rVB      | 254            | 155           | 0.00%           | 0.000%        |
| 16        | 4.967       | 1123          | 1128        | 1129         | rBV2     | 282            | 223           | 0.00%           | 0.000%        |
| 17        | 4.999       | 1135          | 1138        | 1140         | rBV2     | 319            | 215           | 0.00%           | 0.000%        |
| 18        | 5.054       | 1141          | 1155        | 1181         | rVV      | 169821         | 375623        | 1.08%           | 0.563%        |
| 19        | 5.324       | 1237          | 1239        | 1241         | rBV      | 249            | 122           | 0.00%           | 0.000%        |
| 20        | 5.362       | 1249          | 1251        | 1255         | rVB      | 356            | 161           | 0.00%           | 0.000%        |
| 21        | 5.446       | 1274          | 1277        | 1280         | rBV      | 215            | 163           | 0.00%           | 0.000%        |
| 22        | 5.568       | 1314          | 1315        | 1316         | rBV      | 117            | 31            | 0.00%           | 0.000%        |
| 23        | 5.607       | 1326          | 1327        | 1328         | rBV      | 152            | 48            | 0.00%           | 0.000%        |
| 24        | 5.719       | 1340          | 1362        | 1390         | rBV2     | 339148         | 967407        | 2.78%           | 1.451%        |
| 25        | 5.989       | 1445          | 1446        | 1449         | rBV2     | 201            | 81            | 0.00%           | 0.000%        |
| 26        | 6.012       | 1449          | 1453        | 1455         | rBV3     | 665            | 528           | 0.00%           | 0.001%        |
| 27        | 6.079       | 1472          | 1474        | 1476         | rBV      | 235            | 86            | 0.00%           | 0.000%        |
| 28        | 6.243       | 1511          | 1525        | 1545         | rBV      | 293653         | 556403        | 1.60%           | 0.835%        |
| 29        | 6.526       | 1603          | 1613        | 1625         | rVB3     | 6836           | 13226         | 0.04%           | 0.020%        |
| 30        | 6.587       | 1631          | 1632        | 1633         | rBV3     | 217            | 72            | 0.00%           | 0.000%        |
| 31        | 6.632       | 1644          | 1646        | 1647         | rVB      | 133            | 30            | 0.00%           | 0.000%        |
| 32        | 6.687       | 1647          | 1663        | 1680         | rBV      | 213199         | 412163        | 1.18%           | 0.618%        |
| 33        | 6.857       | 1714          | 1716        | 1718         | rVB      | 167            | 45            | 0.00%           | 0.000%        |
| 34        | 6.960       | 1742          | 1748        | 1750         | rBV2     | 1013           | 1063          | 0.00%           | 0.002%        |
| 35        | 7.160       | 1808          | 1810        | 1812         | rBV2     | 314            | 123           | 0.00%           | 0.000%        |
| 36        | 7.176       | 1812          | 1815        | 1816         | rBV      | 335            | 209           | 0.00%           | 0.000%        |

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Integrator: RTE

Smoothing : OFF

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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\SFAMULM033123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 37 | 7.295  | 1849 | 1852 | 1858 | rBV2 | 271     | 268     | 0.00%  | 0.000% |
| 38 | 7.327  | 1858 | 1862 | 1868 | rVB2 | 222     | 192     | 0.00%  | 0.000% |
| 39 | 7.462  | 1901 | 1904 | 1906 | rBV2 | 205     | 145     | 0.00%  | 0.000% |
| 40 | 7.494  | 1912 | 1914 | 1917 | rBV2 | 281     | 148     | 0.00%  | 0.000% |
| 41 | 7.562  | 1922 | 1935 | 1951 | rBV  | 121082  | 215038  | 0.62%  | 0.323% |
| 42 | 7.684  | 1970 | 1973 | 1976 | rBV3 | 565     | 386     | 0.00%  | 0.001% |
| 43 | 7.774  | 1999 | 2001 | 2003 | rBV  | 169     | 67      | 0.00%  | 0.000% |
| 44 | 7.793  | 2003 | 2007 | 2012 | rVB4 | 684     | 731     | 0.00%  | 0.001% |
| 45 | 7.822  | 2012 | 2016 | 2017 | rBV  | 288     | 212     | 0.00%  | 0.000% |
| 46 | 7.893  | 2025 | 2038 | 2053 | rBV  | 451872  | 774402  | 2.23%  | 1.162% |
| 47 | 8.092  | 2096 | 2100 | 2101 | rBV  | 499     | 373     | 0.00%  | 0.001% |
| 48 | 8.134  | 2111 | 2113 | 2114 | rBV  | 183     | 76      | 0.00%  | 0.000% |
| 49 | 8.176  | 2115 | 2126 | 2146 | rVV  | 84713   | 144384  | 0.41%  | 0.217% |
| 50 | 8.301  | 2163 | 2165 | 2169 | rVB2 | 300     | 203     | 0.00%  | 0.000% |
| 51 | 8.455  | 2210 | 2213 | 2214 | rBV  | 385     | 181     | 0.00%  | 0.000% |
| 52 | 8.549  | 2233 | 2242 | 2253 | rBV4 | 8906    | 14393   | 0.04%  | 0.022% |
| 53 | 8.626  | 2255 | 2266 | 2297 | rBV  | 247672  | 454109  | 1.30%  | 0.681% |
| 54 | 9.021  | 2387 | 2389 | 2392 | rBV  | 249     | 139     | 0.00%  | 0.000% |
| 55 | 9.198  | 2442 | 2444 | 2445 | rBV  | 164     | 58      | 0.00%  | 0.000% |
| 56 | 9.275  | 2466 | 2468 | 2471 | rBV  | 145     | 100     | 0.00%  | 0.000% |
| 57 | 9.314  | 2477 | 2480 | 2482 | rVB  | 230     | 117     | 0.00%  | 0.000% |
| 58 | 9.330  | 2482 | 2485 | 2488 | rBV  | 170     | 103     | 0.00%  | 0.000% |
| 59 | 9.443  | 2497 | 2520 | 2551 | rBV  | 3449144 | 6337350 | 18.21% | 9.506% |
| 60 | 9.668  | 2580 | 2590 | 2612 | rVB5 | 14505   | 37004   | 0.11%  | 0.056% |
| 61 | 9.751  | 2613 | 2616 | 2620 | rBV2 | 314     | 277     | 0.00%  | 0.000% |
| 62 | 9.851  | 2645 | 2647 | 2652 | rBV2 | 227     | 103     | 0.00%  | 0.000% |
| 63 | 9.925  | 2668 | 2670 | 2673 | rBV  | 261     | 190     | 0.00%  | 0.000% |
| 64 | 9.967  | 2680 | 2683 | 2684 | rBV  | 224     | 111     | 0.00%  | 0.000% |
| 65 | 9.996  | 2688 | 2692 | 2698 | rVB2 | 263     | 280     | 0.00%  | 0.000% |
| 66 | 10.053 | 2708 | 2710 | 2711 | rBV  | 257     | 121     | 0.00%  | 0.000% |
| 67 | 10.102 | 2715 | 2725 | 2738 | rBV4 | 3248    | 5764    | 0.02%  | 0.009% |
| 68 | 10.214 | 2757 | 2760 | 2763 | rBV  | 303     | 183     | 0.00%  | 0.000% |
| 69 | 10.568 | 2867 | 2870 | 2876 | rVB  | 290     | 220     | 0.00%  | 0.000% |
| 70 | 10.751 | 2915 | 2927 | 2942 | rBV  | 315493  | 501029  | 1.44%  | 0.752% |
| 71 | 10.957 | 2989 | 2991 | 2993 | rVB  | 300     | 115     | 0.00%  | 0.000% |
| 72 | 10.986 | 2997 | 3000 | 3001 | rBV  | 417     | 233     | 0.00%  | 0.000% |
| 73 | 11.082 | 3026 | 3030 | 3032 | rBV  | 875     | 709     | 0.00%  | 0.001% |
| 74 | 11.401 | 3126 | 3129 | 3130 | rBV  | 225     | 129     | 0.00%  | 0.000% |
| 75 | 11.465 | 3144 | 3149 | 3157 | rVB4 | 2260    | 2756    | 0.01%  | 0.004% |
| 76 | 11.680 | 3213 | 3216 | 3220 | rBV3 | 431     | 305     | 0.00%  | 0.000% |

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Integration Parameters: LSCINT.P

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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\SFAMULM033123WMA.M

Title : VOC Analysis

|    |        |      |      |      |      |          |          |         |         |
|----|--------|------|------|------|------|----------|----------|---------|---------|
| 77 | 11.741 | 3220 | 3235 | 3248 | rBV  | 11188937 | 17491665 | 50.26%  | 26.236% |
| 78 | 11.835 | 3249 | 3264 | 3308 | rVB  | 22447122 | 34803120 | 100.00% | 52.202% |
| 79 | 12.079 | 3338 | 3340 | 3343 | rBV3 | 904      | 701      | 0.00%   | 0.001%  |
| 80 | 12.204 | 3361 | 3379 | 3402 | rBV2 | 1151869  | 2468422  | 7.09%   | 3.702%  |
| 81 | 12.491 | 3466 | 3468 | 3469 | rBV2 | 425      | 125      | 0.00%   | 0.000%  |
| 82 | 12.989 | 3622 | 3623 | 3626 | rBV  | 238      | 117      | 0.00%   | 0.000%  |
| 83 | 13.221 | 3685 | 3695 | 3707 | rVB4 | 9025     | 14264    | 0.04%   | 0.021%  |
| 84 | 13.452 | 3763 | 3767 | 3768 | rBV  | 369      | 195      | 0.00%   | 0.000%  |
| 85 | 13.600 | 3811 | 3813 | 3817 | rVB  | 403      | 181      | 0.00%   | 0.000%  |
| 86 | 13.622 | 3817 | 3820 | 3823 | rBV2 | 523      | 461      | 0.00%   | 0.001%  |
| 87 | 13.687 | 3837 | 3840 | 3841 | rBV  | 436      | 297      | 0.00%   | 0.000%  |
| 88 | 13.835 | 3876 | 3886 | 3903 | rBV2 | 85934    | 137585   | 0.40%   | 0.206%  |
| 89 | 14.085 | 3956 | 3964 | 3974 | rBV2 | 10285    | 15274    | 0.04%   | 0.023%  |
| 90 | 14.327 | 4029 | 4039 | 4050 | rBV4 | 15417    | 24757    | 0.07%   | 0.037%  |

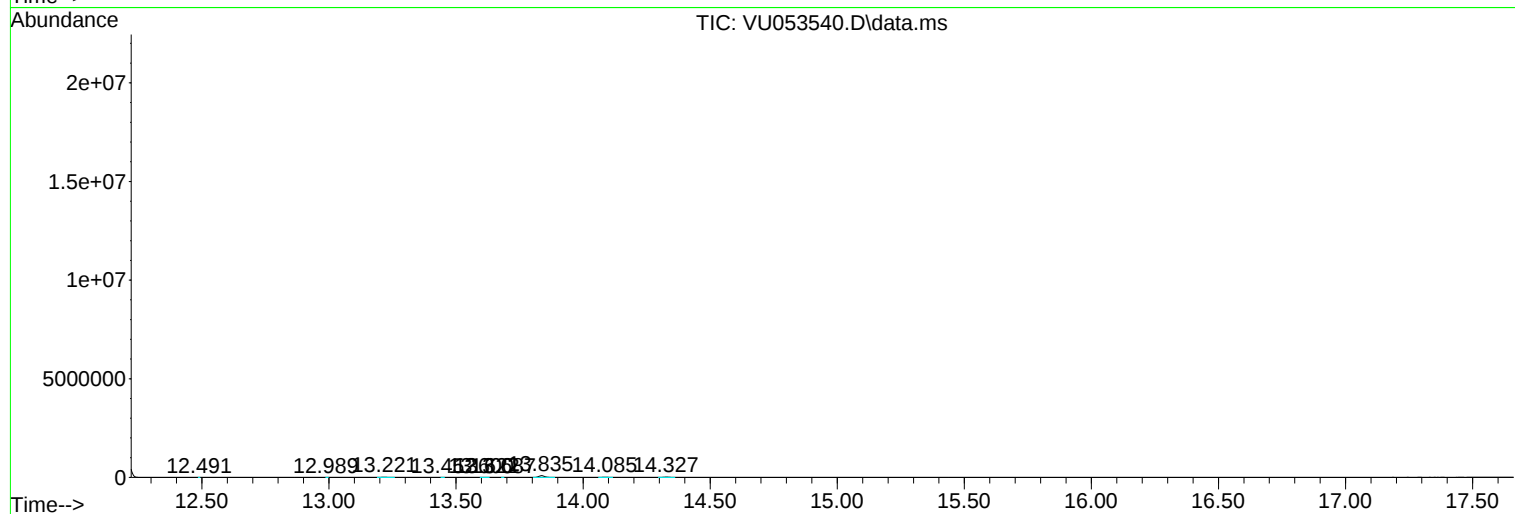
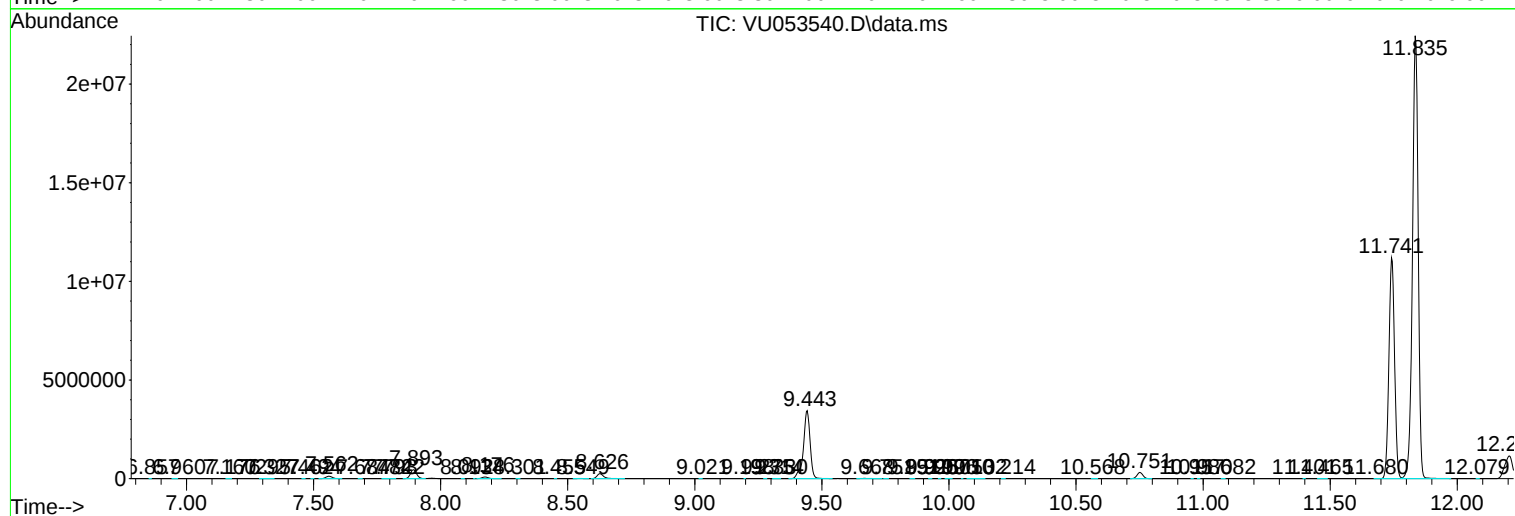
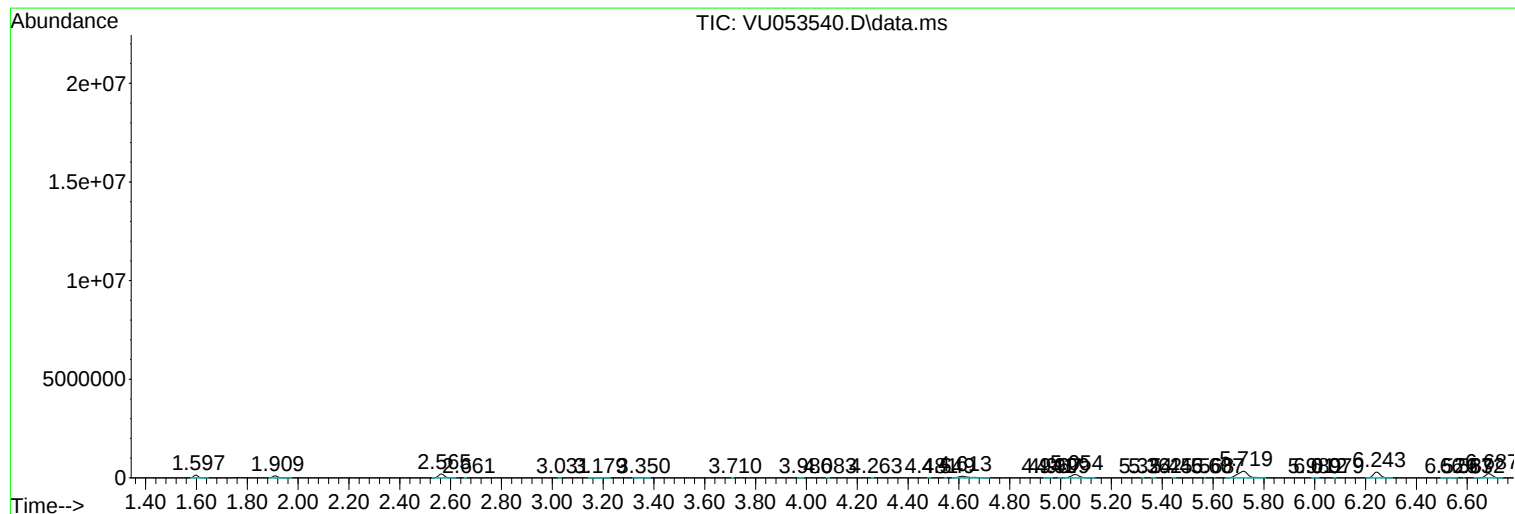
Sum of corrected areas: 66669621

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU040323\  
Data File : VU053540.D  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
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TIC Library : C:\Database\NIST20.L  
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No Library Search Compounds Detected

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