

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU020223\  
 Data File : VU052929.D  
 Acq On : 02 Feb 2023 16:35  
 Operator : JC/MD  
 Sample : 01381-14DL 5X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A44N3DL

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\SFAMULM012623WMA.M  
 Title : VOC Analysis

Signal : TIC: VU052929.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          | 98           | rVB      | 87239          | 110627        | 9.35%           | 1.383%        |
| 2         | 1.819       | 145           | 149         | 150          | rBV3     | 1045           | 747           | 0.06%           | 0.009%        |
| 3         | 1.906       | 169           | 176         | 193          | rBV      | 78280          | 123471        | 10.43%          | 1.544%        |
| 4         | 2.420       | 332           | 336         | 339          | rBV2     | 373            | 299           | 0.03%           | 0.004%        |
| 5         | 2.556       | 366           | 378         | 397          | rVB      | 188702         | 305745        | 25.84%          | 3.822%        |
| 6         | 2.642       | 397           | 405         | 413          | rBV4     | 835            | 1520          | 0.13%           | 0.019%        |
| 7         | 3.041       | 518           | 529         | 545          | rVB      | 6377           | 12627         | 1.07%           | 0.158%        |
| 8         | 3.131       | 552           | 557         | 558          | rBV      | 273            | 226           | 0.02%           | 0.003%        |
| 9         | 3.179       | 558           | 572         | 588          | rBV2     | 8568           | 20409         | 1.72%           | 0.255%        |
| 10        | 3.449       | 654           | 656         | 661          | rVB2     | 289            | 243           | 0.02%           | 0.003%        |
| 11        | 3.575       | 692           | 695         | 700          | rBV      | 198            | 241           | 0.02%           | 0.003%        |
| 12        | 3.642       | 712           | 716         | 717          | rBV      | 210            | 163           | 0.01%           | 0.002%        |
| 13        | 3.829       | 770           | 774         | 777          | rBB      | 195            | 142           | 0.01%           | 0.002%        |
| 14        | 3.887       | 787           | 792         | 795          | rBV      | 207            | 249           | 0.02%           | 0.003%        |
| 15        | 4.057       | 842           | 845         | 847          | rBV      | 167            | 142           | 0.01%           | 0.002%        |
| 16        | 4.102       | 856           | 859         | 862          | rBV      | 181            | 178           | 0.02%           | 0.002%        |
| 17        | 4.208       | 889           | 892         | 895          | rBB      | 216            | 160           | 0.01%           | 0.002%        |
| 18        | 4.276       | 909           | 913         | 916          | rBV      | 214            | 205           | 0.02%           | 0.003%        |
| 19        | 4.334       | 926           | 931         | 937          | rBB      | 241            | 302           | 0.03%           | 0.004%        |
| 20        | 4.436       | 958           | 963         | 965          | rBB2     | 276            | 204           | 0.02%           | 0.003%        |
| 21        | 4.498       | 978           | 982         | 984          | rBV      | 172            | 163           | 0.01%           | 0.002%        |
| 22        | 4.543       | 991           | 996         | 999          | rBB      | 179            | 181           | 0.02%           | 0.002%        |
| 23        | 4.581       | 1004          | 1008        | 1010         | rBV      | 233            | 196           | 0.02%           | 0.002%        |
| 24        | 4.655       | 1010          | 1031        | 1067         | rBV3     | 100976         | 336365        | 28.43%          | 4.205%        |
| 25        | 4.977       | 1128          | 1131        | 1134         | rBV      | 259            | 192           | 0.02%           | 0.002%        |
| 26        | 5.057       | 1138          | 1156        | 1177         | rBV      | 171754         | 379206        | 32.05%          | 4.741%        |
| 27        | 5.157       | 1184          | 1187        | 1192         | rVB2     | 555            | 448           | 0.04%           | 0.006%        |
| 28        | 5.285       | 1223          | 1227        | 1233         | rVB3     | 630            | 730           | 0.06%           | 0.009%        |
| 29        | 5.379       | 1249          | 1256        | 1258         | rBV2     | 284            | 358           | 0.03%           | 0.004%        |
| 30        | 5.446       | 1274          | 1277        | 1281         | rBB2     | 261            | 183           | 0.02%           | 0.002%        |
| 31        | 5.469       | 1282          | 1284        | 1288         | rBB      | 179            | 140           | 0.01%           | 0.002%        |
| 32        | 5.719       | 1340          | 1362        | 1386         | rBV2     | 342709         | 916674        | 77.47%          | 11.460%       |
| 33        | 5.893       | 1414          | 1416        | 1421         | rVB      | 315            | 219           | 0.02%           | 0.003%        |
| 34        | 6.034       | 1457          | 1460        | 1463         | rBV2     | 378            | 342           | 0.03%           | 0.004%        |
| 35        | 6.192       | 1506          | 1509        | 1511         | rBV      | 178            | 147           | 0.01%           | 0.002%        |
| 36        | 6.243       | 1511          | 1525        | 1543         | rVV      | 283966         | 533682        | 45.10%          | 6.672%        |

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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\SFAMULM012623WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.333  | 1551 | 1553 | 1556 | rVB  | 481    | 200    | 0.02%  | 0.003%  |
| 38 | 6.536  | 1604 | 1616 | 1636 | rBV  | 74597  | 142263 | 12.02% | 1.779%  |
| 39 | 6.629  | 1642 | 1645 | 1649 | rBV  | 301    | 271    | 0.02%  | 0.003%  |
| 40 | 6.684  | 1649 | 1662 | 1687 | rVV  | 204874 | 404978 | 34.23% | 5.063%  |
| 41 | 6.768  | 1687 | 1688 | 1693 | rVB  | 321    | 207    | 0.02%  | 0.003%  |
| 42 | 6.803  | 1696 | 1699 | 1704 | rBB2 | 637    | 527    | 0.04%  | 0.007%  |
| 43 | 6.864  | 1714 | 1718 | 1720 | rBB2 | 248    | 187    | 0.02%  | 0.002%  |
| 44 | 7.121  | 1795 | 1798 | 1801 | rBB  | 182    | 145    | 0.01%  | 0.002%  |
| 45 | 7.195  | 1811 | 1821 | 1833 | rBV7 | 1915   | 4697   | 0.40%  | 0.059%  |
| 46 | 7.562  | 1923 | 1935 | 1952 | rBV  | 105364 | 190892 | 16.13% | 2.387%  |
| 47 | 7.645  | 1958 | 1961 | 1966 | rVB2 | 414    | 329    | 0.03%  | 0.004%  |
| 48 | 7.684  | 1969 | 1973 | 1975 | rVV2 | 614    | 381    | 0.03%  | 0.005%  |
| 49 | 7.790  | 2003 | 2006 | 2008 | rBV2 | 269    | 179    | 0.02%  | 0.002%  |
| 50 | 7.893  | 2024 | 2038 | 2055 | rBV  | 409567 | 704016 | 59.50% | 8.802%  |
| 51 | 8.063  | 2087 | 2091 | 2092 | rBV  | 267    | 199    | 0.02%  | 0.002%  |
| 52 | 8.092  | 2097 | 2100 | 2101 | rBV  | 318    | 152    | 0.01%  | 0.002%  |
| 53 | 8.176  | 2115 | 2126 | 2143 | rBV  | 73963  | 129513 | 10.95% | 1.619%  |
| 54 | 8.282  | 2154 | 2159 | 2161 | rBV  | 326    | 307    | 0.03%  | 0.004%  |
| 55 | 8.391  | 2189 | 2193 | 2199 | rBV2 | 262    | 190    | 0.02%  | 0.002%  |
| 56 | 8.472  | 2209 | 2218 | 2226 | rVB3 | 1176   | 2349   | 0.20%  | 0.029%  |
| 57 | 8.530  | 2234 | 2236 | 2239 | rVB2 | 396    | 241    | 0.02%  | 0.003%  |
| 58 | 8.555  | 2240 | 2244 | 2246 | rBB  | 178    | 143    | 0.01%  | 0.002%  |
| 59 | 8.584  | 2251 | 2253 | 2256 | rBV  | 317    | 240    | 0.02%  | 0.003%  |
| 60 | 8.649  | 2258 | 2273 | 2303 | rBV3 | 148031 | 322146 | 27.23% | 4.028%  |
| 61 | 8.886  | 2342 | 2347 | 2350 | rBV  | 247    | 266    | 0.02%  | 0.003%  |
| 62 | 8.957  | 2367 | 2369 | 2373 | rVB  | 276    | 144    | 0.01%  | 0.002%  |
| 63 | 9.189  | 2438 | 2441 | 2444 | rBV  | 164    | 157    | 0.01%  | 0.002%  |
| 64 | 9.266  | 2460 | 2465 | 2468 | rBV  | 319    | 293    | 0.02%  | 0.004%  |
| 65 | 9.321  | 2477 | 2482 | 2483 | rBV  | 178    | 167    | 0.01%  | 0.002%  |
| 66 | 9.414  | 2498 | 2511 | 2545 | rBV2 | 396757 | 933287 | 78.87% | 11.668% |
| 67 | 9.690  | 2594 | 2597 | 2599 | rBV  | 356    | 267    | 0.02%  | 0.003%  |
| 68 | 9.819  | 2634 | 2637 | 2640 | rBV  | 163    | 155    | 0.01%  | 0.002%  |
| 69 | 9.915  | 2664 | 2667 | 2669 | rBV2 | 299    | 216    | 0.02%  | 0.003%  |
| 70 | 10.015 | 2695 | 2698 | 2701 | rBV  | 266    | 226    | 0.02%  | 0.003%  |
| 71 | 10.095 | 2720 | 2723 | 2730 | rVB  | 369    | 446    | 0.04%  | 0.006%  |
| 72 | 10.160 | 2738 | 2743 | 2745 | rBV  | 210    | 229    | 0.02%  | 0.003%  |
| 73 | 10.343 | 2797 | 2800 | 2803 | rBV  | 231    | 216    | 0.02%  | 0.003%  |
| 74 | 10.382 | 2809 | 2812 | 2814 | rBV  | 179    | 148    | 0.01%  | 0.002%  |
| 75 | 10.452 | 2831 | 2834 | 2837 | rVB  | 257    | 168    | 0.01%  | 0.002%  |
| 76 | 10.475 | 2837 | 2841 | 2843 | rBV  | 442    | 345    | 0.03%  | 0.004%  |

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |         |         |
|-----|--------|------|------|------|------|--------|---------|---------|---------|
| 77  | 10.517 | 2849 | 2854 | 2864 | rBB  | 305    | 508     | 0.04%   | 0.006%  |
| 78  | 10.565 | 2865 | 2869 | 2874 | rBB  | 195    | 251     | 0.02%   | 0.003%  |
| 79  | 10.597 | 2875 | 2879 | 2881 | rBV  | 311    | 245     | 0.02%   | 0.003%  |
| 80  | 10.700 | 2908 | 2911 | 2916 | rBV  | 167    | 157     | 0.01%   | 0.002%  |
| 81  | 10.758 | 2916 | 2929 | 2948 | rVV  | 274598 | 439440  | 37.14%  | 5.494%  |
| 82  | 10.886 | 2965 | 2969 | 2977 | rVB3 | 1798   | 2114    | 0.18%   | 0.026%  |
| 83  | 11.021 | 3007 | 3011 | 3015 | rBV2 | 284    | 227     | 0.02%   | 0.003%  |
| 84  | 11.295 | 3093 | 3096 | 3098 | rBV  | 375    | 175     | 0.01%   | 0.002%  |
| 85  | 11.462 | 3144 | 3148 | 3152 | rVB2 | 361    | 407     | 0.03%   | 0.005%  |
| 86  | 11.484 | 3153 | 3155 | 3157 | rBV  | 243    | 161     | 0.01%   | 0.002%  |
| 87  | 11.742 | 3228 | 3235 | 3244 | rBV4 | 6738   | 10022   | 0.85%   | 0.125%  |
| 88  | 11.809 | 3244 | 3256 | 3277 | rBV2 | 410632 | 714861  | 60.41%  | 8.937%  |
| 89  | 12.063 | 3332 | 3335 | 3346 | rVB4 | 1364   | 1595    | 0.13%   | 0.020%  |
| 90  | 12.195 | 3361 | 3376 | 3399 | rBV2 | 502072 | 1183254 | 100.00% | 14.793% |
| 91  | 12.304 | 3408 | 3410 | 3412 | rBV  | 339    | 155     | 0.01%   | 0.002%  |
| 92  | 12.767 | 3549 | 3554 | 3564 | rVB2 | 1054   | 1444    | 0.12%   | 0.018%  |
| 93  | 13.221 | 3686 | 3695 | 3701 | rBV4 | 1230   | 1968    | 0.17%   | 0.025%  |
| 94  | 13.443 | 3761 | 3764 | 3766 | rBV2 | 260    | 158     | 0.01%   | 0.002%  |
| 95  | 13.838 | 3876 | 3887 | 3899 | rBV2 | 27873  | 42663   | 3.61%   | 0.533%  |
| 96  | 14.195 | 3994 | 3998 | 4000 | rBV  | 320    | 245     | 0.02%   | 0.003%  |
| 97  | 14.330 | 4032 | 4040 | 4053 | rBV4 | 4808   | 8476    | 0.72%   | 0.106%  |
| 98  | 14.610 | 4124 | 4127 | 4130 | rBV2 | 406    | 295     | 0.02%   | 0.004%  |
| 99  | 14.944 | 4227 | 4231 | 4234 | rBV2 | 465    | 409     | 0.03%   | 0.005%  |
| 100 | 15.121 | 4283 | 4286 | 4294 | rBV2 | 510    | 724     | 0.06%   | 0.009%  |

Sum of corrected areas: 7998562

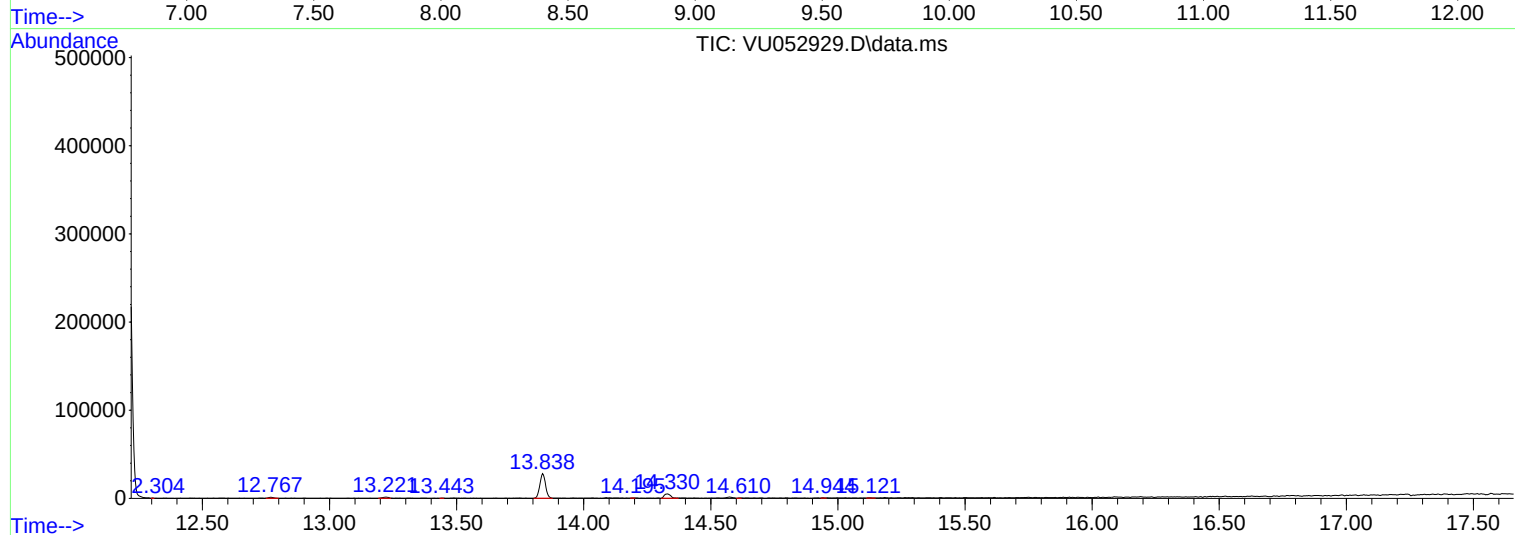
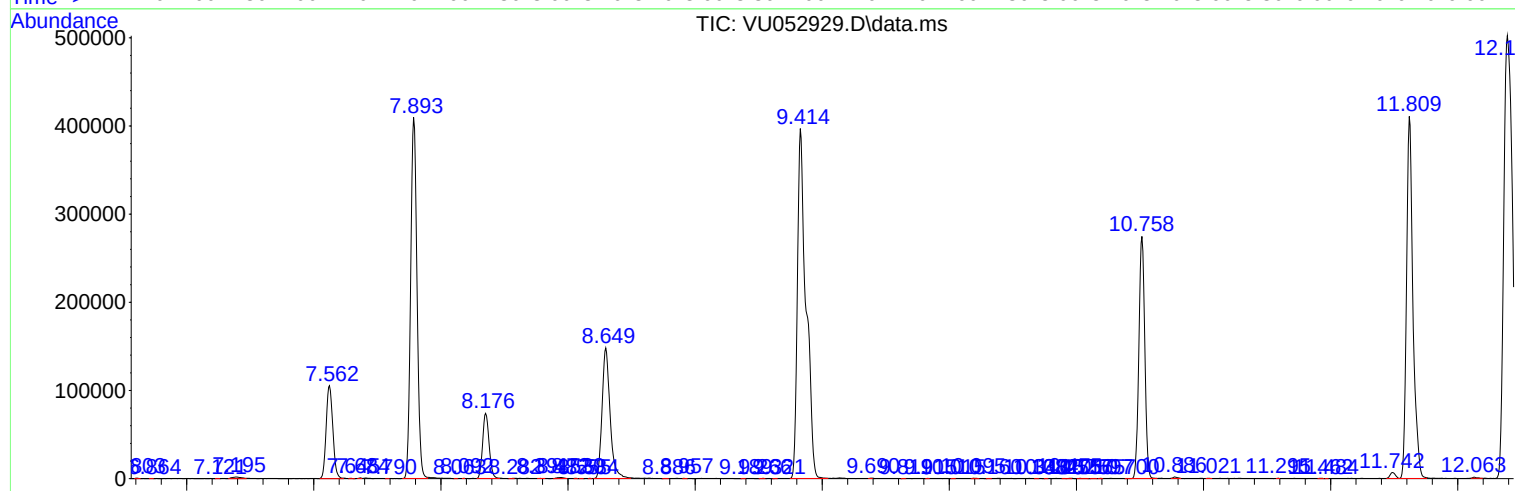
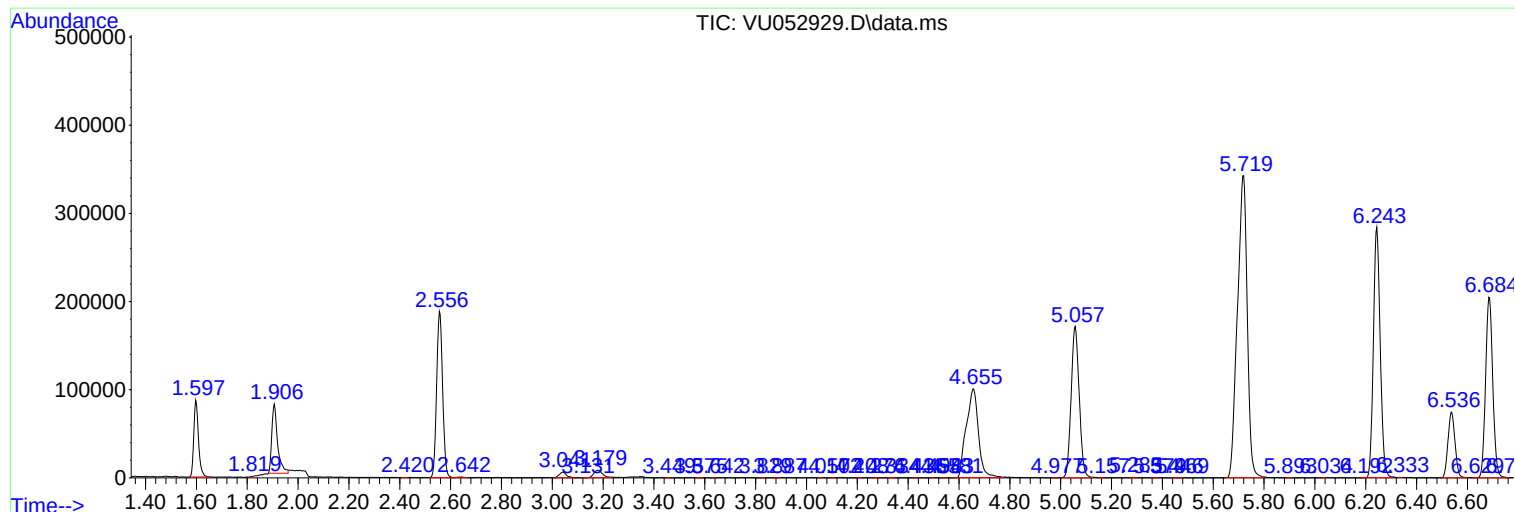
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU020223\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

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

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