

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX112621\  
 Data File : VX025350.D  
 Acq On : 26 Nov 2021 12:52  
 Operator : JC/MD  
 Sample : M4839-06  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ESQN5

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\_X\Method\SFAMXLM112221WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025350.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         | 1.367       | 42            | 46          | 53           | rVB      | 71423          | 68665         | 13.33%          | 1.698%        |
| 2         | 1.666       | 90            | 95          | 105          | rBV      | 53200          | 71127         | 13.81%          | 1.758%        |
| 3         | 2.306       | 194           | 200         | 209          | rBV      | 102463         | 166658        | 32.35%          | 4.120%        |
| 4         | 2.788       | 275           | 279         | 284          | rBV3     | 665            | 1098          | 0.21%           | 0.027%        |
| 5         | 2.965       | 302           | 308         | 316          | rVB2     | 1966           | 4137          | 0.80%           | 0.102%        |
| 6         | 3.105       | 330           | 331         | 332          | rBV      | 167            | 70            | 0.01%           | 0.002%        |
| 7         | 3.282       | 358           | 360         | 362          | rBV      | 127            | 72            | 0.01%           | 0.002%        |
| 8         | 3.684       | 424           | 426         | 428          | rVB      | 156            | 115           | 0.02%           | 0.003%        |
| 9         | 4.038       | 483           | 484         | 487          | rBV      | 116            | 98            | 0.02%           | 0.002%        |
| 10        | 4.068       | 487           | 489         | 491          | rBV      | 131            | 105           | 0.02%           | 0.003%        |
| 11        | 4.458       | 543           | 553         | 569          | rBV      | 47352          | 133483        | 25.91%          | 3.300%        |
| 12        | 4.666       | 585           | 587         | 591          | rVB2     | 150            | 142           | 0.03%           | 0.004%        |
| 13        | 4.849       | 615           | 617         | 618          | rBV2     | 100            | 74            | 0.01%           | 0.002%        |
| 14        | 5.062       | 640           | 652         | 671          | rBV      | 69002          | 208973        | 40.57%          | 5.166%        |
| 15        | 5.330       | 695           | 696         | 697          | rBV      | 121            | 68            | 0.01%           | 0.002%        |
| 16        | 5.379       | 701           | 704         | 705          | rBV2     | 219            | 189           | 0.04%           | 0.005%        |
| 17        | 5.464       | 717           | 718         | 722          | rBV2     | 103            | 101           | 0.02%           | 0.002%        |
| 18        | 5.562       | 728           | 734         | 738          | rBV3     | 472            | 897           | 0.17%           | 0.022%        |
| 19        | 5.611       | 740           | 742         | 743          | rBB2     | 106            | 43            | 0.01%           | 0.001%        |
| 20        | 5.800       | 771           | 773         | 775          | rBV      | 163            | 130           | 0.03%           | 0.003%        |
| 21        | 5.970       | 788           | 801         | 818          | rBV2     | 170600         | 515116        | 100.00%         | 12.735%       |
| 22        | 6.251       | 846           | 847         | 848          | rBB      | 134            | 49            | 0.01%           | 0.001%        |
| 23        | 6.287       | 852           | 853         | 855          | rBV      | 108            | 110           | 0.02%           | 0.003%        |
| 24        | 6.348       | 862           | 863         | 864          | rBV      | 68             | 37            | 0.01%           | 0.001%        |
| 25        | 6.415       | 873           | 874         | 875          | rVB      | 132            | 48            | 0.01%           | 0.001%        |
| 26        | 6.434       | 875           | 877         | 879          | rVB      | 119            | 103           | 0.02%           | 0.003%        |
| 27        | 6.458       | 879           | 881         | 882          | rBV2     | 69             | 36            | 0.01%           | 0.001%        |
| 28        | 6.763       | 922           | 931         | 947          | rBV      | 136358         | 321269        | 62.37%          | 7.943%        |
| 29        | 6.958       | 962           | 963         | 969          | rVB      | 198            | 178           | 0.03%           | 0.004%        |
| 30        | 7.110       | 982           | 988         | 997          | rVB3     | 3071           | 6540          | 1.27%           | 0.162%        |
| 31        | 7.226       | 1004          | 1007        | 1009         | rBV2     | 191            | 233           | 0.05%           | 0.006%        |
| 32        | 7.251       | 1009          | 1011        | 1012         | rVV      | 87             | 48            | 0.01%           | 0.001%        |
| 33        | 7.312       | 1012          | 1021        | 1031         | rVV      | 107218         | 233364        | 45.30%          | 5.769%        |
| 34        | 7.470       | 1045          | 1047        | 1049         | rBV      | 232            | 221           | 0.04%           | 0.005%        |
| 35        | 7.586       | 1064          | 1066        | 1067         | rVB      | 148            | 69            | 0.01%           | 0.002%        |
| 36        | 7.872       | 1112          | 1113        | 1114         | rBV      | 110            | 47            | 0.01%           | 0.001%        |

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 ESQN5

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\_X\Method\SFAMXLM112221WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.933  | 1118 | 1123 | 1129 | rBV2 | 847    | 1547   | 0.30%  | 0.038%  |
| 38 | 8.007  | 1134 | 1135 | 1138 | rBV  | 120    | 64     | 0.01%  | 0.002%  |
| 39 | 8.080  | 1145 | 1147 | 1149 | rBV  | 161    | 147    | 0.03%  | 0.004%  |
| 40 | 8.128  | 1154 | 1155 | 1158 | rVB  | 144    | 79     | 0.02%  | 0.002%  |
| 41 | 8.183  | 1160 | 1164 | 1166 | rBV2 | 98     | 116    | 0.02%  | 0.003%  |
| 42 | 8.256  | 1174 | 1176 | 1179 | rBV2 | 126    | 188    | 0.04%  | 0.005%  |
| 43 | 8.330  | 1181 | 1188 | 1204 | rVV  | 73469  | 124356 | 24.14% | 3.074%  |
| 44 | 8.470  | 1206 | 1211 | 1219 | rVB3 | 641    | 1469   | 0.29%  | 0.036%  |
| 45 | 8.653  | 1234 | 1241 | 1249 | rBV  | 259714 | 415790 | 80.72% | 10.280% |
| 46 | 8.720  | 1249 | 1252 | 1262 | rVB  | 3548   | 5882   | 1.14%  | 0.145%  |
| 47 | 8.951  | 1284 | 1290 | 1300 | rBV  | 56509  | 80230  | 15.58% | 1.984%  |
| 48 | 9.049  | 1303 | 1306 | 1308 | rBV2 | 191    | 227    | 0.04%  | 0.006%  |
| 49 | 9.189  | 1326 | 1329 | 1331 | rBV  | 128    | 125    | 0.02%  | 0.003%  |
| 50 | 9.384  | 1355 | 1361 | 1381 | rBV  | 208024 | 294669 | 57.20% | 7.285%  |
| 51 | 9.555  | 1388 | 1389 | 1391 | rBV  | 144    | 91     | 0.02%  | 0.002%  |
| 52 | 9.878  | 1438 | 1442 | 1443 | rBV2 | 99     | 101    | 0.02%  | 0.002%  |
| 53 | 10.055 | 1465 | 1471 | 1488 | rBV  | 285986 | 379243 | 73.62% | 9.376%  |
| 54 | 10.311 | 1508 | 1513 | 1519 | rBV4 | 509    | 905    | 0.18%  | 0.022%  |
| 55 | 10.439 | 1532 | 1534 | 1537 | rVB2 | 130    | 113    | 0.02%  | 0.003%  |
| 56 | 10.524 | 1547 | 1548 | 1549 | rBV  | 136    | 76     | 0.01%  | 0.002%  |
| 57 | 10.640 | 1565 | 1567 | 1569 | rBV  | 306    | 250    | 0.05%  | 0.006%  |
| 58 | 10.872 | 1604 | 1605 | 1607 | rBV  | 132    | 90     | 0.02%  | 0.002%  |
| 59 | 10.915 | 1610 | 1612 | 1613 | rBV  | 90     | 44     | 0.01%  | 0.001%  |
| 60 | 11.128 | 1642 | 1647 | 1649 | rVB2 | 825    | 1102   | 0.21%  | 0.027%  |
| 61 | 11.195 | 1652 | 1658 | 1665 | rVV  | 212837 | 270992 | 52.61% | 6.700%  |
| 62 | 11.305 | 1671 | 1676 | 1681 | rVV3 | 230    | 448    | 0.09%  | 0.011%  |
| 63 | 11.372 | 1685 | 1687 | 1690 | rVB2 | 177    | 206    | 0.04%  | 0.005%  |
| 64 | 11.457 | 1699 | 1701 | 1703 | rBV2 | 295    | 292    | 0.06%  | 0.007%  |
| 65 | 11.677 | 1735 | 1737 | 1739 | rBV  | 129    | 123    | 0.02%  | 0.003%  |
| 66 | 11.750 | 1746 | 1749 | 1753 | rVB4 | 1098   | 1443   | 0.28%  | 0.036%  |
| 67 | 11.841 | 1762 | 1764 | 1768 | rVB2 | 174    | 217    | 0.04%  | 0.005%  |
| 68 | 11.878 | 1768 | 1770 | 1772 | rBV2 | 161    | 163    | 0.03%  | 0.004%  |
| 69 | 11.933 | 1776 | 1779 | 1784 | rBV2 | 366    | 512    | 0.10%  | 0.013%  |
| 70 | 12.024 | 1789 | 1794 | 1806 | rVB  | 282440 | 355096 | 68.94% | 8.779%  |
| 71 | 12.116 | 1806 | 1809 | 1810 | rBV2 | 175    | 168    | 0.03%  | 0.004%  |
| 72 | 12.231 | 1824 | 1828 | 1831 | rBV2 | 191    | 263    | 0.05%  | 0.007%  |
| 73 | 12.323 | 1837 | 1843 | 1857 | rVB  | 305864 | 371121 | 72.05% | 9.175%  |
| 74 | 12.670 | 1898 | 1900 | 1903 | rBV2 | 202    | 232    | 0.05%  | 0.006%  |
| 75 | 12.737 | 1910 | 1911 | 1912 | rBV  | 141    | 71     | 0.01%  | 0.002%  |
| 76 | 12.908 | 1938 | 1939 | 1940 | rBV  | 203    | 124    | 0.02%  | 0.003%  |

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M

Title : VOC Analysis

|    |        |      |      |      |      |     |     |       |        |
|----|--------|------|------|------|------|-----|-----|-------|--------|
| 77 | 13.164 | 1979 | 1981 | 1983 | rBV  | 118 | 74  | 0.01% | 0.002% |
| 78 | 13.371 | 2011 | 2015 | 2016 | rBV  | 160 | 226 | 0.04% | 0.006% |
| 79 | 13.414 | 2021 | 2022 | 2023 | rBV  | 111 | 50  | 0.01% | 0.001% |
| 80 | 13.475 | 2031 | 2032 | 2035 | rBV2 | 119 | 114 | 0.02% | 0.003% |
| 81 | 13.908 | 2102 | 2103 | 2105 | rVB  | 121 | 50  | 0.01% | 0.001% |
| 82 | 14.133 | 2137 | 2140 | 2143 | rBV2 | 628 | 776 | 0.15% | 0.019% |
| 83 | 14.262 | 2160 | 2161 | 2164 | rBV2 | 198 | 135 | 0.03% | 0.003% |
| 84 | 14.316 | 2168 | 2170 | 2172 | rBV2 | 111 | 115 | 0.02% | 0.003% |
| 85 | 14.396 | 2182 | 2183 | 2186 | rBV  | 190 | 99  | 0.02% | 0.002% |
| 86 | 14.560 | 2207 | 2210 | 2212 | rBV2 | 157 | 176 | 0.03% | 0.004% |
| 87 | 14.597 | 2214 | 2216 | 2218 | rBV  | 200 | 230 | 0.04% | 0.006% |
| 88 | 14.719 | 2234 | 2236 | 2238 | rBV2 | 175 | 141 | 0.03% | 0.003% |
| 89 | 15.017 | 2283 | 2285 | 2286 | rBV2 | 216 | 186 | 0.04% | 0.005% |
| 90 | 15.261 | 2324 | 2325 | 2326 | rVB  | 243 | 89  | 0.02% | 0.002% |
| 91 | 15.310 | 2331 | 2333 | 2336 | rBV  | 287 | 253 | 0.05% | 0.006% |

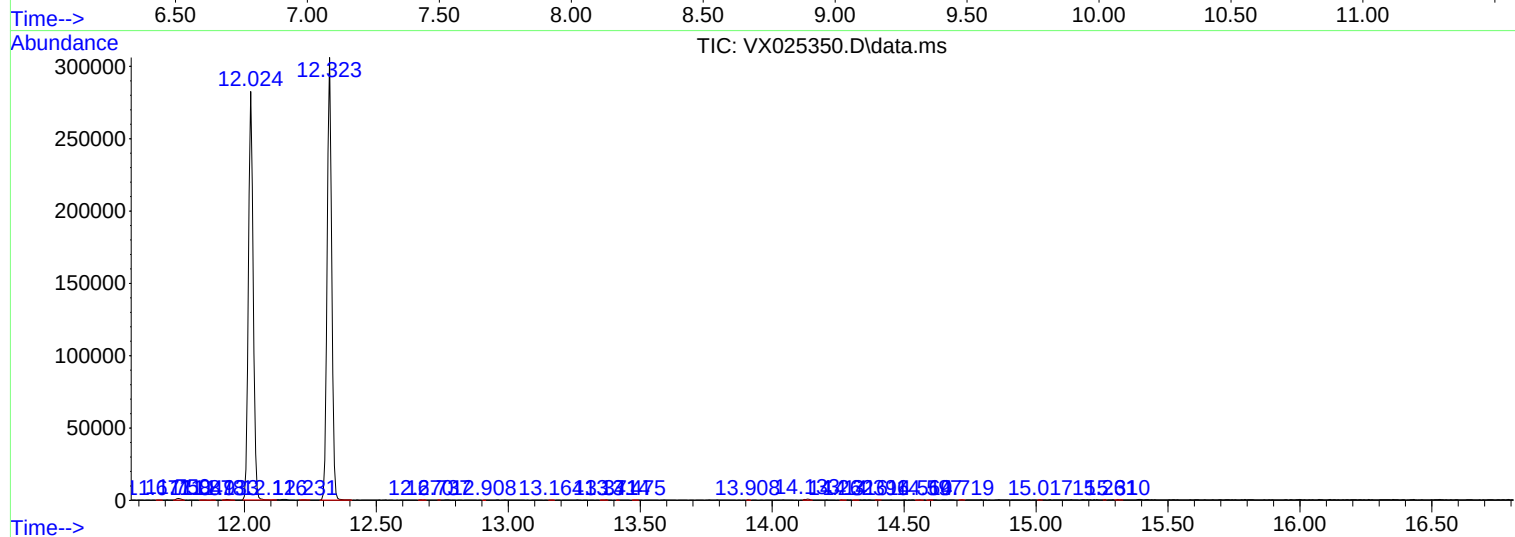
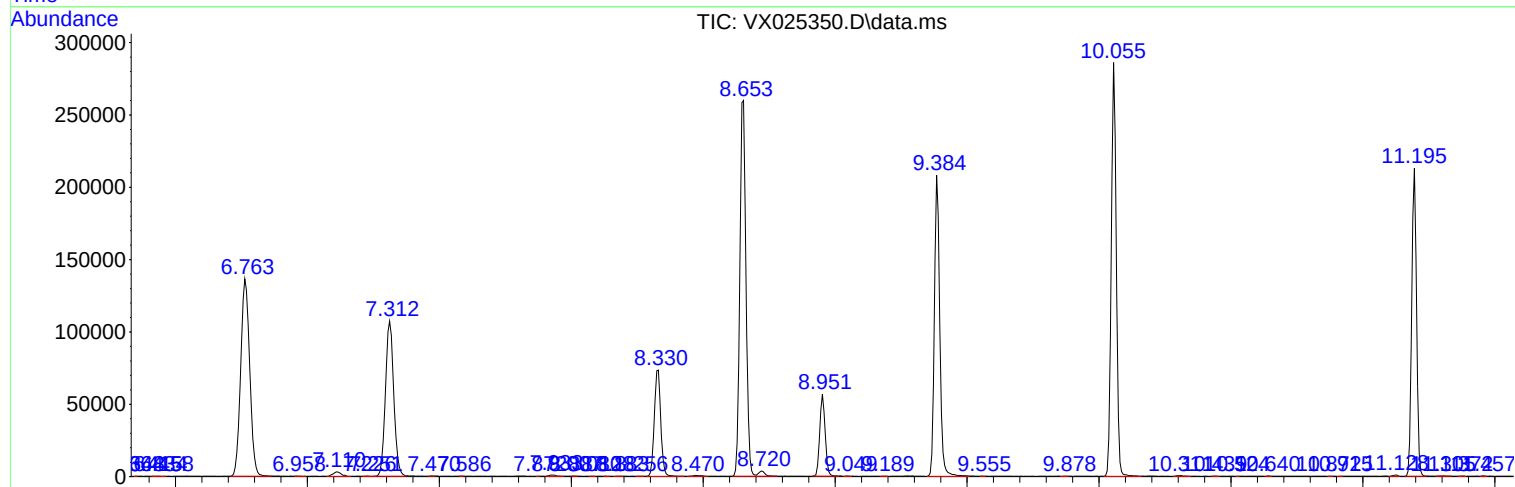
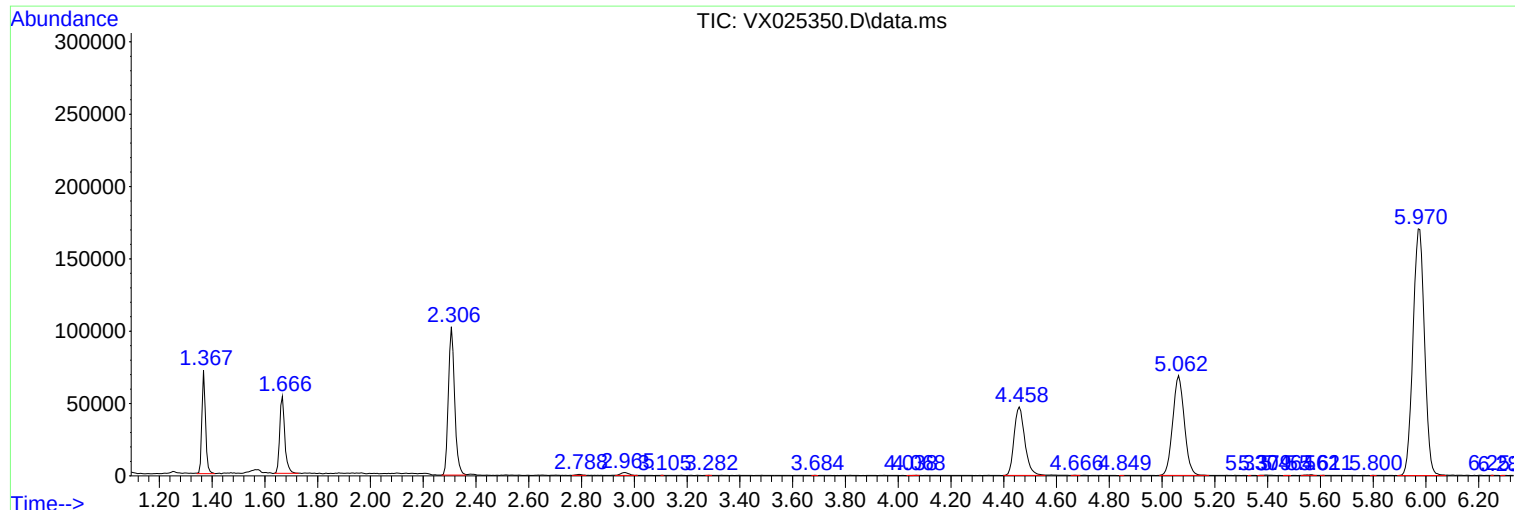
Sum of corrected areas: 4044802

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ClientSampleId :  
ESQN5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX112621\  
Data File : VX025350.D  
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Operator : JC/MD  
Sample : M4839-06  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
ESQN5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML112221WMA.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 |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|