

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX011323\  
 Data File : VX033714.D  
 Acq On : 13 Jan 2023 10:12  
 Operator : JC/MD  
 Sample : VX0113WBL01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK607

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\SFAMXLM122722WMA.M  
 Title : VOC Analysis

Signal : TIC: VX033714.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         | 1.264       | 26            | 29          | 37           | rVB      | 15476          | 13878         | 1.57%           | 0.219%        |
| 2         | 1.368       | 42            | 46          | 60           | rVB      | 101418         | 111745        | 12.67%          | 1.761%        |
| 3         | 1.672       | 91            | 96          | 107          | rBV      | 80943          | 102865        | 11.67%          | 1.621%        |
| 4         | 2.306       | 194           | 200         | 210          | rBV      | 195042         | 303229        | 34.39%          | 4.779%        |
| 5         | 2.514       | 230           | 234         | 239          | rBV      | 1006           | 1569          | 0.18%           | 0.025%        |
| 6         | 2.630       | 252           | 253         | 256          | rBV      | 181            | 160           | 0.02%           | 0.003%        |
| 7         | 2.660       | 256           | 258         | 259          | rVV      | 151            | 98            | 0.01%           | 0.002%        |
| 8         | 2.678       | 259           | 261         | 263          | rVB2     | 194            | 132           | 0.01%           | 0.002%        |
| 9         | 2.794       | 275           | 280         | 284          | rVB2     | 882            | 1384          | 0.16%           | 0.022%        |
| 10        | 2.867       | 291           | 292         | 294          | rBV      | 135            | 112           | 0.01%           | 0.002%        |
| 11        | 2.916       | 298           | 300         | 301          | rBV      | 152            | 140           | 0.02%           | 0.002%        |
| 12        | 3.050       | 319           | 322         | 325          | rBV2     | 163            | 202           | 0.02%           | 0.003%        |
| 13        | 3.099       | 325           | 330         | 335          | rVB3     | 454            | 866           | 0.10%           | 0.014%        |
| 14        | 3.258       | 354           | 356         | 358          | rVB2     | 157            | 100           | 0.01%           | 0.002%        |
| 15        | 3.294       | 360           | 362         | 363          | rVB      | 145            | 74            | 0.01%           | 0.001%        |
| 16        | 3.398       | 377           | 379         | 381          | rVB2     | 201            | 155           | 0.02%           | 0.002%        |
| 17        | 3.416       | 381           | 382         | 384          | rBV      | 157            | 152           | 0.02%           | 0.002%        |
| 18        | 3.471       | 390           | 391         | 393          | rBV      | 187            | 106           | 0.01%           | 0.002%        |
| 19        | 3.739       | 433           | 435         | 437          | rVB      | 133            | 86            | 0.01%           | 0.001%        |
| 20        | 3.764       | 437           | 439         | 441          | rBV      | 111            | 87            | 0.01%           | 0.001%        |
| 21        | 3.812       | 446           | 447         | 448          | rBV      | 143            | 72            | 0.01%           | 0.001%        |
| 22        | 3.831       | 448           | 450         | 453          | rVB2     | 182            | 139           | 0.02%           | 0.002%        |
| 23        | 3.892       | 458           | 460         | 462          | rBV      | 106            | 83            | 0.01%           | 0.001%        |
| 24        | 3.910       | 462           | 463         | 464          | rBV      | 176            | 86            | 0.01%           | 0.001%        |
| 25        | 4.105       | 494           | 495         | 498          | rBV2     | 138            | 139           | 0.02%           | 0.002%        |
| 26        | 4.459       | 544           | 553         | 573          | rBV      | 54699          | 175114        | 19.86%          | 2.760%        |
| 27        | 4.952       | 633           | 634         | 638          | rBV2     | 186            | 243           | 0.03%           | 0.004%        |
| 28        | 5.050       | 638           | 650         | 671          | rVV      | 111266         | 347504        | 39.41%          | 5.476%        |
| 29        | 5.385       | 698           | 705         | 713          | rBV4     | 803            | 2242          | 0.25%           | 0.035%        |
| 30        | 5.544       | 723           | 731         | 741          | rBV2     | 2722           | 8029          | 0.91%           | 0.127%        |
| 31        | 5.617       | 741           | 743         | 745          | rVB      | 175            | 115           | 0.01%           | 0.002%        |
| 32        | 5.964       | 788           | 800         | 820          | rBV2     | 295404         | 881817        | 100.00%         | 13.897%       |
| 33        | 6.275       | 850           | 851         | 855          | rVB      | 127            | 79            | 0.01%           | 0.001%        |
| 34        | 6.391       | 868           | 870         | 871          | rBV      | 173            | 91            | 0.01%           | 0.001%        |
| 35        | 6.409       | 871           | 873         | 875          | rVV      | 147            | 128           | 0.01%           | 0.002%        |
| 36        | 6.458       | 879           | 881         | 883          | rVV2     | 170            | 131           | 0.01%           | 0.002%        |

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Integrator: RTE

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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\_X\Method\SFAMXML122722WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.659  | 912  | 914  | 917  | rBV  | 118    | 150    | 0.02%  | 0.002%  |
| 38 | 6.757  | 920  | 930  | 949  | rBV  | 258920 | 602774 | 68.36% | 9.499%  |
| 39 | 7.037  | 974  | 976  | 978  | rBV  | 151    | 102    | 0.01%  | 0.002%  |
| 40 | 7.110  | 980  | 988  | 995  | rBV3 | 1796   | 3902   | 0.44%  | 0.061%  |
| 41 | 7.306  | 1009 | 1020 | 1034 | rBV  | 181878 | 399741 | 45.33% | 6.300%  |
| 42 | 7.476  | 1044 | 1048 | 1053 | rBV2 | 538    | 885    | 0.10%  | 0.014%  |
| 43 | 7.751  | 1092 | 1093 | 1095 | rVB  | 200    | 77     | 0.01%  | 0.001%  |
| 44 | 7.769  | 1095 | 1096 | 1098 | rVB  | 140    | 83     | 0.01%  | 0.001%  |
| 45 | 7.927  | 1118 | 1122 | 1132 | rBV4 | 1430   | 2879   | 0.33%  | 0.045%  |
| 46 | 8.177  | 1159 | 1163 | 1164 | rBV2 | 120    | 176    | 0.02%  | 0.003%  |
| 47 | 8.214  | 1167 | 1169 | 1172 | rBV  | 173    | 143    | 0.02%  | 0.002%  |
| 48 | 8.257  | 1172 | 1176 | 1177 | rBV2 | 126    | 101    | 0.01%  | 0.002%  |
| 49 | 8.324  | 1180 | 1187 | 1203 | rBV  | 114282 | 191957 | 21.77% | 3.025%  |
| 50 | 8.482  | 1209 | 1213 | 1217 | rBV4 | 1106   | 1635   | 0.19%  | 0.026%  |
| 51 | 8.647  | 1233 | 1240 | 1249 | rBV  | 483308 | 737072 | 83.59% | 11.616% |
| 52 | 8.946  | 1284 | 1289 | 1302 | rBV  | 80576  | 123169 | 13.97% | 1.941%  |
| 53 | 9.275  | 1339 | 1343 | 1347 | rBV2 | 728    | 851    | 0.10%  | 0.013%  |
| 54 | 9.384  | 1355 | 1361 | 1376 | rBV  | 260010 | 377012 | 42.75% | 5.941%  |
| 55 | 9.701  | 1410 | 1413 | 1419 | rVB2 | 577    | 810    | 0.09%  | 0.013%  |
| 56 | 10.055 | 1465 | 1471 | 1486 | rVB  | 494101 | 637540 | 72.30% | 10.047% |
| 57 | 10.195 | 1491 | 1494 | 1500 | rBV3 | 522    | 740    | 0.08%  | 0.012%  |
| 58 | 10.305 | 1508 | 1512 | 1519 | rVV3 | 418    | 688    | 0.08%  | 0.011%  |
| 59 | 10.451 | 1533 | 1536 | 1539 | rBV  | 271    | 376    | 0.04%  | 0.006%  |
| 60 | 10.482 | 1539 | 1541 | 1544 | rVV2 | 94     | 127    | 0.01%  | 0.002%  |
| 61 | 10.659 | 1565 | 1570 | 1578 | rVB5 | 756    | 1709   | 0.19%  | 0.027%  |
| 62 | 10.756 | 1583 | 1586 | 1592 | rVB2 | 163    | 412    | 0.05%  | 0.006%  |
| 63 | 10.805 | 1592 | 1594 | 1595 | rBV  | 142    | 137    | 0.02%  | 0.002%  |
| 64 | 10.860 | 1599 | 1603 | 1606 | rBV2 | 181    | 278    | 0.03%  | 0.004%  |
| 65 | 10.927 | 1612 | 1614 | 1616 | rBV  | 112    | 83     | 0.01%  | 0.001%  |
| 66 | 11.037 | 1630 | 1632 | 1634 | rBV2 | 138    | 133    | 0.02%  | 0.002%  |
| 67 | 11.189 | 1652 | 1657 | 1671 | rBV  | 236268 | 304897 | 34.58% | 4.805%  |
| 68 | 11.451 | 1696 | 1700 | 1705 | rBV3 | 508    | 730    | 0.08%  | 0.012%  |
| 69 | 11.713 | 1741 | 1743 | 1744 | rBV  | 111    | 83     | 0.01%  | 0.001%  |
| 70 | 11.756 | 1746 | 1750 | 1752 | rVV2 | 363    | 400    | 0.05%  | 0.006%  |
| 71 | 11.914 | 1775 | 1776 | 1778 | rBV2 | 102    | 79     | 0.01%  | 0.001%  |
| 72 | 11.969 | 1782 | 1785 | 1788 | rVB3 | 600    | 653    | 0.07%  | 0.010%  |
| 73 | 12.018 | 1788 | 1793 | 1803 | rBV  | 400230 | 503951 | 57.15% | 7.942%  |
| 74 | 12.183 | 1818 | 1820 | 1822 | rBV  | 205    | 132    | 0.01%  | 0.002%  |
| 75 | 12.250 | 1828 | 1831 | 1833 | rVB  | 191    | 179    | 0.02%  | 0.003%  |
| 76 | 12.317 | 1837 | 1842 | 1850 | rBV  | 388086 | 487753 | 55.31% | 7.687%  |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK607

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMXLM122722WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |     |      |       |        |
|-----|--------|------|------|------|------|-----|------|-------|--------|
| 77  | 12.414 | 1857 | 1858 | 1860 | rBV  | 222 | 225  | 0.03% | 0.004% |
| 78  | 12.591 | 1886 | 1887 | 1890 | rBV  | 126 | 87   | 0.01% | 0.001% |
| 79  | 12.744 | 1908 | 1912 | 1913 | rBV  | 176 | 204  | 0.02% | 0.003% |
| 80  | 12.835 | 1924 | 1927 | 1929 | rBV2 | 174 | 245  | 0.03% | 0.004% |
| 81  | 12.853 | 1929 | 1930 | 1933 | rVV2 | 536 | 513  | 0.06% | 0.008% |
| 82  | 13.018 | 1955 | 1957 | 1958 | rBV  | 205 | 108  | 0.01% | 0.002% |
| 83  | 13.115 | 1970 | 1973 | 1979 | rBB4 | 504 | 691  | 0.08% | 0.011% |
| 84  | 13.201 | 1985 | 1987 | 1989 | rBV  | 123 | 84   | 0.01% | 0.001% |
| 85  | 13.493 | 2033 | 2035 | 2038 | rBV2 | 108 | 160  | 0.02% | 0.003% |
| 86  | 13.573 | 2046 | 2048 | 2049 | rBV  | 116 | 83   | 0.01% | 0.001% |
| 87  | 13.591 | 2049 | 2051 | 2056 | rVB3 | 958 | 1184 | 0.13% | 0.019% |
| 88  | 13.676 | 2063 | 2065 | 2066 | rBV  | 168 | 142  | 0.02% | 0.002% |
| 89  | 13.780 | 2078 | 2082 | 2086 | rVB3 | 720 | 1029 | 0.12% | 0.016% |
| 90  | 13.817 | 2086 | 2088 | 2092 | rVB2 | 209 | 214  | 0.02% | 0.003% |
| 91  | 13.847 | 2092 | 2093 | 2094 | rBV  | 133 | 76   | 0.01% | 0.001% |
| 92  | 13.963 | 2109 | 2112 | 2117 | rVB4 | 819 | 1176 | 0.13% | 0.019% |
| 93  | 14.054 | 2125 | 2127 | 2129 | rVB2 | 173 | 151  | 0.02% | 0.002% |
| 94  | 14.073 | 2129 | 2130 | 2135 | rBV2 | 162 | 207  | 0.02% | 0.003% |
| 95  | 14.128 | 2137 | 2139 | 2144 | rVB3 | 163 | 246  | 0.03% | 0.004% |
| 96  | 14.280 | 2162 | 2164 | 2166 | rBV2 | 155 | 138  | 0.02% | 0.002% |
| 97  | 14.688 | 2229 | 2231 | 2232 | rBV  | 130 | 112  | 0.01% | 0.002% |
| 98  | 14.762 | 2238 | 2243 | 2244 | rBV3 | 212 | 356  | 0.04% | 0.006% |
| 99  | 14.829 | 2253 | 2254 | 2257 | rBV2 | 169 | 171  | 0.02% | 0.003% |
| 100 | 15.633 | 2384 | 2386 | 2387 | rBV  | 336 | 172  | 0.02% | 0.003% |

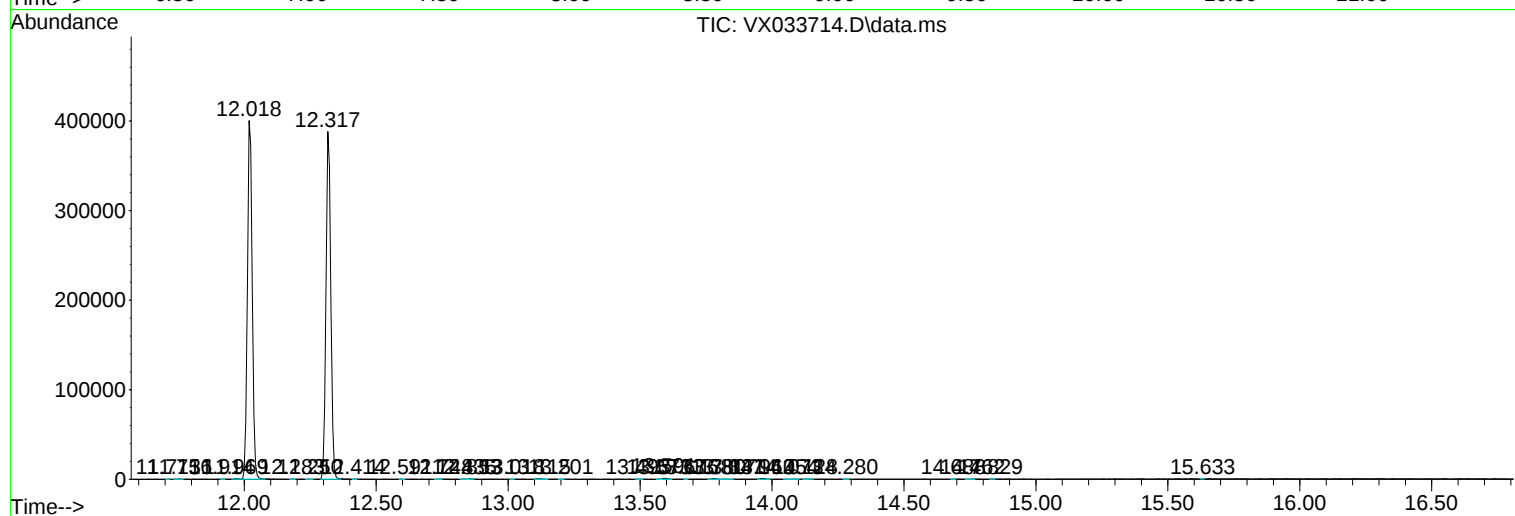
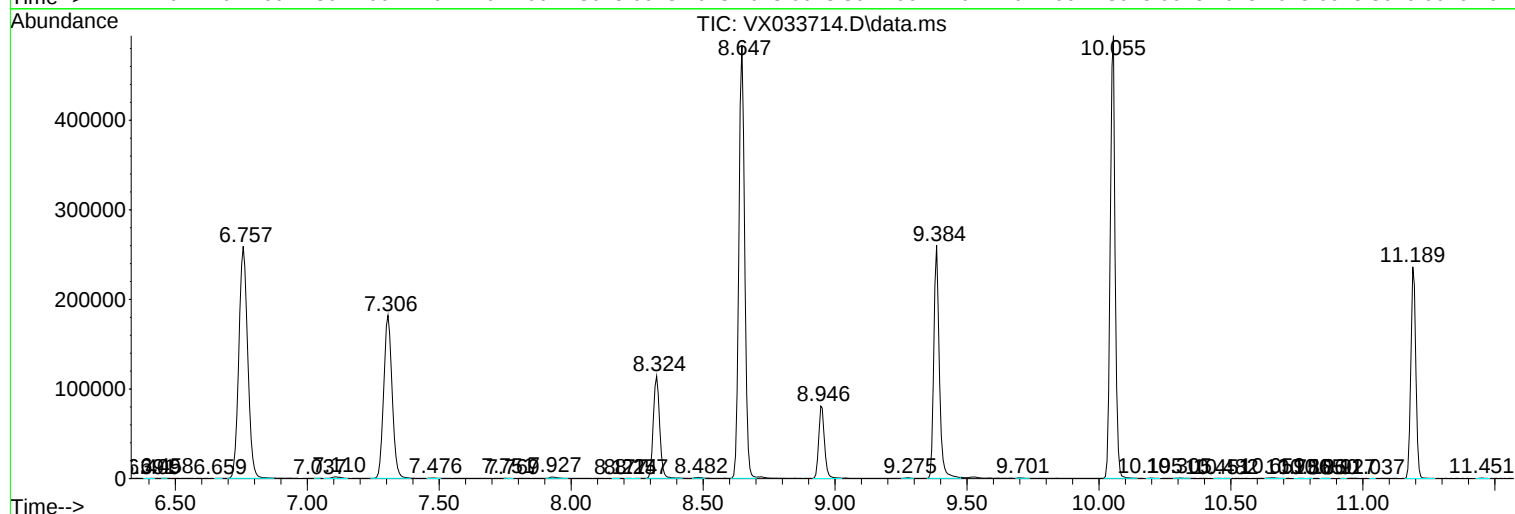
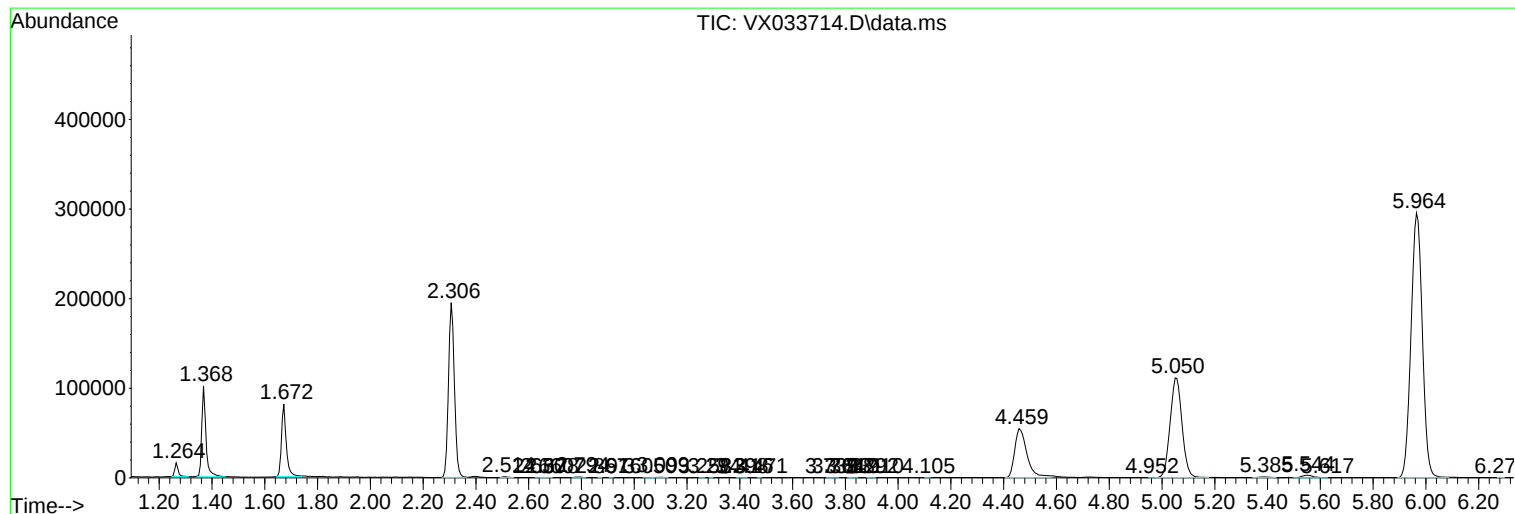
Sum of corrected areas: 6345525

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122722WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX011323\  
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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML122722WMA.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 |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|