

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX111221\  
 Data File : VX025143.D  
 Acq On : 12 Nov 2021 10:09  
 Operator : JC/MD  
 Sample : VX1112WBL01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK637

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\SFAMXLM11121WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025143.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         | 1.368       | 42            | 46          | 52           | rBV      | 102558         | 103495        | 15.11%          | 1.869%        |
| 2         | 1.672       | 92            | 96          | 108          | rVB      | 71618          | 92448         | 13.50%          | 1.669%        |
| 3         | 2.306       | 194           | 200         | 213          | rVB      | 144919         | 238759        | 34.86%          | 4.312%        |
| 4         | 2.483       | 227           | 229         | 230          | rBV2     | 573            | 493           | 0.07%           | 0.009%        |
| 5         | 3.221       | 348           | 350         | 354          | rBV3     | 235            | 298           | 0.04%           | 0.005%        |
| 6         | 3.629       | 415           | 417         | 421          | rBV2     | 300            | 474           | 0.07%           | 0.009%        |
| 7         | 3.678       | 423           | 425         | 427          | rBV2     | 356            | 437           | 0.06%           | 0.008%        |
| 8         | 4.038       | 482           | 484         | 487          | rVB3     | 289            | 320           | 0.05%           | 0.006%        |
| 9         | 4.074       | 487           | 490         | 494          | rBV3     | 418            | 684           | 0.10%           | 0.012%        |
| 10        | 4.465       | 545           | 554         | 568          | rVV      | 56785          | 166721        | 24.34%          | 3.011%        |
| 11        | 4.745       | 599           | 600         | 603          | rBV2     | 321            | 262           | 0.04%           | 0.005%        |
| 12        | 4.782       | 603           | 606         | 608          | rVV3     | 360            | 446           | 0.07%           | 0.008%        |
| 13        | 4.824       | 611           | 613         | 616          | rBV3     | 191            | 275           | 0.04%           | 0.005%        |
| 14        | 4.867       | 618           | 620         | 624          | rVV3     | 373            | 519           | 0.08%           | 0.009%        |
| 15        | 4.916       | 624           | 628         | 630          | rVB3     | 440            | 530           | 0.08%           | 0.010%        |
| 16        | 5.062       | 640           | 652         | 668          | rBV2     | 85942          | 264852        | 38.67%          | 4.783%        |
| 17        | 5.214       | 676           | 677         | 680          | rBV3     | 323            | 393           | 0.06%           | 0.007%        |
| 18        | 5.300       | 690           | 691         | 693          | rVB2     | 344            | 232           | 0.03%           | 0.004%        |
| 19        | 5.324       | 693           | 695         | 698          | rBV3     | 295            | 363           | 0.05%           | 0.007%        |
| 20        | 5.385       | 698           | 705         | 708          | rBV5     | 796            | 1671          | 0.24%           | 0.030%        |
| 21        | 5.489       | 720           | 722         | 724          | rVB2     | 329            | 284           | 0.04%           | 0.005%        |
| 22        | 5.611       | 740           | 742         | 744          | rBV3     | 368            | 287           | 0.04%           | 0.005%        |
| 23        | 5.672       | 749           | 752         | 753          | rBV2     | 448            | 351           | 0.05%           | 0.006%        |
| 24        | 5.726       | 758           | 761         | 762          | rVB2     | 309            | 277           | 0.04%           | 0.005%        |
| 25        | 5.757       | 762           | 766         | 767          | rBV3     | 355            | 481           | 0.07%           | 0.009%        |
| 26        | 5.861       | 781           | 783         | 787          | rVB3     | 501            | 548           | 0.08%           | 0.010%        |
| 27        | 5.897       | 787           | 789         | 790          | rBV2     | 474            | 385           | 0.06%           | 0.007%        |
| 28        | 5.976       | 790           | 802         | 819          | rVV2     | 230099         | 684976        | 100.00%         | 12.370%       |
| 29        | 6.159       | 830           | 832         | 834          | rVB      | 511            | 323           | 0.05%           | 0.006%        |
| 30        | 6.208       | 837           | 840         | 842          | rBV4     | 386            | 297           | 0.04%           | 0.005%        |
| 31        | 6.458       | 878           | 881         | 882          | rBV3     | 435            | 521           | 0.08%           | 0.009%        |
| 32        | 6.525       | 889           | 892         | 893          | rBV2     | 395            | 334           | 0.05%           | 0.006%        |
| 33        | 6.635       | 908           | 910         | 912          | rVB3     | 491            | 364           | 0.05%           | 0.007%        |
| 34        | 6.671       | 912           | 916         | 917          | rBV3     | 365            | 354           | 0.05%           | 0.006%        |
| 35        | 6.763       | 922           | 931         | 945          | rVV      | 182558         | 439245        | 64.13%          | 7.932%        |
| 36        | 6.982       | 966           | 967         | 970          | rVB3     | 303            | 256           | 0.04%           | 0.005%        |

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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\SFAMXLM11121WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.110  | 981  | 988  | 996  | rVV7 | 2724   | 7058   | 1.03%  | 0.127%  |
| 38 | 7.312  | 1012 | 1021 | 1035 | rBV  | 141861 | 310021 | 45.26% | 5.598%  |
| 39 | 7.476  | 1043 | 1048 | 1052 | rBV4 | 745    | 1360   | 0.20%  | 0.025%  |
| 40 | 7.702  | 1081 | 1085 | 1087 | rVV4 | 247    | 275    | 0.04%  | 0.005%  |
| 41 | 7.726  | 1087 | 1089 | 1091 | rVB3 | 437    | 375    | 0.05%  | 0.007%  |
| 42 | 7.757  | 1091 | 1094 | 1097 | rBV2 | 303    | 423    | 0.06%  | 0.008%  |
| 43 | 7.872  | 1111 | 1113 | 1115 | rVB  | 301    | 268    | 0.04%  | 0.005%  |
| 44 | 7.927  | 1118 | 1122 | 1126 | rVV2 | 787    | 1213   | 0.18%  | 0.022%  |
| 45 | 8.007  | 1134 | 1135 | 1138 | rBV  | 366    | 229    | 0.03%  | 0.004%  |
| 46 | 8.324  | 1181 | 1187 | 1198 | rBV  | 110139 | 182529 | 26.65% | 3.296%  |
| 47 | 8.653  | 1234 | 1241 | 1248 | rBV  | 367924 | 587708 | 85.80% | 10.613% |
| 48 | 8.720  | 1249 | 1252 | 1256 | rVB  | 5155   | 7706   | 1.13%  | 0.139%  |
| 49 | 8.830  | 1268 | 1270 | 1271 | rBV  | 262    | 225    | 0.03%  | 0.004%  |
| 50 | 8.952  | 1284 | 1290 | 1302 | rBV  | 83436  | 120672 | 17.62% | 2.179%  |
| 51 | 9.238  | 1333 | 1337 | 1339 | rVB4 | 384    | 547    | 0.08%  | 0.010%  |
| 52 | 9.275  | 1339 | 1343 | 1347 | rBV6 | 475    | 737    | 0.11%  | 0.013%  |
| 53 | 9.384  | 1356 | 1361 | 1374 | rBV  | 271646 | 380942 | 55.61% | 6.879%  |
| 54 | 9.616  | 1397 | 1399 | 1404 | rVB3 | 455    | 543    | 0.08%  | 0.010%  |
| 55 | 9.659  | 1404 | 1406 | 1411 | rBV5 | 403    | 668    | 0.10%  | 0.012%  |
| 56 | 9.750  | 1419 | 1421 | 1427 | rVB4 | 323    | 409    | 0.06%  | 0.007%  |
| 57 | 9.957  | 1451 | 1455 | 1457 | rBV4 | 201    | 245    | 0.04%  | 0.004%  |
| 58 | 9.988  | 1457 | 1460 | 1461 | rBV3 | 345    | 252    | 0.04%  | 0.005%  |
| 59 | 10.055 | 1465 | 1471 | 1481 | rBV  | 389753 | 519578 | 75.85% | 9.383%  |
| 60 | 10.201 | 1491 | 1495 | 1498 | rVB3 | 734    | 1204   | 0.18%  | 0.022%  |
| 61 | 10.238 | 1498 | 1501 | 1503 | rBV3 | 311    | 340    | 0.05%  | 0.006%  |
| 62 | 10.305 | 1508 | 1512 | 1517 | rVV3 | 1243   | 2050   | 0.30%  | 0.037%  |
| 63 | 10.585 | 1556 | 1558 | 1562 | rVB2 | 417    | 369    | 0.05%  | 0.007%  |
| 64 | 10.652 | 1562 | 1569 | 1574 | rBV7 | 974    | 1977   | 0.29%  | 0.036%  |
| 65 | 10.744 | 1582 | 1584 | 1585 | rBV2 | 463    | 415    | 0.06%  | 0.007%  |
| 66 | 10.939 | 1614 | 1616 | 1617 | rBV  | 364    | 318    | 0.05%  | 0.006%  |
| 67 | 10.963 | 1618 | 1620 | 1625 | rVB4 | 631    | 838    | 0.12%  | 0.015%  |
| 68 | 11.079 | 1636 | 1639 | 1640 | rBV3 | 417    | 458    | 0.07%  | 0.008%  |
| 69 | 11.122 | 1643 | 1646 | 1649 | rVV  | 2595   | 2935   | 0.43%  | 0.053%  |
| 70 | 11.195 | 1652 | 1658 | 1666 | rBV  | 269934 | 342415 | 49.99% | 6.183%  |
| 71 | 11.457 | 1694 | 1701 | 1703 | rBV2 | 886    | 1385   | 0.20%  | 0.025%  |
| 72 | 11.579 | 1719 | 1721 | 1724 | rBV4 | 341    | 382    | 0.06%  | 0.007%  |
| 73 | 11.713 | 1741 | 1743 | 1745 | rBV3 | 411    | 394    | 0.06%  | 0.007%  |
| 74 | 11.750 | 1745 | 1749 | 1753 | rVB3 | 2746   | 3664   | 0.53%  | 0.066%  |
| 75 | 11.933 | 1775 | 1779 | 1783 | rBV3 | 1198   | 1534   | 0.22%  | 0.028%  |
| 76 | 11.969 | 1783 | 1785 | 1789 | rBV3 | 1006   | 1007   | 0.15%  | 0.018%  |

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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\SFAMXML111121WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.024 | 1789 | 1794 | 1805 | rVB  | 412828 | 516615 | 75.42% | 9.329% |
| 78  | 12.103 | 1805 | 1807 | 1808 | rBV2 | 390    | 314    | 0.05%  | 0.006% |
| 79  | 12.152 | 1813 | 1815 | 1819 | rVB2 | 1379   | 1455   | 0.21%  | 0.026% |
| 80  | 12.323 | 1836 | 1843 | 1851 | rBV  | 414868 | 517348 | 75.53% | 9.342% |
|     |        |      |      |      |      |        |        |        |        |
| 81  | 12.433 | 1856 | 1861 | 1865 | rBV4 | 809    | 1264   | 0.18%  | 0.023% |
| 82  | 12.536 | 1876 | 1878 | 1880 | rVB3 | 385    | 271    | 0.04%  | 0.005% |
| 83  | 12.609 | 1889 | 1890 | 1892 | rBV  | 443    | 371    | 0.05%  | 0.007% |
| 84  | 12.670 | 1896 | 1900 | 1903 | rVV3 | 545    | 771    | 0.11%  | 0.014% |
| 85  | 12.859 | 1927 | 1931 | 1935 | rBV3 | 773    | 1015   | 0.15%  | 0.018% |
|     |        |      |      |      |      |        |        |        |        |
| 86  | 13.115 | 1970 | 1973 | 1978 | rVB4 | 841    | 1385   | 0.20%  | 0.025% |
| 87  | 13.237 | 1991 | 1993 | 1996 | rBV4 | 364    | 439    | 0.06%  | 0.008% |
| 88  | 13.280 | 1998 | 2000 | 2003 | rVV4 | 198    | 281    | 0.04%  | 0.005% |
| 89  | 13.347 | 2009 | 2011 | 2014 | rVB3 | 322    | 255    | 0.04%  | 0.005% |
| 90  | 13.597 | 2048 | 2052 | 2054 | rBV2 | 1155   | 1279   | 0.19%  | 0.023% |
|     |        |      |      |      |      |        |        |        |        |
| 91  | 13.780 | 2080 | 2082 | 2089 | rVB  | 809    | 1068   | 0.16%  | 0.019% |
| 92  | 13.963 | 2109 | 2112 | 2115 | rVB3 | 663    | 992    | 0.14%  | 0.018% |
| 93  | 13.999 | 2115 | 2118 | 2122 | rVB3 | 260    | 365    | 0.05%  | 0.007% |
| 94  | 14.127 | 2137 | 2139 | 2141 | rVB2 | 361    | 263    | 0.04%  | 0.005% |
| 95  | 14.164 | 2141 | 2145 | 2148 | rBV4 | 337    | 507    | 0.07%  | 0.009% |
|     |        |      |      |      |      |        |        |        |        |
| 96  | 14.688 | 2230 | 2231 | 2234 | rBV2 | 242    | 252    | 0.04%  | 0.005% |
| 97  | 14.975 | 2276 | 2278 | 2281 | rBV3 | 428    | 469    | 0.07%  | 0.008% |
| 98  | 15.072 | 2292 | 2294 | 2297 | rBV4 | 439    | 622    | 0.09%  | 0.011% |
| 99  | 16.194 | 2476 | 2478 | 2485 | rVB5 | 534    | 836    | 0.12%  | 0.015% |
| 100 | 16.603 | 2543 | 2545 | 2548 | rBV4 | 474    | 523    | 0.08%  | 0.009% |

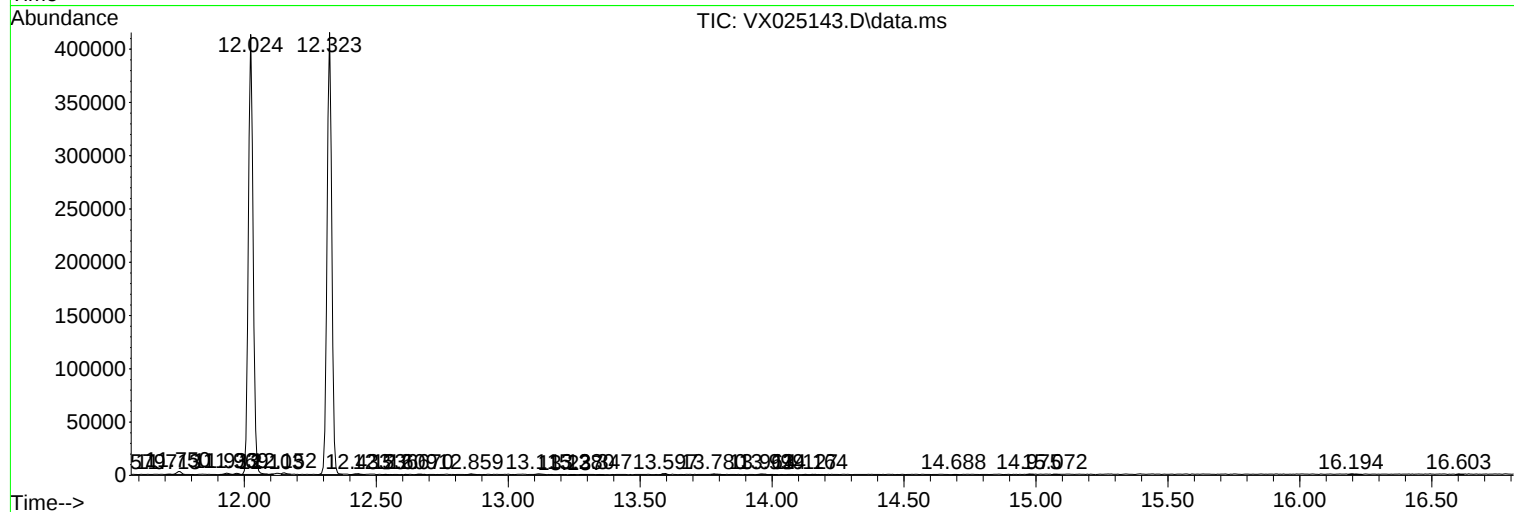
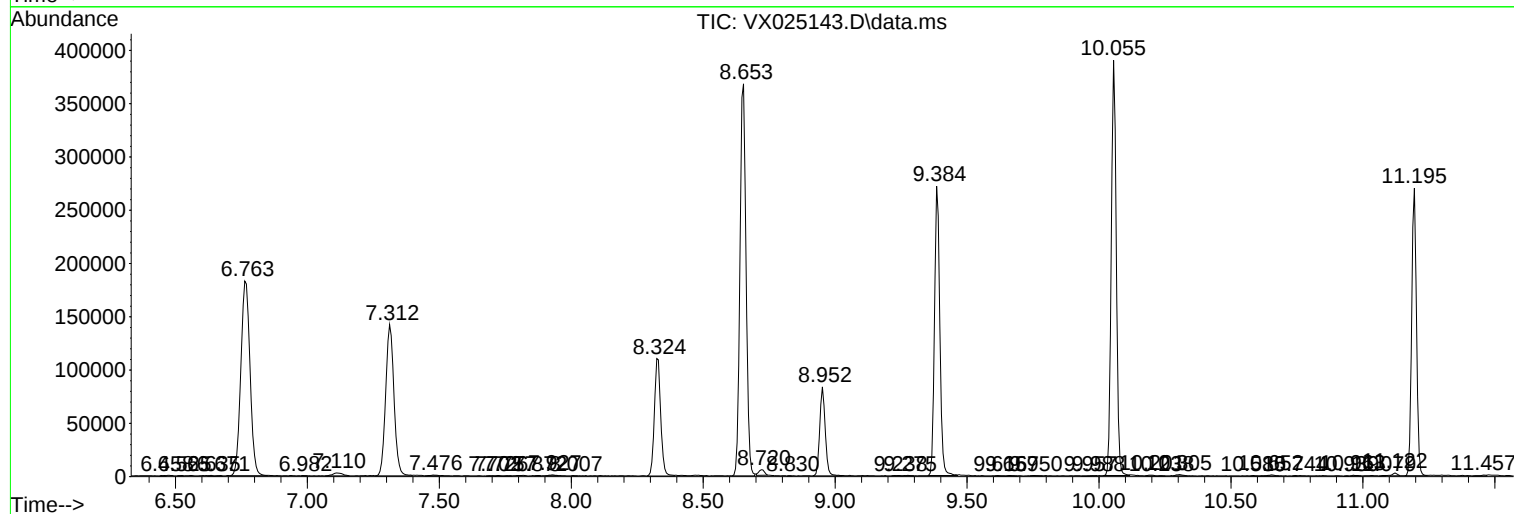
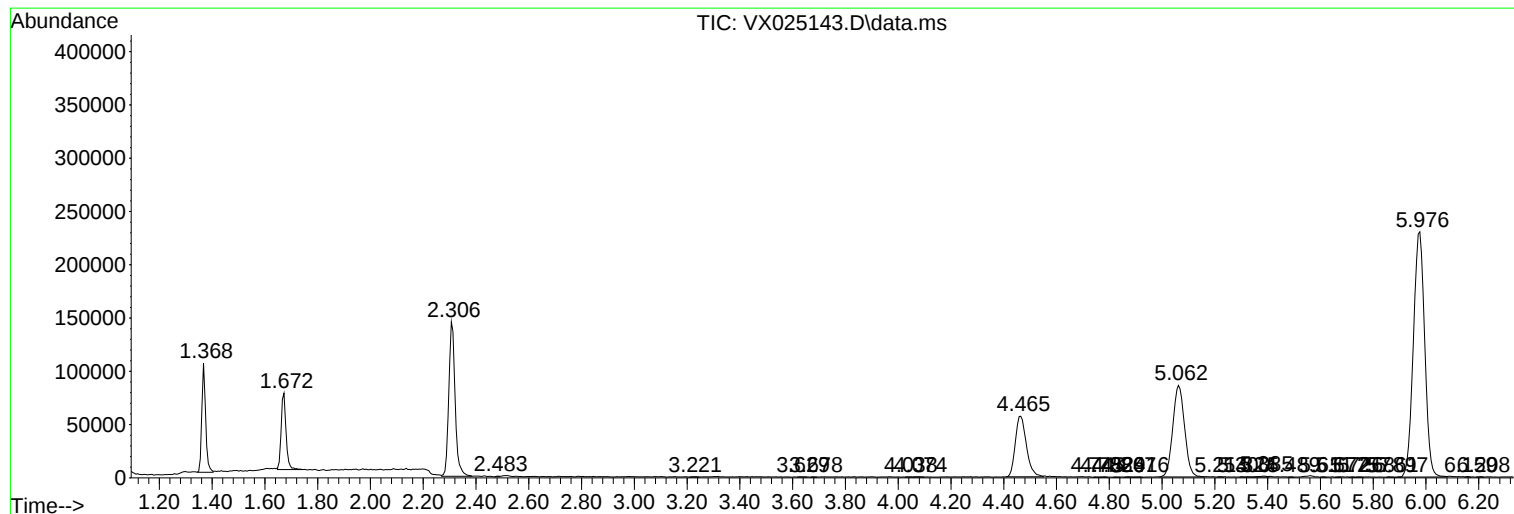
Sum of corrected areas: 5537583

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM111121WMA.M  
Quant Title : VOC Analysis

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



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No Library Search Compounds Detected

\*\*\*\*\*

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