

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121021\  
 Data File : VX025706.D  
 Acq On : 10 Dec 2021 17:01  
 Operator : JC/MD  
 Sample : M4888-20ME  
 Misc : 5.84g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX8C5ME

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: VX025706.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       | 43            | 46          | 52           | rVB      | 43116          | 50175         | 12.52%          | 1.517%        |
| 2         | 1.648       | 89            | 92          | 99           | rVB      | 31209          | 39064         | 9.75%           | 1.181%        |
| 3         | 2.276       | 189           | 195         | 207          | rBV      | 83576          | 141435        | 35.29%          | 4.277%        |
| 4         | 2.654       | 256           | 257         | 258          | rBV      | 493            | 232           | 0.06%           | 0.007%        |
| 5         | 2.946       | 301           | 305         | 317          | rVB2     | 3727           | 9243          | 2.31%           | 0.280%        |
| 6         | 3.550       | 402           | 404         | 405          | rBV      | 354            | 234           | 0.06%           | 0.007%        |
| 7         | 3.605       | 410           | 413         | 416          | rBV2     | 333            | 573           | 0.14%           | 0.017%        |
| 8         | 3.702       | 428           | 429         | 432          | rBV      | 483            | 398           | 0.10%           | 0.012%        |
| 9         | 3.757       | 437           | 438         | 440          | rBV      | 366            | 255           | 0.06%           | 0.008%        |
| 10        | 3.782       | 440           | 442         | 444          | rBV2     | 406            | 292           | 0.07%           | 0.009%        |
| 11        | 3.867       | 454           | 456         | 458          | rBV      | 424            | 410           | 0.10%           | 0.012%        |
| 12        | 3.910       | 461           | 463         | 464          | rBV      | 370            | 308           | 0.08%           | 0.009%        |
| 13        | 4.501       | 550           | 560         | 581          | rBV      | 16609          | 76274         | 19.03%          | 2.307%        |
| 14        | 4.983       | 638           | 639         | 641          | rBV      | 483            | 316           | 0.08%           | 0.010%        |
| 15        | 5.068       | 641           | 653         | 669          | rVV      | 47890          | 162679        | 40.59%          | 4.920%        |
| 16        | 5.745       | 762           | 764         | 766          | rBV2     | 332            | 307           | 0.08%           | 0.009%        |
| 17        | 5.970       | 789           | 801         | 817          | rBV2     | 139521         | 400809        | 100.00%         | 12.121%       |
| 18        | 6.281       | 850           | 852         | 856          | rBV      | 308            | 311           | 0.08%           | 0.009%        |
| 19        | 6.379       | 860           | 868         | 872          | rBV6     | 1871           | 5502          | 1.37%           | 0.166%        |
| 20        | 6.458       | 879           | 881         | 886          | rVB      | 295            | 322           | 0.08%           | 0.010%        |
| 21        | 6.598       | 902           | 904         | 905          | rBV      | 495            | 339           | 0.08%           | 0.010%        |
| 22        | 6.763       | 922           | 931         | 945          | rBV      | 99191          | 256762        | 64.06%          | 7.765%        |
| 23        | 7.031       | 972           | 975         | 978          | rVB      | 358            | 444           | 0.11%           | 0.013%        |
| 24        | 7.129       | 982           | 991         | 1002         | rBV      | 38224          | 89193         | 22.25%          | 2.697%        |
| 25        | 7.311       | 1013          | 1021        | 1040         | rVB      | 74749          | 177968        | 44.40%          | 5.382%        |
| 26        | 7.433       | 1040          | 1041        | 1044         | rBV      | 408            | 303           | 0.08%           | 0.009%        |
| 27        | 7.561       | 1061          | 1062        | 1065         | rVV2     | 480            | 473           | 0.12%           | 0.014%        |
| 28        | 7.592       | 1065          | 1067        | 1069         | rVV      | 298            | 286           | 0.07%           | 0.009%        |
| 29        | 7.635       | 1072          | 1074        | 1075         | rBV      | 427            | 323           | 0.08%           | 0.010%        |
| 30        | 7.708       | 1084          | 1086        | 1089         | rBV2     | 422            | 469           | 0.12%           | 0.014%        |
| 31        | 7.738       | 1089          | 1091        | 1093         | rVB      | 463            | 331           | 0.08%           | 0.010%        |
| 32        | 7.769       | 1093          | 1096        | 1097         | rBV2     | 342            | 376           | 0.09%           | 0.011%        |
| 33        | 7.958       | 1123          | 1127        | 1129         | rBV      | 888            | 1045          | 0.26%           | 0.032%        |
| 34        | 8.006       | 1134          | 1135        | 1137         | rVV      | 387            | 282           | 0.07%           | 0.009%        |
| 35        | 8.055       | 1141          | 1143        | 1147         | rVB      | 278            | 286           | 0.07%           | 0.009%        |
| 36        | 8.134       | 1154          | 1156        | 1159         | rVB      | 368            | 234           | 0.06%           | 0.007%        |

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 EX8C5ME

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Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 8.171  | 1160 | 1162 | 1166 | rVB  | 333    | 369    | 0.09%  | 0.011%  |
| 38 | 8.220  | 1168 | 1170 | 1172 | rBV  | 311    | 385    | 0.10%  | 0.012%  |
| 39 | 8.281  | 1175 | 1180 | 1182 | rBV  | 358    | 589    | 0.15%  | 0.018%  |
| 40 | 8.330  | 1182 | 1188 | 1198 | rBV  | 51344  | 90379  | 22.55% | 2.733%  |
| 41 | 8.537  | 1219 | 1222 | 1223 | rBV2 | 241    | 283    | 0.07%  | 0.009%  |
| 42 | 8.592  | 1229 | 1231 | 1234 | rBV  | 421    | 362    | 0.09%  | 0.011%  |
| 43 | 8.653  | 1234 | 1241 | 1249 | rBV  | 205697 | 331778 | 82.78% | 10.033% |
| 44 | 8.726  | 1249 | 1253 | 1256 | rVB2 | 2371   | 3704   | 0.92%  | 0.112%  |
| 45 | 8.805  | 1263 | 1266 | 1269 | rBV2 | 313    | 434    | 0.11%  | 0.013%  |
| 46 | 8.957  | 1285 | 1291 | 1300 | rBV  | 32514  | 54932  | 13.71% | 1.661%  |
| 47 | 9.025  | 1300 | 1302 | 1305 | rVB3 | 315    | 273    | 0.07%  | 0.008%  |
| 48 | 9.116  | 1314 | 1317 | 1321 | rBV2 | 322    | 534    | 0.13%  | 0.016%  |
| 49 | 9.275  | 1337 | 1343 | 1351 | rBV  | 104197 | 148404 | 37.03% | 4.488%  |
| 50 | 9.403  | 1357 | 1364 | 1377 | rBV  | 98197  | 167775 | 41.86% | 5.074%  |
| 51 | 9.555  | 1387 | 1389 | 1390 | rBV  | 274    | 243    | 0.06%  | 0.007%  |
| 52 | 9.573  | 1390 | 1392 | 1397 | rVB2 | 453    | 432    | 0.11%  | 0.013%  |
| 53 | 9.616  | 1397 | 1399 | 1404 | rVB3 | 681    | 812    | 0.20%  | 0.025%  |
| 54 | 9.659  | 1404 | 1406 | 1409 | rVB  | 346    | 329    | 0.08%  | 0.010%  |
| 55 | 9.683  | 1409 | 1410 | 1412 | rBV  | 295    | 289    | 0.07%  | 0.009%  |
| 56 | 9.762  | 1420 | 1423 | 1426 | rBV2 | 392    | 646    | 0.16%  | 0.020%  |
| 57 | 10.061 | 1466 | 1472 | 1481 | rVV  | 203689 | 300875 | 75.07% | 9.099%  |
| 58 | 10.207 | 1494 | 1496 | 1498 | rVB  | 457    | 326    | 0.08%  | 0.010%  |
| 59 | 10.299 | 1509 | 1511 | 1513 | rBV2 | 442    | 462    | 0.12%  | 0.014%  |
| 60 | 10.616 | 1562 | 1563 | 1566 | rVV2 | 376    | 306    | 0.08%  | 0.009%  |
| 61 | 10.646 | 1566 | 1568 | 1573 | rVB3 | 565    | 877    | 0.22%  | 0.027%  |
| 62 | 10.707 | 1573 | 1578 | 1579 | rBV  | 352    | 525    | 0.13%  | 0.016%  |
| 63 | 10.756 | 1583 | 1586 | 1588 | rBV  | 462    | 379    | 0.09%  | 0.011%  |
| 64 | 10.896 | 1607 | 1609 | 1613 | rBV3 | 359    | 504    | 0.13%  | 0.015%  |
| 65 | 10.933 | 1613 | 1615 | 1616 | rBV  | 284    | 242    | 0.06%  | 0.007%  |
| 66 | 11.122 | 1642 | 1646 | 1649 | rBV3 | 1767   | 2517   | 0.63%  | 0.076%  |
| 67 | 11.201 | 1653 | 1659 | 1669 | rVB  | 141012 | 185282 | 46.23% | 5.603%  |
| 68 | 11.268 | 1669 | 1670 | 1671 | rBV  | 633    | 403    | 0.10%  | 0.012%  |
| 69 | 11.439 | 1695 | 1698 | 1699 | rBV  | 321    | 257    | 0.06%  | 0.008%  |
| 70 | 11.512 | 1708 | 1710 | 1713 | rBV2 | 418    | 410    | 0.10%  | 0.012%  |
| 71 | 11.591 | 1718 | 1723 | 1724 | rBV2 | 208    | 364    | 0.09%  | 0.011%  |
| 72 | 11.609 | 1724 | 1726 | 1730 | rVB2 | 419    | 353    | 0.09%  | 0.011%  |
| 73 | 11.713 | 1741 | 1743 | 1746 | rBV2 | 413    | 563    | 0.14%  | 0.017%  |
| 74 | 11.750 | 1746 | 1749 | 1754 | rVB3 | 1964   | 2536   | 0.63%  | 0.077%  |
| 75 | 12.024 | 1789 | 1794 | 1801 | rBV  | 231729 | 293420 | 73.21% | 8.873%  |
| 76 | 12.280 | 1834 | 1836 | 1837 | rBV  | 431    | 284    | 0.07%  | 0.009%  |

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Integration Parameters: LSCINT.P

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Peak Location: TOP

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Peak separation: 5

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

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.323 | 1838 | 1843 | 1850 | rVB  | 219790 | 283913 | 70.83% | 8.586% |
| 78  | 12.426 | 1857 | 1860 | 1863 | rVB2 | 1353   | 1649   | 0.41%  | 0.050% |
| 79  | 12.457 | 1863 | 1865 | 1867 | rBV2 | 290    | 302    | 0.08%  | 0.009% |
| 80  | 12.859 | 1930 | 1931 | 1935 | rVB  | 355    | 267    | 0.07%  | 0.008% |
| 81  | 12.902 | 1936 | 1938 | 1940 | rBV  | 416    | 320    | 0.08%  | 0.010% |
| 82  | 13.694 | 2067 | 2068 | 2071 | rVB  | 337    | 246    | 0.06%  | 0.007% |
| 83  | 13.957 | 2108 | 2111 | 2113 | rVB  | 394    | 444    | 0.11%  | 0.013% |
| 84  | 14.042 | 2122 | 2125 | 2127 | rVB3 | 633    | 641    | 0.16%  | 0.019% |
| 85  | 14.133 | 2138 | 2140 | 2144 | rVB2 | 600    | 671    | 0.17%  | 0.020% |
| 86  | 14.676 | 2227 | 2229 | 2230 | rBV  | 351    | 297    | 0.07%  | 0.009% |
| 87  | 14.725 | 2234 | 2237 | 2239 | rBV2 | 367    | 508    | 0.13%  | 0.015% |
| 88  | 14.755 | 2239 | 2242 | 2245 | rBV4 | 621    | 947    | 0.24%  | 0.029% |
| 89  | 14.975 | 2276 | 2278 | 2279 | rVB  | 487    | 243    | 0.06%  | 0.007% |
| 90  | 15.078 | 2294 | 2295 | 2298 | rBV3 | 281    | 366    | 0.09%  | 0.011% |
| 91  | 15.133 | 2302 | 2304 | 2308 | rBV  | 367    | 661    | 0.16%  | 0.020% |
| 92  | 15.212 | 2315 | 2317 | 2320 | rVB2 | 445    | 506    | 0.13%  | 0.015% |
| 93  | 15.487 | 2360 | 2362 | 2365 | rVB3 | 576    | 465    | 0.12%  | 0.014% |
| 94  | 15.597 | 2379 | 2380 | 2383 | rBV  | 407    | 290    | 0.07%  | 0.009% |
| 95  | 15.792 | 2411 | 2412 | 2415 | rVB2 | 376    | 257    | 0.06%  | 0.008% |
| 96  | 16.200 | 2477 | 2479 | 2481 | rBV  | 383    | 297    | 0.07%  | 0.009% |
| 97  | 16.224 | 2481 | 2483 | 2485 | rVB  | 451    | 391    | 0.10%  | 0.012% |
| 98  | 16.566 | 2537 | 2539 | 2542 | rBV  | 316    | 268    | 0.07%  | 0.008% |
| 99  | 16.615 | 2545 | 2547 | 2548 | rBV  | 427    | 408    | 0.10%  | 0.012% |
| 100 | 16.688 | 2557 | 2559 | 2560 | rBV  | 382    | 258    | 0.06%  | 0.008% |

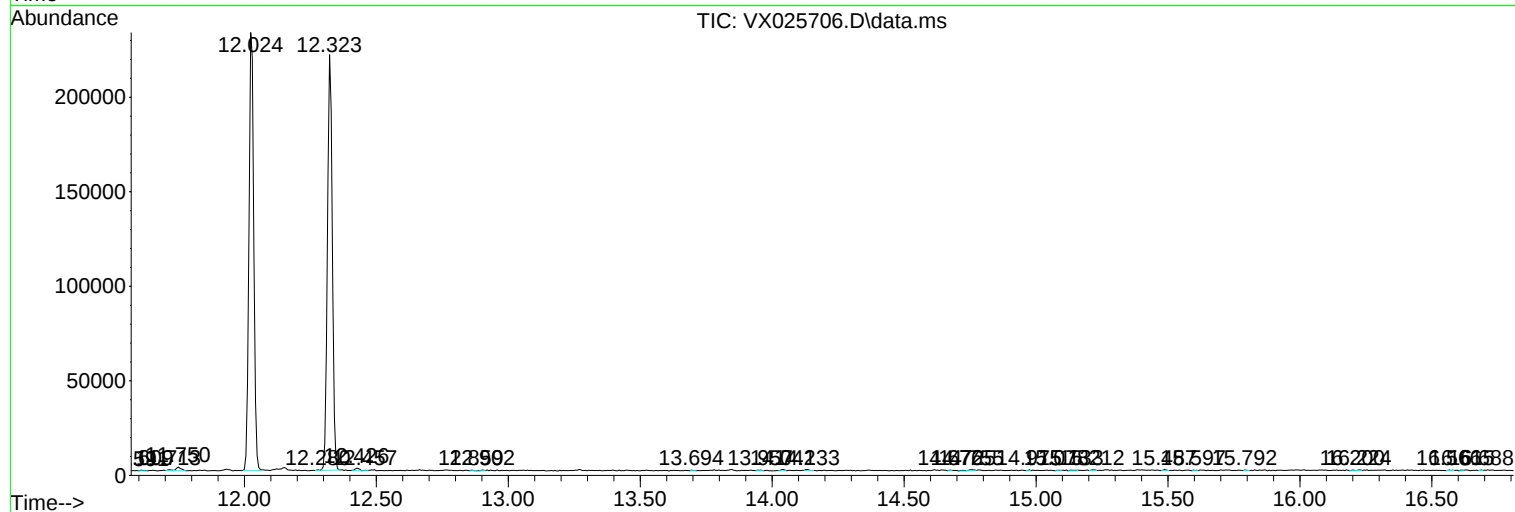
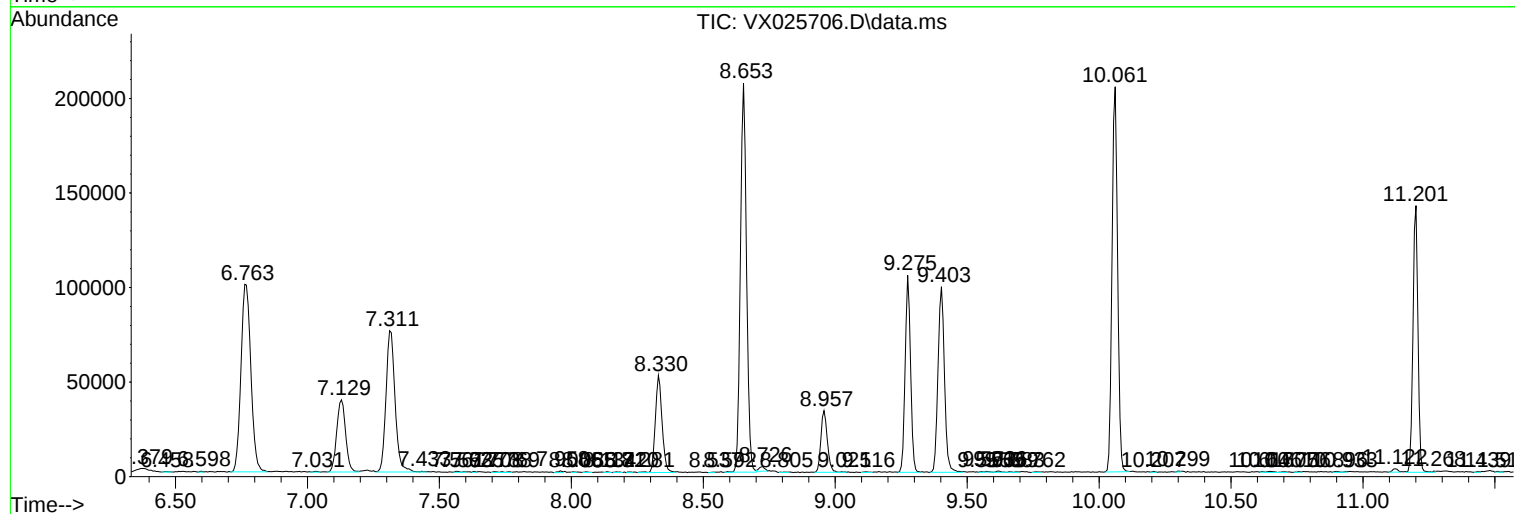
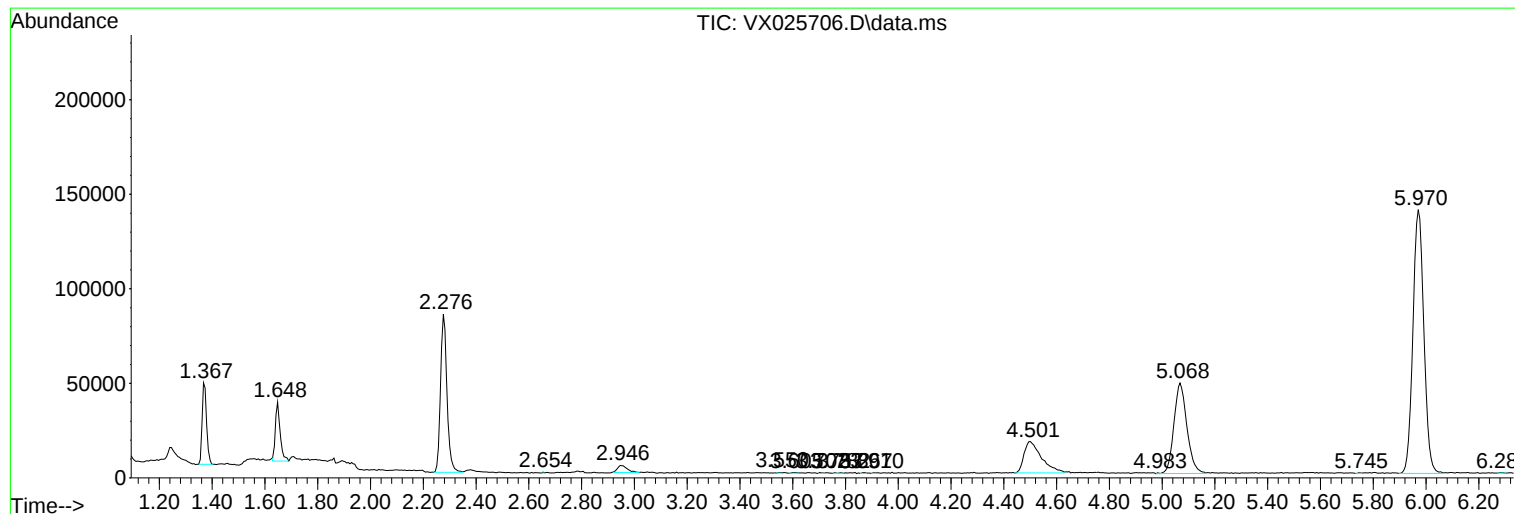
Sum of corrected areas: 3306705

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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



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