

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120721\  
 Data File : VX025575.D  
 Acq On : 07 Dec 2021 13:34  
 Operator : JC/MD  
 Sample : M4881-14ME  
 Misc : 4.40g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EW9F0ME

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: VX025575.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         | 1.246       | 22            | 26          | 33           | rBV2     | 3698           | 8735          | 1.60%           | 0.202%        |
| 2         | 1.368       | 42            | 46          | 53           | rVB      | 58311          | 64811         | 11.86%          | 1.502%        |
| 3         | 1.648       | 70            | 92          | 97           | rBV      | 41280          | 85360         | 15.62%          | 1.978%        |
| 4         | 2.282       | 190           | 196         | 205          | rBV      | 115047         | 183392        | 33.56%          | 4.250%        |
| 5         | 2.953       | 298           | 306         | 314          | rBV      | 4031           | 10257         | 1.88%           | 0.238%        |
| 6         | 3.422       | 379           | 383         | 388          | rVB3     | 664            | 1210          | 0.22%           | 0.028%        |
| 7         | 4.282       | 518           | 524         | 525          | rBV3     | 261            | 532           | 0.10%           | 0.012%        |
| 8         | 4.489       | 547           | 558         | 586          | rBV2     | 25429          | 116930        | 21.40%          | 2.710%        |
| 9         | 5.068       | 640           | 653         | 673          | rBV      | 68969          | 221347        | 40.50%          | 5.130%        |
| 10        | 5.452       | 712           | 716         | 727          | rVB6     | 879            | 2601          | 0.48%           | 0.060%        |
| 11        | 5.611       | 740           | 742         | 746          | rVB3     | 259            | 291           | 0.05%           | 0.007%        |
| 12        | 5.971       | 789           | 801         | 817          | rVV2     | 189233         | 546491        | 100.00%         | 12.665%       |
| 13        | 6.153       | 829           | 831         | 834          | rVB2     | 256            | 285           | 0.05%           | 0.007%        |
| 14        | 6.367       | 858           | 866         | 878          | rVB6     | 2077           | 7159          | 1.31%           | 0.166%        |
| 15        | 6.763       | 921           | 931         | 946          | rBV      | 117948         | 300320        | 54.95%          | 6.960%        |
| 16        | 6.983       | 964           | 967         | 972          | rBV2     | 136            | 246           | 0.05%           | 0.006%        |
| 17        | 7.129       | 982           | 991         | 1000         | rBV      | 38777          | 90415         | 16.54%          | 2.095%        |
| 18        | 7.312       | 1012          | 1021        | 1030         | rBV      | 107023         | 249290        | 45.62%          | 5.777%        |
| 19        | 7.495       | 1047          | 1051        | 1052         | rVV2     | 347            | 381           | 0.07%           | 0.009%        |
| 20        | 7.775       | 1093          | 1097        | 1100         | rVB2     | 303            | 409           | 0.07%           | 0.009%        |
| 21        | 7.952       | 1121          | 1126        | 1127         | rBV3     | 501            | 528           | 0.10%           | 0.012%        |
| 22        | 8.275       | 1173          | 1179        | 1181         | rBV4     | 381            | 702           | 0.13%           | 0.016%        |
| 23        | 8.330       | 1181          | 1188        | 1203         | rVB      | 59065          | 106313        | 19.45%          | 2.464%        |
| 24        | 8.440       | 1203          | 1206        | 1208         | rBV2     | 275            | 270           | 0.05%           | 0.006%        |
| 25        | 8.598       | 1226          | 1232        | 1233         | rBV4     | 1164           | 1454          | 0.27%           | 0.034%        |
| 26        | 8.653       | 1234          | 1241        | 1249         | rVV      | 273093         | 453615        | 83.01%          | 10.513%       |
| 27        | 8.720       | 1249          | 1252        | 1256         | rVB      | 4566           | 6405          | 1.17%           | 0.148%        |
| 28        | 8.909       | 1280          | 1283        | 1285         | rVV2     | 536            | 603           | 0.11%           | 0.014%        |
| 29        | 8.958       | 1285          | 1291        | 1301         | rVV      | 39513          | 68201         | 12.48%          | 1.581%        |
| 30        | 9.275       | 1341          | 1343        | 1346         | rBV      | 383            | 416           | 0.08%           | 0.010%        |
| 31        | 9.397       | 1357          | 1363        | 1374         | rBV      | 156406         | 254174        | 46.51%          | 5.891%        |
| 32        | 9.561       | 1386          | 1390        | 1394         | rVB3     | 931            | 1466          | 0.27%           | 0.034%        |
| 33        | 9.622       | 1394          | 1400        | 1404         | rBV      | 1153           | 1803          | 0.33%           | 0.042%        |
| 34        | 9.714       | 1411          | 1415        | 1418         | rVB2     | 497            | 669           | 0.12%           | 0.016%        |
| 35        | 9.824       | 1428          | 1433        | 1437         | rVB2     | 936            | 1176          | 0.22%           | 0.027%        |
| 36        | 9.915       | 1445          | 1448        | 1451         | rVB2     | 327            | 329           | 0.06%           | 0.008%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 10.055 | 1466 | 1471 | 1480 | rVV  | 236234 | 353848 | 64.75% | 8.201% |
| 38 | 10.201 | 1492 | 1495 | 1499 | rVB2 | 507    | 685    | 0.13%  | 0.016% |
| 39 | 10.305 | 1508 | 1512 | 1517 | rVV  | 2821   | 3914   | 0.72%  | 0.091% |
| 40 | 10.360 | 1517 | 1521 | 1524 | rVB3 | 1086   | 1335   | 0.24%  | 0.031% |
| 41 | 10.494 | 1540 | 1543 | 1549 | rVB2 | 136    | 223    | 0.04%  | 0.005% |
| 42 | 10.586 | 1556 | 1558 | 1561 | rVV2 | 361    | 403    | 0.07%  | 0.009% |
| 43 | 10.653 | 1564 | 1569 | 1574 | rVB4 | 1830   | 2746   | 0.50%  | 0.064% |
| 44 | 10.781 | 1583 | 1590 | 1594 | rBV6 | 832    | 1636   | 0.30%  | 0.038% |
| 45 | 10.854 | 1598 | 1602 | 1605 | rBV3 | 553    | 744    | 0.14%  | 0.017% |
| 46 | 10.896 | 1605 | 1609 | 1612 | rVB2 | 1044   | 1289   | 0.24%  | 0.030% |
| 47 | 11.031 | 1624 | 1631 | 1634 | rBV3 | 368    | 571    | 0.10%  | 0.013% |
| 48 | 11.122 | 1642 | 1646 | 1653 | rVB2 | 2957   | 3668   | 0.67%  | 0.085% |
| 49 | 11.195 | 1653 | 1658 | 1667 | rBV  | 204896 | 267022 | 48.86% | 6.188% |
| 50 | 11.311 | 1673 | 1677 | 1683 | rVB5 | 888    | 1822   | 0.33%  | 0.042% |
| 51 | 11.384 | 1686 | 1689 | 1696 | rVB3 | 769    | 1275   | 0.23%  | 0.030% |
| 52 | 11.451 | 1697 | 1700 | 1701 | rBV2 | 644    | 475    | 0.09%  | 0.011% |
| 53 | 11.476 | 1701 | 1704 | 1708 | rVB3 | 2018   | 2617   | 0.48%  | 0.061% |
| 54 | 11.543 | 1713 | 1715 | 1718 | rVB3 | 455    | 546    | 0.10%  | 0.013% |
| 55 | 11.616 | 1724 | 1727 | 1736 | rVB5 | 492    | 861    | 0.16%  | 0.020% |
| 56 | 11.689 | 1736 | 1739 | 1741 | rBV2 | 330    | 481    | 0.09%  | 0.011% |
| 57 | 11.713 | 1741 | 1743 | 1746 | rVV2 | 2037   | 2328   | 0.43%  | 0.054% |
| 58 | 11.750 | 1746 | 1749 | 1757 | rVB2 | 4145   | 5597   | 1.02%  | 0.130% |
| 59 | 11.817 | 1757 | 1760 | 1762 | rBV2 | 245    | 300    | 0.05%  | 0.007% |
| 60 | 11.841 | 1762 | 1764 | 1768 | rVB2 | 588    | 593    | 0.11%  | 0.014% |
| 61 | 11.939 | 1776 | 1780 | 1784 | rBV3 | 1718   | 2368   | 0.43%  | 0.055% |
| 62 | 11.976 | 1784 | 1786 | 1789 | rBV3 | 235    | 310    | 0.06%  | 0.007% |
| 63 | 12.024 | 1789 | 1794 | 1800 | rBV  | 299258 | 362648 | 66.36% | 8.405% |
| 64 | 12.152 | 1813 | 1815 | 1823 | rVB  | 2321   | 2791   | 0.51%  | 0.065% |
| 65 | 12.323 | 1835 | 1843 | 1850 | rBV  | 343949 | 427095 | 78.15% | 9.898% |
| 66 | 12.427 | 1856 | 1860 | 1864 | rVB2 | 4122   | 4882   | 0.89%  | 0.113% |
| 67 | 12.475 | 1864 | 1868 | 1875 | rVV5 | 952    | 1399   | 0.26%  | 0.032% |
| 68 | 12.664 | 1896 | 1899 | 1902 | rBV4 | 544    | 748    | 0.14%  | 0.017% |
| 69 | 12.762 | 1911 | 1915 | 1920 | rVB3 | 436    | 759    | 0.14%  | 0.018% |
| 70 | 12.805 | 1920 | 1922 | 1923 | rBV  | 274    | 202    | 0.04%  | 0.005% |
| 71 | 12.890 | 1933 | 1936 | 1938 | rVV  | 305    | 372    | 0.07%  | 0.009% |
| 72 | 12.921 | 1938 | 1941 | 1944 | rVV2 | 286    | 375    | 0.07%  | 0.009% |
| 73 | 12.975 | 1947 | 1950 | 1957 | rVV3 | 1041   | 1424   | 0.26%  | 0.033% |
| 74 | 13.042 | 1957 | 1961 | 1963 | rVV4 | 632    | 852    | 0.16%  | 0.020% |
| 75 | 13.091 | 1967 | 1969 | 1974 | rVB  | 247    | 237    | 0.04%  | 0.005% |
| 76 | 13.195 | 1982 | 1986 | 1987 | rBV2 | 214    | 218    | 0.04%  | 0.005% |

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Min Area: 0 % of largest Peak

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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\_X\Method\SFAMXML112221WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |       |       |        |
|-----|--------|------|------|------|------|------|-------|-------|--------|
| 77  | 13.268 | 1992 | 1998 | 2010 | rVB3 | 3504 | 6310  | 1.15% | 0.146% |
| 78  | 13.384 | 2013 | 2017 | 2022 | rBV3 | 1582 | 2048  | 0.37% | 0.047% |
| 79  | 13.628 | 2053 | 2057 | 2061 | rBV4 | 524  | 672   | 0.12% | 0.016% |
| 80  | 13.780 | 2077 | 2082 | 2087 | rVB  | 8243 | 10680 | 1.95% | 0.248% |
|     |        |      |      |      |      |      |       |       |        |
| 81  | 13.847 | 2089 | 2093 | 2096 | rVB  | 3089 | 3665  | 0.67% | 0.085% |
| 82  | 14.042 | 2119 | 2125 | 2129 | rBV  | 3602 | 4403  | 0.81% | 0.102% |
| 83  | 14.134 | 2136 | 2140 | 2146 | rVB2 | 2603 | 3433  | 0.63% | 0.080% |
| 84  | 14.195 | 2146 | 2150 | 2153 | rVB4 | 340  | 506   | 0.09% | 0.012% |
| 85  | 14.250 | 2157 | 2159 | 2162 | rVB2 | 267  | 240   | 0.04% | 0.006% |
|     |        |      |      |      |      |      |       |       |        |
| 86  | 14.506 | 2195 | 2201 | 2208 | rBV3 | 1321 | 2139  | 0.39% | 0.050% |
| 87  | 14.567 | 2208 | 2211 | 2215 | rBV2 | 242  | 293   | 0.05% | 0.007% |
| 88  | 14.615 | 2215 | 2219 | 2221 | rVV  | 1844 | 2617  | 0.48% | 0.061% |
| 89  | 14.640 | 2221 | 2223 | 2229 | rVB  | 3401 | 3690  | 0.68% | 0.086% |
| 90  | 14.756 | 2238 | 2242 | 2244 | rBV2 | 3673 | 4072  | 0.75% | 0.094% |
|     |        |      |      |      |      |      |       |       |        |
| 91  | 15.121 | 2300 | 2302 | 2306 | rBV2 | 283  | 287   | 0.05% | 0.007% |
| 92  | 15.213 | 2313 | 2317 | 2323 | rVV3 | 3969 | 5403  | 0.99% | 0.125% |
| 93  | 15.274 | 2323 | 2327 | 2329 | rVV3 | 848  | 1019  | 0.19% | 0.024% |
| 94  | 15.347 | 2336 | 2339 | 2340 | rVV2 | 428  | 450   | 0.08% | 0.010% |
| 95  | 15.396 | 2343 | 2347 | 2357 | rVB5 | 1152 | 2230  | 0.41% | 0.052% |
|     |        |      |      |      |      |      |       |       |        |
| 96  | 15.487 | 2357 | 2362 | 2368 | rBV4 | 3397 | 5295  | 0.97% | 0.123% |
| 97  | 15.615 | 2378 | 2383 | 2387 | rBV3 | 1044 | 1619  | 0.30% | 0.038% |
| 98  | 16.304 | 2493 | 2496 | 2497 | rBV  | 265  | 253   | 0.05% | 0.006% |
| 99  | 16.371 | 2504 | 2507 | 2513 | rVB6 | 1830 | 3079  | 0.56% | 0.071% |
| 100 | 16.450 | 2518 | 2520 | 2521 | rBV2 | 335  | 266   | 0.05% | 0.006% |

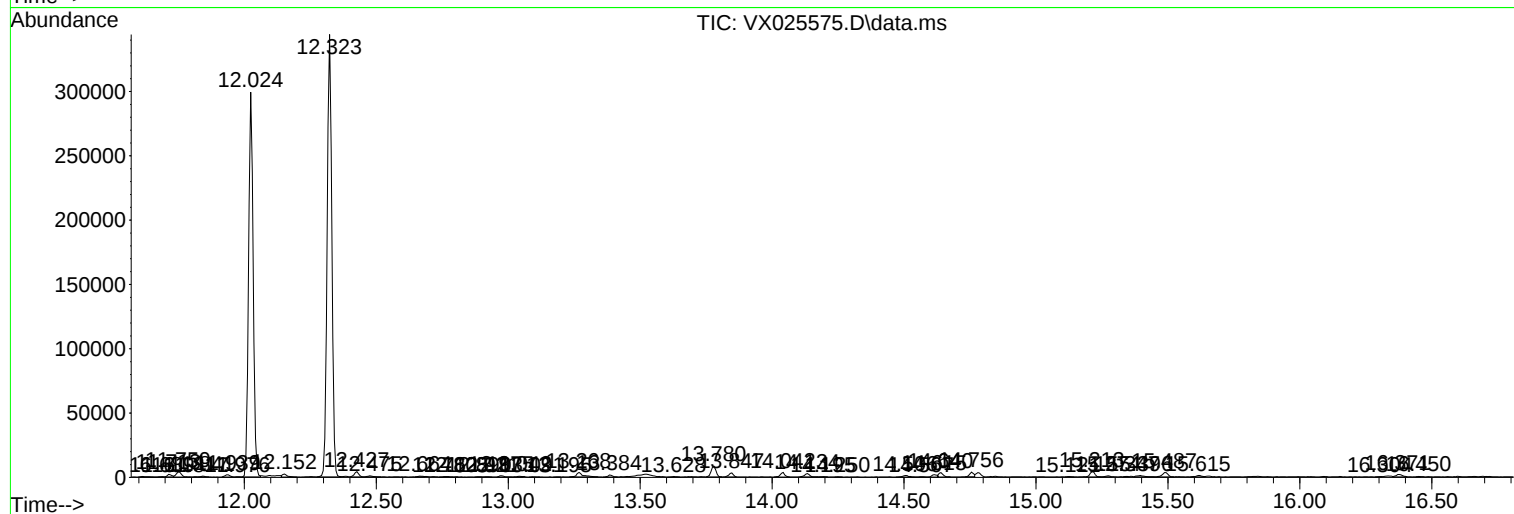
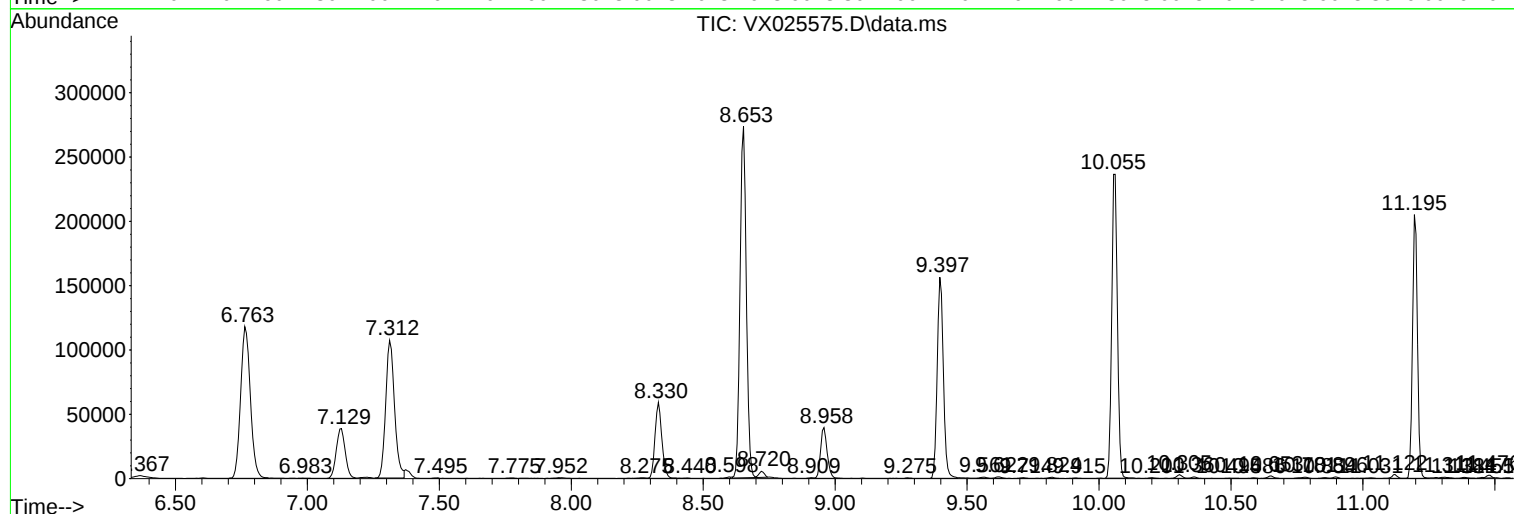
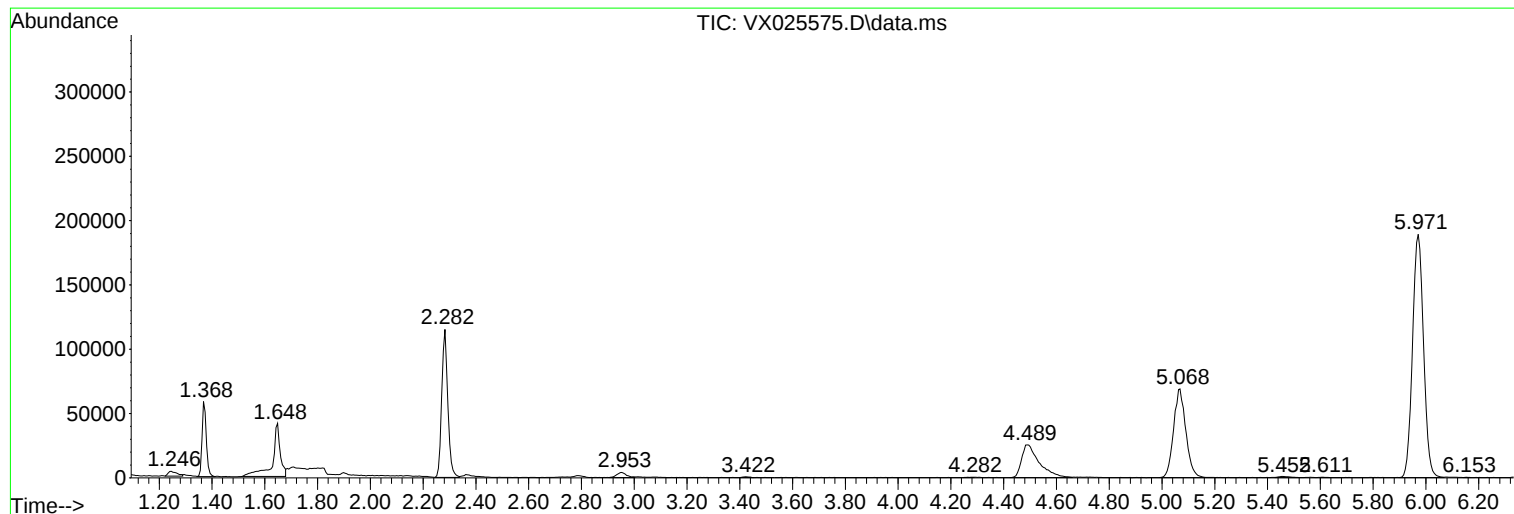
Sum of corrected areas: 4314914

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Instrument :  
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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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No Library Search Compounds Detected

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