

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121823\  
 Data File : VX039330.D  
 Acq On : 18 Dec 2023 22:45  
 Operator : JC/MD  
 Sample : 05835-12 100X  
 Misc : 4.53g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 35 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AQ9

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\SFAMXML120523WMA.M  
 Title : VOC Analysis

Signal : TIC: VX039330.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          | 55           | rBV      | 84972          | 90793         | 11.23%          | 1.389%        |
| 2         | 1.666       | 91            | 95          | 108          | rVB      | 60281          | 88418         | 10.94%          | 1.353%        |
| 3         | 2.306       | 194           | 200         | 210          | rBV      | 163555         | 257142        | 31.81%          | 3.935%        |
| 4         | 2.647       | 255           | 256         | 259          | rVB      | 288            | 183           | 0.02%           | 0.003%        |
| 5         | 2.794       | 274           | 280         | 290          | rVB6     | 1634           | 3661          | 0.45%           | 0.056%        |
| 6         | 2.946       | 298           | 305         | 313          | rVB2     | 5359           | 11580         | 1.43%           | 0.177%        |
| 7         | 3.489       | 390           | 394         | 395          | rBV      | 156            | 202           | 0.02%           | 0.003%        |
| 8         | 3.678       | 423           | 425         | 428          | rBV2     | 168            | 166           | 0.02%           | 0.003%        |
| 9         | 3.824       | 447           | 449         | 453          | rBV2     | 292            | 342           | 0.04%           | 0.005%        |
| 10        | 4.080       | 490           | 491         | 494          | rBV2     | 241            | 254           | 0.03%           | 0.004%        |
| 11        | 4.348       | 533           | 535         | 538          | rVB      | 353            | 268           | 0.03%           | 0.004%        |
| 12        | 4.452       | 542           | 552         | 565          | rBV      | 85729          | 241293        | 29.85%          | 3.692%        |
| 13        | 5.056       | 638           | 651         | 668          | rBV2     | 101057         | 322600        | 39.90%          | 4.936%        |
| 14        | 5.403       | 706           | 708         | 710          | rVB3     | 414            | 300           | 0.04%           | 0.005%        |
| 15        | 5.537       | 728           | 730         | 733          | rBV2     | 241            | 284           | 0.04%           | 0.004%        |
| 16        | 5.836       | 776           | 779         | 780          | rBV2     | 236            | 176           | 0.02%           | 0.003%        |
| 17        | 5.970       | 789           | 801         | 820          | rBV2     | 266624         | 808444        | 100.00%         | 12.371%       |
| 18        | 6.263       | 847           | 849         | 851          | rVB2     | 266            | 179           | 0.02%           | 0.003%        |
| 19        | 6.324       | 858           | 859         | 861          | rBV2     | 249            | 200           | 0.02%           | 0.003%        |
| 20        | 6.494       | 886           | 887         | 892          | rVB2     | 260            | 246           | 0.03%           | 0.004%        |
| 21        | 6.763       | 922           | 931         | 945          | rBV      | 217631         | 524710        | 64.90%          | 8.029%        |
| 22        | 6.982       | 966           | 967         | 970          | rBV2     | 222            | 196           | 0.02%           | 0.003%        |
| 23        | 7.055       | 975           | 979         | 980          | rBV2     | 276            | 360           | 0.04%           | 0.006%        |
| 24        | 7.122       | 983           | 990         | 995          | rVB6     | 1289           | 3027          | 0.37%           | 0.046%        |
| 25        | 7.305       | 1012          | 1020        | 1034         | rBV      | 167538         | 374876        | 46.37%          | 5.736%        |
| 26        | 7.482       | 1047          | 1049        | 1054         | rVB3     | 706            | 790           | 0.10%           | 0.012%        |
| 27        | 7.628       | 1072          | 1073        | 1076         | rVB2     | 267            | 210           | 0.03%           | 0.003%        |
| 28        | 7.659       | 1076          | 1078        | 1081         | rBV2     | 189            | 234           | 0.03%           | 0.004%        |
| 29        | 7.817       | 1103          | 1104        | 1105         | rBV      | 281            | 179           | 0.02%           | 0.003%        |
| 30        | 7.964       | 1123          | 1128        | 1131         | rBV2     | 290            | 384           | 0.05%           | 0.006%        |
| 31        | 8.323       | 1181          | 1187        | 1202         | rBV      | 111841         | 187823        | 23.23%          | 2.874%        |
| 32        | 8.518       | 1217          | 1219        | 1221         | rVB3     | 412            | 337           | 0.04%           | 0.005%        |
| 33        | 8.579       | 1226          | 1229        | 1233         | rBV2     | 435            | 419           | 0.05%           | 0.006%        |
| 34        | 8.646       | 1234          | 1240        | 1255         | rBV      | 391247         | 627756        | 77.65%          | 9.606%        |
| 35        | 8.951       | 1284          | 1290        | 1304         | rBV      | 82594          | 124575        | 15.41%          | 1.906%        |
| 36        | 9.091       | 1311          | 1313        | 1317         | rVB3     | 263            | 231           | 0.03%           | 0.004%        |

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 ALS Vial : 35 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AQ9

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\SFAMXLM120523WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 9.171  | 1324 | 1326 | 1331 | rVB2 | 265    | 307    | 0.04%  | 0.005%  |
| 38 | 9.238  | 1335 | 1337 | 1340 | rVB2 | 228    | 173    | 0.02%  | 0.003%  |
| 39 | 9.274  | 1340 | 1343 | 1345 | rBV2 | 382    | 364    | 0.05%  | 0.006%  |
| 40 | 9.341  | 1352 | 1354 | 1355 | rBV  | 168    | 177    | 0.02%  | 0.003%  |
| 41 | 9.384  | 1355 | 1361 | 1380 | rVV  | 383388 | 553748 | 68.50% | 8.474%  |
| 42 | 9.701  | 1409 | 1413 | 1418 | rVB3 | 669    | 803    | 0.10%  | 0.012%  |
| 43 | 9.738  | 1418 | 1419 | 1421 | rBV  | 297    | 217    | 0.03%  | 0.003%  |
| 44 | 9.811  | 1430 | 1431 | 1433 | rBV2 | 279    | 272    | 0.03%  | 0.004%  |
| 45 | 9.884  | 1441 | 1443 | 1445 | rBV2 | 184    | 180    | 0.02%  | 0.003%  |
| 46 | 9.994  | 1459 | 1461 | 1465 | rVB2 | 194    | 228    | 0.03%  | 0.003%  |
| 47 | 10.055 | 1465 | 1471 | 1482 | rBV  | 471541 | 657007 | 81.27% | 10.054% |
| 48 | 10.195 | 1492 | 1494 | 1499 | rVB3 | 614    | 787    | 0.10%  | 0.012%  |
| 49 | 10.286 | 1506 | 1509 | 1510 | rBV  | 234    | 197    | 0.02%  | 0.003%  |
| 50 | 10.311 | 1510 | 1513 | 1517 | rVB3 | 531    | 735    | 0.09%  | 0.011%  |
| 51 | 10.353 | 1517 | 1520 | 1525 | rBV  | 221    | 370    | 0.05%  | 0.006%  |
| 52 | 10.439 | 1532 | 1534 | 1537 | rVB  | 224    | 197    | 0.02%  | 0.003%  |
| 53 | 10.646 | 1563 | 1568 | 1572 | rBV2 | 530    | 629    | 0.08%  | 0.010%  |
| 54 | 10.683 | 1572 | 1574 | 1577 | rBV  | 162    | 185    | 0.02%  | 0.003%  |
| 55 | 10.963 | 1618 | 1620 | 1624 | rVV2 | 462    | 614    | 0.08%  | 0.009%  |
| 56 | 11.024 | 1628 | 1630 | 1633 | rVB  | 225    | 207    | 0.03%  | 0.003%  |
| 57 | 11.091 | 1638 | 1641 | 1644 | rBV4 | 453    | 705    | 0.09%  | 0.011%  |
| 58 | 11.122 | 1644 | 1646 | 1649 | rVB  | 300    | 198    | 0.02%  | 0.003%  |
| 59 | 11.189 | 1652 | 1657 | 1672 | rVB  | 323207 | 419819 | 51.93% | 6.424%  |
| 60 | 11.457 | 1698 | 1701 | 1708 | rVB3 | 481    | 755    | 0.09%  | 0.012%  |
| 61 | 11.512 | 1708 | 1710 | 1712 | rVB2 | 188    | 172    | 0.02%  | 0.003%  |
| 62 | 11.548 | 1712 | 1716 | 1718 | rBV2 | 263    | 408    | 0.05%  | 0.006%  |
| 63 | 11.695 | 1739 | 1740 | 1742 | rBV  | 289    | 205    | 0.03%  | 0.003%  |
| 64 | 11.762 | 1748 | 1751 | 1755 | rBV2 | 596    | 694    | 0.09%  | 0.011%  |
| 65 | 11.975 | 1783 | 1786 | 1788 | rBV2 | 522    | 529    | 0.07%  | 0.008%  |
| 66 | 12.024 | 1788 | 1794 | 1802 | rVV  | 483338 | 643895 | 79.65% | 9.853%  |
| 67 | 12.237 | 1828 | 1829 | 1832 | rVB2 | 313    | 251    | 0.03%  | 0.004%  |
| 68 | 12.268 | 1832 | 1834 | 1837 | rBV  | 211    | 214    | 0.03%  | 0.003%  |
| 69 | 12.316 | 1837 | 1842 | 1850 | rBV  | 425313 | 565272 | 69.92% | 8.650%  |
| 70 | 12.469 | 1865 | 1867 | 1869 | rBV2 | 238    | 208    | 0.03%  | 0.003%  |
| 71 | 12.762 | 1911 | 1915 | 1919 | rVV2 | 678    | 794    | 0.10%  | 0.012%  |
| 72 | 12.963 | 1946 | 1948 | 1950 | rVV2 | 219    | 191    | 0.02%  | 0.003%  |
| 73 | 13.127 | 1971 | 1975 | 1976 | rBV2 | 212    | 196    | 0.02%  | 0.003%  |
| 74 | 13.176 | 1981 | 1983 | 1985 | rBV  | 203    | 191    | 0.02%  | 0.003%  |
| 75 | 13.255 | 1993 | 1996 | 1997 | rVV2 | 252    | 234    | 0.03%  | 0.004%  |
| 76 | 13.463 | 2027 | 2030 | 2031 | rBV  | 172    | 175    | 0.02%  | 0.003%  |

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 ALS Vial : 35 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AQ9

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\SFAMXML120523WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 13.597 | 2046 | 2052 | 2055 | rBV2 | 490  | 800  | 0.10% | 0.012% |
| 78  | 13.792 | 2078 | 2084 | 2089 | rBV3 | 363  | 825  | 0.10% | 0.013% |
| 79  | 13.969 | 2109 | 2113 | 2117 | rBV  | 439  | 577  | 0.07% | 0.009% |
| 80  | 14.127 | 2136 | 2139 | 2147 | rVB2 | 1234 | 1761 | 0.22% | 0.027% |
| 81  | 14.194 | 2147 | 2150 | 2152 | rBV  | 206  | 262  | 0.03% | 0.004% |
| 82  | 14.261 | 2160 | 2161 | 2163 | rBV  | 273  | 209  | 0.03% | 0.003% |
| 83  | 14.426 | 2186 | 2188 | 2191 | rVB2 | 257  | 215  | 0.03% | 0.003% |
| 84  | 14.645 | 2221 | 2224 | 2227 | rBV2 | 203  | 256  | 0.03% | 0.004% |
| 85  | 14.676 | 2227 | 2229 | 2231 | rBV2 | 265  | 203  | 0.03% | 0.003% |
| 86  | 14.773 | 2242 | 2245 | 2248 | rBV  | 238  | 337  | 0.04% | 0.005% |
| 87  | 14.987 | 2279 | 2280 | 2282 | rBV  | 227  | 203  | 0.03% | 0.003% |
| 88  | 15.182 | 2310 | 2312 | 2314 | rBV2 | 274  | 278  | 0.03% | 0.004% |
| 89  | 15.206 | 2314 | 2316 | 2317 | rVB  | 371  | 217  | 0.03% | 0.003% |
| 90  | 15.224 | 2317 | 2319 | 2320 | rBV  | 315  | 212  | 0.03% | 0.003% |
| 91  | 15.340 | 2334 | 2338 | 2341 | rBV  | 311  | 384  | 0.05% | 0.006% |
| 92  | 15.389 | 2344 | 2346 | 2348 | rBV2 | 512  | 519  | 0.06% | 0.008% |
| 93  | 15.627 | 2383 | 2385 | 2389 | rVB2 | 382  | 367  | 0.05% | 0.006% |
| 94  | 15.773 | 2407 | 2409 | 2410 | rBV2 | 268  | 181  | 0.02% | 0.003% |
| 95  | 15.834 | 2417 | 2419 | 2422 | rBV2 | 240  | 208  | 0.03% | 0.003% |
| 96  | 15.895 | 2428 | 2429 | 2430 | rBV  | 360  | 205  | 0.03% | 0.003% |
| 97  | 16.358 | 2503 | 2505 | 2509 | rVV2 | 308  | 312  | 0.04% | 0.005% |
| 98  | 16.480 | 2521 | 2525 | 2526 | rBV2 | 313  | 282  | 0.03% | 0.004% |
| 99  | 16.578 | 2537 | 2541 | 2542 | rBV3 | 387  | 384  | 0.05% | 0.006% |
| 100 | 16.706 | 2560 | 2562 | 2566 | rBV3 | 386  | 518  | 0.06% | 0.008% |

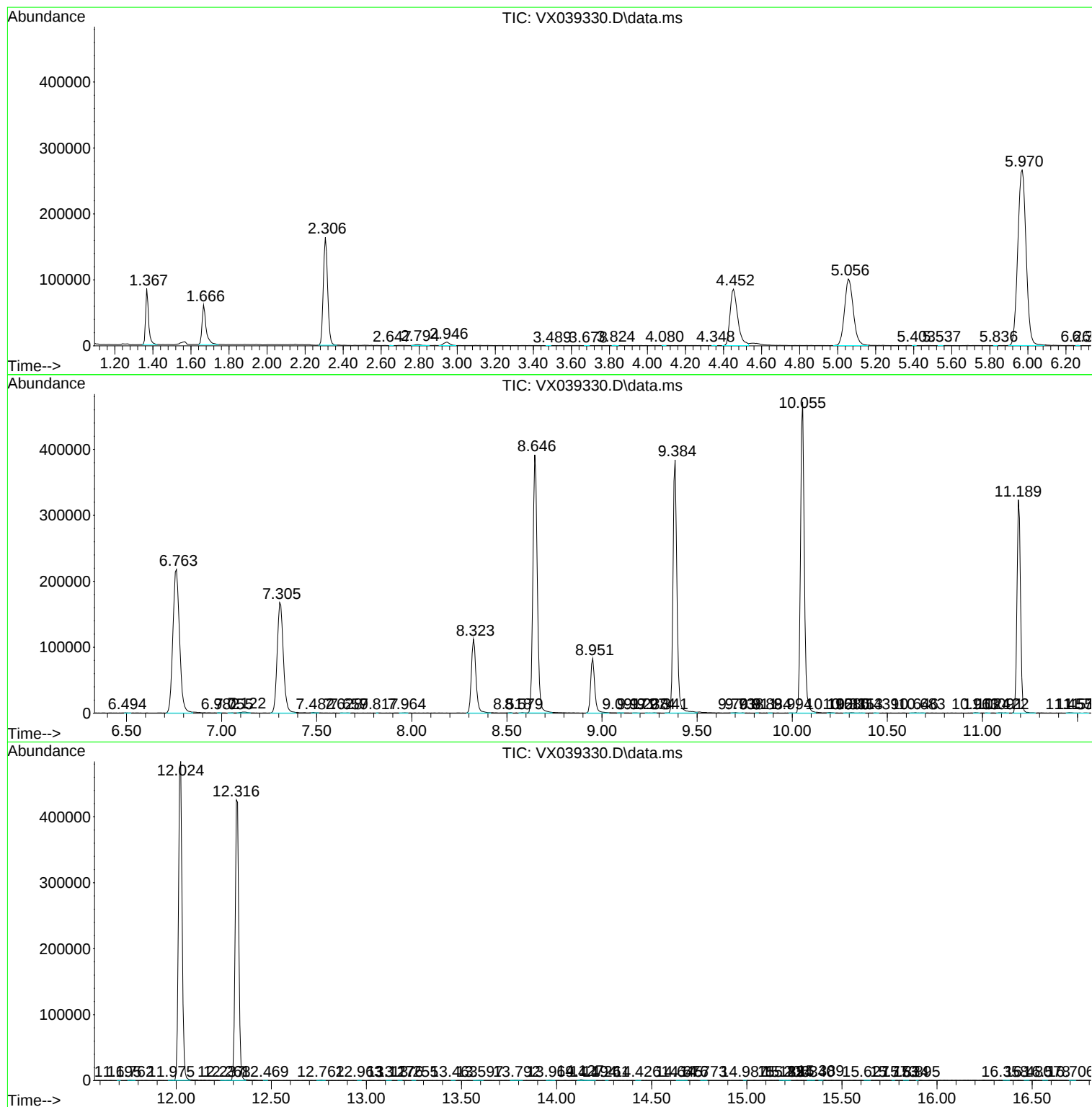
Sum of corrected areas: 6535056

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ALS Vial : 35 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
C0AQ9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121823\  
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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 Top Hit name | RT | EstConc | Units | Response | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |