

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122123\  
 Data File : VX039419.D  
 Acq On : 21 Dec 2023 11:12  
 Operator : JC/MD  
 Sample : 05808-08 20X  
 Misc : 4.19g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0B02

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: VX039419.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       | 43            | 46          | 56           | rVB      | 85778          | 94545         | 11.66%          | 1.228%        |
| 2         | 1.660       | 90            | 94          | 105          | rBV      | 57162          | 87331         | 10.77%          | 1.135%        |
| 3         | 2.306       | 193           | 200         | 210          | rBV      | 164271         | 260184        | 32.09%          | 3.380%        |
| 4         | 2.630       | 251           | 253         | 255          | rVB2     | 295            | 200           | 0.02%           | 0.003%        |
| 5         | 2.648       | 255           | 256         | 259          | rBV      | 200            | 214           | 0.03%           | 0.003%        |
| 6         | 2.697       | 261           | 264         | 265          | rBV2     | 240            | 217           | 0.03%           | 0.003%        |
| 7         | 2.788       | 274           | 279         | 286          | rBV4     | 1311           | 2340          | 0.29%           | 0.030%        |
| 8         | 2.867       | 286           | 292         | 298          | rVV3     | 7490           | 14471         | 1.78%           | 0.188%        |
| 9         | 2.941       | 299           | 304         | 313          | rVB2     | 4693           | 10337         | 1.27%           | 0.134%        |
| 10        | 3.081       | 326           | 327         | 328          | rBV      | 451            | 246           | 0.03%           | 0.003%        |
| 11        | 4.233       | 513           | 516         | 517          | rBV      | 284            | 278           | 0.03%           | 0.004%        |
| 12        | 4.452       | 543           | 552         | 566          | rBV      | 74302          | 218278        | 26.92%          | 2.836%        |
| 13        | 4.855       | 616           | 618         | 619          | rBV2     | 251            | 189           | 0.02%           | 0.002%        |
| 14        | 5.056       | 639           | 651         | 672          | rBV      | 102031         | 325875        | 40.19%          | 4.234%        |
| 15        | 5.391       | 702           | 706         | 708          | rBV3     | 514            | 782           | 0.10%           | 0.010%        |
| 16        | 5.964       | 789           | 800         | 815          | rBV2     | 266561         | 810907        | 100.00%         | 10.535%       |
| 17        | 6.190       | 836           | 837         | 841          | rVB2     | 409            | 341           | 0.04%           | 0.004%        |
| 18        | 6.385       | 867           | 869         | 871          | rVB2     | 257            | 217           | 0.03%           | 0.003%        |
| 19        | 6.653       | 911           | 913         | 915          | rVB      | 277            | 231           | 0.03%           | 0.003%        |
| 20        | 6.684       | 915           | 918         | 919          | rBV2     | 257            | 226           | 0.03%           | 0.003%        |
| 21        | 6.757       | 922           | 930         | 952          | rBV      | 193811         | 471850        | 58.19%          | 6.130%        |
| 22        | 6.970       | 964           | 965         | 971          | rVB2     | 403            | 475           | 0.06%           | 0.006%        |
| 23        | 7.019       | 971           | 973         | 976          | rBV2     | 261            | 249           | 0.03%           | 0.003%        |
| 24        | 7.111       | 983           | 988         | 996          | rVB3     | 1540           | 3110          | 0.38%           | 0.040%        |
| 25        | 7.306       | 1011          | 1020        | 1039         | rBV      | 176849         | 381259        | 47.02%          | 4.953%        |
| 26        | 7.708       | 1084          | 1086        | 1088         | rVB      | 315            | 248           | 0.03%           | 0.003%        |
| 27        | 7.958       | 1123          | 1127        | 1128         | rBV2     | 364            | 323           | 0.04%           | 0.004%        |
| 28        | 8.226       | 1169          | 1171        | 1172         | rBV      | 325            | 191           | 0.02%           | 0.002%        |
| 29        | 8.324       | 1181          | 1187        | 1200         | rBV      | 118774         | 190665        | 23.51%          | 2.477%        |
| 30        | 8.525       | 1215          | 1220        | 1223         | rBV3     | 433            | 792           | 0.10%           | 0.010%        |
| 31        | 8.568       | 1226          | 1227        | 1234         | rBB3     | 357            | 372           | 0.05%           | 0.005%        |
| 32        | 8.647       | 1234          | 1240        | 1258         | rBV      | 401142         | 636934        | 78.55%          | 8.275%        |
| 33        | 8.854       | 1273          | 1274        | 1277         | rBV2     | 235            | 200           | 0.02%           | 0.003%        |
| 34        | 8.946       | 1284          | 1289        | 1299         | rBV      | 79189          | 125312        | 15.45%          | 1.628%        |
| 35        | 9.269       | 1341          | 1342        | 1347         | rVB3     | 529            | 614           | 0.08%           | 0.008%        |
| 36        | 9.384       | 1355          | 1361        | 1379         | rBV      | 353835         | 516736        | 63.72%          | 6.713%        |

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 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0B02

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 | 9.665  | 1404 | 1407 | 1408 | rBV2 | 331    | 291    | 0.04%  | 0.004% |
| 38 | 9.695  | 1409 | 1412 | 1419 | rVB4 | 663    | 1200   | 0.15%  | 0.016% |
| 39 | 9.775  | 1423 | 1425 | 1426 | rVV  | 271    | 181    | 0.02%  | 0.002% |
| 40 | 9.830  | 1432 | 1434 | 1436 | rBV2 | 383    | 341    | 0.04%  | 0.004% |
| 41 | 10.006 | 1462 | 1463 | 1465 | rBV  | 274    | 183    | 0.02%  | 0.002% |
| 42 | 10.049 | 1465 | 1470 | 1488 | rVV  | 412024 | 593995 | 73.25% | 7.717% |
| 43 | 10.189 | 1492 | 1493 | 1499 | rVB3 | 567    | 899    | 0.11%  | 0.012% |
| 44 | 10.262 | 1504 | 1505 | 1509 | rVB  | 229    | 193    | 0.02%  | 0.003% |
| 45 | 10.299 | 1509 | 1511 | 1512 | rBV  | 428    | 419    | 0.05%  | 0.005% |
| 46 | 10.653 | 1564 | 1569 | 1570 | rBV4 | 604    | 818    | 0.10%  | 0.011% |
| 47 | 10.799 | 1590 | 1593 | 1596 | rVB2 | 261    | 320    | 0.04%  | 0.004% |
| 48 | 10.872 | 1602 | 1605 | 1611 | rVB2 | 278    | 408    | 0.05%  | 0.005% |
| 49 | 10.921 | 1611 | 1613 | 1615 | rBV  | 176    | 180    | 0.02%  | 0.002% |
| 50 | 10.970 | 1620 | 1621 | 1626 | rVB2 | 649    | 503    | 0.06%  | 0.007% |
| 51 | 11.098 | 1639 | 1642 | 1646 | rBV2 | 444    | 433    | 0.05%  | 0.006% |
| 52 | 11.189 | 1652 | 1657 | 1671 | rVB  | 337395 | 427410 | 52.71% | 5.553% |
| 53 | 11.311 | 1674 | 1677 | 1682 | rVB3 | 843    | 1286   | 0.16%  | 0.017% |
| 54 | 11.348 | 1682 | 1683 | 1685 | rBV2 | 197    | 194    | 0.02%  | 0.003% |
| 55 | 11.415 | 1691 | 1694 | 1695 | rBV2 | 176    | 196    | 0.02%  | 0.003% |
| 56 | 11.451 | 1697 | 1700 | 1705 | rVB3 | 762    | 1291   | 0.16%  | 0.017% |
| 57 | 11.488 | 1705 | 1706 | 1708 | rBV2 | 340    | 269    | 0.03%  | 0.003% |
| 58 | 11.707 | 1740 | 1742 | 1746 | rVB  | 303    | 416    | 0.05%  | 0.005% |
| 59 | 11.762 | 1746 | 1751 | 1754 | rBV3 | 690    | 1168   | 0.14%  | 0.015% |
| 60 | 11.878 | 1767 | 1770 | 1775 | rBV2 | 256    | 425    | 0.05%  | 0.006% |
| 61 | 11.921 | 1775 | 1777 | 1781 | rBV2 | 152    | 199    | 0.02%  | 0.003% |
| 62 | 11.969 | 1781 | 1785 | 1789 | rBV  | 22965  | 30043  | 3.70%  | 0.390% |
| 63 | 12.018 | 1789 | 1793 | 1805 | rVB  | 487276 | 637392 | 78.60% | 8.281% |
| 64 | 12.317 | 1837 | 1842 | 1853 | rBV  | 490665 | 662638 | 81.72% | 8.609% |
| 65 | 12.616 | 1889 | 1891 | 1895 | rVV2 | 219    | 280    | 0.03%  | 0.004% |
| 66 | 12.646 | 1895 | 1896 | 1900 | rVB  | 307    | 332    | 0.04%  | 0.004% |
| 67 | 12.695 | 1902 | 1904 | 1908 | rBV2 | 256    | 273    | 0.03%  | 0.004% |
| 68 | 12.762 | 1910 | 1915 | 1920 | rBV2 | 4011   | 5656   | 0.70%  | 0.073% |
| 69 | 12.902 | 1934 | 1938 | 1941 | rBV2 | 171    | 273    | 0.03%  | 0.004% |
| 70 | 12.951 | 1943 | 1946 | 1949 | rVB2 | 296    | 324    | 0.04%  | 0.004% |
| 71 | 12.987 | 1949 | 1952 | 1955 | rBV2 | 167    | 278    | 0.03%  | 0.004% |
| 72 | 13.061 | 1959 | 1964 | 1970 | rVB5 | 1690   | 3138   | 0.39%  | 0.041% |
| 73 | 13.109 | 1970 | 1972 | 1976 | rBV3 | 1276   | 1494   | 0.18%  | 0.019% |
| 74 | 13.201 | 1984 | 1987 | 1989 | rVB3 | 873    | 867    | 0.11%  | 0.011% |
| 75 | 13.274 | 1997 | 1999 | 2003 | rBV2 | 255    | 342    | 0.04%  | 0.004% |
| 76 | 13.390 | 2015 | 2018 | 2020 | rVV2 | 299    | 392    | 0.05%  | 0.005% |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0B02

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

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 13.433 | 2023 | 2025 | 2029 | rVB  | 216    | 277    | 0.03%  | 0.004% |
| 78  | 13.487 | 2032 | 2034 | 2038 | rBV2 | 235    | 211    | 0.03%  | 0.003% |
| 79  | 13.585 | 2045 | 2050 | 2064 | rVB  | 518963 | 640179 | 78.95% | 8.317% |
| 80  | 13.780 | 2079 | 2082 | 2087 | rVB2 | 687    | 932    | 0.11%  | 0.012% |
| 81  | 13.957 | 2106 | 2111 | 2123 | rBV  | 164414 | 206118 | 25.42% | 2.678% |
| 82  | 14.128 | 2132 | 2139 | 2145 | rBV  | 7447   | 10252  | 1.26%  | 0.133% |
| 83  | 14.237 | 2155 | 2157 | 2158 | rBV2 | 266    | 191    | 0.02%  | 0.002% |
| 84  | 14.256 | 2158 | 2160 | 2164 | rVV2 | 265    | 331    | 0.04%  | 0.004% |
| 85  | 14.292 | 2164 | 2166 | 2169 | rVV2 | 242    | 240    | 0.03%  | 0.003% |
| 86  | 14.384 | 2180 | 2181 | 2185 | rVB  | 633    | 669    | 0.08%  | 0.009% |
| 87  | 14.432 | 2187 | 2189 | 2190 | rBV  | 315    | 216    | 0.03%  | 0.003% |
| 88  | 14.627 | 2217 | 2221 | 2223 | rVB3 | 522    | 573    | 0.07%  | 0.007% |
| 89  | 14.658 | 2223 | 2226 | 2228 | rBV2 | 194    | 259    | 0.03%  | 0.003% |
| 90  | 14.780 | 2239 | 2246 | 2251 | rVB2 | 30479  | 51255  | 6.32%  | 0.666% |
| 91  | 14.884 | 2261 | 2263 | 2265 | rBV2 | 242    | 213    | 0.03%  | 0.003% |
| 92  | 15.243 | 2316 | 2322 | 2332 | rBV  | 163405 | 236508 | 29.17% | 3.073% |
| 93  | 15.731 | 2400 | 2402 | 2405 | rVB3 | 249    | 258    | 0.03%  | 0.003% |
| 94  | 15.761 | 2405 | 2407 | 2412 | rBV3 | 336    | 379    | 0.05%  | 0.005% |
| 95  | 15.835 | 2417 | 2419 | 2420 | rBV  | 310    | 179    | 0.02%  | 0.002% |
| 96  | 16.127 | 2466 | 2467 | 2470 | rBV  | 304    | 269    | 0.03%  | 0.003% |
| 97  | 16.176 | 2473 | 2475 | 2476 | rVV2 | 355    | 233    | 0.03%  | 0.003% |
| 98  | 16.231 | 2482 | 2484 | 2486 | rBV  | 337    | 277    | 0.03%  | 0.004% |
| 99  | 16.255 | 2486 | 2488 | 2491 | rVV  | 282    | 290    | 0.04%  | 0.004% |
| 100 | 16.505 | 2524 | 2529 | 2538 | rVB5 | 7783   | 13378  | 1.65%  | 0.174% |

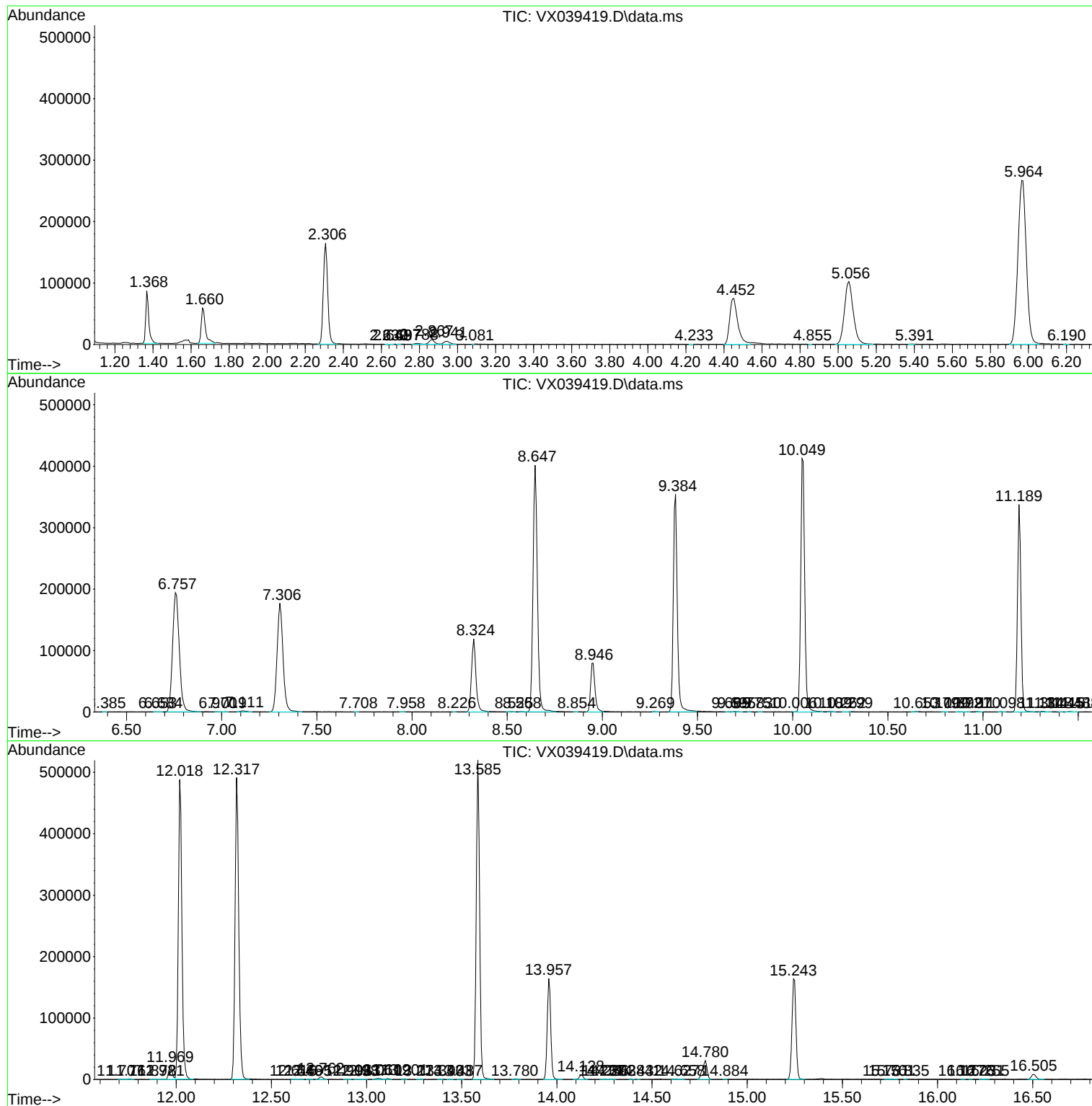
Sum of corrected areas: 7697366

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ALS Vial : 6 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
C0B02

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\VX122123\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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TIC Integration Parameters: LSCINT.P

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