

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX041123\  
 Data File : VX034999.D  
 Acq On : 11 Apr 2023 09:39  
 Operator : JC/MD  
 Sample : VX0411MBL01  
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK619

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\SFAMXML041023WMA.M  
 Title : VOC Analysis

Signal : TIC: VX034999.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          | 58           | rBV      | 209394         | 230470        | 13.25%          | 1.718%        |
| 2         | 1.673       | 91            | 96          | 108          | rBV      | 163177         | 217428        | 12.50%          | 1.621%        |
| 3         | 2.307       | 194           | 200         | 209          | rBV      | 395442         | 598848        | 34.43%          | 4.464%        |
| 4         | 2.514       | 229           | 234         | 240          | rVB      | 2615           | 4338          | 0.25%           | 0.032%        |
| 5         | 2.788       | 274           | 279         | 285          | rVB3     | 1574           | 2853          | 0.16%           | 0.021%        |
| 6         | 2.916       | 298           | 300         | 301          | rVB      | 408            | 192           | 0.01%           | 0.001%        |
| 7         | 2.983       | 309           | 311         | 312          | rBV      | 401            | 225           | 0.01%           | 0.002%        |
| 8         | 3.099       | 323           | 330         | 336          | rVB3     | 1549           | 3269          | 0.19%           | 0.024%        |
| 9         | 3.203       | 345           | 347         | 348          | rBV2     | 240            | 256           | 0.01%           | 0.002%        |
| 10        | 3.258       | 353           | 356         | 357          | rVV2     | 234            | 209           | 0.01%           | 0.002%        |
| 11        | 3.276       | 357           | 359         | 362          | rVV2     | 316            | 304           | 0.02%           | 0.002%        |
| 12        | 3.380       | 372           | 376         | 378          | rBV      | 367            | 487           | 0.03%           | 0.004%        |
| 13        | 3.471       | 389           | 391         | 392          | rVV      | 306            | 198           | 0.01%           | 0.001%        |
| 14        | 3.605       | 412           | 413         | 419          | rVB2     | 303            | 362           | 0.02%           | 0.003%        |
| 15        | 3.849       | 451           | 453         | 454          | rVB      | 276            | 189           | 0.01%           | 0.001%        |
| 16        | 3.873       | 456           | 457         | 460          | rBV2     | 314            | 232           | 0.01%           | 0.002%        |
| 17        | 4.465       | 544           | 554         | 575          | rBV      | 103477         | 346294        | 19.91%          | 2.582%        |
| 18        | 4.885       | 620           | 623         | 625          | rBV3     | 314            | 340           | 0.02%           | 0.003%        |
| 19        | 4.934       | 628           | 631         | 632          | rBV2     | 353            | 431           | 0.02%           | 0.003%        |
| 20        | 4.977       | 635           | 638         | 639          | rBV      | 423            | 414           | 0.02%           | 0.003%        |
| 21        | 5.050       | 639           | 650         | 668          | rVV      | 227174         | 697321        | 40.09%          | 5.198%        |
| 22        | 5.373       | 699           | 703         | 704          | rBV2     | 767            | 1001          | 0.06%           | 0.007%        |
| 23        | 5.458       | 715           | 717         | 718          | rBV      | 302            | 200           | 0.01%           | 0.001%        |
| 24        | 5.556       | 724           | 733         | 737          | rBV3     | 2838           | 7068          | 0.41%           | 0.053%        |
| 25        | 5.763       | 764           | 767         | 768          | rBV2     | 200            | 208           | 0.01%           | 0.002%        |
| 26        | 5.836       | 777           | 779         | 783          | rVB2     | 269            | 313           | 0.02%           | 0.002%        |
| 27        | 5.964       | 787           | 800         | 819          | rBV2     | 579206         | 1739411       | 100.00%         | 12.967%       |
| 28        | 6.214       | 840           | 841         | 843          | rBV2     | 245            | 202           | 0.01%           | 0.002%        |
| 29        | 6.342       | 860           | 862         | 864          | rVB      | 387            | 266           | 0.02%           | 0.002%        |
| 30        | 6.477       | 882           | 884         | 889          | rVV2     | 294            | 393           | 0.02%           | 0.003%        |
| 31        | 6.538       | 889           | 894         | 895          | rVV3     | 310            | 326           | 0.02%           | 0.002%        |
| 32        | 6.556       | 895           | 897         | 898          | rVV      | 280            | 212           | 0.01%           | 0.002%        |
| 33        | 6.666       | 913           | 915         | 918          | rBV      | 375            | 311           | 0.02%           | 0.002%        |
| 34        | 6.757       | 920           | 930         | 947          | rBV      | 516170         | 1246547       | 71.66%          | 9.293%        |
| 35        | 7.111       | 981           | 988         | 1001         | rVB5     | 5915           | 15053         | 0.87%           | 0.112%        |
| 36        | 7.306       | 1011          | 1020        | 1039         | rBV      | 354076         | 796455        | 45.79%          | 5.937%        |

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Integrator: RTE

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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\SFAMXML041023WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |        |         |
|----|--------|------|------|------|------|---------|---------|--------|---------|
| 37 | 7.818  | 1101 | 1104 | 1105 | rBV  | 443     | 386     | 0.02%  | 0.003%  |
| 38 | 7.854  | 1108 | 1110 | 1112 | rBV2 | 244     | 223     | 0.01%  | 0.002%  |
| 39 | 7.940  | 1119 | 1124 | 1126 | rBV4 | 1177    | 1838    | 0.11%  | 0.014%  |
| 40 | 8.086  | 1144 | 1148 | 1153 | rBV2 | 331     | 648     | 0.04%  | 0.005%  |
| 41 | 8.135  | 1153 | 1156 | 1160 | rBV2 | 263     | 441     | 0.03%  | 0.003%  |
| 42 | 8.171  | 1160 | 1162 | 1163 | rVV2 | 242     | 199     | 0.01%  | 0.001%  |
| 43 | 8.208  | 1166 | 1168 | 1171 | rBV  | 279     | 260     | 0.01%  | 0.002%  |
| 44 | 8.324  | 1180 | 1187 | 1204 | rBV  | 228737  | 377847  | 21.72% | 2.817%  |
| 45 | 8.574  | 1225 | 1228 | 1230 | rBV3 | 387     | 497     | 0.03%  | 0.004%  |
| 46 | 8.647  | 1233 | 1240 | 1255 | rBV  | 893795  | 1390663 | 79.95% | 10.367% |
| 47 | 8.830  | 1268 | 1270 | 1272 | rVB3 | 445     | 357     | 0.02%  | 0.003%  |
| 48 | 8.946  | 1284 | 1289 | 1304 | rBV  | 152798  | 237436  | 13.65% | 1.770%  |
| 49 | 9.275  | 1340 | 1343 | 1348 | rVB3 | 1423    | 2004    | 0.12%  | 0.015%  |
| 50 | 9.385  | 1355 | 1361 | 1381 | rBV  | 506003  | 737460  | 42.40% | 5.498%  |
| 51 | 9.763  | 1421 | 1423 | 1426 | rVB2 | 390     | 431     | 0.02%  | 0.003%  |
| 52 | 9.799  | 1426 | 1429 | 1432 | rBV3 | 361     | 528     | 0.03%  | 0.004%  |
| 53 | 9.854  | 1437 | 1438 | 1440 | rVV  | 336     | 223     | 0.01%  | 0.002%  |
| 54 | 9.903  | 1444 | 1446 | 1448 | rVB  | 369     | 270     | 0.02%  | 0.002%  |
| 55 | 10.049 | 1465 | 1470 | 1487 | rBV  | 1001809 | 1412946 | 81.23% | 10.533% |
| 56 | 10.195 | 1491 | 1494 | 1498 | rVB2 | 1820    | 1908    | 0.11%  | 0.014%  |
| 57 | 10.311 | 1505 | 1513 | 1516 | rBV5 | 1467    | 2690    | 0.15%  | 0.020%  |
| 58 | 10.342 | 1516 | 1518 | 1519 | rVV2 | 296     | 248     | 0.01%  | 0.002%  |
| 59 | 10.378 | 1522 | 1524 | 1527 | rVB3 | 209     | 200     | 0.01%  | 0.001%  |
| 60 | 10.512 | 1545 | 1546 | 1549 | rVB2 | 317     | 299     | 0.02%  | 0.002%  |
| 61 | 10.647 | 1562 | 1568 | 1569 | rBV2 | 1640    | 2111    | 0.12%  | 0.016%  |
| 62 | 10.708 | 1577 | 1578 | 1582 | rVB2 | 417     | 291     | 0.02%  | 0.002%  |
| 63 | 10.750 | 1582 | 1585 | 1586 | rBV  | 252     | 251     | 0.01%  | 0.002%  |
| 64 | 10.768 | 1586 | 1588 | 1590 | rVB  | 406     | 273     | 0.02%  | 0.002%  |
| 65 | 10.799 | 1590 | 1593 | 1595 | rVB2 | 485     | 485     | 0.03%  | 0.004%  |
| 66 | 10.842 | 1598 | 1600 | 1603 | rVB2 | 235     | 215     | 0.01%  | 0.002%  |
| 67 | 10.872 | 1603 | 1605 | 1607 | rBV  | 316     | 301     | 0.02%  | 0.002%  |
| 68 | 10.964 | 1617 | 1620 | 1628 | rVV5 | 1552    | 2234    | 0.13%  | 0.017%  |
| 69 | 11.085 | 1638 | 1640 | 1644 | rBV3 | 402     | 594     | 0.03%  | 0.004%  |
| 70 | 11.189 | 1652 | 1657 | 1669 | rBV  | 580119  | 741583  | 42.63% | 5.528%  |
| 71 | 11.305 | 1674 | 1676 | 1678 | rVV3 | 415     | 368     | 0.02%  | 0.003%  |
| 72 | 11.427 | 1692 | 1696 | 1697 | rBV2 | 243     | 266     | 0.02%  | 0.002%  |
| 73 | 11.451 | 1697 | 1700 | 1706 | rVB2 | 1717    | 2223    | 0.13%  | 0.017%  |
| 74 | 11.579 | 1718 | 1721 | 1723 | rVB2 | 437     | 324     | 0.02%  | 0.002%  |
| 75 | 11.604 | 1723 | 1725 | 1726 | rBV2 | 294     | 205     | 0.01%  | 0.002%  |
| 76 | 11.659 | 1732 | 1734 | 1738 | rVV2 | 220     | 293     | 0.02%  | 0.002%  |

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Instrument :  
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Integration Parameters: LSCINT.P

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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\SFAMXLM041023WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |         |         |        |        |
|-----|--------|------|------|------|------|---------|---------|--------|--------|
| 77  | 11.707 | 1740 | 1742 | 1744 | rVV2 | 482     | 466     | 0.03%  | 0.003% |
| 78  | 11.756 | 1746 | 1750 | 1755 | rVB  | 1802    | 2509    | 0.14%  | 0.019% |
| 79  | 11.878 | 1769 | 1770 | 1773 | rBV2 | 261     | 281     | 0.02%  | 0.002% |
| 80  | 11.909 | 1773 | 1775 | 1779 | rVB  | 269     | 260     | 0.01%  | 0.002% |
| 81  | 11.969 | 1782 | 1785 | 1788 | rBV2 | 2467    | 3141    | 0.18%  | 0.023% |
| 82  | 12.018 | 1788 | 1793 | 1803 | rBV  | 1031103 | 1336351 | 76.83% | 9.962% |
| 83  | 12.317 | 1837 | 1842 | 1862 | rVB  | 951443  | 1191639 | 68.51% | 8.884% |
| 84  | 12.744 | 1910 | 1912 | 1914 | rBV2 | 170     | 188     | 0.01%  | 0.001% |
| 85  | 12.914 | 1939 | 1940 | 1944 | rVV  | 354     | 199     | 0.01%  | 0.001% |
| 86  | 12.975 | 1948 | 1950 | 1952 | rVB2 | 393     | 319     | 0.02%  | 0.002% |
| 87  | 13.110 | 1969 | 1972 | 1977 | rVV2 | 7712    | 10840   | 0.62%  | 0.081% |
| 88  | 13.170 | 1980 | 1982 | 1985 | rVV2 | 236     | 196     | 0.01%  | 0.001% |
| 89  | 13.231 | 1991 | 1992 | 1995 | rVB  | 372     | 236     | 0.01%  | 0.002% |
| 90  | 13.542 | 2042 | 2043 | 2045 | rBV2 | 240     | 193     | 0.01%  | 0.001% |
| 91  | 13.591 | 2047 | 2051 | 2058 | rVV  | 7353    | 9465    | 0.54%  | 0.071% |
| 92  | 13.707 | 2068 | 2070 | 2072 | rBV2 | 267     | 245     | 0.01%  | 0.002% |
| 93  | 13.780 | 2077 | 2082 | 2090 | rBV  | 7050    | 9068    | 0.52%  | 0.068% |
| 94  | 13.963 | 2105 | 2112 | 2117 | rVB2 | 7813    | 10662   | 0.61%  | 0.079% |
| 95  | 14.128 | 2137 | 2139 | 2143 | rVB3 | 625     | 694     | 0.04%  | 0.005% |
| 96  | 14.231 | 2154 | 2156 | 2158 | rBV2 | 413     | 385     | 0.02%  | 0.003% |
| 97  | 14.335 | 2169 | 2173 | 2176 | rVB2 | 388     | 630     | 0.04%  | 0.005% |
| 98  | 14.506 | 2199 | 2201 | 2202 | rBV  | 401     | 352     | 0.02%  | 0.003% |
| 99  | 15.024 | 2284 | 2286 | 2289 | rBV3 | 425     | 430     | 0.02%  | 0.003% |
| 100 | 15.091 | 2295 | 2297 | 2302 | rVB2 | 651     | 642     | 0.04%  | 0.005% |

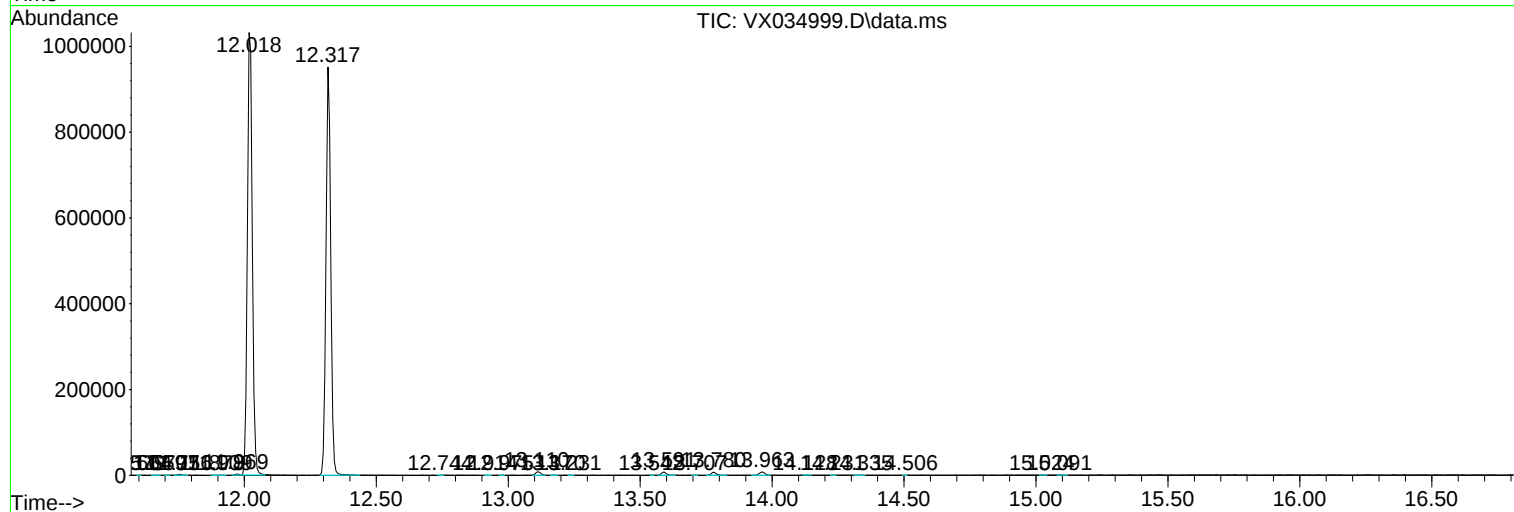
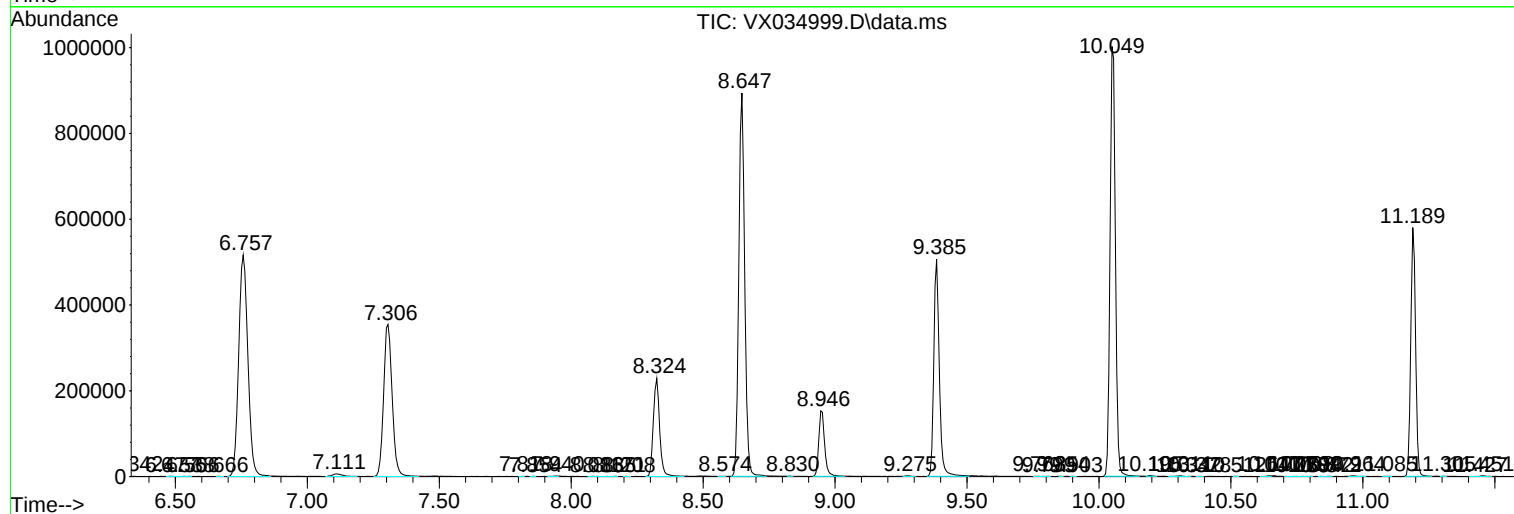
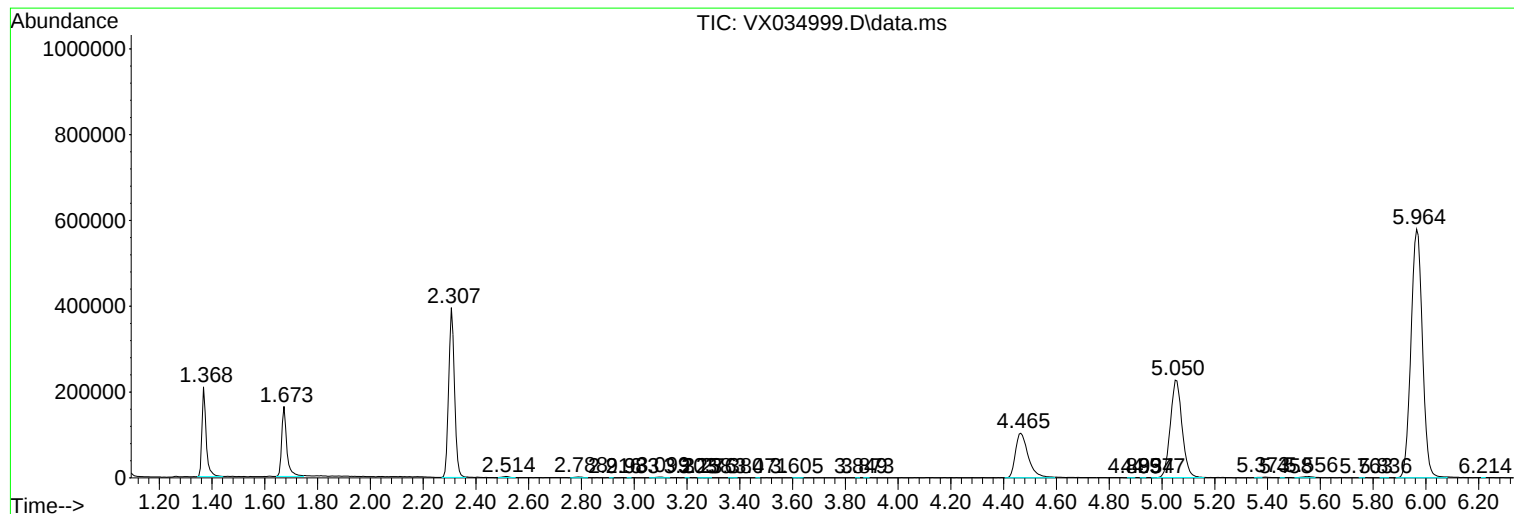
Sum of corrected areas: 13414036

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML041023WMA.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          |