

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121021\  
 Data File : VX025703.D  
 Acq On : 10 Dec 2021 15:51  
 Operator : JC/MD  
 Sample : M4888-11ME  
 Misc : 6.54g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX8B6ME

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\SFAMXML112221WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025703.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          | 55           | rVB      | 42184          | 47606         | 12.45%          | 1.564%        |
| 2         | 1.648       | 88            | 92          | 97           | rBV      | 28409          | 35493         | 9.29%           | 1.166%        |
| 3         | 2.276       | 189           | 195         | 206          | rBV      | 76647          | 130092        | 34.03%          | 4.274%        |
| 4         | 2.855       | 288           | 290         | 291          | rVB      | 385            | 261           | 0.07%           | 0.009%        |
| 5         | 2.953       | 298           | 306         | 322          | rBV      | 5248           | 16040         | 4.20%           | 0.527%        |
| 6         | 3.459       | 387           | 389         | 391          | rBV      | 353            | 369           | 0.10%           | 0.012%        |
| 7         | 3.635       | 416           | 418         | 419          | rBV2     | 406            | 310           | 0.08%           | 0.010%        |
| 8         | 3.776       | 439           | 441         | 442          | rVB      | 506            | 273           | 0.07%           | 0.009%        |
| 9         | 3.806       | 443           | 446         | 448          | rBV      | 296            | 313           | 0.08%           | 0.010%        |
| 10        | 4.129       | 497           | 499         | 501          | rBV      | 381            | 386           | 0.10%           | 0.013%        |
| 11        | 4.263       | 519           | 521         | 522          | rBV      | 430            | 273           | 0.07%           | 0.009%        |
| 12        | 4.507       | 550           | 561         | 587          | rBV      | 15862          | 76334         | 19.97%          | 2.508%        |
| 13        | 4.891       | 621           | 624         | 626          | rBV      | 321            | 369           | 0.10%           | 0.012%        |
| 14        | 4.971       | 635           | 637         | 638          | rBV      | 409            | 285           | 0.07%           | 0.009%        |
| 15        | 5.068       | 641           | 653         | 670          | rBV      | 45743          | 155598        | 40.71%          | 5.112%        |
| 16        | 5.233       | 678           | 680         | 683          | rBV2     | 367            | 504           | 0.13%           | 0.017%        |
| 17        | 5.702       | 755           | 757         | 759          | rBV      | 364            | 340           | 0.09%           | 0.011%        |
| 18        | 5.720       | 759           | 760         | 763          | rVB      | 364            | 351           | 0.09%           | 0.012%        |
| 19        | 5.855       | 780           | 782         | 784          | rBV      | 350            | 330           | 0.09%           | 0.011%        |
| 20        | 5.970       | 791           | 801         | 815          | rVB2     | 133467         | 382241        | 100.00%         | 12.559%       |
| 21        | 6.367       | 860           | 866         | 868          | rBV3     | 1980           | 3932          | 1.03%           | 0.129%        |
| 22        | 6.763       | 922           | 931         | 945          | rBV      | 98755          | 254199        | 66.50%          | 8.352%        |
| 23        | 7.117       | 983           | 989         | 995          | rBV7     | 1900           | 4705          | 1.23%           | 0.155%        |
| 24        | 7.208       | 1001          | 1004        | 1007         | rBV2     | 921            | 1514          | 0.40%           | 0.050%        |
| 25        | 7.312       | 1013          | 1021        | 1039         | rVB      | 72620          | 177231        | 46.37%          | 5.823%        |
| 26        | 7.501       | 1051          | 1052        | 1055         | rBV2     | 299            | 277           | 0.07%           | 0.009%        |
| 27        | 7.629       | 1071          | 1073        | 1077         | rVB      | 366            | 504           | 0.13%           | 0.017%        |
| 28        | 7.708       | 1084          | 1086        | 1089         | rBV2     | 249            | 315           | 0.08%           | 0.010%        |
| 29        | 8.098       | 1146          | 1150        | 1152         | rBV      | 454            | 533           | 0.14%           | 0.018%        |
| 30        | 8.116       | 1152          | 1153        | 1156         | rVV      | 267            | 275           | 0.07%           | 0.009%        |
| 31        | 8.147       | 1156          | 1158        | 1160         | rVV2     | 270            | 279           | 0.07%           | 0.009%        |
| 32        | 8.202       | 1165          | 1167        | 1171         | rVV2     | 256            | 349           | 0.09%           | 0.011%        |
| 33        | 8.275       | 1178          | 1179        | 1182         | rVB      | 483            | 307           | 0.08%           | 0.010%        |
| 34        | 8.330       | 1182          | 1188        | 1199         | rBV      | 51356          | 88937         | 23.27%          | 2.922%        |
| 35        | 8.653       | 1234          | 1241        | 1249         | rBV      | 191240         | 317429        | 83.04%          | 10.430%       |
| 36        | 8.726       | 1249          | 1253        | 1256         | rVB3     | 3107           | 4887          | 1.28%           | 0.161%        |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX8B6ME

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 8.878  | 1275 | 1278 | 1279 | rBV  | 299    | 319    | 0.08%  | 0.010%  |
| 38 | 8.958  | 1285 | 1291 | 1303 | rVB  | 32074  | 54040  | 14.14% | 1.776%  |
| 39 | 9.275  | 1338 | 1343 | 1347 | rVV3 | 4339   | 6213   | 1.63%  | 0.204%  |
| 40 | 9.403  | 1357 | 1364 | 1374 | rBV  | 98990  | 164768 | 43.11% | 5.414%  |
| 41 | 9.561  | 1388 | 1390 | 1395 | rVB4 | 577    | 880    | 0.23%  | 0.029%  |
| 42 | 9.628  | 1395 | 1401 | 1404 | rBV2 | 621    | 1108   | 0.29%  | 0.036%  |
| 43 | 9.915  | 1447 | 1448 | 1451 | rVB  | 495    | 274    | 0.07%  | 0.009%  |
| 44 | 9.957  | 1451 | 1455 | 1456 | rBV  | 459    | 546    | 0.14%  | 0.018%  |
| 45 | 9.976  | 1456 | 1458 | 1462 | rVB  | 400    | 314    | 0.08%  | 0.010%  |
| 46 | 10.061 | 1466 | 1472 | 1480 | rBV  | 206504 | 305135 | 79.83% | 10.026% |
| 47 | 10.171 | 1486 | 1490 | 1491 | rVB2 | 274    | 299    | 0.08%  | 0.010%  |
| 48 | 10.207 | 1491 | 1496 | 1498 | rBV2 | 543    | 770    | 0.20%  | 0.025%  |
| 49 | 10.250 | 1501 | 1503 | 1505 | rVB2 | 301    | 285    | 0.07%  | 0.009%  |
| 50 | 10.275 | 1505 | 1507 | 1508 | rBV2 | 339    | 269    | 0.07%  | 0.009%  |
| 51 | 10.305 | 1508 | 1512 | 1517 | rVB2 | 2390   | 3770   | 0.99%  | 0.124%  |
| 52 | 10.342 | 1517 | 1518 | 1520 | rBV  | 353    | 283    | 0.07%  | 0.009%  |
| 53 | 10.360 | 1520 | 1521 | 1523 | rBV2 | 336    | 271    | 0.07%  | 0.009%  |
| 54 | 10.549 | 1548 | 1552 | 1555 | rBV2 | 287    | 500    | 0.13%  | 0.016%  |
| 55 | 10.646 | 1565 | 1568 | 1575 | rVB2 | 2220   | 2919   | 0.76%  | 0.096%  |
| 56 | 10.701 | 1575 | 1577 | 1580 | rBV  | 231    | 295    | 0.08%  | 0.010%  |
| 57 | 10.787 | 1588 | 1591 | 1593 | rBV  | 406    | 413    | 0.11%  | 0.014%  |
| 58 | 10.811 | 1593 | 1595 | 1600 | rVB2 | 431    | 608    | 0.16%  | 0.020%  |
| 59 | 10.854 | 1600 | 1602 | 1607 | rBV  | 449    | 698    | 0.18%  | 0.023%  |
| 60 | 10.902 | 1607 | 1610 | 1614 | rBV2 | 393    | 477    | 0.12%  | 0.016%  |
| 61 | 10.970 | 1619 | 1621 | 1623 | rVB2 | 491    | 372    | 0.10%  | 0.012%  |
| 62 | 11.085 | 1639 | 1640 | 1643 | rBV  | 214    | 278    | 0.07%  | 0.009%  |
| 63 | 11.122 | 1643 | 1646 | 1650 | rVV4 | 1652   | 2206   | 0.58%  | 0.072%  |
| 64 | 11.195 | 1653 | 1658 | 1667 | rBV  | 135398 | 182316 | 47.70% | 5.990%  |
| 65 | 11.305 | 1674 | 1676 | 1682 | rVB5 | 827    | 1204   | 0.31%  | 0.040%  |
| 66 | 11.384 | 1685 | 1689 | 1694 | rBV3 | 591    | 1144   | 0.30%  | 0.038%  |
| 67 | 11.482 | 1702 | 1705 | 1708 | rVB3 | 717    | 900    | 0.24%  | 0.030%  |
| 68 | 11.616 | 1726 | 1727 | 1730 | rBV2 | 506    | 406    | 0.11%  | 0.013%  |
| 69 | 11.719 | 1740 | 1744 | 1746 | rBV3 | 522    | 845    | 0.22%  | 0.028%  |
| 70 | 11.750 | 1746 | 1749 | 1756 | rVB3 | 2575   | 3778   | 0.99%  | 0.124%  |
| 71 | 11.823 | 1760 | 1761 | 1763 | rBV  | 357    | 269    | 0.07%  | 0.009%  |
| 72 | 11.847 | 1763 | 1765 | 1767 | rBV2 | 359    | 291    | 0.08%  | 0.010%  |
| 73 | 11.933 | 1776 | 1779 | 1783 | rBV2 | 650    | 786    | 0.21%  | 0.026%  |
| 74 | 11.963 | 1783 | 1784 | 1789 | rVB  | 343    | 497    | 0.13%  | 0.016%  |
| 75 | 12.024 | 1789 | 1794 | 1802 | rBV  | 242633 | 298640 | 78.13% | 9.812%  |
| 76 | 12.268 | 1833 | 1834 | 1837 | rBV2 | 359    | 418    | 0.11%  | 0.014%  |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX8B6ME

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

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.323 | 1838 | 1843 | 1850 | rVB  | 219272 | 280639 | 73.42% | 9.221% |
| 78  | 12.427 | 1857 | 1860 | 1864 | rVB4 | 1339   | 1732   | 0.45%  | 0.057% |
| 79  | 12.628 | 1891 | 1893 | 1895 | rBV2 | 311    | 337    | 0.09%  | 0.011% |
| 80  | 12.664 | 1897 | 1899 | 1900 | rBV  | 434    | 394    | 0.10%  | 0.013% |
| 81  | 12.768 | 1913 | 1916 | 1918 | rBV  | 550    | 586    | 0.15%  | 0.019% |
| 82  | 12.969 | 1948 | 1949 | 1953 | rVB2 | 405    | 398    | 0.10%  | 0.013% |
| 83  | 13.054 | 1961 | 1963 | 1966 | rBV2 | 451    | 483    | 0.13%  | 0.016% |
| 84  | 13.183 | 1983 | 1984 | 1987 | rBV  | 304    | 297    | 0.08%  | 0.010% |
| 85  | 13.268 | 1993 | 1998 | 2005 | rBV4 | 857    | 1421   | 0.37%  | 0.047% |
| 86  | 13.475 | 2028 | 2032 | 2033 | rBV  | 376    | 426    | 0.11%  | 0.014% |
| 87  | 13.780 | 2079 | 2082 | 2086 | rVB  | 3190   | 3588   | 0.94%  | 0.118% |
| 88  | 14.042 | 2122 | 2125 | 2127 | rVB2 | 984    | 1004   | 0.26%  | 0.033% |
| 89  | 14.134 | 2136 | 2140 | 2145 | rVB3 | 699    | 1127   | 0.29%  | 0.037% |
| 90  | 14.609 | 2215 | 2218 | 2220 | rBV2 | 854    | 953    | 0.25%  | 0.031% |
| 91  | 14.646 | 2220 | 2224 | 2228 | rVB2 | 897    | 1568   | 0.41%  | 0.052% |
| 92  | 14.755 | 2239 | 2242 | 2244 | rBV2 | 1233   | 1214   | 0.32%  | 0.040% |
| 93  | 14.841 | 2254 | 2256 | 2260 | rBV2 | 465    | 633    | 0.17%  | 0.021% |
| 94  | 15.213 | 2314 | 2317 | 2321 | rVB2 | 1117   | 1081   | 0.28%  | 0.036% |
| 95  | 15.292 | 2328 | 2330 | 2332 | rBV2 | 287    | 274    | 0.07%  | 0.009% |
| 96  | 15.335 | 2335 | 2337 | 2341 | rBV2 | 357    | 327    | 0.09%  | 0.011% |
| 97  | 16.176 | 2473 | 2475 | 2477 | rVB2 | 523    | 458    | 0.12%  | 0.015% |
| 98  | 16.206 | 2477 | 2480 | 2481 | rBV3 | 405    | 438    | 0.11%  | 0.014% |
| 99  | 16.347 | 2502 | 2503 | 2506 | rBV  | 437    | 352    | 0.09%  | 0.012% |
| 100 | 16.694 | 2557 | 2560 | 2563 | rBV  | 354    | 590    | 0.15%  | 0.019% |

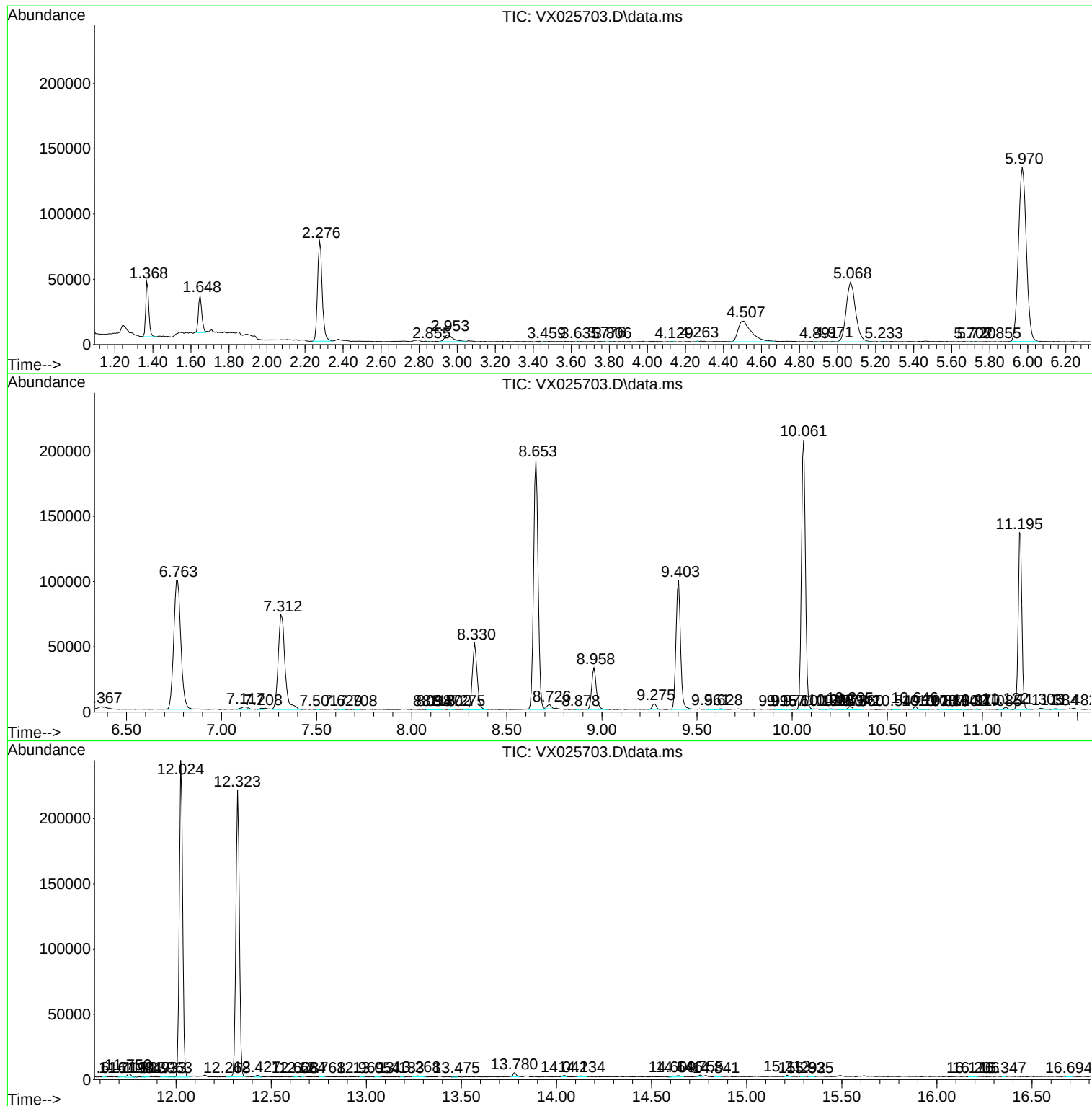
Sum of corrected areas: 3043565

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Instrument :  
MSVOA\_X  
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EX8B6ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121021\  
Data File : VX025703.D  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML112221WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.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 |