

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061322\  
 Data File : VX029454.D  
 Acq On : 14 Jun 2022 07:42  
 Operator : JC/MD  
 Sample : N3311-06  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 56 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0E06

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\SFAMXML061322WMA.M  
 Title : VOC Analysis

Signal : TIC: VX029454.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          | 53           | rVB      | 171417         | 168509        | 5.57%           | 1.224%        |
| 2         | 1.666       | 91            | 95          | 104          | rVB      | 129122         | 155563        | 5.14%           | 1.130%        |
| 3         | 2.313       | 194           | 201         | 211          | rBV2     | 316813         | 593947        | 19.62%          | 4.316%        |
| 4         | 2.709       | 261           | 266         | 268          | rBV2     | 783            | 969           | 0.03%           | 0.007%        |
| 5         | 2.788       | 276           | 279         | 284          | rVB2     | 856            | 1228          | 0.04%           | 0.009%        |
| 6         | 2.940       | 301           | 304         | 309          | rBV3     | 859            | 1548          | 0.05%           | 0.011%        |
| 7         | 3.026       | 316           | 318         | 320          | rBV2     | 420            | 488           | 0.02%           | 0.004%        |
| 8         | 3.099       | 326           | 330         | 332          | rBV2     | 765            | 1016          | 0.03%           | 0.007%        |
| 9         | 3.617       | 409           | 415         | 424          | rVB3     | 2215           | 5720          | 0.19%           | 0.042%        |
| 10        | 3.703       | 427           | 429         | 432          | rBV2     | 301            | 289           | 0.01%           | 0.002%        |
| 11        | 3.818       | 446           | 448         | 451          | rBV2     | 201            | 255           | 0.01%           | 0.002%        |
| 12        | 3.843       | 451           | 452         | 455          | rVB2     | 276            | 247           | 0.01%           | 0.002%        |
| 13        | 3.892       | 457           | 460         | 461          | rBV      | 297            | 285           | 0.01%           | 0.002%        |
| 14        | 4.215       | 509           | 513         | 514          | rBV2     | 363            | 352           | 0.01%           | 0.003%        |
| 15        | 4.251       | 517           | 519         | 520          | rBV      | 302            | 251           | 0.01%           | 0.002%        |
| 16        | 4.324       | 529           | 531         | 534          | rVB2     | 330            | 263           | 0.01%           | 0.002%        |
| 17        | 4.477       | 544           | 556         | 573          | rBV2     | 135280         | 539516        | 17.82%          | 3.920%        |
| 18        | 4.727       | 595           | 597         | 599          | rVB2     | 439            | 295           | 0.01%           | 0.002%        |
| 19        | 4.745       | 599           | 600         | 602          | rBV      | 246            | 235           | 0.01%           | 0.002%        |
| 20        | 4.916       | 625           | 628         | 629          | rBV      | 314            | 233           | 0.01%           | 0.002%        |
| 21        | 4.940       | 629           | 632         | 633          | rBV      | 284            | 241           | 0.01%           | 0.002%        |
| 22        | 5.062       | 639           | 652         | 670          | rBV      | 181509         | 547022        | 18.07%          | 3.975%        |
| 23        | 5.385       | 695           | 705         | 719          | rVB      | 38943          | 118527        | 3.92%           | 0.861%        |
| 24        | 5.483       | 719           | 721         | 725          | rBV3     | 260            | 435           | 0.01%           | 0.003%        |
| 25        | 5.653       | 748           | 749         | 752          | rBV2     | 533            | 435           | 0.01%           | 0.003%        |
| 26        | 5.720       | 759           | 760         | 763          | rVB2     | 314            | 233           | 0.01%           | 0.002%        |
| 27        | 5.800       | 771           | 773         | 774          | rVV      | 362            | 273           | 0.01%           | 0.002%        |
| 28        | 5.970       | 789           | 801         | 817          | rBV2     | 449485         | 1331742       | 43.99%          | 9.677%        |
| 29        | 6.251       | 844           | 847         | 848          | rVB      | 372            | 331           | 0.01%           | 0.002%        |
| 30        | 6.306       | 854           | 856         | 859          | rVB2     | 263            | 245           | 0.01%           | 0.002%        |
| 31        | 6.422       | 874           | 875         | 878          | rBV      | 399            | 362           | 0.01%           | 0.003%        |
| 32        | 6.458       | 878           | 881         | 885          | rVV      | 621            | 690           | 0.02%           | 0.005%        |
| 33        | 6.617       | 901           | 907         | 908          | rBV2     | 302            | 505           | 0.02%           | 0.004%        |
| 34        | 6.678       | 916           | 917         | 920          | rVB      | 356            | 229           | 0.01%           | 0.002%        |
| 35        | 6.763       | 920           | 931         | 942          | rBV      | 348591         | 828090        | 27.36%          | 6.017%        |
| 36        | 7.129       | 981           | 991         | 1012         | rBV      | 1422977        | 3027032       | 100.00%         | 21.995%       |

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 ALS Vial : 56 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0E06

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\SFAMXML061322WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 7.312  | 1012 | 1021 | 1036 | rVB  | 272485 | 594709  | 19.65% | 4.321% |
| 38 | 7.482  | 1045 | 1049 | 1054 | rBV4 | 1048   | 1575    | 0.05%  | 0.011% |
| 39 | 7.616  | 1069 | 1071 | 1073 | rVB2 | 316    | 223     | 0.01%  | 0.002% |
| 40 | 7.836  | 1106 | 1107 | 1109 | rVB2 | 354    | 219     | 0.01%  | 0.002% |
| 41 | 7.933  | 1119 | 1123 | 1125 | rBV3 | 1107   | 1511    | 0.05%  | 0.011% |
| 42 | 8.324  | 1181 | 1187 | 1201 | rBV  | 158904 | 268619  | 8.87%  | 1.952% |
| 43 | 8.482  | 1211 | 1213 | 1214 | rBV2 | 646    | 441     | 0.01%  | 0.003% |
| 44 | 8.580  | 1227 | 1229 | 1232 | rVB2 | 380    | 388     | 0.01%  | 0.003% |
| 45 | 8.653  | 1234 | 1241 | 1249 | rVV  | 688714 | 1068872 | 35.31% | 7.767% |
| 46 | 8.720  | 1249 | 1252 | 1262 | rVB2 | 9631   | 16655   | 0.55%  | 0.121% |
| 47 | 8.848  | 1271 | 1273 | 1276 | rBV3 | 349    | 391     | 0.01%  | 0.003% |
| 48 | 8.952  | 1284 | 1290 | 1297 | rBV  | 114799 | 168423  | 5.56%  | 1.224% |
| 49 | 9.104  | 1313 | 1315 | 1318 | rVB2 | 298    | 267     | 0.01%  | 0.002% |
| 50 | 9.159  | 1318 | 1324 | 1329 | rVB4 | 2099   | 3678    | 0.12%  | 0.027% |
| 51 | 9.202  | 1329 | 1331 | 1334 | rBV2 | 305    | 372     | 0.01%  | 0.003% |
| 52 | 9.275  | 1340 | 1343 | 1347 | rVB4 | 2140   | 2791    | 0.09%  | 0.020% |
| 53 | 9.384  | 1356 | 1361 | 1377 | rBV  | 526353 | 760841  | 25.13% | 5.528% |
| 54 | 9.732  | 1416 | 1418 | 1422 | rVB2 | 291    | 242     | 0.01%  | 0.002% |
| 55 | 9.982  | 1455 | 1459 | 1462 | rBV3 | 390    | 748     | 0.02%  | 0.005% |
| 56 | 10.055 | 1465 | 1471 | 1483 | rVV  | 731858 | 965171  | 31.89% | 7.013% |
| 57 | 10.171 | 1487 | 1490 | 1492 | rVV4 | 979    | 1271    | 0.04%  | 0.009% |
| 58 | 10.195 | 1492 | 1494 | 1496 | rVB2 | 632    | 507     | 0.02%  | 0.004% |
| 59 | 10.305 | 1508 | 1512 | 1517 | rBV4 | 1004   | 1617    | 0.05%  | 0.012% |
| 60 | 10.445 | 1533 | 1535 | 1537 | rVB  | 440    | 283     | 0.01%  | 0.002% |
| 61 | 10.579 | 1553 | 1557 | 1559 | rBV2 | 272    | 391     | 0.01%  | 0.003% |
| 62 | 10.646 | 1566 | 1568 | 1572 | rVB  | 728    | 734     | 0.02%  | 0.005% |
| 63 | 10.677 | 1572 | 1573 | 1575 | rBV2 | 304    | 256     | 0.01%  | 0.002% |
| 64 | 10.976 | 1617 | 1622 | 1624 | rBV3 | 363    | 572     | 0.02%  | 0.004% |
| 65 | 11.030 | 1629 | 1631 | 1633 | rBV  | 482    | 372     | 0.01%  | 0.003% |
| 66 | 11.116 | 1643 | 1645 | 1650 | rVB3 | 1213   | 1603    | 0.05%  | 0.012% |
| 67 | 11.195 | 1652 | 1658 | 1670 | rVV  | 530783 | 689828  | 22.79% | 5.012% |
| 68 | 11.360 | 1683 | 1685 | 1688 | rBV2 | 217    | 234     | 0.01%  | 0.002% |
| 69 | 11.390 | 1688 | 1690 | 1694 | rVB2 | 395    | 455     | 0.02%  | 0.003% |
| 70 | 11.457 | 1699 | 1701 | 1703 | rBV2 | 506    | 432     | 0.01%  | 0.003% |
| 71 | 11.543 | 1714 | 1715 | 1717 | rVB  | 552    | 230     | 0.01%  | 0.002% |
| 72 | 11.604 | 1722 | 1725 | 1726 | rBV2 | 205    | 247     | 0.01%  | 0.002% |
| 73 | 11.689 | 1734 | 1739 | 1740 | rBV2 | 268    | 391     | 0.01%  | 0.003% |
| 74 | 11.713 | 1741 | 1743 | 1746 | rVB  | 415    | 239     | 0.01%  | 0.002% |
| 75 | 11.756 | 1746 | 1750 | 1755 | rBV3 | 2014   | 2619    | 0.09%  | 0.019% |
| 76 | 11.835 | 1761 | 1763 | 1765 | rVB2 | 282    | 226     | 0.01%  | 0.002% |

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 ALS Vial : 56 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

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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\SFAMXML061322WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.933 | 1777 | 1779 | 1783 | rVB2 | 584    | 461    | 0.02%  | 0.003% |
| 78  | 12.024 | 1788 | 1794 | 1803 | rBV  | 754273 | 939256 | 31.03% | 6.825% |
| 79  | 12.225 | 1824 | 1827 | 1829 | rBV2 | 502    | 481    | 0.02%  | 0.003% |
| 80  | 12.262 | 1831 | 1833 | 1836 | rBV2 | 284    | 259    | 0.01%  | 0.002% |
| 81  | 12.323 | 1837 | 1843 | 1853 | rBV  | 718996 | 929381 | 30.70% | 6.753% |
| 82  | 12.457 | 1863 | 1865 | 1868 | rVB2 | 468    | 349    | 0.01%  | 0.003% |
| 83  | 12.494 | 1868 | 1871 | 1872 | rVB2 | 312    | 336    | 0.01%  | 0.002% |
| 84  | 12.518 | 1872 | 1875 | 1877 | rBV2 | 352    | 374    | 0.01%  | 0.003% |
| 85  | 12.542 | 1877 | 1879 | 1881 | rBV2 | 441    | 354    | 0.01%  | 0.003% |
| 86  | 12.792 | 1918 | 1920 | 1922 | rVB  | 353    | 219    | 0.01%  | 0.002% |
| 87  | 12.835 | 1925 | 1927 | 1928 | rBV  | 341    | 268    | 0.01%  | 0.002% |
| 88  | 13.006 | 1952 | 1955 | 1956 | rBV2 | 270    | 248    | 0.01%  | 0.002% |
| 89  | 13.140 | 1976 | 1977 | 1979 | rBV  | 317    | 231    | 0.01%  | 0.002% |
| 90  | 13.280 | 1996 | 2000 | 2001 | rBV2 | 240    | 287    | 0.01%  | 0.002% |
| 91  | 13.359 | 2011 | 2013 | 2015 | rVV  | 243    | 213    | 0.01%  | 0.002% |
| 92  | 13.408 | 2019 | 2021 | 2024 | rBV2 | 307    | 237    | 0.01%  | 0.002% |
| 93  | 13.500 | 2034 | 2036 | 2039 | rBV2 | 268    | 295    | 0.01%  | 0.002% |
| 94  | 13.664 | 2062 | 2063 | 2065 | rBV2 | 280    | 216    | 0.01%  | 0.002% |
| 95  | 13.719 | 2070 | 2072 | 2075 | rBV2 | 405    | 436    | 0.01%  | 0.003% |
| 96  | 13.987 | 2115 | 2116 | 2118 | rBV2 | 494    | 301    | 0.01%  | 0.002% |
| 97  | 14.018 | 2119 | 2121 | 2124 | rVB2 | 558    | 563    | 0.02%  | 0.004% |
| 98  | 14.316 | 2168 | 2170 | 2172 | rVB2 | 377    | 340    | 0.01%  | 0.002% |
| 99  | 15.585 | 2376 | 2378 | 2381 | rBV2 | 572    | 616    | 0.02%  | 0.004% |
| 100 | 16.066 | 2455 | 2457 | 2458 | rBV  | 546    | 355    | 0.01%  | 0.003% |

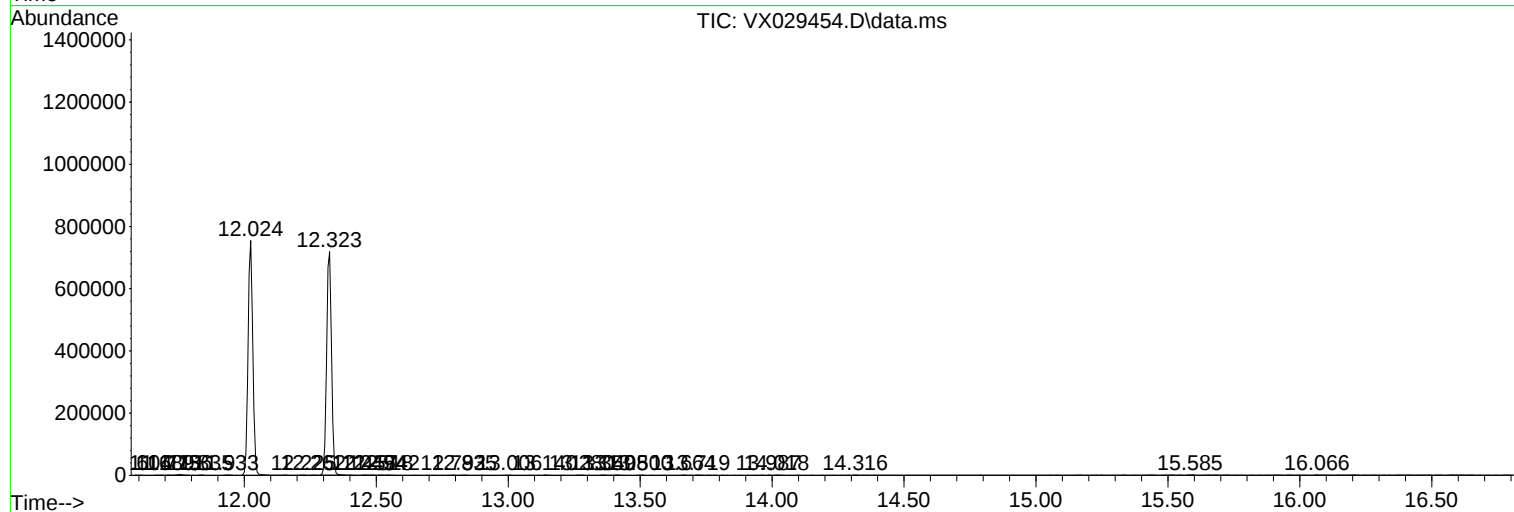
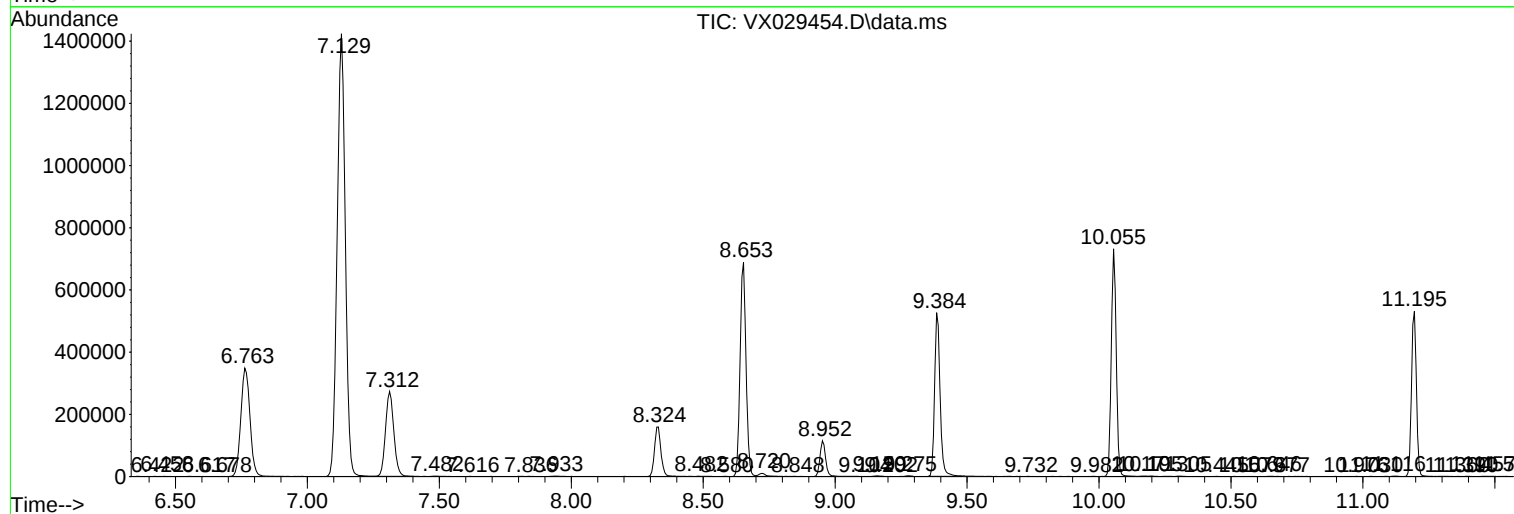
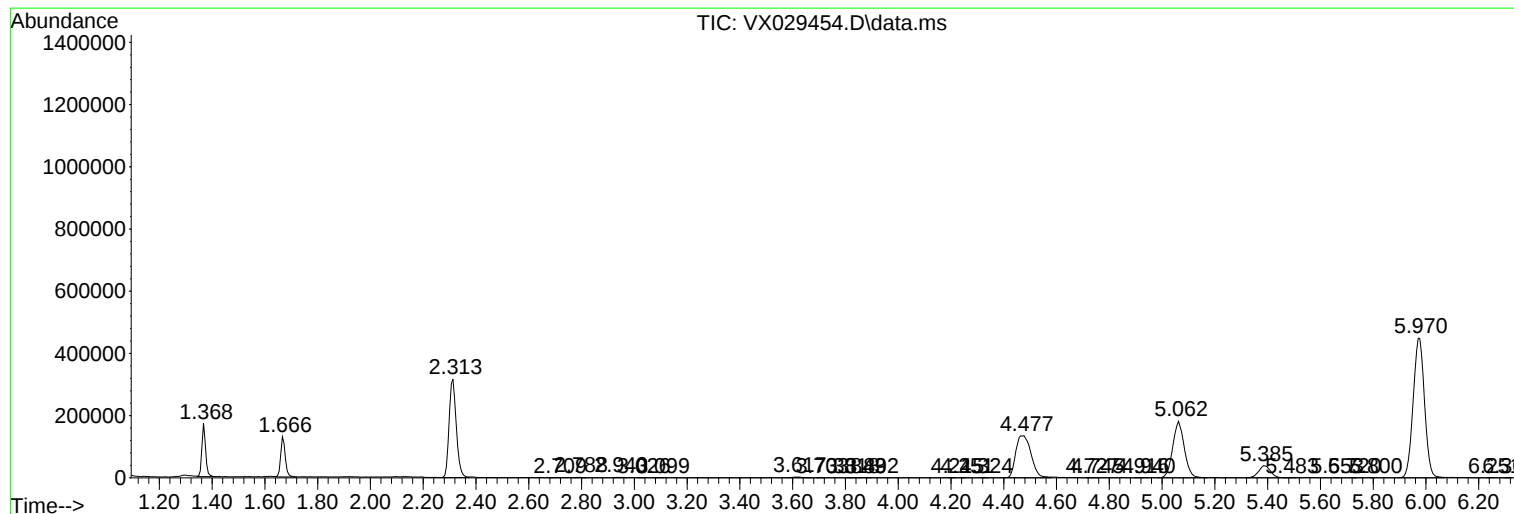
Sum of corrected areas: 13762320

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Instrument :  
MSVOA\_X  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML061322WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061322\  
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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 |