

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX081022\  
 Data File : VX030540.D  
 Acq On : 10 Aug 2022 09:44  
 Operator : JC/MD  
 Sample : VX0810MBL01  
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK677

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\SFAMXML080422WMA.M  
 Title : VOC Analysis

Signal : TIC: VX030540.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          | 56           | rVB      | 150436         | 155271        | 12.53%          | 1.641%        |
| 2         | 1.672       | 91            | 96          | 104          | rBV      | 117219         | 144342        | 11.65%          | 1.525%        |
| 3         | 2.307       | 194           | 200         | 211          | rVB      | 242876         | 380154        | 30.68%          | 4.018%        |
| 4         | 2.508       | 229           | 233         | 237          | rVB4     | 1485           | 2174          | 0.18%           | 0.023%        |
| 5         | 2.599       | 246           | 248         | 252          | rVB3     | 422            | 520           | 0.04%           | 0.005%        |
| 6         | 2.794       | 275           | 280         | 288          | rVV5     | 1880           | 3840          | 0.31%           | 0.041%        |
| 7         | 2.947       | 299           | 305         | 310          | rBV4     | 1905           | 4132          | 0.33%           | 0.044%        |
| 8         | 3.093       | 327           | 329         | 335          | rVB3     | 538            | 1011          | 0.08%           | 0.011%        |
| 9         | 3.160       | 337           | 340         | 342          | rBV2     | 274            | 405           | 0.03%           | 0.004%        |
| 10        | 3.178       | 342           | 343         | 348          | rBV3     | 309            | 441           | 0.04%           | 0.005%        |
| 11        | 3.416       | 381           | 382         | 385          | rBV2     | 490            | 486           | 0.04%           | 0.005%        |
| 12        | 3.514       | 395           | 398         | 401          | rVB3     | 421            | 624           | 0.05%           | 0.007%        |
| 13        | 3.556       | 401           | 405         | 407          | rBV2     | 512            | 619           | 0.05%           | 0.007%        |
| 14        | 3.636       | 416           | 418         | 421          | rVV2     | 455            | 457           | 0.04%           | 0.005%        |
| 15        | 3.678       | 423           | 425         | 428          | rVB2     | 399            | 488           | 0.04%           | 0.005%        |
| 16        | 3.770       | 437           | 440         | 442          | rBV2     | 416            | 406           | 0.03%           | 0.004%        |
| 17        | 3.867       | 452           | 456         | 457          | rVB2     | 427            | 507           | 0.04%           | 0.005%        |
| 18        | 3.879       | 457           | 458         | 460          | rBV2     | 411            | 420           | 0.03%           | 0.004%        |
| 19        | 4.093       | 490           | 493         | 494          | rVB      | 546            | 444           | 0.04%           | 0.005%        |
| 20        | 4.123       | 494           | 498         | 499          | rBV2     | 500            | 572           | 0.05%           | 0.006%        |
| 21        | 4.251       | 515           | 519         | 520          | rBV2     | 454            | 540           | 0.04%           | 0.006%        |
| 22        | 4.471       | 545           | 555         | 570          | rBV      | 109733         | 336403        | 27.15%          | 3.555%        |
| 23        | 5.062       | 640           | 652         | 669          | rVV      | 170671         | 518139        | 41.82%          | 5.476%        |
| 24        | 5.215       | 673           | 677         | 679          | rBV3     | 422            | 581           | 0.05%           | 0.006%        |
| 25        | 5.361       | 699           | 701         | 702          | rBV      | 526            | 391           | 0.03%           | 0.004%        |
| 26        | 5.379       | 702           | 704         | 707          | rBV3     | 988            | 1135          | 0.09%           | 0.012%        |
| 27        | 5.519       | 725           | 727         | 728          | rBV      | 741            | 453           | 0.04%           | 0.005%        |
| 28        | 5.568       | 728           | 735         | 738          | rVV5     | 1640           | 3883          | 0.31%           | 0.041%        |
| 29        | 5.769       | 763           | 768         | 770          | rBV2     | 362            | 720           | 0.06%           | 0.008%        |
| 30        | 5.971       | 789           | 801         | 817          | rBV2     | 425538         | 1238925       | 100.00%         | 13.093%       |
| 31        | 6.245       | 845           | 846         | 849          | rBV      | 435            | 526           | 0.04%           | 0.006%        |
| 32        | 6.409       | 872           | 873         | 875          | rBV      | 568            | 397           | 0.03%           | 0.004%        |
| 33        | 6.763       | 921           | 931         | 943          | rBV      | 310613         | 738956        | 59.64%          | 7.809%        |
| 34        | 6.970       | 964           | 965         | 968          | rVB2     | 460            | 405           | 0.03%           | 0.004%        |
| 35        | 7.056       | 977           | 979         | 981          | rBV2     | 585            | 437           | 0.04%           | 0.005%        |
| 36        | 7.111       | 981           | 988         | 998          | rVB4     | 11290          | 26130         | 2.11%           | 0.276%        |

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Instrument :  
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 VBLK677

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\SFAMXML080422WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.312  | 1010 | 1021 | 1034 | rBV  | 255535 | 575094 | 46.42% | 6.078%  |
| 38 | 7.482  | 1045 | 1049 | 1052 | rVB3 | 774    | 1344   | 0.11%  | 0.014%  |
| 39 | 7.940  | 1122 | 1124 | 1125 | rBV  | 464    | 451    | 0.04%  | 0.005%  |
| 40 | 8.086  | 1147 | 1148 | 1154 | rBV3 | 618    | 791    | 0.06%  | 0.008%  |
| 41 | 8.135  | 1154 | 1156 | 1158 | rVB  | 600    | 537    | 0.04%  | 0.006%  |
| 42 | 8.208  | 1167 | 1168 | 1172 | rVB  | 691    | 647    | 0.05%  | 0.007%  |
| 43 | 8.324  | 1180 | 1187 | 1202 | rBV  | 177072 | 298819 | 24.12% | 3.158%  |
| 44 | 8.562  | 1224 | 1226 | 1228 | rVV2 | 521    | 461    | 0.04%  | 0.005%  |
| 45 | 8.647  | 1234 | 1240 | 1251 | rBV  | 592194 | 948768 | 76.58% | 10.027% |
| 46 | 8.952  | 1283 | 1290 | 1302 | rBV  | 134394 | 201406 | 16.26% | 2.128%  |
| 47 | 9.147  | 1319 | 1322 | 1324 | rBV3 | 714    | 557    | 0.04%  | 0.006%  |
| 48 | 9.269  | 1341 | 1342 | 1346 | rBV4 | 709    | 699    | 0.06%  | 0.007%  |
| 49 | 9.385  | 1356 | 1361 | 1376 | rBV  | 507886 | 726375 | 58.63% | 7.676%  |
| 50 | 9.647  | 1403 | 1404 | 1408 | rVB3 | 769    | 671    | 0.05%  | 0.007%  |
| 51 | 9.702  | 1408 | 1413 | 1420 | rBV3 | 2922   | 4540   | 0.37%  | 0.048%  |
| 52 | 9.830  | 1433 | 1434 | 1437 | rBV  | 538    | 567    | 0.05%  | 0.006%  |
| 53 | 10.055 | 1465 | 1471 | 1483 | rBV  | 648908 | 858690 | 69.31% | 9.075%  |
| 54 | 10.201 | 1493 | 1495 | 1497 | rBV2 | 964    | 546    | 0.04%  | 0.006%  |
| 55 | 10.305 | 1509 | 1512 | 1516 | rVV3 | 1190   | 1721   | 0.14%  | 0.018%  |
| 56 | 10.488 | 1539 | 1542 | 1544 | rVB2 | 387    | 375    | 0.03%  | 0.004%  |
| 57 | 10.598 | 1557 | 1560 | 1561 | rBV2 | 565    | 568    | 0.05%  | 0.006%  |
| 58 | 10.659 | 1564 | 1570 | 1576 | rBV4 | 1077   | 2259   | 0.18%  | 0.024%  |
| 59 | 10.964 | 1618 | 1620 | 1625 | rVB4 | 914    | 1329   | 0.11%  | 0.014%  |
| 60 | 11.085 | 1639 | 1640 | 1644 | rBV2 | 323    | 449    | 0.04%  | 0.005%  |
| 61 | 11.134 | 1646 | 1648 | 1651 | rBV  | 457    | 453    | 0.04%  | 0.005%  |
| 62 | 11.195 | 1652 | 1658 | 1671 | rVB  | 472999 | 600771 | 48.49% | 6.349%  |
| 63 | 11.427 | 1692 | 1696 | 1698 | rBV2 | 444    | 663    | 0.05%  | 0.007%  |
| 64 | 11.451 | 1698 | 1700 | 1704 | rVB2 | 988    | 1316   | 0.11%  | 0.014%  |
| 65 | 11.500 | 1707 | 1708 | 1712 | rBV2 | 526    | 689    | 0.06%  | 0.007%  |
| 66 | 11.579 | 1718 | 1721 | 1723 | rBV2 | 658    | 771    | 0.06%  | 0.008%  |
| 67 | 11.604 | 1723 | 1725 | 1729 | rVV  | 432    | 473    | 0.04%  | 0.005%  |
| 68 | 11.756 | 1746 | 1750 | 1754 | rBV2 | 1063   | 1479   | 0.12%  | 0.016%  |
| 69 | 11.884 | 1768 | 1771 | 1775 | rVB2 | 573    | 657    | 0.05%  | 0.007%  |
| 70 | 11.921 | 1775 | 1777 | 1780 | rBV2 | 427    | 552    | 0.04%  | 0.006%  |
| 71 | 11.976 | 1780 | 1786 | 1788 | rBV4 | 1473   | 2095   | 0.17%  | 0.022%  |
| 72 | 12.024 | 1788 | 1794 | 1804 | rVV  | 660258 | 797512 | 64.37% | 8.428%  |
| 73 | 12.189 | 1815 | 1821 | 1823 | rBV2 | 693    | 1523   | 0.12%  | 0.016%  |
| 74 | 12.219 | 1823 | 1826 | 1833 | rBV6 | 2516   | 3301   | 0.27%  | 0.035%  |
| 75 | 12.323 | 1837 | 1843 | 1849 | rBV  | 642124 | 816596 | 65.91% | 8.630%  |
| 76 | 12.536 | 1876 | 1878 | 1880 | rBV  | 546    | 400    | 0.03%  | 0.004%  |

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 ALS Vial : 3 Sample Multiplier: 1

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

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Smoothing : OFF

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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\SFAMXML080422WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |       |       |        |
|-----|--------|------|------|------|------|------|-------|-------|--------|
| 77  | 12.579 | 1883 | 1885 | 1888 | rVB2 | 572  | 431   | 0.03% | 0.005% |
| 78  | 12.731 | 1908 | 1910 | 1912 | rBV  | 567  | 446   | 0.04% | 0.005% |
| 79  | 12.914 | 1937 | 1940 | 1941 | rVB  | 549  | 392   | 0.03% | 0.004% |
| 80  | 12.969 | 1947 | 1949 | 1952 | rVB2 | 488  | 425   | 0.03% | 0.004% |
| 81  | 13.055 | 1960 | 1963 | 1966 | rBV  | 416  | 389   | 0.03% | 0.004% |
| 82  | 13.116 | 1970 | 1973 | 1977 | rVB3 | 1814 | 2268  | 0.18% | 0.024% |
| 83  | 13.256 | 1995 | 1996 | 1998 | rBV  | 757  | 414   | 0.03% | 0.004% |
| 84  | 13.292 | 1998 | 2002 | 2003 | rBV2 | 490  | 560   | 0.05% | 0.006% |
| 85  | 13.591 | 2047 | 2051 | 2055 | rVB4 | 1978 | 2857  | 0.23% | 0.030% |
| 86  | 13.664 | 2061 | 2063 | 2064 | rBV  | 482  | 458   | 0.04% | 0.005% |
| 87  | 13.737 | 2074 | 2075 | 2077 | rBV  | 387  | 375   | 0.03% | 0.004% |
| 88  | 13.762 | 2077 | 2079 | 2080 | rVV2 | 765  | 580   | 0.05% | 0.006% |
| 89  | 13.780 | 2080 | 2082 | 2086 | rVB3 | 2287 | 2531  | 0.20% | 0.027% |
| 90  | 13.963 | 2109 | 2112 | 2116 | rBV4 | 1878 | 2565  | 0.21% | 0.027% |
| 91  | 14.042 | 2121 | 2125 | 2126 | rBV2 | 676  | 553   | 0.04% | 0.006% |
| 92  | 14.085 | 2130 | 2132 | 2135 | rVV3 | 598  | 672   | 0.05% | 0.007% |
| 93  | 14.128 | 2137 | 2139 | 2141 | rVV2 | 1015 | 707   | 0.06% | 0.007% |
| 94  | 14.341 | 2172 | 2174 | 2177 | rBV2 | 662  | 376   | 0.03% | 0.004% |
| 95  | 14.524 | 2200 | 2204 | 2206 | rBV2 | 638  | 916   | 0.07% | 0.010% |
| 96  | 14.548 | 2206 | 2208 | 2209 | rVB2 | 732  | 445   | 0.04% | 0.005% |
| 97  | 14.627 | 2209 | 2221 | 2225 | rBV6 | 6449 | 19654 | 1.59% | 0.208% |
| 98  | 15.298 | 2329 | 2331 | 2333 | rBV2 | 1065 | 803   | 0.06% | 0.008% |
| 99  | 16.109 | 2463 | 2464 | 2467 | rBV3 | 778  | 646   | 0.05% | 0.007% |
| 100 | 16.274 | 2489 | 2491 | 2492 | rBV  | 870  | 683   | 0.06% | 0.007% |

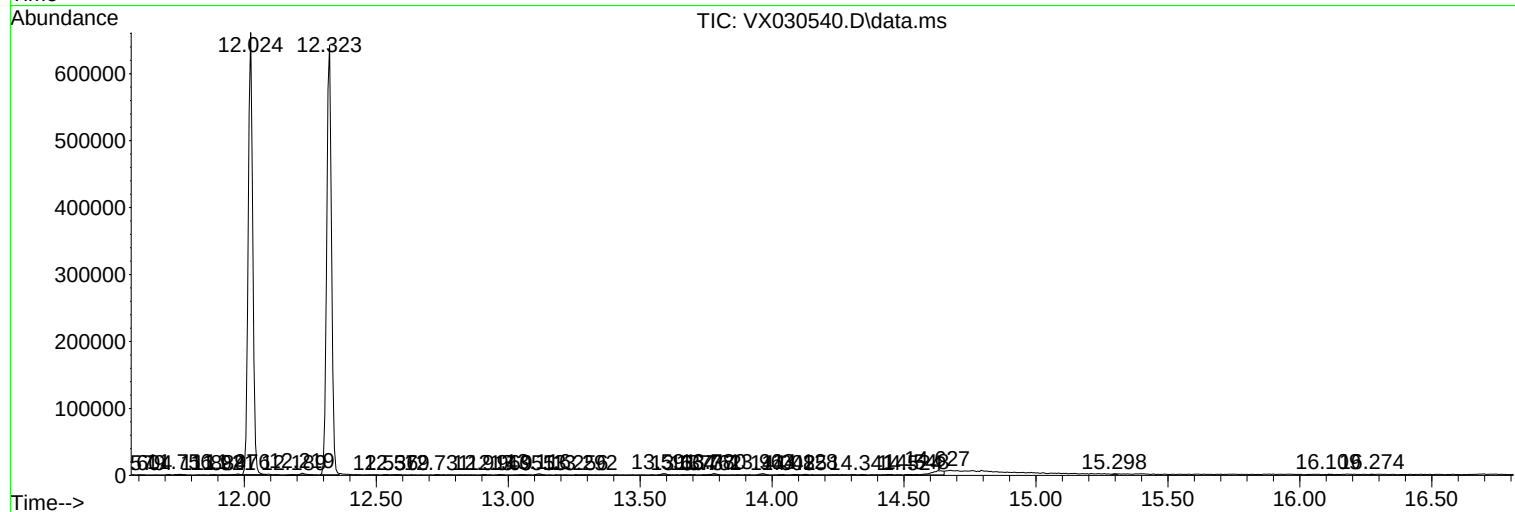
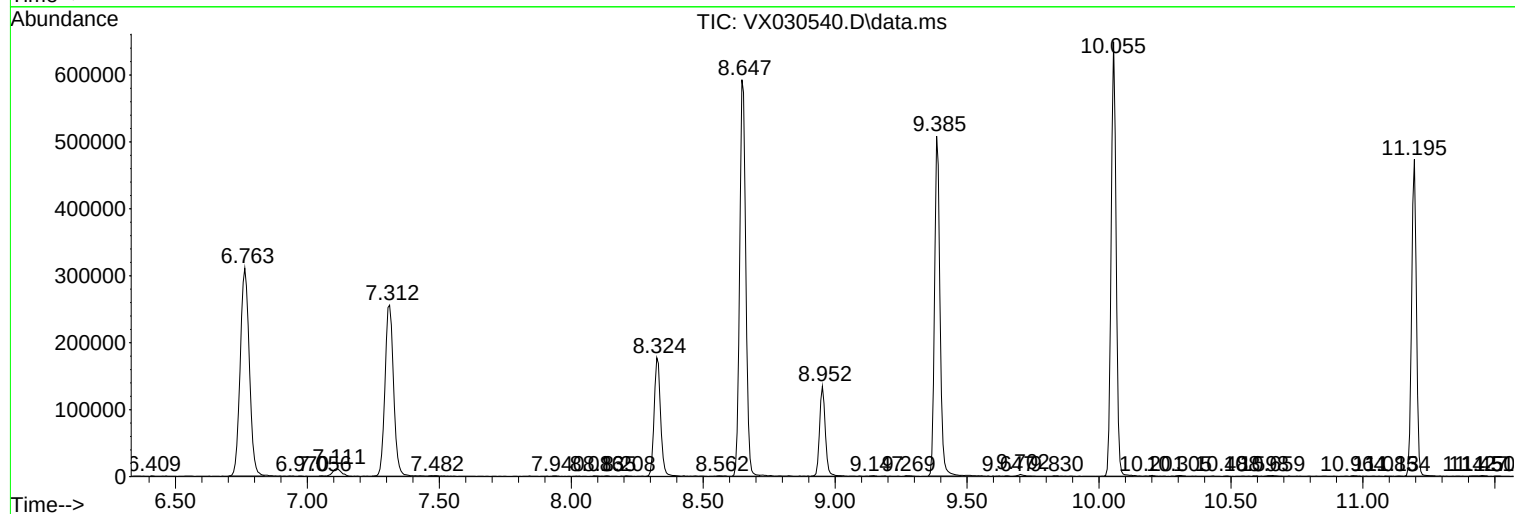
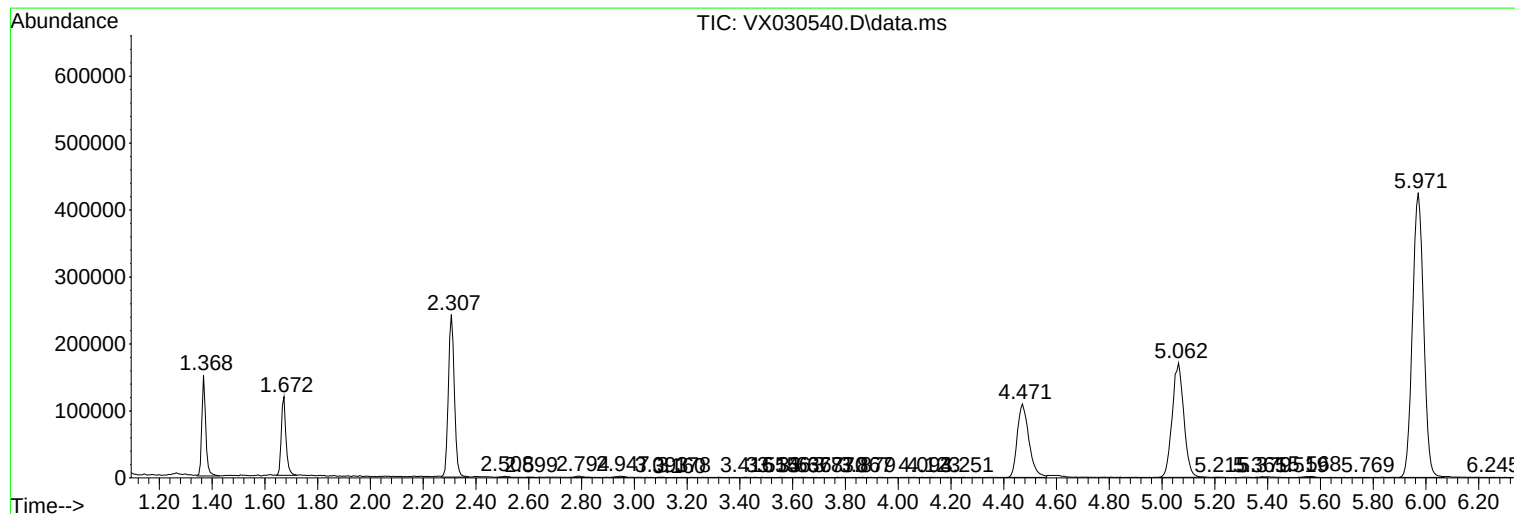
Sum of corrected areas: 9462395

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML080422WMA.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 |