

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU083122\  
 Data File : VU050560.D  
 Acq On : 31 Aug 2022 19:42  
 Operator : SY/MD  
 Sample : N4363-06ME  
 Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DBVW1ME

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\_U\Method\SFAMULM083022WMA.M  
 Title : VOC Analysis

Signal : TIC: VU050560.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         | 1.594       | 72            | 79          | 90           | rBV      | 50611          | 72031         | 5.21%           | 0.827%        |
| 2         | 2.530       | 358           | 370         | 391          | rVB      | 194287         | 319698        | 23.14%          | 3.672%        |
| 3         | 2.800       | 452           | 454         | 458          | rVB2     | 262            | 160           | 0.01%           | 0.002%        |
| 4         | 3.031       | 515           | 526         | 538          | rBV4     | 4877           | 9816          | 0.71%           | 0.113%        |
| 5         | 3.176       | 559           | 571         | 574          | rBV      | 4053           | 6451          | 0.47%           | 0.074%        |
| 6         | 3.298       | 606           | 609         | 613          | rVB2     | 396            | 276           | 0.02%           | 0.003%        |
| 7         | 3.321       | 613           | 616         | 619          | rBV2     | 188            | 164           | 0.01%           | 0.002%        |
| 8         | 3.385       | 632           | 636         | 639          | rVB      | 225            | 122           | 0.01%           | 0.001%        |
| 9         | 3.404       | 640           | 642         | 644          | rBV      | 208            | 127           | 0.01%           | 0.001%        |
| 10        | 3.546       | 683           | 686         | 689          | rBV2     | 168            | 135           | 0.01%           | 0.002%        |
| 11        | 3.562       | 689           | 691         | 697          | rBV      | 236            | 172           | 0.01%           | 0.002%        |
| 12        | 3.610       | 703           | 706         | 711          | rVB2     | 259            | 214           | 0.02%           | 0.002%        |
| 13        | 3.636       | 711           | 714         | 719          | rBV2     | 200            | 174           | 0.01%           | 0.002%        |
| 14        | 3.668       | 719           | 724         | 730          | rBV4     | 822            | 931           | 0.07%           | 0.011%        |
| 15        | 3.713       | 735           | 738         | 739          | rVV      | 300            | 164           | 0.01%           | 0.002%        |
| 16        | 3.742       | 743           | 747         | 751          | rVB      | 286            | 188           | 0.01%           | 0.002%        |
| 17        | 3.800       | 761           | 765         | 771          | rBV2     | 258            | 229           | 0.02%           | 0.003%        |
| 18        | 3.906       | 794           | 798         | 799          | rBV      | 241            | 148           | 0.01%           | 0.002%        |
| 19        | 4.009       | 821           | 830         | 833          | rBV      | 190            | 247           | 0.02%           | 0.003%        |
| 20        | 4.208       | 890           | 892         | 897          | rVB      | 181            | 119           | 0.01%           | 0.001%        |
| 21        | 4.317       | 924           | 926         | 930          | rBV      | 235            | 125           | 0.01%           | 0.001%        |
| 22        | 4.443       | 961           | 965         | 969          | rBV2     | 194            | 169           | 0.01%           | 0.002%        |
| 23        | 4.533       | 985           | 993         | 997          | rBV2     | 439            | 666           | 0.05%           | 0.008%        |
| 24        | 4.649       | 1015          | 1029        | 1074         | rBV      | 66769          | 254084        | 18.39%          | 2.918%        |
| 25        | 5.060       | 1141          | 1157        | 1180         | rBV      | 173104         | 411806        | 29.81%          | 4.729%        |
| 26        | 5.221       | 1204          | 1207        | 1211         | rVB2     | 202            | 178           | 0.01%           | 0.002%        |
| 27        | 5.288       | 1219          | 1228        | 1235         | rBV3     | 668            | 1272          | 0.09%           | 0.015%        |
| 28        | 5.343       | 1241          | 1245        | 1248         | rBV2     | 175            | 138           | 0.01%           | 0.002%        |
| 29        | 5.362       | 1248          | 1251        | 1254         | rBV2     | 467            | 400           | 0.03%           | 0.005%        |
| 30        | 5.430       | 1269          | 1272        | 1276         | rBV2     | 209            | 161           | 0.01%           | 0.002%        |
| 31        | 5.478       | 1285          | 1287        | 1290         | rBV      | 140            | 114           | 0.01%           | 0.001%        |
| 32        | 5.555       | 1307          | 1311        | 1313         | rBV      | 242            | 158           | 0.01%           | 0.002%        |
| 33        | 5.581       | 1313          | 1319        | 1322         | rBV2     | 191            | 252           | 0.02%           | 0.003%        |
| 34        | 5.716       | 1341          | 1361        | 1399         | rBV2     | 421560         | 1067852       | 77.31%          | 12.264%       |
| 35        | 5.912       | 1419          | 1422        | 1424         | rBV3     | 297            | 198           | 0.01%           | 0.002%        |
| 36        | 5.980       | 1434          | 1443        | 1455         | rBV5     | 6533           | 14908         | 1.08%           | 0.171%        |

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 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
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 DBVW1ME

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\_U\Method\SFAMULM083022WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |         |         |
|----|-------|------|------|------|------|--------|---------|---------|---------|
| 37 | 6.073 | 1470 | 1472 | 1474 | rVV  | 264    | 109     | 0.01%   | 0.001%  |
| 38 | 6.163 | 1498 | 1500 | 1505 | rVB  | 196    | 114     | 0.01%   | 0.001%  |
| 39 | 6.195 | 1505 | 1510 | 1511 | rBV  | 262    | 169     | 0.01%   | 0.002%  |
| 40 | 6.247 | 1512 | 1526 | 1558 | rVV  | 295944 | 595386  | 43.10%  | 6.838%  |
| 41 | 6.449 | 1587 | 1589 | 1593 | rVB2 | 284    | 203     | 0.01%   | 0.002%  |
| 42 | 6.533 | 1602 | 1615 | 1627 | rBV6 | 3758   | 7245    | 0.52%   | 0.083%  |
| 43 | 6.607 | 1629 | 1638 | 1648 | rVV3 | 3020   | 6631    | 0.48%   | 0.076%  |
| 44 | 6.690 | 1649 | 1664 | 1687 | rVB  | 232872 | 479427  | 34.71%  | 5.506%  |
| 45 | 6.906 | 1729 | 1731 | 1737 | rBV2 | 192    | 168     | 0.01%   | 0.002%  |
| 46 | 6.941 | 1739 | 1742 | 1746 | rVB  | 149    | 150     | 0.01%   | 0.002%  |
| 47 | 6.986 | 1752 | 1756 | 1757 | rBV  | 338    | 195     | 0.01%   | 0.002%  |
| 48 | 7.028 | 1765 | 1769 | 1773 | rBV2 | 219    | 190     | 0.01%   | 0.002%  |
| 49 | 7.047 | 1773 | 1775 | 1780 | rVB  | 211    | 129     | 0.01%   | 0.001%  |
| 50 | 7.070 | 1780 | 1782 | 1785 | rBV  | 299    | 202     | 0.01%   | 0.002%  |
| 51 | 7.234 | 1818 | 1833 | 1845 | rBV8 | 2923   | 7252    | 0.53%   | 0.083%  |
| 52 | 7.301 | 1850 | 1854 | 1855 | rBV  | 311    | 234     | 0.02%   | 0.003%  |
| 53 | 7.353 | 1868 | 1870 | 1872 | rBV  | 263    | 140     | 0.01%   | 0.002%  |
| 54 | 7.568 | 1924 | 1937 | 1957 | rBV  | 100235 | 196907  | 14.26%  | 2.261%  |
| 55 | 7.674 | 1966 | 1970 | 1973 | rVB2 | 313    | 231     | 0.02%   | 0.003%  |
| 56 | 7.700 | 1973 | 1978 | 1981 | rBV2 | 330    | 317     | 0.02%   | 0.004%  |
| 57 | 7.758 | 1988 | 1996 | 2001 | rBV3 | 306    | 387     | 0.03%   | 0.004%  |
| 58 | 7.896 | 2026 | 2039 | 2060 | rBV  | 449022 | 819420  | 59.32%  | 9.411%  |
| 59 | 8.124 | 2106 | 2110 | 2113 | rBV  | 262    | 215     | 0.02%   | 0.002%  |
| 60 | 8.182 | 2116 | 2128 | 2150 | rVV2 | 65934  | 131900  | 9.55%   | 1.515%  |
| 61 | 8.292 | 2159 | 2162 | 2167 | rBV  | 148    | 136     | 0.01%   | 0.002%  |
| 62 | 8.423 | 2200 | 2203 | 2204 | rBV2 | 208    | 138     | 0.01%   | 0.002%  |
| 63 | 8.552 | 2229 | 2243 | 2261 | rBV  | 798239 | 1381318 | 100.00% | 15.864% |
| 64 | 8.664 | 2262 | 2278 | 2307 | rVB2 | 183704 | 532716  | 38.57%  | 6.118%  |
| 65 | 8.877 | 2341 | 2344 | 2345 | rBV2 | 212    | 120     | 0.01%   | 0.001%  |
| 66 | 8.922 | 2355 | 2358 | 2359 | rBV  | 269    | 118     | 0.01%   | 0.001%  |
| 67 | 8.935 | 2360 | 2362 | 2364 | rVV2 | 430    | 187     | 0.01%   | 0.002%  |
| 68 | 8.960 | 2367 | 2370 | 2375 | rVB2 | 207    | 158     | 0.01%   | 0.002%  |
| 69 | 8.983 | 2375 | 2377 | 2380 | rVB  | 278    | 156     | 0.01%   | 0.002%  |
| 70 | 9.002 | 2381 | 2383 | 2387 | rBV  | 308    | 242     | 0.02%   | 0.003%  |
| 71 | 9.025 | 2388 | 2390 | 2395 | rVB  | 232    | 123     | 0.01%   | 0.001%  |
| 72 | 9.105 | 2411 | 2415 | 2417 | rBV2 | 225    | 207     | 0.01%   | 0.002%  |
| 73 | 9.182 | 2437 | 2439 | 2441 | rBV  | 183    | 114     | 0.01%   | 0.001%  |
| 74 | 9.230 | 2450 | 2454 | 2456 | rBV2 | 172    | 125     | 0.01%   | 0.001%  |
| 75 | 9.285 | 2469 | 2471 | 2474 | rVB  | 224    | 140     | 0.01%   | 0.002%  |
| 76 | 9.420 | 2499 | 2513 | 2534 | rBV  | 366988 | 700084  | 50.68%  | 8.040%  |

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 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DBVW1ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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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\_U\Method\SFAMULM083022WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 9.571  | 2558 | 2560 | 2562 | rVB  | 457    | 221    | 0.02%  | 0.003% |
| 78  | 9.642  | 2579 | 2582 | 2584 | rBV  | 208    | 145    | 0.01%  | 0.002% |
| 79  | 9.767  | 2618 | 2621 | 2624 | rBV2 | 156    | 111    | 0.01%  | 0.001% |
| 80  | 9.790  | 2624 | 2628 | 2632 | rBV2 | 233    | 239    | 0.02%  | 0.003% |
| 81  | 9.963  | 2680 | 2682 | 2686 | rBV2 | 195    | 197    | 0.01%  | 0.002% |
| 82  | 10.050 | 2705 | 2709 | 2714 | rBV2 | 241    | 217    | 0.02%  | 0.002% |
| 83  | 10.160 | 2740 | 2743 | 2746 | rBV2 | 226    | 146    | 0.01%  | 0.002% |
| 84  | 10.340 | 2796 | 2799 | 2806 | rVV2 | 205    | 196    | 0.01%  | 0.002% |
| 85  | 10.375 | 2806 | 2810 | 2817 | rVB2 | 242    | 300    | 0.02%  | 0.003% |
| 86  | 10.584 | 2872 | 2875 | 2883 | rVB  | 273    | 258    | 0.02%  | 0.003% |
| 87  | 10.764 | 2918 | 2931 | 2952 | rBV  | 312614 | 535090 | 38.74% | 6.145% |
| 88  | 10.989 | 2998 | 3001 | 3004 | rBV  | 185    | 135    | 0.01%  | 0.002% |
| 89  | 11.115 | 3036 | 3040 | 3046 | rVB5 | 1544   | 1531   | 0.11%  | 0.018% |
| 90  | 11.295 | 3093 | 3096 | 3100 | rBV  | 271    | 209    | 0.02%  | 0.002% |
| 91  | 11.632 | 3198 | 3201 | 3202 | rBV  | 211    | 130    | 0.01%  | 0.001% |
| 92  | 11.815 | 3246 | 3258 | 3275 | rBV  | 331039 | 521195 | 37.73% | 5.986% |
| 93  | 11.947 | 3296 | 3299 | 3303 | rBV  | 448    | 305    | 0.02%  | 0.004% |
| 94  | 11.976 | 3303 | 3308 | 3315 | rVB2 | 469    | 460    | 0.03%  | 0.005% |
| 95  | 12.198 | 3364 | 3377 | 3394 | rBV  | 379466 | 617511 | 44.70% | 7.092% |
| 96  | 12.655 | 3516 | 3519 | 3522 | rBV2 | 270    | 213    | 0.02%  | 0.002% |
| 97  | 12.787 | 3557 | 3560 | 3563 | rBV2 | 238    | 164    | 0.01%  | 0.002% |
| 98  | 12.922 | 3600 | 3602 | 3605 | rBV  | 301    | 189    | 0.01%  | 0.002% |
| 99  | 13.163 | 3675 | 3677 | 3680 | rVB  | 420    | 208    | 0.02%  | 0.002% |
| 100 | 13.510 | 3780 | 3785 | 3791 | rBV2 | 404    | 595    | 0.04%  | 0.007% |

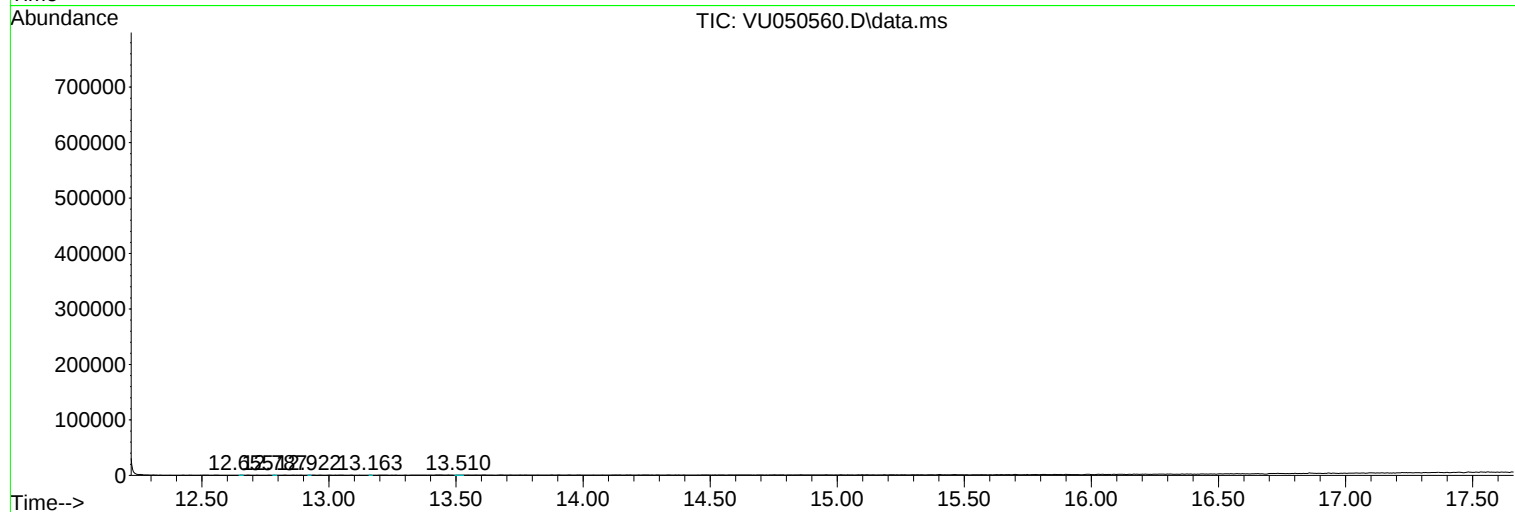
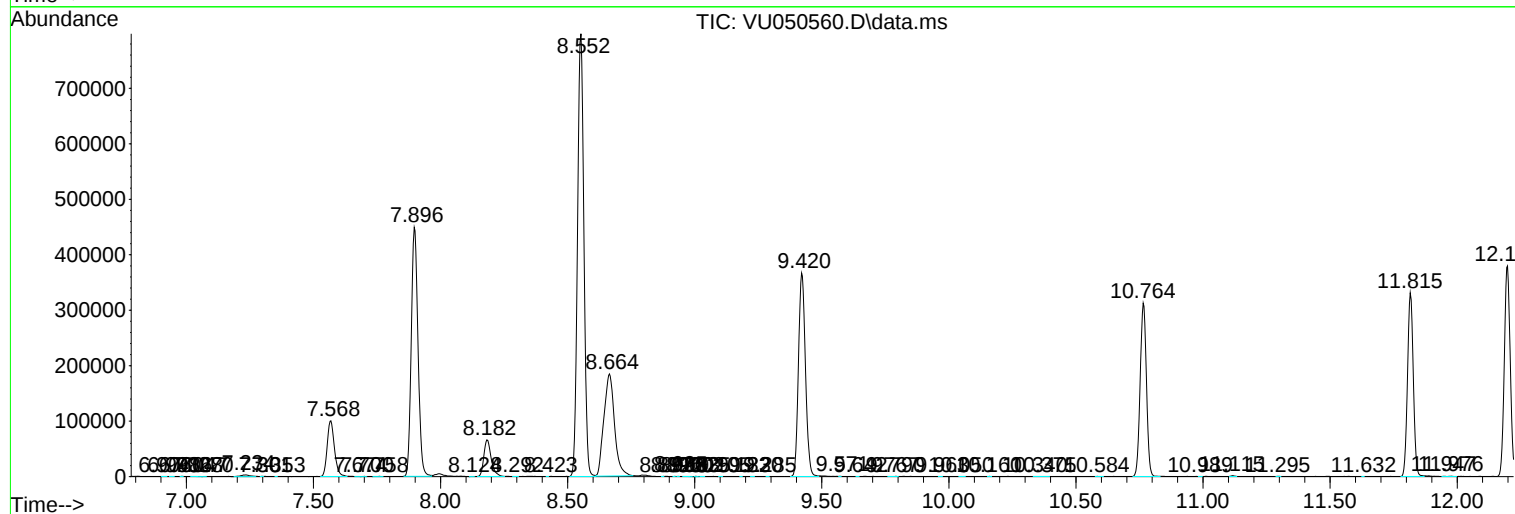
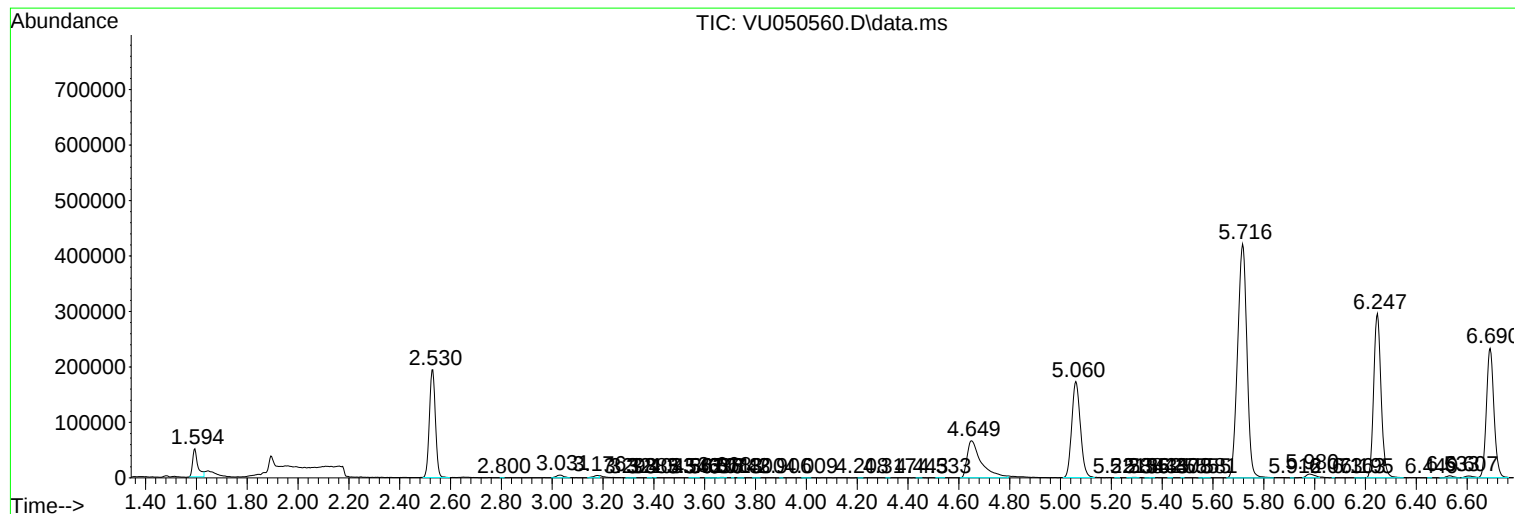
Sum of corrected areas: 8707415

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Instrument :  
MSVOA\_U  
ClientSampleId :  
DBVW1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM083022WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU083122\  
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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 |