

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050823\  
 Data File : VU054075.D  
 Acq On : 08 May 2023 13:00  
 Operator : JC/MD  
 Sample : VU0508MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK091

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\SFAMULM042923WMA.M  
 Title : VOC Analysis

Signal : TIC: VU054075.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         | 1.597       | 72            | 80          | 96           | rVB      | 96978          | 118859        | 12.74%          | 1.754%        |
| 2         | 1.806       | 140           | 145         | 147          | rBV4     | 2290           | 2086          | 0.22%           | 0.031%        |
| 3         | 1.906       | 167           | 176         | 193          | rVB      | 80347          | 114499        | 12.27%          | 1.690%        |
| 4         | 2.295       | 295           | 297         | 299          | rBV      | 512            | 218           | 0.02%           | 0.003%        |
| 5         | 2.376       | 319           | 322         | 326          | rBV3     | 514            | 455           | 0.05%           | 0.007%        |
| 6         | 2.433       | 338           | 340         | 344          | rVB2     | 563            | 382           | 0.04%           | 0.006%        |
| 7         | 2.459       | 344           | 348         | 353          | rBV3     | 447            | 485           | 0.05%           | 0.007%        |
| 8         | 2.485       | 353           | 356         | 362          | rVB2     | 361            | 409           | 0.04%           | 0.006%        |
| 9         | 2.562       | 368           | 380         | 397          | rBV      | 183326         | 296800        | 31.81%          | 4.380%        |
| 10        | 2.630       | 397           | 401         | 402          | rBV2     | 697            | 478           | 0.05%           | 0.007%        |
| 11        | 2.790       | 444           | 451         | 456          | rVB4     | 898            | 1319          | 0.14%           | 0.019%        |
| 12        | 2.819       | 456           | 460         | 461          | rBV2     | 220            | 169           | 0.02%           | 0.002%        |
| 13        | 2.938       | 494           | 497         | 501          | rBV2     | 339            | 319           | 0.03%           | 0.005%        |
| 14        | 2.999       | 511           | 516         | 519          | rBV2     | 286            | 278           | 0.03%           | 0.004%        |
| 15        | 3.038       | 520           | 528         | 529          | rBV3     | 3496           | 3597          | 0.39%           | 0.053%        |
| 16        | 3.170       | 562           | 569         | 572          | rBV      | 1148           | 1437          | 0.15%           | 0.021%        |
| 17        | 3.356       | 621           | 627         | 631          | rVB4     | 597            | 606           | 0.06%           | 0.009%        |
| 18        | 3.382       | 631           | 635         | 644          | rBV2     | 256            | 385           | 0.04%           | 0.006%        |
| 19        | 3.437       | 649           | 652         | 654          | rBV      | 258            | 166           | 0.02%           | 0.002%        |
| 20        | 3.752       | 746           | 750         | 752          | rBV2     | 271            | 205           | 0.02%           | 0.003%        |
| 21        | 3.797       | 762           | 764         | 768          | rVB2     | 251            | 174           | 0.02%           | 0.003%        |
| 22        | 3.890       | 790           | 793         | 798          | rBV      | 348            | 340           | 0.04%           | 0.005%        |
| 23        | 4.047       | 838           | 842         | 848          | rBV      | 190            | 262           | 0.03%           | 0.004%        |
| 24        | 4.224       | 894           | 897         | 902          | rVB      | 254            | 189           | 0.02%           | 0.003%        |
| 25        | 4.276       | 908           | 913         | 915          | rBV2     | 237            | 222           | 0.02%           | 0.003%        |
| 26        | 4.404       | 950           | 953         | 958          | rBV2     | 195            | 172           | 0.02%           | 0.003%        |
| 27        | 4.485       | 974           | 978         | 981          | rVB2     | 223            | 210           | 0.02%           | 0.003%        |
| 28        | 4.617       | 1007          | 1019        | 1039         | rBV      | 74735          | 182594        | 19.57%          | 2.694%        |
| 29        | 4.935       | 1115          | 1118        | 1122         | rBV2     | 252            | 273           | 0.03%           | 0.004%        |
| 30        | 4.990       | 1131          | 1135        | 1137         | rBV2     | 205            | 190           | 0.02%           | 0.003%        |
| 31        | 5.057       | 1139          | 1156        | 1179         | rVV      | 167435         | 371826        | 39.85%          | 5.487%        |
| 32        | 5.395       | 1257          | 1261        | 1265         | rBB      | 177            | 164           | 0.02%           | 0.002%        |
| 33        | 5.472       | 1277          | 1285        | 1287         | rBV2     | 412            | 584           | 0.06%           | 0.009%        |
| 34        | 5.719       | 1339          | 1362        | 1395         | rBV2     | 337740         | 933071        | 100.00%         | 13.769%       |
| 35        | 5.944       | 1429          | 1432        | 1437         | rVB3     | 207            | 181           | 0.02%           | 0.003%        |
| 36        | 5.967       | 1437          | 1439        | 1443         | rVB2     | 306            | 211           | 0.02%           | 0.003%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\_U\Method\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.118  | 1483 | 1486 | 1489 | rBV3 | 307    | 268    | 0.03%  | 0.004%  |
| 38 | 6.176  | 1500 | 1504 | 1507 | rBV2 | 358    | 402    | 0.04%  | 0.006%  |
| 39 | 6.244  | 1511 | 1525 | 1547 | rBV  | 262540 | 498747 | 53.45% | 7.360%  |
| 40 | 6.462  | 1590 | 1593 | 1597 | rVB2 | 341    | 303    | 0.03%  | 0.004%  |
| 41 | 6.526  | 1604 | 1613 | 1622 | rVV6 | 3061   | 5245   | 0.56%  | 0.077%  |
| 42 | 6.562  | 1622 | 1624 | 1628 | rVB  | 229    | 171    | 0.02%  | 0.003%  |
| 43 | 6.684  | 1648 | 1662 | 1683 | rVV  | 217985 | 423588 | 45.40% | 6.251%  |
| 44 | 6.797  | 1695 | 1697 | 1698 | rBV  | 315    | 164    | 0.02%  | 0.002%  |
| 45 | 6.861  | 1715 | 1717 | 1720 | rVB2 | 287    | 161    | 0.02%  | 0.002%  |
| 46 | 6.983  | 1747 | 1755 | 1760 | rBV2 | 236    | 346    | 0.04%  | 0.005%  |
| 47 | 7.009  | 1760 | 1763 | 1766 | rBV2 | 182    | 176    | 0.02%  | 0.003%  |
| 48 | 7.047  | 1771 | 1775 | 1777 | rBV  | 268    | 254    | 0.03%  | 0.004%  |
| 49 | 7.150  | 1802 | 1807 | 1812 | rBV  | 328    | 457    | 0.05%  | 0.007%  |
| 50 | 7.186  | 1814 | 1818 | 1821 | rVV2 | 812    | 847    | 0.09%  | 0.012%  |
| 51 | 7.198  | 1821 | 1822 | 1826 | rVB3 | 644    | 369    | 0.04%  | 0.005%  |
| 52 | 7.266  | 1834 | 1843 | 1844 | rBV2 | 213    | 282    | 0.03%  | 0.004%  |
| 53 | 7.559  | 1922 | 1934 | 1961 | rVV2 | 118530 | 212506 | 22.77% | 3.136%  |
| 54 | 7.694  | 1971 | 1976 | 1979 | rBV2 | 687    | 668    | 0.07%  | 0.010%  |
| 55 | 7.793  | 2002 | 2007 | 2008 | rBV2 | 565    | 482    | 0.05%  | 0.007%  |
| 56 | 7.893  | 2024 | 2038 | 2065 | rBV  | 420605 | 732889 | 78.55% | 10.815% |
| 57 | 8.173  | 2114 | 2125 | 2140 | rBV  | 84896  | 144287 | 15.46% | 2.129%  |
| 58 | 8.272  | 2153 | 2156 | 2159 | rBV3 | 284    | 256    | 0.03%  | 0.004%  |
| 59 | 8.427  | 2201 | 2204 | 2207 | rBV2 | 240    | 193    | 0.02%  | 0.003%  |
| 60 | 8.546  | 2237 | 2241 | 2248 | rVB3 | 848    | 942    | 0.10%  | 0.014%  |
| 61 | 8.575  | 2248 | 2250 | 2255 | rBV2 | 262    | 165    | 0.02%  | 0.002%  |
| 62 | 8.629  | 2255 | 2267 | 2294 | rBV2 | 214120 | 400925 | 42.97% | 5.916%  |
| 63 | 8.829  | 2326 | 2329 | 2332 | rBV2 | 232    | 207    | 0.02%  | 0.003%  |
| 64 | 9.144  | 2422 | 2427 | 2432 | rBV2 | 176    | 255    | 0.03%  | 0.004%  |
| 65 | 9.311  | 2476 | 2479 | 2482 | rBV2 | 184    | 188    | 0.02%  | 0.003%  |
| 66 | 9.411  | 2498 | 2510 | 2534 | rBV  | 350576 | 592237 | 63.47% | 8.739%  |
| 67 | 9.999  | 2690 | 2693 | 2696 | rBV  | 247    | 214    | 0.02%  | 0.003%  |
| 68 | 10.153 | 2739 | 2741 | 2751 | rVB  | 220    | 289    | 0.03%  | 0.004%  |
| 69 | 10.240 | 2765 | 2768 | 2773 | rVB  | 254    | 209    | 0.02%  | 0.003%  |
| 70 | 10.266 | 2773 | 2776 | 2779 | rBV  | 442    | 354    | 0.04%  | 0.005%  |
| 71 | 10.475 | 2838 | 2841 | 2845 | rBV2 | 649    | 591    | 0.06%  | 0.009%  |
| 72 | 10.642 | 2888 | 2893 | 2895 | rBV3 | 473    | 299    | 0.03%  | 0.004%  |
| 73 | 10.751 | 2914 | 2927 | 2942 | rBV  | 283883 | 466428 | 49.99% | 6.883%  |
| 74 | 10.841 | 2952 | 2955 | 2958 | rVB  | 310    | 201    | 0.02%  | 0.003%  |
| 75 | 10.954 | 2988 | 2990 | 2995 | rVB2 | 292    | 253    | 0.03%  | 0.004%  |
| 76 | 10.980 | 2995 | 2998 | 3001 | rBV2 | 270    | 233    | 0.02%  | 0.003%  |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\_U\Method\SFAMULM042923WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.044 | 3014 | 3018 | 3021 | rBV  | 263    | 256    | 0.03%  | 0.004% |
| 78  | 11.089 | 3028 | 3032 | 3036 | rVB2 | 499    | 486    | 0.05%  | 0.007% |
| 79  | 11.153 | 3045 | 3052 | 3054 | rBV2 | 203    | 233    | 0.02%  | 0.003% |
| 80  | 11.465 | 3144 | 3149 | 3157 | rBV  | 958    | 1177   | 0.13%  | 0.017% |
| 81  | 11.620 | 3194 | 3197 | 3201 | rBV2 | 179    | 188    | 0.02%  | 0.003% |
| 82  | 11.745 | 3230 | 3236 | 3243 | rVB2 | 1458   | 1652   | 0.18%  | 0.024% |
| 83  | 11.806 | 3243 | 3255 | 3274 | rBV  | 346136 | 557799 | 59.78% | 8.231% |
| 84  | 11.925 | 3288 | 3292 | 3297 | rVB4 | 445    | 473    | 0.05%  | 0.007% |
| 85  | 12.189 | 3361 | 3374 | 3400 | rBV  | 400961 | 660761 | 70.82% | 9.751% |
| 86  | 12.388 | 3433 | 3436 | 3443 | rBV2 | 282    | 265    | 0.03%  | 0.004% |
| 87  | 12.462 | 3453 | 3459 | 3461 | rBV2 | 272    | 296    | 0.03%  | 0.004% |
| 88  | 12.867 | 3581 | 3585 | 3589 | rBV2 | 371    | 408    | 0.04%  | 0.006% |
| 89  | 12.928 | 3601 | 3604 | 3607 | rBV  | 261    | 185    | 0.02%  | 0.003% |
| 90  | 13.221 | 3690 | 3695 | 3707 | rVB6 | 2296   | 3565   | 0.38%  | 0.053% |
| 91  | 13.529 | 3788 | 3791 | 3792 | rBV  | 249    | 170    | 0.02%  | 0.003% |
| 92  | 13.616 | 3815 | 3818 | 3822 | rVB2 | 302    | 208    | 0.02%  | 0.003% |
| 93  | 13.636 | 3822 | 3824 | 3828 | rBV2 | 197    | 168    | 0.02%  | 0.002% |
| 94  | 13.841 | 3881 | 3888 | 3896 | rBV3 | 4177   | 6283   | 0.67%  | 0.093% |
| 95  | 13.970 | 3925 | 3928 | 3933 | rVB2 | 394    | 301    | 0.03%  | 0.004% |
| 96  | 14.089 | 3956 | 3965 | 3975 | rBV2 | 7465   | 12389  | 1.33%  | 0.183% |
| 97  | 14.330 | 4031 | 4040 | 4048 | rBV6 | 5002   | 7676   | 0.82%  | 0.113% |
| 98  | 14.693 | 4152 | 4153 | 4159 | rBV2 | 372    | 305    | 0.03%  | 0.005% |
| 99  | 15.417 | 4375 | 4378 | 4381 | rBV2 | 524    | 360    | 0.04%  | 0.005% |
| 100 | 15.462 | 4390 | 4392 | 4394 | rBV  | 431    | 204    | 0.02%  | 0.003% |

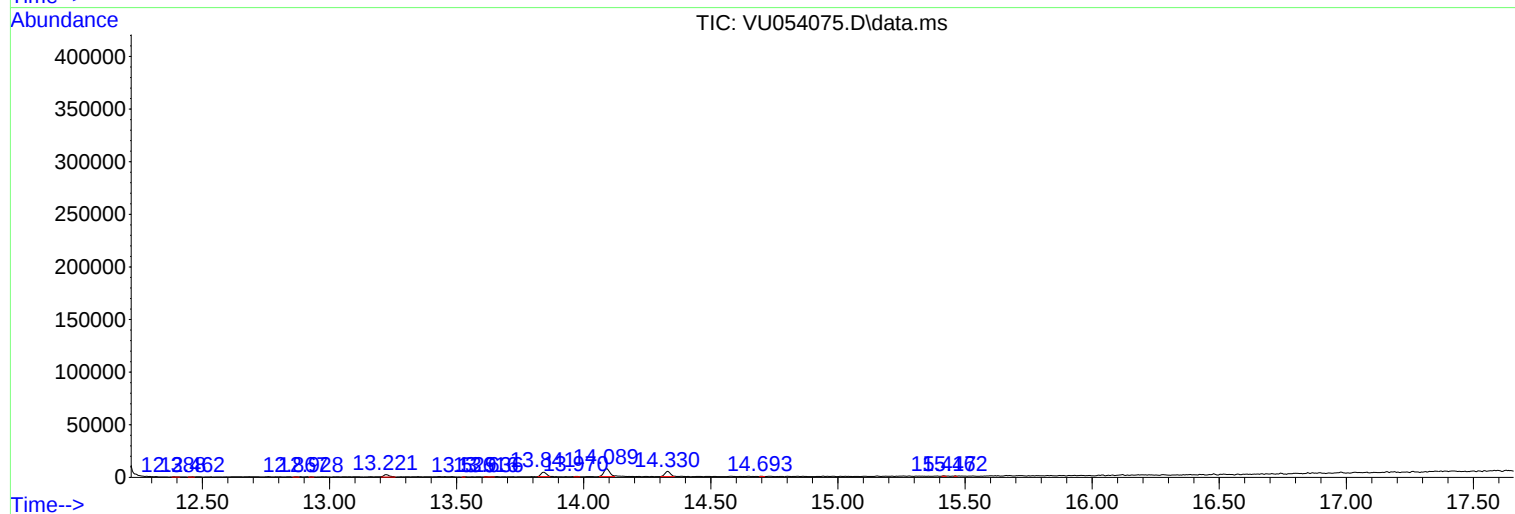
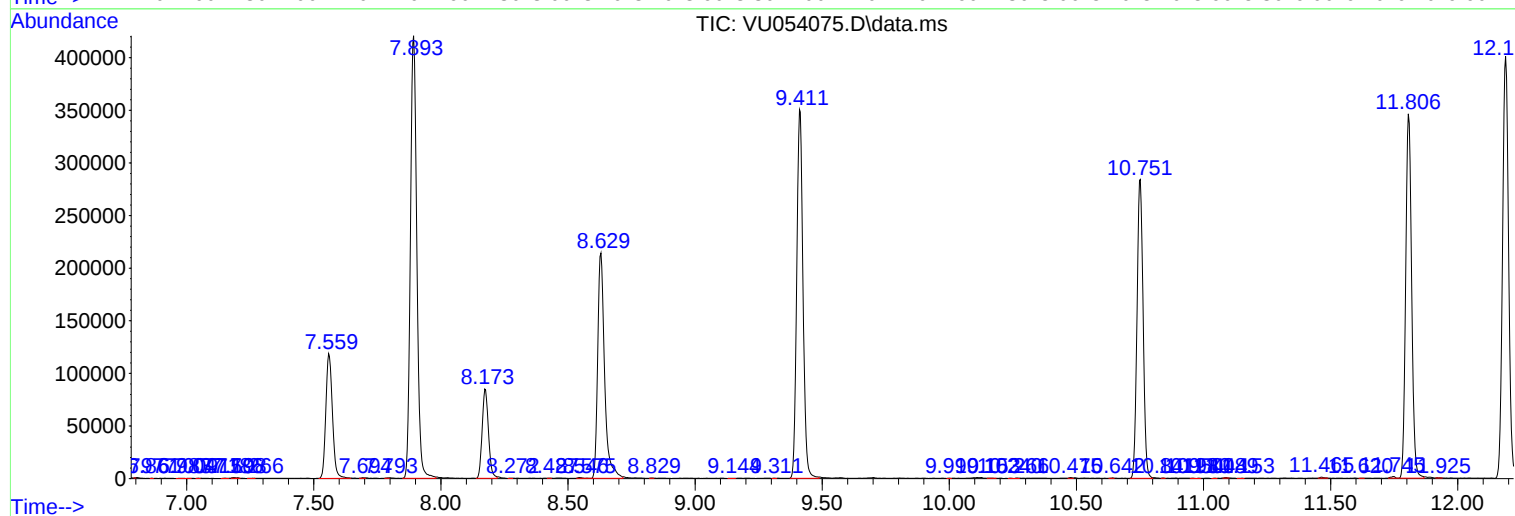
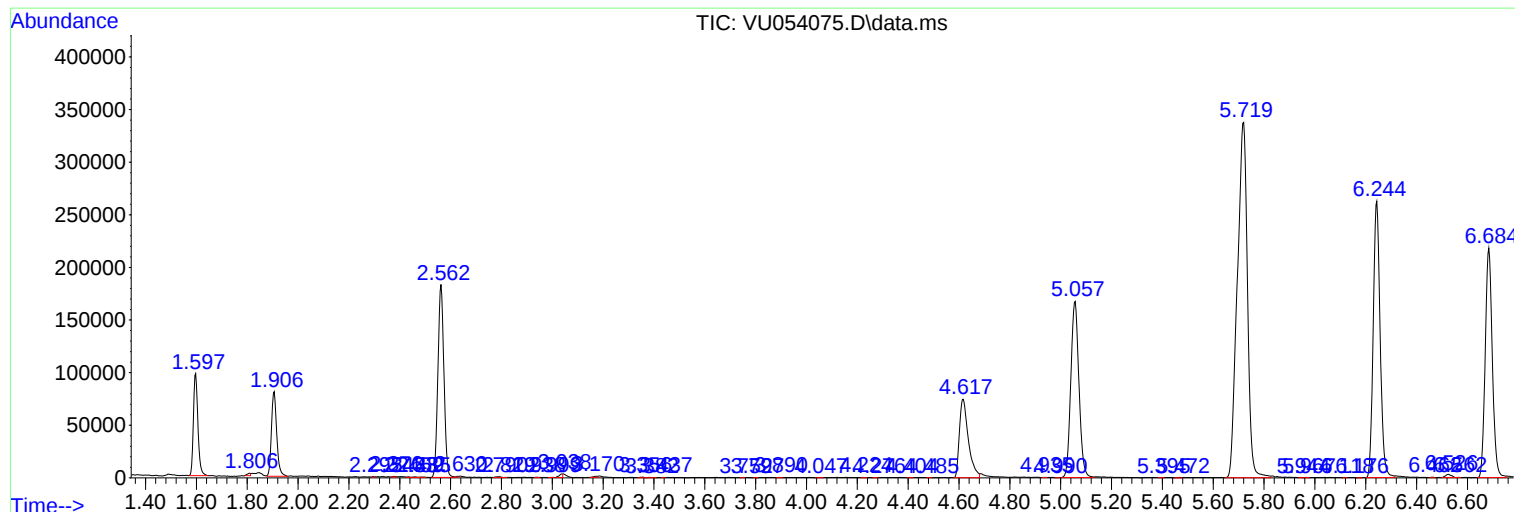
Sum of corrected areas: 6776674

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Instrument :  
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VBLK091

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050823\  
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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 |