

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101723\  
 Data File : VU055786.D  
 Acq On : 17 Oct 2023 11:37  
 Operator : MD/SY  
 Sample : VU1017MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK109

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\SFAMULM101023WMA.M  
 Title : VOC Analysis

Signal : TIC: VU055786.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         | 1.599       | 88            | 96          | 112          | rBV      | 213254         | 261273        | 12.69%          | 1.619%        |
| 2         | 1.885       | 178           | 185         | 205          | rVB      | 173517         | 264255        | 12.83%          | 1.637%        |
| 3         | 2.512       | 378           | 380         | 382          | rBV3     | 624            | 358           | 0.02%           | 0.002%        |
| 4         | 2.557       | 382           | 394         | 412          | rVV      | 385318         | 627315        | 30.46%          | 3.886%        |
| 5         | 2.750       | 452           | 454         | 459          | rBV4     | 485            | 442           | 0.02%           | 0.003%        |
| 6         | 2.792       | 462           | 467         | 470          | rVB6     | 1288           | 1141          | 0.06%           | 0.007%        |
| 7         | 2.894       | 494           | 499         | 502          | rVB3     | 504            | 453           | 0.02%           | 0.003%        |
| 8         | 3.036       | 533           | 543         | 556          | rVB6     | 3567           | 6544          | 0.32%           | 0.041%        |
| 9         | 3.155       | 577           | 580         | 582          | rBV2     | 440            | 330           | 0.02%           | 0.002%        |
| 10        | 3.174       | 583           | 586         | 588          | rVV      | 524            | 358           | 0.02%           | 0.002%        |
| 11        | 3.232       | 601           | 604         | 608          | rBV2     | 385            | 293           | 0.01%           | 0.002%        |
| 12        | 3.293       | 620           | 623         | 626          | rVB2     | 433            | 306           | 0.01%           | 0.002%        |
| 13        | 3.322       | 626           | 632         | 634          | rBV2     | 311            | 384           | 0.02%           | 0.002%        |
| 14        | 3.374       | 641           | 648         | 652          | rBV2     | 321            | 329           | 0.02%           | 0.002%        |
| 15        | 3.496       | 683           | 686         | 689          | rVV2     | 327            | 274           | 0.01%           | 0.002%        |
| 16        | 3.512       | 689           | 691         | 696          | rVV2     | 400            | 378           | 0.02%           | 0.002%        |
| 17        | 3.538       | 696           | 699         | 705          | rVB2     | 507            | 509           | 0.02%           | 0.003%        |
| 18        | 3.624       | 723           | 726         | 731          | rVB2     | 257            | 270           | 0.01%           | 0.002%        |
| 19        | 3.702       | 747           | 750         | 757          | rVB2     | 640            | 481           | 0.02%           | 0.003%        |
| 20        | 3.956       | 825           | 829         | 834          | rVB2     | 277            | 330           | 0.02%           | 0.002%        |
| 21        | 4.081       | 864           | 868         | 871          | rBV2     | 300            | 272           | 0.01%           | 0.002%        |
| 22        | 4.132       | 879           | 884         | 887          | rBV2     | 388            | 296           | 0.01%           | 0.002%        |
| 23        | 4.615       | 1023          | 1034        | 1080         | rBV      | 166918         | 474771        | 23.05%          | 2.941%        |
| 24        | 4.939       | 1131          | 1135        | 1137         | rBV      | 590            | 392           | 0.02%           | 0.002%        |
| 25        | 5.055       | 1155          | 1171        | 1197         | rBV      | 371316         | 829556        | 40.28%          | 5.139%        |
| 26        | 5.290       | 1241          | 1244        | 1248         | rVB4     | 787            | 579           | 0.03%           | 0.004%        |
| 27        | 5.328       | 1248          | 1256        | 1258         | rBV5     | 841            | 1003          | 0.05%           | 0.006%        |
| 28        | 5.718       | 1353          | 1377        | 1408         | rBV2     | 753556         | 2059575       | 100.00%         | 12.759%       |
| 29        | 5.955       | 1448          | 1451        | 1453         | rBV3     | 556            | 374           | 0.02%           | 0.002%        |
| 30        | 5.975       | 1453          | 1457        | 1459         | rBV3     | 728            | 638           | 0.03%           | 0.004%        |
| 31        | 6.026       | 1468          | 1473        | 1474         | rBV3     | 407            | 340           | 0.02%           | 0.002%        |
| 32        | 6.045       | 1477          | 1479        | 1482         | rVV2     | 571            | 401           | 0.02%           | 0.002%        |
| 33        | 6.078       | 1485          | 1489        | 1493         | rVB3     | 321            | 275           | 0.01%           | 0.002%        |
| 34        | 6.116       | 1493          | 1501        | 1505         | rBV4     | 523            | 835           | 0.04%           | 0.005%        |
| 35        | 6.245       | 1527          | 1541        | 1563         | rBV      | 612240         | 1184010       | 57.49%          | 7.335%        |
| 36        | 6.412       | 1591          | 1593        | 1597         | rVB2     | 1343           | 913           | 0.04%           | 0.006%        |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK109

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\SFAMULM101023WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 6.438  | 1597 | 1601 | 1604 | rVB4 | 415    | 331     | 0.02%  | 0.002% |
| 38 | 6.528  | 1618 | 1629 | 1643 | rBV4 | 24719  | 48503   | 2.36%  | 0.300% |
| 39 | 6.685  | 1663 | 1678 | 1708 | rBV  | 477083 | 942100  | 45.74% | 5.836% |
| 40 | 6.878  | 1734 | 1738 | 1743 | rVB5 | 609    | 541     | 0.03%  | 0.003% |
| 41 | 7.013  | 1777 | 1780 | 1784 | rBV2 | 372    | 358     | 0.02%  | 0.002% |
| 42 | 7.193  | 1825 | 1836 | 1847 | rBV8 | 3856   | 9714    | 0.47%  | 0.060% |
| 43 | 7.238  | 1847 | 1850 | 1857 | rVV4 | 1312   | 1440    | 0.07%  | 0.009% |
| 44 | 7.271  | 1857 | 1860 | 1864 | rVB2 | 491    | 429     | 0.02%  | 0.003% |
| 45 | 7.505  | 1930 | 1933 | 1938 | rBV2 | 516    | 438     | 0.02%  | 0.003% |
| 46 | 7.563  | 1938 | 1951 | 1978 | rBV  | 248665 | 458223  | 22.25% | 2.839% |
| 47 | 7.708  | 1990 | 1996 | 2011 | rVB8 | 1989   | 4016    | 0.19%  | 0.025% |
| 48 | 7.798  | 2021 | 2024 | 2026 | rBV2 | 569    | 297     | 0.01%  | 0.002% |
| 49 | 7.894  | 2040 | 2054 | 2088 | rBV  | 890804 | 1573288 | 76.39% | 9.746% |
| 50 | 8.177  | 2131 | 2142 | 2168 | rBV  | 178426 | 308026  | 14.96% | 1.908% |
| 51 | 8.351  | 2190 | 2196 | 2199 | rVB4 | 598    | 485     | 0.02%  | 0.003% |
| 52 | 8.441  | 2221 | 2224 | 2226 | rBV2 | 430    | 311     | 0.02%  | 0.002% |
| 53 | 8.553  | 2254 | 2259 | 2262 | rBV2 | 653    | 636     | 0.03%  | 0.004% |
| 54 | 8.637  | 2272 | 2285 | 2320 | rBV5 | 464424 | 1224148 | 59.44% | 7.584% |
| 55 | 8.910  | 2365 | 2370 | 2372 | rBV3 | 490    | 376     | 0.02%  | 0.002% |
| 56 | 9.241  | 2470 | 2473 | 2477 | rVB4 | 605    | 343     | 0.02%  | 0.002% |
| 57 | 9.274  | 2477 | 2483 | 2485 | rBV2 | 464    | 434     | 0.02%  | 0.003% |
| 58 | 9.287  | 2485 | 2487 | 2490 | rVB  | 539    | 306     | 0.01%  | 0.002% |
| 59 | 9.415  | 2514 | 2527 | 2557 | rBV  | 919892 | 1560560 | 75.77% | 9.668% |
| 60 | 9.566  | 2572 | 2574 | 2579 | rVB4 | 940    | 474     | 0.02%  | 0.003% |
| 61 | 9.627  | 2588 | 2593 | 2595 | rBV2 | 421    | 435     | 0.02%  | 0.003% |
| 62 | 9.685  | 2609 | 2611 | 2613 | rVV2 | 707    | 426     | 0.02%  | 0.003% |
| 63 | 9.698  | 2613 | 2615 | 2623 | rVV3 | 1602   | 1555    | 0.08%  | 0.010% |
| 64 | 9.859  | 2660 | 2665 | 2670 | rVB  | 376    | 377     | 0.02%  | 0.002% |
| 65 | 10.277 | 2791 | 2795 | 2798 | rVB  | 419    | 311     | 0.02%  | 0.002% |
| 66 | 10.344 | 2813 | 2816 | 2820 | rBV  | 402    | 290     | 0.01%  | 0.002% |
| 67 | 10.373 | 2820 | 2825 | 2828 | rBV2 | 357    | 388     | 0.02%  | 0.002% |
| 68 | 10.405 | 2832 | 2835 | 2841 | rVB2 | 524    | 556     | 0.03%  | 0.003% |
| 69 | 10.434 | 2841 | 2844 | 2846 | rBV2 | 396    | 294     | 0.01%  | 0.002% |
| 70 | 10.753 | 2927 | 2943 | 2967 | rBV  | 731802 | 1222849 | 59.37% | 7.576% |
| 71 | 10.859 | 2973 | 2976 | 2983 | rVB3 | 773    | 680     | 0.03%  | 0.004% |
| 72 | 10.891 | 2983 | 2986 | 2989 | rBV2 | 495    | 338     | 0.02%  | 0.002% |
| 73 | 10.975 | 3010 | 3012 | 3016 | rVV2 | 458    | 287     | 0.01%  | 0.002% |
| 74 | 11.023 | 3022 | 3027 | 3030 | rVB2 | 696    | 607     | 0.03%  | 0.004% |
| 75 | 11.415 | 3147 | 3149 | 3151 | rBV2 | 588    | 320     | 0.02%  | 0.002% |
| 76 | 11.476 | 3162 | 3168 | 3172 | rBV4 | 809    | 832     | 0.04%  | 0.005% |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
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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\SFAMULM101023WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 11.502 | 3174 | 3176 | 3182 | rVB  | 360    | 299     | 0.01%  | 0.002% |
| 78  | 11.592 | 3200 | 3204 | 3208 | rBV  | 527    | 425     | 0.02%  | 0.003% |
| 79  | 11.753 | 3249 | 3254 | 3259 | rVB4 | 1282   | 1250    | 0.06%  | 0.008% |
| 80  | 11.811 | 3259 | 3272 | 3297 | rBV  | 936609 | 1502019 | 72.93% | 9.305% |
| 81  | 11.981 | 3322 | 3325 | 3328 | rBV3 | 600    | 415     | 0.02%  | 0.003% |
| 82  | 12.190 | 3375 | 3390 | 3414 | rBV  | 907802 | 1533295 | 74.45% | 9.499% |
| 83  | 12.450 | 3469 | 3471 | 3474 | rBV2 | 505    | 290     | 0.01%  | 0.002% |
| 84  | 12.476 | 3476 | 3479 | 3485 | rVB2 | 917    | 523     | 0.03%  | 0.003% |
| 85  | 12.528 | 3491 | 3495 | 3497 | rBV2 | 743    | 400     | 0.02%  | 0.002% |
| 86  | 12.704 | 3547 | 3550 | 3554 | rVB3 | 701    | 543     | 0.03%  | 0.003% |
| 87  | 12.740 | 3556 | 3561 | 3563 | rBV3 | 594    | 530     | 0.03%  | 0.003% |
| 88  | 13.010 | 3641 | 3645 | 3647 | rBV2 | 862    | 631     | 0.03%  | 0.004% |
| 89  | 13.064 | 3659 | 3662 | 3665 | rBV2 | 609    | 434     | 0.02%  | 0.003% |
| 90  | 13.116 | 3675 | 3678 | 3681 | rBV2 | 752    | 421     | 0.02%  | 0.003% |
| 91  | 13.232 | 3710 | 3714 | 3716 | rBV3 | 620    | 509     | 0.02%  | 0.003% |
| 92  | 13.357 | 3750 | 3753 | 3754 | rBV  | 532    | 290     | 0.01%  | 0.002% |
| 93  | 13.862 | 3904 | 3910 | 3920 | rVB7 | 2664   | 4051    | 0.20%  | 0.025% |
| 94  | 13.965 | 3940 | 3942 | 3944 | rBV2 | 460    | 263     | 0.01%  | 0.002% |
| 95  | 14.109 | 3981 | 3987 | 3989 | rBV3 | 1906   | 1985    | 0.10%  | 0.012% |
| 96  | 14.344 | 4052 | 4060 | 4069 | rBV7 | 2138   | 3916    | 0.19%  | 0.024% |
| 97  | 14.563 | 4126 | 4128 | 4131 | rBV3 | 763    | 544     | 0.03%  | 0.003% |
| 98  | 14.833 | 4210 | 4212 | 4218 | rBV3 | 694    | 517     | 0.03%  | 0.003% |
| 99  | 15.032 | 4272 | 4274 | 4279 | rBV4 | 1485   | 1173    | 0.06%  | 0.007% |
| 100 | 15.138 | 4304 | 4307 | 4311 | rBV3 | 863    | 840     | 0.04%  | 0.005% |

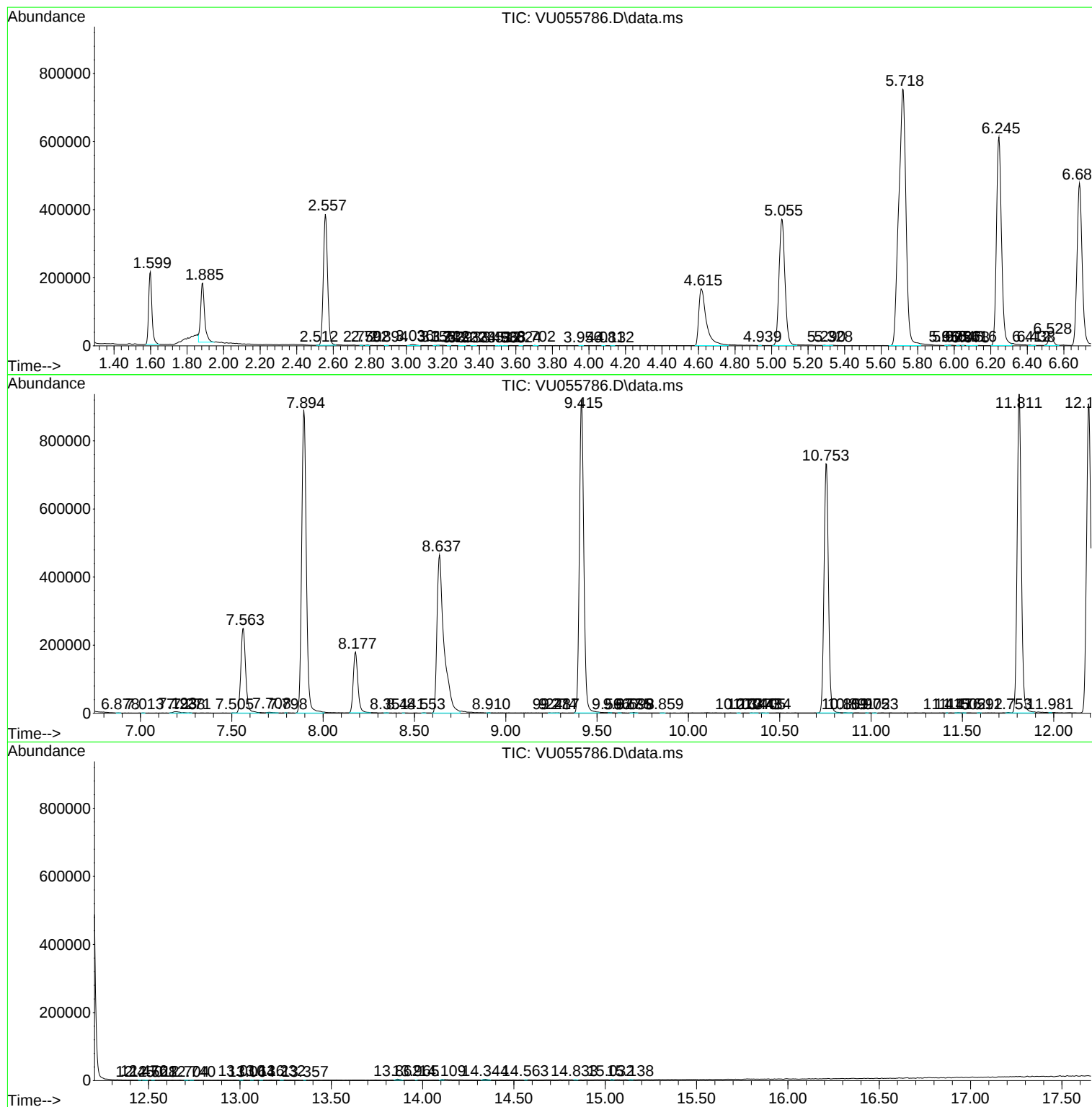
Sum of corrected areas: 16142138

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ALS Vial : 4 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
VBLK109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM101023WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101723\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM101023WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
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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 |