

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU102523\  
 Data File : VU055868.D  
 Acq On : 25 Oct 2023 10:30  
 Operator : MD/SY  
 Sample : VU1025MBL01  
 Misc : 5.00g/5.00mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK115

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: VU055868.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       | 89            | 96          | 110          | rVB      | 230198         | 265317        | 11.63%          | 1.501%        |
| 2         | 1.892       | 180           | 187         | 206          | rVB      | 171700         | 269310        | 11.81%          | 1.524%        |
| 3         | 2.561       | 382           | 395         | 412          | rBV      | 409419         | 674411        | 29.56%          | 3.815%        |
| 4         | 2.782       | 455           | 464         | 475          | rBV3     | 2665           | 4965          | 0.22%           | 0.028%        |
| 5         | 2.827       | 475           | 478         | 480          | rVB2     | 714            | 401           | 0.02%           | 0.002%        |
| 6         | 2.850       | 480           | 485         | 487          | rBV3     | 708            | 521           | 0.02%           | 0.003%        |
| 7         | 2.908       | 498           | 503         | 504          | rBV2     | 582            | 418           | 0.02%           | 0.002%        |
| 8         | 3.040       | 533           | 544         | 556          | rBV6     | 4218           | 8799          | 0.39%           | 0.050%        |
| 9         | 3.178       | 579           | 587         | 592          | rBV4     | 1376           | 1866          | 0.08%           | 0.011%        |
| 10        | 3.297       | 619           | 624         | 627          | rBV3     | 625            | 588           | 0.03%           | 0.003%        |
| 11        | 3.345       | 636           | 639         | 641          | rBV      | 796            | 571           | 0.03%           | 0.003%        |
| 12        | 3.387       | 648           | 652         | 656          | rBV3     | 354            | 356           | 0.02%           | 0.002%        |
| 13        | 3.416       | 656           | 661         | 665          | rVB4     | 564            | 487           | 0.02%           | 0.003%        |
| 14        | 3.554       | 697           | 704         | 707          | rBV2     | 300            | 377           | 0.02%           | 0.002%        |
| 15        | 3.612       | 718           | 722         | 725          | rBV2     | 393            | 330           | 0.01%           | 0.002%        |
| 16        | 4.557       | 1009          | 1016        | 1018         | rBV2     | 385            | 422           | 0.02%           | 0.002%        |
| 17        | 4.612       | 1022          | 1033        | 1068         | rBV      | 186015         | 488118        | 21.40%          | 2.762%        |
| 18        | 4.831       | 1099          | 1101        | 1104         | rVB2     | 886            | 438           | 0.02%           | 0.002%        |
| 19        | 4.966       | 1141          | 1143        | 1147         | rVB3     | 508            | 367           | 0.02%           | 0.002%        |
| 20        | 5.056       | 1155          | 1171        | 1197         | rBV      | 418788         | 933599        | 40.93%          | 5.282%        |
| 21        | 5.290       | 1239          | 1244        | 1245         | rBV3     | 841            | 765           | 0.03%           | 0.004%        |
| 22        | 5.322       | 1251          | 1254        | 1255         | rBV2     | 1637           | 917           | 0.04%           | 0.005%        |
| 23        | 5.490       | 1300          | 1306        | 1310         | rBV2     | 594            | 674           | 0.03%           | 0.004%        |
| 24        | 5.512       | 1310          | 1313        | 1320         | rBV4     | 516            | 644           | 0.03%           | 0.004%        |
| 25        | 5.718       | 1355          | 1377        | 1412         | rBV2     | 819575         | 2281203       | 100.00%         | 12.906%       |
| 26        | 5.962       | 1450          | 1453        | 1457         | rVV5     | 1369           | 1214          | 0.05%           | 0.007%        |
| 27        | 5.994       | 1461          | 1463        | 1467         | rVV3     | 852            | 491           | 0.02%           | 0.003%        |
| 28        | 6.039       | 1469          | 1477        | 1482         | rBV7     | 899            | 1316          | 0.06%           | 0.007%        |
| 29        | 6.245       | 1527          | 1541        | 1567         | rBV      | 641868         | 1254207       | 54.98%          | 7.096%        |
| 30        | 6.525       | 1619          | 1628        | 1631         | rBV6     | 4054           | 6072          | 0.27%           | 0.034%        |
| 31        | 6.576       | 1641          | 1644        | 1645         | rBV2     | 871            | 383           | 0.02%           | 0.002%        |
| 32        | 6.686       | 1662          | 1678        | 1702         | rBV      | 522219         | 1039575       | 45.57%          | 5.881%        |
| 33        | 6.850       | 1727          | 1729        | 1734         | rVB3     | 935            | 581           | 0.03%           | 0.003%        |
| 34        | 6.892       | 1739          | 1742        | 1745         | rVB2     | 719            | 420           | 0.02%           | 0.002%        |
| 35        | 6.943       | 1751          | 1758        | 1761         | rBV2     | 608            | 517           | 0.02%           | 0.003%        |
| 36        | 7.049       | 1787          | 1791        | 1795         | rBV2     | 412            | 332           | 0.01%           | 0.002%        |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK115

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 | 7.184  | 1820 | 1833 | 1848 | rBV6 | 8135    | 20236   | 0.89%  | 0.114% |
| 38 | 7.412  | 1901 | 1904 | 1908 | rBV2 | 632     | 432     | 0.02%  | 0.002% |
| 39 | 7.483  | 1922 | 1926 | 1928 | rBV  | 488     | 361     | 0.02%  | 0.002% |
| 40 | 7.560  | 1936 | 1950 | 1970 | rBV  | 282017  | 506723  | 22.21% | 2.867% |
| 41 | 7.695  | 1984 | 1992 | 2002 | rBV5 | 2927    | 5471    | 0.24%  | 0.031% |
| 42 | 7.798  | 2017 | 2024 | 2032 | rBV5 | 1839    | 2799    | 0.12%  | 0.016% |
| 43 | 7.895  | 2040 | 2054 | 2091 | rBV  | 1001077 | 1759659 | 77.14% | 9.955% |
| 44 | 8.174  | 2130 | 2141 | 2172 | rVB  | 197514  | 343921  | 15.08% | 1.946% |
| 45 | 8.342  | 2190 | 2193 | 2196 | rVB2 | 685     | 375     | 0.02%  | 0.002% |
| 46 | 8.399  | 2208 | 2211 | 2216 | rVB5 | 620     | 486     | 0.02%  | 0.003% |
| 47 | 8.451  | 2223 | 2227 | 2228 | rBV2 | 759     | 456     | 0.02%  | 0.003% |
| 48 | 8.464  | 2228 | 2231 | 2232 | rBV3 | 818     | 505     | 0.02%  | 0.003% |
| 49 | 8.547  | 2253 | 2257 | 2264 | rVB5 | 1527    | 1568    | 0.07%  | 0.009% |
| 50 | 8.631  | 2270 | 2283 | 2319 | rBV  | 677571  | 1325126 | 58.09% | 7.497% |
| 51 | 8.917  | 2369 | 2372 | 2375 | rBV4 | 967     | 749     | 0.03%  | 0.004% |
| 52 | 8.978  | 2387 | 2391 | 2395 | rBV4 | 617     | 576     | 0.03%  | 0.003% |
| 53 | 8.998  | 2395 | 2397 | 2403 | rVB5 | 678     | 604     | 0.03%  | 0.003% |
| 54 | 9.055  | 2411 | 2415 | 2418 | rBV3 | 579     | 558     | 0.02%  | 0.003% |
| 55 | 9.075  | 2418 | 2421 | 2423 | rVV2 | 937     | 489     | 0.02%  | 0.003% |
| 56 | 9.091  | 2423 | 2426 | 2429 | rVB3 | 496     | 369     | 0.02%  | 0.002% |
| 57 | 9.129  | 2435 | 2438 | 2442 | rVB4 | 553     | 389     | 0.02%  | 0.002% |
| 58 | 9.226  | 2464 | 2468 | 2471 | rBV3 | 490     | 440     | 0.02%  | 0.002% |
| 59 | 9.242  | 2471 | 2473 | 2478 | rVB2 | 427     | 322     | 0.01%  | 0.002% |
| 60 | 9.277  | 2481 | 2484 | 2489 | rVB  | 639     | 458     | 0.02%  | 0.003% |
| 61 | 9.300  | 2489 | 2491 | 2495 | rBV  | 797     | 614     | 0.03%  | 0.003% |
| 62 | 9.342  | 2501 | 2504 | 2508 | rVB2 | 823     | 550     | 0.02%  | 0.003% |
| 63 | 9.412  | 2513 | 2526 | 2550 | rBV  | 937734  | 1581170 | 69.31% | 8.945% |
| 64 | 9.547  | 2566 | 2568 | 2571 | rBV5 | 489     | 331     | 0.01%  | 0.002% |
| 65 | 9.673  | 2602 | 2607 | 2609 | rBV3 | 974     | 957     | 0.04%  | 0.005% |
| 66 | 9.769  | 2631 | 2637 | 2639 | rBV2 | 459     | 528     | 0.02%  | 0.003% |
| 67 | 9.837  | 2653 | 2658 | 2661 | rBV2 | 484     | 417     | 0.02%  | 0.002% |
| 68 | 9.891  | 2673 | 2675 | 2680 | rBV2 | 603     | 553     | 0.02%  | 0.003% |
| 69 | 10.052 | 2716 | 2725 | 2730 | rBV3 | 473     | 785     | 0.03%  | 0.004% |
| 70 | 10.178 | 2760 | 2764 | 2768 | rBV3 | 583     | 509     | 0.02%  | 0.003% |
| 71 | 10.293 | 2793 | 2800 | 2803 | rBV2 | 581     | 541     | 0.02%  | 0.003% |
| 72 | 10.422 | 2835 | 2840 | 2843 | rVB2 | 648     | 520     | 0.02%  | 0.003% |
| 73 | 10.486 | 2853 | 2860 | 2869 | rVB5 | 1111    | 1855    | 0.08%  | 0.010% |
| 74 | 10.563 | 2880 | 2884 | 2887 | rVB  | 441     | 337     | 0.01%  | 0.002% |
| 75 | 10.625 | 2899 | 2903 | 2910 | rBV2 | 526     | 649     | 0.03%  | 0.004% |
| 76 | 10.753 | 2928 | 2943 | 2962 | rBV  | 835436  | 1365045 | 59.84% | 7.723% |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK115

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  | 10.879 | 2975 | 2982 | 2985 | rBV4 | 996     | 1268    | 0.06%  | 0.007%  |
| 78  | 10.904 | 2988 | 2990 | 2997 | rVB4 | 1097    | 1145    | 0.05%  | 0.006%  |
| 79  | 11.097 | 3043 | 3050 | 3052 | rBV2 | 864     | 1098    | 0.05%  | 0.006%  |
| 80  | 11.229 | 3087 | 3091 | 3095 | rBV  | 513     | 381     | 0.02%  | 0.002%  |
| 81  | 11.470 | 3163 | 3166 | 3168 | rBV3 | 1225    | 855     | 0.04%  | 0.005%  |
| 82  | 11.743 | 3246 | 3251 | 3252 | rBV2 | 2260    | 1480    | 0.06%  | 0.008%  |
| 83  | 11.808 | 3259 | 3271 | 3292 | rBV  | 1002217 | 1640594 | 71.92% | 9.282%  |
| 84  | 12.123 | 3366 | 3369 | 3371 | rBV2 | 676     | 528     | 0.02%  | 0.003%  |
| 85  | 12.190 | 3376 | 3390 | 3413 | rBV  | 1081498 | 1810377 | 79.36% | 10.242% |
| 86  | 12.444 | 3466 | 3469 | 3470 | rBV2 | 603     | 372     | 0.02%  | 0.002%  |
| 87  | 12.731 | 3555 | 3558 | 3561 | rBV2 | 715     | 542     | 0.02%  | 0.003%  |
| 88  | 12.782 | 3569 | 3574 | 3576 | rBV3 | 610     | 596     | 0.03%  | 0.003%  |
| 89  | 12.837 | 3587 | 3591 | 3596 | rVB2 | 604     | 555     | 0.02%  | 0.003%  |
| 90  | 13.001 | 3640 | 3642 | 3650 | rVB6 | 1017    | 1018    | 0.04%  | 0.006%  |
| 91  | 13.110 | 3672 | 3676 | 3681 | rBV2 | 699     | 619     | 0.03%  | 0.004%  |
| 92  | 13.219 | 3704 | 3710 | 3722 | rBV8 | 3043    | 5672    | 0.25%  | 0.032%  |
| 93  | 13.557 | 3812 | 3815 | 3818 | rBV3 | 568     | 537     | 0.02%  | 0.003%  |
| 94  | 13.660 | 3844 | 3847 | 3854 | rVB3 | 891     | 911     | 0.04%  | 0.005%  |
| 95  | 13.846 | 3897 | 3905 | 3917 | rBV8 | 5561    | 9682    | 0.42%  | 0.055%  |
| 96  | 14.094 | 3976 | 3982 | 3998 | rBV2 | 7207    | 15058   | 0.66%  | 0.085%  |
| 97  | 14.335 | 4049 | 4057 | 4069 | rVB8 | 6155    | 11368   | 0.50%  | 0.064%  |
| 98  | 14.476 | 4099 | 4101 | 4104 | rVB2 | 1115    | 563     | 0.02%  | 0.003%  |
| 99  | 14.505 | 4108 | 4110 | 4113 | rBV2 | 714     | 592     | 0.03%  | 0.003%  |
| 100 | 15.161 | 4312 | 4314 | 4317 | rBV4 | 965     | 393     | 0.02%  | 0.002%  |

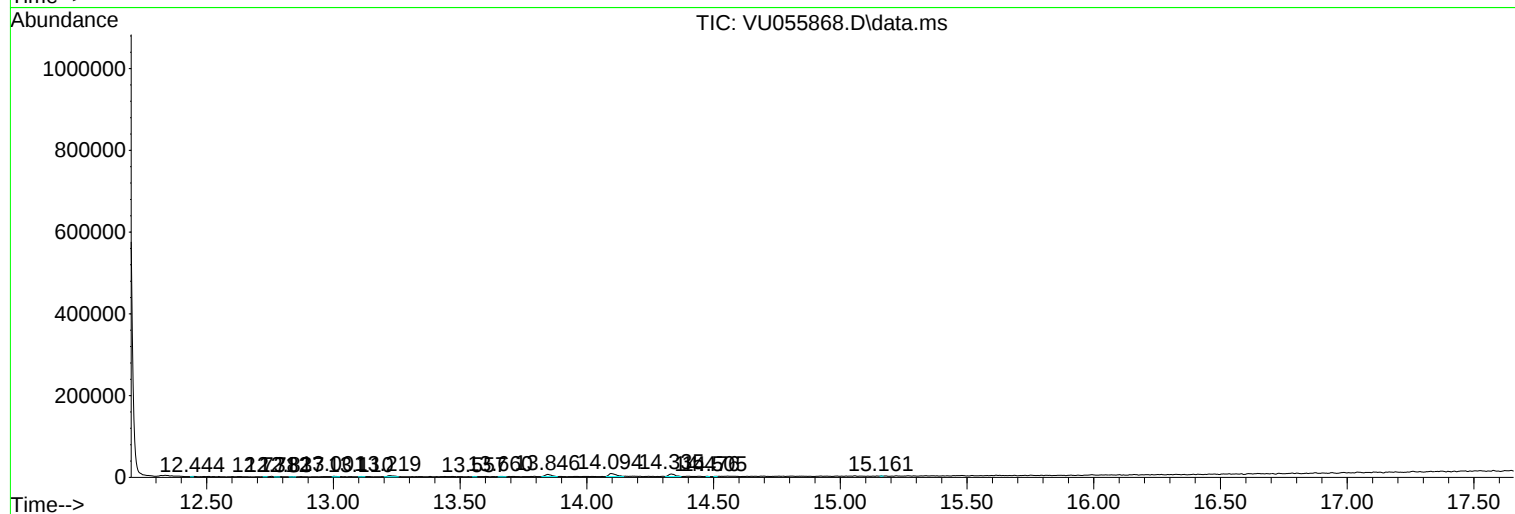
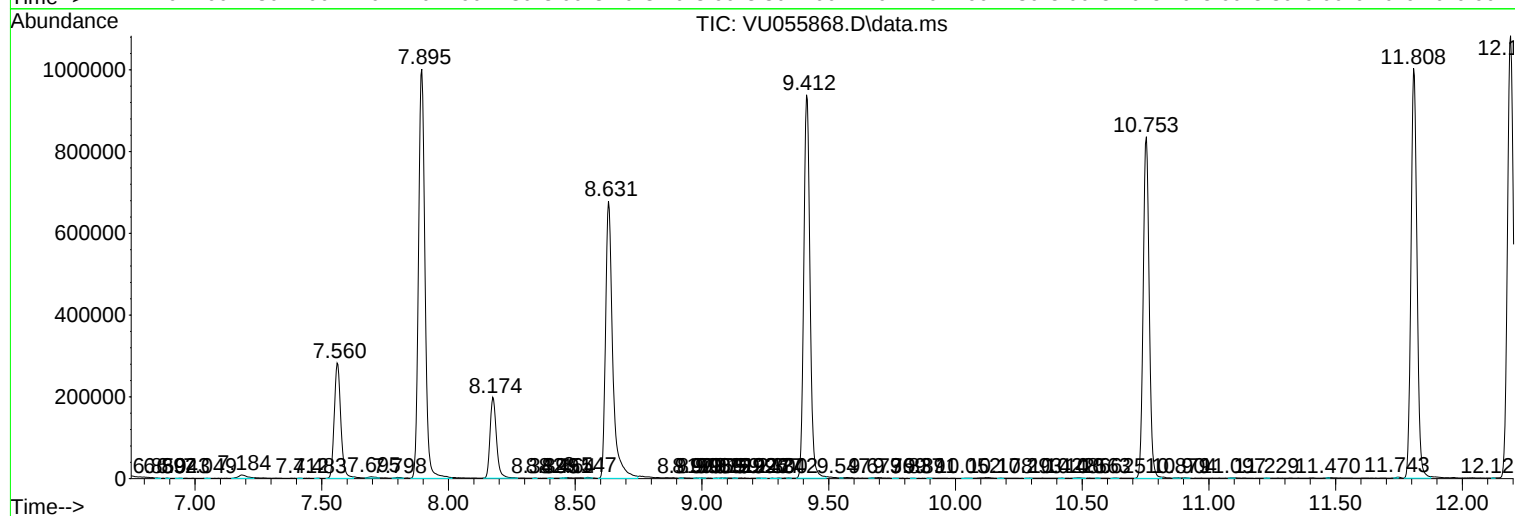
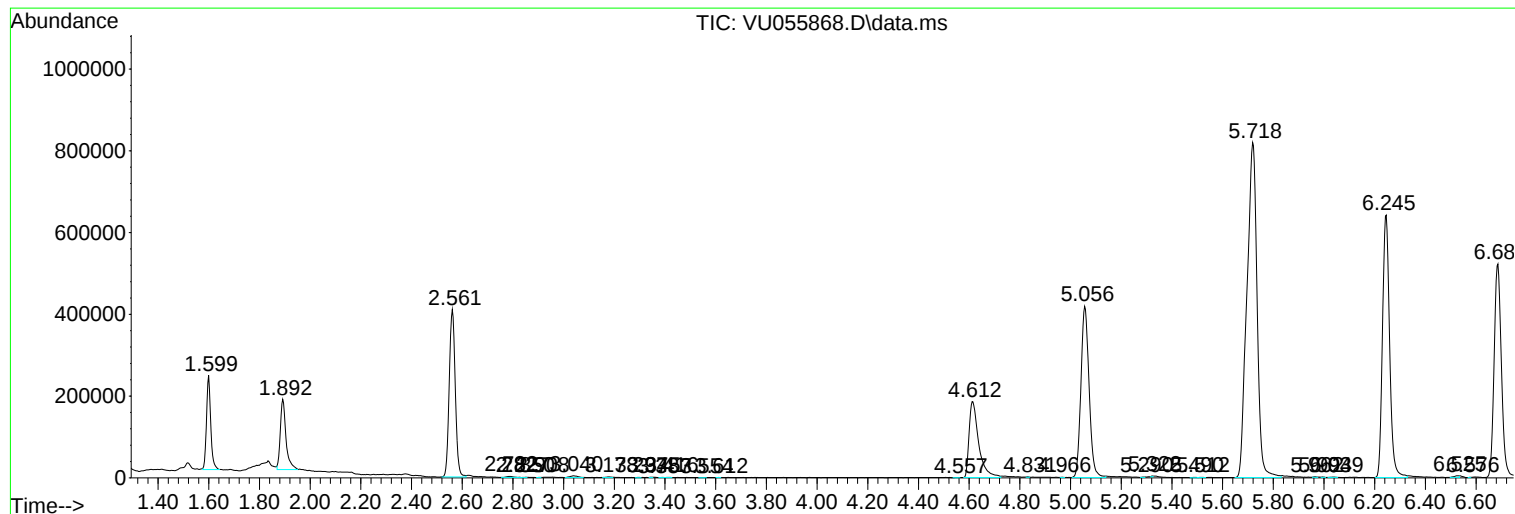
Sum of corrected areas: 17675609

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Instrument :  
MSVOA\_U  
ClientSampleId :  
VBLK115

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\VU102523\  
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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 |