

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042821\  
 Data File : VV021203.D  
 Acq On : 28 Apr 2021 15:51  
 Operator : SY/MD  
 Sample : M2165-12DL 10000X  
 Misc : 6.07g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GB3F3DL

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\_V\Method\SFAMVLM042121WMA.M  
 Title : VOC Analysis

Signal : TIC: VV021203.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         | 1.307       | 77            | 83          | 100          | rVB      | 409714         | 412981        | 14.76%          | 1.693%        |
| 2         | 1.571       | 157           | 165         | 179          | rVB      | 329320         | 375696        | 13.43%          | 1.540%        |
| 3         | 2.111       | 322           | 333         | 370          | rVB      | 699877         | 1058202       | 37.83%          | 4.337%        |
| 4         | 2.358       | 409           | 410         | 412          | rBV      | 768            | 338           | 0.01%           | 0.001%        |
| 5         | 2.413       | 425           | 427         | 429          | rBV3     | 556            | 286           | 0.01%           | 0.001%        |
| 6         | 2.455       | 437           | 440         | 441          | rBV2     | 1251           | 657           | 0.02%           | 0.003%        |
| 7         | 2.577       | 475           | 478         | 483          | rVB3     | 1161           | 750           | 0.03%           | 0.003%        |
| 8         | 2.603       | 483           | 486         | 489          | rBV3     | 786            | 666           | 0.02%           | 0.003%        |
| 9         | 2.651       | 498           | 501         | 502          | rBV2     | 489            | 227           | 0.01%           | 0.001%        |
| 10        | 2.667       | 504           | 506         | 510          | rVB3     | 581            | 293           | 0.01%           | 0.001%        |
| 11        | 2.776       | 536           | 540         | 543          | rBV3     | 718            | 677           | 0.02%           | 0.003%        |
| 12        | 2.873       | 569           | 570         | 573          | rVB2     | 855            | 302           | 0.01%           | 0.001%        |
| 13        | 2.908       | 579           | 581         | 584          | rVB      | 497            | 259           | 0.01%           | 0.001%        |
| 14        | 2.928       | 584           | 587         | 589          | rBV      | 878            | 547           | 0.02%           | 0.002%        |
| 15        | 2.940       | 589           | 591         | 596          | rVV2     | 504            | 473           | 0.02%           | 0.002%        |
| 16        | 2.989       | 604           | 606         | 608          | rBV      | 1013           | 491           | 0.02%           | 0.002%        |
| 17        | 3.114       | 642           | 645         | 647          | rBV3     | 577            | 308           | 0.01%           | 0.001%        |
| 18        | 3.140       | 651           | 653         | 656          | rBV2     | 338            | 205           | 0.01%           | 0.001%        |
| 19        | 3.172       | 661           | 663         | 666          | rBV2     | 703            | 552           | 0.02%           | 0.002%        |
| 20        | 3.268       | 690           | 693         | 696          | rBV      | 937            | 538           | 0.02%           | 0.002%        |
| 21        | 3.336       | 711           | 714         | 718          | rVB2     | 1009           | 623           | 0.02%           | 0.003%        |
| 22        | 3.362       | 718           | 722         | 724          | rBV      | 610            | 401           | 0.01%           | 0.002%        |
| 23        | 3.384       | 726           | 729         | 730          | rBV      | 396            | 179           | 0.01%           | 0.001%        |
| 24        | 3.416       | 735           | 739         | 741          | rBV      | 544            | 350           | 0.01%           | 0.001%        |
| 25        | 3.510       | 766           | 768         | 770          | rBV      | 314            | 178           | 0.01%           | 0.001%        |
| 26        | 3.564       | 783           | 785         | 788          | rBV3     | 330            | 222           | 0.01%           | 0.001%        |
| 27        | 3.593       | 791           | 794         | 797          | rBV2     | 401            | 313           | 0.01%           | 0.001%        |
| 28        | 3.654       | 812           | 813         | 816          | rBV      | 319            | 185           | 0.01%           | 0.001%        |
| 29        | 3.709       | 826           | 830         | 833          | rBV2     | 566            | 484           | 0.02%           | 0.002%        |
| 30        | 3.725       | 833           | 835         | 840          | rVV3     | 365            | 332           | 0.01%           | 0.001%        |
| 31        | 3.780       | 849           | 852         | 854          | rBV3     | 438            | 226           | 0.01%           | 0.001%        |
| 32        | 3.850       | 871           | 874         | 875          | rBV2     | 671            | 415           | 0.01%           | 0.002%        |
| 33        | 3.899       | 879           | 889         | 927          | rBV      | 153865         | 526928        | 18.84%          | 2.160%        |
| 34        | 4.252       | 997           | 999         | 1001         | rBV      | 747            | 289           | 0.01%           | 0.001%        |
| 35        | 4.352       | 1014          | 1030        | 1060         | rBV2     | 471195         | 1169396       | 41.80%          | 4.793%        |
| 36        | 4.593       | 1103          | 1105        | 1106         | rBV2     | 882            | 371           | 0.01%           | 0.002%        |

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Instrument :  
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 ClientSampleId :  
 GB3F3DL

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\_V\Method\SFAMVLM042121WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |         |         |         |         |
|----|-------|------|------|------|------|---------|---------|---------|---------|
| 37 | 4.702 | 1137 | 1139 | 1141 | rBV2 | 501     | 224     | 0.01%   | 0.001%  |
| 38 | 4.776 | 1160 | 1162 | 1166 | rVB4 | 665     | 419     | 0.01%   | 0.002%  |
| 39 | 4.841 | 1180 | 1182 | 1186 | rBV4 | 583     | 465     | 0.02%   | 0.002%  |
| 40 | 4.985 | 1225 | 1227 | 1229 | rBV3 | 498     | 253     | 0.01%   | 0.001%  |
| 41 | 5.050 | 1229 | 1247 | 1287 | rBV2 | 1089913 | 2797411 | 100.00% | 11.466% |
| 42 | 5.622 | 1408 | 1425 | 1452 | rBV  | 868760  | 1744200 | 62.35%  | 7.149%  |
| 43 | 5.911 | 1507 | 1515 | 1533 | rVB4 | 32159   | 69970   | 2.50%   | 0.287%  |
| 44 | 6.075 | 1553 | 1566 | 1595 | rBV  | 610940  | 1238883 | 44.29%  | 5.078%  |
| 45 | 6.362 | 1652 | 1655 | 1658 | rBV5 | 1075    | 667     | 0.02%   | 0.003%  |
| 46 | 6.455 | 1681 | 1684 | 1686 | rBV3 | 984     | 589     | 0.02%   | 0.002%  |
| 47 | 6.519 | 1702 | 1704 | 1706 | rBV3 | 646     | 300     | 0.01%   | 0.001%  |
| 48 | 6.535 | 1706 | 1709 | 1710 | rBV2 | 751     | 372     | 0.01%   | 0.002%  |
| 49 | 6.657 | 1744 | 1747 | 1749 | rBV2 | 530     | 370     | 0.01%   | 0.002%  |
| 50 | 6.728 | 1764 | 1769 | 1772 | rBV3 | 903     | 904     | 0.03%   | 0.004%  |
| 51 | 6.770 | 1780 | 1782 | 1785 | rVB3 | 400     | 201     | 0.01%   | 0.001%  |
| 52 | 6.818 | 1793 | 1797 | 1803 | rVB4 | 984     | 1089    | 0.04%   | 0.004%  |
| 53 | 6.992 | 1839 | 1851 | 1879 | rBV  | 326050  | 617335  | 22.07%  | 2.530%  |
| 54 | 7.262 | 1932 | 1935 | 1939 | rVB3 | 1573    | 1111    | 0.04%   | 0.005%  |
| 55 | 7.320 | 1940 | 1953 | 1972 | rBV  | 1346517 | 2328095 | 83.22%  | 9.543%  |
| 56 | 7.625 | 2038 | 2048 | 2069 | rBV  | 242764  | 420804  | 15.04%  | 1.725%  |
| 57 | 7.815 | 2105 | 2107 | 2109 | rBV  | 1200    | 393     | 0.01%   | 0.002%  |
| 58 | 7.863 | 2120 | 2122 | 2123 | rBV  | 509     | 192     | 0.01%   | 0.001%  |
| 59 | 7.895 | 2130 | 2132 | 2136 | rVB2 | 1272    | 543     | 0.02%   | 0.002%  |
| 60 | 7.979 | 2145 | 2158 | 2180 | rBV  | 1476083 | 2470186 | 88.30%  | 10.125% |
| 61 | 8.095 | 2184 | 2194 | 2229 | rVV  | 614493  | 1164385 | 41.62%  | 4.773%  |
| 62 | 8.657 | 2366 | 2369 | 2371 | rBV3 | 780     | 505     | 0.02%   | 0.002%  |
| 63 | 8.763 | 2400 | 2402 | 2406 | rVB3 | 973     | 504     | 0.02%   | 0.002%  |
| 64 | 8.857 | 2419 | 2431 | 2459 | rBV  | 1342700 | 2172637 | 77.67%  | 8.905%  |
| 65 | 9.146 | 2513 | 2521 | 2522 | rBV5 | 1633    | 1791    | 0.06%   | 0.007%  |
| 66 | 9.313 | 2570 | 2573 | 2574 | rBV2 | 949     | 451     | 0.02%   | 0.002%  |
| 67 | 9.339 | 2579 | 2581 | 2583 | rBV  | 804     | 371     | 0.01%   | 0.002%  |
| 68 | 9.455 | 2615 | 2617 | 2618 | rBV  | 520     | 248     | 0.01%   | 0.001%  |
| 69 | 9.541 | 2642 | 2644 | 2645 | rBV2 | 594     | 256     | 0.01%   | 0.001%  |
| 70 | 9.635 | 2671 | 2673 | 2677 | rVB2 | 982     | 518     | 0.02%   | 0.002%  |
| 71 | 9.754 | 2708 | 2710 | 2711 | rBV  | 432     | 190     | 0.01%   | 0.001%  |
| 72 | 9.786 | 2717 | 2720 | 2721 | rBV  | 401     | 213     | 0.01%   | 0.001%  |
| 73 | 9.815 | 2727 | 2729 | 2734 | rVB3 | 858     | 681     | 0.02%   | 0.003%  |
| 74 | 9.837 | 2734 | 2736 | 2737 | rBV  | 502     | 259     | 0.01%   | 0.001%  |
| 75 | 9.879 | 2747 | 2749 | 2752 | rVB2 | 531     | 275     | 0.01%   | 0.001%  |
| 76 | 9.895 | 2752 | 2754 | 2755 | rBV  | 764     | 223     | 0.01%   | 0.001%  |

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Instrument :  
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Integration Parameters: LSCINT.P

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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\_V\Method\SFAMVLM042121WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |         |         |        |        |
|-----|--------|------|------|------|------|---------|---------|--------|--------|
| 77  | 9.927  | 2761 | 2764 | 2766 | rBV  | 525     | 361     | 0.01%  | 0.001% |
| 78  | 9.988  | 2779 | 2783 | 2785 | rBV  | 728     | 476     | 0.02%  | 0.002% |
| 79  | 10.037 | 2796 | 2798 | 2803 | rVB3 | 825     | 561     | 0.02%  | 0.002% |
| 80  | 10.059 | 2803 | 2805 | 2807 | rBV  | 339     | 188     | 0.01%  | 0.001% |
| 81  | 10.078 | 2808 | 2811 | 2814 | rBV3 | 913     | 765     | 0.03%  | 0.003% |
| 82  | 10.133 | 2820 | 2828 | 2836 | rBV5 | 6683    | 9252    | 0.33%  | 0.038% |
| 83  | 10.223 | 2843 | 2856 | 2877 | rBV  | 905682  | 1440085 | 51.48% | 5.903% |
| 84  | 10.458 | 2925 | 2929 | 2931 | rBV3 | 799     | 598     | 0.02%  | 0.002% |
| 85  | 10.487 | 2936 | 2938 | 2939 | rBV  | 676     | 309     | 0.01%  | 0.001% |
| 86  | 10.538 | 2950 | 2954 | 2958 | rBV3 | 839     | 772     | 0.03%  | 0.003% |
| 87  | 10.570 | 2959 | 2964 | 2967 | rBV3 | 1074    | 1097    | 0.04%  | 0.004% |
| 88  | 10.795 | 3031 | 3034 | 3035 | rBV2 | 785     | 378     | 0.01%  | 0.002% |
| 89  | 10.837 | 3044 | 3047 | 3048 | rBV  | 1018    | 533     | 0.02%  | 0.002% |
| 90  | 10.927 | 3065 | 3075 | 3081 | rBV4 | 6329    | 8779    | 0.31%  | 0.036% |
| 91  | 11.017 | 3101 | 3103 | 3107 | rBV3 | 580     | 406     | 0.01%  | 0.002% |
| 92  | 11.152 | 3140 | 3145 | 3150 | rBV5 | 2678    | 3123    | 0.11%  | 0.013% |
| 93  | 11.255 | 3165 | 3177 | 3203 | rBV  | 1352330 | 2103481 | 75.19% | 8.622% |
| 94  | 11.631 | 3282 | 3294 | 3316 | rBV  | 1407970 | 2228578 | 79.67% | 9.135% |
| 95  | 11.934 | 3386 | 3388 | 3389 | rBV  | 716     | 349     | 0.01%  | 0.001% |
| 96  | 12.863 | 3675 | 3677 | 3679 | rBV  | 587     | 350     | 0.01%  | 0.001% |
| 97  | 12.995 | 3715 | 3718 | 3720 | rBV2 | 439     | 264     | 0.01%  | 0.001% |
| 98  | 13.046 | 3732 | 3734 | 3735 | rBV2 | 759     | 327     | 0.01%  | 0.001% |
| 99  | 13.709 | 3937 | 3940 | 3942 | rBV  | 1398    | 830     | 0.03%  | 0.003% |
| 100 | 14.085 | 4054 | 4057 | 4061 | rBV2 | 1011    | 1020    | 0.04%  | 0.004% |

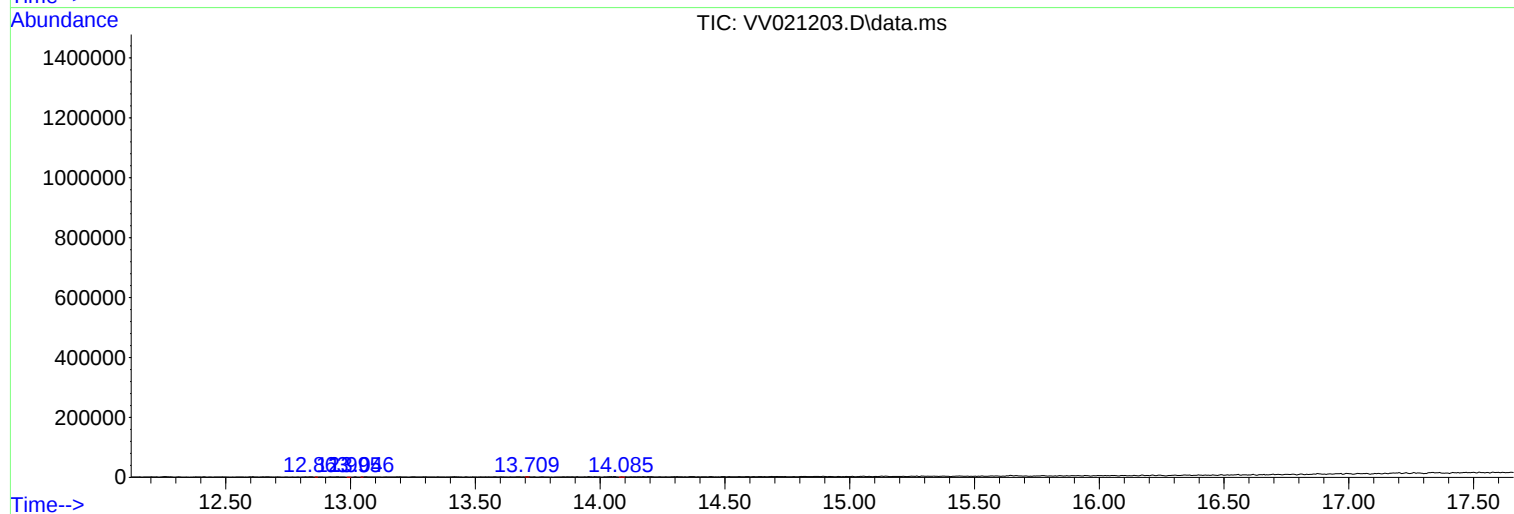
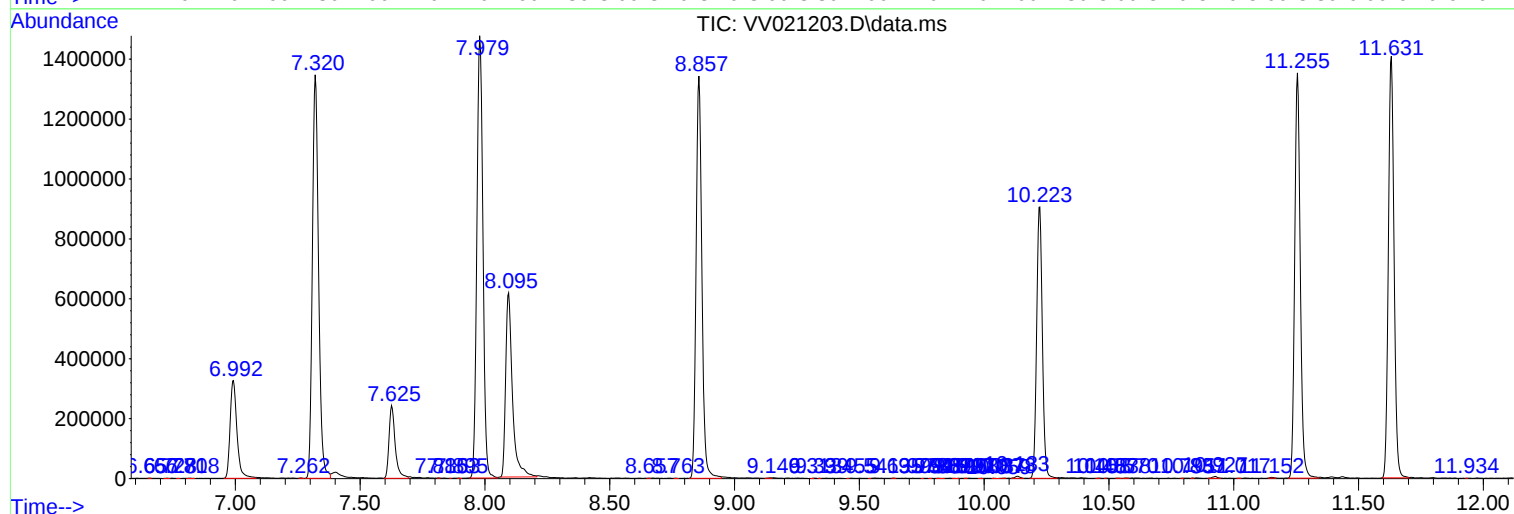
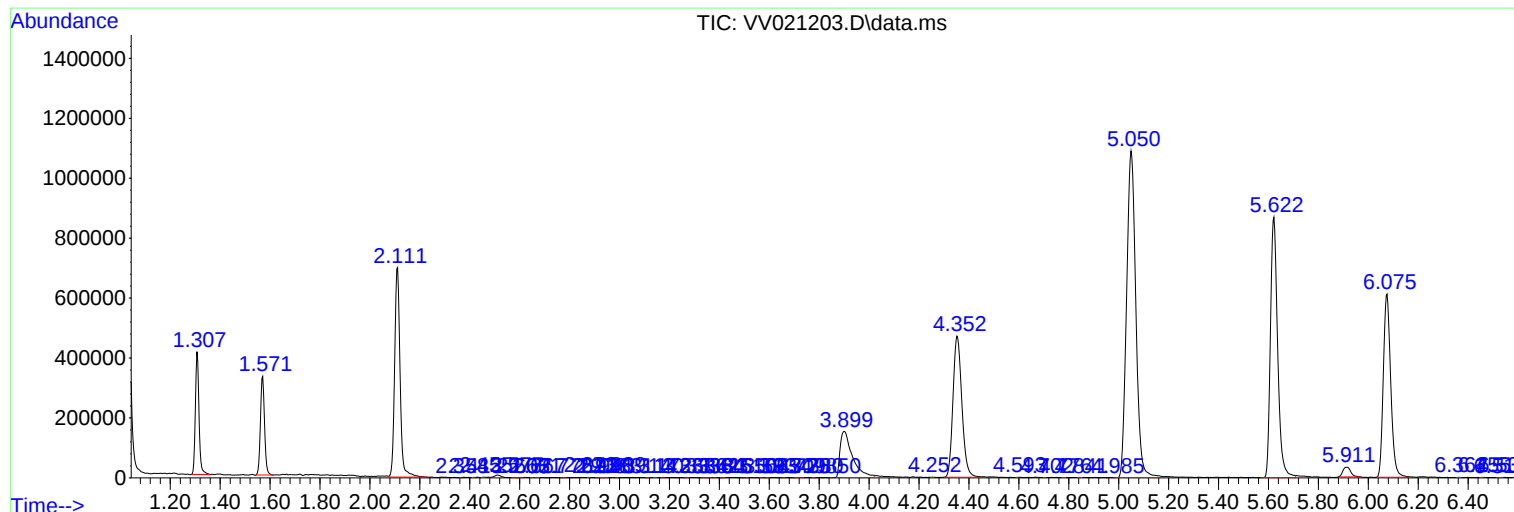
Sum of corrected areas: 24396705

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GB3F3DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM042121WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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No Library Search Compounds Detected

\*\*\*\*\*

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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|