

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU070224\  
 Data File : VU059746.D  
 Acq On : 02 Jul 2024 17:53  
 Operator : MD/SY  
 Sample : P3010-21ME  
 Misc : 3.35g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A4BD0ME

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\SFAMULM070224WMA.M  
 Title : VOC Analysis

Signal : TIC: VU059746.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         | 1.593       | 87            | 94          | 118          | rVB      | 58284          | 100442        | 13.19%          | 1.599%        |
| 2         | 2.538       | 377           | 388         | 409          | rVB      | 145640         | 239688        | 31.48%          | 3.816%        |
| 3         | 2.827       | 475           | 478         | 485          | rVB2     | 443            | 486           | 0.06%           | 0.008%        |
| 4         | 2.856       | 485           | 487         | 489          | rBV2     | 266            | 152           | 0.02%           | 0.002%        |
| 5         | 2.949       | 509           | 516         | 528          | rBV3     | 2947           | 4985          | 0.65%           | 0.079%        |
| 6         | 3.175       | 572           | 586         | 604          | rBV2     | 9958           | 25799         | 3.39%           | 0.411%        |
| 7         | 3.316       | 628           | 630         | 633          | rVB      | 264            | 135           | 0.02%           | 0.002%        |
| 8         | 3.570       | 706           | 709         | 710          | rBV      | 216            | 100           | 0.01%           | 0.002%        |
| 9         | 3.612       | 719           | 722         | 726          | rBV2     | 280            | 279           | 0.04%           | 0.004%        |
| 10        | 3.779       | 772           | 774         | 776          | rBV      | 119            | 72            | 0.01%           | 0.001%        |
| 11        | 3.978       | 833           | 836         | 839          | rVB2     | 357            | 245           | 0.03%           | 0.004%        |
| 12        | 3.998       | 839           | 842         | 844          | rBV      | 196            | 116           | 0.02%           | 0.002%        |
| 13        | 4.123       | 879           | 881         | 883          | rBV2     | 136            | 71            | 0.01%           | 0.001%        |
| 14        | 4.274       | 925           | 928         | 933          | rBV2     | 215            | 233           | 0.03%           | 0.004%        |
| 15        | 4.351       | 949           | 952         | 957          | rVB      | 420            | 371           | 0.05%           | 0.006%        |
| 16        | 4.383       | 957           | 962         | 965          | rBV2     | 323            | 189           | 0.02%           | 0.003%        |
| 17        | 4.400       | 965           | 967         | 970          | rBV2     | 176            | 143           | 0.02%           | 0.002%        |
| 18        | 4.464       | 984           | 987         | 990          | rBV      | 172            | 121           | 0.02%           | 0.002%        |
| 19        | 4.522       | 1002          | 1005        | 1009         | rVB2     | 228            | 135           | 0.02%           | 0.002%        |
| 20        | 4.544       | 1009          | 1012        | 1015         | rBV2     | 192            | 160           | 0.02%           | 0.003%        |
| 21        | 4.625       | 1026          | 1037        | 1083         | rBV      | 55908          | 174622        | 22.93%          | 2.780%        |
| 22        | 5.049       | 1155          | 1169        | 1191         | rBV2     | 131826         | 293502        | 38.54%          | 4.673%        |
| 23        | 5.174       | 1204          | 1208        | 1211         | rBV3     | 283            | 263           | 0.03%           | 0.004%        |
| 24        | 5.313       | 1248          | 1251        | 1255         | rBV2     | 295            | 224           | 0.03%           | 0.004%        |
| 25        | 5.383       | 1270          | 1273        | 1275         | rBV      | 109            | 73            | 0.01%           | 0.001%        |
| 26        | 5.470       | 1297          | 1300        | 1304         | rBV      | 226            | 149           | 0.02%           | 0.002%        |
| 27        | 5.490       | 1304          | 1306        | 1309         | rVB2     | 222            | 128           | 0.02%           | 0.002%        |
| 28        | 5.567       | 1328          | 1330        | 1335         | rVB2     | 383            | 251           | 0.03%           | 0.004%        |
| 29        | 5.609       | 1340          | 1343        | 1346         | rBV2     | 233            | 216           | 0.03%           | 0.003%        |
| 30        | 5.711       | 1356          | 1375        | 1406         | rBV2     | 287849         | 761507        | 100.00%         | 12.125%       |
| 31        | 5.975       | 1450          | 1457        | 1460         | rBV4     | 1037           | 1541          | 0.20%           | 0.025%        |
| 32        | 6.094       | 1489          | 1494        | 1499         | rBV2     | 222            | 283           | 0.04%           | 0.005%        |
| 33        | 6.239       | 1527          | 1539        | 1566         | rBV      | 285877         | 561275        | 73.71%          | 8.937%        |
| 34        | 6.512       | 1620          | 1624        | 1625         | rBV2     | 1478           | 904           | 0.12%           | 0.014%        |
| 35        | 6.596       | 1640          | 1650        | 1663         | rBV3     | 2115           | 4941          | 0.65%           | 0.079%        |
| 36        | 6.682       | 1664          | 1677        | 1696         | rVV      | 167082         | 333729        | 43.82%          | 5.314%        |

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 ClientSampleId :  
 A4BD0ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMULM070224WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.779  | 1705 | 1707 | 1710 | rVB2 | 562    | 295    | 0.04%  | 0.005%  |
| 38 | 6.801  | 1711 | 1714 | 1718 | rBV4 | 546    | 422    | 0.06%  | 0.007%  |
| 39 | 6.978  | 1762 | 1769 | 1773 | rBV2 | 432    | 498    | 0.07%  | 0.008%  |
| 40 | 7.020  | 1779 | 1782 | 1783 | rBV  | 138    | 101    | 0.01%  | 0.002%  |
| 41 | 7.062  | 1790 | 1795 | 1801 | rBV2 | 265    | 452    | 0.06%  | 0.007%  |
| 42 | 7.094  | 1801 | 1805 | 1807 | rBV  | 152    | 143    | 0.02%  | 0.002%  |
| 43 | 7.139  | 1817 | 1819 | 1821 | rBV2 | 214    | 119    | 0.02%  | 0.002%  |
| 44 | 7.190  | 1832 | 1835 | 1837 | rBV3 | 578    | 367    | 0.05%  | 0.006%  |
| 45 | 7.309  | 1871 | 1872 | 1877 | rBV  | 96     | 83     | 0.01%  | 0.001%  |
| 46 | 7.354  | 1880 | 1886 | 1889 | rBV2 | 150    | 211    | 0.03%  | 0.003%  |
| 47 | 7.461  | 1916 | 1919 | 1920 | rBV  | 194    | 123    | 0.02%  | 0.002%  |
| 48 | 7.560  | 1938 | 1950 | 1969 | rBV  | 87966  | 162343 | 21.32% | 2.585%  |
| 49 | 7.715  | 1989 | 1998 | 1999 | rBV2 | 390    | 533    | 0.07%  | 0.008%  |
| 50 | 7.772  | 2012 | 2016 | 2018 | rBV2 | 628    | 440    | 0.06%  | 0.007%  |
| 51 | 7.846  | 2035 | 2039 | 2040 | rBV  | 195    | 143    | 0.02%  | 0.002%  |
| 52 | 7.891  | 2040 | 2053 | 2075 | rBV  | 344259 | 605422 | 79.50% | 9.640%  |
| 53 | 8.104  | 2116 | 2119 | 2122 | rBV2 | 273    | 141    | 0.02%  | 0.002%  |
| 54 | 8.174  | 2130 | 2141 | 2164 | rBV2 | 60607  | 112246 | 14.74% | 1.787%  |
| 55 | 8.306  | 2179 | 2182 | 2184 | rBV2 | 170    | 142    | 0.02%  | 0.002%  |
| 56 | 8.457  | 2226 | 2229 | 2231 | rBV2 | 269    | 185    | 0.02%  | 0.003%  |
| 57 | 8.551  | 2252 | 2258 | 2262 | rBV4 | 944    | 1167   | 0.15%  | 0.019%  |
| 58 | 8.641  | 2273 | 2286 | 2310 | rBV  | 171758 | 384241 | 50.46% | 6.118%  |
| 59 | 8.985  | 2386 | 2393 | 2395 | rBV2 | 228    | 309    | 0.04%  | 0.005%  |
| 60 | 9.007  | 2398 | 2400 | 2402 | rVB2 | 182    | 72     | 0.01%  | 0.001%  |
| 61 | 9.039  | 2408 | 2410 | 2412 | rBV2 | 179    | 107    | 0.01%  | 0.002%  |
| 62 | 9.126  | 2431 | 2437 | 2441 | rBV2 | 336    | 393    | 0.05%  | 0.006%  |
| 63 | 9.284  | 2481 | 2486 | 2487 | rBV2 | 138    | 100    | 0.01%  | 0.002%  |
| 64 | 9.412  | 2512 | 2526 | 2544 | rBV  | 416481 | 731056 | 96.00% | 11.640% |
| 65 | 9.567  | 2570 | 2574 | 2576 | rBV2 | 737    | 600    | 0.08%  | 0.010%  |
| 66 | 9.692  | 2605 | 2613 | 2614 | rBV2 | 3161   | 2591   | 0.34%  | 0.041%  |
| 67 | 9.785  | 2640 | 2642 | 2645 | rVB2 | 199    | 120    | 0.02%  | 0.002%  |
| 68 | 9.853  | 2658 | 2663 | 2668 | rBV2 | 348    | 395    | 0.05%  | 0.006%  |
| 69 | 9.878  | 2669 | 2671 | 2674 | rBV2 | 177    | 110    | 0.01%  | 0.002%  |
| 70 | 9.959  | 2692 | 2696 | 2699 | rBV2 | 209    | 188    | 0.02%  | 0.003%  |
| 71 | 10.001 | 2707 | 2709 | 2712 | rBV  | 151    | 124    | 0.02%  | 0.002%  |
| 72 | 10.203 | 2770 | 2772 | 2774 | rBV  | 158    | 114    | 0.01%  | 0.002%  |
| 73 | 10.235 | 2779 | 2782 | 2786 | rBV2 | 208    | 138    | 0.02%  | 0.002%  |
| 74 | 10.258 | 2786 | 2789 | 2792 | rBV2 | 205    | 157    | 0.02%  | 0.002%  |
| 75 | 10.274 | 2792 | 2794 | 2796 | rBV2 | 231    | 115    | 0.02%  | 0.002%  |
| 76 | 10.306 | 2801 | 2804 | 2807 | rBV2 | 219    | 165    | 0.02%  | 0.003%  |

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 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
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 ClientSampleId :  
 A4BD0ME

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\SFAMULM070224WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 10.351 | 2815 | 2818 | 2820 | rVB  | 221    | 137    | 0.02%  | 0.002%  |
| 78  | 10.431 | 2841 | 2843 | 2844 | rBV  | 321    | 98     | 0.01%  | 0.002%  |
| 79  | 10.676 | 2915 | 2919 | 2921 | rBV  | 232    | 202    | 0.03%  | 0.003%  |
| 80  | 10.753 | 2930 | 2943 | 2962 | rBV  | 280595 | 457058 | 60.02% | 7.278%  |
| 81  | 10.936 | 2996 | 3000 | 3003 | rBV2 | 179    | 193    | 0.03%  | 0.003%  |
| 82  | 10.959 | 3004 | 3007 | 3012 | rBV2 | 307    | 231    | 0.03%  | 0.004%  |
| 83  | 11.100 | 3048 | 3051 | 3052 | rBV  | 251    | 152    | 0.02%  | 0.002%  |
| 84  | 11.197 | 3078 | 3081 | 3084 | rBV  | 178    | 140    | 0.02%  | 0.002%  |
| 85  | 11.322 | 3117 | 3120 | 3123 | rBV  | 242    | 198    | 0.03%  | 0.003%  |
| 86  | 11.380 | 3133 | 3138 | 3140 | rBV2 | 329    | 281    | 0.04%  | 0.004%  |
| 87  | 11.441 | 3149 | 3157 | 3160 | rBV2 | 324    | 375    | 0.05%  | 0.006%  |
| 88  | 11.560 | 3191 | 3194 | 3198 | rBV  | 168    | 156    | 0.02%  | 0.002%  |
| 89  | 11.583 | 3198 | 3201 | 3204 | rVB  | 286    | 192    | 0.03%  | 0.003%  |
| 90  | 11.615 | 3209 | 3211 | 3218 | rVB2 | 263    | 290    | 0.04%  | 0.005%  |
| 91  | 11.650 | 3218 | 3222 | 3225 | rBV2 | 369    | 315    | 0.04%  | 0.005%  |
| 92  | 11.685 | 3230 | 3233 | 3238 | rBV2 | 244    | 217    | 0.03%  | 0.003%  |
| 93  | 11.714 | 3238 | 3242 | 3245 | rBV2 | 278    | 259    | 0.03%  | 0.004%  |
| 94  | 11.808 | 3259 | 3271 | 3292 | rBV  | 432436 | 713685 | 93.72% | 11.364% |
| 95  | 12.190 | 3377 | 3390 | 3410 | rBV  | 357688 | 590920 | 77.60% | 9.409%  |
| 96  | 12.374 | 3445 | 3447 | 3450 | rBV2 | 262    | 115    | 0.02%  | 0.002%  |
| 97  | 12.492 | 3481 | 3484 | 3486 | rBV  | 194    | 105    | 0.01%  | 0.002%  |
| 98  | 12.592 | 3510 | 3515 | 3516 | rBV2 | 305    | 252    | 0.03%  | 0.004%  |
| 99  | 13.634 | 3836 | 3839 | 3844 | rBV2 | 351    | 303    | 0.04%  | 0.005%  |
| 100 | 15.000 | 4261 | 4264 | 4266 | rBV  | 422    | 256    | 0.03%  | 0.004%  |

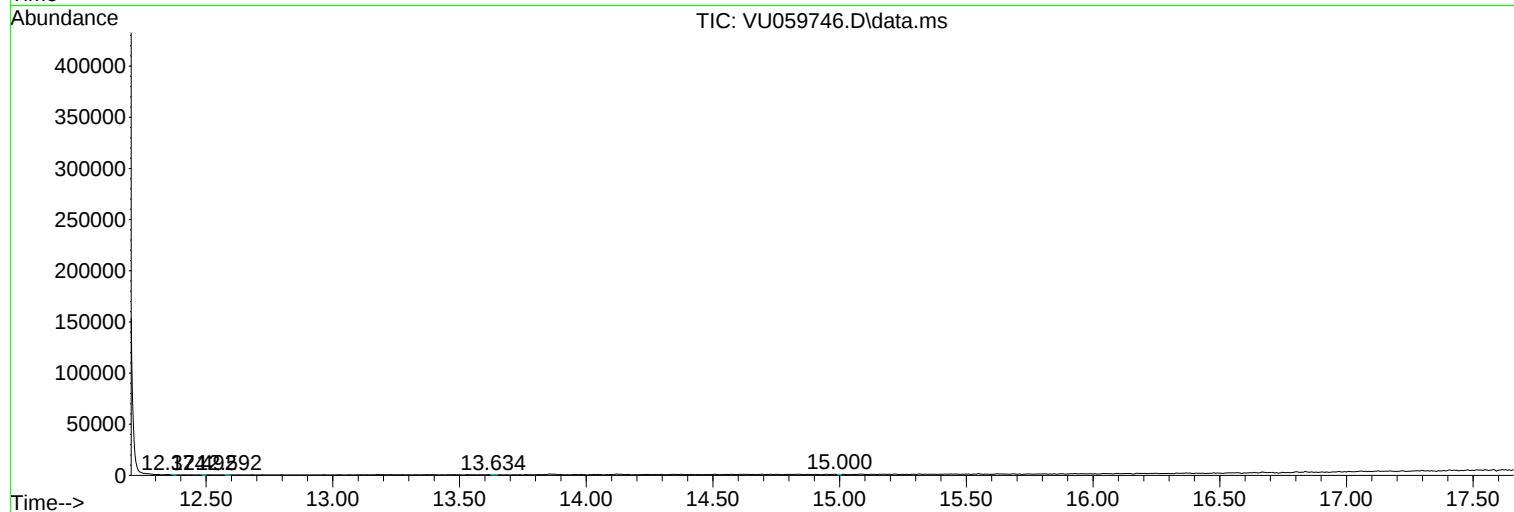
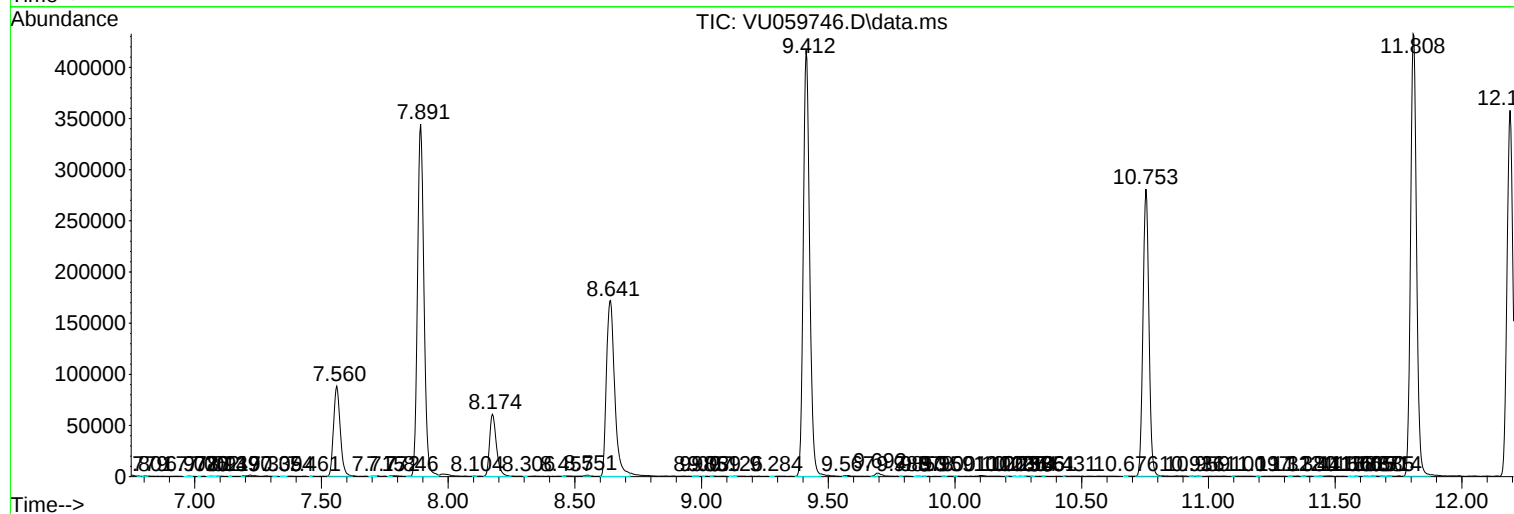
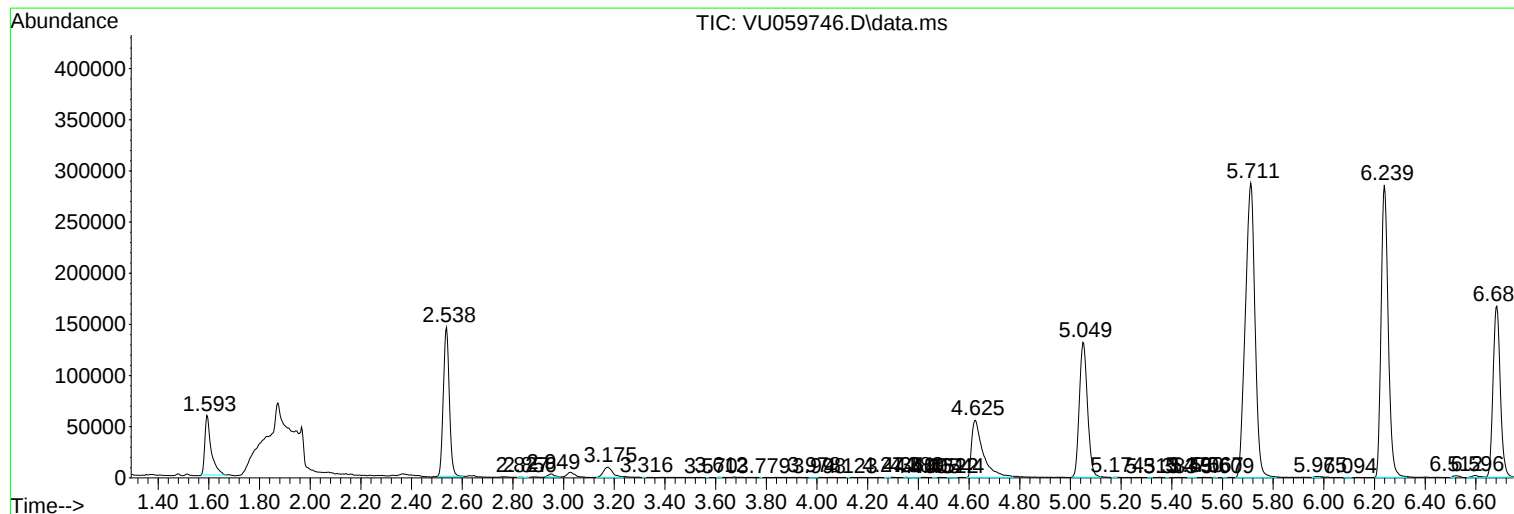
Sum of corrected areas: 6280331

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Instrument :  
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A4BD0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM070224WMA.M  
Quant Title : VOC Analysis

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



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No Library Search Compounds Detected

\*\*\*\*\*

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