

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV062923\  
 Data File : VV031611.D  
 Acq On : 29 Jun 2023 10:37  
 Operator : SY/MD  
 Sample : VV0629MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 VBLK362

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\SFAMVLM061423WMA.M

Title : VOC Analysis

Signal : TIC: VV031611.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         | 1.282       | 68            | 75          | 90           | rVB      | 105097         | 115286        | 14.82%          | 1.790%        |
| 2         | 1.536       | 147           | 154         | 169          | rVB      | 98761          | 120439        | 15.48%          | 1.870%        |
| 3         | 2.063       | 308           | 318         | 336          | rBV      | 203866         | 295381        | 37.97%          | 4.586%        |
| 4         | 2.240       | 369           | 373         | 376          | rBV4     | 782            | 655           | 0.08%           | 0.010%        |
| 5         | 2.452       | 429           | 439         | 449          | rBV5     | 2807           | 4290          | 0.55%           | 0.067%        |
| 6         | 2.587       | 478           | 481         | 487          | rVB3     | 494            | 455           | 0.06%           | 0.007%        |
| 7         | 2.629       | 492           | 494         | 497          | rBV2     | 354            | 218           | 0.03%           | 0.003%        |
| 8         | 2.703       | 513           | 517         | 519          | rBV3     | 847            | 637           | 0.08%           | 0.010%        |
| 9         | 2.780       | 539           | 541         | 548          | rVB2     | 347            | 217           | 0.03%           | 0.003%        |
| 10        | 2.889       | 571           | 575         | 582          | rBV2     | 367            | 472           | 0.06%           | 0.007%        |
| 11        | 3.044       | 618           | 623         | 626          | rBV3     | 256            | 258           | 0.03%           | 0.004%        |
| 12        | 3.124       | 645           | 648         | 653          | rVB4     | 439            | 372           | 0.05%           | 0.006%        |
| 13        | 3.146       | 653           | 655         | 660          | rBV2     | 324            | 301           | 0.04%           | 0.005%        |
| 14        | 3.195       | 667           | 670         | 677          | rVB      | 541            | 526           | 0.07%           | 0.008%        |
| 15        | 3.230       | 677           | 681         | 683          | rBV2     | 231            | 221           | 0.03%           | 0.003%        |
| 16        | 3.243       | 683           | 685         | 689          | rVV2     | 344            | 270           | 0.03%           | 0.004%        |
| 17        | 3.278       | 694           | 696         | 700          | rVB2     | 345            | 268           | 0.03%           | 0.004%        |
| 18        | 3.526       | 767           | 773         | 775          | rBV2     | 493            | 458           | 0.06%           | 0.007%        |
| 19        | 3.606       | 792           | 798         | 799          | rBV      | 290            | 218           | 0.03%           | 0.003%        |
| 20        | 3.642       | 805           | 809         | 813          | rBV2     | 237            | 230           | 0.03%           | 0.004%        |
| 21        | 3.728       | 834           | 836         | 839          | rVB2     | 389            | 257           | 0.03%           | 0.004%        |
| 22        | 3.796       | 847           | 857         | 887          | rBV2     | 57219          | 164972        | 21.20%          | 2.561%        |
| 23        | 4.198       | 977           | 982         | 984          | rBV2     | 330            | 298           | 0.04%           | 0.005%        |
| 24        | 4.256       | 984           | 1000        | 1031         | rVV      | 135447         | 347924        | 44.72%          | 5.402%        |
| 25        | 4.564       | 1093          | 1096        | 1097         | rBV      | 379            | 222           | 0.03%           | 0.003%        |
| 26        | 4.690       | 1132          | 1135        | 1139         | rVB2     | 439            | 354           | 0.05%           | 0.005%        |
| 27        | 4.963       | 1202          | 1220        | 1248         | rBV3     | 287729         | 778012        | 100.00%         | 12.079%       |
| 28        | 5.195       | 1288          | 1292        | 1296         | rVB3     | 478            | 447           | 0.06%           | 0.007%        |
| 29        | 5.317       | 1326          | 1330        | 1332         | rBV3     | 288            | 232           | 0.03%           | 0.004%        |
| 30        | 5.471       | 1375          | 1378        | 1382         | rBV2     | 238            | 227           | 0.03%           | 0.004%        |
| 31        | 5.539       | 1387          | 1399        | 1424         | rBV      | 248925         | 514311        | 66.11%          | 7.985%        |
| 32        | 5.825       | 1484          | 1488        | 1490         | rBV3     | 1287           | 1171          | 0.15%           | 0.018%        |
| 33        | 5.995       | 1528          | 1541        | 1560         | rBV      | 185738         | 383261        | 49.26%          | 5.951%        |
| 34        | 6.223       | 1608          | 1612        | 1615         | rBV2     | 259            | 281           | 0.04%           | 0.004%        |
| 35        | 6.317       | 1635          | 1641        | 1644         | rVB2     | 422            | 352           | 0.05%           | 0.005%        |
| 36        | 6.577       | 1718          | 1722        | 1725         | rVV3     | 393            | 443           | 0.06%           | 0.007%        |

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 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 VBLK362

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\SFAMVLM061423WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.728  | 1765 | 1769 | 1772 | rVB4 | 582    | 377    | 0.05%  | 0.006%  |
| 38 | 6.789  | 1784 | 1788 | 1791 | rVB3 | 348    | 230    | 0.03%  | 0.004%  |
| 39 | 6.918  | 1816 | 1828 | 1861 | rBV2 | 87291  | 169796 | 21.82% | 2.636%  |
| 40 | 7.121  | 1888 | 1891 | 1896 | rBV3 | 690    | 440    | 0.06%  | 0.007%  |
| 41 | 7.249  | 1919 | 1931 | 1955 | rBV  | 298189 | 530385 | 68.17% | 8.235%  |
| 42 | 7.487  | 2001 | 2005 | 2007 | rBV  | 476    | 284    | 0.04%  | 0.004%  |
| 43 | 7.558  | 2016 | 2027 | 2050 | rBV  | 76585  | 141525 | 18.19% | 2.197%  |
| 44 | 7.677  | 2062 | 2064 | 2076 | rVB4 | 1148   | 1433   | 0.18%  | 0.022%  |
| 45 | 7.728  | 2076 | 2080 | 2083 | rBV3 | 375    | 300    | 0.04%  | 0.005%  |
| 46 | 7.793  | 2092 | 2100 | 2104 | rBV4 | 682    | 862    | 0.11%  | 0.013%  |
| 47 | 7.892  | 2129 | 2131 | 2137 | rVB3 | 564    | 395    | 0.05%  | 0.006%  |
| 48 | 7.921  | 2137 | 2140 | 2141 | rBV  | 432    | 246    | 0.03%  | 0.004%  |
| 49 | 8.030  | 2164 | 2174 | 2199 | rBV  | 229137 | 412776 | 53.06% | 6.409%  |
| 50 | 8.301  | 2256 | 2258 | 2260 | rVB2 | 645    | 232    | 0.03%  | 0.004%  |
| 51 | 8.420  | 2292 | 2295 | 2299 | rVB3 | 598    | 466    | 0.06%  | 0.007%  |
| 52 | 8.532  | 2326 | 2330 | 2333 | rVB3 | 556    | 268    | 0.03%  | 0.004%  |
| 53 | 8.789  | 2398 | 2410 | 2432 | rBV  | 436292 | 721338 | 92.72% | 11.199% |
| 54 | 8.956  | 2460 | 2462 | 2467 | rBV3 | 607    | 537    | 0.07%  | 0.008%  |
| 55 | 9.088  | 2495 | 2503 | 2506 | rBV5 | 629    | 902    | 0.12%  | 0.014%  |
| 56 | 9.133  | 2512 | 2517 | 2521 | rBV4 | 462    | 463    | 0.06%  | 0.007%  |
| 57 | 9.262  | 2556 | 2557 | 2562 | rVB2 | 345    | 231    | 0.03%  | 0.004%  |
| 58 | 9.873  | 2741 | 2747 | 2751 | rBV3 | 541    | 748    | 0.10%  | 0.012%  |
| 59 | 10.005 | 2785 | 2788 | 2792 | rVB  | 373    | 236    | 0.03%  | 0.004%  |
| 60 | 10.046 | 2795 | 2801 | 2806 | rBV3 | 676    | 656    | 0.08%  | 0.010%  |
| 61 | 10.156 | 2823 | 2835 | 2857 | rVV  | 293912 | 466000 | 59.90% | 7.235%  |
| 62 | 10.281 | 2869 | 2874 | 2876 | rVB2 | 360    | 301    | 0.04%  | 0.005%  |
| 63 | 10.326 | 2886 | 2888 | 2893 | rVB4 | 540    | 462    | 0.06%  | 0.007%  |
| 64 | 10.352 | 2893 | 2896 | 2899 | rBV3 | 440    | 350    | 0.04%  | 0.005%  |
| 65 | 10.484 | 2933 | 2937 | 2938 | rBV2 | 818    | 670    | 0.09%  | 0.010%  |
| 66 | 11.024 | 3101 | 3105 | 3107 | rBV  | 314    | 227    | 0.03%  | 0.004%  |
| 67 | 11.130 | 3132 | 3138 | 3144 | rVB3 | 1805   | 2085   | 0.27%  | 0.032%  |
| 68 | 11.191 | 3145 | 3157 | 3180 | rBV  | 425198 | 640630 | 82.34% | 9.946%  |
| 69 | 11.426 | 3226 | 3230 | 3233 | rBV3 | 288    | 304    | 0.04%  | 0.005%  |
| 70 | 11.567 | 3262 | 3274 | 3291 | rBV  | 359505 | 560267 | 72.01% | 8.699%  |
| 71 | 11.709 | 3315 | 3318 | 3320 | rBV2 | 311    | 223    | 0.03%  | 0.003%  |
| 72 | 12.448 | 3546 | 3548 | 3555 | rBV2 | 541    | 498    | 0.06%  | 0.008%  |
| 73 | 12.532 | 3569 | 3574 | 3581 | rBV3 | 444    | 605    | 0.08%  | 0.009%  |
| 74 | 12.590 | 3586 | 3592 | 3599 | rBV4 | 2896   | 3539   | 0.45%  | 0.055%  |
| 75 | 12.805 | 3656 | 3659 | 3665 | rBV2 | 504    | 419    | 0.05%  | 0.007%  |
| 76 | 12.908 | 3688 | 3691 | 3695 | rBV2 | 298    | 234    | 0.03%  | 0.004%  |

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 Sample : VV0629MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 VBLK362

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\SFAMVLM061423WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 13.178 | 3773 | 3775 | 3776 | rBV  | 484   | 229   | 0.03% | 0.004% |
| 78  | 13.204 | 3776 | 3783 | 3794 | rVV3 | 4098  | 6226  | 0.80% | 0.097% |
| 79  | 13.352 | 3824 | 3829 | 3830 | rBV  | 310   | 263   | 0.03% | 0.004% |
| 80  | 13.390 | 3837 | 3841 | 3843 | rBV2 | 420   | 304   | 0.04% | 0.005% |
| 81  | 13.448 | 3851 | 3859 | 3871 | rBV  | 12904 | 19307 | 2.48% | 0.300% |
| 82  | 13.503 | 3874 | 3876 | 3880 | rVB3 | 507   | 348   | 0.04% | 0.005% |
| 83  | 13.570 | 3892 | 3897 | 3898 | rBV2 | 333   | 238   | 0.03% | 0.004% |
| 84  | 13.689 | 3925 | 3934 | 3945 | rVB6 | 7051  | 10573 | 1.36% | 0.164% |
| 85  | 13.844 | 3978 | 3982 | 3985 | rBV2 | 470   | 435   | 0.06% | 0.007% |
| 86  | 13.931 | 4005 | 4009 | 4012 | rVB3 | 431   | 353   | 0.05% | 0.005% |
| 87  | 13.992 | 4023 | 4028 | 4037 | rVB5 | 1613  | 2012  | 0.26% | 0.031% |
| 88  | 14.111 | 4063 | 4065 | 4068 | rVB3 | 642   | 223   | 0.03% | 0.003% |
| 89  | 14.336 | 4133 | 4135 | 4139 | rVB2 | 439   | 264   | 0.03% | 0.004% |
| 90  | 14.374 | 4144 | 4147 | 4150 | rBV2 | 424   | 319   | 0.04% | 0.005% |
| 91  | 14.410 | 4155 | 4158 | 4160 | rBV3 | 609   | 420   | 0.05% | 0.007% |
| 92  | 14.484 | 4175 | 4181 | 4183 | rBV  | 759   | 745   | 0.10% | 0.012% |
| 93  | 14.628 | 4222 | 4226 | 4227 | rBV2 | 485   | 277   | 0.04% | 0.004% |
| 94  | 14.741 | 4259 | 4261 | 4265 | rBV3 | 456   | 250   | 0.03% | 0.004% |
| 95  | 14.779 | 4271 | 4273 | 4278 | rVB3 | 463   | 290   | 0.04% | 0.005% |
| 96  | 14.853 | 4294 | 4296 | 4298 | rBV  | 459   | 246   | 0.03% | 0.004% |
| 97  | 14.959 | 4326 | 4329 | 4331 | rBV4 | 565   | 428   | 0.06% | 0.007% |
| 98  | 15.001 | 4340 | 4342 | 4344 | rBV2 | 628   | 230   | 0.03% | 0.004% |
| 99  | 15.377 | 4457 | 4459 | 4464 | rBV4 | 902   | 521   | 0.07% | 0.008% |
| 100 | 15.461 | 4482 | 4485 | 4486 | rBV2 | 607   | 434   | 0.06% | 0.007% |

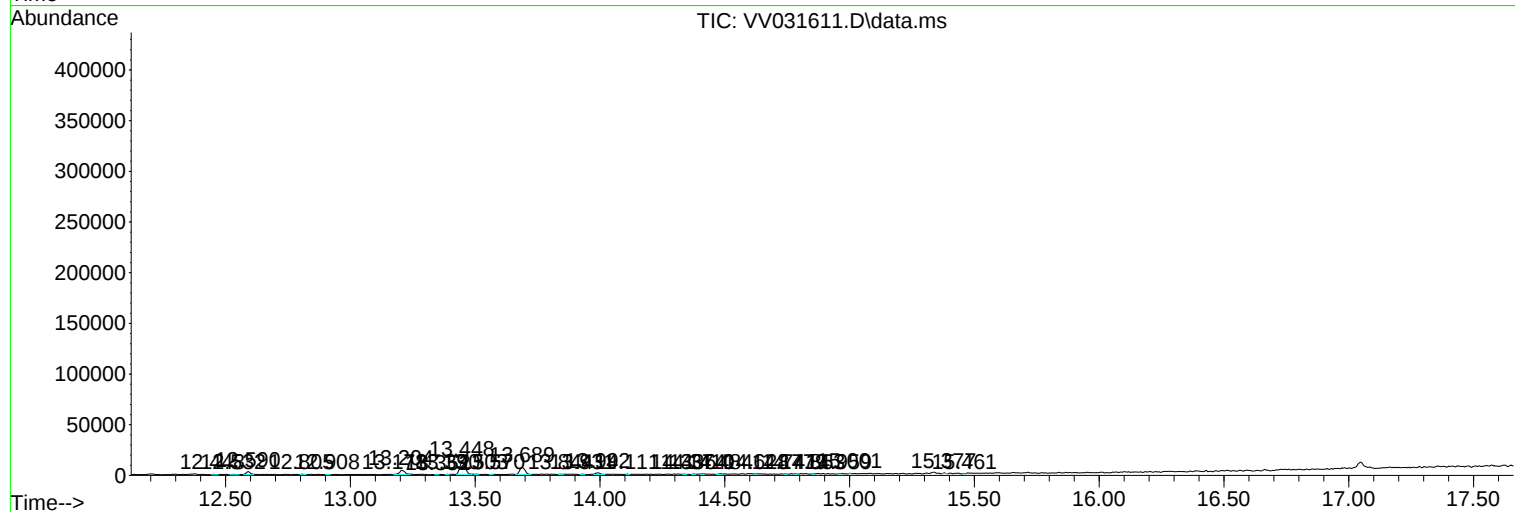
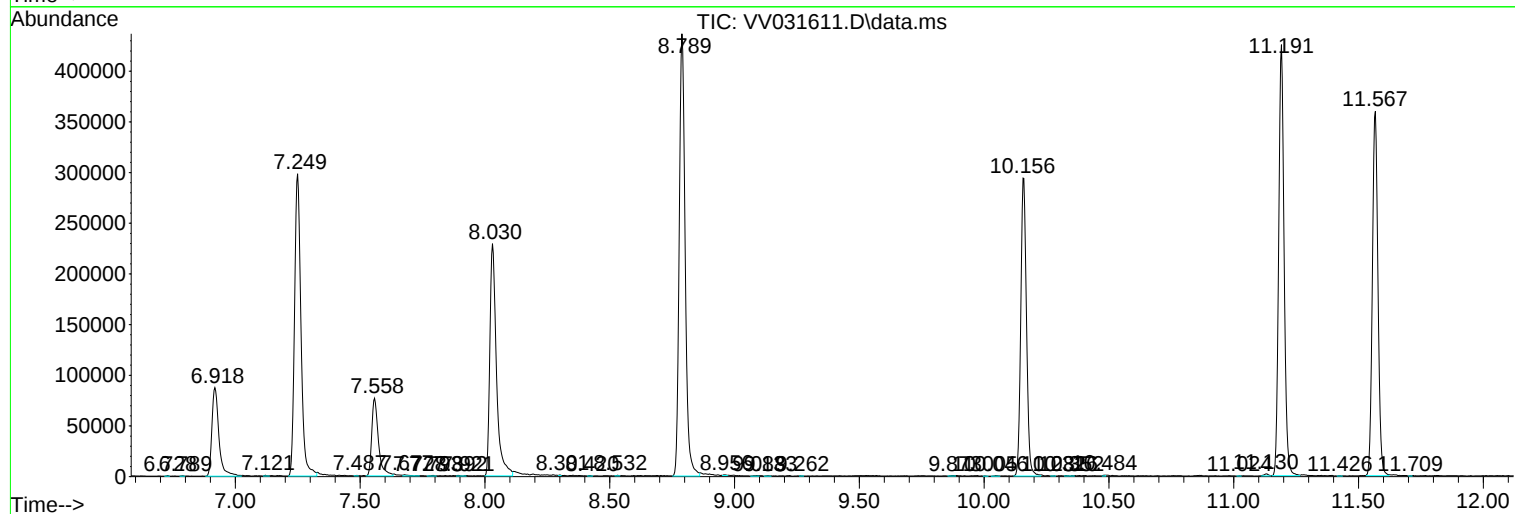
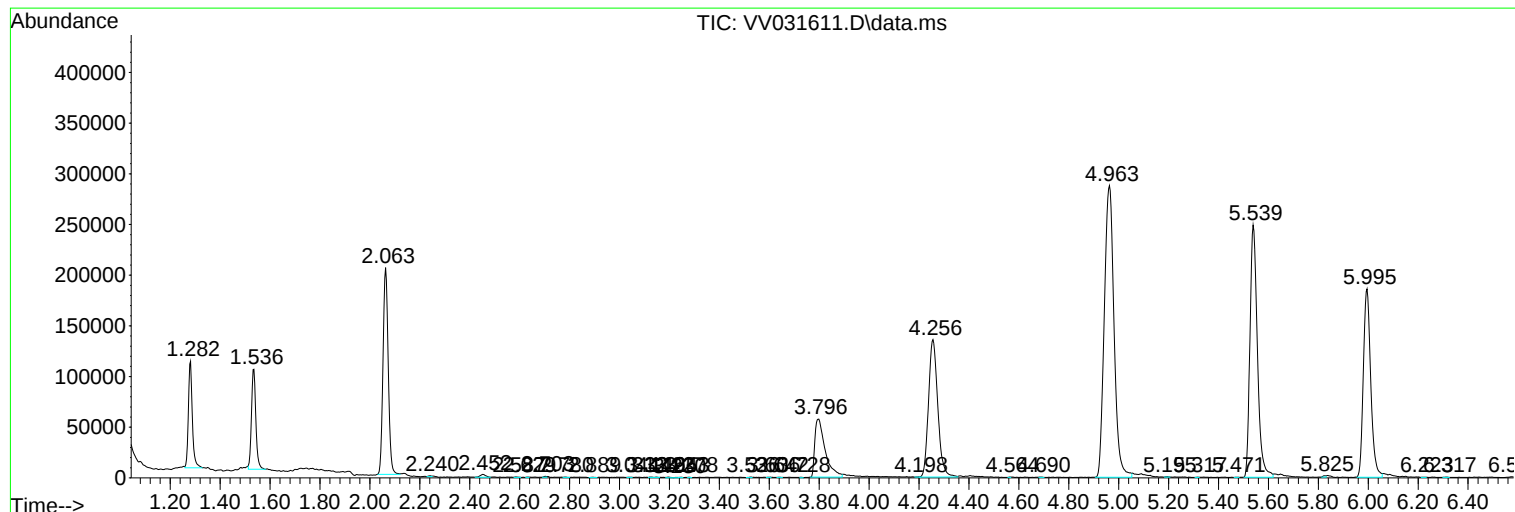
Sum of corrected areas: 6440811

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VBLK362

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM061423WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV062923\  
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No Library Search Compounds Detected

\*\*\*\*\*

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