

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121123\  
 Data File : VX039146.D  
 Acq On : 11 Dec 2023 16:08  
 Operator : JC/MD  
 Sample : 05646-19DL 200X  
 Misc : 2.18g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AS6DL

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\_X\Method\SFAMXLM120523WMA.M  
 Title : VOC Analysis

Signal : TIC: VX039146.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         | 1.246       | 23            | 26          | 31           | rBV3     | 2746           | 5795          | 0.35%           | 0.056%        |
| 2         | 1.368       | 42            | 46          | 56           | rVB      | 130872         | 135890        | 8.20%           | 1.308%        |
| 3         | 1.666       | 91            | 95          | 111          | rVB      | 82044          | 120861        | 7.29%           | 1.163%        |
| 4         | 2.306       | 194           | 200         | 214          | rVB      | 231611         | 361849        | 21.83%          | 3.482%        |
| 5         | 2.739       | 269           | 271         | 273          | rBV      | 274            | 189           | 0.01%           | 0.002%        |
| 6         | 2.940       | 298           | 304         | 308          | rBV2     | 1245           | 2562          | 0.15%           | 0.025%        |
| 7         | 3.062       | 321           | 324         | 325          | rVV2     | 251            | 188           | 0.01%           | 0.002%        |
| 8         | 3.166       | 338           | 341         | 342          | rBV2     | 311            | 359           | 0.02%           | 0.003%        |
| 9         | 3.233       | 350           | 352         | 354          | rBV2     | 181            | 165           | 0.01%           | 0.002%        |
| 10        | 3.477       | 391           | 392         | 395          | rVB      | 274            | 207           | 0.01%           | 0.002%        |
| 11        | 3.544       | 401           | 403         | 406          | rVB2     | 143            | 150           | 0.01%           | 0.001%        |
| 12        | 3.770       | 438           | 440         | 442          | rBV      | 211            | 192           | 0.01%           | 0.002%        |
| 13        | 4.050       | 484           | 486         | 487          | rBV2     | 245            | 186           | 0.01%           | 0.002%        |
| 14        | 4.337       | 532           | 533         | 536          | rBV2     | 221            | 238           | 0.01%           | 0.002%        |
| 15        | 4.446       | 543           | 551         | 566          | rBV      | 99254          | 280043        | 16.89%          | 2.695%        |
| 16        | 5.056       | 640           | 651         | 671          | rBV      | 133958         | 425973        | 25.70%          | 4.099%        |
| 17        | 5.330       | 693           | 696         | 698          | rBV3     | 243            | 338           | 0.02%           | 0.003%        |
| 18        | 5.379       | 702           | 704         | 705          | rBV2     | 472            | 358           | 0.02%           | 0.003%        |
| 19        | 5.470       | 717           | 719         | 722          | rVB2     | 235            | 196           | 0.01%           | 0.002%        |
| 20        | 5.531       | 726           | 729         | 730          | rBV2     | 271            | 329           | 0.02%           | 0.003%        |
| 21        | 5.690       | 753           | 755         | 758          | rBV2     | 205            | 180           | 0.01%           | 0.002%        |
| 22        | 5.830       | 777           | 778         | 783          | rVB2     | 226            | 194           | 0.01%           | 0.002%        |
| 23        | 5.964       | 788           | 800         | 821          | rBV2     | 358279         | 1112122       | 67.09%          | 10.701%       |
| 24        | 6.178       | 833           | 835         | 838          | rBV2     | 274            | 257           | 0.02%           | 0.002%        |
| 25        | 6.202       | 838           | 839         | 842          | rVB2     | 371            | 230           | 0.01%           | 0.002%        |
| 26        | 6.300       | 852           | 855         | 861          | rBV2     | 251            | 561           | 0.03%           | 0.005%        |
| 27        | 6.458       | 880           | 881         | 883          | rVB      | 303            | 150           | 0.01%           | 0.001%        |
| 28        | 6.476       | 883           | 884         | 887          | rBV2     | 321            | 237           | 0.01%           | 0.002%        |
| 29        | 6.598       | 903           | 904         | 909          | rVB      | 379            | 476           | 0.03%           | 0.005%        |
| 30        | 6.635       | 909           | 910         | 912          | rBV2     | 183            | 162           | 0.01%           | 0.002%        |
| 31        | 6.757       | 920           | 930         | 949          | rBV      | 270644         | 659492        | 39.78%          | 6.346%        |
| 32        | 6.988       | 966           | 968         | 972          | rBV2     | 262            | 262           | 0.02%           | 0.003%        |
| 33        | 7.110       | 983           | 988         | 997          | rBV5     | 1761           | 4091          | 0.25%           | 0.039%        |
| 34        | 7.305       | 1012          | 1020        | 1037         | rBV      | 223865         | 497347        | 30.00%          | 4.785%        |
| 35        | 7.482       | 1046          | 1049        | 1051         | rBV3     | 753            | 931           | 0.06%           | 0.009%        |
| 36        | 7.580       | 1064          | 1065        | 1071         | rBV      | 349            | 252           | 0.02%           | 0.002%        |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AS6DL

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\_X\Method\SFAMXLM120523WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |         |         |
|----|--------|------|------|------|------|--------|---------|---------|---------|
| 37 | 7.696  | 1081 | 1084 | 1089 | rVB2 | 270    | 479     | 0.03%   | 0.005%  |
| 38 | 7.793  | 1099 | 1100 | 1103 | rVB  | 197    | 149     | 0.01%   | 0.001%  |
| 39 | 7.897  | 1116 | 1117 | 1123 | rVB2 | 156    | 218     | 0.01%   | 0.002%  |
| 40 | 7.964  | 1123 | 1128 | 1130 | rBV2 | 263    | 419     | 0.03%   | 0.004%  |
| 41 | 7.988  | 1130 | 1132 | 1134 | rVB  | 187    | 153     | 0.01%   | 0.001%  |
| 42 | 8.135  | 1155 | 1156 | 1160 | rVV  | 215    | 170     | 0.01%   | 0.002%  |
| 43 | 8.183  | 1162 | 1164 | 1166 | rBV  | 210    | 236     | 0.01%   | 0.002%  |
| 44 | 8.324  | 1181 | 1187 | 1201 | rBV  | 165564 | 274349  | 16.55%  | 2.640%  |
| 45 | 8.598  | 1230 | 1232 | 1234 | rBV2 | 329    | 426     | 0.03%   | 0.004%  |
| 46 | 8.647  | 1234 | 1240 | 1255 | rVV  | 560281 | 867601  | 52.34%  | 8.348%  |
| 47 | 8.952  | 1284 | 1290 | 1302 | rBV  | 117861 | 182504  | 11.01%  | 1.756%  |
| 48 | 9.080  | 1309 | 1311 | 1314 | rBV3 | 256    | 331     | 0.02%   | 0.003%  |
| 49 | 9.232  | 1333 | 1336 | 1337 | rBV  | 284    | 243     | 0.01%   | 0.002%  |
| 50 | 9.275  | 1340 | 1343 | 1347 | rBV3 | 459    | 592     | 0.04%   | 0.006%  |
| 51 | 9.378  | 1355 | 1360 | 1377 | rBV  | 433875 | 649358  | 39.17%  | 6.248%  |
| 52 | 9.701  | 1409 | 1413 | 1418 | rVB4 | 867    | 1398    | 0.08%   | 0.013%  |
| 53 | 9.842  | 1435 | 1436 | 1438 | rBV  | 327    | 248     | 0.01%   | 0.002%  |
| 54 | 10.055 | 1465 | 1471 | 1489 | rBV2 | 563493 | 1051795 | 63.45%  | 10.120% |
| 55 | 10.573 | 1554 | 1556 | 1559 | rVB2 | 163    | 165     | 0.01%   | 0.002%  |
| 56 | 10.713 | 1577 | 1579 | 1580 | rBV  | 163    | 153     | 0.01%   | 0.001%  |
| 57 | 10.805 | 1589 | 1594 | 1595 | rBV  | 246    | 321     | 0.02%   | 0.003%  |
| 58 | 10.866 | 1603 | 1604 | 1606 | rBV2 | 289    | 152     | 0.01%   | 0.001%  |
| 59 | 11.091 | 1638 | 1641 | 1648 | rBV3 | 662    | 886     | 0.05%   | 0.009%  |
| 60 | 11.189 | 1652 | 1657 | 1666 | rVV  | 423649 | 528916  | 31.91%  | 5.089%  |
| 61 | 11.457 | 1699 | 1701 | 1702 | rBV  | 296    | 166     | 0.01%   | 0.002%  |
| 62 | 11.494 | 1706 | 1707 | 1709 | rVB  | 300    | 161     | 0.01%   | 0.002%  |
| 63 | 11.591 | 1720 | 1723 | 1726 | rBV  | 270    | 237     | 0.01%   | 0.002%  |
| 64 | 11.658 | 1730 | 1734 | 1736 | rBV  | 258    | 231     | 0.01%   | 0.002%  |
| 65 | 11.738 | 1743 | 1747 | 1749 | rBV  | 201    | 196     | 0.01%   | 0.002%  |
| 66 | 11.823 | 1759 | 1761 | 1763 | rBV2 | 189    | 153     | 0.01%   | 0.001%  |
| 67 | 11.841 | 1763 | 1764 | 1766 | rBV  | 232    | 152     | 0.01%   | 0.001%  |
| 68 | 11.933 | 1777 | 1779 | 1780 | rBV  | 238    | 245     | 0.01%   | 0.002%  |
| 69 | 11.969 | 1780 | 1785 | 1788 | rVV  | 26325  | 31981   | 1.93%   | 0.308%  |
| 70 | 12.036 | 1788 | 1796 | 1805 | rVB2 | 770999 | 1657709 | 100.00% | 15.950% |
| 71 | 12.231 | 1827 | 1828 | 1831 | rVB  | 300    | 210     | 0.01%   | 0.002%  |
| 72 | 12.317 | 1837 | 1842 | 1853 | rBV2 | 593816 | 879176  | 53.04%  | 8.459%  |
| 73 | 12.616 | 1889 | 1891 | 1895 | rVB2 | 199    | 205     | 0.01%   | 0.002%  |
| 74 | 12.646 | 1895 | 1896 | 1899 | rBV2 | 218    | 176     | 0.01%   | 0.002%  |
| 75 | 12.756 | 1912 | 1914 | 1916 | rBV2 | 405    | 438     | 0.03%   | 0.004%  |
| 76 | 12.847 | 1927 | 1929 | 1932 | rBV  | 381    | 318     | 0.02%   | 0.003%  |

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Instrument :  
 MSVOA\_X  
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 C0AS6DL

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\_X\Method\SFAMXML120523WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.951 | 1943 | 1946 | 1948 | rBV2 | 139    | 151    | 0.01%  | 0.001% |
| 78  | 13.061 | 1959 | 1964 | 1970 | rBV4 | 4270   | 7680   | 0.46%  | 0.074% |
| 79  | 13.250 | 1993 | 1995 | 1999 | rVB2 | 249    | 271    | 0.02%  | 0.003% |
| 80  | 13.585 | 2045 | 2050 | 2063 | rBV  | 354447 | 435908 | 26.30% | 4.194% |
| 81  | 13.780 | 2078 | 2082 | 2086 | rBV3 | 219    | 462    | 0.03%  | 0.004% |
| 82  | 13.957 | 2106 | 2111 | 2119 | rBV  | 133482 | 167360 | 10.10% | 1.610% |
| 83  | 14.066 | 2128 | 2129 | 2131 | rBV2 | 172    | 151    | 0.01%  | 0.001% |
| 84  | 14.201 | 2147 | 2151 | 2152 | rBV2 | 154    | 208    | 0.01%  | 0.002% |
| 85  | 14.353 | 2174 | 2176 | 2180 | rVB2 | 221    | 287    | 0.02%  | 0.003% |
| 86  | 14.383 | 2180 | 2181 | 2185 | rBV  | 302    | 265    | 0.02%  | 0.003% |
| 87  | 14.524 | 2202 | 2204 | 2206 | rVV3 | 243    | 199    | 0.01%  | 0.002% |
| 88  | 14.615 | 2217 | 2219 | 2220 | rBV  | 420    | 271    | 0.02%  | 0.003% |
| 89  | 14.646 | 2220 | 2224 | 2226 | rVV  | 173    | 282    | 0.02%  | 0.003% |
| 90  | 14.780 | 2241 | 2246 | 2252 | rBV3 | 4338   | 6434   | 0.39%  | 0.062% |
| 91  | 14.975 | 2274 | 2278 | 2279 | rBV2 | 245    | 300    | 0.02%  | 0.003% |
| 92  | 15.121 | 2300 | 2302 | 2304 | rBV2 | 250    | 228    | 0.01%  | 0.002% |
| 93  | 15.164 | 2308 | 2309 | 2312 | rBV  | 328    | 205    | 0.01%  | 0.002% |
| 94  | 15.249 | 2318 | 2323 | 2331 | rVB2 | 16267  | 24021  | 1.45%  | 0.231% |
| 95  | 15.713 | 2397 | 2399 | 2402 | rVB  | 385    | 356    | 0.02%  | 0.003% |
| 96  | 15.938 | 2435 | 2436 | 2439 | rBV  | 347    | 198    | 0.01%  | 0.002% |
| 97  | 16.267 | 2488 | 2490 | 2492 | rBV3 | 295    | 241    | 0.01%  | 0.002% |
| 98  | 16.322 | 2497 | 2499 | 2502 | rBV4 | 449    | 540    | 0.03%  | 0.005% |
| 99  | 16.566 | 2537 | 2539 | 2542 | rVB2 | 510    | 409    | 0.02%  | 0.004% |
| 100 | 16.718 | 2562 | 2564 | 2569 | rBV3 | 343    | 555    | 0.03%  | 0.005% |

Sum of corrected areas: 10393010

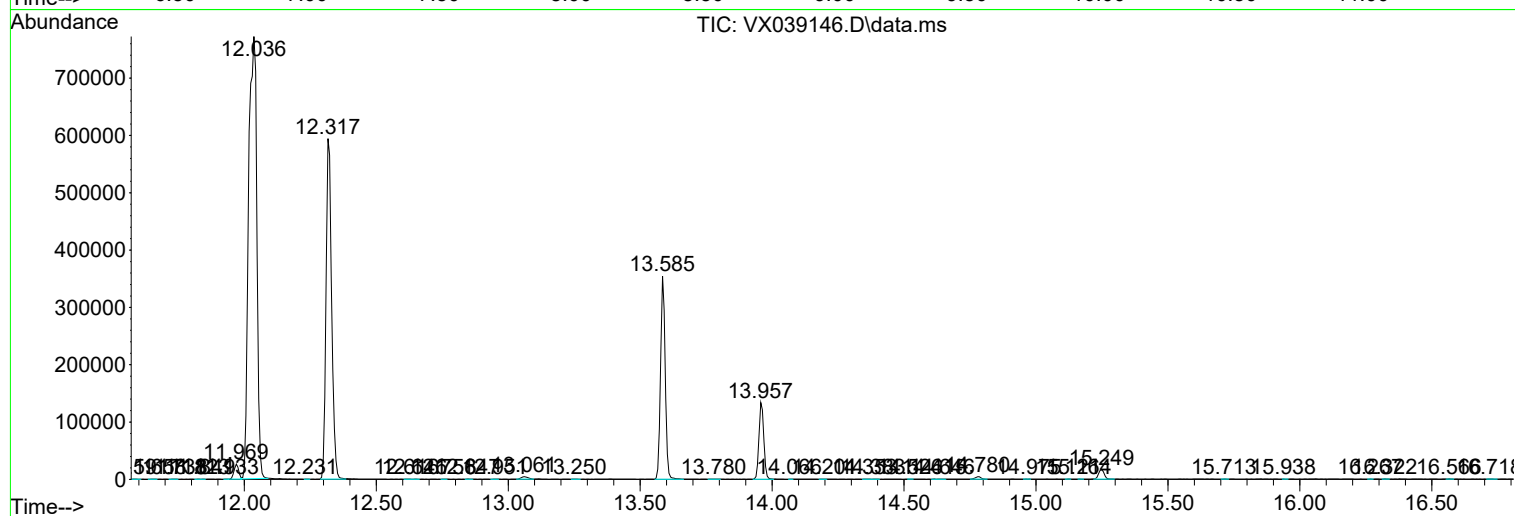
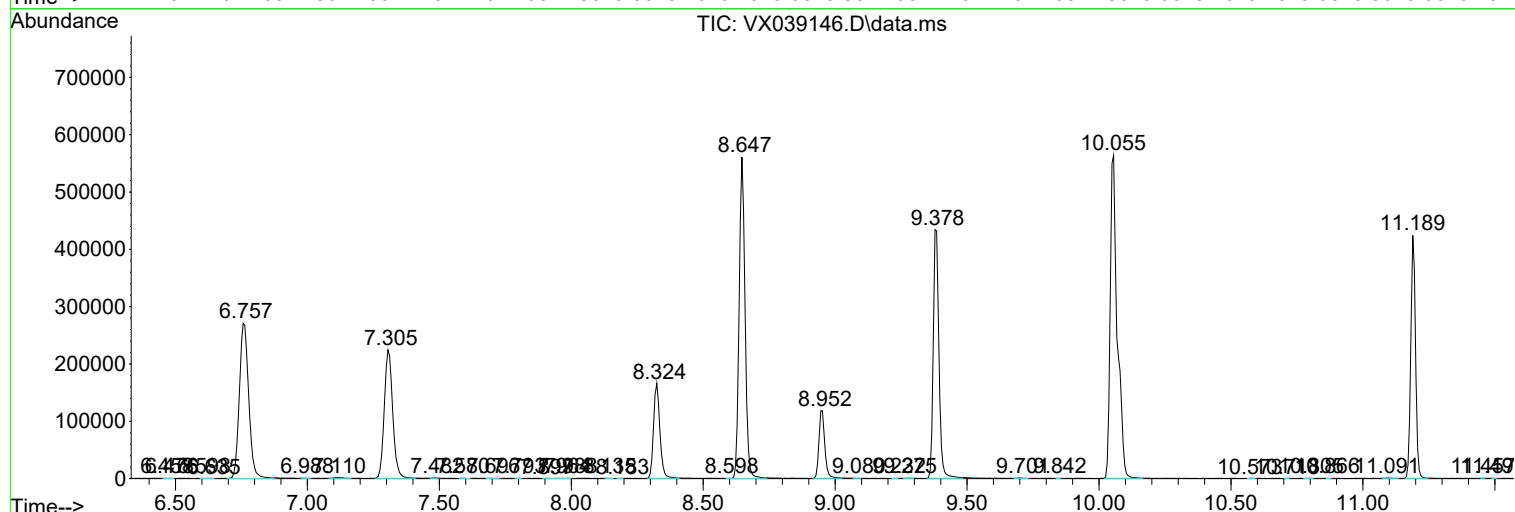
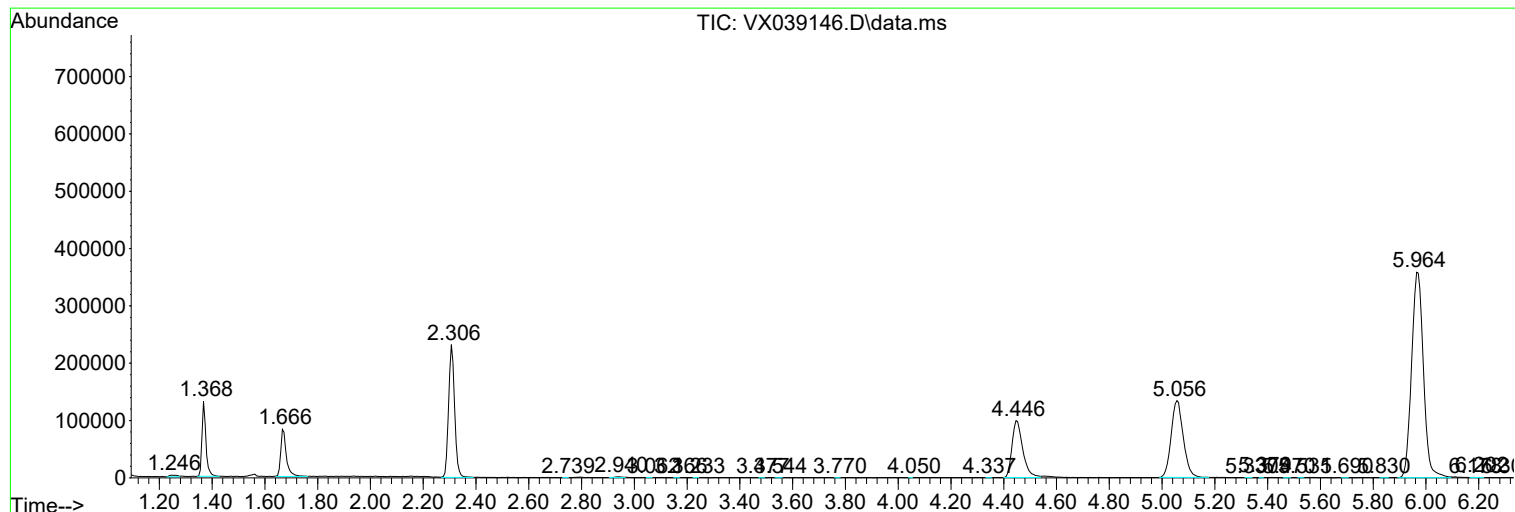
Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121123\  
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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121123\  
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No Library Search Compounds Detected

\*\*\*\*\*

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