Cc1cn2c(CN(C)C(=O)c3ccc(F)cc3C)c(C)nc2s1 Cc1cc(F)ccc1C(=O)N(C)Cc1c(C)nc2scc(C)n12

Figure 1. Two almost identical molecules with markedly different canonical SMILES in RDKit. The edit distance between two strings is 22 (50.5% of the whole sequence).

```
Minimal DFS codes:
[[0,
       1,
            6,
                 0,
                     6], [1,
                                 2,
                                     6,
                                          0,
                                              7], [2,
                                                          3,
                                                              7,
                                                                   0,
                                                                       6],
 [ 3,
                 0,
                     6], [4,
                                 5,
                                     6,
                                          2,
                                              6],
                                                   [ 5,
                                                          6,
                                                              6,
                                                                   0,
                                                                       61,
            6,
 [ 5,
      7,
                 2,
                     6], [7,
                                              6], [8,
            6,
                                 8,
                                     6,
                                          2,
                                                          9,
                                                              6,
                                                                       9],
 [ 8, 10,
            6,
                 2,
                     6], [10, 11,
                                     6,
                                          2,
                                              6], [11,
                                                          4,
                                                              6,
                                                                   2,
                                                                       6],
                     8], [ 2, 13,
                                              6], [ 0, 14,
 [ 3, 12,
            6,
                 1,
                                     7,
                                          Ο,
                                                              6,
                                                                       6],
 [14, 15,
                 Ο,
                     6], [14, 16,
                                     6,
                                          2,
                                              7], [16, 17,
                                                              7,
                                                                   2,
            6,
                                                                       6],
                                              6], [18, 19,
 [17, 18,
            6,
                 2,
                     7], [18,
                               Ο,
                                     7,
                                          2,
                                                              7,
                                                                   2,
 [19, 20,
           6,
                2,
                     6], [20, 21,
                                     6,
                                          0,
                                              6], [20, 22,
                                                              6,
 [22, 17, 16,
                 2,
                     611
and
                                        0,
[[0,
       1,
            6,
                 Ο,
                     6],[1,
                               2,
                                    6,
                                             7],[2,
                                                       3,
                                                            7,
                                                                 0,
                                                                     6],
                               5,
 [ 3,
       4,
            6,
                 Ο,
                     6],[4,
                                    6,
                                        2,
                                             6],[5,
                                                       6,
                                                            6,
                                                                     6],
      7,
 [ 5,
            6,
                 2,
                     6],[7,
                               8,
                                    6,
                                        2,
                                             6],[8,
                                                                     9],
                2,
 [ 8, 10,
                     6],[10, 11,
                                             6],[11,
            6,
                                    6,
                                        2,
                                                       4,
                                                                 2,
                                                                     6],
 [ 3, 12,
            6,
                 1,
                     8],[2,13,
                                    7,
                                        Ο,
                                             6],[0,14,
                                                            6,
                                                                 2,
                                                                     6],
                     6],[14, 16,
 [14, 15,
            6,
                Ο,
                                    6,
                                        2,
                                             7],[16, 17,
                                                            7,
                                                                 2,
                                                                     61,
                     7],[18, 0,
                                   7,
                                             6],[18, 19,
 [17, 18,
            6,
                 2,
                                        2,
                                                            7,
                                                                 2,
                                                                     6],
 [19, 20,
                     6],[19, 21,
                                             6],[21, 22,
            6,
                0,
                                   6,
                                        2,
                                                            6,
                                                                 2, 16],
 [22, 17, 16,
                 2,
                     611
```

Example from <a href="https://arxiv.org/pdf/1802.04364.pdf">https://arxiv.org/pdf/1802.04364.pdf</a>

## Junction Tree Variational Autoencoder for Molecular Graph Generation