Report I : Learning to Extend Molecular Scaffolds with Structural Motifs

Irem Begüm Gündüz - 7026821

Contents

Overview of the Approach

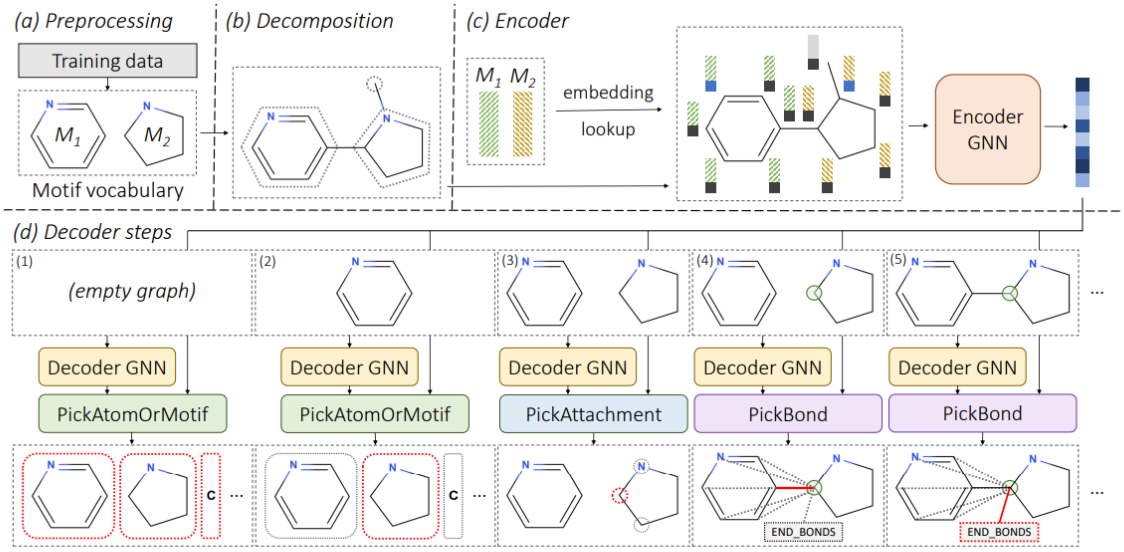

Figure 1: Overview of our approach. We discover motifs from data (a) and use them to decompose an input molecule (b) into motifs and single atoms. In the encoder (c), atom features (bottom) are combined with motif embeddings (top), making the motif information available at the atom level. Decoder steps (d) are only conditioned on the encoder output and partial graph (hence independent) and have to select one of the valid options (shown below, correct choices marked in red).

Figure 1: Overwiew of the methdology.

Discussion

Existed methodologies are limited with scaffold and, this study is proven to overcome the limitations of scaffold predictions which requires a known existed scaffold.

References