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(54) Title: GRAPH EDIT DISTANCE DETERMINATION IN DRUG-LIKE CHEMICAL SPACES

(57) Abstract: Systems and methods for estimating graph edit distance (GED) between compounds are provided. A first graph representing a first compound comprises a plurality of nodes and a plurality of edges. Atoms of the first compound are represented by the nodes and bonds of the first compound are represented by the edges of the first graph. A second graph representing a second compound also comprises a plurality of nodes and a plurality of edges. Atoms of the second compound are represented by the nodes and bonds of the second compound are represented by edges of the second graph. The first graph is inputted into a model to generate a first latent embedding. The second graph is inputted into the model to generate a second latent embedding. An estimate (GED) between the two compounds is determined as the difference between the two latent embeddings.