PhectorMatch: Contrastive Learning Enables Fast Virtual Screening with 3D Pharmacophore Models

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3D pharmacophore-based virtual screening is an established method in drug discovery[1] but its applicability to massive datasets is limited due to the computationally expensive alignment of query pharmacophores to database ligands. We propose a novel approach inspired by neural subgraph matching[2] that formulates alignment as approximate subgraph matching within an order embedding space[3]. Pharmacophores are encoded into vector representations using a graph neural network, enabling efficient querying of pre-encoded conformational databases via the order embedding space, thereby bypassing traditional alignment (Figure 1). This significantly accelerates virtual screening, demonstrating promising results for the screening of massive datasets.

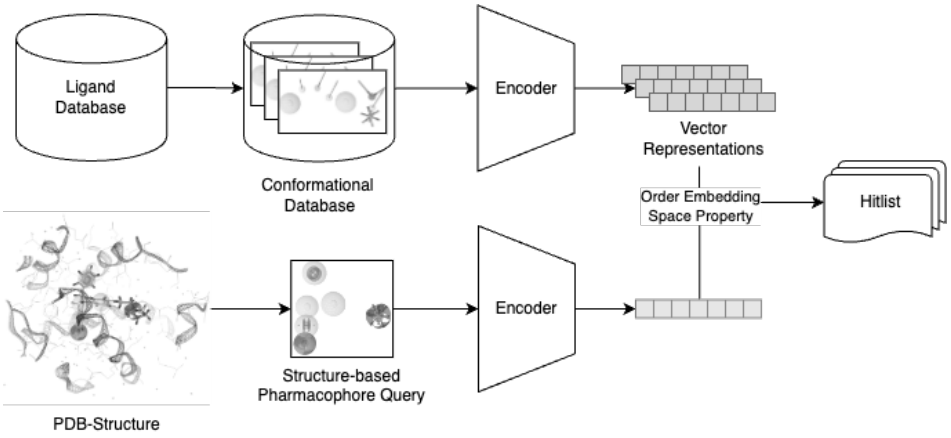

Figure 1: Schematic overview of the proposed method.

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