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Generative model based on 3D molecule structure driven Atom-pair map

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Recently, data on hundreds of thousands to millions of compounds are being accumulated due to the rapidly developing computer technology and experimental technology. The scope of application of AI techniques has expanded in large-scale data analysis, and attempts to discover new drugs by combining them with abundant experimental data are attracting attention. For AI-based drug virtual search, conventional chemical representations have a limitation in that they cannot express the three-dimensional spatial information and physicochemical properties that have an important effect on the binding of the target protein to the drug. Atom-pair map is a method which represents chemical compound by counting combination of physicochemical properties and distance between atom pair that composes a chemical compound. More intuitive interpretation of binding sites between drug and protein target is possible through our proposed generative model based on atom-pair maps. By transforming rich fragment information in the library to atom-pair map representation, the model learns reasonable drug-target matches on each corresponding fragment, ultimately presenting complete molecule structures. The model was validated on benchmark databases, including PDB, by scoring generated structures for fragment similarity and novelty.