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Exploring Scoring Function Space: Developing Computational Models for Drug Discovery

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Abstract

Background: The idea of scoring function space established a systems-level approach to address the development of models to predict the affinity of drug molecules by those interested in drug discovery.

Objective: Our goal here is to review the concept of scoring function space and how to explore it to develop machine learning models to address protein-ligand binding affinity.

Methods: We searched the articles available in PubMed related to the scoring function space. We also utilized crystallographic structures found in the protein data bank (PDB) to represent the protein space.

Results: The application of systems-level approaches to address receptor-drug interactions allows us to have a holistic view of the process of drug discovery. The scoring function space adds

flexibility to the process since it makes it possible to see drug discovery as a relationship involving mathematical spaces.

Conclusion: The application of the concept of scoring function space has provided us with an integrated view of drug discovery methods. This concept is useful during drug discovery, where we see the process as a computational search of the scoring function space to find an adequate model to predict receptor-drug binding affinity.