Pharmacophore-based molecular docking for drug discovery.

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Abstract

Pharmacophore-based molecular docking is a powerful computational tool that plays an important role in drug discovery. This approach allows researchers to predict how small molecules or ligands will bind to protein targets. This is essential in the design of new drugs.

Keywords: Molecular docking, Pharmacophore, Ligands, Protein targets.

Introduction

Pharmacophore-based molecular docking uses computer algorithms to simulate the binding of small molecules to protein targets. A pharmacophore is a three-dimensional model that represents the essential properties of a ligand required for binding to a particular receptor or enzyme. These features include hydrogen bond donors and acceptors, hydrophobic regions, and other chemical groups that interact with proteins [1].

The first step in pharmacophore-based molecular docking is the development of a ligand pharmacophore model. This model is then used to screen small-molecule libraries to identify potential drug candidates that share the same key properties as the original ligand. The next step is to dock the ligand of choice to the protein target using a molecular docking algorithm that predicts the binding conformation and affinity of the ligand to the protein [2].

Pharmacophore-based molecular docking has several advantages over traditional molecular docking approaches. One of its major advantages is that it allows the identification of ligands that may not be structurally similar to the original ligand but share the same key pharmacophore functions. This is particularly useful for identifying new drug candidates with different chemical structures from existing drugs [3].

Another advantage of pharmacophore-based molecular docking is that it can be used to predict binding modes of ligands to multiple protein targets simultaneously. This is particularly useful for identifying drugs that target multiple proteins or have multi-pharmacological effects.

Pharmacophore-based molecular docking has been successfully applied in several drug discovery projects. For example, the development of HIV protease inhibitors uses pharmacophore-based molecular docking to screen libraries of compounds for potential inhibitors. This approach identified several promising drug candidates, which later developed into clinically approved agents [4].

Another study used pharmacophore-based molecular docking to identify novel inhibitors of human dihydroorotate dehydrogenase (DHODH), an enzyme involved in pyrimidine nucleotide biosynthesis. This research led to the discovery of a new class of DHODH inhibitors with potential to treat autoimmune diseases [5].

Conclusion

Pharmacophore-based molecular docking is a valuable tool in drug discovery. This enables the identification of new drug candidates with different chemical structures from existing drugs, and predicts the binding modes of ligands to multiple protein targets simultaneously. This approach has been successfully applied in several drug discovery projects and is expected to continue to play an important role in new drug development in the future.

References

1. Joseph-McCarthy D, Thomas IV BE, Belmarsh M, et al. Pharmacophore-based molecular docking to account for ligand flexibility. Proteins: Struct Funct Bioinformat. 2003;51(2):172-88.
2. Sun H. Pharmacophore-based virtual screening. Curr Med Chem. 2008;15(10):1018-24.
3. Gao Q, Yang L, Zhu Y. Pharmacophore based drug design approach as a practical process in drug discovery. Curr Comput-Aid Drug. 2010;6(1):37-49.
4. Hu B, Lill MA. PharmDock: A pharmacophore-based docking program. J Cheminform. 2014;6:1-4.
5. Jiang L, Rizzo RC. Pharmacophore-based similarity scoring for DOCK. J Phys Chem B. 2015;119(3):1083-102.

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