Molecular docking and drug discovery in ?-adrenergic receptors

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Background: Evolution in computer engineering, availability of increasing amounts of data and the development of new and fast docking algorithms and software have led to improved molecular simulations with crucial applications in virtual high-throughput screening and drug discovery. Moreover, analysis of protein-ligand recognition through molecular docking has become a valuable tool in drug design. Objective: In this review, we focus on the applicability of molecular docking on a particular class of G protein-coupled receptors: the ?-adrenergic receptors, which are relevant targets in clinic for the treatment of asthma and cardiovascular diseases. Results: We describe the binding site in ?-adrenergic receptors to understand key factors in ligand recognition along with the proteins activation process. Moreover, we focus on the discovery of new lead compounds that bind the receptors, on the evaluation of virtual screening using the active/inactive binding site states, and on the structural optimization of known families of binders to improve ?-adrenergic affinity. We also discussed strengths and challenges related to the applicability of molecular docking in ?-adrenergic receptors. Conclusion: Molecular docking is a valuable technique in computational chemistry to deeply analyze ligand recognition and has led to important breakthroughs in drug discovery and design in the field of ?-adrenergic receptors. © 2017 Bentham Science Publishers.

Drug design

Drug discovery

G proteincoupled receptors

Molecular docking

Virtual screening

?-adrenergic receptors

adrenergic receptor

beta 1 adrenergic receptor

beta 2 adrenergic receptor

beta 3 adrenergic receptor

beta adrenergic receptor

beta adrenergic receptor blocking agent

beta adrenergic receptor stimulating agent

boron derivative

beta adrenergic receptor

beta adrenergic receptor blocking agent

beta adrenergic receptor stimulating agent

drug binding site

drug conformation

drug design

drug protein binding

drug screening

human

ligand binding

molecular docking

Review

algorithm

asthma

cardiovascular disease

chemistry

drug development

high throughput screening

metabolism

software

Adrenergic beta-Agonists

Adrenergic beta-Antagonists

Algorithms

Asthma

Cardiovascular Diseases

Drug Discovery

High-Throughput Screening Assays

Humans

Molecular Docking Simulation

Receptors, Adrenergic, beta

Software