Applications of multi-target computer-aided methodologies in molecular design of CNS drugs

Raevsky O.A.

Mukhametov A.

Grigorev V.Y.

Ustyugov A.

Tsay S.-C.

Hwu R.J.-R.

Yarla N.S.

Barreto G.E.

Aliev G.

Bachurin S.O.

The discovery of drugs for diseases of the central nervous system (CNS) faces high attrition rates in clinical trials. Neural diseases are extremely complex in nature and typically associated with multiple drug targets. A conception of multi-target directed ligands (MTDL), widely applied to the discovery of cancer pharmaceuticals, may be a perspective solution for CNS diseases. Special bioinformatics approaches have been developed which can assist the medicinal chemists in identification and structural optimization of MTDL. In this review, we analyze the current status of the development of multi-target approaches in quantitative structure-activity relationships (mt-QSAR) for CNS drug discovery; and describes applications of multi-target approaches in molecular modelling (which can be called mt-MM), as well as perspectives for multi-target approaches in bioinformatics in relation to Alzheimer?s disease.

Alzheimer?s disease

Bioinformatics

Cheminformatics

Molecular modelling

MTDL

Multi-target

QSAR

central nervous system agents

ligand

central nervous system agents

algorithm

Alzheimer disease

bioinformatics

computer aided design

drug design

drug targeting

human

methodology

molecular docking

molecular model

nonhuman

process optimization

quantitative structure activity relation

Review

Alzheimer disease

biology

central nervous system disease

chemistry

pathology

Alzheimer Disease

Central Nervous System Agents

Central Nervous System Diseases

Computational Biology

Drug Design

Humans

Ligands

Models, Molecular

Quantitative Structure-Activity Relationship