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On the Chirality of Drugs and Biomacromolecule Structures

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Abstract: As a phenomenon associated with the homochirality of monomers that make up the essential classes of biological macromolecules, symmetry is of fundamental importance not only for all molecular biology as a systemic factor of its organization but also for pharmacology as well as a systemic factor of drug stereospecificity. Enantiomers, including pharmaceuticals, may exhibit utterly different chemical specificity in processes involving chiral compounds, as well as different bioactivity. It is crucial to consider the peculiarities of interaction of enantiomers with asymmetric compounds of the organism when creating drugs since it may turn out that just one drug form has a therapeutic effect. At the same time, the other could be less active or even cause severe side effects, being toxic.

More than half of the drugs currently in use are chiral, and most of the last ones are marketed as racemates. More than half of the drugs developed in recent years consist of chiral molecules. Chiral drugs are used in the treatment of a wide range of diseases, including cardiovascular and gastrointestinal. Obtaining optically pure forms of the substance is a complicated and expensive task, but their use in many cases could reduce the dosage and the number of side effects. The therapeutic activity of enantiomers, their pharmacokinetics, and pharmacodynamics are currently intensively studied. However, the physical nature of the differences in the therapeutic effects of enantiomers has not yet totally been established.

The stereospecific drug-target interaction should be considered more broadly than only local complementarity. Here, to develop the concept of chirality's role in the structure formation of biological macromolecules, we discuss the bioactivity of chiral drugs and make assumptions about the possible relationship between the drug chirality and the drug effect on a specific chiral molecular target.

Keywords: chirality; enantiomers, chiral drugs, stereospecificity, structure hierarchies

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