Ligand and Structure-Based Descriptors of some Chiral Anti-inflammatory Drugs

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Résumé

The inflammation is a normal defense of the organism against foreign agents. However, when the inflammatory response is chronically prolonged; it may negatively affect the organism.
For a long time, non stero´idal anti-inflammatory drugs (NSAIDs) were used for the treatment of inflammation, because of the inhibition of an enzyme called cyclooxygenase (COX). Among these drugs such as profens are a racemic mixture of two isoforms: R and S, one of which can be toxic.

In order to obtain pure enantiomers of these NSAIDs, it is necessary to investigate which enantiomer is responsible for COX inhibitory activity.

The aim of our study is to understand the difference in the biological response between two enantiomers with anti-inflammatory activity. We have selected in literature some potential NSAIDs with one asymmetric center and available activity. Each compound was modeled before simulation by the molecular docking in the COX-2 enzyme. The focus is on generating descriptors for this set of ligands that are docked to a receptor using Schr´odinger programs.

The analysis of the results can explain the anti-inflammatory activity of each enantiomer. These descriptors will be used to generate a QSAR model which will be used to predict the most active enantiomer in the racemic mixture.

Mots-Clés: Cyclooxygenase, NSAIDs, Enantiomers, Docking, Descriptors

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