

## ***IN SILICO* STUDY OF PHYSICOCHEMICAL, PHARMACOKINETIC AND TOXICOLOGICAL PROPERTIES OF 5-LIPOXYGENASE INHIBITORS**

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5-Lipoxygenase (5-LO) is an important enzyme involved in the production of leukotrienes, arachidonic acid metabolites which directly affect the development of the inflammatory reaction associated with numerous pathophysiological conditions. As a result, the discovery and development of selective 5-LO inhibitors for therapeutic use became a subject of active research. The study aimed to conduct first a literature review of the most potent synthetic 5-LO inhibitors (with  $IC_{50}$  values below 1  $\mu M$ ), focusing on their chemical structure, and then an *in silico* study of their basic physicochemical, pharmacokinetic and toxicological properties. The results showed that the investigated 5-LO inhibitors differed significantly in their physicochemical, pharmacokinetic and toxicological profiles. About half of the investigated 5-LO inhibitors fulfilled Lipinski's rule of five and Veber's rule, i.e., their good oral bioavailability was predicted, and were also predicted as compounds with no risk of mutagenic, tumorigenic, reproductive and/or irritant effects. The ability to permeate through Caco-2 cells, the possibility of intestinal absorption and the possibility of passing through the blood-brain barrier were predicted for a small number of tested compounds. Taken together, favorable physicochemical and toxicological properties were predicted for 32 out of a total of 99 tested compounds, while the most favorable pharmacokinetic profile was shown by the benzylidene derivative **22**.

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**Key words:** *5-lipoxygenase, in silico study, physicochemical properties, pharmacokinetic properties, toxicological properties*