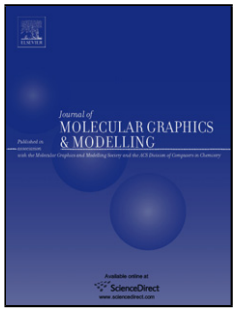

Title: Sterols and triterpenoids as potential anti-inflammatories: Molecular docking studies for binding to some enzymes involved in inflammatory pathways

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Title.

Sterols and triterpenoids as potential anti-inflammatories: Molecular docking studies for binding to some enzymes involved in inflammatory pathways

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Abstract

Triterpenes and sterols are good candidates for the development of anti-inflammatory drugs and use in chemoprevention or chemotherapy of cancer via the interaction with therapeutic targets related to inflammation, such as COX-1 and -2; LOX-5; MPO, PLA2 and *i*-NOS. In this study, we use molecular docking to evaluate the potential binding of a database of selected sterol and triterpenoid compounds with several skeletons against enzymes related to inflammation to propose structural requirements beneficial for anti-inflammatory activity that can be used for the design of more potent and selective anti-inflammatory and antitumor drugs. Our results suggest that the substitution pattern is important and that there is an important relationship between the class of sterol or triterpenoid skeleton and enzyme binding.

Highlights

- We performed docking studies of key triterpenoids to enzymes involved in inflammation.
- We determined the relationship between the skeleton type and the inhibited enzyme.
- Both skeleton and substitution pattern are important for enzyme binding.
- Our results support the use of triterpenoids as potential leads for drug design.

Graphical abstract.