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# Virtual screening of a library of natural compounds against COX-2 protein

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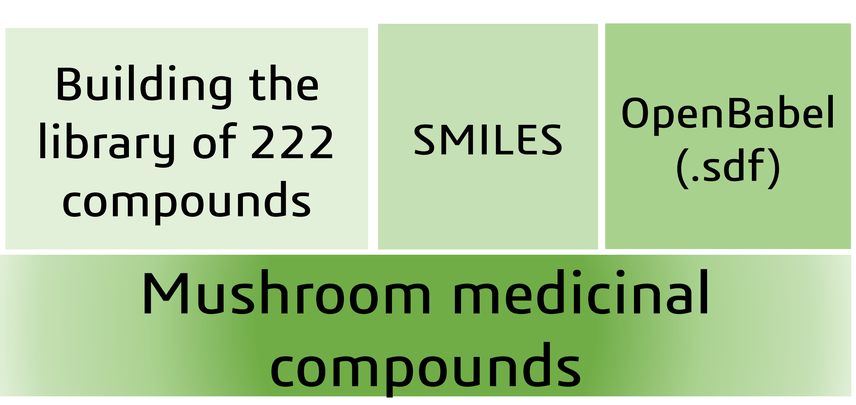
## Motivation

The use of nonsteroidal anti-inflammatory drugs (NSAIDs) in treating inflammatory diseases has been widespread, especially in treating rheumatoid arthritis. NSAIDs act mainly by promoting the inhibition of cyclooxygenase enzymes (COX-1 and COX-2), inducing significant anti-inflammatory, analgesic, and antipyretic activity. However, recent data show that prolonged use of NSAIDs can lead to cardiovascular side effects. Thus, the present work aims to identify COX-2 inhibitors alternatives from natural sources, specifically mushrooms, as an alternative to conventional inhibitors.

## Methods

In this study, virtual screening of a library of 211 low molecular weight compounds present in mushrooms was performed. Molecular Docking studies were completed against a COX-2 protein structure using GOLD docking software with the GoldScore function [1]. The crystallographic ligand meclofenamic acid was also docked against COX-2 protein. For library preparation, Openbabel was used to obtain the compounds in .sdf format [2], and docking results were analyzed with Discovery Studio software [3].

## Results




## Conclusion

The docking results obtained showed that of the 211 compounds, Gerronemin E (**Figure 1A**) and Gerronemin D (**Figure 1B**), both compounds from the *Genorrema* species mushroom, presented better predicted inhibition ability, with scores of 87.3 and 83.5, respectively. Gerronemin E and Gerronemin D are predicted to be promising natural COX-2 inhibitors with anti-inflammatory potential.

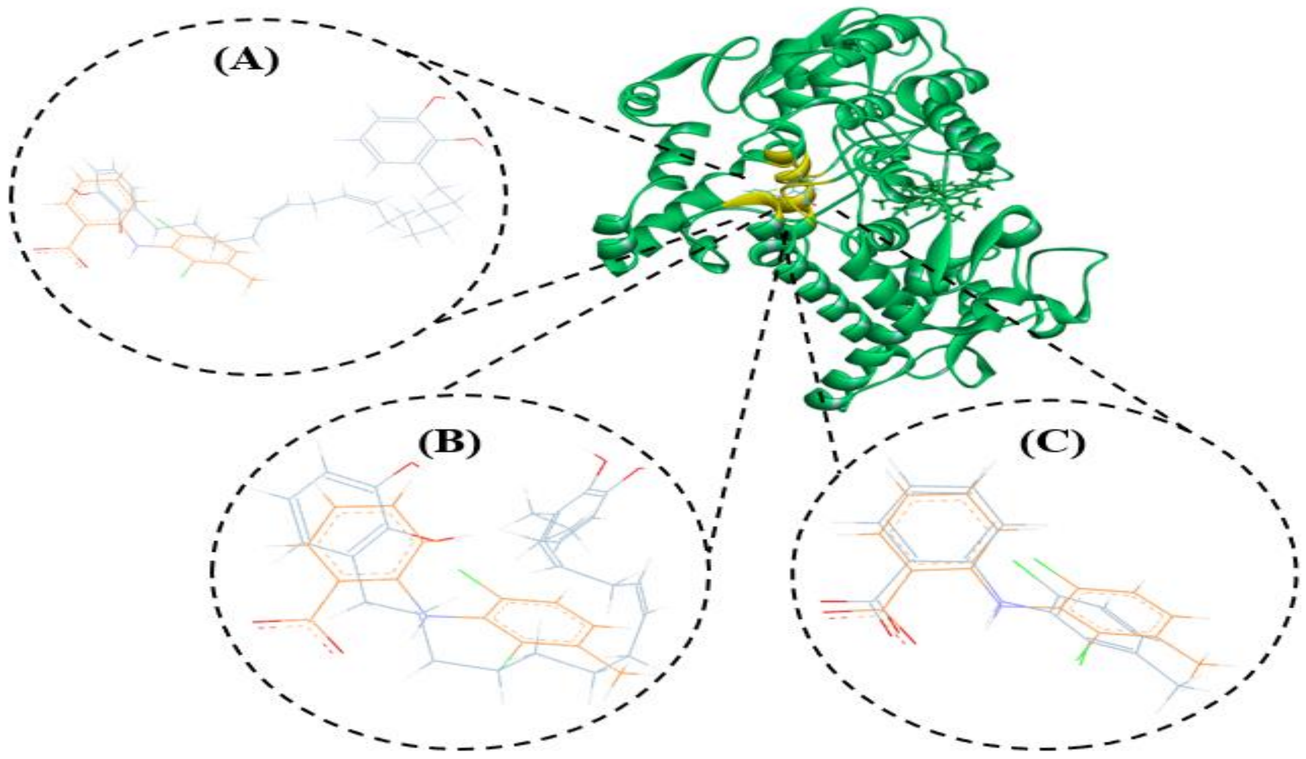



**Figure 1:** Docking conformation of: Gerronemin E (A), Gerronemin D (B), and Meclofenamic acid (C) against COX-2 experimental structure (PDB: 5IKQ). The crystallographic conformation of Meclofenamic acid is presented in orange color and docking conformations in blue color.

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