Abstract

In the last years, the development of the drug for the treatment of inflammation is very fast. The inflammation is a first-rate example of a disease that symbolizes turmoil in normal host defense systems. COX-2 is an oxido-reductase having a role in prostaglandin biosynthesis, inflammatory responses and in cardiovascular events. COX-2 has gained special focus on research since past few decades. The compounds isolated from plants have good inhibitory effects against cyclooxygenase. In this study, Molecular modeling and docking analysis were
used to predict and understand interactions between COX-2 and some compounds isolated from Artemisia arborescensL. The approach is applicable in engineering 3D structures of enzymatic models, and studying interactions of active site residues with ligands show that the three compounds: L9, L8 and L4 give the best results, so they may be effective as the potential inhibitor compound against COX-2 protein and can be evaluated as anti-inflammatory drug molecule using clinical trials.

References

Docking Studies on Cyclooxygenases-2 Inhibitors based On Potential Ligand Binding Sites


- Arômes library of Laboratory of Chemistry of Natural Products (1987-2011). University of Corse, Corte, France. UMR CNRS. p 6134.


Docking Studies on Cyclooxygenases-2 Inhibitors based On Potential Ligand Binding Sites

- 1CX2: 3-dimensional structure downloaded from http://www.rcsb.org/pdb.
- ISIS Draw, a 2-dimensional chemical molecule drawing software: http://www.mdl.com/


Index Terms

Computer Science

Applied Sciences
Keywords
Anti-inflammation  COX-2  Cycloprodigiosin  Molecular docking  Artemisia arborescensL
Interactions