Document details

‹ Back to results | 1 of 1

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Synthesis, In silico molecular docking modeling and pharmacophore mapping of (E)-3-(4-hydroxy-2,6-dimethoxyphenyl)-1-phenylprop-2-en-1- one as potential new inhibitor of microsomal prostaglandin E_2 synthase-1 (Book Chapter)

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Abstract

View references (10)

The discovery of potent anti-inflammatory agents through inhibition of prostaglandin E2 (PGE2) via microsomal prostaglandin E2 synthase-1 (mPGES-1) blocking has been proven to be an important game changer in pharmaceutical industry in recent years. In this study, new chalcone derivative has been successfully synthesized via Claisen-Schmidt condensation reaction. The compound was then docked into mPGES-1 active site to predict anti-inflammatory properties through ligand-enzyme interaction investigation. The data collected from in silico molecular docking simulation and pharmacophore modeling studies provide important insight on the molecular conformation and further shed light towards structural modification of the future novel mPGES-1 inhibitor. © 2020 Trans Tech Publications Ltd, Switzerland.

Author keywords

Chalcone derivative | Docking | mPGES-1 | Pharmacophore

Indexed keywords

Engineering controlled terms: Condensation reactions | Lipids | Pharmacodynamics

Engineering uncontrolled terms: Anti-inflammatory agents | Claisen Schmidt condensation | Microsomal prostaglandin | Molecular conformation | Molecular docking simulations | Pharmaceutical industry | Pharmacophore modeling | Structural modifications

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