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Optimization of the indole – pyrimidine – chrysin hybrid as the lead molecule for anti-inflammatory drugs

Jagroop Kaur and **Palwinder Singh**
Guru Nanak Dev University, India

By using the multi-target-directed drug designing strategy, a highly promising anti-inflammatory agent capable to inhibit cyclooxygenase-2 (COX-2) and lipoxygenase (5-LOX) enzymes of arachidonic acid metabolic pathway is developed. The strategic design of the molecules; linking together indole, chrysin and barbituric acid (pharmacophores of different medicinal agents) through propanol and methine moieties, was based on the results of molecular docking and molecular dynamics studies. The title compound 1 exhibited IC_{50} 1nM and 1.5nM for COX-2 and 5-LOX, respectively. The results of UV-VIS spectral studies and isothermal titration calorimetry experiments indicated appreciable interactions of the compound with these two cellular targets. Further, the *in-vivo* investigations on Swiss Albino mice using capsaicin induced paw lickings and dextran induced inflammation models showed that these compounds possess appreciable analgesic and anti-inflammatory activities. The details of all the experiments including those in support of mode of action of the compound with its cellular targets will be presented.

Biography

Jagroop Kaur graduated from BBK DAV College (for women), Amritsar with BSc in Medical Bioinformatics in 2009. After completing her MSc in Applied Chemistry (Pharmaceuticals) from Guru Nanak Dev University, Amritsar in May 2012, she started her PhD under the supervision of Prof. Palwinder Singh in the same University. Her research interests include medicinal chemistry, various characterization techniques, bio-evaluation of synthesized compounds and computer aided drug designing.

jagroop321@gmail.com

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