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Effect of novel nitric oxide donor N-aryl piperamide derivatives on neuroinflammation and degeneration diseases and the prediction of ADMET profiles

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Through discovery of the various pathophysiological and physiological processes involving nitric oxide (NO), the most attempts were focused on developing new drugs with capability to modulate NO production directly and/or indirectly for therapeutic purposes such as NO-releasing drugs, NO-inhibiting drugs, and phosphodiesterase V inhibitors. NO donor drugs showed an important therapeutic effect in the treatment of many diseases such as arteriopathies, various acute and chronic inflammatory conditions, and several degenerative diseases (Alzheimer's disease and cancer). Nitric oxide (NO)-releasing anti-inflammatory drugs are the prototypes of novel class of compounds that, combining the pharmacological activities of anti-inflammatory and antinociceptive of drugs with those of NO (vasodilator, anti-aggregant, antimicrobial and immune modulator agent), possess potential therapeutic applications in a great variety of diseases. The anti-inflammatory activity of different N-Aryl Piperamides (NAP) have been screened and verified in our previous study and different other reports. In this study, we designed and predicted the biological activity by targeting cyclooxygenase type 2 and pharmacological profiling along with toxicity predictions of various NAPs linked via an ester bond to a spacer that is bound to a Nitric Oxide (NO)-releasing moiety (-ONO2). The result of ADMET and Docking study indicated that among 44 designed molecules, 2-((2E,4E)-5-(benzo[d][1,3]dioxol-5-yl)-N-(4-(1-hydroxyethyl) phenyl)penta-2,4-dienamido) ethyl nitrate with code number 2e showed the best binding potential in both substrate and inhibitory binding pocket of COX-2 enzyme with affinity values -9.33 and -5.12 for PDB ID:1CVU and 3LN1 respectively, thereby, having the potential to be developed as therapeutic agent.

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Conscientious awareness of pharmacists and pharmaceutical sciences

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For manufacturing any dosage form, it has to be stable, safe, effective and most of all Elegant to comply with the patient requirements. The topic of this event is "Conscientious Awareness of Pharmacists and Pharmaceutical Sciences". Therefore, it is a good opportunity to discuss points missed in pharmacopoeias in QC of all dosage forms. The score marked tablet, their QC guidelines not solved yet in all pharmacopoeias except EP. As far as we know, tablets are the most commonly manufactured dosage form, for ease of mass production, more stable, easily stored and easily transported. The presence of a score mark in tablet implies to a patient that a tablet can be split and can be subdivided into smaller doses. Patients expect that the split tablet will provide the same quality, safety and efficacy profile as a whole tablet of equivalent dose. Currently no standards for the performance of subdivisions of scored tablets. In addition, stability studies for divided dose are not found in stability study file for the product. The fatal occurrence if the API is sensitive and easily decomposed after crushing. Finally, harmonization between the pharmacopoeias regarding the weight uniformity testing of split tablets is a necessary requirement.

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