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Selective inhibition of cyclooxygenase-2 (COX-2) as a novel phyto-drug design against inflammation: *In-silico* and *in-vivo* studies

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N on-steroidal anti-inflammatory drugs (NSAIDs) competitively inhibit cyclooxygenase (COX), the enzyme that catalyzes the conversion of arachidonic acid to prostaglandins (PGs). In addition to the outstanding anti-inflammatory potential of the NSAIDs, the associated side effects of the current NSAIDs have limited their therapeutic benefits. The therapeutic mechanism of action of NSAIDs is through the inhibition of COX-2 and COX-1, however, side effects of NSAIDs arise from the inhibition of COX-1. Hence, the need to search for novel compounds (phytochemicals) that can selectively inhibit COX-2. In the present study, Virtual High Throughput Screening techniques were employed to screen eight hundred and fifty (850) phytochemicals from seventeen medicinal plants, the lead phytochemicals (Citrostadienol from Nicotiana tabacum and Eriodictyol from Sorghum bicolor, with binding energies of -10.9kcal/mol and -11.1kcal/mol respectively) that selectively inhibit COX-2 were selected. The pharmacological kinetic analyses of the lead phytochemicals were determined. Moreover, Citrostadienol and Eriodictyol down-regulated the expressions of pro-anti-inflammatory cytokines genes (TNF-α, IL-6, COX-2, and CRP) in HCl/ethanol-induced inflammation in male Wistar rats. *In-vivo* biochemical assays carried out also give credence to the anti-inflammatory potentials of the lead compounds.

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