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Impact of novel N-aryl piperamide on NF- B translocation in neuro-inflammation: Rational drug designing, synthesis, and biological evaluation

Sajad Shahbazi[1], Shikha Singh[2] and Ranbir Chander Sobti[1, 3]
[1]Panjab University, India
[2]Siksha O Anusandhan University, India
[3]Babasaheb Bhimrao Ambedkar University, India

The discovery of the role nitric oxide (NO) in the various pathophysiological and physiological processes leaded to develop new drugs for modulation of the nitric oxide (NO) production directly and/or indirectly, for therapeutic purposes such as NO-releasing drugs, NO-inhibiting drugs, and phosphodiesterase V inhibitors. There are numbers of 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). The NO donor anti-inflammatory drugs are a novel class of compounds in which NO combined to an anti-inflammatory agent to improve the efficacies and reduce the side effects. They are combining the pharmacological activities of anti-inflammatory and antinociceptive of drugs with those of NO (vasodilator, anti-aggregant, anti-microbial and immune modulator agent). In our pervious study, the anti-inflammatory activity of different alkyl nitrate derivatives of the various types of N-Aryl Piperamides (NAP) have been screened and verified. In this study, we are investigating the biological activity by targeting NF- B subunits and Cyclooxygenase-2 *in silico and in vitro*, and pharmacological profiling along with toxicity predictions of various NAPs linked via an ester bond to a spacer that is bound to a NO -releasing moiety (-ONO2). The result in *silico* investigation indicated that among 51 designed molecules, 3-((2E,4E) -5-(benzo [d] [1,3] dioxol-5-yl) -N-(4-(hydroxymethyl) phenyl) Penta-2,4-dienamido) propyl nitrate with code number PA-3'K showed the best anti-inflammatory potential. These findings have been tested and supported by the *in vitro* investigation and will presenting along with.

e: siavosh.farma@gmail.com