Synthesis, biological evaluation and molecular docking studies of novel 3,5-disubstituted 2,4-thiazolidinediones derivatives

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Thiazolidinediones (TZDs) are a new class of antidiabetic drugs, having an insulin sensitizing effect in patients with type 2 diabetes. We report here the synthesis A series of thirteen 2,4-thiazolidinedione derivatives. The 2,4-thiazolidinedione ring's fifth position was used as a site for Knoevenagel condensation to generate the compounds listed in the title. The synthesised derivatives were characterised using a variety of physicochemical and spectral analyses, including IR, Mass, 1H-NMR, ^{13}C-NMR, and elemental analysis. By using the carrageenan-induced rat paw edoema method, the alloxan-induced diabetes in wistar rats method, and the FRAP (ferric reducing antioxidant power) method, respectively, the derivatives were examined for their *in vivo* anti-diabetic, *in vivo* anti-inflammatory, and *in vitro* free radical scavenging activities. Some of the compounds showed promise as powerful anti-inflammatory, anti-free radical, and anti-diabetic medications. The most effective anti-diabetic compounds, NB7, NB12, and NB13, were docked using MOE software to study some potential structural insights into the potential binding patterns with the target PPAR active sites (PDB ID: 2PRG). The dichloro derivative chemical NB-7 has demonstrated strong anti-inflammatory and antioxidant potential in the current investigation in addition to having the highest anti-diabetic efficacy.