

## Synthesis, characterization, molecular docking, ADMET properties and *in vitro* anti-inflammatory screening of some isoxazoline derivatives

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This paper describes the synthesis of isoxazoline derivatives using Bi<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> nanocatalyst. The (E)-3-(2-amino-3,5-dibromophenyl)-1-(substituedphenyl)prop-2-en-1-one have been treated with hydroxylamine hydrochloride in the presence of nanocatalyst Bi<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> and ethanol as solvent to yield 2,4-dibromo-6-(3-(substituedphenyl)-4,5-dihydroisoxazol-5-yl)aniline **8-14**. The final product has been separated and purified by ethanol recrystallization. The obtained final product **8-14** has been characterized by elemental analysis, FT-IR, <sup>1</sup>H and <sup>13</sup>C NMR spectral studies. Synthetic transformation details, small catalytic amounts, excellent product yields and suitable solvent for the formation of these isoxazoline scaffolds are elucidated. Synthesized derivatives have been screened for their *in vitro* anti-inflammatory activity using HRBC method. The obtained *in vitro* results have been compared with the molecular docking with protein, DNA Gyrase (PDB ID: 3U2D), Cyclooxygenase-1 (PDB ID: 3N8V) and Cyclooxygenase-2 (PDB ID: 3LN1) enzyme using Schrodinger suit Maestro 11.2 version. *In silico* ADMET screening has also been performed by qikprop module of Schrodinger suit.

**Keywords:** Bi<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> nano catalyst, Docking, ADMET