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Synthesis, molecular docking, molinspiration and anti-oxidant studies of novel N-ethylbenzimidazolylisoxazole derivatives

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A pandemic of acute respiratory disease known as "coronavirus disease 2019" (COVID-19) has been caused by coronavirus 2 (SARS-CoV-2), a highly transmissible and pathogenic coronavirus that first appeared in late 2019. This disease poses a hazard to public health and safety. A series of novel benzimidazolylisoxazoles have been synthesized from 1,2-diaminobenzene and lactic acid. It is expected that they will exhibit a wide range of biological activities. Synthesised compounds have been characterised by FT-IR, ^{1}H NMR and mass spectroscopy. Docking studies have also been carried out by using PyRx and visualized by PyMoL software. Molecular properties and bioactivity of the compounds have been predicted using molinspiration online software. Anti-oxidant activities of the synthesised compounds have been determined using DPPH scavenging assay.

Keywords: SARS-CoV-2, Docking, Molinspiration, Anti-oxidant, DPPH