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RESEARCH LETTER

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Synthesis, molecular docking, QSTR and in-silico ADME studies of novel 1,3-thiazolidine-amide derivatives as hybrid bioactive heterocycles

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Abstract

In this article, we described synthesis of 1,3-thiazolidine - amide hybrid derivatives by two different methods from (*S*)-2-amino-3-(4-(benzyloxy)phenyl)-1-(thiazolidin-3-yl)propan-1-one (4). In first method, catalytic amidation was carried out under microwave irradiation using Ceric Ammonium Nitrate (CAN) as a green catalyst where as in second conventional method; CDI was used as a significant coupling reagent to optimize reaction condition and yield of product. All new compounds were well characterized by ^{1}H NMR, ^{13}C NMR, IR and ESMS spectral techniques and evaluated in vitro antibacterial and antifungal activity. The molecular docking study revealed that the designed compounds snuggly fit in the active site of 4WMZ protein. In addition, the QSTR study of new compounds were carried out with the help of Toxicity Estimation Software Tool (T.E.S.T). The results showed slight toxic nature of new compounds. *In-silico* ADME studies significant values of pharmacokinetic parameters and demonstrated good drug like characteristics based on Lipinski's rule of five.

KEYWORDS

antimicrobial, CDI, ceric ammonium nitrate, green approach, microwave irradiation, molecular docking, QSTR study

1 | INTRODUCTION

One of the most serious problem regarding public health is antimicrobial resistance (AMR). It poses crucial challenge to the effective prevention and treatment of various infections. Antimicrobial resistance is generally caused by spontaneous evolution, bacterial mutation, and horizontal gene transfer or resistant of bacteria. The bacteria that causes a common or severe infections would develop resistance to new pharmacophores. Despite the various steps implemented in the last few decades to address this problem, there is no declination in trends. To overcome this threat, designing of hybrid drugs with multifunctional profiles is a significant strategy against drug resistance (Saadeh & Mubarak, 2017). Heterocyclic scaffolds can be developed by combining two or more bioactive pharmacophores with enhanced bioactivity. This molecular hybridization diversify the drug molecules to transform their physicochemical, pharmacokinetic, and pharmacodynamics properties and refrains the microbial resistance (Dadgostar, 2019; Hogberg et al., 2010). Considering the biological importance of new antimicrobial medications with innovative mechanisms of action, we report here amide containing hybrid heterocyclic compounds with significant antimicrobial activity (Abdelhafez et al., 2023; Kushwaha et al., 2011; Ozdemir, 2013).

