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RESEARCH ARTICLE

In-silico and *in-vitro* evaluation of diazenyl compounds as anti-bacterial agents

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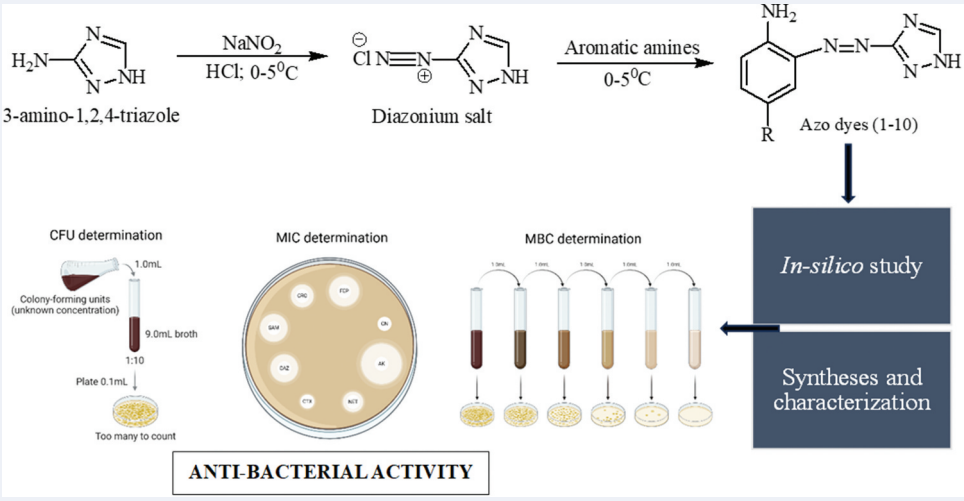
ABSTRACT

Aim: The diazenyls are interesting scaffold in medicinal chemistry displaying a wide range of pharmacological activities including anti-microbial, anti-cancer, anti-inflammatory, and analgesic-antipyretic, among others. These diverse attributes have reinitiated the interest of the researchers in them. Studies suggest that incorporating heterocyclic ring system into diazenyl scaffold helps to improve the biological property of the drug-like substances. The present study aims to synthesize novel diazinyl-triazole adducts, with an intent to obtain compounds with enhanced anti-bacterial potential.

Materials and methods: All synthesized compounds were characterized using physicochemical methods and spectroscopic techniques. The compounds were evaluated *in-vitro* against two Gram-positive and two Gram-negative bacterial strains, demonstrating good to moderate efficacy. *In-silico* prediction study was also carried out for the synthesized series of compounds.

Results and conclusion: The molecular docking data are aligned with the *in-vitro* experimental results. The ADMET predictions suggested the compounds are both efficacious and safe. The study presents new compounds as potential anti-bacterial agents with desirable pharmacological profile.



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Diazenyl; triazole; anti-bacterial activity; *in-vitro*; molecular docking; ADMET studies

1. Introduction

The outbreak of antimicrobial resistance along with lack of development of new antimicrobial drugs has resulted in an alarming situation for human and animal health care globally [1]. It is pertinent to mention that the success of modernized healthcare system, right from care of preterm babies, organ transplant, cancer remedy, or any other advanced major surgery, is not possible without effective antibiotic chemotherapy [2]. Hence, there is an urgent need for finding newer antimicrobial drugs with the ability of overcoming resistance [3]. In this regard, the development of compounds utilizing a hybrid approach may prove beneficial.

The compounds possessing the azo group (-N=N-) are broadly called diazenyl compounds [4]. Because of the vivid colors [5] in which they exist, they are commonly referred to as azo dyes. Their pharmaceutical applications include their usage as cell staining and imaging agents [6], in addition to their potential as anti-microbial, anti-viral and anti-cancer agents, when incorporated in some important heterocyclic scaffolds *viz*. thiazole, benzothiazole, imidazole, pyrazole, thiophene, and quinoline [7]. These are also useful as carriers in prodrug strategy [8], besides being widely used in textile, cosmetics, paper printing industries [9], light and weather-fastness [10], and food industry [11].

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