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Experimental and Theoretical Studies for Noncovalent Interactions Analysis of 2-Mercaptopyrimidine Derivative and Their Antimicrobial Activities

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Abstract—Here, we have synthesized the 2-mercaptopyrimidine derivative for noncovalent interactions and their antimicrobial activities. The non-covalent interactions have been carried out by crystallographic studies, revealed that it showed different interactions such as C–H···N, C–H···S and S···π. Further, these intermolecular interactions have also been quantified by Hirshfeld surface analysis, and NIC calculation. Chimera 1.17.3 software is used for molecular docking studies with (protein ID: 1JIJ) and Discovery Studio is used for analyzing the docking results. The in vitro antifungal activity has been done against two fungal strains (*C. albicans* and *A. niger*) and antimicrobial activity has been done against two strains (*S. aureus* and *P. aeruginosa*).

Keywords: crystal structure, Hirshfeld surface analysis, antifungal activity, antimicrobial activity, intermolecular interaction energy calculation

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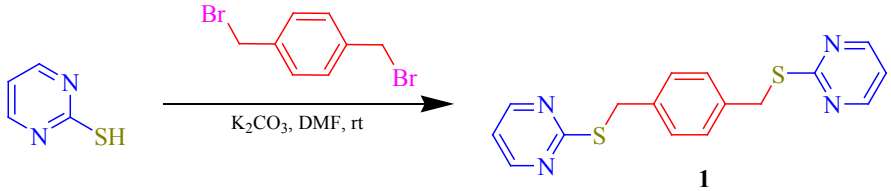
INTRODUCTION

Pyrimidine are known to be vital and to play a significant role in pharmacological importance as therapeutics in clinical applications [1, 2]. The pyrimidine derivatives possess significant biological activities such as antifungal [3–9], antibacterial [10, 11], anticancer [12–14], antitumor [15], antiinflammatory [16], antiparkinsonian [17], antihyperlipidemic agents [18], antimicrobial [19, 20].

RESULTS AND DISCUSSION

As a result of the previously mentioned discovery, we have synthesized the dimmer of 2-mercaptopyrimidine derivatives (Scheme 1) in order to study noncovalent interactions and antifungals activity. These compounds, which contain the pyrimidine core, display a range of potential biological activities. The pyrimidine core serves as a key structural component in these compounds, contributing to their diverse biological effects. These types of compounds extensively, uncovering their

Scheme 1.



1