

Poster Presentations

Synthesis, DFT and antibacterial studies of new Schiff base derived from nicotinohydrazide

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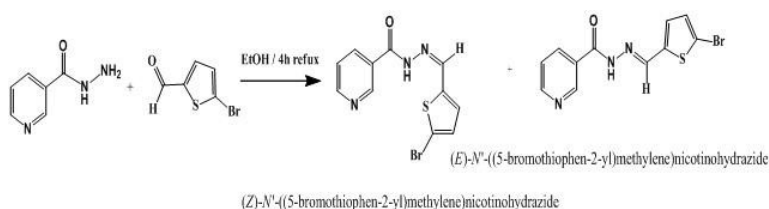
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Abstract

A new Schiff base N'-(5-bromothiophen-2-yl)methylene) nicotinohydrazide was isolated and characterized as Z- isomer as seen in the Scheme.



The synthetic condensation reaction was monitored by FT-IR and UV-visible as well as DFT calculation. The structure of desired compound was experimentally analyzed based on: elemental analysis, EI-MS, UV-visible, FT-IR spectral, TG/DTG. ¹H-NMR and DFT-computational calculation supported Z-isomer as favored product over E one. Good agreement between experimental and theoretical calculation were obtained. The antibacterial results obtained using the desired compound indicates a promising result against human pathogenic bacteria.

Keywords: FT-IR, condensation, TG, Schiff bases, DFT.