Indian Journal of Chemistry
Vol. 64, July 2025, pp. 663-669
DOI: 10.56042/ijc.v64i7.11086

Synthesis, characterization, PASS prediction, molecular docking and ADME study of benzo[*b*]thiophen-5-amine based biologically active Schiff bases

Raksha V Zala[a], Chandresh S Vaya*[a,b] & Rakesh Jani[a,c]

[a] Department of Chemistry, Kamani Science College and Prataprai Arts College, Amreli 365 601, Gujarat, India

[b] GMB Polytechnic, Rajula 365 560, Gujarat, India

[c] Lalan Science College, Bhuj 370 001, Gujarat, India

E-mail: c.s.vaya2011@gmail.com

Received 22 June 2024; accepted (revised) 13 June 2025

Adopting the potentiality of benzo[*b*]thiophene moiety and Schiff base compounds, a series of Schiff base compounds namely, 2-{[(1-benzothiophen-5-yl)imino]methyl}phenol *i.e.* **5a**, 3-{[(1-benzothiophen-5-yl)imino]methyl}benzene-1,2-diol *i.e.* **5b**, 2-{[(1-benzothiophen-5-yl)imino]methyl}-6-methoxyphenol *i.e.* **5c**, 2-{[(1-benzothiophen-5-yl)imino]methyl}-5-methoxyphenol *i.e.* **5d**, 2-{[(1-benzothiophen-5-yl)imino]methyl}-4-nitrophenol *i.e.* **5e** and 2-{[(1-benzothiophen-5-yl)imino]methyl}-4-chlorophenol *i.e.* **5f** have been synthesized in good yields and characterized by FT-IR, ^{1}H and ^{13}C NMR, and mass spectroscopy. Biological activity has been checked after performing antimicrobial and antifungal activity studies of synthesized compounds using the Minimum Inhibitory Concentration (MIC) determination technique. Computational studies like PASS (Prediction of Activity Spectra for Substances) prediction, molecular docking, and an ADME (Absorption, Distribution, Metabolism, Excretion) study have been performed to gain insight into the synthesized molecules' *in silico* properties.

Keywords: ADME, Antimicrobial Activity, Antifungal activity, Benzo[*b*]thiophen-5-amine, Molecular docking, PASS prediction, Schiff base

In the class of sulfur heterocycles, benzo[b]thiophene