Indian Journal of Chemistry
Vol. 65, May 2026, pp. 493-519
DOI: 10.56042/ijc.v65i5.29167

Synthesis, spectral QSAR, molecular docking, DFT, ADMET studies and anti-microbial activity evaluation of some benzodioxin pyrazolines

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Received 26 February 2026; accepted (revised) 14 May 2026

A series of nine 4,5-dihydro-3-(2,3-dihydrobenzo[b][1,4]dioxin-7-yl)-1,5-(substitutedphenyl)-1*H*-pyrazolines have been synthesized by treating (*E*)-1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-3-phenylprop-2-en-1-ones with phenyl hydrazine hydrochloride in the presence of sodium acetate *via* cyclization reaction by cyclo-condensation process. These synthesized products have been characterized by FT-IR, ^{1}H and ^{13}C NMR spectral data. The infrared spectral frequencies C=N, N-N and C-X (ν, cm^{-1}), along with NMR chemical shifts (δ, ppm) of H_a, H_b, H_c protons, and the C=N, C-N, C-X, CH_2 carbons of 4,5-dihydro-3-(2,3-dihydrobenzo[b][1,4]dioxin-7-yl)-1,5-(substitutedphenyl)-1*H*-pyrazoline have been assigned and related to utilizing single and multi-regression analysis with Swain-Lupton's parameters and Hammett substituent constants. The *in vitro* antimicrobial assay of all compounds has been evaluated with two-gram positive bacterial species: *Staphylococcus Aureus, Streptococcus Pneumonia* and two-gram negative bacterial species: *Pseudomonas aeruginosa, Escherichia coli*, fungal species: *Candida albicans, Candida auris*. The highest values of zone of inhibition have been recorded for compound **1**, followed by the compound **4** and **8**, which exhibit good zones of inhibition both in bacterial and fungal strains. *In silico* analysis like molecular docking studies of potent antibacterial compounds (**1, 4** and **8**) indicate strong binding affinities to the receptors *Streptococcus aureus*-7S54, *Escherichia coli*-9R2Z, *Candida albicans*-5HW8. Employing DFT(B3LYP) with 6-311G(d,p) basis set for *in-silico* evaluations confirm favourable drug-likeness and pharmacokinetic properties for all pyrazolines. The ADMET properties further demonstrate that these compounds possess a good therapeutic application in combating bacterial and fungal infections.

Keywords: Pyrazolines, Hammett correlation, Anti-microbial activity, ADMET, pharmacokinetics