Conclusion The synthesis of indolyl–triazole hybrid molecules (IT1–8) has been successfully achieved, with their structures confirmed by advanced spectroscopic techniques.These compounds exhibit promising antimicrobial properties, particularly against bact- erial strains, due to the structural features of halogenated phenyl rings and indolyl moieties.Computational analyses using PASS and Molinspiration predicted significant antitubercular and anticancer activities, identifying compounds IT1 and IT2 as potential GPCR ligands and enzyme inhibitors.This research demonstrates the potential of indolyl- triazoles as effective antimicrobial agents and empha- sizes the importance of integrating experimental and comput- ational approaches in drug development.However, the in silico predictions did not fully align with experimental anti- microbial results, underscoring the complexity of drug inter- actions and the limitations of computational tools alone.The toxicological assessments highlighted IT5 as a compound with favourable safety profiles, while others demonstrated varying levels of toxicity.Further investigations into the structure–activity relationships is essential to optimize these compounds for the clinical .applications