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Docking, synthesis and antibacterial Studies on N-(5-bromo/nitro-pyridin-2-yl)-sulfonamide analogues as FtsZ inhibitors

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The cytoskeletal filamentous temperature-sensitive protein Z (FtsZ) plays a pivotal role in prokaryotic cell division and is 👢 present in majority of the bacterial species. In recent years, inhibitors of FtsZ have been identified that may function as lead compounds for the development of novel antimicrobials. A series of 5-(bromo/nitro-pyridin-2-yl) sulphonamide derivatives have been designed and docked with MtbFtsZ. On the basis of cavity detection analysis of MtbFtsZ, it was found that the allosteric site was the possible binding site for these inhibitors. The designed inhibitors were docked into the allosteric binding pockets and the best docked poses were selected based on ranked Ligandfit dock score and binding energy analysis. The docked complexes were then submitted for molecular dynamics simulation to retrieve the stable structures. Hydrogen bonding and hydrophobic interactions were observed as the stabilizing force of protein-ligand complexes. The molecules showing potential during docking studies were synthesized, purified and evaluated for their antibacterial activity against a variety of bacterial strains, like B. subtilis (NCIM-2156), S. aureus (NCIM-2079), S. epidermis (NCIM-2493), P. aeruginosa (NCIM-2036), E. coli (NCIM-2065) and P. vulgaris (NCIM 2027) following broth dilution method using ciprofloxacin and vancomycin as reference. Antibacterial results indicated that these molecules possessed promising activity against the tested bacterial strains.

Biography

Ramendra K. Singh, an associate Professor of chemistry, is director of Nucleic Acids & Antiretroviral Research Laboratory in the University of Allahabad, India. He is member of several national bodies, editor to different international journals and referee to a dozen of national/international journals. He has been recipient of various awards/fellowships, like Young Scientists' Award, India, XVI IUBMB fellowship, India, Jawaharlal Nehru Visiting fellowship, India, UNESCO fellowship, Japan, Post-Doc fellowship, Japan, INSA International Exchange fellowship, Poland and Fulbright fellowship, USA. He has published more than 50 research articles/book chapters in journals/books of national and international repute.

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