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An efficient synthesis of annulated novel pyrimido[4,5-d]pyrimidine derivatives: DFT, docking, SAR and antimicrobial evaluation

Manojkumar K Rathod¹ and Mohsin A Jamadar²¹Marwadi University, India²Adarsh Nivasi Shala, Bharuch, India

A simple green synthetic approach was developed to synthesize medicinally important heterocyclic novel pyrimido[4,5-d]pyrimidine (PP) derivatives by using heterogeneous solid acid catalyst, through single reaction chamber. This green process offer high yields within short reaction time. *In silico* proficiency of Lipinski's, DFT, docking and SAR study have been carried out in order to get target drug like novel PP molecules with desired activity through multidisciplinary green approach. Computer aided drug designing (CADD), molsoft and Osiris tool were used to predict PP structural parameters of Lipinski rule which meant to find molecular membrane permeability, oral bioavailability, drug-likeness and drug score. In addition, DFT method was employed to calculate the PP structural geometries, molecular stability and electronics structures using online tool. Moreover, the docking method was used to determine voltage-dependent calcium channel blockers receptor-PP ligand interactions and molecular surface bonding were performed by online tool. The synthesized products were characterized by FT-IR, ¹H NMR and ¹³C NMR spectral analysis. The synthesized analogs have also been evaluated for their bioassay against bacterial and fungal strains. SAR study relates features of PP structure to a property, effect and biological activity associated within moiety. In this summary, theoretical and experimental approaches brought together in order to synthesize target PP molecules with desired activity will serve as vital aid for future researchers working in the area of drug design.

Biography

Manojkumar K Rathod completed his MSc, MPhil in Bioinformatics; BSc, MSc in Chemistry and; PhD in Chemistry at Sardar Vallabhbhai National Institute of Technology, Surat, India. At present, he works as an Assistant Professor in Department of Chemistry at Marwadi University, Gujarat, India. He has two years of experience as an Assistant Professor and Head of Department of Chemistry at S S Agrawal College of Commerce & Management, Gujarat, India. He received scientific awards by RSC (2014) and BTISNET, DBT (2012). He has published four research paper and presented research article in nine national & international conference.

manojrathod13@gmail.com

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