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QSAR study of benzimidazole type of fluconazole analogues invoking quantum mechanical density functional based descriptors

Recently Hui-Zhen Zhang *et al.* reported a series of benzimidazole type of fluconazoles which have potent antimicrobial activity. They synthesized and characterized 27 analogs invoking 1H NMR, 13C NMR, IR, MS and HRMS spectra. An antimicrobial activity of all the newly synthesized compounds has been done *in vitro* conditions by using two-fold serial dilution technique. The derivative 3,5-bis(trifluoromethyl)phenyl benzimidazoles exhibits comparable and even stronger antibacterial and antifungal efficiency in comparison with reference drugs such as chloromycin, norfloxacin and fluconazole. In this venture, we have tried to make a qualitative correlation between experimental antimicrobial activity and computed Density Functional Theory (DTF) based global quantum mechanical descriptors of instant bio-active compounds. The effect of substitutions on the experimental activities is explained invoking global descriptors. Local descriptors have been used to identify site selectivity and mechanistic pathways of bio-active molecules. Finally we have adopted multi linear regression analysis methodology to model the experimental activities of instant organic bio active compounds in terms of DFT based descriptors through Quantitative Structure Activity Relationship/Quantitative Structure Property Relationship (QSAR/QSPR) analysis.

Biography

Tanmoy Chakraborty has completed his PhD from University of Kalyani, West-Bengal. He did his PhD on QSAR/QSPR analysis of Bio-Active molecules invoking DFT based Descriptors. He has been carrying his research in domain of Theoretical and Computational Chemistry since 9 years. Presently, he is the Associate Professor at Department of Chemistry, Manipal University Jaipur, Rajasthan and also serving as Deputy Registrar of the University. He has published more than 22 research papers in reputed journals and is serving as an International Editorial Board Member of International Journal of Chemoinformatics and Chemical Engineering, IGI-Global, USA. He is the Editor-In-Chief of research book: "Computational Quantum chemistry, Developments and Applications" (published by Apple Academic Press and distributed by Taylor & Francis Group, USA).

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