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In Silico ADME prediction on calcium channel blockers using QSPkR studies

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The use of in silico approaches for successful prediction of pharmacokinetic properties of compounds during new drug discovery has been increasing exponentially. These in silico models, for the prognosis of absorption, distribution, metabolism, and excretion (ADME) are invariably based upon the implementation of quantitative structure pharmacokinetic relationship (QSPkR) techniques. The primary aim of QSPkR studies is to enable drug designer to modify the chemical structure of a pharmacodynamically active drug in such a manner as to alter its pharmacokinetic properties without diminishing its pharmacodynamic potential. Once such relationship is ascertained with adequate statistical degree of confidence, it can be of valuable assistance in the prognosis of behavior of new molecules, even before these are actually synthesized.

An early assessment of ADME properties will help pharmaceutical scientists to select the best drug candidate as well as to reject those with a low probability of success. It not only saves considerable amount of time, money, animal life and involvement of "normally, healthy and drug-free human volunteers" required for conducting experimental pharmacokinetic studies, but also the expertise of pharmacokinetists and drug designers. Construction of a typical QSPkR involves pharmacokinetic parameters, structural parameters (descriptors) and multivariate statistical techniques.

The in silico QSPkR concept would be illustrated using the case studies from the dry lab experimental findings carried out in our laboratories on calcium channel blockers congeneric and non-congeneric drug series using diverse molecular descriptors viz. lipophilic, steric, electronic, electrostatic, constitutional, topological, geometric, polarizability and quantum-chemical. The in silico approaches yielded high degree of ADME prognosis and successful validation using the leave-one-out (LOO) procedures.

Biography

During his three decades of dedicated experience, Prof. Bhupinder Singh Bhoop has earned to his credit over 140 publications in peer-reviewed journals, 9 book chapters, 3 patents, 13 research projects, 20 Best Paper Awards, 170 Conference presentations and over 130 invited talks delivered in India, US, and China. His work fetched several awards & accolades like, Leading Educators of World (UK), Best Pharma Personality 2008, Shiksha Rattan Award and Founder Coordinator: Student Research Convention by Association of Indian Universities. He is on Editorial Board of over dozen journals and reviewer of over 30 journals. Lately, he has been assigned as Coordinator of UGC NanoSciTech Centre at Panjab University.

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