doi:10.4172/0975-0851.1000027

TITLE

IN SILICO ADME PREDICTION USING QSPR STUDIES

Dr Yash Paul Singla

Principal, Lord Shiva College of Pharmacy
Sirsa (Haryana), India.

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 (QSPR) techniques. The primary aim of QSPR 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 QSPR involves pharmacokinetic parameters, structural parameters (descriptors) and multivariate statistical techniques.

The *in silico* QSPR concept would be illustrated using the case studies from the dry lab experimental findings carried out in our laboratories on several 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.