

11th Global Experts Meeting on

CHEMISTRY AND COMPUTATIONAL CATALYSIS

May 18-19, 2018 Singapore

The role of computational chemistry in drug discovery and development**Vishakha A Mali, Dhara S Soni and Keyuri K Bhatt**

Parul University, India

Quantitative Structure-Activity Relationships (QSAR) represent an attempt to correlate structural or property descriptors of compounds with activities. QSAR attempts to find consistent relationship between biological activity and molecular properties, so that these rules can be used to evaluate the activity of new compounds. Earlier, drugs were designed by systemic modification of chemical precursors using standard tools of medicinal chemistry. But, the approach of Edisonian research for synthesizing organic molecules with an objective of obtaining medicinal compounds with desired biological activities is not effective in the present days. As in the process, the prospective drug substances have to cross long and rigid methodologies of tests and should satisfy all the requirements which make the probability of success very little. The rational approach of drug designing is, therefore, a natural choice to enhance probability of success as well as to minimize labor, time and cost. The QSAR is based on Structure Activity Relation (SAR) approach. It uses physicochemical properties based on Hansch analysis and Hammett equation once a 3D QSAR model is generated further optimized by molecular docking to predict the interaction mode between the high/low potent ligands and protein (enzyme/receptor) parameters. Lipophilic parameters two parameters are commonly used to relate drug absorption and distribution with biological activity, namely, the partition coefficient (P) and the lipophilic substituent constant (p).

Biography

Vishakha A Mali is the scholar of Department of Pharmaceutical Chemistry Parul University. She with her two other colleagues got scholarship approx. 1,10,000 INR because of their good academic index and their dedication towards research during their undergraduate study. Presently she is assigned work related to anticancer activity and antidiabetic activity. She is self-motivated and connecting to the world with their research ability.

vishakha.mali@yahoo.in, sonidhara104@gmail.com, keyubhatt@gmail.com

Notes: