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**A Concise Review on the Significance of QSAR in Drug Design**

Hiteshi Tandona, **Tanmoy Chakrabortyb,**Vandana Suhagc

a. Department of Chemistry, Manipal University Jaipur, Jaipur, India

**b. Department of Chemistry, School of Engineering, Presidency University, Bengaluru, India**

c. Department of Applied Sciences, BML Munjal University, Gurgaon, India

**Abstract**

Drug designing is a crucial step in the exploration of novel drugs which requires potent methodologies. One of such methodologies is Quantitative Structure Activity Relationship (QSAR) which is a widely used statistical tool that correlates the structure of a molecule to a biological activity as a function of molecular descriptors, thereby, playing an essential role in the drug designing. QSAR utilizes Density Functional Theory (DFT) based chemical descriptors for this purpose. The selection of such significant molecular descriptors from various available descriptors is the foremost challenge in a QSAR as structural descriptors are representative of the molecular characteristics accountable for the relevant activity. Recently, new QSAR approaches have been introduced which further enhance the study of the activities. Further, the constructed QSAR models also need to be tested and validated for their efficiency and practical usage. As the QSAR models are structure specific, they may not be universally applicable. However, because of their high precision and efficacy, they have a promising future in the world of drug design. This review briefly summarizes the role of descriptor based QSAR in drug design in conjunction with existing QSAR approaches and also the utility as well as constraints of this approach in drug design.

**Keywords:**

QSAR, Density Functional Theory (DFT), Quantum Chemical Descriptors, Drug Design

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