In-Silico Computational Tools in Effective Product Design and Pharmacokinetics Optimization

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Editorial

A lot of data has been generated from the lab-based experiments for physical and chemical characterization of the different chemicals such as drugs, excipients, polymers, solvents and surfactants. This big data is of very important for designing the new drug product but it is very difficult to extract the information manually from this huge source. Now days a new ways of data mining and processing are on focus of the scientists such as Machine Learning (ML), Deep Learning (DL) and Artificial Intelligence (AI). Therefore, in the era of artificial intelligence (AI) and computer revolution, the conventional methods of product design seem to be irrelevant as personalized medicines are now getting more attention. Now the conventional approach of "one drug-fits all" have been replacing by the "customizable dosage forms" based on the individual needs. So a large scale updation of pharmaceutical sector is indeed required to adopt for innovative engineering and processing methods of formulation development. Induction of computer simulation and computational approaches such as Quality by Design (QbD) concept, statistical analysis and simulation software's now shifted the paradigm from lab-based research to *in-silico* research where majority of the research activities related to product development are performed on the computer simulated mathematical models with high degree of accuracy covering the interaction of all the process variables. *In silico* approach eliminates the irrelevant sets of experiments and only provides the best suitable ones using AI based simulated model. The areas of application of AI approach in formulation development can be formulation optimization and pharmacokinetic evaluation as discussed one by one in the coming sections. The data of physicochemical properties of the different drugs, chemicals and excipients is stored in the AI enabled computer software. The AI algorhythm in the computer system find the expected results of the mutual interaction of any given set of excipients and drug by the aid of algorhythm based mathematical calculations and predict the characteristics of the resulting formulation. Here we can optimize the formulation for the desired results as defined by the QbD tools by varying the concentrations of the excipients without performing the actual experimentation. Statistical tools such as Central Composite Design (CCD), box-behnken design or others provide us with the different formulations with the varying concentration ranges of polymers which may have the desired and optimized formulation. Using computer algorhythm a blend of raw materials can be designed based on the physical and chemical properties of the drug and excipients to produce the product with desired characteristics. This saves the cost and time of research and increase the confidence on the quality of product. The customization of the dosage forms based on the individual needs is also possible through *in-silico* approach. The customization is done to adjust the pharmaceutical, pharmacokinetic and therapeutic characteristics of the product as per the need of the individual patients i.e., based on the behavior of the drug in individual patients due to different genetic makeup and different body physiology. AI based evaluation of pharmacokinetics parameters is the necessary and important part of the formulation development as it reduces the attrition rate and failure of drug compounds during the clinical studies. AI based techniques predicts the ADME profile of the drug in a particular dosage form that not only help in drug optimization but also in drug repurposing. Establishing an *In Vitro-In Vivo* Correlation (IVIVC) predicts the pharmacokinetic behavior of the drug inside the body in earlier phase of the study before going in to the actual experimentation. In this manner a product can be designed from initial step to final optimized formulation using the computer simulated algorhythm. After validation of the final design, the product is developed in the lab and tested for its characteristics to check if these are as per the given specifications or not.

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