Research and Reviews: Drug Delivery

Brief Overview on Pharmacokinetic Software and Toxicokinetic Modeling

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Commentary

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ABOUT THE STUDY

Pharmacokinetics is the study of movement of foreign substances (xenobiotics) as they transit through the body, and it includes absorption, distribution, biotransformation/metabolism, and excretion kinetics (ADME). It can simply be defined as the body's response to xenobiotics. Pharmacokinetics describes the time course of ADME of xenobiotics in the body using mathematical equations (models), allowing us to better understand, interpret, and even anticipate the nature and magnitude of biological effects (therapeutic or harmful) of xenobiotics.

To characterize the destiny of xenobiotics in the body, pharmacokinetics uses a variety of techniques, including viewing the body as one or more homogeneous compartments based on mathematical fitting or physiological features. The ability to comprehend and anticipate the fate of xenobiotics inside the body is improved by describing the rates at which they migrate into tissues. The reader will be introduced to the fundamental concepts and

principles of pharmacokinetic analysis using both compartmental and physiologically based models.

Pharmacokinetic software

Noncompartmental, compartmental, and physiological approaches are used to analyse pharmacokinetic data. In addition, nonlinear mixed effects models and maximum likelihood estimation methods are used to undertake population pharmacokinetic studies. The noncompartmental technique uses the trapezoidal rule to measure the area under the plasma drug concentration–time curve and is based on the idea of statistical moments. It has few underlying assumptions.

The compartmental technique calculates PK parameters by evaluating the plasma drug concentration–time curve with kinetic models. As a result, graph plotting and lengthy mathematical calculations are required for ADME and drug concentration–time data interpretation. As a result, a number of software tools for pharmacokinetic data processing, Non-Compartmental Analysis (NCA), nonlinear model fitting, and sophisticated pharmacokinetic/pharmacodynamic modelling have been developed and verified.

For PK modelling and simulation, a variety of commercially available software such as Phoenix WinNonlin/NLME, Kinetica, GastroPlus, SimCyp, and NONMEM are commonly utilised. Other cost-effective PK data analysis software are available, including Microsoft Excel, ADAPT, and SAAM II, which are open-source and frequently used for pharmacokinetic data analysis. Software like MATLAB, S-Plus, SAS, and R, which are widely used in science and engineering, are increasingly being employed in pharmacokinetic modelling and simulations.

These pharmacokinetic data analysis programmes make painstaking computations easier and provide quick answers to complex pharmacokinetic equations. Additionally, pharmacokinetic data analysis software can be used for experimental study designs, statistical data analysis, data manipulation, graphical data display, pharmacokinetic model simulation, and drug ADME and drug effect prediction. As a result, pharmacokinetic data analysis software has aided in the better understanding of drug ADME during drug research and development, as well as drug use in clinical settings.

Toxicokinetic modeling

The transport of a foreign substance through the body is mathematically described by pharmacokinetic and toxicokinetic models. These models define the kinetic characteristics that govern a chemical's absorption, distribution, metabolism, and excretion from the body. Pharmacokinetic models that are compartmental and physiologically based can help anticipate a variety of characteristics related to a chemical's toxicity. The following are some of these elements: (1) determining the dose–response relationship of a chemical; (2) predicting xenobiotic concentrations in organs/tissues; (3) assisting in the selection of an animal species to act as a proxy for human toxicity; and (4) determining whether an overdose intervention is necessary.