Metabolism: Investigating and predicting how biology changes molecules and their properties

Robert C Glen

Unilever Centre for Molecular Science Informatics Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW, United Kingdom.

Most molecules are transformed and transported by specific metabolising enzymes and transporters resulting in changes in their bioactivities, pharmacokinetics and toxicity profiles. This is a key consideration in the design of drugs. Ideally, when medicines have performed their task; they need to fade away gracefully, and not introduce unexpected or untoward biological effects. Some examples of predictive metabolism, transport and interesting design considerations of drugs are described.