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Molecular modelling of ligands, receptors and enzymes for in silico drug discovery

Tuesday, 5 December 2017 11:00 (30 minutes)

Over the past two decades, computational or in silico methods have been increasingly applied to the process of drug development and testing. These methods include the use of quantitative structure-activity relationships, database searching, pharmacophores, homology models and other molecular modeling approaches. With the advent of cheminformatics techniques in drug design, molecules with promising efficacy can be developed in a comparatively short time span. Public chemical databases can be screened and the compounds predicted for behaviour as inhibitors or activators. The highly sophisticated pharmacoinformatics tools available can assist in the generation of even subatomic descriptors that provide high predictivity for activity.

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