

Chawla / Singh / Dua

Computational Drug Delivery

Molecular Simulation for Pharmaceutical Formulation

The book bridges the gap between pharmaceuticals and molecular modelling at the micro, meso and macro scale. It covers Lipinski's rule of five, nanoparticulate drug delivery, computational prediction of drug solubility and ability to cross blood brain barrier, computer-based simulation of pharmacokinetic parameters, virtual screening of mucoadhesive polymers, QSPR modelling, designing of 2D nanomaterials and role of principal component analysis.

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