

Computational Pharmaceutics Application Of Molecular Modeling In Drug Delivery Advances In Pharmaceutical Technology

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Computational methods that are already successfully used to calculate solubility include classical molecular simulation for solvation free energies , , while partition coefficient calculations (log P) are used to predict solubility ratios or to provide a molecular understanding of the compound compartmentalization after solubilization .

Molecular simulation as a computational pharmaceutics tool ...

Ke, Peng, Qi, Sheng, Sadowski, Gabriele and Ouyang, Defang (2015) Computational Pharmaceutics: Application of Molecular Modeling in Drug Delivery:Solid dispersion - a pragmatic method to improve the bioavailability of poorly soluble drugs. Wiley. ISBN 978-1-118-57399-0 Full text not available from this repository. (Request a copy)

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Predicting the effects of molecular motions on NMR by MD ...

Bunker, A. (2015). "Molecular modeling as a tool to understand the role of Poly(Ethylene) glycol in drug delivery." in Computational pharmaceutics: Applications of Molecular modelling in Drug Delivery, eds D. Ouyang and S. C. Smith (Hoboken, NJ: John Wiley & Sons), 217:234. doi: 10.1002/9781118573983.ch11. CrossRef Full Text | Google Scholar

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