

Computational drug design : a guide for computational and medicinal chemists / David C. Young

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Abstrak

There are books that talk about drug design tools, algorithms, and mathematical functions, and books that give some results showing that one compound worked better than another for inhibiting a particular enzyme. However, these books spend surprisingly little time discussing the process that the chemist goes through to actually design a new drug molecule. This book is oriented around the way that computational techniques are utilized in the drug design process.