

Computational drug design : a guide for computational and medicinal chemists

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Abstrak

Helps you choose the right computational tools and techniques to meet your drug design goals. Computational Drug Design covers all of the major computational drug design techniques in use today, focusing on the process that pharmaceutical chemists employ to design a new drug molecule. The discussions of which computational tools to use and when and how to use them are all based on typical pharmaceutical industry drug design processes. Following an introduction, the book is divided into three parts: Part One, The Drug Design Process, sets forth a variety of design processes suitable for a.