Quantum medicinal chemistry / edited by Paolo Carloni and Frank Alber

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Abstrak

Computational methods are transforming the work of chemical and pharmaceutical laboratories. Increasingly faster and more exact simulation algorithms have made quantum chemistry a valuable tool in the search for active substances.
Written by a team of leading international quantum chemists, this book is aimed at both beginners as well as experienced users of quantum chemical methods. All commonly used quantum chemical methods are treated here, including Density Functional Theory, quantum and molecular mechanical approaches. Numerous examples illustrate the use of these methods for dealing with problems in pharmaceutical practice, whether the study of inhibitor binding, identifying the surface load of active substances or deriving molecular descriptors using quantum chemical tools.