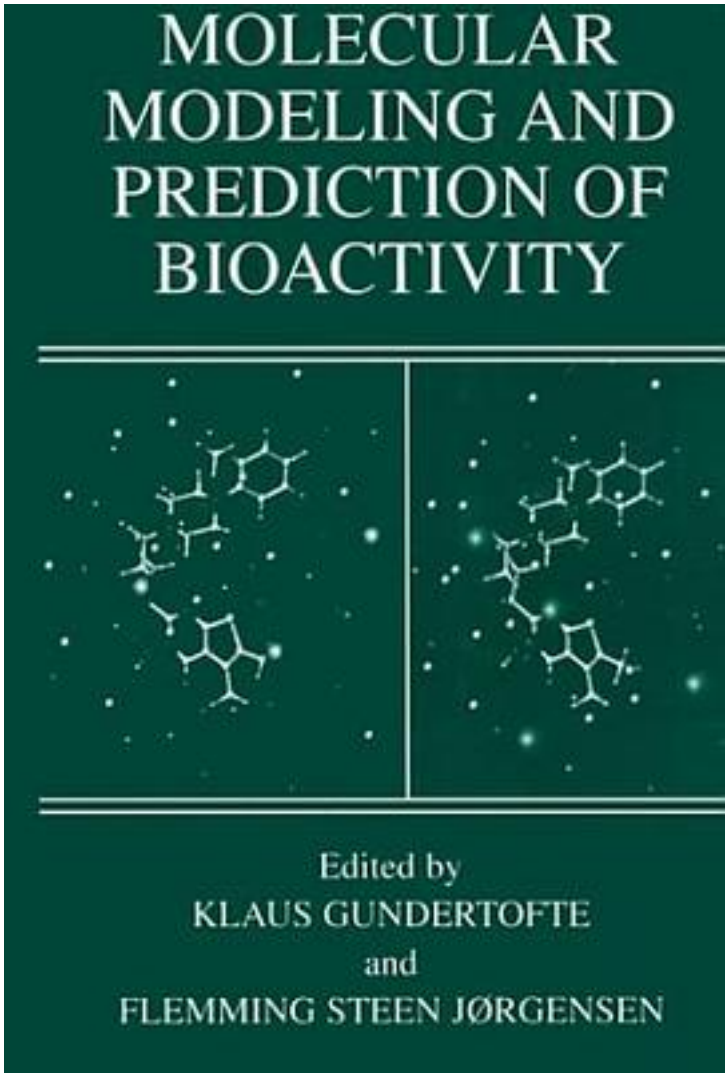
Molecular Modeling and Prediction of Bioactivity



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The book covers highly important topics in the challenging process from lead finding to drug candidates. Focus is upon the potential usefulness of methods for design of lead discovery libraries, lead optimisation, computational chemistry methods for the calculation of energetics of protein-ligand interaction, and computer simulations of biological activities. Important topics include new developments in chemometrics and rational molecular design as well as different aspects of structure representation, knowledge-based approaches to structure identification, and information handling.

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