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Sommario/riassunto

The Reviews in Computational Chemistry series brings together leading authorities in the field to teach the newcomer and update the expert on topics centered around molecular modeling, such as computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics in Volume 28 include: Free-energy Calculations with Metadynamics Polarizable Force Fields for Biomolecular Modeling Modeling Protei