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Computational Molecular Modelling in Structural Biology

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Molecular Modeling methods have received a fast growth over the last years due to the developments in CPU speed, the development of GPUs, the growth in High Performance Computing capabilities and new computational algorithms and theories. The present volume of Advances in Protein Chemistry and Structural Biology is focused on some of the recent applications of computational modeling methods in the area of structural biology. Contributions from leading researchers in the field were selected to provide good balance between the development of the computational methods and their implementations in the areas of structural biology, drug design and enzymology.

Cover image: The figure highlights the multidisciplinary nature and interrelated topics around QSAR, KDD-OECD and summarizes a predictive model of LD50 toxicity values of benzimidazole pesticides (top right), internal validation (bottom left graph), external validation (bottom right), an equation of the model (bottom).

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