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Journal of Molecular Graphics and Modelling 24 (2006) 413
Journal of Molecular Graphics and Modelling
www.elsevier.com/locate/JMGM

Preface

Understanding protein–ligand interactions

This special issue of the *Journal of Molecular Graphics and Modeling* is derived from a symposium titled *Understanding Protein–Ligand Interactions* held at the spring 2005 National ACS Meeting in San Diego, CA. I would like to acknowledge my conference co-organizer, Professor Kenneth M. Merz of the University of Florida, for his assistance in putting that program together. Modeling the interactions of small molecule ligands with their protein targets is perhaps the most fundamental goal of computational chemistry as applied to drug discovery. This special issue is a broad sampling of approaches for understanding and modeling protein–ligand binding. Some of the topics explored in this issue include: building and using structural databases for analysis of protein–ligand binding, applying MD simulations to study the dynamic properties of enzyme active sites, empirical and (at the other extreme) quantum mechanical methods for modeling interaction energies, and finally modeling ligand binding in important drug discovery targets. I would like to thank Andy Holder, Egbert Wezenbeek, Mary Liddy, and the production staff at Elsevier for their assistance in assembling this special issue. Most of all, I thank the authors for their contributions to the symposium and this collection.

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Available online 5 December 2005

doi:10.1016/j.jmgm.2005.11.001