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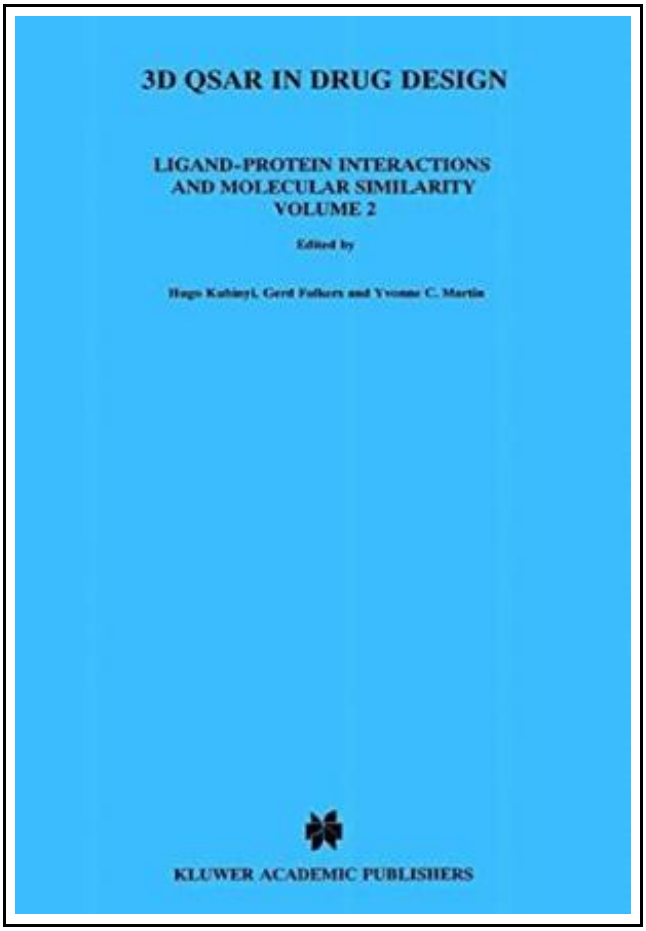

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Book Condition: New. Publisher/Verlag: Springer Netherlands | Volume 2: Ligand-Protein Interactions and Molecular Similarity | Significant progress has been made in the study of three-dimensional quantitative structure-activity relationships (3D QSAR) since the first publication by Richard Cramer in 1988 and the first volume in the series. 3D QSAR in Drug Design. Theory, Methods and Applications, published in 1993. The aim of that early book was to contribute to the understanding and the further application of CoMFA and related approaches and to facilitate the appropriate use of these methods. Since then, hundreds of papers have appeared using the quickly developing techniques of both 3D QSAR and computational sciences to study a broad variety of biological problems. Again the editor(s) felt that the time had come to solicit reviews on published and new viewpoints to document the state of the art of 3D QSAR in its broadest definition and to provide visions of where new techniques will emerge or new appli- tions may be found. The intention is not only to highlight new ideas but also to show the shortcomings, inaccuracies, and abuses of the methods. We hope this book will enable others to separate trivial from visionary approaches and me-too methodology from in- vative techniques. These concerns guided our choice of contributors. To our delight, our call for papers elicited a great many manuscripts. | Volume 2: Section 1: Ligand-Protein Interactions. Progress in Force Field Calculations of Molecular Interaction Fields and Intermolecular Interactions; T. Liljefors. Comparative Binding Energy Analysis; R.C. Wade, et al. Receptor-Based Prediction of Binding Affinities; T.I. Oprea, G.R. Marshall. A Priori Prediction of Ligand Affinity by Energy Minimization; M.K. Holloway. Rapid Estimation of Relative Binding Affinities of Enzyme Inhibitors; M.R. Reddy, et al. Binding Affinities and Non-Bonded Interaction Energies; R.M.A. Knegtel, P.D.J. Grootenhuis. Molecular Mechanics Calculations on Protein-Ligand...

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