
Preface

Fragment-based methods for drug discovery have been investigated in one form or another for several decades, but there has been increased interest in the last 10 years in their practical application in drug discovery. This is partly due to some of the recent successes of the field and their contribution to drug discovery, as well as an expansion in the number and availability of methods and improved computational resources. This volume will cover the techniques necessary for a successful fragment-based drug design project, beginning from defining the problem in terms of preparing the protein model, identifying potential binding sites, and the consideration of various candidate fragments for simulation. The second part of this volume discusses the technical aspects that various methods have used to simulate fragment binding to a target protein using Monte Carlo, molecular dynamics, and docking algorithms. After simulations, fragments are assembled into molecules using a variety of approaches, which are explored next. A discussion of design strategies and consideration of drug-like properties is included as part of the design process at this stage. Finally, several examples of successful fragment-based drug design projects are presented.

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