

---

# Contents

<i>Preface</i> . . . . .	<i>v</i>
<i>Contributors</i> . . . . .	<i>ix</i>
PART I PREPARATION	
1 Solvation Methods for Protein–Ligand Docking . . . . . <i>Rachelle J. Bienstock</i>	3
2 Binding Site Druggability Assessment in Fragment-Based Drug Design. . . . . <i>Yu Zhou and Niu Huang</i>	13
3 Generating “Fragment-Based Virtual Library” Using Pocket Similarity Search of Ligand–Receptor Complexes . . . . . <i>Raed S. Khashan</i>	23
4 Virtual Fragment Preparation for Computational Fragment-Based Drug Design. . . . . <i>Jennifer L. Ludington</i>	31
5 Fragment Library Design: Using Cheminformatics and Expert Chemists to Fill Gaps in Existing Fragment Libraries . . . . . <i>Peter S. Kutchukian, Sung-Sau So, Christian Fischer, and Chris L. Waller</i>	43
PART II SIMULATION	
6 Protocol for Fragment Hopping . . . . . <i>Kevin B. Teuscher and Haitao Ji</i>	57
7 Site Identification by Ligand Competitive Saturation (SILCS) Simulations for Fragment-Based Drug Design. . . . . <i>Christina E. Faller, E. Prabhu Raman, Alexander D. MacKerell, Jr., and Olgun Guvench</i>	75
8 A Computational Fragment-Based De Novo Design Protocol Guided by Ligand Efficiency Indices (LEI) . . . . . <i>Álvaro Cortés-Cabrera, Federico Gago, and Antonio Morreale</i>	89
9 Scoring Functions for Fragment-Based Drug Discovery. . . . . <i>Jui-Chih Wang and Jung-Hsin Lin</i>	101
PART III DESIGN	
10 Computational Methods for Fragment-Based Ligand Design: Growing and Linking . . . . . <i>Rachelle J. Bienstock</i>	119
11 Design Strategies for Computational Fragment-Based Drug Design . . . . . <i>Zenon D. Konteatis</i>	137

12	Protein Binding Site Analysis for Drug Discovery Using a Computational Fragment-Based Method. . . . .	145
	<i>Jennifer L. Ludington</i>	
PART IV CASE STUDIES		
13	Fragment-Based Design of Kinase Inhibitors: A Practical Guide. . . . .	157
	<i>Jon A. Erickson</i>	
14	Designing a Small Molecule Erythropoietin Mimetic. . . . .	185
	<i>Frank Guarnieri</i>	
15	Designing an Orally Available Nontoxic p38 Inhibitor with a Fragment-Based Strategy. . . . .	211
	<i>Frank Guarnieri</i>	
	<i>Index. . . . .</i>	227



<http://www.springer.com/978-1-4939-2485-1>

Fragment-Based Methods in Drug Discovery

Klon, A.E. (Ed.)

2015, IX, 230 p. 68 illus., 53 illus. in color., Hardcover

ISBN: 978-1-4939-2485-1

A product of Humana Press