

CONTENTS

1.	Database Searching: Past, Present, and Future	1
	Techniques	
2.	Crystallographic Databases and Their Use for Studying Intermolecular Interactions	19
3.	Automated Three-Dimensional Structure Generation	47
4.	The Principles and Practice of Three-Dimensional Database Searching	73
5.	Integration of Molecular Modeling and Database Searching	97
	Applications	
6.	Pharmacophore Mapping	121
7.	Structure Generation for De Novo Design	149
8.	Docking: Predicting the Structure and Binding Affinity of Ligand-Receptor Complexes	175
9.	Calculation of Three-Dimensional Similarity	199
10.	3D-QSAR Methods	219
11.	Summary and Future Developments	253
	Index	261