

Contents

Introduction to Fragment-Based Drug Discovery	1
Daniel A. Erlanson	
Fragment Screening Using X-Ray Crystallography	33
Thomas G. Davies and Ian J. Tickle	
Hsp90 Inhibitors and Drugs from Fragment and Virtual Screening	61
Stephen Roughley, Lisa Wright, Paul Brough, Andrew Massey, and Roderick E. Hubbard	
Combining NMR and X-ray Crystallography in Fragment-Based Drug Discovery: Discovery of Highly Potent and Selective BACE-1 Inhibitors	83
Daniel F. Wyss, Yu-Sen Wang, Hugh L. Eaton, Corey Strickland, Johannes H. Voigt, Zhaoning Zhu, and Andrew W. Stamford	
Combining Biophysical Screening and X-Ray Crystallography for Fragment-Based Drug Discovery	115
Michael Hennig, Armin Ruf, and Walter Huber	
Targeting Protein–Protein Interactions and Fragment-Based Drug Discovery	145
Eugene Valkov, Tim Sharpe, May Marsh, Sandra Greive, and Marko Hyvönen	
Fragment Screening and HIV Therapeutics	181
Joseph D. Bauman, Disha Patel, and Eddy Arnold	
Fragment-Based Approaches and Computer-Aided Drug Discovery	201
Didier Rognan	
Index	223