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Nota di contenuto	Fragment-based Drug Discovery: Lessons and Outlook; Contents; Contributors; Preface; A Personal Foreword; Part I: The Concept of Fragment-based Drug Discovery; 1. The Role of Fragment-based Discovery in Lead Finding; 1.1 Introduction; 1.2 What is FBLD?; 1.3 FBLD: Current Practice; 1.3.1 Using Fragments: Conventional Targets; 1.3.2 Using Fragments: Unconventional Targets; 1.4 What do Fragments Bring to Lead Discovery?; 1.5 How did We Get Here?; 1.5.1 Evolution of the Early Ideas and History; 1.5.2 What has Changed Since the First Book was Published in 2006? 1.6 Evolution of the Methods and Their Application Since 2005 1.6.1 Developments in Fragment Libraries; 1.6.2 Fragment Hit Rate and Druggability; 1.6.3 Developments in Fragment Screening; 1.6.4 Ways of Evolving Fragments; 1.6.5 Integrating Fragments Alongside Other Lead-Finding Strategies; 1.6.6 Fragments Can be Selective; 1.6.7 Fragment Binding Modes; 1.6.8 Fragments, Chemical Space, and

Novelty; 1.7 Current Application and Impact; 1.8 Future Opportunities; References; 2. Selecting the Right Targets for Fragment-Based Drug Discovery; 2.1 Introduction
2.2 Properties of Targets and Binding Sites 2.3 Assessing Druggability; 2.4 Properties of Ligands and Drugs; 2.5 Case Studies; 2.5.1 Case Study 1: Inhibitors of Apoptosis Proteins (IAPs); 2.5.2 Case Study 2: HCV-NS3; 2.5.3 Case Study 3: PKM2; 2.5.4 Case Study 4: Soluble Adenylate Cyclase; 2.6 Conclusions; References; 3. Enumeration of Chemical Fragment Space; 3.1 Introduction; 3.2 The Enumeration of Chemical Space; 3.2.1 Counting and Sampling Approaches; 3.2.2 Enumeration of the Chemical Universe Database GDB; 3.2.3 GDB Contents; 3.3 Using and Understanding GDB; 3.3.1 Drug Discovery
3.3.2 The MQN System 3.3.3 Other Fingerprints; 3.4 Fragments from GDB; 3.4.1 Fragment Replacement; 3.4.2 Shape Diversity of GDB Fragments; 3.4.3 Aromatic Fragments from GDB; 3.5 Conclusions and Outlook; Acknowledgment; References; 4. Ligand Efficiency Metrics and their Use in Fragment Optimizations; 4.1 Introduction; 4.2 Ligand Efficiency; 4.3 Binding Thermodynamics and Efficiency Indices; 4.4 Enthalpic Efficiency Indices; 4.5 Lipophilic Efficiency Indices; 4.6 Application of Efficiency Indices in Fragment-Based Drug Discovery Programs; 4.7 Conclusions; References
Part II: Methods and Approaches for Fragment-based Drug Discovery 5. Strategies for Fragment Library Design; 5.1 Introduction; 5.2 Aims; 5.3 Progress; 5.3.1 BDDP Fragment Library Design: Maximizing Diversity; 5.3.2 Assessing Three-Dimensionality; 5.3.3 3DFrag Consortium; 5.3.4 Commercial Fragment Space Analysis; 5.3.5 BDDP Fragment Library Design; 5.3.6 Fragment Complexity; 5.3.6.1 Diversity-Oriented Synthesis-Derived Fragment-Like Molecules; 5.4 Future Plans; 5.5 Summary; 5.6 Key Achievements; References
6. The Synthesis of Biophysical Methods In Support of Robust Fragment-Based Lead Discovery
