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Autore	Lee Wen Ho
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Nota di contenuto	Contents; A Personal Introduction; Chapter 1 Small Molecules for Chemogenomics-based Drug Discovery Edgar Jacoby, Ansgar Schuffenhauer, Kamal Azzaoui, Maxim Popov, Sigmar Dressler, Meir Glick, Jeremy Jenkins, John Davies and Silvio Roggo; 1. Introduction; 2. Compound Categories; 2.1. Natural products and derivatives; 2.2. Primary metabolites, co-substrates, co-factors, and marketed drugs; 2.3. Peptides and peptido-mimetics; 2.4. Diversity oriented synthesis molecules; 3. Designing Comprehensive Chemogenomics Screening Compound Collections 4. Essential Properties and Selection Processes along the Discovery Pipeline5. Molecular Information Systems and Annotated Compound Libraries; 6. Conclusion; Acknowledgements; References; Chapter 2 Mapping the Chemogenomic Space Jordi Mestres; 1. The Chemogenomic Space; 2. Annotation and Classification Schemes for Proteins; 2.1. Enzymes; 2.2. Receptors; 2.2.1. Channel receptors; 2.2.2. G Protein-coupled receptors; 2.2.3. Nuclear receptors; 3. Structural

Representativity of Protein Families; 4. Annotation and Classification Schemes for Molecules; 5. Mapping the Molecule-Protein Space
6. Exploiting the Chemogenomic Space 7. Conclusions; References; Chapter 3 Natural Product Scaffolds and Protein Structure Similarity Clustering (PSSC) as Inspiration Sources for Compound Library Design in Chemogenomics and Drug Development Frank J. Dekker, Stefan Wetzel and Herbert Waldmann; 1. Introduction; 2. Biological Relevance in Compound Library Design; 2.1. Compound libraries as sources for small molecule modulators of protein function; 2.2. Annotated libraries; 2.3. Natural products as inspiration sources for library design; 2.4. Library design based on privileged structures
3. Natural Product Inspired Compound Library Synthesis 4. Target Clustering as Strategy in Drug Discovery; 4.1. Target clustering; 4.2. Target clustering based on structural and functional similarity; 5. PSSC as Guiding Principle for Compound Library Design; 5.1. Protein structure similarity clustering (PSSC); 5.2. PSSC based reanalysis of the development of leukotriene A4 hydrolase inhibitors; 5.3. PSSC based reanalysis of the development of nuclear hormone receptor ligands
5.4. Application of PSSC for de novo ligand development for the protein cluster Cdc25A phosphataseacetylcholinesterase-11-hydroxysteroid dehydrogenase5.5. Position of the PSSC concept in drug development and chemogenomics; 6. Conclusions; Acknowledgments; References; Chapter 4 A Reductionist Approach to Chemogenomics in the Design of Drug Molecules and Focused Libraries Roger Crossley and Martin Slater; 1. Introduction; 2. Molecular Recognition and Vicinity AnalysisTM; 3. Thematic AnalysisTM; Examples of Themes; 4. Family B and C GPCRs; 5. Classification of GPCRs; 6. Pharmacophore Maps
7. Library Design Using Thematic AnalysisTM

Sommario/riassunto

Devoted to the subject of shape charge design using numerical methods, this book offers the defense and commercial industries unique material not contained in any other single volume. The coverage of the Lagrangian and Eulerian methods as well as the equation of state provides first hand help to engineers working on shape charge problems.The book includes detailed descriptions of oil-well perforation not available from any other sources and, coupled with the material flow physics discussed in Chapters 2 and 3 and Appendix B, readers can design the fuel rod configurations for a nuclear reactor