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Nota di contenuto	Pharmacophores and Pharmacophore Searches; Contents; Preface; A Personal Foreword; List of Contributors; Part I Introduction; 1 Pharmacophores: Historical Perspective and Viewpoint from a Medicinal Chemist; 1.1 Definitions; 1.1.1 Functional Groups Considered as Pharmacophores: the Privileged Structure Concept; 1.2 Historical Perspective; 1.2.1 Early Considerations About Structure-Activity Relationships; 1.2.2 Early Considerations About the Concept of Receptors; 1.2.3 Ehrlich's "Magic Bullet"; 1.2.4 Fischer's "Lock and Key"; 1.3 Pharmacophores: the Viewpoint of a Medicinal Chemist 1.3.1 Two-dimensional Pharmacophores1.3.1.1 Sulfonamides and PABA; 1.3.1.2 Estrogens; 1.3.2 An Early Three-dimensional Approach: the Three-point Contact Model; 1.3.2.1 Clonidine and Its Interaction with the -Adrenergic Receptor; 1.3.3 Criteria for a Satisfactory Pharmacophore Model [32]; 1.3.4 Combination of Pharmacophores; 1.4 Conclusion; References; Part II Pharmacophore Approaches; 2 Pharmacophore Model Generation Software Tools; 2.1 Introduction; 2.2

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Sommario/riassunto

This handbook is the first to address the practical aspects of this novel method. It provides a complete overview of the field and progresses from general considerations to real life scenarios in drug discovery research. Starting with an introductory historical overview, the authors move on to discuss ligand-based approaches, including 3D pharmacophores and 4D QSAR, as well as the concept and application of pseudoreceptors. The next section on structure-based approaches includes pharmcophores from ligand-protein complexes, FLIP and 3D protein-ligand binding interactions. The whole is rounded