

Pharmacophores and pharmacophore searches

Deskripsi Lengkap: <https://lib.ui.ac.id/detail?id=20395917&lokasi=lokal>

Abstrak

This handbook is 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 pharmacophores from ligand-protein complexes, FLIP and 3D protein-ligand binding interactions. The whole is rounded off with a complete section devoted to applications and examples, including modeling of ADME properties.