



Designing Bioactive Molecules: Three-Dimensional Techniques and Applications (Computer Applications in Chemistry Collection)

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Three-dimensional structural information often provides the key to discovering or designing bioactive molecules and compounds. This volume covers the principal computational techniques for processing three-dimensional structures of small molecules and compounds. It describes database construction and searching, analysis of structure-activity relationships by pharmacophore mapping and QSAR, prediction of biological potency of small molecules and compounds by QSAR and by docking to macromolecular targets. The book also includes a chapter on *de novo* design of ligands to fit a macromolecular target.

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