The study of drugs binding to specific receptor sites is nowaday one of the most promising fields in structure-properties relationships. Two different facts, the unknown nature of receptors and the ascertained stereospecificity of drug-receptor interactions, concur to focus our attention on the molecular structure of drugs as the only way for obtaining valuable information on the geometry of the receptor itself.

Unfortunately this simple idea often fails owing to the extraordinary complexity of the mechanisms of action of biological systems. Future developments will depend on the following factors: 1. The formulation of a wider concept of 'structure', including stereochemical as well electronic and lipophilic aspects; 2. A better understanding of non-bonded forces responsible for the drug-receptor interaction; 3. A more precise definition of molecular 'properties' in biological systems by complementing the pharmacological profile with 'in vitro' binding studies and 'in vivo' pharmacokinetics data.

Examples will be taken from drugs exerting their action on the GABA/benzodiazepine/barbiturate receptor chloride channel complex which is postsynaptically localized in the inhibitory GABAergic synapses of the central nervous system. In particular the new classes of compounds chemically unrelated to benzodiazepines but binding to their receptor will be discussed. Rather surprisingly they display a spectrum of pharmacological properties ranging from full benzodiazepine-like properties (agonists) to opposite ones (inverse agonists) through pure binding to the receptor without any 'per se' effect (antagonists). These compounds seem to propose a well-defined stereochemical problem as agonists, antagonists and inverse agonists must possess a common chemical moiety responsible for the binding to the same receptor site while agonists and inverse agonists should have additional and different stereochemical features able to trigger opposite pharmacological effects.