



Quantum Pharmacology

W. G. Richards

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Quantum Pharmacology, Second Edition discusses molecular pharmacology, molecular quantum mechanics, and the applications of theory to experiment. The book reviews molecular and quantitative pharmacology, as well as acetylcholines, catecholamines, and histamines. The text also discusses the central nervous system in relation to monoamines, acetylcholines, amino acids, and peptides. The book explains wave functions and orbitals, secular equations, matrix elements, and self-consistent molecular orbitals. One way to improve wave functions as a result of a self-consistent field or as an approximate calculation, is to permit different configurations to interact. Linear mixing will lead to improved wave functions. The investigator can compute wave functions and energies of molecules for any set of nuclear coordinates. Quantum chemical calculations treat conformation as similar with geometry; calculations are performed for a series of positions in one part of a molecule relative to another. The investigator can then compare the energies found in each position. The book points out that calculations of conformational internal energy surfaces for flexible pharmacological molecules treating the molecule or ion as isolated in space fit in with observed results of crystallographic experiments. The text is suitable for pharmacologists, and scientists involved in molecular pharmacology, medicinal chemistry, and quantum chemistry.

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