Molecular Orbital Studies in Chemical Pharmacology. Edited by LEMONT B. KIER. Springer-Verlag, New York, NY 10010, 1970. v + 290 pp. 18 × 26 cm. Price $9.40.

This volume is a collection of eleven contributions presented at a Battelle Seattle Research Center symposium dealing with applications of the molecular orbital approaches of quantum chemistry to studies in chemical pharmacology.

In an introductory lecture, B. Pullman outlines the history of the calculations on the electronic structure of the purine and pyrimidine bases making up the nucleic acids. The impact of the development of techniques of calculation on the nature and significance of the results is discussed by the analysis of the results for four representative problems concerning the properties of these bases: electronic charge distribution, molecular ionization potential, hydrogen-bonding and stacking intermolecular interactions, and purine tautomerism as a possible mechanism for mutations.

In the next lecture, J. R. Hoyland presents a valuable critical analysis of the nature, merits, and demerits of the most common "all valence-electrons" molecular orbital approaches. The "extended" and "iterative extended" Hückel methods, the non-empirical approaches (NEMO methods), the semi-empirical approaches in which atomic orbital differential overlap is neglected (CNDO, INDO, and MINDO methods), are discussed in detail. Deeply analyzed is the probable correctness which can be expected from each of these methods when applied to problems on molecular geometries, relative conformational energies, charge distribution, ionization potentials, hydrogen-bond strengths, heats of dimer formation, and reaction rates.

Three of the subsequent contributions are concerned with problems involving the calculations of the energy of molecular systems. R. Rein and his coworkers discuss the feasibility of a direct physical interaction between an amino acid and a nucleotide base as a primitive transcription mechanism in the recognition process required by the genetic code. This is done by calculating the total interaction energies between glycine and the nucleotide bases guanine, cytosine, adenine, and uracil. Rein's group, in a second contribution, considers the mechanism of thymine photodimerization to gain insight into the possible dimerization modes in DNA. Calculations are made for all the interaction energies as two ground state thymine molecules approach to within bonding distances, and these energies are compared to the interaction energies obtained when one of the thymine molecules is in an excited state. L. B. Kier and J. M. George present a study of the energetically preferred conformations of nine amino acid residues. This is done with the hope that the proper assemblage of the conformationally preferred residues may result in a structure which has some significance in relation to polypeptide conformation. Bradykinin structure is specifically approached in this way.

The other six contributions are more closely related to specific pharmacological problems. They are entitled:

- The Correlation of Electronic Structures of Indole Derivatives With Their Biological Activities, by J. P. Green and S. Kang.
- The Application of Hückel and Extended Hückel Molecular Orbital Calculations to Biochemical Problems, by W. B. Neely.
- Quantitative Structure-Activity Relationships and Molecular Orbitals in Medicinal Chemistry, by W. P. Purcell and J. M. Clayton
- Quantum Perturbation Theory and Linear Free-Energy Relationships in the Study of Drug Action, by A. Cammarata.
- Psychedelic Drug Activity: Electronic, Steric and Biochemical Correlates, by S. M. Snyder, and
- Molecular Orbital Theory and Pharmacologic Receptor Theory as Integrated Experimental Tools (which is a study of the mechanism of action of antihypertensive agents), by A. J. Wohl.

Apart from some conformational considerations, these contributions make use of the molecular orbital approaches to calculate a variety of quantum chemical electronic indexes. These are subsequently applied to gain correlations between drug activities (measured at different levels of biological complexity) and the calculated electronic index, used individually or in equations which may be subjected to multiple regression analyses. In several cases the electronic indexes are combined with free-energy related physicochemical parameters. The utilization of these empirically derived regression equations to gain insight into pharmacological problems (structure–activity relationships, rational drug design, submolecular mechanism of drug action and drug–receptor interaction) are discussed. Since, if it is not an established consequence of physical laws, it is incorrect to imply causality from a correlation, however high the correlation may be, discussions are also begun regarding the possible physical meaning of such correlations.

This book, dedicated to the first symposium dealing with the subject of quantum pharmacology, provides a good appreciation of the present state of knowledge in this difficult field, which is in an early, pioneering stage of development. A useful bibliography is provided for those theoreticians and experimentalists interested in doing more detailed studies in this emerging discipline.

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Chromatographic and Microscopic Analysis of Drugs. Edited by EGON STAHL. Gustav Fischer Verlag, Stuttgart, West Germany, 1970. vii + 195 pp. 17 × 24.5 cm. (*German*)

This book bears the subheading "A useful supplementation for the European Pharmacopoeiae." In the preface, the author refers to the actual task of pharmacognosy, *i.e.*, the identification and evaluation of drugs and their corresponding mixtures and preparations. For many drugs of the pharmacopoeia, the macroscopic and microscopic examination was the only possibility of analytical evaluation. It was only a small number of drugs which got an additional determination of value. The evaluation of chromatography, especially of thin-layer chromatography, enabled an analytical statement by separation and subsequent identification of such mixtures. This statement has reached an importance just as great as the classic microscopy. For this reason, the chromatography of drugs was already integrated into modern pharmacopeias, for example, into the European Pharmacopoeia.

The author succeeded in representing the microscopic and chromatographic features, classified according to their substances into "chromatographic groups," in a precise and valuable form both for lectures and in practice.

The book is divided into 3 sections.

Part A describes in well-arranged and clear form the basis of the methods of thin-layer chromatography according to the procedure TAS, the sensory-physiological examination, and the microscopic analysis of drugs.

Part B describes the microscopic characters, the chromatographic analysis, and, provided that they are integrated into the European Pharmacopoeia, the quantitative determinations of more than 80 drugs. Further drugs of the different groups of active agents are summarized in tables.

In Part C, a list of reagents informs the reader about the various reagents necessary for microscopic and chromatographic analysis.

In this representation of classic and modern methods of drug examinations, the book represents a valuable contribution to the training of pharmacy students and can be recommended highly both to the pharmacist working in the chemist's shop and in industry.

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