MOLECULAR ORBITAL THEORY
IN DRUG RESEARCH
MEDICINAL CHEMISTRY
A Series of Monographs

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In Preparation
JULIUS A. VIDA. Anticonvulsants
To my wife
Martha
and my children
Sarah, Lemont, Jr., Andrew, Peter, Katherine
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It is apparent from a survey of the literature of the past decade that a growing number of scientists are employing theoretical chemistry to probe biological events at the molecular level. The increasing use of molecular orbital theory in medicinal chemistry, chemical pharmacology, and biochemistry directed toward drug studies has made it desirable to incorporate a presentation and review of the subject in one source.

This book evolved from a series of lectures I presented to graduate students in medicinal chemistry at the University of Michigan. It is directed to the advanced undergraduate or graduate student in medicinal chemistry or pharmacology, to the practicing scientist interested in acquiring some understanding of this approach, and to the theoretical chemist seeking information on biological phenomena amenable to semiempirical molecular orbital study.

The chapters dealing with the applications of molecular orbital theory have been organized on the basis of physical chemical phenomena concluded from the studies described to be involved in the biological activity. Discussion of the chemistry or pharmacology relating to the studies is limited to information pertinent to a background description of the problem and to the validity of the predictions. Major emphasis is placed on the use of molecular orbital theory in each case and the conclusions drawn.

A large number of colleagues have been consulted on many of the topics discussed in the book. Grateful acknowledgment is made to Mr. Gordon Amidon, Dr. Richard Falb, Dr. James Hoyland, Dr. Jackson Lynn, Mr. Victor Marquez, Dr. Brian Myhr, Miss Judith Raisch, Dr. Edward Roche, Mr. Richard Stein, Dr. James Stubbins, and Dr. Edward Truitt. I would also like to gratefully acknowledge the excellent typing done by Mrs. Lucyle Arrowsmith. Finally I want to thank my wife for her patience and understanding.
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