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11. Receptor-Guided Structure-Activity Modeling of Inhibitors of Juvenile Hormone Epoxide Hydrolases12. Structural Studies of Juvenile Hormone Binding Proteins; 13. In Silico Stereoelectronic Profile and Pharmacophore Similarity Analysis of Juvenile Hormone, Juvenile Hormone Mimics (IGRs), and Insect Repellents May Aid Discovery and Design of Novel Arthropod Repellents; 14. Use of Multicriteria Analysis for Selecting Candidate Insecticides for Vector Control

Sommario/riassunto

Juvenile hormones play a key role in the control of larval development and metamorphosis of insects as well as the various aspects of the reproduction of adults. The book presents modeling approaches that can be used to study the mechanism of action of juvenile hormones (JHs) in insects and to estimate the adverse effects and the environmental fate of the manmade chemicals that mimic the actions of JHs. The text aims to provide a deeper understanding of the juvenile hormones mechanism of action, which may help to control the population of insects. Leading contributors address various topics that underscore the important role of natural compounds in the discovery and development of new human medicines--
Series Introduction The correlation between the toxicity of molecules and their physicochemical properties can be traced to the nineteenth century. Indeed, in a French thesis entitled Action de l'alcool amylique sur l'organisme (Action of amyl alcohol on the body), which was presented by A. Cros before the Faculty of Medicine at the University of Strasbourg in 1863, an empirical relationship was made between the toxicity of alcohols, their number of carbon atoms, as well as their solubility. In 1875, Dujardin-Beaumetz and Audigier the first to stress the mathematical character of the relationship between the toxicity of alcohols and their chain length and molecular weight. In 1899, Hans Horst Meyer and Fritz Baum, at the University of Marburg, showed that narcosis or hypnotic activity was in fact linked to the affinity of substances to water and lipid sites within the organism. At the same time at the University of Zurich, Ernest Overton came to the same conclusion providing the foundation of the lipoid theory of narcosis. The next important step was made in the 1930s by Lazarev in St. Petersburg, who first demonstrated that different physiological and toxicological effects of molecules were correlated with their oil- water partition coefficient through formal mathematical equations in the following form: log C = a logPoil/water + b. Thus, the quantitative structure-activity relationship (QSAR) discipline was born. Its foundations were definitively fixed in the early 1960s by the seminal works contributed by C. Hansch and T. Fujita--