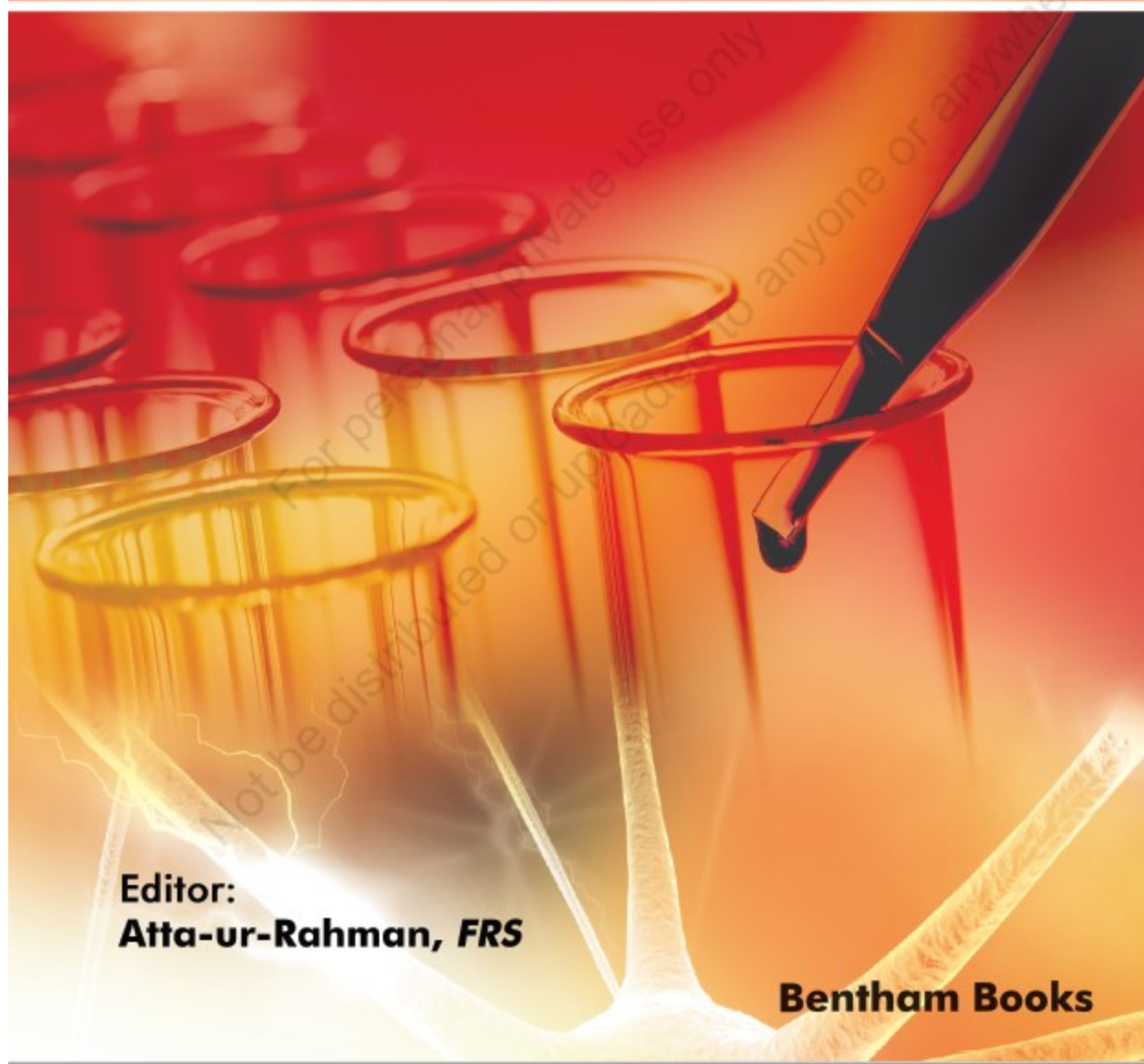


Frontiers in Clinical Drug Research  
**Anti Allergy Agents**

Editor:  
**Atta-ur-Rahman, FRS**

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**Frontiers in Clinical Drug  
Research – Anti Allergy Agents**

*(Volume 4)*

**Edited by**

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## *In-Silico* Approaches in Drug Discovery and Design of Anti-Allergic Agents

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**Abstract:** The process of drug discovery is a long back episode appearing from the ancient times. The therapeutic applications of plants, mineral were recorded in ancient civilizations like Chinese, Hindus, and European. The development of the new drug from lead/hit molecules is a very expensive event considering money, manpower as well as time. The traditional approach includes the synthesis of compounds in laboratory which is a time-consuming process and their testing in *in-vivo* biological assays. The *in silico* approaches are often known as high throughput screening methods (HTS) virtual screening mainly applied in the early phases of drug discovery. It helps the researchers to go deep into *in silico* simulation prior to wet laboratory experiments. The statistics highlighted that there is a shift from 10% to 20% by the pharmaceutical industries in pharmaceutical R&D on computer modeling and simulations. In late 1990s FDA identified that poor pharmacokinetic parameters (ADME/Tox) were one of the major cause of late stage failure of drug candidates for clinical trials. In the past decade, there was a remarkable growth of computational approach in bridging the chemical and biological process in drug discovery pipeline. The advent of the arena of *in silico* approaches was made possible by the advancement of software and hardware computational ability and a further increase in precision and accuracy. The incidents of allergic diseases like bronchial asthma, allergic rhinoconjunctivitis and atopic dermatitis are increasing. Drugs in this categories act through different targets like inhibitors of histaminic receptors, leukotrienes, thromboxane-A2 inhibitors, mast cell stabilizer. In this context, the chapter tries to give emphasis on different recent targets for antiallergic agents and a brief overview on *in silico* methods as well as computational studies carried out for the targets in accelerating the drug discovery for the antiallergic agents for controlling the above-mentioned disease.

**Keywords:** ADME/T, Antiallergic Agents, HTS, *in Silico*.

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