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# 1 Introduction to Drug Design and Discovery

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## 1.1 MEDICINAL CHEMISTRY: AN INTERDISCIPLINARY SCIENCE

Therapeutic agents are chemical entities that prevent disease, assist in restoring health to the diseased, or alleviate symptoms associated with disease conditions. Medicinal chemistry is the scientific discipline that makes such drugs available either through discovery or design processes. Throughout history, drugs were primarily discovered by empirical methods, investigating substances or preparations of materials, such as plant parts or plant extracts, found in the local environment. Over the previous centuries, chemists developed methods for the isolation and purification of the active principles in medicinal plants. The purification and structure determination of natural products like morphine, hyoscyamine, quinine, and digitalis glycosides represent milestones in the field of drug discovery and the beginning of medicinal chemistry as a fascinating independent field of research (Figure 1.1).

In the twentieth century, a very large number of biologically active natural products were structurally modified in order to optimize their pharmacology and drug properties in general, and novel drugs were prepared by an increasing use of advanced synthetic methods. Moreover, the rapidly growing understanding of the nature of disease mechanisms, how cells function, and how drugs interact with cellular processes has led to the rational design, synthesis, and pharmacological evaluation of new drug candidates. Most recently, new dimensions and opportunities have emerged from a deeper understanding of cell biology, genetics, and biostructures.

Modern medicinal chemistry draws upon many scientific disciplines, with organic chemistry, physical chemistry, and pharmacology being of fundamental importance. But other disciplines such as biochemistry, molecular biology, toxicology, genetics, cell biology, biophysics, physiology, pathology, and computer modeling approaches play important roles. The key research objective of medicinal chemistry is to investigate relationships between chemical structure and biological effects. When the chemical structure of a particular drug candidate has been optimized to interact