# Preface

The use of computers to collect, store, and manipulate chemical information is at the heart of chemoinformatics. The "tools of the trade" in this emerging area, whose main target thus far has been the pharmaceutical field, are general and can be applied to other types of chemical datasets, such as those containing food chemicals. *Foodinformatics: Applications of Chemical Information to Food Chemistry* collects together a number of studies where chemoinformatics tools have been applied in answering questions about food-related compounds. Chapter 1 presents a didactic introduction to the concepts of molecular similarity and chemical spaces, which are cornerstones of chemoinformatics. Chapters 2 and 3 discuss practical applications of chemical space and molecular similarity studies, respectively. Chapters 4 and 5 describe two concepts of current interest, namely, reverse pharmacognosy and epigenetics. While Chap. 4 concerns the discovery of new health-related applications for existing food ingredients, Chap. 5 focuses on the exploration of molecular determinants and the pharmacological role of food and food-derived compounds as modulators of epigenetics and metabolism. Chapters 6, 7, 8 and 9 exemplify the use of molecular and/or statistical models to analyze food-related compound collections for biological activities or organoleptic properties. Finally, Chap. 9 provides a compilation of software resources and databases that have been used or can be used in the food chemistry field; it also presents a perspective of *Foodinformatics*.

While the use of chemical information methodologies to address food-related challenges is still in its infancy, interest is growing and will continue to do so as the methods prove useful, particularly for providing practical solutions to food industry challenges. This book attempts to give an overview of basic concepts, applications, tools, and perspectives.

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