CHEMOINFORMATICS OF NATURAL PRODUCTS VOLUME 1: FUNDAMENTAL CONCEPTS

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Volume 1 of *Chemoinformatics of Natural Products* lays down the fundamental concepts of chemical informatics and is exclusively dedicated to the investigation of natural products (NPs) or secondary metabolites (SMs), the main source of lead compounds for drug discovery.
Several experts in the field, working in different continents and from diverse backgrounds have contributed. The book is divided into four parts; Part I examines the foundational concepts and begins with a description of various structural classes of NPs, their structural diversity, bioactivity, and ecological functions. In Part II, tools and methods for natural product structure elucidation, focusing on mass spectrometry (MS) and nuclear magnetic resonance (NMR) tools are discussed. Part III is dedicated to drug discovery proper, i.e. lead compound discovery and development while Part IV is dedicated to case studies.
This book will help chemists investigate new problems and organize and analyze scientific data in order to develop novel compounds, materials, and processes through the application of information technology.

- Overview of natural products chemistry and computational methods.
- Reviews tools for structure elucidation, drug property prediction, natural product databases, metabolite biosynthesis, etc.
- Contains Glossary of Terms Used in Chemoinformatics of Natural Products

Fidele Ntie-Kang
teaches physical, computational and medicinal chemistry at the University of Buea, Cameroon and in several summer schools. He has been awarded several fellowships and distinctions and has published above 70 journal articles and book chapters, with about 1200 citations.

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CHEMOINFORMATICS OF NATURAL PRODUCTS

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