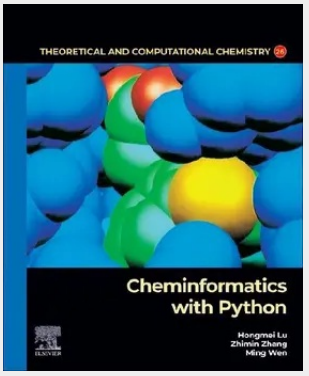
Lu / Wen

# Cheminformatics with Python

Volume 26

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Cheminformatics with Python provides a ground-up, practical introduction that helps reader make effective use of the software. In four parts, including programming, data, methods, and applications, the book provides a brief introduction to Python language and related scientific computing, cheminformatics, machine learning, and deep learning packages and presents a systematic study of the representation of instrumental data, including molecular structures and common chemical databases. The methods section covers analytical signal processing, multivariate calibration, multivariate resolution, classical machine learning, and deep learning methods. Finally, the application section presents case studies of successful applications of cheminformatics in analytical chemistry, metabolomics, drug discovery, and more. A supporting appendix section and the necessary mathematical, statistical, and information theory-related theories are provided, along with practical tips such as code editors and source code management. Online coding materials on GitHub and an individual Jupyter notebook for each chapter further support practical learning. This book will be a great resource for senior undergraduate students, graduate students, post-docs, and professors primarily in the field of computational and analytical chemistry.

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