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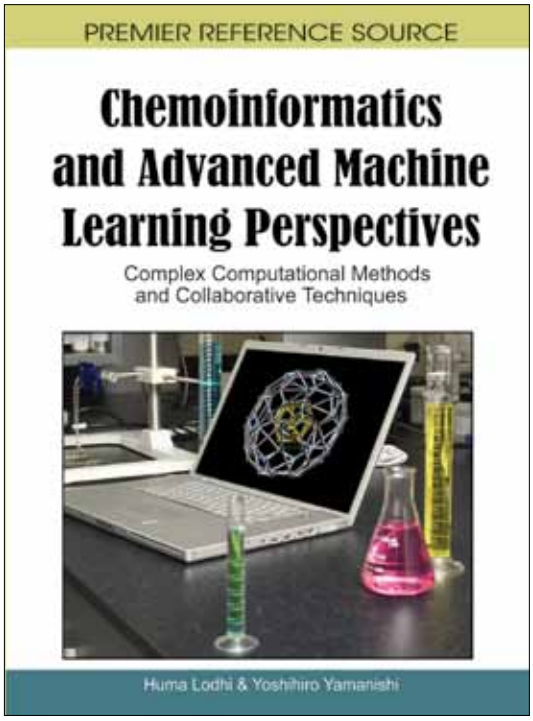
Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques



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Chemoinformatics is a scientific area that endeavours to study and solve complex chemical problems using computational techniques and methods.

Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques provides an overview of current research in machine learning and applications to chemoinformatics tasks. As a timely compendium of research, this book offers perspectives on key elements that are crucial for complex study and investigation.

Topics Covered:

- Graph kernels for chemoinformatics
- Support vector machines
- Similarity fusion for virtual screening
- Graph mining in chemoinformatics
- Advanced PLS techniques in chemometrics
- Nonlinear partial least squares
- Bayesian statistics
- Machine leaning in drug discovery and development
- Compound-protein interactions with machine learning methods
- Chemoinformatics on metabolic pathways

Market: This premier publication is essential for all academic and research library reference collections. It is a crucial tool for academicians, researchers, and practitioners and is ideal for classroom use.

Huma Lodhi obtained her Ph.D. in computer science from University of London. She is a researcher with the department of Computing, Imperial College London. She has published in leading international journals, books, conference proceedings and has edited a volume **Elements of Computational Systems Biology** (Wiley Series in Bioinformatics), (2010) by Huma M Lodhi and Stephen H Muggleton (Editors), Wiley. Her research interests are machine learning and data mining and their application to tasks in bioinformatics, chemoinformatics and computation systems biology.

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