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| Collana                 | Computational Methods in Engineering & the Sciences, , 2662-4877  |
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| Soggetti                | Toxicology<br>Machine learning<br>Artificial intelligence<br>Machine Learning<br>Artificial Intelligence  |
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| Nota di bibliografia    | Includes bibliographical references.  |
| Nota di contenuto       | Machine Learning and Deep Learning Promotes Predictive Toxicology for Risk Assessment of Chemicals -- Multi-Modal Deep Learning Approaches for Molecular Toxicity prediction -- Emerging Machine Learning Techniques in Predicting Adverse Drug Reactions -- Drug Effect Deep Learner Based on Graphical Convolutional Network -- AOP Based Machine Learning for Toxicity Prediction -- Graph Kernel Learning for Predictive Toxicity Models -- Optimize and Strengthen Machine Learning Models Based on in vitro Assays with Mechanistic Knowledge and Real-World Data -- Multitask Learning for Quantitative Structure-Activity Relationships: A Tutorial -- Isalos Predictive Analytics Platform: Cheminformatics, Nanoinformatics and Data Mining Applications -- ED Profiler: Machine Learning Tool for Screening Potential Endocrine Disrupting Chemicals -- Quantitative Target-specific Toxicity Prediction Modeling (QTTPM): Coupling Machine Learning with Dynamic Protein-Ligand Interaction Descriptors (dyPLIDs) to Predict Androgen Receptor-mediated Toxicity -- Mold2 Descriptors |

Facilitate Development of Machine Learning and Deep Learning Models for Predicting Toxicity of Chemicals -- Applicability Domain  
Characterization for Machine Learning QSAR Models -- Controlling for Confounding in Complex Survey Machine Learning Models to Assess Drug Safety and Risk. .

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#### Sommario/riassunto

This book is a collection of machine learning and deep learning algorithms, methods, architectures, and software tools that have been developed and widely applied in predictive toxicology. It compiles a set of recent applications using state-of-the-art machine learning and deep learning techniques in analysis of a variety of toxicological endpoint data. The contents illustrate those machine learning and deep learning algorithms, methods, and software tools and summarise the applications of machine learning and deep learning in predictive toxicology with informative text, figures, and tables that are contributed by the first tier of experts. One of the major features is the case studies of applications of machine learning and deep learning in toxicological research that serve as examples for readers to learn how to apply machine learning and deep learning techniques in predictive toxicology. This book is expected to provide a reference for practical applications of machine learning and deep learning in toxicological research. It is a useful guide for toxicologists, chemists, drug discovery and development researchers, regulatory scientists, government reviewers, and graduate students. The main benefit for the readers is understanding the widely used machine learning and deep learning techniques and gaining practical procedures for applying machine learning and deep learning in predictive toxicology. .

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