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| Titolo                  | Advances in Computational Toxicology : Methodologies and Applications in Regulatory Science // edited by Huixiao Hong  |
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| Descrizione fisica      | 1 online resource (416 pages)  |
| Collana                 | Challenges and Advances in Computational Chemistry and Physics, , 2542-4491 ; ; 30   |
| Disciplina              | 025.066159   |
| Soggetti                | Chemoinformatics<br>Pharmacology<br>Bioinformatics<br>Computational biology<br>Chemistry, Physical and theoretical<br>Bioinformatics<br>Computer Applications in Chemistry<br>Pharmacology/Toxicology<br>Computer Appl. in Life Sciences<br>Theoretical and Computational Chemistry<br>Computational Biology/Bioinformatics  |
| Lingua di pubblicazione | Inglese  |
| Formato                 | Materiale a stampa   |
| Livello bibliografico   | Monografia   |
| Nota di contenuto       | Computational Toxicology Promotes Regulatory Science -- Tasks, Major Challenges and Emerging Modelling Methods for Computational Toxicology -- Xenobiotic Metabolism by Cytochrome P450s: Insights Gained from Molecular Simulations -- Applications of Molecular Modeling to Probe the Mechanism of Endocrine Disruptor Action -- Mixture Toxicity -- Towards reproducible in silico practice via OpenTox -- Combining Machine Learning and Multilayer Networks for Toxicity Prediction -- Matrix and tensor factorization for toxicity modelling -- Network-based In Silico Assessment of Drug Cardiotoxicity -- Mode-of-action-guided chemical toxicity prediction: A novel in silico |

approach for predictive toxicology -- Machine learning methods for toxicity analysis -- Predictive modeling of Tox21 data -- The NTP DrugMatrix Toxicogenomics Database and Analysis Tool -- Applications of Computational Toxicology for Risk Assessment of Food Ingredients and Indirect Food Additives -- In silico prediction of the point of departure (POD) with high throughput data -- The application of topic modeling on drug safety signal detection and analysis -- Molecular dynamics simulations and applications in computational toxicology -- Computational modeling for prediction of drug-induced liver injury in humans -- Genomics in vitro to in vivo extrapolation (GIVIVE) for drug safety evaluation.

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### Sommario/riassunto

This book provides a comprehensive review of both traditional and cutting-edge methodologies that are currently used in computational toxicology and specifically features its application in regulatory decision making. The authors from various government agencies such as FDA, NCATS and NIEHS industry, and academic institutes share their real-world experience and discuss most current practices in computational toxicology and potential applications in regulatory science. Among the topics covered are molecular modeling and molecular dynamics simulations, machine learning methods for toxicity analysis, network-based approaches for the assessment of drug toxicity and toxicogenomic analyses. Offering a valuable reference guide to computational toxicology and potential applications in regulatory science, this book will appeal to chemists, toxicologists, drug discovery and development researchers as well as to regulatory scientists, government reviewers and graduate students interested in this field.

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