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Nota di contenuto	Water quality and contaminants of emerging concern (CECs) / Antonio Juan Garcia-Fernandez, Silvia Espin, Pilar Gomez-Ramirez, Pablo Sanchez-Virosta, Isabel Navas -- The effects of contaminants of emerging concern on water quality / Heiko L. Schoenfuss -- Chemometrics : multivariate statistical analysis of analytical chemical and biomolecular data / Richard Brereton -- Chemometrics and cheminformatics--an introduction / Chanin Nantasenamat -- An introduction to some basic chemometric tools / Lennart Eriksson, Erik Johansson, Johan Trygg -- From data to models : mining experimental values with machine learning tools / G. Gini, E. Benfenati -- Machine learning approaches in computational toxicology studies / Pravin Ambure, Stephen Jones Barigye, Rafael Gozalbes -- Counter-propagation neural networks for modelling and read across in aquatic (fish) toxicity / Marjan Vracko, Viktor Drgan -- Aiming high versus aiming all : aquatic toxicology and QSAR multitarget models / Ana S. Moura and M. Natalia D.S. Cordeiro -- Chemometric approaches to evaluate interspecies relationships and extrapolation in aquatic toxicity / S. Raimondo, C.M. Lavelle, M.G. Barron -- The QSAR paradigm to

explore and predict aquatic toxicity / Fotios Tsopelas, Anna Tsantili-Kakoulidou -- Application of cheminformatics to model fish toxicity / Sorin Avram, Simona Funar-Timofei, Gheorghe Ilia -- Chemometric modeling of algal and daphnia toxicity / Luminita Crisan, Ana Borota, Alina Bora, Simona Funar-Timofei, Gheorghe Ilia -- Chemometric modeling of algal toxicity / Gulcin Tugcu, Serli Onlu, M.T. Sacan -- Chemometric modelling of daphnia toxicity / Amit Kumar Halder and M. Natalia D.S. Cordeiro -- Chemometric modeling of Daphnia toxicity : quantum-mechanical insights / Reenu and Vikas -- Chemometric modeling of toxicity of chemicals to tadpoles / Kabiruddin Khan and Kunal Roy -- Chemometric modeling of chemical toxicity to marine bacteria / Kabiruddin Khan and Kunal Roy -- Chemometric modeling of pesticide aquatic toxicity / Alina Bora, Simona Funar-Timofei -- Contribution of chemometric modeling to chemical risks assessment for aquatic plants : state of the art / Mabrouk Hamadache, Abdeltif Amrane , Othmane Benkortbi, Salah Hanini -- Application of 3D QSAR approaches to classification and prediction of aquatic toxicity / S. Lee, M.G. Barron -- Aquatic ecotoxicity QSAR methods for cationic polymers / Hans Sanderson, Pathan Mohsin Khan, Supratik Kar, Kunal Roy, Anna Magdalene Brun Hansen, Kristin Connors, Scott Belanger -- In silico platforms for predictive ecotoxicology : from machine learning to deep learning / Yong Oh Lee, Baeckkyoung Sung -- The use and evolution of web tools for aquatic toxicology studies / Renata Priscila Costa Barros, Luana de Moraes e Silva, Natalia Ferreira de Sousa, Luciana Scotti, Marcus Tullius Scotti -- The tools for aquatic toxicology within the VEGAHUB system / A. Lombarodo, D. Baderna, E. Benfenati -- Aquatic toxicology databases / Supratik Kar, Kerzy Leszczynski -- Computational tools for the assessment and substitution of biocidal active substances of ecotoxicological concern : the COMBASE project / Maria Blazquez, Oscar Andreu-Sanchez, Arantxa Ballesteros, Maria Luisa Fernandez-Cruz, Carlos Fito, Sergi Gomez-Ganau, Rafael Gozalbes, David Hernandez-Moreno, Anna Lombardo, Marco Marzo, Irati Ranero, Emilio Benfenati -- Image analysis and deep learning web services for nanoinformatics / Anastasios G. Papadiamantis, Antreas Afantitis, Andreas Tsoumanis, Pantelis Karatzas, Philip Doganis, Dimitra-Danai Varsou, Haralambos Sarimveis, Laura-Jayne A. Ellis, Eugenia Valsami-Jones, Iseult Lynch, Georgia Melagraki.

Sommario/riassunto

"This book introduces readers to the existing and emerging problems of contamination of the aquatic environment due to various metal and organic pollutants (including industrial chemicals, pharmaceuticals, cosmetics, biocides, nanomaterials, pesticides, surfactants, dyes, etc.) and resultant effects on water quality, chemical threat to the aquatic organisms and consequent effects on human health. The book discusses different chemometric (classification and pattern recognition tools, clustering techniques, principal component analysis, multivariate regression analysis, etc.) and cheminformatic (toxicophore, QSAR, data mining, etc.) tools for the non-experts and their application in analyzing and modeling toxicity data of chemicals (including metal and organic contaminants) to various aquatic organisms. Split into four sections the book covers chemometric and cheminformatic tools and protocols, case studies and literature reports, and tools and databases. Multispecies aquatic toxicity modeling will demonstrate the data gap filling in absence of toxicity data for a particular aquatic species. Various aquatic toxicity databases and chemometric software tools and web servers are covered and practical examples of model development with illustrations are provided"--