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Autore	Porretta, Sebastiano
Titolo	L'analisi sensoriale / Sebastiano Porretta
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Titolo	Advances in QSAR Modeling : Applications in Pharmaceutical, Chemical, Food, Agricultural and Environmental Sciences / / edited by Kunal Roy
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Collana	Challenges and Advances in Computational Chemistry and Physics, , 2542-4491 ; ; 24
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Soggetti	Chemistry, Physical and theoretical Pharmaceutical technology Environmental chemistry Food—Biotechnology Pharmaceutical chemistry Agriculture Theoretical and Computational Chemistry Pharmaceutical Sciences/Technology Environmental Chemistry Food Science Medicinal Chemistry
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Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Performance parameters and validation practices in QSAR modeling -- Towards interpretable QSAR models -- The use of topological indices in QSAR and QSPR modeling -- The Maximum Common Substructure (MCS) search as a new tool for SAR and QSAR -- The universal approach for structural and physico-chemical interpretation of QSAR/QSPR models -- Generative Topographic Mapping approach -- Monte Carlo methods for solution of tasks in Environmental Sciences -- QSAR in Environmental Research -- QSAR applications for environmental chemical prioritization: Biotransformation of chemicals -- QSAR modeling in environmental risk assessment: application to the

prediction of pesticide toxicity -- Counter propagation artificial neural network (CP ANN) models for prediction of carcinogenicity of non congeneric chemicals for regulatory uses -- Strategy for identification of critical nanomaterials properties linked to biological impacts: interlinking of experimental and computational approaches -- QSAR/QSPR modeling in the design of drug candidates with balanced pharmacodynamics and pharmacokinetic properties -- Molecular modeling of food chemicals as potential bioactive compounds -- On application QSARs in Food and Agricultural Sciences: History and Recent Developments.

Sommario/riassunto

The book covers theoretical background and methodology as well as all current applications of Quantitative Structure-Activity Relationships (QSAR). Written by an international group of recognized researchers, this edited volume discusses applications of QSAR in multiple disciplines such as chemistry, pharmacy, environmental and agricultural sciences addressing data gaps and modern regulatory requirements. Additionally, the applications of QSAR in food science and nanoscience have been included – two areas which have only recently been able to exploit this versatile tool. This timely addition to the series is aimed at graduate students, academics and industrial scientists interested in the latest advances and applications of QSAR.
