1. Record Nr. UNINA9910298635503321 Autore Roy Kunal Titolo A Primer on QSAR/QSPR Modeling: Fundamental Concepts / / by Kunal Roy, Supratik Kar, Rudra Narayan Das Pubbl/distr/stampa Cham:,: Springer International Publishing:,: Imprint: Springer,, 2015 **ISBN** 3-319-17281-6 Edizione [1st ed. 2015.] Descrizione fisica 1 online resource (129 p.) Collana SpringerBriefs in Molecular Science, , 2191-5407 543.0072 Disciplina Soggetti Chemistry, Physical and theoretical Chemometrics **Bioinformatics** Computational biology Theoretical and Computational Chemistry Math. Applications in Chemistry Computer Appl. in Life Sciences Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Description based upon print version of record. Nota di bibliografia Includes bibliographical references at the end of each chapters. Nota di contenuto QSAR/QSPR Modeling: Introduction -- Statistical methods in QSAR/QSPR -- QSAR/QSPR Methods -- Newer directions in QSAR/QSPR. Sommario/riassunto This brief goes back to basics and describes the Quantitative structureactivity/property relationships (QSARs/QSPRs) that represent predictive models derived from the application of statistical tools correlating biological activity (including therapeutic and toxic) and properties of chemicals (drugs/toxicants/environmental pollutants) with descriptors representative of molecular structure and/or properties. It explains how the sub-discipline of Cheminformatics is used for many applications such as risk assessment, toxicity prediction, property prediction and regulatory decisions apart from drug discovery and lead optimization. The authors also present, in basic terms, how QSARs and related

> chemometric tools are extensively involved in medicinal chemistry, environmental chemistry and agricultural chemistry for ranking of potential compounds and prioritizing experiments. At present, there is

no standard or introductory publication available that introduces this important topic to students of chemistry and pharmacy. With this in mind, the authors have carefully compiled this brief in order to provide a thorough and painless introduction to the fundamental concepts of QSAR/QSPR modelling. The brief is aimed at novice readers.