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Autore	Li, Hong Xing
Titolo	Fuzzy sets and fuzzy decision-making / Hong Xing Li and Vincent C. Yen
Pubbl/distr/stampa	Boca Raton [etc.] : CRC, c1995
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Altri autori (Persone)	Yen, Vincent C.
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Autore	Roy Kunal
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Collana	SpringerBriefs in Molecular Science, , 2191-5407
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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 structure-activity/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.