
Contents

<i>Dedication</i>	v
<i>Preface</i>	vii
<i>Contributors</i>	xiii

PART I WHERE WE ARE AND WHERE WE ARE GOING TO

1 Molecular Descriptors for Structure–Activity Applications: A Hands-On Approach	3
<i>Francesca Grisoni, Davide Ballabio, Roberto Todeschini, and Viviana Consonni</i>	
2 The OECD QSAR Toolbox Starts Its Second Decade	55
<i>Terry W. Schultz, Robert Diderich, Chanita D. Kuseva, and Ovanes G. Mekenyan</i>	
3 QSAR: What Else?	79
<i>Giuseppina Gini</i>	
4 (Q)SARs as Adaptations to REACH Information Requirements	107
<i>Toni Alasuvanto, Andrea Gissi, Tomasz Sobanski, Panagiotis Karamertzanis, and Mike Rasenberg</i>	

PART II MOLECULAR AND DATA MODELING

5 Machine Learning Methods in Computational Toxicology	119
<i>Igor I. Baskin</i>	
6 Applicability Domain: A Step Toward Confident Predictions and Decidability for QSAR Modeling	141
<i>Supratik Kar, Kunal Roy, and Jerzy Leszczynski</i>	
7 Molecular Similarity in Computational Toxicology	171
<i>Matteo Floris and Stefania Olla</i>	
8 Molecular Docking for Predictive Toxicology	181
<i>Daniela Trisciuzzi, Domenico Alberga, Francesco Leonetti, Ettore Novellino, Orazio Nicolotti, and Giuseppe F. Mangiatordi</i>	
9 Criteria and Application on the Use of Nontesting Methods within a Weight of Evidence Strategy	199
<i>Anna Lombardo, Giuseppa Raitano, Domenico Gadaleta, and Emilio Benfenati</i>	
10 Characterization and Management of Uncertainties in Toxicological Risk Assessment: Examples from the Opinions of the European Food Safety Authority	219
<i>Alberto Mantovani</i>	

PART III IMPACT IN DRUG DISCOVERY AND DEVELOPMENT

- 11 Computational Toxicology and Drug Discovery 233
Catrin Hasselgren and Glenn J. Myatt
- 12 Approaching Pharmacological Space: Events and Components 245
*Giulio Vistoli, Alessandro Pedretti, Angelica Mazzolari,
and Bernard Testa*
- 13 Computational Toxicology Methods in Chemical Library
Design and High-Throughput Screening Hit Validation 275
Kirk E. Hevener
- 14 Enalos Suite: New Cheminformatics Platform for Drug Discovery
and Computational Toxicology 287
*Dimitra-Danai Varsov, Spyridon Nikolakopoulos, Andreas Tsoumanis,
Georgia Melagraki, and Antreas Afantitis*
- 15 Ion Channels in Drug Discovery and Safety Pharmacology 313
*Paola Imbrici, Orazio Nicolotti, Francesco Leonetti, Diana Conte,
and Antonella Liantonio*
- 16 Computational Approaches in Multitarget Drug Discovery 327
*Luciana Scotti, Hamilton Mitsugu Ishiki, Marcelo Cavalcante Duarte,
Tiago Branquinho Oliveira, and Marcus T. Scotti*
- 17 Nanoformulations for Drug Delivery: Safety, Toxicity, and Efficacy 347
Antonio Lopalco and Nunzio Denora
- 18 Toxicity Potential of Nutraceuticals 367
Ramesh C. Gupta, Ajay Srivastava, and Rajiv Lall
- 19 Impact of Pharmaceuticals on the Environment: Risk Assessment
Using QSAR Modeling Approach 395
Supratik Kar, Kunal Roy, and Jerzy Leszczynski

PART IV PREDICTING HUMAN HEALTH TOXICOLOGY ENDPOINTS

- 20 (Q)SAR Methods for Predicting Genotoxicity and Carcinogenicity:
Scientific Rationale and Regulatory Frameworks 447
*Cecilia Bossa, Romualdo Benigni, Olga Tcheremenskaia,
and Chiara Laura Battistelli*
- 21 Stem Cell-Based Methods to Predict Developmental Chemical Toxicity 475
Hiroki Takahashi, Xian-Yang Qin, Hideko Sone, and Wataru Fujibuchi
- 22 Predicting Chemically Induced Skin Sensitization by Using
In Chemico/In Vitro Methods 485
Laura H. Rossi and Janine Ezendam
- 23 Hepatotoxicity Prediction by Systems Biology Modeling
of Disturbed Metabolic Pathways Using Gene Expression Data 505
Oriol López-Massaguer, Manuel Pastor, Ferran Sanz, and Pablo Carbonell
- 24 Nontest Methods to Predict Acute Toxicity: State of the Art
for Applications of In Silico Methods 519
Ronan Bureau

25	Predictive Systems Toxicology	535
	<i>Narsis A. Kiani, Ming-Mei Shang, Hector Zenil, and Jesper Tegner</i>	
26	Chemoinformatic Approach to Assess Toxicity of Ionic Liquids	559
	<i>Anita Sosnowska, Anna Rybinska-Fryca, Maciej Barycki, Karolina Jagiello, and Tomasz Puzyn</i>	
27	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results.....	573
	<i>Andrey A. Toropov, Alla P. Toropova, Alessandra Roncaglioni, and Emilio Benfenati</i>	
	Index.....	585