

Contents

Preface — V

Chapter 1

Toxicity Assessment — 1

- 1.1 Toxicity Measurements and Predictions — 1
 - 1.1.1 Dose Descriptors and In Silico Tools — 1
 - 1.1.2 Aquatic Toxicity — 2
- 1.2 Quantitative Structure–Activity/Property/Toxicity Relationships (QSAR QSPR/QSTR)/ — 4
- 1.3 Statistical Parameters for Assessment of QSAR/QSPR/QSTR Models — 5
- 1.4 Common Organic Solvents and Their Toxicities — 6
 - 1.4.1 Section of Solvents for Polymers with Less Toxicity — 7
 - 1.4.2 The Use of a Simple Approach for Selection Solvents of Polymers — 7
 - 1.4.3 General Comments on Using Solvents — 10
- 1.5 Toxicities of Polycyclic Aromatic Hydrocarbons — 11
 - 1.5.1 Carcinogenicity of PAHs — 11
 - 1.5.2 Octanol/Water Partition Coefficient (K_{ow}) — 12
- 1.6 Organophosphate Pesticides and Their Toxicities — 12
- 1.7 Prediction of Henry's Law Constant of Pesticides, Solvents, Aromatic Hydrocarbons, and Persistent Pollutants — 15
- 1.8 Common Process for Removal of Organic Compounds in the Environment — 23
- 1.9 Summary — 24

Chapter 2

Toxicity of Small Data Sets of Organic Compounds — 27

- 2.1 Nitroaromatic Compounds — 27
 - 2.1.1 QSAR/QSTR Studies on Bacteria — 28
 - 2.1.2 QSAR/QSTR Studies on Rodents — 29
- 2.2 Aromatic Aldehydes — 30
 - 2.2.1 Two Descriptors $\log K_{ow}$ and the Maximum Acceptor Superdelocalizability in a Molecule — 31
 - 2.2.2 $\log K_{ow}$ and Molecular Connectivity Index — 32
 - 2.2.3 $\log K_{ow}$ as well as Electronic and Topological Descriptors — 33
- 2.3 Amino Compounds — 34
 - 2.3.1 Estimation of *ISTP* — 34
 - 2.3.2 Prediction of *DSTP* — 35
 - 2.3.3 Different Effects of –OH and –N = O — 35
- 2.4 Halogenated Phenols — 36

2.4.1	The DFT-B3LYP Method with the Basis Set 6-31G (d, p), and log K_{ow} — 36
2.4.2	Two-Dimensional (2D) and Two Three-Dimensional (3D) QSAR/QSTR Models — 36
2.4.3	Wastewater-Derived Halogenated Phenolic Disinfection By-Products — 38
2.5	Organophosphate Compounds — 39
2.6	Polychlorinated Naphthalenes — 41
2.7	Assessment of the Agonistic Activity of Dibenzazepine Derivatives — 43
2.8	Summary — 48

Chapter 3

Toxicity of Medium-Sized Data Sets — **51**

3.1	Polycyclic Aromatic Hydrocarbons (PAHs) — 51
3.2	Benzene Derivatives — 52
3.2.1	3D-QSAR/QSTPR Studies Using CoMFA, CoMSIA, and VolSurf Approaches — 52
3.2.2	Atom-Based Nonstochastic and Stochastic Linear Indices — 53
3.2.3	Semiempirical Descriptors — 55
3.3	Phenol Derivatives — 56
3.4	Benzoic Acid Derivatives — 57
3.4.1	Predicting Toxicity Through Mouse via Oral LD_{50} — 57
3.4.2	Estimating Toxicity Through Rats via Oral LD_{50} — 58
3.5	Assessment of Antitrypanosomal Activity of Sesquiterpene Lactones — 60
3.6	Assessment of Activities of Thrombin Inhibitors — 65
3.7	Assessing the Psychotomimetic Activity of the Substituted Phenethylamines — 75
3.8	Summary — 79

Chapter 4

Toxicity of Large Data Sets — **83**

4.1	Aromatic Compounds — 83
4.1.1	Regression-Based QSTR and Read-Across Algorithm — 83
4.1.2	Acute Toxicity of Aromatic Chemicals in Tadpoles of the Japanese Brown Frog (<i>Rana japonica</i>) Using Correlation Weights — 89
4.1.3	Chemometric Modeling of Acute Toxicity of Diverse Aromatic Compounds Against <i>Rana japonica</i> — 91
4.1.4	Toxicity of Different Substituted Aromatic Compounds to the Aquatic Ciliate <i>Tetrahymena pyriformis</i> — 93
4.1.5	Toxicity of Aromatic Pollutants and Photooxidative Intermediates in Water — 95

4.1.6	Risk Assessment of Aromatic Compounds to <i>Tetrahymena pyriformis</i> by a Simple QSAR/QSTR Model — 98
4.1.7	Toxicity Toward <i>Chlorella vulgaris</i> of Organic Aromatic Compounds in Environmental Protection — 105
4.2	Organic Compounds — 110
4.2.1	Chemical Toxicity to <i>Tetrahymena pyriformis</i> with Four Descriptor Models — 110
4.2.2	Ecotoxicological QSAR/QSTR Modeling of Organic Compounds Against Fish — 112
4.3	Summary — 125

Chapter 5

Toxicity of Ionic Liquids — 127

5.1	Toxicity of ILs Based on <i>Vibrio fischeri</i> Through the Structure of Cations with Specific Anions — 141
5.2	Relationships of the Toxicity with the Structure and the 1-Octanol–Water Partition Coefficient of ILs — 146
5.3	Using a Simple Group Contribution Method for Some ILs — 147
5.4	Using Atomic Electrostatic Potential Descriptors for Predicting the Ecotoxicity of ILs Toward Leukemia Rat Cell Line (ICP-81) — 149
5.5	Summary — 158

List of Symbols — 161

Answers to Problems — 171

References — 175

About the Author — 195

Index — 197