Appendix D.
Thematic Bibliography

In this appendix, bibliographic references are collected for some special topics of general interest. These references are in addition to those already quoted in the main text of the book.

Topics for which additional references are provided here are listed in alphabetic order; moreover, for each topic, bibliographic references are reported according to their publication year.

Note that these topics do not necessarily correspond to entries in the book; in most of the cases, they are indeed specific topics of a more general subject (i.e., entry of the book) for which only some bibliographic references are given to provide the reader with a starting point for further investigation of the topic of interest. Addition of these specific topics allowed a more rational partition of all (sometimes a huge number) the bibliographic references concerning an entry of the book and, hence, allowed an easier retrieval. Selection of the topics was based on the most frequent keywords encountered in the publications about molecular descriptors and related research fields.

In this appendix of the book, the reader should not be expected to find an exhaustive bibliography concerning the topic, because most of the quoted references concern only with studies related to molecular descriptors and applications in QSAR/QSPR fields and the references to the earliest and most significant publications dealing with a topic have already been reported in the main text of the book.

Topics
ADME properties
Artificial Neural Networks (ANNs)
chemical compound classes
- alcohols
- amines
- conjugated systems
- flavonoids
- halocompounds
- hydrocarbons, alkane, cycloalkanes, alkenes
- PCB, PCDD, PCDF
- pesticides
- solvents

Molecular Descriptors for Chemoinformatics, Volume II: Appendices, References
Roberto Todeschini and Viviana Consonni
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classification methods
chromatographic descriptors
CODESSA descriptors
Comparative Molecular Field Analysis (CoMFA)
connectivity indices
- biological activities and toxicological indices
- bioconcentration factor
- chromatographic properties
- lipophilicity
- soil sorption coefficients
- solubility
- various physicochemical properties
- other applications

DRAGON descriptors
drug design
electronic substituent constants
electrotopological state indices
graph invariants
GRID method
Hansch analysis
Hosoya *Z* index
hydrogen-bonding descriptors
Linear Solvation Energy Relationships
pharmacological topics
- acetylcholine neurotransmitter, AChe
- antibacterial activity
- anticonvulsant activity
- anti-inflammatory activity
- antihypertensive activity
- antimalarial activity
- antitumor activity
- benzodiazepines
- Blood–Brain Barrier, BBB
- CACO-2 permeability
- DiHydroFolate Reductase enzyme, DHFR
- dopamine agonists
- Human Immunodeficiency Virus, HIV
- skin sensitization potential
- skin permeability potential
- steroids

physicochemical properties
- boiling point
- equilibrium constants

- log *P*
- melting point
- molar refractivity
- solubility

QSAR philosophy, history and methodologies
quantum-chemical descriptors
regression methods
Self-Organizing Maps (SOMs)
similarity/diversity analysis
toxicological end-points
- aquatic toxicity (in general)
- aquatic toxicity against *Tetrahymena pyriformis*
- aquatic toxicity against *Daphnia magna*
- aquatic toxicity against fathead minnow
- carcinogenic and mutagenic effects
- various toxicological studies and end-points

validation techniques
variable selection
virtual screening and library design
WHIM descriptors
Wiener index

ADME Properties

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