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
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, ACh
  • 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 \textit{Tetrahymena pyriformis}
- aquatic toxicity against \textit{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

\section*{ADME Properties}


Chen Gang, Zheng Suxin, Luo Xiaomin, Shen Jianhua, Zhu Weiliang, Liu Hong, Gui Chunshen,


Artificial Neural Networks (ANNs)


Appendix D. Thematic Bibliography


Arupijoti S. and Iragavarapu S. (1998). New electrotopological descriptor for prediction of boiling points of alkanes and aliphatic alcohols through artificial neural network and multiple


Appendix D. Thematic Bibliography


Chemical Compound Classes
(C: Alcohols)


Chemical Compound Classes (amines)


### Chemical Compound Classes

(© Conjugated Systems)


Kekulé A. (1866). Lehrbuch der Organischen Chemie. Erlangen (Germany).


Mekenyan O., Bonchev D. and Balaban A. T. (1984). Hierarchically Ordered Extended Connectivities. Reflection in the $^{1}$H NMR Chemical Shifts of...


Appendix D. Thematic Bibliography


Appendix D. Thematic Bibliography


Appendix D. Thematic Bibliography


He Linnan, Jurs P. C., Custer L. L., Durham S. K. and Pearl G. M. (2003). Predicting the Genotoxicity of


Appendix D. Thematic Bibliography


Chemical Compound Classes

Flavonoids


### Chemical Compound Classes (Halocompounds)


Appendix D. Thematic Bibliography


Richard A. M. and Hunter E. S. (1996). Quantitative Structure-Activity Relationships for the...
Appendix D. Thematic Bibliography
Appendix D. Thematic Bibliography


Chemical Compound Classes (⊙ Hydrocarbons, Alkanes, Cycloalkanes, Alkenes)


Optimum Semi-Empirical Topological Index, for Methyl-Branch Alkanes Produced by Insects. Chromatographia, 55, 707–713.


**Chemical Compound Classes (© PCB, PCDD, PCDF)**


### Chemical Compound Classes (Pesticides)


Appendix D. Thematic Bibliography


Okamoto Y., Inukai T. and Brown H. C. (1958). Rates of Solvolysis of Phenylidimethylcarbinyl Chlorides


Classification Methods


Lather V. and Madan A. K. (2004). Models for the prediction of adenosine receptors binding activity


**Chromatographic Descriptors**


Appendix D. Thematic Bibliography


Appendix D. Thematic Bibliography

Graph Descriptors. SAR & QSAR Environ. Res., 11, 419–452.
descriptors to QSRR and QSAR analysis of


**CODESSA Descriptors**


**Comparative Molecular Field Analysis (CoMFA)**


Appendix D. Thematic Bibliography


Demyttenaere-Kovatcheva A., Cronin M. T. D., Benfenati E., Roncaglioni A. and LoLiparo E.

Connectivity Indices (☐ Biological Activities and Toxicological End-Point)

skin pathogens. *Arzneim. Forsch. (German)*, 32, 1515–1517.


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Connectivity Indices

(1) Bioconcentration Factor


Connectivity Indices

(2) Chromatographic Properties


**Connectivity Indices ( Lipophilicity)**

**Connectivity Indices ( Soil Sorption Coefficients)**


### Connectivity Indices (Solubility)


### Connectivity Indices (Various Physico-Chemical Properties)


### Connectivity Indices

**Other Applications**


Appendix D. Thematic Bibliography


### DRAGON Descriptors


Casañola-Martín G. M., Marrero-Ponce Y., Khan M. T. H., Ather A., Khan K. M., Torrens F. and
Drug Design


Appendix D. Thematic Bibliography

Motoc I., Eds.), Springer-Verlag, Berlin (Germany), vol. 114, pp. 7–19.
Appendix D. Thematic Bibliography


Electronic Substituent Constants


Okamoto Y., Inukai T. and Brown H. C. (1958). Rates of Solvolysis of Phenylmethylcarbiny1 Chlorides...
Appendix D. Thematic Bibliography


Graph Invariants


Kirby E. C. (1994). Sensitivity of Topological Indices to Methyl Group Branching in Octanes and...


Appendix D. Thematic Bibliography


**GRID Method**


Chiu Ting-Lan and So Sung-Sau (2004). Development of Neural Network QSPPR Models for


**Hosoya Z Index**


Hosoya Z(Ch) Index of a Molecular Graph. Rev. Roum. Chim., 43, 481–484.

**Hydrogen-Bonding Descriptors**


**Appendix D. Thematic Bibliography**


#### Linear Solvation Energy Relationships


Pharmacological Topics (_permsAcetylcholine Neurotransmitter, ACh)


Pharmacological Topics (Antibacterial Activity)


Pharmacological Topics (Anticonvulsant Activity)


**Pharmacological Topics (Antihypertensive Activity)**


### Pharmacological Topics (Antimalarial Activity)


### Pharmacological Topics (Antitumor Activity)


### Pharmacological Topics

#### Benzodiazepines


Pharmacological Topics (©: Blood-Brain Barrier, BBB)


### Pharmacological Topics (© CACO-2 Permeability)


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Pharmacological Topics (© Dihydrofolate Reductase Enzyme, DHFR)


\section{Pharmacological Topics (\textcircled{D} Dopamine Agonists)}


Between Clozapine and Substituted 
[4-Phenylpiperazinyl]-methyl] benzamides: 
Hoffman B., Cho Sung Jin, Zheng Weifan, Wyrick 
S. D., Nichols D. E., Mailman R. B. and Tropsha A. 
(1999). Quantitative structure-activity relationship 
modeling of dopamine D-1 antagonists using 
comparative molecular field analysis, genetic 
algorithms-partial least-squares, and K nearest 
Molecular Similarity: Method and Algorithms. 
Babes-Bolyai 
Studia Univ. 
Dopamine Receptor Antagonists.
Multi-conformational Ligand Representation in 
4D-QSAR: Reducing the Bias Associated with 
Ligand Alignment. Quant. Struct. -Act. Relat., 19, 
149–161.
Mariussen E., Andersson P. L., Tysklind M. and 
Biphenyls on the Uptake of Dopamine into Rat 
Brain Synaptic Vesicles: A Structure–Activity 
Kulkarni S. K., Newman A. H. and Houlihan W. J. 
(2002). Three-Dimensional Quantitative Structure– 
Activity Relationships of Mazindol Analogues at 
the Dopamine Transporter Binding. Validation of the Model for a Small Data Set. 
Multi-conformational Ligand Representation in 
4D-QSAR: Reducing the Bias Associated with 
Ligand Alignment. Quant. Struct. -Act. Relat., 19, 
149–161.
Boström J., Böhm M., Gundertofte K. and Klebe G. 
(2003). A 3D QSAR Study on a Set of Dopamine D4 
43, 1020–1027.
Ursu O. and Diudea M. V. (2005). 3D Molecular 
Similarity: Method, Algorithms and Case Study on 
Dopamine Receptor Antagonists. Studia Univ. 
Babes-Bolyai, 50, 175–184.
Molecular Similarity: Method and Algorithms. 
J. Comp. Chem. (Japan), 5, 39–46.
Xu Lu, Zhang Jing-You, Wang Jun and Dong Lin 
(2006). Extended topological indices and prediction 
of activities of chiral compounds. Chemom. Intell. 
Lab. Syst., 82, 37–43.
Zheng Fang, Bayram E., Sumithran S. P., Ayers J. T., 
Zhan Chang-Guo, Schmitt J. D., Dwoskin L. P. and 
bi-quaternary ammonium salts that act as agonists 
at neuronal nicotinic acetylcholine receptors 
14, 3017-3037.

Pharmacological Topics (Human 
Immunodeficiency Virus, HIV)
indexes and their applications in evaluating 
antileukemic activity of 9-anilinoacridines and the 
activity of 2',3'-dideoxy-nucleosides against HIV. 
1165–1169.
Debnath A. K., Jiang S., Strick N., Lin K., Haberfield 
Structure-Activity Analysis of a Series of Porphyrin 
Derivatives with Anti HIV-1 Activity Targeted to the 
V3 Loop of the gp120 Envelope Glycoprotein of the 
Human Immunodeficiency Virus Type 1. J. Med. 
Chem., 37, 1099–1108.
Joao H. C., Devreese K., Pauwels R., Declercq E., 
Quantitative Structural-Activity Relationship Study of 
bis-Tetraazacyclic Compounds. A Novel Series of 
HIV-1 and HIV-2 Inhibitors. J. Med. Chem., 38, 
3865–3873.
Molecular Modeling and Quantitative Structure– 
Activity Studies of Anti HIV-1 2- 
3D-Quantitative Structure-Activity Relationships of 
Human Immunodeficiency Virus Type-1 
Proteinase Inhibitors: Comparative Molecular 
Field Analysis of 2-Heterobridged Statine 
Derivatives - Implications for the Design of Novel 
Gussio R., Pattabiraman N., Zaharevitz D. W., 
Kellogg G. E., Topol I. A., Rice W. G., Schaeffer C. 
Models for the Nonnucleoside Binding Site of 
HIV-1 Reverse Transcriptase Complexed with 
39, 1645–1650.
Hannongbua S., Lawtrakul L. and Limtrakul J. 
(1996). Structure-Activity Correlation Study of


### Pharmacological Topics (Skin Sensitization)


Pharmacological Topics (Skin Permeability)


Pharmacological Topics (Skin Permeability)


Appendix D. Thematic Bibliography


**Physico-Chemical Properties (△ Boiling Point)**


Arupiyoti S. and Iragavarapu S. (1998). New electrotopological descriptor for prediction of boiling points of alkanes and aliphatic alcohols through artificial neural network and multiple


### Physico-Chemical Properties (Equilibrium Constants)


**Physico-Chemical Properties (ς: Log P)**


### Physico-Chemical Properties (Melting Point)


Physico-Chemical Properties (© Molar Refractivity)


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Physico-Chemical Properties

Solubility


Appendix D. Thematic Bibliography


### QSAR Phylosophy, History and Methodologies


### Quantum-Chemical Descriptors


Appendix D. Thematic Bibliography


Chen Jingwen, Quan Xie, Schramm K.-W., Kettrup A. and Yang Fenglin (2001). Quantitative structure-property relationships (QSPRs) on direct photolysis of PCDDs. Chemosphere, 45, 151–159.


Regression Methods

Appendix D. Thematic Bibliography


Appendix D. Thematic Bibliography


### Self-Organizing Maps (SOMs)


Domine D., Devillers J., Wiencek D. and Buydens L. (1996). Test Series Selection from Nonlinear...


Appendix D. Thematic Bibliography | 161


Similarity/Diversity Analysis


Menard P. R., Mason J. S., Morize I. and Liu Dong Xiang, Jiang Hua Liang, Chen Kai Xian and Kunz M. and Radl Z. (1998). Distributions of


Appendix D. Thematic Bibliography

Eds.), Kluwer/ESCOM, Dordrecht
(The Netherlands), vol. 2, pp. 226–252.

Kunz M. and Radl Z. (1998). Distributions of

Liu Dong Xiang, Jiang Hua Liang, Chen Kai Xian and Ji Ru Yun (1998). A New Approach to Design
Virtual Combinatorial Library with Genetic

Menard P. R., Mason J. S., Morize I. and Bauserschmidt S. (1998). Chemistry Space metrics in Diversity Analysis, Library Design, and


Rarey M. and Dixon J. S. (1998). Feature Trees: A New Molecular Similarity Measure Based on Tree

Triple Density Molecular Quantum Similarity


Recursive Partitioning to Analyze a Large SAR Data


Agrafiotis D. K. and Lobanov V. S. (1999). An Efficient Implementation of Distance-Based Diversity

Bayada D. M., Hemersma H. and van Geerestein V. J. (1999). Molecular Diversity and Representativity in

Multilevel Neighborhoods of Atoms: Definition and


Schur D. (1999). Design and Diversity Analysis of
Large Combinatorial Libraries Using Cell-Based

Stanton D. T., Morris T. W., Roychoudhury S. and
Parker C. N. (1999). Application of Nearest-
Neighbor and Cluster Analyses in Pharmaceutical

Chuman H., Goto S., Karasawa M., Sasaki M.,
Three-Dimensional Structure-Activity
Relationships of Synthetic Pyrethroids: 1.
Similarity in Bioactive Conformations and Their

Combination of molecular similarity measures

Combinatorial Preferences Affect Molecular
Similarity/Diversity Calculations Using Binary

Golbraikh A. (2000). Molecular Dataset Diversity
Indices and Their Applications to Comparison of

molecular similarity method correlated with


Simple knowledge-based descriptors to
predict protein-ligand interactions. Methodology


Appendix D. Thematic Bibliography


Toxicological End-Points (© Aquatic Toxicity in General)


Toxicological End-Points (Aquatic Toxicity Against *Tetrahymena Pyriformis*)


 Toxicological End-Points (© Aquatic Toxicity Against Daphnia Magna)


## Toxicological End-Points (Aquatic Toxicity Against Fathead Minnow)


### Toxicological End-Points (Carcinogenic and Mutagenic Effects)


### Toxicological END-POINTS (Various Toxicological Studies and End-Points)


support vector machine (SVM) for prediction toxic activity of different data sets. *Toxicology*, 217, 105–119.


### Validation Techniques


Variable Selection


Prediction Ability and Interpretability of Three-


Salt D. W., Maccari L., Botta M. and Ford M. G. (2004). Variable selection and specification of robust QSAR models from multicollinear data: arylpiperazinyl derivatives with affinity and


### Virtual Screening and Library Design


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**Wiener Index**


Appendix D. Thematic Bibliography


Gutman I., Marković S., Popović L., Spalević Z. and Pavlović L. (1997). The Relation Between the


