

Index

A

acquired immunodeficiency syndrome (AIDS) 26, 75, 85
active learning (AL) 2-3, 5-8, 26, 30, 36, 39, 44, 48, 52, 65, 74, 77, 79, 83, 89, 93-106, 112-119, 142-143, 152, 154, 156-157, 162, 165, 168-169, 171-172, 220-221, 232, 235, 237-239, 243, 247-267, 283, 289, 292, 295-296, 308, 320, 326, 334-342, 344, 349-352, 356-357, 365-366, 369, 371, 373, 381-385, 388-392, 396, 399-400
Agency for Toxic Substances and Disease Registry (ATSDR) 381, 402
amide hydrolysis 280, 298, 312-313
Amino Acid Sequence Autocorrelations (AASA) 221
aminolysis of esters 280, 300, 313
analysis of variance (ANOVA) 192
anti-human immunodeficiency virus (HIV) 25-27, 57, 61, 81, 84, 107, 222, 225
aromaticity 165, 167
artificial neural networks (ANN) 193-196, 226, 321, 368, 404
aryltriazolylhydroxamates (ATHs) 25, 27, 61, 64, 71, 84
Atomic Force Microscopy (AFM) 255-256, 273, 275
autocatalator 200
autocatalyst decay 201

B

Balaban index 220
basis-set superposition error (BSSE) 284, 292
Beer-Lambert spectroscopy 168
Belousov-Zhabotinsky reaction 199
benzyl halides 304

Binding Affinity 41, 81, 222, 224, 333-334, 336-339, 344

bioinformatics 72-74, 76-79, 81-87, 90, 189, 197, 225, 227, 333-334, 338, 343

Blasius equation 201, 204

Bond-Atom Graph (BAG) 221

Broto-Moreau autocorrelation 220

Brownian enzymic reactions 168-169, 181

C

carbon nanotubes (CNT) 89, 96-97, 101, 108-109

charge transfer 6-7, 261, 287, 292, 295

chemical complete graph 153

chemical graph 152-154, 156, 166-167, 190, 198, 220, 228, 241, 401, 410

Chemical Graph Theory 153, 166-167, 190, 198, 220, 228, 241, 401, 410

chemical pseudographs 151-154

chemoinformatics 22, 219, 228, 328, 333-334, 337, 343-344, 399, 406

chemometrics 83, 166, 189, 194, 225, 321, 328

chlorophenols (CPs) 1, 3-5, 7-8, 13-21, 23

Cognitive Sciences 140

colony forming unit (CFU) 267

compartmental systems 348-351, 353-357, 359-368, 371, 374, 376

competitive inhibition 178, 181

complete graph 152-153, 167

computational chemistry 21, 75-76, 81, 91, 167, 198, 225-227, 311, 317-324, 328, 331, 337, 345-346, 404

conceptual DFT 1, 8, 20, 187

cookbookery 324

coupled cluster (CC) theory 95, 98, 134, 137, 160

cubic-autocatalysis 199-200

cubic autocatalytic reactions 200, 204

curse of dimensionality 190, 192

D

Data Analysis 5, 7, 79, 83, 90, 140, 242, 370, 406
data mining technology 111-112
decision trees (DT) 194-195, 338
density functional theory (DFT) 1-3, 8, 20-21, 23, 95, 99, 187, 191, 281, 290, 292, 300, 304, 307, 311, 315, 317
descriptor relevance 189-190, 195-196
descriptors 1-4, 7-9, 13, 15-20, 22-23, 41, 80, 85, 92, 95, 97-103, 105, 108-110, 138-146, 148-150, 165-167, 189-196, 198, 219-221, 223-228, 234, 242, 245, 283, 288-290, 293, 295, 301, 304, 312, 314, 320-322, 327, 342-344, 380-382, 384-386, 388, 391-392, 395-396, 399-400, 403-408, 410
discovery 20, 41, 77, 80, 82-83, 85, 90, 109, 111-114, 118, 131, 134, 136-137, 150, 166, 171, 181, 222, 226, 230, 238-245, 263-264, 289, 330, 333-334, 344, 380-382, 384-385
Duffing equation 201
dye-sensitized solar cells 261, 264-266, 275-276, 278

E

ecotoxicity 1, 4, 9, 19-20, 23, 395
electronegativity 2, 5, 23, 220, 316, 389-390, 392-394
electrophilicity 1-9, 13, 15, 20-21, 23-24, 281, 299, 302-304, 315, 317
electrostatic potential at nuclei (EPN) 280-285, 288-289, 291-292, 295-296, 300-302, 304, 306-308, 310, 312
electrotopological state 151, 166, 324, 403, 405
entropy production 27, 29, 36, 61, 65, 68, 88
enzyme kinetics 168, 170, 172-173, 185-187, 367, 369
enzyme-linked immunoassays (ELISAs) 174
enzyme-product (EP) 169-171, 173, 175, 177-178, 182
enzyme-substrate (ES) 77, 106, 157, 169-173, 175, 177-179, 182, 186, 295-297, 359, 362, 370, 382
enzymic activity 168
enzymology 181, 184, 187, 242, 313
epistemology 318, 322, 326, 329, 331-332
EPN descriptor 280
EPN index 280, 282-283, 296
equipartition conjecture 25, 27, 29, 36, 61, 65, 68
equipartition line 29
evolutionary algorithms (EA) 114, 159, 194-196

Extended Topochemical Atom (ETA) Indices 380, 382, 388, 391-393, 395-397, 399-400, 408-410

F

feature selection 80, 115, 149, 189-190, 192-194, 197-198, 226
Form Recognitions 140
free energy calculations 333, 341
free energy perturbation (FEP) 338-339, 341-342

G

genetic algorithms (GA) 80, 100, 134, 140, 194, 196-198, 234, 323, 342
Goodness of Fit (GOF) 119, 125, 129, 132
graph-theoretical indices 151
Graph Theory 143, 153, 157, 166-167, 190, 198, 219-220, 225, 228, 241, 343, 367, 384, 401, 403, 410
Gray-Scott model 199
grouping rule 28

H

halocompounds 157-158
Hansch equation 320, 383-384
Harary numbers 220
Hartree-Fock (HF) 4, 7-9, 11, 95, 108, 283-287, 304, 313-314
hashed fingerprints 143
heterogeneous catalysis 111-114, 135
hierarchical tree 29
highest occupied molecular orbital (HOMO) 52, 91, 95, 103, 143, 320
high-throughput 65, 72, 83, 86, 111, 135, 239-241, 244
high throughput (HT) technology 113-114, 116-117, 131
Homotopy Perturbation Method (HPM) 199-206, 208
human rhinovirus (HRV) 223
hydrogen-bonded clusters 286-287
hydrogen bonding (HB) 146, 159, 161, 221-222, 280-283, 287-289, 291-296, 310-314, 316, 400
hydrophobicity 70, 96, 324, 383

I

inductive logic programming (ILP) 194
information entropy 25, 28-30, 61, 65, 68, 70-71, 75, 89
Information Theory 28, 143, 220, 343, 385, 401

International Chemical Identifier (InChI) 98-99, 110

K

Kier's molecular connectivity indices (MCI) 329, 388
 kinetic equations 348, 350-351, 357, 361-362, 364-366, 369, 372
 Knn 139, 144-145, 148
 knowledge discovery in databases (KDD) 112, 136-137
 Kohonen networks 139-140, 144-145

L

ligand 26-27, 57, 71, 78, 178, 283, 321-322, 326, 334-342, 359, 362, 365
 Lighthill equation 201
 linear decay 199-200
 linear discriminant analysis (LDA) 192, 240, 243-244
 Linear Interaction energy 333, 338
 linear interaction energy (LIE) method 338-339
 linear response approximation (LRA) theory 338-339
 logistic function 168
 lowest unoccupied molecular orbital (LUMO) 95, 103, 143, 320

M

Macromolecule 219
 Markov Chains Theory 220
 mass spectra (MS) 105, 223
 Mathematical modeling 199, 204
 mathematistry 324
 Mean Residence Time (MRT) 349, 372
 Michaelis-Menten kinetics 168, 171, 173, 183
 molecular connectivity theory 151-153, 167
 Molecular Descriptor 100, 219
 Molecular docking 222, 241, 333-335, 337, 344
 molecular dynamics (MD) 26, 71, 75-76, 184, 240-241, 322, 336, 339, 341-342, 371
 molecular electrostatic potential (MEP) 281-282, 284, 286-288, 293, 297, 313
 molecular field analysis (MFA) 41, 61, 81, 314, 320
 molecular shape analysis (MSA) 41, 80
 molecular surface electrostatic potential (MSEP) 283, 285, 291, 315
 Moller-Plesset perturbation theory (MP2) 95, 283-284, 304
 mutual information feature selection (MIFS) 193

N

nanomaterials 92-94, 96, 102, 104-110, 187, 247, 262, 275
 nanoparticles 89, 92-96, 102-108, 110, 246-248, 253, 255, 260, 264, 266-267, 273, 278
 nanostructures 70, 102, 247, 254, 277
 net electrophilicity 1, 3, 6, 20
 neural networks 22, 77, 79, 116, 131, 139-140, 144, 193-195, 197-198, 223-224, 226, 318, 321, 327
 non-linear reaction-diffusion equations 199
 normal mode analysis (NMA) 341
 Nuclear Magnetic Resonance (NMR) 222, 232, 410
 Nucleotide or Amino acid Adjacency Networks (NAANs) 221-222

O

out of the bag (OOB) 195

P

Parr electrophilicity index 281, 299
 photocatalytic decolorization 261, 264
 phylogenetic tree 25, 36, 44, 46-48, 50-52, 54-56, 68, 70, 77, 81, 84, 91
 physico-chemical effects 95
 Pimentel Report 281
 Platt index 385
 Poisson-Boltzmann (PB) equation 128, 340
 polyaromatic hydrocarbons (PAHs) 3
 Post hoc 190, 192, 194-196
 principal component analysis (PCA) 30, 32, 68, 71-72, 86, 88, 192, 196
 probiotics 32, 82
 pseudoconnectivity indices 151, 153, 155-156
 pseudograph 151-155, 164, 227

Q

QSAR techniques 320-323, 327-329, 333, 342, 344, 382
 QSAR Theory 219-220, 222-223
 Quantitative Structure-Activity Relationships (QSAR) 1-4, 7, 9, 15, 19-24, 27, 41, 65, 78, 80-83, 85-86, 92-93, 103, 105-109, 134, 136-137, 142-143, 149, 151, 157, 164-167, 189-198, 219-228, 234, 241-244, 283, 289, 312, 314, 318, 320-333, 342-344, 380-384, 388-389, 392, 396, 399-400, 402-410
 Quantitative Structure-Binding Relationships (QSBR) 222

Quantitative-Structure-Toxicity-Relationship (QSTR) 1, 8, 13, 20, 22, 381-382, 384, 388, 392, 395-396, 400, 408-409
quantum chemical descriptors (QCDs) 2-4, 20, 191, 221, 343-344
Quantum Mechanical Polarized ligand Docking (QPLD) 337
Quantum Mechanics 169, 220, 319, 323, 332, 337, 341
quantum tunneling 168-169, 171, 177-178, 183
quasi-steady-state-approximation (QSSA) 171, 173

R

Randic connectivity indices 220
random forests (RF) 194-195, 197, 248, 278-279
reactivity 1, 3-5, 13, 15, 20-24, 94, 96, 106, 114, 143, 183, 187, 261, 280-284, 286-293, 295-296, 299-302, 304-310, 312-317
receptor surface analysis (RSA) 41
Registration, Evaluation and Authorization of Chemicals (REACH) program 111, 118, 140, 251, 261, 329, 381, 402
RELIEF algorithm 193
reverse transcriptase (RT) 26-27, 71, 75, 80, 83-84, 86-87, 340, 342
root mean square deviation (rmsd) 336-337

S

Sal'nikov thermokinetic oscillator 199
Sampling 111, 113-119, 121, 124, 128, 130-131, 234, 311, 321-322, 336-337
Scanning Electron Microscopy (SEM) 255-259, 264-265
Schrödinger equation 319
Secondary Topology Graphs (STG) 221
Self Organizing Maps (SOM) 139-140, 145, 148
Similarity 27-28, 30, 32, 41, 44, 48, 52, 57, 70, 74, 81, 91, 139-142, 144, 148-150, 155, 222, 226-227, 231, 234-235, 239, 243-245, 316, 404
similarity indices 27
simple chemical graphs 157
simple graph 153
simple random sampling (SRS) 114, 118, 121, 123-125, 130-132
simplified molecular input line entry system (SMILES) 97-99, 102, 109, 327
simulated annealing (SA) 194, 196, 338-341
Sol-Gel Process 246, 249-250, 252-254, 264-265, 272-275, 278-279

solvent accessible surface area (SASA) 339-340, 344
space structure 111, 114, 119
Special Substrates 246, 255, 260-261, 272
spectrophotometry techniques 174
steady state 169, 188, 200, 202, 348, 366-368, 370-372
stochastic methods 30, 195
structural substitutions 30
structure-activity relationships (SARs) 2, 7, 21, 24, 80, 93, 107-108, 189-190, 192, 197, 219, 312, 321, 329-331, 343, 382, 400, 402-403, 405, 408, 410
styrylquinolines (SQs) 25, 27, 61, 63, 71, 80
substituent constants 22, 280-281, 304, 307-308, 310, 313, 317, 401, 403-404, 411
substructure keys 143
Successive Interference Fringes Method (SIFM) 246, 249, 268, 272
Support Vector Machines (SVM) 107, 117, 140, 149, 192, 224, 327
Symbolic Machine Learning 140

T

TiO₂ Nanoparticles 246, 253, 255, 260, 264, 266-267, 278
titanium dioxide nanostructured thin films 246, 254
topochemically arrived unique (TAU) scheme 382, 388, 391-393, 407, 409
topographic indices (TPGIs) 220, 222-223
topological indices (TIs) 99-100, 142-143, 166, 220-226, 275, 381, 385, 388, 400, 404, 410
toxicity 1-4, 7-9, 11-13, 15-24, 41, 71, 92-96, 102-109, 167, 173, 190, 239, 242, 319, 325, 333, 342, 380-382, 384, 388, 391, 396, 400, 402, 406, 408-411
toxicology 20-24, 106-107, 110, 166, 193, 197, 245, 318, 321, 327, 329, 345, 400, 402, 406
transient phase 186, 348, 362, 366-367, 370-372
transition state theory (TST) 169
Transmission Electron Microscopy (TEM) 255
Trichomonas vaginalis 25, 27, 30, 83

U

ultrametric distance 141
unbalanced 111, 114, 121
uncompetitive inhibition 179-180

V

valence connectivity indices 220
valence molecular connectivity indices 151, 153,
 155
variation ultrametric 141
vector of properties 27
Verification and Validation (V&V) 318, 326
vertex degree of general and complete graphs 151
vibrational enhancement 170
vibrationally enhanced ground-state tunneling
 theory (VEGST) 170
virtual sifting 139-140

W

Wiener index 220, 385, 405
W-Lambert function 168, 172, 174

X

X-ray Diffraction (XRD) 255, 257-258

Y

Young's modulus (YM) 102, 109, 258-259

Z

Zagreb indices 220