

Index

a

ab initio methods 268, 303, 304, 320, 327–333, 335–337
ab initio molecular dynamics (MD) 303, 304
absorption band 168
acidity 128, 130, 336
activity cliffs 458, 468, 470
addition reaction 141
adjacency matrix 18–21, 367
ADME (absorption, distribution, metabolism and excretion) 384, 466
advanced interatomic potentials 290–291
adverse drug reactions (ADRs) 479
agglomerative HCA 420
ALADDIN 362
algorithms
 backtracking 83, 236–239, 251, 258
 brute force 237
 complexity 232
 deep learning 453
 depth-first search 238
 dynamic programming 256–258
 efficiency 232
 hash 49
 heuristic 415
 leapfrog 304
 learning 380, 453, 458, 529
alignment
 global 256
 local 258
 pair-wise 254
 target-template 516

allosteric 315, 382
AMBER 280, 281, 283, 284, 286, 288, 293–295, 303, 304, 311, 312, 315, 316
AM1 326, 327
analytical chemistry 214, 399, 423, 434
angle bending 283–284, 289, 295
antimalarial 479, 480
antioxidation 369
applicability domain (AD) 158, 346, 434, 450, 466, 468, 475–478
application programming interface (API) 71, 222
Arabidopsis Information Resource 207
arithmetic mean 288, 402, 414, 433
aromaticity 29, 48, 79, 109, 110, 144, 193
aromatization 469, 484, 486
artificial intelligence (AI) 166, 168, 453
artificial neural network (ANN) 345, 346, 438, 442–451, 467
asphericity 378
association coefficients 247, 248
atom-by-atom 163, 164, 237, 243
atomic mean force potentials 517
atomic orbitals (AOs) 321–325, 327–329
atom pairs (AP) 249, 283, 287, 288, 303, 304, 352, 359–362
atom surface assignments (ASA) 381
atropisomers 32
attenuation models 271–277, 384
augmented annealing 445
augmented atoms (AA) 249

- Augmented Connectivity Molecular Formula (ACMF) 162
- autocorrelation vectors 249, 370, 378
- automorphism searching 74, 241–242
- autoscaling 408, 470
- average linkage 420
- average predictive ability 414, 415
- b**
- backtracking algorithm 83, 236–239, 251, 258
- bagging 432
- Balaban index 234, 364
- Ball-and Stick Model 101–102
- barrier of rotation 284
- basicity 336
- basis set 157, 321, 324, 327–329
- Bayes
- information criterion 400, 414
 - rule 457
- Bayesian
- methods 456
 - probability 359
 - regularization 445, 457
- Bayesian neural network (BNN) 459–461
- Beilstein Registry Number (BRN) 234
- B-factor 314
- bias 186, 413, 444, 455
- bibliographic databases 213, 214
- full text 216, 217
 - patent 214, 215
 - searching 216
- Big Data 159, 453, 466, 526
- binary QSAR 467
- Bingo 222
- binning 250, 359
- bioactivity 192, 199, 209, 481, 486, 487
- biochemical reactions 123, 136, 148, 360
- bioinformatics 479–518
- Bioinformatics Links Directory 207, 208
- BioJava 109
- Biological Abstracts (BIOSIS) 214
- biological activity 4, 33, 35, 58, 91, 155, 169, 174, 192, 202, 358, 359, 362, 366, 375, 381, 384, 385, 456, 458, 466, 471, 475, 478
- biological information 192, 206, 207, 501
- biological macromolecules 44, 102–103, 307
- biomolecular systems 294, 308, 316
- biopolymers 195–198, 207, 208, 293
- BIOVIA 71, 134, 220, 222
- bit collisions 240
- bitmap 160
- bit string 160, 239, 366
- bit vectors 160, 163, 239–241, 246, 247, 249, 250, 252, 356
- biuniqueness 11, 12, 25
- BLAST 195–197, 258, 259, 503, 505–507, 509, 516
- blastn 509
- blastp 503, 505
- blastx 509
- blood-brain barrier 366
- BLOSUM matrices 256, 503–509
- Boltzmann constant 304
- bond counts 359, 364, 377
- bond–electron (BE) matrix 21–23
- bond increments 287
- bond rotation 96, 250, 284, 302
- bond stretching 282–283, 289, 295
- Boolean array 160, 353
- bootstrap 416, 430, 431
- Born free energy of solvation 307
- Born–Oppenheimer approximation 280
- boxplot 401, 402, 433
- box scaling 170
- BRENDA (Braunschweiger Enzymdatenbank) 208
- brute force algorithm 237
- Buckingham potential 288
- Burden matrix 367
- c**
- CACTVS 58, 71, 75, 86, 222
- Cahn–Ingold–Prelog (CIP) rules 34, 57, 86–88
- calcium channel 360

- calibration 6, 175, 294, 404, 406, 411–414, 423, 429
 Cambridge Crystallographic Data Centre (CCDC) 67
 Cambridge Structural Database (CSD) 91, 99, 199
 canonical ensemble 309
 numbering 77, 233
 numeration 485
 canonicalization 25, 48, 76–78
 CAplus 189, 206, 210, 213–216, 218–220
 Capped Sticks Model 101
 cardinality 16
 Cartesian coordinates 36, 50, 51, 55, 58, 63, 94, 98, 159, 160, 280, 303, 307, 308, 379–381
 CAS numbers 485
 CASREACT 189, 210–212, 216
 CAST 87
 catalog databases 190, 200
 cell membranes 315
 cell organelles 315
 centering 6, 404, 407–408
 centroid 407, 420, 421, 429
 Certara 48, 53, 384
 charge distribution 126–127, 145, 147, 271–272, 274, 275, 286, 290, 295, 333
 net atomic 286, 334–335, 338
 charge–charge interactions 286, 306
 charged polar surface area (CPSA) 336
 CHARMM 283, 286, 288, 293–295, 303
 CHARTS 47
 CHELP 335
 ChemAxon 70, 222, 469, 470, 484
 ChEMBL 208, 234, 482, 483
 ChemBridge 479
 CHEMCATS 189, 200
 Chemical Abstracts Service (CAS) registry 12, 77, 91, 162, 188, 189, 191, 194–197, 201, 202, 204, 206, 209, 215, 216, 482
 chemical–biological read across (CBRA) 471
 chemical compound representation 6, 363, 527
 Chemical Markup Language (CML) 44, 45, 68, 135, 244
 chemical nomenclature 11–12
 chemical notations 12–14
 chemical reactions 121–151
 chemical space 244, 246, 249, 251
 Chemical Structure Lookup Service (CSLS) 192
 ChemInform RX database 146
 Chemistry Development Kit (CDK) 47, 70, 109, 222, 485, 486
 CHEMLIST 189
 CHEMnetBASE 201, 204
 chemogenomics 483–485
 chemometrics 175, 399, 400, 406, 418, 423, 425, 431
 chemotypes 68, 69, 244–245, 356–358, 484
 Chemspider 192, 200, 201, 234, 485
 chirality 33–36, 86–88, 198 characterization 47
 codes 376, 377, 387, 388
 descriptors 375
 CHIRON 86
 chord 80, 83, 86
 CHORTLES 47
 chromatographic data 203, 204
 CHUCKLES 47
 CIF2PDB 70
 CIFTEX 67
 CIFTr 70
 citation databases 212–219
 city-block distance 247, 409
 classification trees (CART) 429, 432, 433
 clinical trials 208, 209
 Clustal Omega 196, 511
 Clustal X 509
 Clustal W 509
 cluster analysis 406, 412, 417, 419–420
 cluster detection 419
 clustering 145, 419, 421
 coarse graining 290

- coefficient
 adjusted squared correlation 414
 association 247, 248
 correlation 247, 404, 407, 429
 cosine 247, 355, 356
 distance 247
 distribution 366
 energy 129
 Fourier 167, 175
 Hadamard 167
 Hamming 356
 Jaccard similarity 410
 orbital 129, 130, 275
 Pearson correlation 414, 424, 472
 probabilistic 247
 regression 423–425, 450
 simple matching 248, 404
 Tanimoto 248, 253, 254, 356, 358,
 485, 486
 wavelet transformation 175
 combinatorial chemistry 28, 272
 combinatorial libraries 48, 134, 231,
 243, 377, 379, 479
 command-driven (retrieval language)
 systems 187, 188
 comparative molecular field analysis
 (ComFA) 364, 383, 467
 comparative molecular similarity
 analysis (CoMSIA) 384
 comparative molecular surface analysis
 (ComSA) 382
 complete linkage 420, 423
 complete neglect of differential overlap
 (CNDO) 325, 326
 completeness and non-redundancy
 232
 complexity exponential 238
 compound databases 191–206
 computational chemistry 267–339,
 345
 computer-aided drug design (CADD)
 315
 CONCORD 250
 configuration interaction (CI) 330, 331
 conformation 250, 302, 361, 376
 conformational analysis 96, 302
 conformational ensemble 385
 conformational flexibility 251
 conformational space 96, 280
 conformer generation 94, 251
 connection table (CT) 23–25, 28–31,
 36, 51–54, 71, 76, 93, 135, 140,
 150, 156, 159, 191, 195, 232, 367
 Connolly surface 104–106
 ConQuest 199
 consensus models 459
 consensus prediction 468, 478, 479
 constant energy 308–311
 continuum solvent models 306
 coordinate system 36, 37, 50, 159
 CORINA 92, 250, 321, 361, 427
 correct classification rate (CCR) 471,
 473
 correlation
 adjusted squared 414
 coefficient 247, 400, 429, 472
 electron 330–332, 337
 Kendall tau 404
 Pearson 414, 424, 472
 Spearman rank 404
 COSMOS DB 222
 cost function 456
 Coulomb energy 306, 383
 Coulomb's law 286, 307, 310
 Coulson analysis 334
 counter-propagation ANN 442,
 445–447
 coupled cluster (CC) method 331
 covariance matrix 375, 400, 407, 410,
 418, 424, 430
 CPK model 102
 cross-correlation 360
 cross entropy 432
 cross terms 281, 289, 408
 cross-validation 415–416, 470–472,
 475
 CrossFire 188, 189
 cryo-electron microscopy 107, 198
 Crystallographic Information File (CIF)
 45, 65, 198
 Crystallography 66, 135, 198
 Crystallography Open Database 192,
 199
 C1s-ESCA shift 274

- CSRML (Chemical Subgraphs and Reactions Markup Language) 68–69, 244, 245, 356
- CTfile, 52, 53
- cut-off 288, 302, 304, 308, 310, 384, 477
- cyclomatic number 81
- d**
- DAT file 171
- data
- accuracy 170, 483
 - analysis methods 6, 345, 387, 528
 - chromatographic 203, 204
 - curation 7, 346, 466, 470, 482–487
 - cycle 346, 356, 481–483, 487, 488
 - mining 68, 110, 156, 158, 163, 171, 172, 356, 480, 481, 488
 - processing 12, 44, 109, 167, 204, 481, 482
 - science 481, 487, 488
 - thermochemical 202–204, 268
 - thermodynamic 202–204, 291, 312
 - transformation 175, 176
 - types 156–170, 177, 222, 351, 363
- databases 185–223
- mining 467, 478
 - search 160, 177, 187, 191, 244–245, 254, 258, 353, 499, 507–509
 - substance 191
 - system 74, 185–191, 200, 205, 208, 219, 222, 353
- data complexity 173–174
- dataset curation 467, 469–470
- data storage 169–175, 406
- data type
- bit vector 160–164
 - chemical reactions 164–165
 - molecular spectra 165–168
 - molecular structures 159–160
 - numerical data 157–159
- Daylight Chemical Information Systems 134–135
- DDAT file 171
- deep learning 6, 346, 453–461, 528
- deep neural network (DNN) 454–459
- degree-of-fit 476
- deletion 17, 255, 506
- delocalization 29–30, 127, 193
- DelPhi 307
- dendograms 417, 419, 420, 423
- denoising smoothing (DS) 176
- density functional theory (DFT) 6, 282, 320, 325, 332–334
- density matrix 335
- depth-first search algorithm 238
- Derwent Drug File 214–215
- Derwent Patents Citation Index (DPCI) 219
- Derwent World Patent Index (WPI) 28, 219
- descriptor 6, 36, 79, 158, 163, 170, 171, 246, 247, 250, 252, 277, 335, 349–389, 423, 427, 458, 467, 480, 485
- 0D molecular descriptors 363, 364
 - 1D molecular descriptors 363, 364
 - 2D molecular descriptors 352–361, 365–369
 - 3D molecular descriptors 361–363, 369–375, 387
 - 4D molecular descriptors 384–385
- atom pair 359, 361
- BCUT 364, 367–368
- biological 471
- CATS2D (Chemically Advanced Template Search) 360–362
- CATS3D 361–362
- CHARGE3D 361–362
- chemical structure 385–387
- chirality 375–382
- classification 351
- coding 249–250
- E-state 367
- EVA 375
- fragment 367
- molecular shape 377–378, 385
- molecular surfaces 377–378
- pharmacophores 362
- physicochemical 146–148, 360, 361, 369
- quantum chemical 126, 295, 363, 385
- RDF code 371–375

- descriptor (*contd.*)
 selection 249–250
 surface 336
 topological 21, 352, 364–366, 387, 388
 TPSA 366, 382
 WHIM 364, 375
- Design Institute for Physical Property Research (DIPPR) 202–203
- Detherm 202, 203
- DGEOM 92
- diagram method 255
- diastereoisomers 32, 87
- Dice 247, 248
- dictionary definition language (DDL) 66
- dielectric constant 27, 286, 306, 307, 383
- Diels–Alder reaction 124, 129
- digital object identifier (DOI) 217
- dipole moment 90, 274, 275, 326, 335, 364, 385
- discriminant partial least squares (D-PLS) 406–407
- dispersion 288, 294, 333, 359
- dissimilarity 355, 473
- distance
 coefficients 247
 matrix 20–21, 87, 254, 365, 420
 topological 20, 249, 368, 447
- distribution coefficient 366
- divide and conquer (D&C) 337
- Django 222
- DNA codon 508
- DNA Data Bank of Japan (DDBJ) 197, 499
- docking 37, 91, 199, 316, 340
- Document Type Definition (DTD) 66, 68
- Dortmund Data Bank (DDB) 202, 203
- dot matrix analysis 255
- double cross-validation (dCV) 413, 416
- Dragon 427
- Dreiding model 101
- drug design 37, 106, 171, 199, 208, 315, 356, 362, 366, 379, 453, 458, 466, 527–529
- drug discovery 2, 7, 26, 31, 44, 103, 108, 164, 316, 453, 454, 460–461, 466, 479, 480, 484, 529
- drug target 200, 208, 209, 254, 316, 503
- dynamic programming algorithm 256–258
- e**
- eccentricity 364, 378
- EC code 361
- EclipseLink 222
- effective prediction domain (EPD) 476
- eigenvalue (EVA) 322, 323, 331, 336, 367, 368, 375
- eigenvectors 322–324, 331, 418
- electrocyclic reaction 141, 149
- electron affinity 272, 325, 336, 385
- electron density 37, 103, 106, 107, 126, 280, 323, 327–329, 332–336, 362–363
- electron diffraction 91, 369–372
- electron donating 145
- electronegativity 126, 127, 272–274, 276, 277, 280, 286, 287, 339, 360
- electronic journals 187, 219–220
- electronic laboratory notebooks (ELN) 137, 138, 156
- electrophilic aromatic substitution 124, 141
- electrostatics 37, 280, 282, 294, 304
 interactions 287, 288, 305, 307, 311
 potential 107, 108, 321
 shielding 307
- elimination reaction 124, 125, 141
- EMBASE 214
- eMolecules 190, 200
- EMPIRE 337
- empirical cumulative probability density function (ECDF) 401, 402
- empirical formulas 9, 12–14, 25, 234
- empirical models 399, 412–417
- enantiomers 32–36, 204, 210, 375–377, 387
- enCIFer 67

- encyclopedias 221
 energy
 correlation 330
 force field 282, 303
 kinetic 304, 309, 311, 312, 332
 minimization 294, 517
 molecular orbital (MO) 302
 potential 95, 96, 99, 279–285, 295,
 301, 303–305, 308–312
 of protonation 385
 total 282, 304, 309, 311, 312, 329
 van der Waals 104
 zero-point 302
 Entrez Gene 207
 enumeration 17, 28, 74, 75
 environmental information 210
 enzymatic reactions 338, 369
 equilibrium constant 27, 130, 131
 EROS 142
 error back-propagation (EBP) ANN
 443–445
 essential set of essential rings (ESER)
 83
 eTOX database 222
 Euclidean distance 253, 355, 360, 370,
 409, 417, 420, 423, 429, 430, 432,
 477
 Euclidean metric 251
 Euclidean space 458
 European Bioinformatics Institute (EBI)
 196
 European Nucleotide Archive (ENA)
 197, 499
E-value 507, 508
 exchange-correlation (XC) energy 332
 excited state 301, 330, 331
 ExPASy 197, 207, 208, 513
 experimental design 169, 481
 explicit solvation model 307
 extended connectivities 77, 78, 164,
 364, 366
 extended Hückel theory (EHT) 323

f
 false negative 415, 514
 false positive 164, 415, 514
 Fast Fourier transformation (FFT) 175
 fast sequence searching 258
 FASTA 196, 258, 259, 503
 federated database system (FDBS) 222
 file formats 5, 36, 43–70, 72, 94, 109,
 134, 171, 172
 fingerprint 160, 163, 239, 247, 249,
 350, 352, 353
 biological 471
 circular 354, 364, 366
 extended connectivity fingerprints
 (ECP) 164, 364, 366
 hashed 240, 241, 250
 MACCS 353
 Fisher discriminant analysis 430
 Fisher weight 405
 FlexX 369
 flux balance analysis 150
FlyBase 207
 force field 94, 280, 292, 302, 304
 Allinger 280
 AMBER 283, 284, 294
 CFF 284, 289
 CGenFF 294
 CHARMM 283, 294
 GLYCAM 293
 GROMOS 283, 294
 MARTINI 290
 MM2, MM3, MM4 280, 292
 MMFF 284
 OPLS 295
 protein 294
 TINKER 293
 UFF 292
 Urey–Bradley 289
 Fourier coefficients 175
 free energy 280
 Langevin dipoles 307
 perturbation 316
 of solvation 307
 Friedel–Crafts alkylation 146
 frontier molecular orbital theory (FMO)
 128
 full structure search 161, 162,
 232–235, 251
 full-text databases 219–221
 fully integrated database systems 188

- functional groups 13, 14, 28, 124, 138, 145, 146, 163, 212, 240, 292, 295, 352, 469, 486
- g**
- gap penalty 506
 - gas chromatography 204, 205
 - Gaussian functions 323, 326, 328, 384
 - Gaussian type orbital (GTO) 328
 - GenBank 197, 254, 497, 499–501
 - Generic Match Algorithm (GMA) 238
 - general citation databases 218
 - generalized Born (GB) method 306
 - generalized gradient approximation (GGA) 333
 - genetic algorithms (GA) 98, 301, 427, 445, 529
 - genome 207, 497–499, 511
 - GenomeQuest 196
 - Gibbs free energy 131
 - Gini index 432
 - global minimum 95, 96, 301, 415
 - global optimum 449
 - Glycan Structures Database 208
 - GlycomeDB 208
 - glycomics 207
 - Google Patents 214, 221
 - Google Scholar 213, 218
 - graph 15, 44, 79, 80, 150, 157, 232, 251, 252, 365
 - isomorphism problem 74, 251
 - graph theory 16–20
 - GRid-INdependent descriptors (GRIND) 384
 - grid search 96
 - Groningen Molecular Simulation (GROMOS) 283, 294, 303
 - Grubb's tests 470
- h**
- Hadamard coefficient 167
 - Hamming distance 256, 356
 - Hammond's postulate 246
 - harmonic potential 282–285, 289, 290
 - Hartree–Fock (HF) 159, 325
 - hash algorithm 49
 - heat capacity 269
 - hash codes 87, 144, 160–162, 234, 235
 - hashed fingerprints 240, 241, 250
 - hashing 161, 162, 164, 234, 235, 240, 352, 353
 - heat of formation 58, 269, 385
 - heuristic algorithms 415
 - HHsearch 516
 - Hibernate 222
 - hidden layers 443, 445, 454, 455, 457, 458
 - hidden-Markov models (HMMs) 514
 - hierarchical cluster analysis (HCA) 406, 420, 473
 - HORACE 145–146
 - highest occupied molecular orbital (HOMO) 107, 128, 331, 336, 385
 - high-scoring segment pair (HSP) 503
 - high-throughput screening (HTS) 372, 379, 471
 - Hill order 194
 - histograms 99, 100, 359, 362, 401, 402
 - HomoloGen 197, 207
 - homologous proteins 502, 503, 505, 509, 515–517
 - homology modeling 515–518
 - homology searching 195, 254
 - Hooke's law 268, 283, 284
 - hosts 187, 188, 190, 196, 210, 213–215, 218, 383
 - Hückel matrix 274, 275, 322–324
 - Hückel molecular orbital (HMO) 6, 274, 320–324
 - human genome 497
 - hybrid functionals 333
 - hybridization states 92, 270–271, 275, 280, 369
 - hydrogen bond donor 58, 251, 271, 360, 362
 - hydrogen bonding 27, 108, 364, 379
 - hydrogen motions 305
 - hydrophobicity potential 37, 108, 364, 379
 - hyperconjugation effect 276, 277
 - hypersurface 95, 301, 309

i

- iAMOEBA 290
 image recognition 454, 529
 implicit solvation models 307
 implicitly polarized Q (IPolQ) 293
 InChI 48, 50, 135, 191
 InChIKey 14, 48–50, 75, 135, 234
 incidence matrix 19–20
 index(ing)
 branching 365
 charge-related topological index (CTI) 234
 Jaccard 248
 topological 87
 induced subgraph 17
 inductive effect 127, 128, 131, 147, 272, 274, 276
 inductive learning 3–6, 124, 132, 268, 345, 349, 527
 InfoChem 143–144, 213
 infrared spectra 166–168, 175
 Inorganic Crystal Structure Database (ICSD) 198, 199
 INPADOC 215
 interaction
 charge–charge 286, 306
 Coulomb 286, 310
 dispersion 288
 electrostatic 286–288, 303, 304, 306, 310
 intermolecular 281
 van der Waals 286–289, 303, 333
 interchangeability classes (ICs) 83–85
 intermediate neglect of differential overlap (INDO) 326
 internal coordinates 36, 37, 45, 51, 52, 95, 97, 98, 159, 160, 289
 International Nucleotide Sequence Database Collaboration (INSDC) 197, 499
 International Pharmaceutical Abstracts (IPA) 214
 International Union of Crystallography (IUCr) 66
 International Union of Pure and Applied Chemistry (IUPAC) 11, 165
 InterPro 207

InterProScan 514

- interquartile range (IQR) 400, 403
 ionization potentials 30, 31, 272, 320, 324–326, 336, 337, 385
 iScienceSearch 192, 200
 isomers 13, 25–27, 31–33, 73–74, 86, 89, 188, 234
 isomorphism 73–74, 163, 235–239, 241, 243, 244, 251, 252
 isosurfaces 107–108
 isovalue-based electron density 106

j

- Jaccard similarity coefficient 410
 Jacobi rotation 418
 Java Persistence API (JPA) 222
 JavaScript Molecular Editor (JSME) 71, 72, 135, 136
 JCAMP-CS 44, 45
 JCAMP-DX 44, 171–172
 JChem 70, 222, 484
 JME 72, 135
 JOELib 70
 Journal Impact Factor 218

k

- KAGGLE datasets 459
 Karlin–Altschul parameters 508
 Kennard–Stone clustering 473
 kinetic energy 304, 309, 311, 312, 332
 k-means clustering 419, 421
 k-nearest neighbors (kNN) 147, 407, 430–431, 467
 Knime 100, 484
 Kohonen artificial neural network 146–148, 360, 379, 445, 447, 448
 Kohonen map 147, 148, 170, 419
 Koopmans’ theorem 336, 337
 K-rings 83
 Kyoto Encyclopedia of Genes and Genomes (KEGG) 199

l

- labeled data records (LDR) 171
 Langevin equation 307
 Laplacian, of electron density 335
 LCAO-approximation 323, 329, 334

- Leapfrog algorithm 304
 learning
 algorithms 380, 453, 458, 529
 cost-sensitive 474
 inductive 3–6, 124, 132, 268, 345,
 349, 527
 methods 176, 346
 rate 445, 449
 leave-one-out (LOO) 415, 470
 Lee–Richards surface 106
 Lennard–Jones potential 287, 288,
 295, 310, 383
 Lexika 221
 LHASA 86
 library design 467
 LigandBox 199
 LigandScout 362
 LigPrep 484
 linear combination of atomic orbitals
 (LCAO) 321, 323, 327, 329, 334
 linear discriminant analysis (LDA) 33,
 412, 418, 429, 430
 linear free energy relationships (LFER)
 130–132, 306
 linear latent variables 410–412, 417,
 423, 424, 430
 linear scaling methods 337–338
 line notation 14, 44, 48, 87, 134, 232,
 233, 243, 244
 lipophilicity 364, 366
 liquid chromatography 377
 loading
 matrix 400, 418
 plot 412, 417, 422
 local density approximation (LDA)
 333
 local ionization potential 336–337
 localized molecular orbital (LMO)
 technique 338
 local minimum 285, 301, 449
 local optima 450, 455
 DIALOG 187
 lone pairs 30, 326, 328, 329, 338
 long-range electrostatics 291, 302,
 306, 310
 long-range forces 303, 310–311
 Lorentz–Berthelot 288
 lowest unoccupied molecular orbitals
 (LUMO) 107, 128, 331, 335
- m**
- MACCS keys 353
 machine learning 145, 158, 434, 454,
 458, 459, 461, 488
 macromolecular Crystallographic
 Information File (mmCIF) 65,
 67–68, 70
 macromolecules 44, 48, 58, 62, 67,
 102–103, 107, 231, 283, 284, 307
 Mahalanobis distance 407, 410
 Manhattan distance 247, 355, 409
 mapping 67, 74, 134–136, 138, 210,
 211, 234–238, 241, 242, 252, 380,
 381, 419, 439–441, 451
 atom-to-atom 134–136, 139, 244,
 254
 Markush structures 27, 47, 192, 193,
 215, 243
 MARPAT 28, 189, 215
 mass spectroscopy 166, 204, 205, 404,
 421–423, 432–433
 materials design 294, 458, 461
 mathematical methods 346, 406, 408
 matrix 18, 20, 21, 90, 140, 170, 253,
 256, 367, 400, 406, 418, 430,
 503–506, 509
 adjacency 18–19
 bond 21
 bond–electron (BE) 21–23, 140
 distance 20
 hat 476
 incidence 19
 permutation 89
 matrix reaction 140
 maximal segment pair (MSP) 503
 maximum common substructure (MCS)
 242–243, 250–254
 Maxwell distribution 304
 mBed algorithm 511
 MDL 44, 52, 53, 94, 134, 143, 163, 165,
 353
 mean absolute error (MAE) 473
 mean-centered matrix 175, 404, 407,
 418, 423, 424

- mean field approximation 325, 330, 331
 mean squared error (MSE) 413, 414
 median 402, 403, 408, 427, 428
 median absolute deviation (MAD) 400, 403, 408
 medical information 208–209
 Medical Subject Heading (MeSH) 213
 medicinal chemistry 208, 231, 232, 366, 468, 483
 Medline 189, 191, 206, 213, 214, 216
 membranes 291, 292, 315
 memory complexity 232
Merck Index 208, 221
 Merck Molecular Activity 459
 mesomeric effect 128, 274
 mesomerism 27, 193, 274
 metabolic flux analysis 150
 metabolic information 135, 208
 Metabolic Information Input System (METIS) 135, 136
 metabolic pathways 150, 208
 metadata 44, 65–69, 167
 meteorite 421–423, 432–433
 Metropolis Monte Carlo (MC) 98
 Michael addition 124, 146
 microcanonical ensemble 308
 MIMUMBA 98
 MINDO 326
MineSoft PatBase 215
Minkowski distance 409
 MLR 440, 450
 mmcCIF File Format 67–68, 70
 MMFF 287, 293
 MM2/MM3/MM4 280, 286, 292
 MNDO-ESP 335
 modelability 467–471
 modeling 68, 345, 440
 QSAR/QSAR 345, 346
 quantitative 453
 MODELLER 515, 519
 model validation 467, 468, 472, 478, 480, 481, 517
 Modified Neglect of Diatomic Overlap (MNDO) 326, 327, 335
 Mol2 45
 molar refraction 269
 MolConverter 470
 molecular descriptors 36, 58, 79, 163, 164, 170, 249, 345, 349–351, 359, 363, 388, 406, 423, 454, 484
 molecular diameter 378
 molecular dynamics (MD) 98, 280, 302–317, 385
 molecular electrostatic potential (MEP) 108, 335, 378, 380
 molecular graph 70, 74, 79–82, 85, 86, 100–102, 365, 369
 molecular interaction fields 384
 molecular mechanics 280–292, 339
 molecular modeling 71, 100, 199, 293, 340, 481, 488
 Molecular Operating Environment (MOE) 470
 molecular orbital (MO) theory 28, 107, 270, 320–327
 ab initio 320, 327–333
 energies 302
 molecular representation 5, 10, 11, 14, 157, 364
 molecular self-assembly 316
 molecular shape analysis 385
 molecular span 378
 molecular structure 6, 10, 23, 25, 28–29, 36, 44, 48, 51, 58, 69, 101, 103, 159–161, 232, 301, 321, 345, 351, 385, 527
 molecular surface 6, 37, 103–108, 336, 337, 378–382, 388
 molecular volume 336
 molecular weights 58, 155, 234, 269, 386
 molecularity 124, 537
 molecule editor 48, 57, 70–73, 135, 525
 molecule viewer 70, 71, 73
 Molfile 44, 52–58, 134
 MOLGEO 92
 Moller-Plesset (MP) theory 331
 MOLMAP 369
 Monte Carlo (MC)
 search 302
 simulation 98, 280, 296
 Morgan algorithm 48, 77, 87, 233, 366

- Morgan algorithm (*contd.*)
 stereochemically extended (SEMA)
 162
- Morse function 282, 283
- Mulliken population analysis 271, 334
- Multi-level Neighborhoods of Atoms (MNA) 358–359
- multilinear regression 440
- multi-variate data representation
 439–441
- multigraph 16
- multiple sequence alignment (MSA)
 509, 511
- multipole expansion 286
- multipole moments 287, 335
- multivariate calibration 406, 413, 423,
 429
- multivariate classification
 binary classification 429
 classification trees 429, 432
 discriminant PLS 430
 k-nearest neighbor 430
 linear discriminant analysis 430
 multicategory classification 429
 multivariate similarity 429
 pattern recognition 429
 regression methods 429
 support vector machine 429, 431
- multivariate data
 cluster analysis 406
 linear latent variables 410–412
 matrix 406
 multivariate calibration 406
 multivariate classification 407
 object distance 408–410
 preprocessing 407–408
 multivariate data analysis 346,
 399–402
- mutation 255, 311, 504, 509, 515
- n**
- natural atomic orbital-point charge (NAO-PC) 335
- natural population analysis (NPA) 334,
 335
- Needleman and Wunsch 256
- neglect of diatomic differential overlap (NDDO) 326, 327
- net atomic charges 286, 334–336, 338
- neural network 166, 167, 360, 454–457
 architecture 455
 artificial 438
 back propagation 457
 counter-propagation 445
 deep 453, 454
 error-back propagation 443
 feed-forward 457, 458
 self-organizing 146, 360, 379, 381
 shallow 453, 454
 neuron 147, 442–450, 458
- Newton equation 303
- Newtonian mechanics 292
- NIPALS 418, 425
- NIST Data Gateway 203
- NMR chemical shifts 274
- NMR spectra 58, 87, 91, 198, 204–206,
 291, 304, 315, 369, 374, 386, 526
- nmrshiftdb2* 206
- noise 169, 426, 456
- nomenclature 11–12, 34, 73, 234, 324,
 328
- non-bonded electrostatic interactions 303
- nonlinear mapping 417, 419, 422, 441
- non-polynomial (NP)-complete problem 235
- normalization 6, 48, 170, 222, 355,
 408, 484
- notation 12, 14, 73, 400
- nucleic acids 58, 62, 195, 200, 207,
 254–259, 293, 294
- Nucleic Acid Database (NDB) 199,
 200, 254–259
- nucleophilic aliphatic substitutions 124, 128, 141, 148
- o**
- octet rule 23
- OEChem 69
- OELib 70
- ONIOM superimposition 338
- Online Public Access Catalogue (OPAC) 217, 220

- ontology 156, 208
 Open Babel 70, 109, 470
 OpenEye 47, 69
 optical character recognition (OCR) 220
 optimization 159, 232, 236, 259, 432, 442, 450, 455–458, 515
 algorithms 467
 backtracking algorithm 238
 geometry 302
 global 294
 Optimized Potentials for Liquid Simulations (OPLS) 293, 295, 303, 425
 orbitals 30
 coefficients 129, 275
 electron densities 385
 electronegativity 272
 energies 337
 OrChem 222
 ORCID 216
 ordinary least-squares (OLS) regression 407, 418, 423–425, 430
 organometallic 31, 92, 212, 484
 orthologs 502
 outliers 174–175, 404, 470, 477
 out-of-plane bending 285
 overfitting 176, 412, 431, 432, 445, 450, 455, 457, 467, 475
 oversampling 474
 overtraining 176, 450, 451, 455
- p**
 parachor 269
PARAFAC 419
 paralogs 502
 parameterization 280–282, 284, 288, 291–295, 305, 327, 335
 partial atomic charges 127, 271, 280, 292, 356, 362, 366, 368, 374, 376, 382
 partial equalization of orbital electronegativities (PEOE) 127, 272–275
 partial least-squares (PLS) 383, 385, 406, 423
 discriminant analysis 430
 regression (PLSR) 383, 406, 407, 425–426
 particle mesh Ewald (PME) method 310, 311
 partitioning 239, 385, 419
 patents 196, 214, 220, 221
 databases 28, 189, 214, 215, 219
 Patent Chemistry Database (PCD) 189
 path 17, 240
 counts 250, 253
 number 365
 patterns 512
 matching 75, 83, 85
 recognition 345, 346, 351, 429
 PatternHunter 259
 Pauli principle 288
 PDB file format 44, 58–65, 94
 PDB2CIF 70
 Pearson correlation coefficient 404, 407, 414, 424
 Pearson product-moment correlation coefficient (PPMCC) 247, 404
percentiles 403
 Perception Reaction Center 138–139
 periodic boundary conditions 308, 310, 311
 permutation 35, 74, 88–90, 149
 perturbation theory 130, 331
 PFAM 207, 514
 pharmaceutical and medical information 208–209
 pharmaceutical excipients 209
 pharmacophore 160, 251, 360, 362, 367, 385
 screening 75
 searching 251, 252
 physical properties 35, 37, 187, 201–202, 209, 232, 308, 335, 386, 502, 509
 physicochemical effect 126–128, 145, 368
 physicochemical properties 68, 159, 185, 244, 249, 356, 368, 369, 376, 384, 387
 π -charge distribution 274
 PLS2 425

- PM3 327
 PM5-PM7 328
 PMML 171–172
 point accepted mutations (PAM) 256, 504, 505
 point charges 286, 307
 Poisson–Boltzmann equation 307
 Poisson equation 307
 polar surface area (PSA) 336, 366, 382
 polarity 126, 504
 polarizability 108, 128, 271, 275–277, 290, 335, 336, 360, 363, 368, 369
 polarizability effect 127, 128, 147, 271, 275–277
 polarization 274, 290, 291, 294, 308, 329, 337–339
 POL5-TZ 290
 polycyclic aromatic compounds (PAC) 427–429
 polymers 47–49, 191, 194, 204, 324, 385, 386, 527
 Pople diagram 329, 330, 332
 Pople-Pariser-Parr (PPP) 325
 population analysis 271, 334
 PostgreSQL 222
 potential energy 95, 96, 279, 282–284, 295, 301, 304, 308, 309, 311
 potential energy function (PEF) 99, 281, 303–305, 310, 311
 prediction 423, 440
 chemical reactivity 128
 data 176
 properties 345, 347
 Prediction of Activity Spectra of Substances (PASS) 358, 359
 Predictive Model Markup Language (PMML) 172–173
 predictive power 451, 459, 461, 467, 474, 478, 513, 514
 predictivity 450, 455–460, 473, 485
 pre-processing 6, 236, 239, 407–412, 438
 primary literature 61, 186–189, 191, 196, 206, 212
 principal component analysis (PCA) 375, 406, 407, 412, 417–419, 422–425, 430
 principal component regression (PCR) 423–425
 principal moments of inertia 378
 3D printing 103
 probabilistic coefficients 247
 probability 37, 98, 161, 323, 359, 405, 457, 504, 514
 probability density function (PDF) 401, 402
 problem-related transformation 408
 PROCHECK 517
 3D profiles 517
 projection 33, 103, 159, 379, 411, 412, 417, 419, 440, 442, 447
 ProQuest DIALOG 187, 208, 214
 PROSITE 207, 512–514
 Protein characteristics 509–514
 Protein Data Bank (PDB) 44, 58, 199, 200, 311, 313, 501
 protein families 7, 207, 499, 508, 509, 512, 514, 518
 protein folding 303, 316
 protein information resource (PIR) 196, 501
 protein-ligand docking 316
 protomers 470
 protonation 275, 276, 281, 385
 protonation states 281
 prototropy 26
 pruning 432, 457
 pseudo-isomerism 195
 PubChem 75, 191, 192, 208, 234, 353, 482, 483, 485, 486
 PubMed 191, 192, 213, 220, 500
 Python 69, 161, 222
- q**
quantiles 403
 quantitative structure-activity relationships (QSAR) 335, 345–347, 384, 406, 458, 465–488
 quantitative structure-property relationships (QSPR) 334, 345–347, 349, 406, 427, 465–488
 quantum chemistry 126, 159

- quantum mechanics 51, 107, 271, 280, 281, 286, 306, 320–340, 362, 527
query sequence 505, 507–509
- r**
- racemates 36
racemization 149, 305
radial basis function artificial neural network (RBF ANN) 440
radial distribution function (RDF) 134, 371–376, 387
radicals 30, 108, 145, 194
radius of gyration 378
Randic connectivity index 234, 365–366
random forests 429, 432, 458, 473, 475, 478
randomization of response 475
random weight drop out 457, 458
RDfiles 52
RDKit 109, 222, 484, 485
reactions 68, 121–151
 biochemical 123, 148
 center 125, 135, 138, 139
 chemical 164
 classification 139, 141, 143
 editor 135
 equation 122, 133
 mechanism 125
 networks 149
 organic 90, 141, 142, 146, 212
 oxidation 142
 parallel 123, 133, 165, 537
 path 149
 photochemical 146, 149, 369
 prediction 142
 rate 131
 representation 121
 reduction 142
 search 138, 244
 site 138
 SMILES 134
 type 123, 145
reaction database 133–138, 210–212
reactive force field (ReaxFF) 290
reactivity chemical 126–132
reagent 122, 126, 128, 133, 164, 165, 191, 210–212
real world data 173–175
Reaxys 165, 187–191, 193, 194, 198, 200–206, 208–218, 220
receptor 106, 251, 315, 362, 371, 374, 381–384, 468, 474, 528
regioselectivity 130
regression 424, 455, 476
 coefficients 423, 450, 455
regularization 445, 455–458, 460
relational database management system (RDBMS) 185, 186, 222
relaxation 77, 78, 239, 241, 309, 310, 315
relevance vector machines 455, 458
relevant cycles 83, 84
Representational State Transfer (REST) 71, 222
repulsion 104, 288, 322, 325, 326, 330
 electron-electron 323
resampling 415, 416
residual 127, 274, 276, 413, 414, 423, 424, 476
residual standard deviation (RSD) 476
residue-based fluctuation analysis 313
resonance 27, 29–30, 128, 244, 274
 effect 127, 132, 145
RESP 335
REST API 222
retention indices 382, 427–428
RGfiles 52
ribosomes 107, 315
RInChI (International Chemical Identifier for Reactions) 49, 135
ring perception 16, 17, 79–86
RNAs 197, 200
robustness 450, 455
Römpf Online 221
root mean square (RMS) 97, 100, 251, 310, 311, 313, 314
root mean squared error (RMSE) 414, 448, 449, 473, 499
ROSDAL (Representation of Organic Structures Description Arranged Linearly) 14, 233
rotamers 316, 516

- rotatable bond 94–96, 99, 100, 363
 ROTATE 97, 98, 100
 rotational barrier 95, 302
 Remote Procedure Call (RPC) 71
 RXNfiles 52
 RXN format 134
- S**
- saccharomyces genome database 207
 safety information 206–207, 209–210
 Sammon’s nonlinear mapping (NLM)
 417, 419, 422, 423
 scalars 107, 400
 scaling methods 337, 407
 scatter plots 417, 418, 433
 Science Citation Index (SCI) 187, 213,
 216, 218–220
 Science of Synthesis (SoS) 212, 219
 Scientific Technical Network
 International (STN) 188–190,
 195, 196, 200, 208, 210, 215, 218,
 221
 scientometrics 218
SciFinder 165, 188–189–191, 193, 194,
 198, 201, 206, 211, 216, 217
Scopus 190, 213, 214, 216, 218, 220
 scoring 411
 distance 410
 function 517
 matrix 255, 257, 400, 418, 503
 plot 412
 screening 91, 162, 163, 239–241, 250,
 272, 379, 467, 483, 487, 517, 518
 scree plot 418
 SDF Toolkit 70
 SDfiles 52, 53, 57–58, 69, 70, 94
 SEAL algorithm 384
 Search(ing) 231–260
 3D similarity 252
 3D structure 250
 atom-by-atom 237
 automorphism 241
 bibliographic databases 216
 chemical structures 231
 depth-first 238
 full structure 161, 232
 fuzzy-substructure 244
 homology 254
 maximum common substructure
 242
 pharmacophore 251, 252
 reaction 244
 sequence 254, 258, 502
 similarity 162, 245, 252–254, 350,
 352
 substructure 162, 243
 superstructure 241
 secondary literature 187, 212
 secondary structure 58, 83, 103, 107,
 314
 self-consistent-field (SCF) 325, 327,
 329–331, 333
 self-organizing map (SOM) 147, 360,
 361, 380, 419, 451
 self-organizing network 369, 379
 semiempirical 6, 51, 107, 130, 320,
 324–327, 331–339
 sensitivity 130, 168, 258, 259, 415, 432,
 471, 473, 503, 514
 sequence 195, 254, 497
 alignment 254, 502
 biopolymers 195–198
 DNA/RNA 499
 homology 502
 protein 499
 search 255–259
 similarity 255, 502
 sequence database search 499–508
 sequence signature 512
 set of all rings 81–82
 SHAKE 305
 shallow neural network (BNN)
 454–459
 Shannon entropy 174, 359
 Shannon equation 174
 shape indices 359
 similarity 148, 232, 245, 354, 369, 377,
 408, 430, 468, 477, 485
 coefficients 248
 indices 363
 matrix 254
 measures 247–248, 250, 355
 search 232, 245–250, 252–254, 350,
 470

- Simple Object Access Protocol (SOAP) 71
 SIMPLS 425
 simulated annealing 98
 singlet 30
 singular value decomposition (SVD) 418
 Slater-type orbitals (STOs) 327, 328, 330
 smallest set of smallest rings (SSSR) 82–84
 SMARTS 47–48, 79, 82, 83, 134, 243, 244, 514
 SMILES 14, 44–48, 58, 71, 134–135, 233, 243, 485
 SMIRKS 47, 134–135, 244
 Smith and Waterman 258, 259
 solvation shell 291
 solvent-accessible surface 104–106, 307, 336
 solvent effect 276, 290, 305–308
 solvent-excluded surface 104
 space-filling model 102, 104
 spatial distance 370
 SPC 290, 308
 specificity 353, 415, 471, 473, 474
 SpecInfo 205
 spectra 137, 165, 170, 204, 386, 420, 439
 calculation 332
 experimental 170, 206
 simulation 74
 Spectral Database for Organic Compounds (SDBS) 206
 spectral library 203, 247
 spectroscopic database systems 205
 sphere exclusion 472, 473
 spin density 108
 spin state 280
SPRESI 211
 standard deviation 400, 402, 403, 405, 407, 408, 413, 418, 476, 477, 483
 standard error of calibration (SEC) 414, 424
 standard error of prediction (SEP) 412–414, 427, 428, 459
 standardizer 469, 484
 STAR (Self-defining Text Archive and Retrieval) file 65–67
 statistical data evaluation 402–405
 statistical mechanics 309
 statistics 218, 336, 346, 400, 407, 424, 450, 455, 467, 472, 475
 stereoaxes 31
 stereocenters 31, 33, 86–88, 485
 Stereochemical Extension of Morgan Algorithm (SEMA) 87, 162
 stereochemistry 14, 19, 31, 33–35, 47, 49, 56, 57, 87, 89–90, 148–149, 162, 485
 stereodescriptors 57, 88, 90
 stereoelectronic effect 127, 128, 538
 stereoisomerism 32, 47, 470
 stereoisomers 25, 33, 87, 88, 90, 192, 375, 470, 485
 stereoplanes 31
 steric effect 127, 128, 131
 Stevens–Johnson Syndrome (SJS) 479
 stoichiometry 13, 133, 139, 528
 STRAPS 47
 structural biology 315
 structural fingerprints 164, 232, 239
 structural function 305
 structural key 162–163, 239, 350, 352, 353, 359
 structural transition 316
 structure checker 469
 structure diagram 10, 15, 24, 27, 33, 70, 72, 100, 352, 358
 3D structures 45, 51, 57, 60, 72, 73, 86–103, 198–200, 250–252, 361, 369–370, 375, 376, 386, 503, 515, 526
 Structured Query Language (SQL) 158, 196, 222
 structure elucidation 4, 44, 73, 91, 232, 243
 structure generator 55, 72, 73, 91, 92, 98, 361, 370
 structure isomers 73–74
 structure keys 160, 163, 164, 250, 356
 structure-searchable database 222, 223
 subgraphs 17, 18, 68, 244, 356

- substitution 124, 128, 141, 148, 195, 255, 256, 504, 505, 509
 substructure 6, 54, 68, 94, 162–164, 200, 201, 212, 232, 352
 substructure search 211, 235–245
 supergraph 17, 18
 supermolecule 303–307
 superstructure 6, 93, 94, 156, 241
 supervised method 429, 439, 440
 support vector machine (SVM) 429, 431–432, 455, 458, 467
 SureChEMBL 214
 Surfaces 106, 337
 SWISS-MODEL 515, 516
 Swiss-Prot 196, 501, 513
 SYBYL line notation (SLN) 48, 243
 symmetry group 74
 synthesis design 3, 44, 142, 147, 272
 synthetic methodology databases 212
 synthetic polymers 191, 194, 204
 System Development Corporation (SDC) 187
- t**
- Tanimoto coefficient 247, 248, 250, 253, 356, 410, 420, 485
 tautomerism 26–27, 43, 48, 74–76, 109, 188, 193, 291, 469, 470, 484
 tblastn 509
 T-COFFEE program 511
 temperature factor 63, 311, 314, 374
 tertiary literature 187, 219, 221
 test set 412, 461, 467, 468, 472, 473
 text mining 525
 thermodynamic and thermochemical data 202–204
 thermodynamical properties 283
 threshold moving 474
 Tikhonov regularization 456
 TINKER 293
 TIP3P 290, 295, 305, 308
 TIP4P-FQ 290
 toolkits 109–110, 222, 485
 topography 10, 25
 topology 10, 25, 74, 145, 162, 198, 232
 autocorrelation vectors 368
 index 87, 234
 torsions 249
 torsion angles 100, 251, 285, 286
 total electrostatic free energy 306
 toxicity 69, 191, 209–210, 244, 466, 478, 487, 528
 toxicity, environmental, safety information 209, 210
 toxicology 2, 209, 356, 471, 480, 487, 529
 TOXNET 209
 ToxPrint 69, 244, 245, 356
 training set 412–416, 423, 430, 448, 461, 467, 468, 472, 475, 477, 479
 trajectory 106, 279, 309, 312, 313
 transformation 63, 134, 159, 168, 170, 244, 346, 351, 404, 408, 424, 438
 transition metal 324, 327, 332, 333
 transition state 126, 139, 289, 301
 TrEMBL 196, 501
 triplet 30, 251
 Tripos 48, 53, 384
 trivial name 10–12, 192, 234
 true positive 415
t-statistic 405
- u**
- Ugi's Scheme 140–143
 unambiguous 11, 25, 33, 47, 76–79, 162, 186, 235, 373, 502
 underfitting 412, 455
 undersampling 474
UniCarb-KB 208
UniGene 207
 UniParc 501
 UniProt (Universal Protein Resource) 196, 201, 499, 501
 UniProt Knowledgebase (UniProtKB) 501, 503, 507, 515
 Unique Ring Families (URFs) 85
 UniRef 501
 unit cell 61, 63, 200, 308
 united-atom force field parameterizations 305
 universal approximation theorem 458–459
 universal force field (UFF) 292–293

- unsupervised learning 146, 147, 381, 417, 439, 440
 Urey-Bradley force fields 289
 user-defined weighting factors 253
 USMILES 47
- V**
 valence electron 21–23, 141, 246
 Valence Shell Electron Pair Repulsion (VSEPR) 93
 valence shell ionization energy (VSIE) 324
 valence states 143, 272
 validation 156, 415, 444, 449, 461, 471, 475, 481
 van der Waals 282, 304
 interactions 288, 290, 304, 334
 radii 37, 102, 104, 288, 306
 surface 104
 volume 104, 369
 variable selection 405, 424, 426–427, 467, 471, 550
 variance 158, 401, 403, 404, 407, 417, 418, 456
 vectors 400
 Boolean 353
 vector field 107, 108
 Verlet algorithm 304
 vertices 15–18, 20, 21, 74, 80–83
 VESPA 335
 vibration 63, 87, 289, 292, 303, 375
 vibrational circular dichroism (VCD) 87
 vibrational frequencies 292, 375
 vibrational spectra 289
 viewers 33, 70, 71, 73, 103
 virtual libraries 28, 110, 479
 virtual orbital 321, 331
 virtual reality 103
 virtual screening 91, 199, 315, 360, 467, 468, 479–482, 487, 518
 visualization 37, 43, 60, 100–103, 107, 108, 159, 199, 200, 218, 381, 401, 412, 418
 voice recognition 453, 454
 VolSurf 384
 volumetric properties 107, 108
- W**
 WABA 259
 walk 17, 236, 243
 Ward linkage 420
 water models 291, 306
 wavefunction 37, 51, 108, 280, 330–332
 wavelet transformation 175–176
Web of Science 190, 218, 219
 WHATCHECK 517
 Wiener index 365
 wire frame model 101
 Wiswesser line notation (WLN) 14
 Wittig–Horner reaction 145
 WOMBAT 481
 Worldwide Protein Data Bank (wwPDB) 58, 200
WormBase 207
- X**
 XDfiles 52
 XML 44, 52, 65, 66, 68, 70, 71, 135, 172, 244, 245, 356
 X-ray 198, 283
 crystal diffraction 63
 crystallography 304, 518
 diffraction 58
 XSMILES 47
 XYZ-Format 50
- Y**
 Y-randomization 475
- Z**
 zero-point energy 302
 ZINC 198, 466
 Z-Matrix 37, 45, 51–52
z-transformation 408

Substance Index

a

- acetylcholine 381
N-acetyl-p-aminophenol (APAP) 167
 adamantane 35
 α -conotoxin PNI1 polypeptide 60
 aniline 270, 274

b

- benzene 27, 29, 95, 132, 163, 320, 331
 benzodiazepine 368
 benzoic acid ester 130
 2*R*-benzylsuccinate 95
 binaphthalene 87
 binaphthyl 35
 Boranes 31
 bovine pancreatic trypsin inhibitor (BPTI) 310
 1,3-butadiene 29, 129, 149, 322–324

c

- cannabinoid receptor 460
 Carbohydrates 208, 291, 293
 (2*R*,3*E*)-4-chlorobut-3-en-2-ol 53
 chloromethane 36
 corticosteroid-binding globulin (CBG)
 receptor 371, 379
 cubane 82–85
 cyanoanilines 382
 cyclobutene 149

d

- dipeptidyl peptidase 460
 dopamine 368

f

- Ferrocene 31

g

- GGG{2-10}R{5-10}R{5-10}RGAGA
 195
 glyceraldehyde 34

h

- helicenes 32
 herbicides 375
 2-hydroxy-propionic acid 33, 34
 hypochlorous acid (ClOH) 76

i

- isoleucine 305, 505

l

- lactic acid 33–35
 lidocaine 192, 193
 lysozyme 102, 104

m

- membranes 291, 292, 315
 metallocenes 195
 2-methoxy-1,3-butadiene 129
 4-methylcyclohexene 233
 methyl ester 130, 131
N-methylpyrrole 159, 168
 muscarinic receptor 381, 382

n

- nicotinic receptor 381

nitroanilines 382

nitrophenol 123

nucleic acids 58, 62, 195, 200, 207,
254–259, 293, 294

o

orexin receptor 460

p

paracetamol 166, 190

paracyclophane 35

r

RNAs 197, 200

s

sulfamide 58

sulfuric diamide 58

t

tetracycline repressor 311, 313

thrombin 360, 460

triazine 375

