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List of Abbreviations

Abbreviation	Full Form
3D	Three-dimensional
5-CV	5-fold cross-validation accuracy
10-CV	10-fold cross-validation accuracy
A	Balanced accuracy
Aβ	Amyloid beta
Ach	Acetylcholine
AChE	Acetylcholinesterase
AD	Alzheimer's disease
ADMET	Absorption, distribution, metabolism, excretion, and toxicity
AI	Artificial intelligence
ARIA	Amyloid-related imaging abnormalities
ASCII	American standard code for information interchange
AUC	Area under the curve
BOA	Bayesian optimization algorithm
CADD	Computer-aided drug design
CDSS	Clinical decision support systems
ChAT	Choline acetyltransferase
CNS	Central nervous system
COX-1	Cyclooxygenase-1
COX-2	Cyclooxygenase-2
CSF	Cerebrospinal fluid
DA	Dopamine
DAPK1	Death-associated protein kinase 1
DCM	Dichloromethane
DL	Deep learning
DT	Decision tree
EGF	Epidermal growth factor
EF	Enrichment factor
EEG	Electroencephalography

EOAD	Early-onset Alzheimer’s disease
FAD	Familial Alzheimer’s disease
FPR	False positive rate
FP	False positive
FRET	Fluorescence resonance energy transfer
GANs	Generative adversarial networks
GABA	Gamma-aminobutyric acid
GH	Goodness of hit
GMQE	Global model quality estimation
GNNs	Graph neural networks
HBAs	Hydrogen bond acceptors
HBDs	Hydrogen bond donors
HTVS	High-throughput virtual screening
ICV	Intracerebroventricular
InChI	IUPAC international chemical identifier
IRLS	Iteratively reweighted least squares
LBDD	Ligand-based drug design
LE	Ligand efficiency
LGA	Lamarckian genetic algorithm
LOAD	Late-onset Alzheimer’s disease
LR	Logistic regression
LRR	Leucine-rich repeat
MBD	Membrane-binding domain
MAE	Mean absolute error
MAP	Microtubule-associated protein
MCC	Matthews correlation coefficient
MD	Molecular dynamics
MDD	Major depressive disorder
MDL	Minimal description length
MM-GBSA	Molecular mechanics–Generalised Born surface area
MM-PBSA	Molecular mechanics-Poisson-Boltzmann surface area
MMSE	Mini-mental state examination

MTLDs	Multi-target-directed ligands
NA	Noradrenaline
NIA-AA	National institute on aging and Alzheimer's association
NFTs	Neurofibrillary tangles
NMR	Nuclear magnetic resonance
NO	Nitric oxide
NOD	The nucleotide-binding oligomerization domain
OA	Overall accuracy
PAINS	Pan-assay interference compounds
PBS	Phosphate buffer saline
PI	Propidium iodide
PK/PD	Pharmacokinetic and pharmacodynamic
PR	Precision
QMEAN	Qualitative model energy analysis
QSAR	Quantitative structure-activity relationships
QSPR	Quantitative structure--property relationship
Rg	Radius of gyration
REOS	Rapid Elimination of Swill
RF	Random Forest
RC	Recall
RDF	Radial distribution function
ROC	Receiver Operating Characteristic
RoF	Rule of Five
RNNs	Recurrent neural networks
RMSD	Root-mean-square deviation
RMSF	Root mean square fluctuation
SBDD	Structure-based drug design
SCO	Scopolamine hydrobromide
SCMC	Sodium carboxymethylcellulose
SL	Supervised learning
TBA	Thiobarbituric acid
TBARS	Thiobarbituric acid reactive substance

TDP	Transactive response DNA-binding protein
TEA	triethylamine
TMS	transcranial magnetic stimulation
TN	true negative
TP	true positive
tDCS	Transcranial direct current stimulation
TPSA	topological polar surface area
UFF	universal force field
UMAP	uniform manifold approximation and projection
VAEs	variational autoencoders
WHO	World Health Organization
XGB	Extreme Gradient Boosting

List of Symbols

Symbol	Meaning
α	Alpha
β	Beta
δ	Delta
Δ	Delta
ε	Epsilon
λ	Lambda
ºC	Degree Celsius
Å	Angstrom
©	Copyright
g	Gram
mg	Milligram
µg	Microgram
ng	Nanogram
mmol	Millimole
µM	Micromolar
nM	Nanomolar
mM	Millimolar
mL	Millilitre
µL	Microlitre
µm	Micrometer
mm	Millimetre
cm	Centimetre
mV	Millivolt
h	Hour
s	Second; Singlet
nm	Nanometre
ppm	Parts per million
rpm	Revolutions per minute
Kcal	Kilocalories
Hz	Hertz
MHz	Megahertz
J	Coupling constant
d	Doublet
t	Triplet

Symbol	Meaning
m	Multiplet
dd	Doublet of doublet
m/z	Mass-to-charge ratio
%	Percent
pH	Potential of hydrogen
≤	Less than or equal
<	Less than
>	More than
±	Plus or minus