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List of abbreviations

Abbreviation	Full Form
3D	Three dimensional
ACh	Acetylcholine
AChE	Acetylcholinesterase
AD	Alzheimer's disease
AI	Artificial intelligence
Aβ	Amyloid-β
APP	Amyloid precursor protein
AS	Anionic site
ATP	Adenosine triphosphate
AUC	Area under the curve
BBB	Blood-brain permeability
BChE	Butyrylcholinesterase
BLAST	Basic local alignment search tool
CaMKII	Ca+2/calmodulin dependent protein kinase II
CAT	Catalase
ChAT	Choline acetyl transferase
ChE	Cholinesterase
CNN	Convolutional neural network
CNS	Central nervous system
CT	Computed tomography
DNP	Donepezil
EAAT2	Excitatory amino acid transporter 2
EC	Enzyme classification
FN	False negative
FP	False positive
GAFF	Generalised amber force field
GSK3	Glycogen synthase kinase-3
iGluRs	ligand-gated ionotropic glutamate receptors
JNK3	c-Jun N-terminal kinase 3
KNN	K-nearest neighbors
LBDD	Ligand based drug design
LDA	Linear discriminant analysis
LGA	Lamarckian Genetic Algorithm
LR	Logistic regression
MACCS	Molecular access system
MD	Molecular dynamics
MEKK	Mitogen-activated Protein/ERK Kinase Kinases
ML	Machine learning
MLP	Multi-layer perceptron
MRI	Magnetic resonance imaging
MSME	Mini-Mental state exam
Nct	Nicastrin
NFT	Neurofibrillary tangle

NMDA	N-methyl D-aspartate
PAC	Passive-aggressive classifier
PAINS	Pan-assay interference compounds
PAM	Positive allosteric modulator
PAMPA	Parallel artificial membrane assay
PAS	Peripheral anionic site
PBL	Porcine brain lipid
PLIP	Protein ligand interaction profiler
PS1	Presenilin 1
PS2	Presenilin 2
QDA	quadratic discriminant analysis
QSAR	Quantitative structure-activity relationship
R_f	Retention factor
RF	Random forest
Rg	Radius of gyration
RMSD	Root mean square deviation
RMSF	Root mean square fluctuation
RO5	Lipinski rule of five
ROC	Receiver operation characteristic
ROS	Reactive oxygen species
RT	Room Temperature
SAR	Structure activity relationship
SASA	Solvent accessible surface area
SBDD	Structure-based drug design
SBVS	Structure based virtual screening
SCO	Scopolamine hydrobromide
SEM	Standard error of mean
SF	Scoring function
SOD	Superoxide dismutase
SVC	Support vector classifier
SVM	Support vector machine
SVR	Support vector regression
TI	Thermodynamic integration
TN	True negative
TP	True positive