

## List of Abbreviations/Acronyms

Abbreviation/Acronyms	Full Form
A	Hydrogen-bond acceptor
A $\beta$	$\beta$ -Amyloid protein
ACh	Acetylcholine
AChE	Acetylcholinesterase
AChEI	Acetylcholinesterase inhibitor
AD	Alzheimer's disease
ADME	Absorption, distribution, metabolism and excretion
ADP	Adenosine diphosphate
ALS	Amyotrophic lateral sclerosis
AMU	Atomic mass unit
APP	Amyloid precursor protein
ATP	Adenosine triphosphate
AUAC	Area under accumulation curve.
AVM	Arteriovenous malformation
BBB	Blood-brain barrier
BEDROC	Boltzmann-enhanced discrimination of receiver operating characteristic
BFGS	Broyden-Fletcher-Goldfarb-Shanno algorithm
BuChE	Butyrylcholinesterase
CAS	Catalytic anionic site
CDCl <sub>3</sub>	Deuterated chloroform
Cdk5/GSK3 $\beta$	Cyclin-dependent kinase 5/glycogen synthase kinase 3 $\beta$
CHCl <sub>3</sub>	Chloroform
CK	Casein kinase
CNS	Central nervous system
D	Hydrogen-bond donor
DCCD	N, N-Dicyclohexyl carbodiimide
DCM	Dichloromethane
DFG motif	Asp-Phe-Gly motif
DFT	Density functional theory
DMEM-F12	Dulbecco's modified Eagle's medium nutrient mixture F-12
DMF	Dimethyl formamide

DMSO	Dimethyl sulfoxide
DMSO-d6	Deuterated dimethyl sulfoxide
3D-QSAR	3-Dimensional-quantitative structure activity relationship
DTNB	5,5'-Dithiobis-(2-nitrobenzoic acid)
ECM	Extra cellular matrix
EDCI	1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide
EF	Enrichment factor
EGTA	Ethylene glycol-bis( $\beta$ -aminoethyl ether)-N,N,N',N'-tetraacetic acid
e-Pharmacophore	Energy-optimized structure-based pharmacophore
EPS	Electrostatics potential charges
ES	Enzyme-substrate
Et <sub>2</sub> O	Diethyl ether
Et <sub>3</sub> N	Triethylamine
FBDD	Fragment based drug design
FBS	Fetal bovine serum
FTD	Frontotemporal dementia
GH	Goodness of hit
HD	Huntington's disease
HOBt	Hydroxybenzotriazole
HOMO	High occupied molecular orbital
HTS	High throughput screening
HTVS	High throughput virtual screening
IC <sub>50</sub>	Inhibitory concentration required to kill 50% of the population
IFD	Induced fit docking
2KC	3-({5-[(4-Methylpiperidin-1-yl)methyl]pyrrolo[2,1-f][1,2,4]triazin-4-yl}phenol
K <sub>2</sub> CO <sub>3</sub>	Potassium carbonate
KH <sub>2</sub> PO <sub>4</sub>	Potassium dihydrogen phosphate
KI	Potassium iodide
Ki	Inhibitor constant
KOH	Potassium hydroxide
LGA	Lamarckian genetic algorithm
LOO	leave one out
LUMO	Low unoccupied molecular orbital
MAO	Monoamine oxidases

MD	Molecular dynamics
MESP	Molecular electrostatic potential
MeOH	Methanol
MG	Myasthenia gravis
MM-GBSA	Molecular mechanic-generalized Born surface area
MMP	Matrix metalloproteinase
MTT	3-(4,5-Dimethyl-2-thiazolyl)-2,5-diphenyl-tetrazolium bromide
N	Negative ionizable group
N73	(S)-N-Isopropoxy-N-(3-methyl-1-nitroso-1-oxobutan-2-yl)-[1,1'-biphenyl]-4-sulfonamide]
NaCl	Sodium chloride
NCCS	National Centre for Cell Science
NFT	Neurofibrillary tangles
NMR	Nuclear magnetic resonance
NTP	Normal temperature and pressure
NTV	Normal temperature and volume
OPLS	Optimized potential for liquid simulations
P	Positive ionizable
PAS	Peripheral anionic site
PAINS	Pan-assay interference compounds
PAMPA	Parallel artificial membrane permeability assay
PBL	Porcine brain lipid
PD	Parkinson's disease
PDB	Protein Data Bank
Pe	Permeability
PHF	Paired helical filament
PLS	Partial least-squares
R	Aromatic ring
RIE	Robust initial enhancement.
RMSD	Root mean square deviation
RMSF	Root mean square fluctuation
ROC	Receiver operating characteristic curve
SAR	Structure-activity relationship
SCA	Spinocerebellar ataxia
SD	Standard deviation

SEM	Standard error of mean
SI	Selectivity index
SP	Standard precision
THA	Tacrine
THF	Tetrahydrofuran
TIP3P	Transferable intermolecular potential with 3 points
TLC	Thin-layer chromatography
TTBK	Tau-tubulin kinase
TSA	Total surface area
TPSA	Topological polar surface area
USFDA	United States Food and Drug Administration
UV	Ultraviolet
vdW	van der Waals
VS	Virtual screening
WHO	World Health Organization
XP	Extra precision
1YL	(1R)-1,6-Dimethyl-1,2-dihydrophenanthro[1,2-b]furan-10,11-dione
ZBG	Zinc-binding group

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