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## **List of Abbreviations**

| <b>Abbreviation</b> | <b>Full Form</b>                                              |
|---------------------|---------------------------------------------------------------|
| 3D                  | Three-dimensional                                             |
| 5-CV                | 5-fold cross-validation accuracy                              |
| 10-CV               | 10-fold cross-validation accuracy                             |
| A                   | Balanced accuracy                                             |
| A $\beta$           | 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           |
| R <sub>g</sub> | 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                |
|--------------------|------------------------|
| $\alpha$           | Alpha                  |
| $\beta$            | Beta                   |
| $\delta$           | Delta                  |
| $\Delta$           | Delta                  |
| $\varepsilon$      | Epsilon                |
| $\lambda$          | Lambda                 |
| $^{\circ}\text{C}$ | Degree Celsius         |
| $\text{\AA}$       | Angstrom               |
| ©                  | Copyright              |
| g                  | Gram                   |
| mg                 | Milligram              |
| $\mu\text{g}$      | Microgram              |
| ng                 | Nanogram               |
| mmol               | Millimole              |
| $\mu\text{M}$      | Micromolar             |
| nM                 | Nanomolar              |
| mM                 | Millimolar             |
| mL                 | Millilitre             |
| $\mu\text{L}$      | Microlitre             |
| $\mu\text{m}$      | 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 |
| $\leq$ | Less than or equal    |
| $<$    | Less than             |
| $>$    | More than             |
| $\pm$  | Plus or minus         |