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LIST OF ABBREVIATIONS

2D	Two-dimensional
3D	Three-dimensional
4D	Four-dimensional
5D	Five-dimensional
6D	Six-dimensional
ADMET	Absorption, Distribution, Metabolism, Excretion, and Toxicity
ARG	Arginine
BA	Biological Activity
CADD	Computer Aided Drug Design
CPH	Common Pharmacophore Hypothesis
CoMFA	Comparative Molecular Field Analysis
CoMSIA	Comparative Molecular Similarity Indices Analysis
CYP51	Cytochrome P450 lanosterol 14α-demethylase
DMSO	Dimethyl sulphoxide
DDE	Dipole and Dipole energy
GFA	Genetic Function Approximation
Glide	Grid-based Ligand Docking with Energetics
Glide SP	Glide single precision docking
Glide XP	Glide extra precision docking
^{1}H-NMR	Proton Nuclear Magnetic Resonance
HOMO	Highest Occupied Molecular Orbital
IR	Infrared Spectra
IC_{50}	Half maximal inhibitory concentration
IUPAC	International Union of Pure and Applied Chemistry
LBDD	Ligand Based Drug Design
LOO	Leave one out method
LHO	Leave Half Out
LOF	Lack of fit
LUMO	Lowest Unoccupied Molecular Orbital
MET	Methionine
MLR	Multiple linear regression
MIC	Minimum Inhibitory Concentration
m.p.	Melting Point
MR	Molar Refractivity

NCEs	New Chemical Entities
Nmt	N -myristoyltransferase
ONC	Optimum number of components
OPLS	Optimized Potential for Liquid Simulation
PDB	Protein data bank
PHASE	Pharmacophore Alignment and Scoring Engine
PHE	Phenylalanine
PLS	Partial Least Square Analysis
q^2	Cross-validated correlation coefficient by leave one out method
QSAR	Quantitative structure-activity relationship
r^2_{bs}	Average r^2 from a bootstrapping
r^2_{ncv}	Non-cross-validated correlation coefficient
r^2_{cv}	Cross-validated correlation coefficient
r^2_{pred}	Predicted correlation coefficient
RMSD	Root mean square deviation
SAR	Structure-activity relationship
SBDD	Structure Based Drug Design
SD	Standard deviation
SEE	Standard Error of Estimate
SEP	Standard Error of Prediction
SER	Serine
TLC	Thin Layer Chromatography
TYR	Tyrosine
VDW	Van Der Waals