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LIST OF ABBREVIATION

2D	=	Two-dimension
3D-QSAR	=	Three-dimensional quantitative structure-activity relationship
Ala (A)	=	Alanine
Asn (N)	=	Asparagine
Arg (R)	=	Arginine
Asp (D)	=	Aspatic acid
B3LYP	=	Beck's three parameter hybrid functional using the LYP correlation functional
BSSE-CP	=	Basis set superposition error based on the counterpoise scheme
CoMFA	=	Comparative molecular field analysis
Comp	=	Compounds
C_{sp3} (+1)	=	Carbon sp3-hybridization with plus 1 charge probe atom
Cys (C)	=	Cysteine
Cyc	=	Cycloguanil
DNA	=	Deoxyribonucleic acid
DHF	=	Dihydrofolate
DHFR	=	Dihydrofolate reductase
dTMP	=	Deoxythymidylate
Gly (G)	=	Glycine
H (+1)	=	Hydrogen plus 1 charge probe atom
HF	=	Hartree-fock theory
HIV-1	=	Human immunodeficiency virus type 1
HQ	=	High level of quantum chemical calculations
Ile (I)	=	Isoleucine
K_i	=	Inhibition constant
Leu (L)	=	Leucine
LOO	=	Leave-one-out
LQ	=	Low level of quantum chemical calculations
Lys (K)	=	Lysine

LIST OF ABBREVIATION (Continued)

MD	=	Molecular dynamics
Met (M)	=	Methionine
MLR	=	Multiple linear regression
MM	=	Molecular mechanics
MP2	=	Second order Möller-plesset
NAD	=	Nicotinamide adenine dinucleophide
Noc	=	Number of component
ONIOM	=	Our own n-layer intergrated molecular orbital molecular mechanics
O_{sp3} (-1)	=	Oxygen sp3-hybridization with minus 1 charge probe atom
PDB	=	Protein data bank
Pf	=	*Plasmodium falciparum*
*Pf*DHFR	=	*Plasmodium falciparum* dihydrofolate reductase
Phe (F)	=	Phenylalanine
p*Ki*	=	Negative logarithm of inhibition constant
PLS	=	Partial least square
PM3	=	Modified neglect of diatomic overlap, parametric method number 3
PME	=	Particle mesh ewald
PRESS	=	Prediction error sum of squares
Pro (P)	=	Proline amino acid
Pyr	=	Pyrimethamine
QM	=	Quantum mechanics
QM/MM	=	Quantum mechanical/molecular mechanical method
QSAR	=	Quantitative structure-activity relationship
r^2_{cv}	=	Predictive ability of cross-validation
r^2_{nv}	=	Predictive ability of no-validation
RMS	=	Root mean square
RMSD	=	Root mean square deviation

LIST OF ABBREVIATION (Continued)

Ser (S)	=	Serine
SHMT	=	Serine hydroxymethyltransferase
S_{press}	=	Uncertainty of the prediction
SSY	=	Variance of the data around the mean value
THF	=	Tetrahydrofolate
Thr (T)	=	Threonine
Trp (W)	=	Tryptophan
TS	=	Thymidylate synthase
Tyr (Y)	=	Tyrosine
Val (V)	=	Valine
UFF	=	universal force field