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LIST OF ABBREVIATIONS

3D database	=	Three-dimensional database
3D-pharmacophore	=	Three-dimensional pharmacophore
3D-QSAR	=	Three-dimensional quantitative structure-activity relationships
ACD	=	Available Chemicals Directory
Ala (A)	=	Alanine
Asn (N)	=	Asparagine
Asp (D)	=	Aspartic acid
CK2	=	Casein kinase II
Cys (C)	=	Cysteine
DNA	=	Deoxyribonucleic acid
dNTP	=	Deoxyribonucleotide triphosphate
ER	=	Estrogen receptor
F7	=	Coagulation factor VIIa
GA	=	Genetic algorithm
Glu (E)	=	Glutamic acid
Gly (G)	=	Glycine
HA	=	Hemagglutinin
His (H)	=	Histidine
HIV-1	=	Human immunodeficiency virus type-1
HTS	=	High-throughput screening
IC ₅₀	=	Inhibitory concentration 50%
ICM	=	Integrated Care Management
IGFBP-5	=	Insulin-like growth factor-I-binding protein-5
IGF-I	=	Insulin-like growth factor-I
Ile (I)	=	Isoleucine
Leu (L)	=	Leucine
LGA	=	Lamarckian genetic algorithm
LS	=	Local search

LIST OF ABBREVIATIONS (Continued)

Lys (K)	=	Lysine
MC	=	Monte Carlo
mRNA	=	Messenger ribonucleic acid
NA	=	Neuraminidase
NCI	=	National Cancer Institute
Neu5Ac	=	N-acetylneuraminic acid
NIs	=	Neuraminidase inhibitors
NMR	=	Nuclear magnetic resonance
PCR	=	Polymerase chain reaction
Phe (F)	=	Phenylalanine
PIs	=	Protease inhibitors
PLP	=	Piecewise linear potential
PM3	=	Parametric method number 3
PMF	=	The Presidential Management Fellows
Pro (P)	=	Proline
pfDHFR	=	The Plasmodium falciparum dihydrofolate reductase
PTP1B	=	Protein tyrosine phosphatase-1B
QM	=	Quantum mechanics
QSARs	=	Quantitative structure-activity relationships
RCSB PDB	=	The research collaboratory for structural bioinformatics (RCSB), the non-profit consortium that manages the Protein Data Bank (PDB)
rmsd	=	Root mean square deviation
RNA	=	Ribonucleic acid
RNP	=	Ribonucleoprotein
Ser (S)	=	Serine
TGT	=	Eubacterial tRNA-guanine transglycosylase
Thr (T)	=	Threonine
TK	=	Thymidine kinase

LIST OF ABBREVIATIONS (Continued)

tRNA	=	Transfer ribonucleic acid
Trp (W)	=	Tryptophan
Tyr (Y)	=	Tyrosine
Val (V)	=	Valine
VLS	=	Virtual ligand screening