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ABBREVIATIONS

AIDS	=	Acquired Immune Deficiency Syndrome
AM1	=	Austin Model 1
AOs	=	Atomic Orbitals
Asp (D)	=	Aspartic acid
B3LYP	=	Becke's three parameter hybrid functional using the LYP correlation functional
BBF	=	Backbone Atoms Fixing
BLYP	=	Beck-Lee-Yang-Parr functional
BE	=	Binding Energy
Cys (C)	=	Cysteine
DEF	=	Deformation Energy
DFT	=	Density Functional Theory
Glu (E)	=	Glutamic acid
Gly (G)	=	Glycine
GTO	=	Gaussian-Type Orbital
HAART	=	The Highly Active Anti-Retroviral Therapy
HAF	=	Heavy Atoms Fixing
HIV-1	=	Human Immunodeficiency Virus Type 1
His (H)	=	Histidine
HF	=	Hartree-Fock
IC ₅₀	=	Inhibitory Concentration 50%
Ile (I)	=	Isoleucine
INT	=	Interaction Energy
LCAO	=	Linear Combination of Atomic Orbitals
LCAO-MO	=	Linear Combination of Atomic Orbitals to Molecular Orbitals
LDA	=	Local Density Approximation
Leu (L)	=	Leucine
LSD	=	Local Spin Density Approximation
LYP	=	Lee-Yang-Parr functional
Lys (K)	=	Lysine

MC/FEP	=	Monte Carlo/free energy perturbation
Met (M)	=	Methionine
MM	=	Molecular Mechanics
MM-PBSA	=	Molecular Mechanics Poisson-Boltzmann/surface area
MNDO	=	Modified Neglect of Diatomic Overlap
MO	=	Molecular Orbital
MP2	=	The second-order Møller-Plesset perturbation theory
NNIBP	=	Non-Nucleoside Inhibitor Binding Pocket
NNRTIs	=	Non-Nucleoside Reverse Transcriptase Inhibitors
NRTIs	=	Nucleoside Reverse Transcriptase Inhibitors
ONIOM	=	Our <i>N</i> -layered Integrated Molecular Orbital plus Molecular Mechanics Method
Phe (F)	=	Phenylalanine
Pro (P)	=	Proline
PM3	=	MNDO Parametric Method number 3
QM	=	Quantum Mechanics
RT	=	Reverse Transcriptase
SCF	=	Self-Consistent Field
SCRf	=	Self-Consistent Reaction Field
STO	=	Slater Type Orbital
STO-3G	=	Slater Type Orbital approximated by 3 Gaussian type orbitals
S-Value test	=	The Substituent-Value test
Trp (W)	=	Tryptophan
Tyr (Y)	=	Tyrosine
Val (V)	=	Valine