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ABBREVIATION

ABNR = Adopted basis Newton-Raphson

Ade = Adenine

AIDS = Acquired Immune Deficiency Syndrome

Ala(A) = Alanine

AM1 = Austin Model 1
AOs = Atomic Orbitals

Asn(N) = Asparagine

Arg(R) = Arginine

Asp(D) = Aspatic acid

Beck's three parameter hybrid functional using the LYP

B3LYP = correlation functional

CD4 = Cluster of differentiation 4

Cyt = Cytosine Cys(C) = Cysteine

DFT = Density Functional Theory

DNA = Deoxyribonucleic acid

dNTP = Deoxynucleoside triphosphate

dsDNA = Double-standed deoxyribonucleic acid

dTTP = Deoxythymidine triphosphate

Gln(Q) = Glutamine

Glu(E) = Glutamic acid

Gly (G) = Glycine
Gua = Guanine

H-transfer = Proton transfer

HF = Hartree-Fock theory

His (H) = Histidine

HIV-1 = Human Immunodeficiency Virus Type 1

Ile (I) = Isoleucine Leu (L) = Leucine LCAO = Linear combination of atomic orbitals

LCAO-MO = Linear combination of atomic orbitals to molecular Orbitals

Lys(K) = Lysine

MD = Molecular Dynamics

Met(M) = Methionine

MLR = Multiple linear regression
MM = Molecular Mechanics

MNDO = Modified neglect of diatomic overlap

MO = Molecular Orbitals

MOs = Molecular Orbital

MP2 = Second order Möller-Plesset mRNA = Messenger ribonucleic acid

NDO = Neglect of diatomic differential overlap

NNRTIS = Non-Nucleoside Reverse Transcriptase Inhibitors

NRTIs = Nucleoside Reverse Transcriptase Inhibitors

Phe (F) = Phenylalanine

PM3 = Modified neglect of diatomic overlap, parametric method

number 3

PPi = Pyrophosphate

Pro (P) = Proline amino acid QM = Quantum Mechanics

QM/MM = Quantum Mechanical/Molecular Mechanical method

RMS = Root Mean Square

RMSD = Root Mean Square Deviation

RNA = Ribonucleic acid RNaseH = Ribonuclease H

RT = Reverse Transcriptase

SBMD = Stochastic Boundary Molecular Dynamics method

SD = Steepest descent

Ser(S) = Serine

SCF = Self-consistent field

Thr (T) = Threonine

tRNA = Transfer ribonucleic acid

Trp (W) = Tryptophan Tyr (Y) = Tyrosine Thy = Thymine

UNAIDS = The Joint United Nations Programme on HIV/AIDS

Val (V) = Valine

WHO = World Heath Organization