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LIST OF ABBREVIATIONS

B3LYP	=	Beck's three parameter hybrid functional using the LYP correlation functional
DFT	=	Density function theory
FT-IR	=	Fourier Transform Infrared spectroscopy
HF	=	Hartree Fock
NMR	=	Nuclear Magnetic Resonance
AM1	=	Austin Model 1
ONIOM	=	The Our own N-layered Integrated Molecular Orbital Molecular Mechanics
kcal/mol	=	Kilocalorie per mol
SD	=	Standard Deviation
RMSD	=	Root Mean Squares Deviation
NRTIs	=	Nucleoside Reverse Transcriptase Inhibitors
NNRTIs	=	Non-Nucleoside Reverse Transcriptase Inhibitors
RT	=	Reverse Transcriptase
HIV-1	=	Human Immunodeficiency Virus Type 1
MD	=	Molecular Dynamics
MK	=	Merz-Kollman Singh Charge Method
MM	=	Molecular Mechanics
NEV	=	Nevirapine
GIAO	=	Gauge including atomic orbitals
SCRF	=	Self-consistent reaction field
IEFPCM	=	Integral equation formalism polarized continuum
ASC	=	Apparent surface charge
RDF	=	Radial distribution function
gHMBC	=	Gradient-selected versions Heteronuclear Multiple Bond Coherence