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List of Abbreviations

Å	:	Angstrom
ACE	:	Atomic contact Energy
AF-1	:	Activation function-1
AFM	:	Atomic Force Microscopy
AIB1	:	Amplified in Breast Cancer
AMBER	:	Assisted Model Building with Energy Refinement
ATP	:	Adenosine Triphosphate
BPTI	:	Bovine Pancreatic Trypsin Inhibitor
CAPRI	:	Critical Assessment of Prediction of Interaction
COM	:	Centre of Mass
CDK5	:	Cyclin-dependent kinase 5
3-D	:	3-Dimensional
DBD	:	DNA-binding domain
DNA	:	Deoxyribonucleic Acid
EPKs	:	Eukaryotic protein kinases
ER	:	Estrogen receptor
FFT	:	Fast Fourier Transform
FTIR	:	Fourier-transform Infrared Spectroscopy
GAFF	:	General Amber force field
GBSA	:	Generalized Born generalized Born and surface area continuum solvation
GRB2	:	Growth factor receptor bound protein
HER2	:	Human epidermal growth factor receptor 2
HR	:	Hormone receptors
HTVS	:	High throughput virtual screening
IDP	:	Intrinsically Disordered Protein
KFC	:	Knowledge-based FADE and Contacts
LBD	:	Ligand binding domain
LGA	:	Lamarckian genetic algorithm
LMTK3	:	Lemur Tyrosine Kinase 3
LTP	:	Long-term Potentiation
I-TASSER	:	Iterative Threading ASSembly Refinement
MD	:	Molecular Dynamics
MM	:	Molecular Mechanics
ns	:	nanosecond
NMR	:	Nuclear Magnetic Resonance Spectroscopy
ps	:	picosecond
PBC	:	Periodic boundary condition
PBSA	:	Poisson–Boltzmann surface area continuum solvation
PDB	:	Protein Data Bank
PKA	:	Protein kinase A
PME	:	Particle Mesh Ewald
PMF	:	Potential of Mean Force
PPIs	:	Protein-protein interaction
PR	:	Progesterone receptor
QM	:	Quantum Mechanics
RBVI	:	Resource for Biocomputing Visualization, and

List of Abbreviations

		Informatics
RC	:	Reaction Coordinate
Rg	:	Radius of Gyration
RMSD	:	Root Mean Square Deviation
RMSF	:	Root Mean Square Fluctuation
RTKs	:	Receptor tyrosine kinases
SH	:	SRC homology
SP	:	Standard precision
SPC	:	Simple Point Charge
SRF	:	Serum response factor
TIP3P	:	Transferable Intermolecular Potential Three-point
US	:	Umbrella Sampling
VMD	:	Visual Molecular Dynamics
WHAM	:	Weighted Histogram Analysis Method
XP	:	Extra precision