

# Abbreviations

2D	2-dimensional
3D	3-dimensional
AIDS	acquired immune deficiency syndrome
APV	amprenavir
CMO	contact map overlap
CVT	centroidal Voronoi tessellation
DNA	deoxyribonucleic acid
HIV	human immunodeficiency virus
HIVPI	HIV-1 protease inhibitor
HMC	hybrid Monte Carlo
IDV	indinavir
ILP	integer linear programming
LPV	lopinavir
MC	Monte Carlo
MCES	maximum common edge subgraph
MCIS	maximum common induced subgraph
MCS	maximum common subgraph
MD	molecular dynamics
MEP	molecular electrostatic potential
MMFF	Merck molecular force field
NFV	nelfinavir
PDB	Protein Data Bank
rms	root mean square
RNA	ribonucleic acid
RTV	ritonavir
SAR	structure activity relationship
SES	solvent excluded surface
SQV	saquinavir
TPV	tipranavir
QSAR	quantitative structure activity relationship

