

## LIST OF ABBREVIATIONS

Ach	=	Acetylcholine
AChE	=	Acetylcholinesterase
AM1	=	Austin model 1
BCh	=	Butyrylcholine
B3LYP	=	Beck's three parameter hybrid functional using the LYP correlation functional
BChE	=	Butyrylcholinesterase
BTC	=	Butyrylthiocholine
ChE	=	Cholinesterase
CS	=	Catalytic substrate binding site
DFT	=	Density functional theory
ES	=	Enzyme substrate complex
EVB	=	Empirical valence bond
HF	=	Hartree-Fock
IMOMM	=	Integrated molecular orbital and molecular mechanics method
INT	=	Intermediate
kcal/mol	=	Kilocalorie per mol
LBHBs	=	Low-barrier hydrogen bonds
LYP	=	Lee-Yang-Parr functional
MD	=	Molecular dynamics
MM	=	Molecular mechanics
MM-PB	=	Molecular-mechanics-Poisson-Boltzmann
MO	=	Molecular orbital
MP2	=	The second-order Møller-Plesset perturbations theory
ONIOM	=	Our-own-N-layered Integrated molecular Orbital and molecular Mechanics
PAS	=	The peripheral anionic site
PCM	=	Polarizable continuum method
PM3	=	Paranetric method number 3