QM = Quantum mechanics

QM/MM = Quantum mechanical/molecular mechanical

OPs = Organophosphates

SCRF = Self-consistent reaction field

SIMOMM = Surface Integrated Molecular Orbital/Molecular Mechanics

TcAChE = Torpedo californica Acetylcholinesterase

TS = Transition state

## **AMINO ACID CODES**

Ala = Alanine

Val = Valine

Leu = Leucine

Ile = Isoleucine

Pro = Proline

Phe = Phenylanaline

 $Trp \hspace{1cm} = \hspace{1cm} Trptophan$ 

Met = Methionine

Gly = Glycine

Ser = Serine

Thr = Threonine

Cys = Cysteine

Tyr = Tyrocine

Asn = Asparagine

Gln = Glutamine

Asp = Aspartic acid

Glu = Glutamic acid

Lys = Lysine

Arg = Arginine

His = Histidine