List of Tables

List of Figures

Abbreviations used in the Thesis

ADME	Absorption Distribution Metabolism Excretion
ADME-TOX	Absorption Distribution Metabolism Excretion and Toxicity
A	Adenine
BSSE	Basis set superposition errors
BLYP	Becke-Lee-Yang-Parr
BB	Blood Brain
CPT	Camptothecin
CNS	Central nervous system
CDDP	*cis*-diamiminedichloroplatinum(II)
CGF	Core contracted gaussain functions
R^2	Correlation coefficient
CLs	Cross-links
C	Cytosine
DFT	Density functional theory
DNA	Deoxyribonucleic acid
DNP	Double numeric polarization
DN	Double numerical
DND	Double-numerical + d-DNP basis
DZ	Double-zeta
ECP	Effective Core Potential
EA	Electron affinity
ESI	Electrospray Ionization
E_{LUMO}	Energy of lowest unoccupied orbital
E_{NL}	Energy of next LUMO
F	Fisher significance ratio
FMO	Frontier molecular orbital
FF	Fukui function
GTO	Gaussain Type Orbitals

GGA	Generalized Gradient Approximation
G	Guanine
HCTH	Handy's family of functionals
HF	Hartee-Fock Method
HOMO	Highest occupied molecular orbital
HIA	Human intestinal absorption
HE	Hydration energy
IR	Infrared
IM	Intermediate
ICLs	Interstrand cross-links
IRC	Intrinsic reaction coordinate
IP	Ionization potential
KS	Kohn-Sham
LOO	Leave one out
LCAO	Linear combination of atomic orbitals
LDA	Local Density Approximation
R^2_{CV}	LOO cross validated squared correlation coefficient
LANL2DZ	Los Alamos National Laboratory ECP plus Double-zeta
LUMO	Lowest unoccupied molecular orbital
MHP	Maximum hardness principle
MEP	Minimum electrophilicity principle
MR	Molar refractivity
MM	Molecular Mechanics
MO	Molecular orbital
MVD	Molegro Virtual Docker
MLR	Multiple linear regression
NMR	Nucler magnetic resonance
PBE	Perdew-Burke-Ernzerhof
PW91	Perdew-Wang 91
P-gp	*p*-glycoprotein
Pol	Polarizability

CPCM	Polarized continuum-model
PES	Potential energy surface
Q	Quality factor
QSAR	Quantitative structure-activity relationship
QSPR	Quantitative structure-property relationship
QSTR	Quantitative structure-toxicity relationship
QM	Quantum mechanics
QM/MM	Quantum mechanics/molecular mechanics
RHF	Restricted Hartee-Fock
ROHF	Restricted Open Shell Hartee-Fock
SE	Standard error
STO	Stater Type Orbitals
SAR	Structure Activity Relationship
SA	Surface area
T	Thymine
TS	Transition states
TNP	Triple numeric polarization
TZ	Triple-zeta
UHF	Unrestriced Hartee-Fock
WHO	World Health Organization
ZPE	Zero-point energy

List of Symbols used in the Thesis

Å	Angstrom
¦	Chemical hardness
«	Chemical potential,
°	Electron Density
S	Electron spin
χ	Electronegativity
ω	Electrophilicity
$\Delta_r H^0$	Enthalpy of reaction

v	External potential
f_k^+ and f_k^-	Fukui functions
$\Delta G^{\#}$	Gibbs free energy of activation
$\hat{H}$	Hamiltonian operator
®	Pi
$\Delta_r G^0$	Reaction free energies