

DECLARATION

I, **Dharitri Das**, bearing Ph. D. Registration Number, **Ph. D./1189/2010 dt 15.09.2010**, hereby declare that the thesis entitled “**Structure and reactivity of ruthenium based anticancer drugs and their interaction with biomolecules: A density functional approach**” submitted to Assam University, Silchar for the partial fulfillment of the degree of Doctor of Philosophy in Chemistry is the record of original research work done by me under the supervision of Dr. Paritosh Mondal, Department of Chemistry, Assam University, Silchar. I further declare that the contents of this thesis have not formed the basis for the award of any other degree/diploma.

Place: Assam University, Silchar

(Dharitri Das)

Date: 15.06.2015

Dedicated to

My

Father Tarun Chandra Das

&

Mother Ila Prava Das

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ABBREVIATIONS

- FDA : American Food and Drugs Administration
- GG : guanine-guanine
- DNA : deoxyribonucleic acid
- DFT : density functional theory
- BLYP : Becke-Lee-Yang-Parr
- DNP : double numerical with polarization
- GGA : generalized gradient approximation
- LST : linear synchronous transit
- CG : conjugated gradient
- QST : quadratic synchronous transit
- IRC : intrinsic reaction coordinate
- MM : molecular mechanics
- QM : quantum mechanics
- QM/MM : quantum mechanics/molecular mechanics
- ONIOM : our Own N-layer Integrated molecular Orbital
molecular Mechanics
- GA : genetic algorithm
- apo-Tf : apo-transferrin
- QSAR : quantitative structure-activity relationship
- HT-29 : human Colorectal Adenocarcinoma Cell Line
- DMSO : dimethylsulfoxide
- im : imidazole
- IC₅₀ : concentration of a compound that induces 50% growth
inhibition of cells compared to untreated cells
- CPCM : conductor-like polarizable continuum model
- his : histidine
- ser : serine
- cys : cysteine
- HSA : human serum albumin
- RCSB : research collaboratory for structural bioinformatics

- pdb : protein data bank
- HOMO : highest occupied molecular orbital
- LUMO : lowest unoccupied molecular orbital
- UFF : universal force field
- NO : nitric oxide
- ZPE : zero-point vibrational effects
- NBO : natural bond orbital

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