CURRICULAM-VITAE

PERSONAL DETAILS

:

NAME: AISHWARYA DHAR

DATE OF BIRTH: 05/09/1991

LANGUAGES KNOWN: ENGLISH, HINDI, BENGALI

ADDRESS: 41, DOLLY LODGE ROAD, RABINDRANAGAR, ASANSOL, WEST BENGAL, INDIA. PIN-713304

CONTACT DETAILS:

Mobile No: +91 9673084990

Email I.D: dhar.aishwarya@gmail.com

EDUCATIONAL QUALIFICATIONS:

Sr. No.	QUALIFICATION	BOARD/ UNIVERSITY	YEAR OF PASSING	PERCENTAGE/GRADE
1.	SSC	ICSE	2008	86
2.	HSC	CBSE	2010	80
3.	B.Sc.(Hons) Chemistry	DELHI UNIVERSITY	2014	69
4.	M.Sc. Biochemistry	S.P PUNE UNIVERSITY	2016	60

AREAS OF SPECIALIZATION:

Biomolecules, Enzymology and biophysical techniques, Microbiology and cell biology, Bioenergetics and metabolism, Biostatistics, Computers and bioinformatics, Genetics and membrane biochemistry, Molecular biology, Medicinal biochemistry, Immunology, Neurochemistry, Toxicology, Plant biochemistry, Biochemistry of specialized tissues, Clinical biochemistry

Experimental: Analytical biochemistry, Molecular biology, clinical biochemistry

Computation: Fortran coding, GROMACS, Molecular dynamics simulations, Umbrella sampling, PyMol, GLIDE Schrodinger

ACHIEVEMENTS AND AWARDS:

Summer Fellowship, the Institute of Mathematical Sciences (IMSc Chennai), Chennai, India. [May-July, 2015]

Master's Project, University of Pune,Pune, India.

To unravel the molecular mechanism of HRI kinase inhibitor. Supervisor: Dr Manali Joshi, Pune university. [Jan-April, 2016]

Junior Research Fellow, Indian Institute of Technology, Jodhpur, India. Project: Study of calcium oxalate crystal-peptide interactions using molecular dynamics simulations. Supervisor: Dr Ananya Debnath, Indian Institute of Technology, Jodhpur. [Aug2016- -present]

RESEARCH EXPERIENCE:

Project: To unravel the molecular mechanism of HRI kinase inhibitor. Supervisor: Dr Manali Joshi, Pune University. [Jan-April, 2016].

By using molecular docking techniques, our goal was to use calculations to support the future rational identification of more potent small molecule inhibitors of HRI kinases. The The heme-regulated eIF-2α kinase (HRI) regulates globin synthesis in response to heme levels in reticulocytes and erythroid cells in bone marrow. Inhibitors of HRI are proposed to lead to an increased rate of globin production leading to a corresponding increase in hemoglobin benefitting anemia patients.

The aim of this project was to unravel the mechanism of binding of the inhibitors using molecular docking. The hope was to use calculations to support future rational identification of more potent small molecule inhibitors.The experimental data of a series of indeno[1,2-c pyrazole] derivatives were obtained from the literature, including pIC50 values. I sketched the structures using Marvin Sketch and prepared the ligands using the Ligprep module of Maestro. Subsequently, 300 ns of MD simulation data of HRI was made available from previous work in the lab. I clustered the simulation data based on RMSD with respect to the crystal structure and the 100^{th} frame was found to provide the most representative structure. The 100th frame was then prepared using Protein preparation wizard in Maestro. A grid was generated that encompassed the ATP binding site. The prepared ligands were docked using GlideXP. The scores and binding modes of the ligands were analysed. All structured were observed to docked in the ATP binding pocket. The docking scores and pIC-50 values obtained were in good agreement, which indicated a good correlation between experimental and computational values. This gives us confidence in our docking predictions, which can now be used to provide molecular insights into the inhibition.

Project: Study calcium oxalate crystal-peptide interactions using molecular dynamics simulations. Supervisor: Dr Ananya Debnath, Indian Institute of Technology, Jodhpur. [Aug2016- -present].

The majority of human kidney stones are composed primarily of calcium oxalate monohydrate. (COM) crystals. Thus, determining the molecular modulation of COM crystallization by urinary constituents is crucial for understanding and controlling renal stone disease.Interactions between proteins and crystals are thought to be of great importance in many, if not all, forms of biomineral-ization. Such interactions have been proposed to be responsible for the nucleation of crystals in mineralizing tissues, the inhibition of crystallization in soft tissues formation of particular crystalline polymorphs,and biological control over crystal orientation,growth habit.

I examined the interactions between aspartic acid and calcium oxalate to determine the binding energy between the two species. The binding energy is formulated on the basis of the potential mean force, which is obtained from a specialized technique, namely umbrella sampling as implemented in GROMACS.

Project:

The work is to understand protein dynamics and conformational changes in ASC-kaempferol complex we employ MD simulation.This can correlate ligand binding of different binding sites of protein which can modulate certain activities of protein-kaemperol.

This can correlate ligand binding of different binding sites of protein which can modulate certain activities .

The objective of our work was to see

Ligand Binding can cause conformational changes in protein dynamics. Contribution of bindiing domain toward dynamics. The effect of protein conformation on binding affinity.

CONFERENCE ATTENDANCE:

Attended a school on “Advances in Mathematical Biology” held at the Indian Institute of Science

and Research PUNE by the International Centre for Theoretical Sciences-Indian Institute of Science and Research-Pacific Institute of Mathematical Sciences. [Dec 7-16 , 2014]

National Network for Mathematical and Comptational Biology Instructional School held at Indian Institute of Science. [May 23-31, 2016]

REFERENCES:

1. Prof S Sabharwal, Department of Chemistry
S P Pune University, Pune [020- 5601401, Phone]
ssab@chem.unipune.ac.in

2. Prof Manali Joshi, Department of Bioinformatics
S P Pune University, Pune [020-25601395, Phone]
manalijoshi@unipune.ac.in

3. Dr Ananya Debnath, Department of Chemistry
Indian Institute of Technology, Jodhpur [291-2449026, Phone]
ananya@iitj.ac.in

DECLARATION:

I, Miss Aishwarya Dhar, hereby declare that the above information given is true to my knowledge and I will be responsible for any false information.

Place: Jodhpur **Signature: Aishwarya Dhar**
Date: 13-12-16