UNIVERSITÀ DEGLI STUDI DI MILANO

TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO   **ID CODE 4456**

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B fellowship at **Dipartimento di Bioscienze dell'Università degli Studi di Milano**

Scientist- in – charge: **Prof. Carlo Camilloni**

Amit Kumawat

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	Kumawat
Name	Amit
Date of birth	20-11-1989

PRESENT OCCUPATION

Appointment	Structure
Research Associate-I (September 2019 – Present)	Department of Chemical, Biological & Macromolecular Sciences S. N. Bose National Center for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata-700106, West Bengal, India

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Bachelors degree (B.Sc.)	Microbiology	University of Pune, Pune, India	2012
Masters degree (M.Sc.)	Bioinformatics	University of Pune, Pune, India	2014
PhD Broad Area of Research: Computational Biophysical Chemistry	Chemical Sciences	AcSIR - Academy of Scientific & Innovative Research, India	2019
PhD Thesis Title: "Molecular Thermodynamic View of Biomolecular Signaling: Allostery and Protein-Protein Interactions" Advisor: Dr. Suman Chakrabarty Department of Chemical, Biological & Macromolecular Sciences S. N. Bose National Center for Basic Sciences, Kolkata, India			

FOREIGN LANGUAGES

Languages	level of knowledge
English	Fluent

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AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2017	NCL-RF Dr. Krishnan Award for "Best Published Research Paper in Computational Science" titled "Hidden Electrostatic Basis of Dynamic Allostery in a PDZ domain in the journal *Proc. Natl. Acad. Sci. U.S.A*" for the year 2017.
2017	NCL-RF Keerthi Sangoram Memorial Endowment Award for "Best Research Scholar" 2017 in Physical Chemistry Division.
2017	International Travel Grant by Department of Biotechnology, India for attending WATOC-2017 held in Munich, Germany.
2017	Best poster award at Indo-German Workshop on Computing in Chemistry, Biology and Medicine (2017) organized by CCNSB, IIIT, Hyderabad, India
2016	Third Prize for Poster and Oral presentation at Symposium on Accelerating Biology 2016: Decoding the Deluge, organized by CDAC, Pune, India.
2016	Best poster award at 15th Indian Theoretical Chemistry Symposium (2016), University of Hyderabad, India.
2016	Best poster award at National Science Day (2016), CSIR-NCL, Pune, India.
2014	Department of Biotechnology- Research Fellowship (DBT-JRF) awarded for Ph.D. program.
2014	Prof. Kolaskar Gold Medal for standing 1st in M.Sc. (Post graduation) Bioinformatics at University of Pune, India.
2012- 2014	IGIB-G.N. Ramachandran fellowship during M.Sc. Bioinformatics course (2012- 2014) at University of Pune, India.

TRAINING OR RESEARCH ACTIVITY

Research Interest:
- ➤ Molecular basis of signal transduction, allosteric modulation and protein-protein interactions using protein electrostatics.
- ➤ Exploring rare events in biological macromolecules using enhanced sampling techniques and reconstruction of conformational free energy landscape.
- ➤ Molecular docking and ligand binding studies in terms of binding free energy calculations.

Technical Skills:
- • Molecular dynamics simulations and rare event sampling:
  Carried out MD simulation studies of proteins using Gromacs package and enhanced sampling to generate free energy landscape using Metadynamics (PLUMED package).
- • Programming languages: C, Perl programming, Bash scripting.
  - ➤ Developed Unix/Shell and Perl scripts to automate compiling and execution of C programs, interface to retrieve PDB files and protein sequences from web services.
  - ➤ Developed programs in C to read GROMACS trajectory and use the coordinates information for the calculation of various quantities at every time step such as dihedral angles of protein residues, dipole moment, orientational time correlation function (OTCF), autocorrelation function, residence time of water molecules around a particular atom/residue and hydrogen bond occupancy (%) between residues.

- Molecular docking (Auto Dock Vina), Binding free energy calculations (MM-PBSA method), Molecular visualisation softwares: VMD and Pymol.
- Bioinformatics tools: Sequence alignment tools, sequence analysis and phylogenetic studies based tools, and proteins structure prediction tools (MODELLER), Data mining using machine learning software (WEKA)

PROJECT ACTIVITY

Year	Project
Sept.2019 - Present	**Research Associate -I** S. N. Bose National Center for Basic Sciences, Kolkata, India Project title: "Inhibition mechanism of AChE using organoselenides using molecular dynamics simulations" Advisor: Dr. Suman Chakrabarty S. N. Bose National Center for Basic Sciences, Kolkata, India
Sep.2017 - Sep.2019	**Guest Researcher, working remotely:** NIH-National Cancer Institute, Frederick, MD, U.S.A. Project title: "Molecular dissociation mechanism of Rho GTPase- RhoGDI complex upon phosphorylation" Advisor: Dr. Ruth Nussinov (Senior Principal Scientist) NIH-National Cancer Institute, Frederick, MD, U.S.A.
Dec.2013 – Jun.2014	**Master thesis project:** CSIR-National Chemical Laboratory, Pune, India Project title: "Molecular dynamics simulation studies on Rho GTPases reveal conformational sub-states of Switch-I region" Advisor: Dr. Kiran Kulkarni, Dr. Suman Chakrabarty CSIR-National Chemical Laboratory, Pune, India

CONGRESSES AND SEMINARS

Year	Title and Place
2017	11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC-2017), Munich, Germany.
2017	2nd Recent Advances in Modelling Rare Events (RARE), organized by IIT Kanpur and University of Maryland at Agra, India.
2017	Indo-German Workshop on Computing in Chemistry, Biology and Medicine organized by CCNSB, IIIT, Hyderabad, India.
2017	Workshop on Computational Modeling Techniques in Structural Biology, Indian Institute of Science (IISc), Bangalore, India.
2016	15th Indian Theoretical Chemistry Symposium, University of Hyderabad, India.
2016	Symposium on Accelerating Biology 2016: Decoding the Deluge, CDAC, Pune, India.
2016	Elsevier Author Workshop, CSIR-NCL, Pune, India.
2015	NNMCB National Meeting, IISER, Pune, India.
2014	Parallel Computing Workshop, IISER, Pune, India.

PUBLICATIONS

Articles :
1. Hidden electrostatic basis of dynamic allostery in a PDZ domain. A. Kumawat and S. Chakrabarty, Proc. Nat. Acad. Sci. USA., 114, E5825 - E5834 (2017).
2. Nucleotide dependent switching in Rho GTPase: Conformational heterogeneity and competing molecular interactions. A. Kumawat, S. Chakrabarty, K. Kulkarni, Scientific Reports., 7, 45829 (2017).
3. pH dependent allosteric regulation in a PDZ domain: Insights into universal response network. A. Kumawat and S. Chakrabarty (Manuscript under review).
4. Molecular insights into the regulation of Rac1 by selective phosphorylation of RhoGDI. A. Kumawat, H. Jang, S. Chakrabarty and R. Nussinov (Manuscript under submission).
5. Inhibition mechanism of AChE using organoselenides through computational and experimental tools. A. Kumawat and S. Chakrabarty (Manuscript under submission).
6. Addressing the role of structural stability and dynamics of a1-helix in PDZ2 domain. A. Kumawat and S. Chakrabarty (Manuscript under submission).

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

Place and date: **Kolkata**, **04/01/2020**

SIGNATURE

(Amit Kumawat)