

Curriculum Vitae

Amit Kumawat

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DATE OF BIRTH 20th November 1989

CURRENT POSITION

- **Fixed-term Researcher** (Ricercatore a tempo determinato “lettera a” (RTDa) (September 2023 – Present), Department of Physics, University of Cagliari, Sardinia, Italy.

EDUCATION

- **Ph.D.** (Faculty of Chemical Science, July 2014 – November 2019)
CSIR-National Chemical Laboratory, Pune, India
Broad Area of Research: Computational Biophysical Chemistry
Thesis Title: “Molecular Thermodynamic View of Biomolecular Signaling: Allostery and Protein-Protein Interactions”
- **Master of Science** (Bioinformatics), 2012 – 2014
Bioinformatics Centre, University of Pune, India.
- **Bachelor of Science** (Microbiology), 2009 – 2012
M.E.S. Abasaheb Garware College, University of Pune, India.

RESEARCH EXPERIENCE

- **Postdoctoral Fellow** (February 2021 – August 2023)
Department of Biosciences, University of Milan, Italy
- **Postdoctoral fellow** (May 2020 – January 2021)
Indian Institute of technology, Kanpur, India
- **Research Associate – I** (September 2019 – March 2020)
S. N. Bose National Centre for Basic Sciences, Kolkata, India
- **Guest Researcher** (September 2017 – December 2019)
NIH-National Cancer Institute, Frederick, MD, U.S.A.

PUBLICATIONS

- **A. Kumawat**, E. Tavazzani, G. Lentini, A. Trancuccio, D. Kukavica, M. Denegri, S.G. Priori, C. Camilloni, Molecular insights into the rescue mechanism of an hERG activator against severe LQT2 mutations, *bioRxiv* (2024) 2024.03.13.584147. <https://doi.org/10.1101/2024.03.13.584147>.
- S. Costa, A. Minucci, **A. Kumawat**, *et. al.*, Pathogenic G6PD variants: Different clinical pictures arise from different missense mutations in the same codon, *Br J Haematol* (2024). <https://doi.org/https://doi.org/10.1111/bjh.19775>.
- K. Sinha, **A. Kumawat**, S. Chakrabarty, Elucidating the microscopic origin of observed anti-correlation between the protein-protein and protein-water interaction energies, *Chemical Physics Impact* 8 (2024) 100421.
- K. Sinha, **A. Kumawat**, H. Jang, R. Nussinov, S. Chakrabarty, Molecular mechanism of regulation of RhoA GTPase by phosphorylation of RhoGDI, *Biophys J* 123 (2024) 57–67.
- G. Milani, R. Budriesi, E. Tavazzani, *et. al.*, hERG stereoselective modulation by mexiletine-derived ureas: Molecular docking study, synthesis, and biological evaluation, *Arch Pharm (Weinheim)* 356 (2023) 2300116.
- **A. Kumawat**, S. Namsani, D. Pramanik, S. Roy, J.K. Singh, Integrated docking and enhanced

sampling-based selection of repurposing drugs for SARS-CoV-2 by targeting host dependent factors, J Biomol Struct Dyn 40 (2022) 9897–9908.

- **A. Kumawat**, S. Raheem, F. Ali, T.A. Dar, S. Chakrabarty, M.A. Rizvi, Organoselenium compounds as acetylcholinesterase inhibitors: Evidence and mechanism of mixed inhibition, J Phys Chem B 125 (2021) 1531–1541.
- **A. Kumawat**, S. Chakrabarty, Protonation-induced dynamic allostery in PDZ domain: evidence of perturbation-independent universal response network, J Phys Chem Lett 11 (2020) 9026–9031.
- **A. Kumawat**, S. Chakrabarty, Hidden electrostatic basis of dynamic allostery in a PDZ domain, Proceedings of the National Academy of Sciences 114 (2017) E5825–E5834.
- **A. Kumawat**, S. Chakrabarty, K. Kulkarni, Nucleotide dependent switching in rho GTPase: conformational heterogeneity and competing molecular interactions, Sci Rep 7 (2017) 45829.

TECHNICAL SKILLS

- Molecular dynamics simulations and rare event sampling technique such as metadynamics, molecular docking and free energy calculations.
- Experience in cheminformatics and drug discovery software: Schrodinger Suite (Maestro, HTVS, ADME Prediction, Multiple parameter optimisation (MPO)).
- Programming and bioinformatics tools: Sequence alignment tools, sequence analysis and phylogenetic studies-based tools, and protein structure prediction tools.
- Use of HPC resources, github.

AWARDS & DISTINCTIONS

- Fondazione AIRC Postdoctoral fellowship (2024 - 2026).
- Best poster prize in XXI Scientific Convention organised by Fondazione Telethon, Riva del Garda, Italy (2023).
- NCL-RF Keerthi Sangoram Memorial Endowment Award for “Best Research Scholar” in Physical Chemistry Division, CSIR-NCL, Pune, India (2018).
- International Travel Fellowship by Department of Biotechnology, India for attending WATOC-2017, Munich, Germany (2017).
- Best poster award at Indo-German Workshop on Computing in Chemistry, Biology and Medicine (2017) organized by CCNSB, IIIT, Hyderabad, India
- Third Prize for Poster and Oral presentation at Symposium on Accelerating Biology: Decoding the Deluge (2016), organized by CDAC, Pune, India.
- Best poster award at 15th Indian Theoretical Chemistry Symposium (2016), University of Hyderabad, India.
- Best poster award at National Science Day (2016), CSIR-NCL, Pune, India.
- Department of Biotechnology - Research Fellowship awarded for Ph.D. program (August 2014 – July 2019).
- Prof. Dr. Kolaskar Gold Medal for standing 1st in M.Sc. Bioinformatics at University of Pune (2014).
- IGIB-G.N. Ramachandran fellowship during M.Sc. Bioinformatics course (2012- 2014).

GRANTS, CONFERENCES, WORKSHOP & COURSES

Computational Grants

- Principal investigator for IS CRA-C Computational Grant of 96000 GPU core-hours on HPC system Leonardo: *“Tumor-specific targeting of RhoGDI upregulation and downregulation via in silico approaches”*.
- Principal investigator for IS CRA-C Computational Grant of 32000 GPU core-hours on HPC system Marconi (M100): *“Structural and functional characterization of HERG potassium channels’ enhancers as a novel therapeutic strategy for Long QT Syndrome”*.

Oral Presentations

- Physics of Biomolecules: Structure, Dynamics and Function organised by Università degli Studi di Milano and Università degli Studi di Padua, Bressanone, Italy (September 2022).

- Invited talk at Conference on “Recent Trends in Bioinformatics” organized by Bioinformatics Centre, S. P. Pune University, Pune, India (January 2019).
- Symposium on Accelerating Biology 2016: Decoding the Deluge, organized by Centre for Development of Advanced Computing, Pune, India (January 2016).

Poster Presentation

- XXI Scientific Convention organised by Fondazione Telethon, Riva del Garda, Italy (March 2023).
- 67th Biophysical Society Annual Meeting, San Diego, USA (February 2023)
- EMBO/FEBS lecture course on ion channels and transporters in Erice, Italy (May 2022).
- 2nd Recent Advances in Modelling Rare Events (RARE), organized by IIT Kanpur and University of Maryland at Agra, India. (December 2017).
- Indo-German Workshop on Computing in Chemistry, Biology and Medicine organized by CCNSB, International Institute of Information Technology, Hyderabad, India (November 2017).
- 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Munich, Germany (August 2017).
- Workshop on Computational Modeling Techniques in Structural Biology, Indian Institute of Science, Bangalore, India (August 2017).
- 15th Indian Theoretical Chemistry Symposium, University of Hyderabad, India (December 2016).
- NNMCB National Meeting, Indian Institutes of Science Education and Research, Pune, India (2015).

Workshops and Courses

- Introduction to Molecular Modeling in Drug Discovery - Computational Chemistry course by Schrodinger (November 2021).
- Elsevier Author Workshop, organised by CSIR-National Chemical Laboratory, Pune, India (December 2016).
- Parallel Computing Workshop, Indian Institutes of Science Education and Research, Pune, India (July 2014).

OTHER SKILLS

- Co-supervising Activities
Supervision of 1 Master student project thesis at University of Milan, Italy.
- Language Proficiency
English – Bilingual Proficiency
Italian – Limited Working Proficiency (CEFR certificate A2).
German – Beginner (A1)