Lata Rani

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Qualification

- Ph.D. (Chemistry) (7.18) (June 2021)
  Indian Institute of Technology Gandhinagar
- M.S. Pharm. **(**Pharmacoinformatics) (8.96) (June 2013)
  National Institute of Pharmaceutical Education and Research (NIPER-SAS Nagar)
- B.Pharmacy **(**70.75%) (May 2011)
  Delhi Institute of Pharmaceutical Sciences and Research (DIPSAR), New Delhi
- D.Pharmacy **(**71.42%) (May 2007)
  Delhi Institute of Pharmaceutical Sciences and Research (DIPSAR), New Delhi

Grant

- Rajiv Gandhi National Fellowship (UGC) for Ph.D. (April 2015-March 2020)

Award

- Overseas research experience fellowship by IIT Gandhinagar for 6 months internship at Lehigh University, PA, USA. (March 2018-August 2018)
  I worked on intrinsically disordered protein Tau using advanced simulation sampling technique known as parallel tempering well-tempered ensemble (PT-WTE). Setup the simulations for Tau peptide and Tau fibrils to analyze conformational change in the system upon post translational modification.

Work Experience

- Junior Research Analyst (Drug Discovery), NovoInformatics Pvt. Ltd., IIT Delhi
  (October 2013-January 2014)
  Designed research and developed protocols for an in-house software designed to analyze the pharmacokinetic profile of drugs.

Research Experience

Ph.D. project is based on comparative analysis of conformational preferences in peptide upon phosphorylation and O-GlcNAcylation. The study included protein database analysis to reveal structural trends observed in crystal structures; extensive Quantum Mechanical calculations on model peptides; extensive MD simulations on post-translationally modified dipeptides, model α-helices, and Tau fragments to gain insight on the secondary structure preference upon modifications.

Publications

- **Rani, L.**; Mallajosyula, S. S., Phosphorylation-induced structural reorganization in Tau-paired helical filaments. ACS Chemical Neuroscience 2021, 12 (9), 1621-1631.
- **Rani, L.**, Mittal J., Mallajosyula S. S., "Effect of Phosphorylation and O-GlcNAcylation on Proline-rich domain of Tau" *Journal of Physical Chemistry B,* 2020, 124 (10), 1909–1918.

- **Rani, L.**, Mallajosyula S. S., "Phosphorylation versus O-GlcNAcylation: Computational Insights into the Differential Influences of the Two Competitive Post-Translational Modifications" *Journal of Physical Chemistry B*, 2017, 121 (47), 10618–10638.
- **Rani, L.**, Mallajosyula S. S., "Site specific stabilization and destabilization of alanine rich α-helical peptide upon Phosphorylation and O-GlcNAcylation" (under review).
- **Rani, L.**, Arora A., Majhi, S., Patel, D. A., Mishra, A., Mallajosyula, S. S., "Experimental and simulation studies reveal mechanism of action of human defensin derivatives" (under review).

Expertise

- Computational Chemistry, MD simulations using GROMACS, CHARMM
- Computational Quantum mechanical analysis with DFT technique using Gaussian
- Molecular modeling, molecular docking, in-silico drug design, cheminformatics, CADD
- OS: Linux and Windows
- Literature Searches: PubMed, Medline, Embase
- Referencing: EndNote, Mendeley

Management and organization

- Managed several projects and collaborations in parallel, planned work to achieve goals and targets on time
- Organized in-house symposium "Researchers ferret confab 2015" covering broadly Chemistry and Chemical and Material Engineering, March 2015

Conference/Workshop

- ISCBC-NIPiCON-2020 conference on "Integrating Chemical, Biological and Pharmaceutical Sciences for Innovations in Health care", NIRMA University, January 2020.
- Gordon Research Conference (GRC) on "Computational Chemistry ", Mount Snow in West Dover, VT United States, July 2018
- Symposium on "Accelerating biology 2018: Digitizing life" at C-DAC, Pune, India, Jan 2018
- Symposium on "Japan-India Symposium on Material Science", JAIST, Japan, 2017
- International conference on "Theoretical Chemistry Symposium" (TCS), University of Hyderabad, India, 2016
- Workshop on "Gaussian09", Chennai, India, 2015
- International symposium on "Drug Metabolism and Pharamcokinetics" (DMPK), NIPER, India, 2012-13
- International conference on "Modeling Chemical and Biological Reactions" (MCBR3), NIPER, India, 2013

Personal details

- Date of birth: 5th August, 1987
- Gender: Female
- Marital status: Married
- Nationality: Indian

References

Dr. Sairam Swaroop Mallajosyula
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