Prasun Kumar

Present Address

Assistant Professor
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Professional Appointments

Oct 2024–present	Assistant Professor Department of Biological Sciences and Engineering IIT, Palakkad
Dec 2023 – Oct 2024	Senior Bioinformatics Person T-Therapeutics Ltd. Cambridge, UK
Jan 2017 – Nov 2023	Postdoctoral Research Associate Department of Chemistry University of Bristol Bristol, UK

Education

Aug 2011–Jun 2016	Ph.D. in Computational Biology, Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India
Aug 2005–May 2009	B.Tech. in Bioinformatics, SASTRA University, Thanjavur, India

Publications

- **Research Publications in Journals**

1. An atlas of protein homo-oligomerization across domains of life. H. Schweke, T. Levin, M. Pacesa, C. A. Goverde, **P. Kumar**, et al, (2024) ***Cell,*** 187, 999-1010.
2. CC+: A Searchable Database of Validated Coiled coils in PDB Structures and AlphaFold2 Models. **P. Kumar***, R. Petrenas, W.M. Dawson, H. Schweke, E.D. Levy and D. N. Woolfson*, (2023) ***Protein Science*****,** e4789.
3. De novo design of discrete, stable 3_{10}-helix peptide assemblies. **P. Kumar***, N.G. Paterson, J. Clayden and D. N. Woolfson*, (2022) ***Nature***, 607, 387–392.
4. Socket2: A Program for Locating, Visualising, and Analysing Coiled-coil Interfaces in Protein Structures. **P. Kumar*** and D. N. Woolfson*, (2021) ***Bioinformatics***, 37, 23, 4575–4577.
5. RNAHelix: computational modeling of nucleic acid structures with Watson-Crick and non-canonical base pairs. D Bhattacharyya, S Halder, S Basu, D Mukherjee, **P. Kumar** and M.Bansal, (2017) ***Jl of Computer-Aided Molecular Design***, 1–17.
6. Identification of structural and functional analyses of PolyProline-II helices in globular proteins. **P. Kumar** and M.Bansal, (2016) ***Jl of Structural Biology***, 196, 3, 414–425.

7. Dissecting π-helices: Sequence, Structure and Function. **P. Kumar** and M.Bansal, (2015) ***FEBS Journal***, 282, 22, 4415–4432.
8. Identification of local variations within secondary structures of proteins. **P. Kumar** and M.Bansal, (2015) ***Acta Crystallographica Section D*** 71, 5, 1077–1086.
9. MolBridge: A program for identifying non-bonded interactions in small molecules and biomolecular structures. **P. Kumar**, S. Kailasam, S. Chakraborty and M. Bansal (2014) ***J Appl Crystallogr*** 47, 5, 1772–1776.
10. HELANAL-Plus: a web server for analysis of helix geometry in protein structures. **P. Kumar** and M.Bansal, (2012) ***J Biomol Struct Dyn.***, 30,773–783.
11. Identification, Activity and Disulfide connectivity of C-di-GMP Regulating proteins in M. tuberculosis. K. Gupta, **P. Kumar** and D. Chatterji, (2010) ***PLoS ONE*** 5, e15072.

- **Chapters in Books**
  1. Biomolecular Structures: Prediction, Identification and Analyses. **P. Kumar**, S. Halder and M. Bansal in Reference Module in Life Sciences, 2019, Vol 3, pp. 504–534.
  2. Defining α-helix geometry by Cα atom trace vs (φ-ψ) torsion angles: a comparative analysis. A. Shelar[#], **P. Kumar**[#] and M.Bansal in 'Biomolecular Forms and Functions' (Ed. M. Bansal and N.Srinivasan) IISc, Bangalore, 2013, pp.116–127.

**** corresponding author***
#both authors contributed equally
Google Scholar Citations: 400 (as of October 2024)

Technical Skills

- Computational Skills
  1. Programming/Scripting: Perl, Python, Fortran77, R, C^{++}
  2. Data analysis & Statistics: R, MATLAB, Python
  3. AI/ML based approach to design proteins
  4. Domain expertise: Protein design and engineering, Protein structure modeling, homology modeling, binding site analysis, function prediction, protein-protein interaction, sequence analysis
  5. Web development: HTML, CSS, CGI, JavaScript
  6. Software tools: AI based protein structure prediction tools like AlphaFold, Modeller, Rosetta, OpenBabel, NCBI tools and databases, CCP4 suite, Phenix
  7. Databases & OS: MySQL, Postgres, MongoDB, Linux, Mac
- Wet lab Skills
  1. Solid phase peptide synthesis
  2. HPLC
  3. Biophysical characterization: Circular Dichroism, Analytical Ultracentrifugation, SEC
  4. X-ray crystallography

Teaching & Mentoring Experience

2022	Mentored MSci student for his final year project.
2012 & 2013	Teaching Assistant for “Structural Bioinformatics” course in the Molecular Biophysics Unit department at Indian Institute of Science

Grants, Fellowships & Honors

2022	Travel award from "Generate: Biomedicine" for attending "8th Alpbach Workshop on Coiled-coil, Fibrous and Repeat Proteins", Alpbach, Austria
2015	Best Poster Prize for the poster titled "Intrinsic variations in the structures of spacer regions can critically influence the transcription" in MBU In-House symposium, IISc, Bangalore, India
2014	International Travel Support Grant from Department of Science and Technology, Government of India to attend Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery: Bridging Experiments and Computations, Istanbul, Turkey
2013	Awarded Senior Research Fellowship (SRF) by the DBT-BINC
2011	Secured 97.8 percentile in the Graduate Aptitude Test in Engineering
2010	Awarded Junior Research Fellowship (JRF) by the DBT-BINC
2009	Secured AIR-9 in DBT-BINC examination
2008	Awarded Indian academy of science fellowship.
2005—2009	Dean's list, SASTRA University

Conferences & Symposia

- **Oral Presentations**

1. Socket2 and CC$^+$ 2022: Bioinformatics resources for assigning and analyzing coiled-coil structures and models. 8th Alpbach Workshop on Coiled-coil, Fibrous and Repeat Proteins, Alpbach, Austria (2022)
2. A de novo designed 3_{10}-helical bundle. Focal Point organized by school of biochemistry, University of Bristol, Bristol, UK (2021)
3. Identification of local variations within secondary structures of proteins. MBU In-House symposium, IISc, Bangalore, India (2015)
4. Do not Call Me α, I am π-helix. Humboldtkolleg on Interdisciplinary Science: Catalyst for Sustainable Progress, NIAS Auditorium, IISc Campus, Bangalore, India (2014)

- **Poster Presentations**

1. Constructing synthetic-peptide assemblies from de novo designed 3_{10} helices. 8th Alpbach Workshop on Coiled-coil, Fibrous and Repeat Proteins, Alpbach, Austria (2022)
2. Peptides to proteins: Computational Design of a De Novo Three-helix Bundle. Synthetic Biology UK 2018, Bristol, UK (2018)
3. Do not Call Me α, I am π-helix. EMBO Practical Course - CEM3DIP 2016, Thiruvananthapuram, India (2016)
4. Identification of local variations within secondary structures of proteins. MBU In-House symposium, IISc, Bangalore, India (2015)
5. Do not Call Me α, I am π-helix. Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery: Bridging Experiments and Computations, Istanbul, Turkey (2014)

6. Intrinsic variations in the structures of spacer regions can critically influence the transcription. Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery: Bridging Experiments and Computations, Istanbul, Turkey (2014)
7. Amino acid distribution in 3_{10}-helices and their significance for helix stabilization. International Conference on Biomolecular Forms and functions (ICBFF): A celebration of 50 years of the Ramachandran map", Bangalore, India (2013)
8. ASSIGN-A program for assigning regular secondary structure in the protein. 7th Asian Biophysics Association (ABA) Symposium, New Delhi, India (2011)
9. Albumin as a crosslinker in Hydrogels for sustained drug release - A Mathematical analysis. XVI International conference of Society for Biomaterials and Artificial Organs, New Delhi, India (2006)

- **Flash presentation**

1. Constructing synthetic-peptide assemblies from de novo designed 3_{10} helices. 8th Alpbach Workshop on Coiled-coil, Fibrous and Repeat Proteins, Alpbach, Austria (2022)

Outreach & Administrative Services

2019	Data Scientist PI: Challenge proposal for Turing Data Study Group organized by Alan Turing Institute between 5th August-11th August
2018 & 2019	Organizer: ISAMBARD tutorial at CCPBioSim workshop, University of Bristol, Bristol, UK
2013	Organizer: Molecular Biophysics Unit in-house symposium, Indian Institute of Science, Bangalore, India
2013	Volunteer: 'International Conference on Biomolecular Forms and Functions (ICBFF): A Celebration of 50 Years of Ramachandran Map', Indian Institute of Science, Bangalore, India
2012	Volunteer: Indian National Science Academy Annual Meeting, Indian Institute of Science, Bangalore, India
2010	Volunteer: 8th Asia-Pacific Bioinformatics Conference, Indian Institute of Science, Bangalore, India

Professional Activities

- Reviewer for >20 manuscripts for journals: BMC Microbiology, Acta Crystallographica Section F, 3Biotech, Frontiers in Genetics, Archives of Microbiology, Computational Biology and Chemistry & Evolutionary Bioinformatics
- Review Editor for Computational Genomics section of Frontiers in Genetics and Protein Bioinformatics section of Frontiers in Bioinformatics

Scientific Society Membership

2013–present	Indian Biophysical Society
2018–present	Biochemical Society