**Dr. Jhimli Dasgupta**
**Qualification:** M.Sc. (Chemistry),
Ph.D. in (Structural Biology)
**Current Position:** Associate Professor, Postgraduate and Research Department of Biotechnology
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## Honors/Awards

1. '**Innovative Young Biotechnologist Award (IYBA 2010)**' from the Ministry of Science and Technology, **DBT**, Govt. of India.
2. '**Sir P. C. Ray Research Award-2004'** for best thesis from University of Calcutta, India.

## Research experience

- Postdoctoral Research Associate, University of Southern California, CA, USA
- Postdoctoral fellow, Kasha Laboratory, Florida State University, USA
- PhD in Structural Biology, Saha Institute of Nuclear Physics, Kolkata, India

## Research interests and the projects running in the lab

**(1) Structural and functional insights of the molecular motors such as $\sigma^{54}$-dependent transcription activators, involved in flagellar gene transcription and biofilm formation of motile bacteria.**

**(2) Investigating the mechanisms of sensor Histidine kinases that play pivotal roles in flagellar synthesis and motility of motile pathogenic bacteria**

**(2) Understanding the mechanism of nutrient uptake by pathogenic bacteria using ABC transporters to target 'Trojan horse mechanism' of drug delivery**

## Teaching

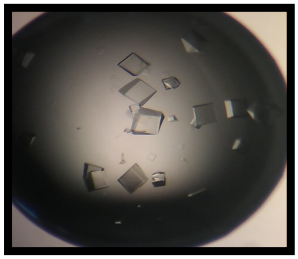
**(a) Theory modules:**

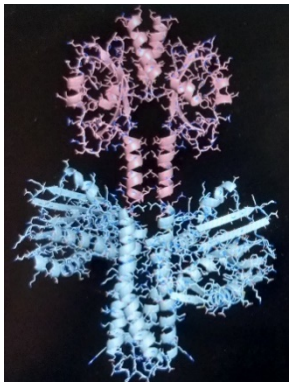
1. Chemical kinetics
2. Enzymology
3. Structural Biology: X-ray crystallography, Cryo-EM, SAXS
4. Bioinformatics
5. Proteomics

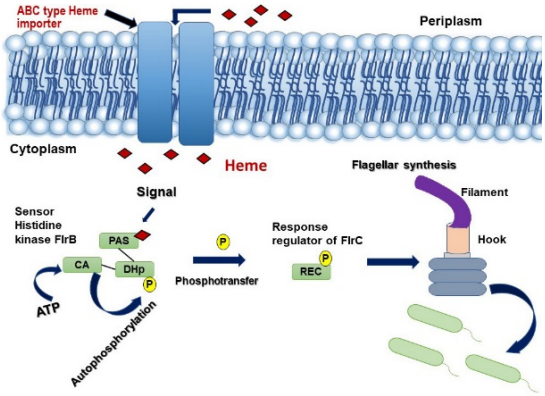
**(b) Practical modules:**

1. Recombinant DNA technology
2. Enzymology
3. Bioinformatics

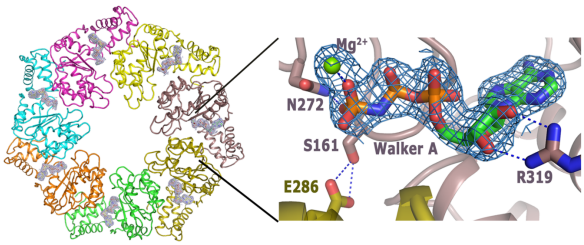
## Glimpse of Research:

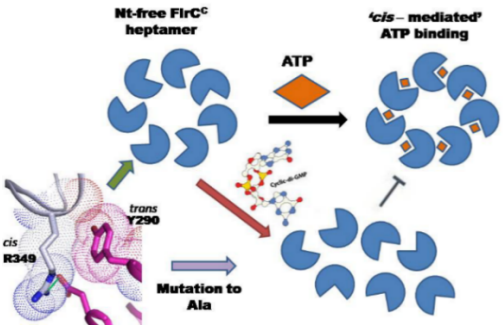


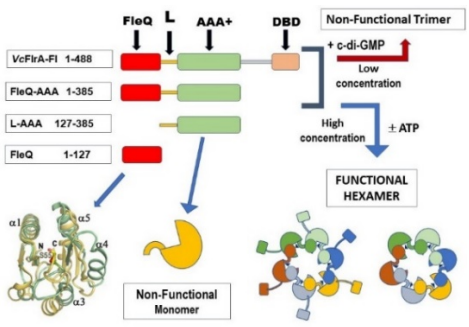


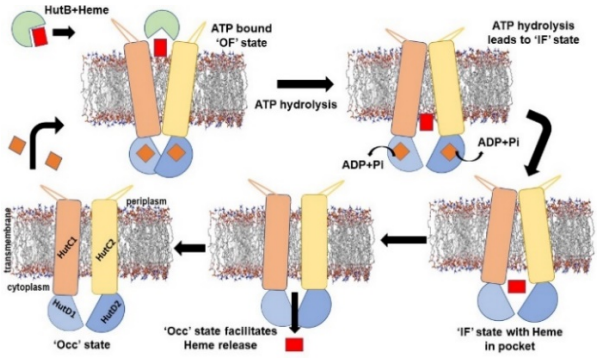



**Structure of Histidine kinase implicated in Flagellar Synthesis**


**c-di-GMP mediated regulation of FlrA**

**Heme transportation through ABC importer HutCD**

**Publications**

1. Mukherjee P, Agarwal S, Mallick SB, Dasgupta J. PAS domain of flagellar histidine kinase FlrB has a unique architecture and binds heme as a sensory ligand in an unconventional fashion. ***Structure***. **2024** Feb 1;32(2):200-216.e5. doi: 10.1016/j.str.2023.11.014. [COVER ARTICLE]

2. Saha I, Ghosh B, Dasgupta J. Structural insights in to the atypical type-I ABC Glucose-6-phosphate importer VCA0625-27 of Vibrio cholerae. ***Biochem Biophys Res Commun***. 2024 Jul 5;716:150030. doi: 10.1016/j.bbrc.2024.150030.

3. Shrestha Chakraborty, Shubhangi Agarwal,Arindam Bakshi, Sanjay Dey, Maitree Biswas, Biplab Ghosh, Jhimli Dasgupta. The N-terminal FleQ domain of the Vibrio cholerae flagellar master regulator FlrA plays pivotal structural roles in stabilizing its active state. ***FEBS Lett.*** **2023 Jul 4.** doi: 10.1002/1873-3468.14693 Epub ahead of print.

4. Saha I, Chakraborty S, Agarwal S, Mukherjee P, Ghosh B, Dasgupta J. Mechanistic insights of ABC importer HutCD involved in heme internalization by *Vibrio cholerae*. ***Sci Rep***. **2022** May 3;12(1):7152. doi:10.1038/s41598-022-11213-9.

5. Chakraborty S, Biswas M, Dey S, Agarwal S, Chakrabortty T, Ghosh B, Dasgupta J. The heptameric structure of the flagellar regulatory protein FlrC is indispensable for ATPase activity and disassembled by cyclic-di-GMP. ***J Biol Chem.*** **2020** Dec 11;295(50):16960-16974. doi: 10.1074/jbc.RA120.014083.

6. Nsp7 and Spike Glycoprotein of SARS-CoV-2 are envisaged as Potential Targets of Vitamin D and Ivermectin. J Dasgupta, U Sen, A Bakshi, A Dasgupta, K Manna, C Saha, RK De, **Preprints. 2020** May 5. doi: 10.20944/preprints202005.0084.v1

7. Agarwal S, Dey S, Ghosh B, Biswas M, Dasgupta J. Mechanistic basis of vitamin B12 and cobinamide salvaging by the Vibrio species. ***Biochim Biophys Acta Proteins Proteom.*** **2019** Feb;1867(2):140-151. doi: 10.1016/j.bbapap.2018.11.004.

8. Agarwal S, Dey S, Ghosh B, Biswas M, Dasgupta J. Structure and dynamics of Type III periplasmic proteins VcFhuD and VcHutB reveal molecular basis of their distinctive ligand binding properties. ***Sci Rep. 2017*** Feb 20;7:42812.

9. Dey S, Biswas M, Sen U, Dasgupta J. Unique ATPase Site Architecture Triggers cis-Mediated Synchronized ATP Binding in Heptameric AAA+-ATPase Domain of Flagellar Regulatory Protein FlrC. ***J Biol Chem***. **2015** Apr 3;290(14):8734-47.

10. Agarwal S, Biswas M, Dasgupta J. Purification, crystallization and preliminary X-ray analysis of the periplasmic haem-binding protein HutB from *Vibrio cholerae*. ***Acta Crystallogr F***. **2015** Apr;71(Pt 4):401-4.

11. Biswas M, Dey S, Khamrui S, Sen U, Dasgupta J. Conformational barrier of CheY3 and inability of CheY4 to bind FliM control the flagellar motor action in *Vibrio cholerae*. ***PLoS One.*** **2013** Sep 16;8(9):e73923.

12. Richards KF, Bienkowska-Haba M, Dasgupta J, Chen XS, Sapp M. Multiple heparan sulfate binding site engagements are required for the infectious entry of human papillomavirus type 16. ***J Virol***. **2013** Nov;87(21):11426-37.

13. Dey S, Dasgupta J. Purification, crystallization and preliminary X-ray analysis of the AAA+ σ54 activator domain of FlrC from Vibrio cholerae. ***Acta Crystallogr Sect F***. **2013** Jul;69(Pt 7):800-3

14. Majumder S, Khamrui S, Dasgupta J, Dattagupta JK, Sen U. Role of remote scaffolding residues in the inhibitory loop pre-organization, flexibility, rigidification and enzyme inhibition of serine protease inhibitors. ***Biochim Biophys Acta***. **2012** Jul;1824(7):882-90.

15. Biswas M, Khamrui S, Sen U, Dasgupta J. Overexpression, purification, crystallization and preliminary X-ray analysis of CheY4 from Vibrio cholerae O395. ***Acta Crystallogr Sect F*. 2011** Dec 1;67(Pt 12):1645-8.

16. Dasgupta J, Bienkowska-Haba M, Ortega ME, Patel HD, Bodevin S, Spillmann D, Bishop B, Sapp M, Chen XS. Structural basis of oligosaccharide receptor recognition by human papillomavirus. ***J Biol Chem*. 2011** Jan 28;286(4):2617-24.

17. Khamrui S, Biswas M, Sen U, Dasgupta J. Cloning, overexpression, purification, crystallization and preliminary X-ray analysis of CheY3, a response regulator that directly interacts with the flagellar 'switch complex' in *Vibrio cholerae*. ***Acta Crystallogr Sect F*. 2010** Aug 1;66(Pt 8):944-7.

18. Khamrui S, Majumder S, Dasgupta J, Dattagupta JK, Sen U. Identification of a novel set of scaffolding residues that are instrumental for the inhibitory property of Kunitz (STI) inhibitors. ***Protein Sci.* 2010** Mar;19(3):593-602.

19. Tsai SJ, Sen U, Zhao L, Greenleaf WB, Dasgupta J, Fiorillo E, Orrú V, Bottini N, Chen XS. Crystal structure of the human lymphoid tyrosine phosphatase catalytic domain: insights into redox regulation. ***Biochemistry*. 2009** Jun 9;48(22):4838-45.

20. Orrú V, Tsai SJ, Rueda B, Fiorillo E, Stanford SM, Dasgupta J, Hartiala J, Zhao L, Ortego-Centeno N, D'Alfonso S; Italian Collaborative Group, Arnett FC, Wu H, Gonzalez Gay MA, Tsao BP, Pons-Estel B, Alarcon-Riquelme ME, He Y, Zhang ZY, Allayee H, Chen XS, Martin J, Bottini N. A loss-of-function variant of PTPN22 is associated with reduced risk of systemic lupus erythematosus. ***Hum Mol Genet*. 2009** Feb 1;18(3):569-79.

21. Thomas M, Dasgupta J, Zhang Y, Chen X, Banks L. Analysis of specificity determinants in the interactions of different HPV E6 proteins with their PDZ domain-containing substrates. ***Virology*. 2008** Jul 5;376(2):371-8.

22. Dasgupta J, Dattagupta JK. Structural determinants of *V. cholerae* CheYs that discriminate them in FliM binding: comparative modeling and MD simulation studies. ***J Biomol Struct Dyn*. 2008** Apr;25(5):495-503.

23. Bishop B, Dasgupta J, Klein M, Garcea RL, Christensen ND, Zhao R, Chen XS. Crystal structures of four types of human papillomavirus L1 capsid proteins: understanding the specificity of neutralizing monoclonal antibodies. ***J Biol Chem*. 2007** Oct 26;282(43):31803-11.

24. Zhang Y#, Dasgupta J#, Ma RZ, Banks L, Thomas M, Chen XS. Structures of a human papillomavirus (HPV) E6 polypeptide bound to MAGUK proteins: mechanisms of targeting tumor suppressors by a high-risk HPV oncoprotein. ***J Virol*. 2007** Apr;81(7):3618-26.

25. Bishop B#, Dasgupta J#, Chen XS. Structure-based engineering of papillomavirus major capsid l1: controlling particle assembly. ***Virol J*. 2007** Jan 8;4:3.

26. Dasgupta J, Khamrui S, Dattagupta JK, Sen U. Spacer Asn determines the fate of Kunitz (STI) inhibitors, as revealed by structural and biochemical studies on WCI mutants. ***Biochemistry*. 2006** Jun 6;45(22):6783-92.

27. Khamrui S, Dasgupta J, Dattagupta JK, Sen U. Single mutation at P1 of a chymotrypsin inhibitor changes it to a trypsin inhibitor: X-ray structural (2.15 A) and biochemical basis. ***Biochim Biophys Acta*. 2005** Aug 31;1752(1):65-72.

28. Sen U, Dasgupta J, Choudhury D, Datta P, Chakrabarti A, Chakrabarty SB, Chakrabarty A, Dattagupta JK. Crystal structures of HbA2 and HbE and modeling of hemoglobin delta 4: interpretation of the thermal stability and the antisickling effect of HbA2 and identification of the ferrocyanide binding site in Hb. ***Biochemistry*. 2004** Oct 5;43(39):12477-88.

29. Dasgupta J, Sen U, Dattagupta JK. In silico mutations and molecular dynamics studies on a winged bean chymotrypsin inhibitor protein. ***Protein Eng*. 2003** Jul;16(7):489-96.

30. Dasgupta J, Sen U, Choudhury D, Datta P, Chakrabarti A, Chakrabarty SB, Chakrabarty A, Dattagupta JK. Crystallization and preliminary X-ray structural studies of hemoglobin A2 and hemoglobin E, isolated from the blood samples of beta-thalassemic patients. ***Biochem Biophys Res Commun***. **2003** Apr 4;303(2):619-23.

**Book Publication:**

Chapter 3. Structural Insights of Cobalamin and Cobinamide Uptake by ABC Importer of *Vibrio* Species. Arunima Bhattacharya[1#], Samriddhi Bhattacharya[1#], Shubhangi Agarwal[1,2] and Jhimli Dasgupta[1]. [1]Post Graduate Department of Biotechnology, St. Xavier's College (Autonomous), Kolkata, West Bengal, India; [2]Weill Cornell Medicine, Department of Anaesthesiology, New York, USA. In: Advances in Health and Disease. Volume 57; Editor: Lowell T. Duncun. ISBN:979-8-88697-098-2. © **2022 Nova Science Publishers, Inc.**

**# Equal contribution.**

**Research Grants [Ongoing]**

(1) Elucidating yet unknown mechanism behind protagonist act of the GTPase, FlhF for flagellar synthesis of Vibrio cholerae by probable modulation of the TCS FlrB-FlrC. Funding: Anusandhan National Research Foundation (**ANRF-ARG**). Sanctioned in April, 2026. Status: Running.

**Research Grants [Completed]**

**(1)** Investigating the mechanistic basis of downstream-enhancer-binding and c-di-GMP mediated transcription regulation of *Vibrio cholerae* FlrC. Granting agency: **DAE(BRNS).** Duration: 2021-2025

**(2)** Investigating structure function relationship of the ATPase-GTPase duo FlhFG that critically regulates flagellar gene transcription and chemotaxis of *Vibrio cholerae*. Granting agency: **MHRD-STARS,** Duration: 2020-2024

**(3)** Understanding the molecular basis of autophosphorylation and phosphotransfer activities of a unique cytosolic sensor Histidine kinase, FlrB, that regulates flagellar synthesis and colonization in *Vibrio cholerae*. Granting Agency: **WBDBT,** Duration: 2016-2021

**(4)** Investigating the molecular mechanism of heme uptake and translocation by ABC transporter system HutB-CD of *Vibrio cholerae*. Granting Agency: **UGC(DAE)-CSR**, Duration: 2016-2021

**(5)** Structural and mechanistic insights of the bacterial enhancer binding proteins FlrA and VpsR of *Vibrio cholerae* and their regulation by second messenger c-di-GMP. Granting Agency: **DST(SERB)**, Duration: 2016-2020

**(6)** Structure and functional insights into the periplasmic Fe(III) and heme binding proteins FhuD and HutB of *Vibrio cholerae* to unravel the mechanism of iron uptake in survival strategy. Granting Agency: **DAE (BRNS),** Duration: 2013-2016

**(7)** Structural and functional studies on transcriptional activator FlrC and its cognate kinase FlrB in *V. cholerae*: a step to understand their role in motility and colonization. Granting Agency: **DBT (IYBA),** Duration: 2011-2015

**(8)** Understanding the role of multiple copies of chemotaxis response regulators (CheYs) present in *Vibrio cholerae*, and their interactions with motor protein FliM: Structural and functional studies. Granting Agency: **CSIR,** Duration: 2009-2012

## CURRENT LAB MEMBERS

**Ruchira Das**

**Arnab Pal**

**Ankita Nanda**

## Lab Alumni

**Dr. Maitree Biswas**
Ph.D awarded: 2016
Former Postdoctoral fellow, University of British Columbia, Canada
Current position: Scientist, Primary Peptides Inc., Unit F142, 2211 Westbrook Mall, Vaccouver BC V6T 2B5, Canada

**Dr. Sanjay Dey**
Ph.D awarded: 2016
Postdoctoral fellow, IGBMC, Alsace, France;
Former Postdoctoral fellow, Penn State University, USA

**Dr. Shubhangi Agarwal**
Ph.D Awarded: 2018
Former Postdoctoral fellow, University of Stuttgart-Hohenheim, Germany
Postdoctoral fellow, Weill Cornell Medicine, Department of Anesthesiology, NY 10065
Current position: Staff Scientist, NYSBC, USA

**Dr. Shrestha Chakraborty**
Ph.D Awarded: 2023
Postdoctoral Research Associate, University of Cambridge, UK

**Dr. Indrila Saha**
Ph.D Awarded: 2024
Postdoctoral Fellow, University of British Columbia, Canada

**Dr. Peeali Mukherjee**
Ph.D Awarded: 2025
Postdoctoral Fellow, IIT Roorkee, India