



## **Dr. Jhimli Dasgupta**

**Department:** Biotechnology

**Qualification:** M.Sc (Chemistry), Ph.D  
(Structural Biology)

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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, India

### **Teaching**

#### **(a) Theory modules:**

1. Chemical kinetics and Structural Enzymology
2. Protein chemistry and Biophysical techniques to understand protein-protein, Protein-DNA interactions
3. Bioinformatics
4. Overview of Protein crystallography and structure function paradigm
5. Proteomics

#### **(b) Practical modules:**

1. Recombinant DNA technology
2. Enzymology
3. Bioinformatics project

### **Research interests and the projects running in the lab**

#### **1. Structural and functional insights of molecular motors such as bacterial enhancer binding protein (bEBPs):**

(a) Structural and functional aspects of AAA<sup>+</sup> ATPase FlrC and its cognate kinase FlrB of *Vibrio cholerae* that control flagellar synthesis and biofilm formation.

(b) FlrA, the master transcription regulator of *Vibrio cholerae* flagellar synthesis: Structural insights, oligomerisation, functional implications and regulation by the second messenger c-di-GMP.

2. **'Trojan horse mechanism' of drug delivery through ABC transporters:**

(a) Structural and functional insights into the periplasmic Fe(III) and heme binding proteins FhuC and HutB of *Vibrio cholerae* to unravel the mechanism of iron uptake in survival strategy.

(b) Unraveling the molecular mechanism of vitamin B12 and norspermidine uptake by *Vibrio cholerae* periplasmic binding proteins BtuF and NspS.

3. **Understanding the role of multiple copies of chemotaxis response regulators (CheYs) and their interactions with kinase CheA to control flagellar motion of *Vibrio cholerae*.**

**Publications**

1. Chakraborty S, Biswas M, Dey S, Agarwal S, Chakraborty 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.

2. 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

3. 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.

4. 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.

5. 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.

6. 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.

7. 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.

8. 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.

9. Dey S, **Dasgupta J**. Purification, crystallization and preliminary X-ray analysis of the AAA+  $\sigma 54$  activator domain of FlrC from *Vibrio cholerae*. *Acta Crystallogr Sect F*. 2013 Jul;69(Pt 7):800-3.

10. 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.
11. 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.
12. **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.
13. 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.
14. 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.
15. 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.
16. 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.
17. 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.
18. **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.
19. 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.
20. 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.
21. Bishop B#, **Dasgupta J**#, Chen XS. Structure-based engineering of papillomavirus major capsid I1: controlling particle assembly. *Viol J*. 2007 Jan 8;4:3.
22. **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.
23. 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 Å) and biochemical basis. *Biochim Biophys Acta*. 2005 Aug 31;1752(1):65-72.

24. 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.
25. **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.
26. **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.

# Equal contribution.

## Research Grants

### Running:

- (1) 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.
- (2) 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
- (3) Investigating the molecular mechanism of heme uptake and translocation by ABC transporter system HutB-CD of *Vibrio cholerae*. Granting Agency: UGC(DAE)-CSR

### Completed:

- (4) 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: 2016-2019
- (5) 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
- (6) 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
- (7) Understanding the role of multiple copies of chemotaxis response regulators (CheYs) present in *Vibrio cholerae*, and their interactions with motor protein FlhM: Structural and functional studies. Granting Agency: CSIR, Duration: 2009-2012

**Current Lab Members:**



**Shrestha Chakraborty**  
SRF: DST (SERB)



**Peeali Mukherjee**  
DST-INSPIRE Fellow



**Indrila Saha**  
SRF: UGC(DAE)



**Ojorshy Basak**  
JRF: MHRD-STARS

**Lab Alumni:**



**Dr. Maitree Biswas**  
PhD awarded: 2016  
Current position: Postdoctoral fellow,  
University of British Columbia, Canada



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



**Dr. Shubhangi Agarwal**  
Ph.D. Awarded: 2018  
Postdoctoral fellow, Cornell University, USA  
Former Postdoctoral fellow, University of  
Stuttgart-Hohenheim, Germany