

## Personal details

### Dr. Parth Sarthi Sen Gupta

Postdoctoral research fellow (PDRF),

DOB – 27.06.1986

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## Current Position

**Postdoctoral Research fellow** in the Department of Chemistry, *Institute of Science Education and Research (IISER)* Berhampur, Berhampur, Odisha, India since 13th April 2018.

## Academic Credentials

**Ph.D., 2018**, in the Department of Biotechnology, DBT (govt. of India), The University of Burdwan.  
The title of my Ph.D. thesis “*Mechanism of amino acids substitution and substitution model: theory and practice by bioinformatical approach*”.

### **M.Sc. (Biotechnology), 2011**

Burdwan University, Burdwan; 77%

### **B.Sc. (Biotechnology), 2009**

Burdwan University, Burdwan; 70%

### **Higher Secondary, 2004**

Central Board of Secondary Education; 72.8%

### **Senior Secondary, 2002**

Central Board of Secondary Education; 75%

## Experience

- Research experience (6 years) June 2012-2018 in Department of Biotechnology, Burdwan University
- Post-doc and teaching in *IISER Berhampur* since April 2018.
- Teaching experience (3 years) 2011-2014 in Institute for Advanced Studies (*IFAS*)

## Awards and Fellowships

- Cleared Graduate Aptitude Test in Engineering (GATE) in 2010 with 540 All India Rank (out of 13262 candidates).

## Research Highlights

- I have published more than **30 research articles** in reputed journals having *h-index* of **13**, *i10-index* of **15** with **395** citations.

- Our research work on COVID19 has been highlighted by more than 30 (National and international) **news agencies** and also recognized by **world health organizations (WHO)**.
- In the world top scientist ranking, I have been ranked **2nd** from Chemical sciences, IISER Berhampur.
- We have already filed application for two **patents**. Details: **1)** filed International standard full patent **“An IoT Based Medicine”** Carrier vide application number **2022/03540** under patent registration office, IPR of Republic of South Africa. **2)** filed Indian full patent **“DESIGNING SINGLE POTENTIAL VACCINE ABHISCOVAC THROUGH IMMUNOINFORMATICS AND IMMUNE SIMULATION APPROACHES”** vide Patent Application No: **202231020075**.

### **List of Research Articles**

1. Choudhury A, **Gupta PS**, Panda SK, Rana MK, Mukherjee S. Designing AbhiSCoVac - a single potential vaccine for all ‘corona culprits’: Immuno-informatics and immune simulation approaches. *Journal of Molecular Liquids*. 2022 Jan 31. **(IF: 6.16)**
2. Ray AK, **Gupta PS**, Panda SK, Rana MK. Repurposing of FDA-approved drugs as potential inhibitors of the SARS-CoV-2 main protease: Molecular insights into improved therapeutic discovery, *Computers in Biology and Medicine*, 2021, 105183, **(IF: 4.6)**
3. Bhattacharya U, Panda SK, **Gupta PS**, Rana MK. Inhibitors of Heptosyltransferase I to prevent heptose transfer against antibiotic resistance of E. coli: Energetics and stability analysis by DFT and molecular dynamics. *Journal of Molecular Structure*. 2021 Dec 24:132258. **(IF: 3.42)**
4. Panda SK, Saxena S, **Gupta PS**, Rana MK. Inhibitors of Plasmeprin X Plasmodium falciparum: Structure-based pharmacophore generation and molecular dynamics simulation. *Journal of Molecular Liquids*. 2021 Jun 30:116851. **(IF: 6.16)**
5. Banerjee S, **Gupta PS\***, Islam RN, Bandyopadhyay AK. Intrinsic basis of thermostability of prolyl oligopeptidase from *Pyrococcus furiosus*. *Scientific reports*. 2021 Jun 2;11(1):1-4. **(IF: 4.42)**
6. Das NC, **Gupta PS\***, Biswal S, Patra R, Rana MK, Mukherjee S. In-silico evidences on filarial cystatin as a putative ligand of human TLR4. *Journal of biomolecular structure & dynamics*.:1-7. **(IF: 3.33)**
7. Panda, S. K., **Gupta, P. S. S\***, Biswal, S., Ray, A. K., & Rana, M. K. (2020). ACE-2-derived Biomimetic Peptides for the Inhibition of Spike Protein of SARS-CoV-2. *J. Proteome Res.* 2021, 20, 2, 1296–1303. **(IF: 4.47)**
8. Das NC, Patra R, **Gupta PS**, Ghosh P, Bhattacharya M, Rana MK, Mukherjee S. Designing of a novel multi-epitope peptide-based vaccine against *Brugia malayi*: An in-silico approach. *Infection, Genetics and Evolution*. 2020 Nov 9:104633. **(IF: 3.42)**
9. **Sen Gupta, Parth Sarthi**, et al. "Binding mechanism and structural insights into the identified protein target of COVID-19 and importin- $\alpha$  with in-vitro effective drug ivermectin." *Journal of Biomolecular Structure and Dynamics* (2020). **(IF: 3.33)**
10. Srivastava R, Gupta SK, Naaz F, **Gupta PS**, Yadav M, Singh VK, Singh A, Rana MK, Gupta SK, Schols D, Singh RK. Alkylated benzimidazoles: Design, synthesis, docking, DFT analysis, ADMET property, molecular dynamics and activity against HIV and YFV. *Computational biology and*

- chemistry. 2020 Dec 1; 89:107400. (IF: 2.88)
11. **Sen Gupta, Parth Sarthi**, and Malay Kumar Rana. "Ivermectin, Famotidine, and Doxycycline: A Suggested Combinatorial Therapeutic for the Treatment of COVID-19." ACS Pharmacology & Translational Science (2020).
  12. **Gupta, Parth Sarthi Sen**, et al. "Computer-aided discovery of bis-indole derivatives as multi-target drugs against cancer and bacterial infections: DFT, docking, virtual screening, and molecular dynamics studies." Journal of Molecular Liquids (2020): 114375. (IF: 6.16)
  13. **Parth Sarthi Sen Gupta**, Shyamashree Banerjee, Sudipta Mondal, Rifat Nawaz Ul Islam, Buddhadev Mondal, Amal Kumar Bandyopadhyay. PHYSICO: An UNIX based Standalone Procedure for Computation of Individual and Group Properties of Protein Sequences. Bioinformatics. 2014, 10 (2), 105.
  14. **Sen Gupta, Parth Sarthi**, et al. "Binding insight of clinically oriented drug famotidine with the identified potential target of SARS-CoV-2." Journal of Biomolecular Structure and Dynamics (2020): 1-7. (IF: 3.33)
  15. Singh VK, Srivastava R, **Gupta PS**, Naaz F, Chaurasia H, Mishra R, Rana MK, Singh RK. Anti-HIV potential of diarylpyrimidine derivatives as non-nucleoside reverse transcriptase inhibitors: Design, synthesis, docking, TOPKAT analysis and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics. 2020 Apr 8:1-7. (IF: 3.33)
  16. **Sen Gupta, Parth Sarthi**, et al. "Screening and molecular characterization of lethal mutations of human homogentisate 1, 2 dioxygenases." Journal of Biomolecular Structure and Dynamics (2020): 1-11. (IF: 3.33)
  17. Haamid Bhat; **Parth Sarthi Sen Gupta**; Satyaranjan Biswal; Malay Kumar Rana. Anion Sensing by Novel Triarylboranes Containing Boraanthracene: DFT Benchmarking, Selective Interactions, and Mechanism Demonstration. 2019. ACS Omega (IF: 3.33).
  18. Sahini Banerjee, Buddhadev Mondal, Rifat Nawaz Ul Islam, **Parth Sarthi Sen Gupta**, Debanjan Mitra, Amal Kumar Bandyopadhyay. POWAINDv1. 0: A Program for Protein- Water Interactions Determination. 2018. Bioinformatics. 14 (9). 530-539. (Projected IF: 5.9)
  19. Rifat Nawaz Ul Islam, Debanjan Mitra, **Parth Sarthi Sen Gupta**, Sahini Banerjee, Buddhadev Mondal, Amal Kumar Bandyopadhyay. AUTOMINv1. 0: an automation for minimization of Protein Data Bank files and its usage. Bioinformatics. 2018. 14 (9). 525- 529 (Projected IF: 5.9)
  20. Rifat Nawaz UL Islam\*, Chittran Roy\*, **Parth Sarthi Sen Gupta\***, Shyamashree Banerjee\*, Amal Kumar Bandyopadhyay\*. PROPAB: Computation of Propensities and Other. Properties from Segments of 3D structure of Proteins. 2018. Bioinformatics 14 (5). 190-193. (Projected IF: 5.9)
  21. Inul Ansary, Arijit Das, **Parth Sarthi Sen Gupta**, Amal Kumar Bandyopadhyay. Synthesis, Molecular Modeling of N-acyl Benzoazetines and their Docking Simulation on Fungal Modeled Target. Synthetic Communication. 2017. 47 (15), 1375-1386. (IF: 2.00).
  22. Banerjee Shyamashree, **Parth Sarthi Sen Gupta**, and Amal Kumar Bandyopadhyay. "Insight into SNPs and epitopes of E protein of newly emerged genotype-I isolates of JEV from Midnapur, West Bengal, India." BMC immunology 18, no. 1 (2017): 13. (IF: 3.62).
  23. **Parth Sarthi Sen Gupta**, Shyamashree Banerjee, Rifat Nawaz Ul Islam, Vishma Pratap Sur, and Amal K. Bandyopadhyay. "Substitutional Analysis of Orthologous Protein Families Using BLOCKS." Bioinformatics 13, no. 1 (2017): 1-7. (Projected IF: 5.9)
  24. Buddhadev Mondal, **Parth Sarthi Sen Gupta**, Chittran Roy, Niladri Hazra, Amal Kumar

- Bandyopadhyay. Comparative Studies on Sequence, Structure and SNPS of E1 Envelope Glycoprotein of Chikungunya Circulating in Maharashtra and West Bengal States of India. IJPBS, (2016), 7(2), 406-417.
25. Arnab Nayek\*, **Parth Sarthi Sen Gupta\***, Shyamashree Banerjee\*, Biswa Pratap Sur, Pratay Seth, Sunit Das, Nathan A Baker, Amal K Bandyopadhyay. ADSETMEAS: Automated Determination of Salt-bridge Energy Terms and Micro Environment from Atomic Structures using APBS method, version 1.0. PROTEIN SCIENCE, (2015), 24, 216-217. (IF: 6.72).
  26. Arnab Nayek\*, **Parth Sarthi Sen Gupta\***, Shyamashree Banerjee\*, Sunit Das, Vishma Pratap Sur, Pratay Seth, Rifat Nawaz Ul Islam and Amal K bandyopadhyay. ADSBET2-- Automated Determination of Salt-bridge Energy Terms version 2. Bioinformation. (2015), 11(8), 413-415.
  27. Shyamashree Banerjee\*, **Parth Sarthi Sen Gupta\***, Arnab Nayek\*, Sunit Das, Vishma Pratap Sur, Pratay Seth, Rifat Nawaz Ul Islam, & Amal K Bandyopadhyay. PHYSICO2: An UNIX based Standalone Procedure for Computation of Physicochemical, Window- dependent and Substitution Based Evolutionary Properties of Protein Sequences along with Automated Block Preparation Tools, Version 2. Bioinformation. (2015), 11(7), 366-368. (Projected IF: 5.9).
  28. Arnab Nayek, **Parth Sarthi Sen Gupta**, Shyamashree Banerjee, Sunit Das, Vishma Pratap Sur, Pratay Seth, Rifat Nawaz Ul Islam and Amal K bandyopadhyay. ADSBET-- Automated Determination of Salt-bridge Energy Terms. IJIPLS. (2015), 5(3), 28-36.
  29. **Sen Gupta Parth Sarthi**, Banerjee Shyamashree, Mondal Sudipta, Mondal Buddhadev, Bandyopadhyay Amal Kumar. An insight into structure and function of chalcone synthase from the sequence of Solanum Tuberosum. Journal of Advanced Bioinformatics application research. (2014), 5(1), 8.
  30. **Sen Gupta Parth Sarthi**, Mondal Buddhadev and Bandyopadhyay Amal Kumar. In silico characterization of human cyclooxygenase using computational tools and servers. IJIPLS. (2013), 3(6), 124.
  31. **Sen Gupta Parth Sarthi**, Mondal Buddhadev and Bandyopadhyay Amal Kumar. In silico characterization of human tyrosinase using computational tools and servers. IJPBS. (2013), 4(3), 181.
  32. **Sen Gupta Parth Sarthi**, Banerjee Shyamashree and Bandyopadhyay Amal Kumar, Sequence, Structural and Functional Characterization of Homogentisate-1, 2-dioxygenase of homo sapiens: An in-silico Analysis. American Journal of Bioinformatics Research. (2013), 3, 42-61.
  33. Arnab Nayek, **Parth Sarthi Sen Gupta**, Shyamashree Banerjee, Buddhadev Mondal, Amal K. Bandyopadhyay Salt-Bridge Energetics in Halophilic Proteins. Plos One. 2014,9(4), e93862 (IF: 3.24)
  34. **Parth Sarthi Sen Gupta**, Arnab Nayek, Shyamashree Banerjee, Pratay Seth, Sunit Das, Vishma Pratap Sur, Chitran Roy & Amal Kumar Bandyopadhyay. SBION2: Analyses of Salt-Bridges from Multiple Structure Files, Version 2. Bioinformation. 2015,11 (1), 039- 042 (Projected IF: 5.9)
  35. **Parth Sarthi Sen Gupta**, Sudipta Mondal, Buddhadev Mondal, Rifat Nawaz Ul Islam, Shyamashree Banerjee & Amal K Bandyopadhyay. SBION: A Program for Analyses of Salt-Bridges from Multiple Structure Files. Bioinformation. 2014,10 (3), 164 (Projected IF: 5.9)

\*Authors contributed equally

➤ Academic Profiles

[ResearchGate](#)

[Google Scholar](#)

### ➤ Symposium/Seminars Presentation (selected)

- **Parth Sarthi Sen Gupta** and Amal K Bandyopadhyay. Odd Amino Acid Substitution Matrices Are Really Odd. FIMB 2012, IISER Kolkata.
- Arnab Nayek\*, **Parth Sarthi Sen Gupta\***, Shyamashree Banerjee\* and Amal K Bandyopadhyay. ADSETMEAS: Automated Determination of Salt Bridge Energy Terms and Microenvironment from Atomic Structures using APBS Method, Version 1.0. The proceedings of 29<sup>th</sup> Annual Symposium, Spain. July 2015.
- **Parth Sarthi Sen Gupta**, Rifat Nawaz UI Islam, Vishma Pratap Sur, Sahini Banerjee and Amal K Bandyopadhyay. New Method to Assess Substitutions and Variability of Different Sites of Protein. 21st CRSI national symposium in chemistry with American Chemical Society (ACS). July 14-16, 2017
- **Parth Sarthi Sen Gupta** and Amal K Bandyopadhyay. Alteration of Codes in the Common Shared Region of Halophilic Ferredoxin for its Adaptation in High Salt. 21st CRSI national symposium in chemistry with American Chemical Society (ACS). July 14-16, 2017

### ➤ Developed Software

1. PHYSICO2 (<http://sourceforge.net/projects/physico2/>)
2. SBION2 (<http://sourceforge.net/projects/sbion2/>)
3. ADSBET (<http://sourceforge.net/projects/adsbet/>)
4. APBEST (<http://sourceforge.net/projects/apbest/>)
5. GENBLOSUMxx (<http://sourceforge.net/projects/genblosumxx/>)
6. ADSBET2 (<http://sourceforge.net/projects/adsbet2/>)
7. PROPAB (<http://sourceforge.net/projects/propab/>)
8. AUTOMINv1.0 (<http://sourceforge.net/projects/automin/>)
9. POWAINDv1.0 (<http://sourceforge.net/projects/automin/>)

### List of three References:

1. **Dr. Amal Kumar Bandyopadhyay**,  
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2. **Dr. Malay Kumar Rana**,  
Assistant Professor, Department of Chemical Sciences, IISER Berhampur, Berhampur-760010, Odisha, India. Phone: +91 680 2227 753, Email: [mrana@iiserbpr.ac.in](mailto:mrana@iiserbpr.ac.in).
3. **Dr. Chandan Goswami**,  
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