Sankar Chandra Basu

Male, Indian, Born on 22.12.1983
Ph.D (Science) from University of Calcutta, India 2014
Computational Biology / Bioinformatics
Doctoral thesis carried out from Saha Institute of Nuclear Physics, Kolkata, India
Post Doc's from (i) FfAME, FL, USA, 2014
(ii) Linkoping University, Sweden, 2014-2016
(iii) DST-SERB National Post Doctoral Fellow, India, 2016-2018
(iv) Computational Biophysics (Delphi) group, Clemson University, USA, 2018
(v) 3BIO, ULB, Brussels, Belgium, 2019
Current: Assistant Professor, Asutosh College, Dept. of Microbiology
under Calcutta University, Kolkata, India (August, 2019 -)
&
External Scientific Collaborator at Prof. Marianne Rooman's group, 3BIO, ULB, Brussels, Belgium (2019-2022)

Permanent Address:

Native:
Lake Residency
343, Dumdum Park, Flat No. 102
Kolkata - 700055
West Bengal, India

Whatsaap: +91-6292210249

Passport Number. R6924295 (India)

valid till 14th Dec, 2027

Email: nemo8130@gmail.com **(primary)**
sankarchandra.basu@asutoshcollege.in **(Official)**

Google_Scholar: **https://scholar.google.com/citations?user=Q5sSUTIAAAAJ&hl=en**
Github: **https://github.com/nemo8130**

ORCID: 0000-0003-1393-1982
Scopus Author ID: 57204428411
Personal Homepage: www.scinetmol.in

h-index: 16
i10-index: 19
(as of to March, 2023)

➔ Statements on Teaching and Research Interests:

◆ Research Objective / Major Interests:

1. Protein Design / Engineering / Peptide Architectonics.
2. Applying Machine Learning, Image Processing, Deep Learning methods to contemporary challenging problems in modern biology and related different interdisciplinary areas.
3. Protein dynamics / Breathing / Molten Globule / Intrinsic Disorder.
4. Structural analysis of membrane proteins, membrane embedding, Drugging of Membrane Proteins
5. Macromolecular structure validation, ranking and scoring, strategies for conformational sampling in molecular docking. Probing protein-protein / protein-nucleic acid interactions using alternative knowledge based semi-empirical functions (e.g., Complementarity) as opposed to energy functions.
6. Classical problems in Graph Theory and its applications in understanding Biological Networks
7. Structure-based functional annotations of proteins. Macromolecular Evolution.
8. Rational Drug design. Scoring protein - small molecule interactions, Virtual Screening

Currently deeply engaged in research on Membrane Proteins (energetics & geometry), COVID19 (Alternative Biotherapeutics & in-depth molecular events), Intrinsically Disordered Proteins (Dynamics & Statistical Mechanics) as well as structural bioinformatics application development (Docking scoring, tools for protein design and study of salt-bridges in ordered and disordered proteins).

◆ Teaching:

To the best of my knowledge and belief, I feel myself competent in teaching a broad range of (both traditional and advanced) topics from Bioinformatics, Biophysics, Biochemistry, Microbiology to Biotechnology having a special emphasize on applications (both computational as well as transnational). My education and research has genuinely had an interdisciplinary component all throughout my academic persuasion.

◆ Teaching Experience:

1. Currently (since, August, 16th, 2019) teaching in the Department of Microbiology as an Assistant Professor at Asutosh College, affiliated to University of Calcutta, Kolkata, India Kolkata. Taught / teaching courses: Metabolism, Expression and regulation of genes, Bacterial growth and nutrition, Microbial control, Fungi, Recombinant DNA technology, Proteins, and, Bioenergetics, Applied Virology, Viral genomes and transmission, Therapeutic and Industrial Biotechnology, Biotransformation, Microbial Products and their recovery. Also teaching environmental science and Interdisciplinary Courses (Microbiology) under the new 4 year NEP UG courses.

2. Taking (annually) a skill enhancement certificate course (https://asutoshcollege.in/new-web/about-bioinformatics.html) on Bioinformatics and Computational Biology for Asutosh College, affiliated to University of Calcutta, Kolkata, India Kolkata.

3. Delivered extended lectures as an invited guest faculty for department of Zoology, Asutosh College, M.Sc, Sem-II, IV, Bioinformatics: Theory and Hands on, May, 2022

4. Took a full course of Bioinformatics practical (M.Sc, Biochemistry, University of Calcutta), January-February, 2017.

5. Took a special paper course (M.Sc, Biochemistry, University of Calcutta) on ‘Molecular Recognition and Docking’, March-May, 2013.

University Examination Duties Performed:

1. Acted as paper setter for the B.Sc Semester V Hons (CBCS) Examination 2020 (syllabus 2018-19) under Calcutta University for the paper Microbiology (MCBA) – DSE-A-2 (Advances in Microbiology) Theory.

2. Acted as paper setter for the B.Sc Semester-IV Hons. (CBCS) Examination 2022 (syllabus 2018-19) under Calcutta University for the paper Microbiology (MCBA) – SEC-B2 (Microbiological analysis of Air and Water) Theory.

3. Acted as paper setter for the B.Sc Semester-IV Hons. (CBCS) Examination 2023 (syllabus 2018-19) under Calcutta University for the paper Microbiology (MCBA) – SEC-B2 (Microbiological analysis of Air and Water) Theory.

4. Acted as paper setter for the B.Sc Semester-IV Hons. (CBCS) Examination 2023 (syllabus 2018-19) under Calcutta University for the paper Microbiology (MCBA) – CC-14 (Medical Microbiology) Theory.

5. Acted as examiner for the B.Sc Semester-IV Hons. (CBCS) Examination 2023 (syllabus 2018-19) under Calcutta University for the paper Microbiology (MCBA) – CC-14 (Medical Microbiology) Theory.

6. Acted as an examiner for the B.Sc Semester-IV Hons. (CBCS) Examination 2023 (syllabus 2018-19) under Calcutta University for the paper Microbiology (MCBA) – SEC-B2 (Microbiological analysis of Air and Water) Theory.

◆ Advanced and Interdisciplinary Courses most willing to teach:

- Protein Folding, Design and Dynamics, Conformational Analysis (Including vector analysis and linear algebra), Use of Machine Learning, Image Processing and Deep Learning Techniques in Biology, Molecular Dynamics: force-fields, energy calculation and minimization, Docking, scoring, ranking, Non-linear Dynamics and systems biology, Bioenergetics, extremophiles and cold adapted enzymes

- Computer architecture, Algorithms and Data Structure, Flow-charts etc. Programming: C, Fortran90, PERL, C++, MATLAB, R, Python, HTML, PHP, webservers (apache), cgi-PERL, web-interacting PERL scripts, API, Graph Theory: Theory and applications in biological networks, Probability theory, PDFs: Binomial, Poisson, Normal distributions, t-test, chi-square etc. Numerical methods: ode solvers, integrals, Linear Algebra: Eigen values and vectors, Vector space, metric, determinants and matrix operations, applications in conformational analysis: third and forth atom fixation, superposition and threading, translation and rotation, internal and global frames of reference, Cartesian to polar, Symmetry operations

- Bioinformatics (sequence data mining, alignment: local & global, profiles), Orthologs & Paralogs, Shannon Entropy, Cloning, Recombinant DNA technology, genetic mapping and engineering

◆ Courses **developed** (& taught) by:

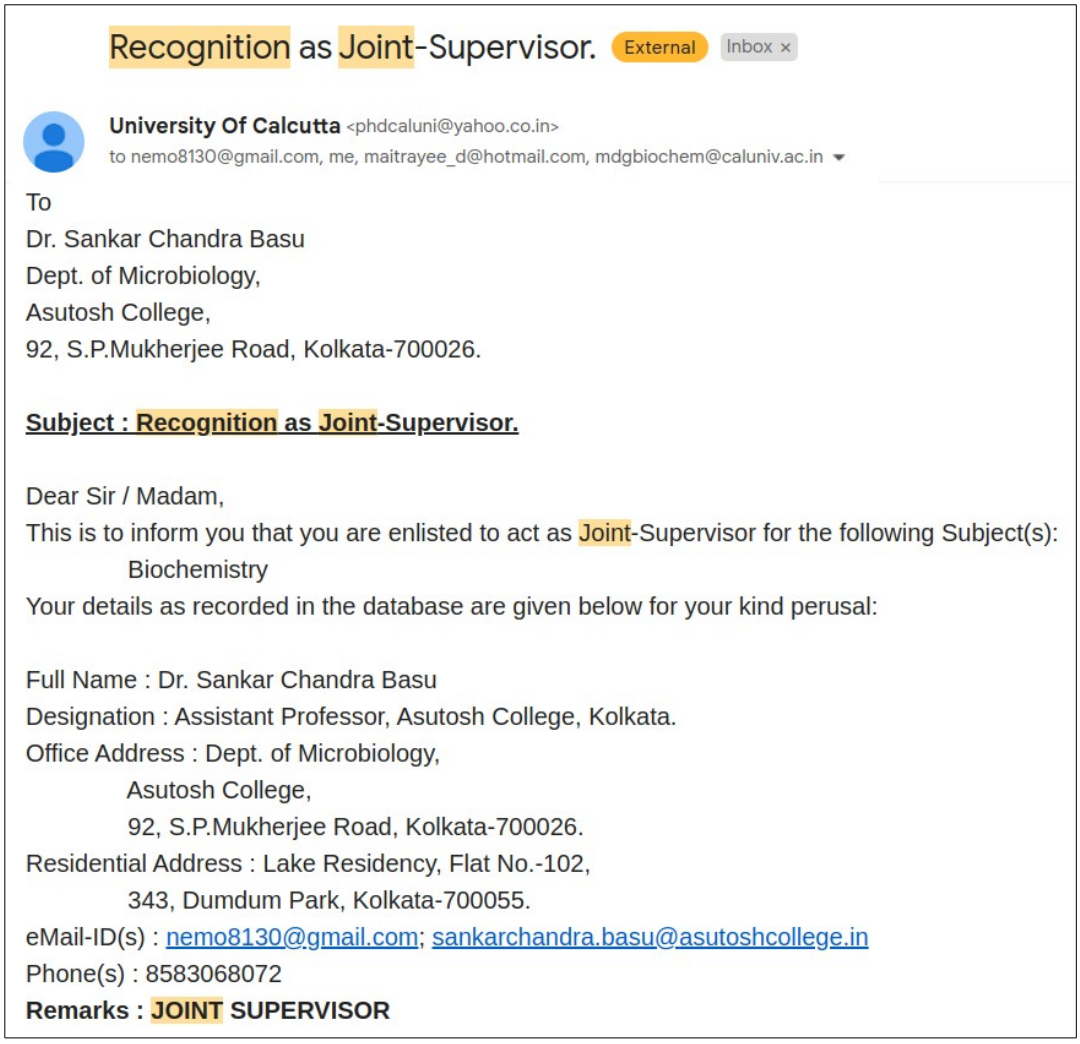
- **BIOINFORMATICS AND COMPUTATIONAL BIOLOGY (6-month Certificate Course, under Asutosh College)** March-August, 2022
https://asutoshcollege.in/new-web/about-bioinformatics.html

◆ Mentorship Experiences:

➢ Guided and supervised the Masters' thesis entitled "**Selecting drug targets in contemporary Human pathogenic diseases and screening them across a database of antimicrobial peptides for plausible therapeutic interventions**" by Ms. Puspita Giri, Department of Bioinformatics (Reg. No. 213001817810017, Roll No. 30017821017), Maulana Abul Kalam Azad University Of Technology, West Bengal as part of the partial fulfillment of her degree of Master of Science during the year 2023.

➢ Co-guiding and joint-supervising the doctoral thesis entitled "**Temperature Dependent Conformers of SYMRK and their Structure-Function Relationship**" by Mr. Souparno Adhikary (**02885/Ph.D. (Sc.) Proceed/2023; 27th April, 2023**) with Prof. Maitrayee DasGupta, Department of Biochemistry, University of Calcutta, Kolkata, India.

- Recognized and enlisted to act as Joint-Supervisor for Department of Biochemistry, University of Calcutta, Kolkata.



Recognition as Joint-Supervisor. External Inbox ×

University Of Calcutta <phdcaluni@yahoo.co.in>
to nemo8130@gmail.com, me, maitrayee_d@hotmail.com, mdgbiochem@caluniv.ac.in

To
Dr. Sankar Chandra Basu
Dept. of Microbiology,
Asutosh College,
92, S.P.Mukherjee Road, Kolkata-700026.

Subject : Recognition as Joint-Supervisor.

Dear Sir / Madam,
This is to inform you that you are enlisted to act as Joint-Supervisor for the following Subject(s):
Biochemistry
Your details as recorded in the database are given below for your kind perusal:

Full Name : Dr. Sankar Chandra Basu
Designation : Assistant Professor, Asutosh College, Kolkata.
Office Address : Dept. of Microbiology,
Asutosh College,
92, S.P.Mukherjee Road, Kolkata-700026.
Residential Address : Lake Residency, Flat No.-102,
343, Dumdum Park, Kolkata-700055.
eMail-ID(s) : nemo8130@gmail.com; sankarchandra.basu@asutoshcollege.in
Phone(s) : 8583068072
Remarks : JOINT SUPERVISOR

➔ List of Publications:

Online access:
https://scholar.google.com/citations?user=Q5sSUTIAAAAJ&hl=en
https://scinetmol.in/sb_homepage/publist.html

Papers in Journals, Book-chapters:

1. Mapping the distribution of packing topologies within protein interiors shows predominant preference for specific packing motifs.
Sankar Basu, Dhananjay Bhattacharyya and Rahul Banerjee*
BMC Bioinformatics 2011, **12**: 195. (ISSN: 1471-2105)
DOI: https://doi.org/10.1186/1471-2105-12-195
PMID: 21605466
Publishers: BMC (Part of Springer Nature)
Journal IF: 3.169

2. Self Complementarity within proteins: bridging the gap between binding and folding.
Sankar Basu, Dhananjay Bhattacharyya and Rahul Banerjee*
Biophysical Journal 2012, **102** (11): 2605-2614. (ISSN: 0006-3495)
DOI: https://doi.org/10.1016/j.bpj.2012.04.029
PMID: 22713576
Publishers: Cell Press
Journal IF: 4.033

3. SARAMA: A Standalone Suite of Programs for the Complementarity Plot – A Graphical Structure Validation Tool for Proteins.
Sankar Basu*, Dhananjay Bhattacharyya and Rahul Banerjee*
Journal of Bioinformatics and Intelligent Control 2013, **2** (4): 321-323. (ISSN: 2326-7496)
DOI: https://doi.org/10.1166/jbic.2013.1059
Publishers: American Scientific Publishers

4. polDNAmelt: Local Melting Within Polymeric DNA—An Improved Method and Its Applications.
Sankar Basu and Dhananjay Bhattacharyya*
Journal of Bioinformatics and Intelligent Control 2013, **2** (4): 316-320. (ISSN: 2326-7496)
DOI: https://doi.org/10.1166/jbic.2013.1058
Publishers: American Scientific Publishers

5. Applications of Complementarity Plot in error detection and structure validation of proteins.
Sankar Basu, Dhananjay Bhattacharyya and Rahul Banerjee*
Indian Journal of Biochemistry and Biophysics, 2014, **51** (June) : 188-200. (ISSN: 0975-0959)
DOI: http://nopr.niscair.res.in/handle/123456789/29083
PMID: 25204080
Publishers: NISCAIR
Journal IF: 1.476

6. Equilibrium unfolding of cyclophilin from Leishmania donovani: Characterization of intermediate states
Sourav Roy, Sankar Basu, Alok K. Datta, Dhananjay Bhattacharyya, Dipak Dasgupta*, and Rahul Banerjee*
International Journal of Biological Macromolecules, 2014, **69**: 353-360. (ISSN: 0141-8130)
DOI: https://doi.org/10.1016/j.ijbiomac.2014.05.063
PMID: 24887548
Publishers: Elsevier
Journal IF: 8.025

7. Analysis of Stacking Overlap in Nucleic Acid Structures: Algorithm and Application
Pavan Kumar Pingali, Sukanya Halder, Debasish Mukharjee, Sankar Basu, Rahul Banerjee, Devapriya Choudhuri and Dhananjay Bhattacharyya*
Journal of Computer-Aided Molecular design, 2014, **28**:851–867 (ISSN: 1573-4951)
DOI: https://doi.org/10.1007/s10822-014-9767-6
PMID: 24990628
Publishers: Springer Nature
Journal IF: 3.686

8. SARAMAint: The Complementarity Plot for Protein-Protein Interface
Sankar Basu, Dhananjay Bhattacharyya, and Bjorn Wallner*
Journal of Bioinformatics and Intelligent Control, 2014, **3:**309-314**.** (ISSN: 2326-7496)
DOI: https://doi.org/10.1166/jbic.2014.1103
Publishers: American Scienctific Publishers

9. The unfolding MD-simulations of Cyclophilin: Analysed by Surface Contact Networks and their associated matrices
Sourav Roy, Sankar Basu, Dipak Dasgupta, Dhananjay Bhattacharyya*, and Rahul Banerjee*
PLOS ONE, 2015, **10**(11): e0142173. (ISSN: 1932-6203)
DOI: https://doi.org/10.1371/journal.pone.0142173
PMID: 26545107
Publishers: PLOS
Journal IF: 3.752

10. Finding correct protein-protein docking models using ProQDock
Sankar Basu, Bjorn Wallner*
Bioinformatics. 2016, **32** (12): i262-i270. (ISSN: 1460-2059)
DOI: https://doi.org/10.1093/bioinformatics/btw257
PMID: 27307625
Publishers: Oxford Press
Journal IF: 6.937

11. DockQ: A quality measure for protein-protein docking models.
Sankar Basu, Bjorn Wallner*
PLOS ONE, 2016, **11**(8): e0161879 (ISSN: 1932-6203)
DOI: https://doi.org/10.1371/journal.pone.0161879
PMID: 27560519
Publishers: PLOS
Journal IF: 3.752

12. RNAHelix: Computational Modeling of Nucleic Acid Structures with Watson-Crick and Non-canonical Base pairs
Dhananjay Bhattacharyya*, Sukanya Halder, Sankar Basu, Prasun Kumar, Debasish Mukherjee, Manju Bansal*
Journal of Computer-Aided Molecular Design, 2017, **31**(2): 219-235 (ISSN: 1573-4951)
DOI: https://doi.org/10.1007/s10822-016-0007-0
PMID: 28102461
Publishers: Springer Nature
Journal IF: 3.686

13. Proteus: A Random Forest Classifier that Predicts Disorder-to-Order Transitioning Binding Regions in Intrinsically Disordered Proteins
Sankar Basu, Fredrik Söderqvist, Björn Wallner*
Journal of Computer-Aided Molecular Design, 2017, **31**(5): 453–466 (ISSN: 1573-4951)
DOI: https://doi.org/10.1007/s10822-017-0020-y
PMID: 28365882
Publishers: Springer Nature
Journal IF: 3.686

14. Salt-bridge Networks within Globular and Disordered Proteins - Characterizing Trends for Designable Interactions.
Sankar Basu* and Debasish Mukharjee
Journal of Molecular Modeling, 2017, **23**:206 (ISSN: 0948-5023)
DOI: https://doi.org/10.1007/s00894-017-3376-y
PMID: 28626846
Publishers: Springer Nature
Journal IF: 1.81

15. Nitric oxide sensing by chlorophyll-a
Abhishek Bhattacharya, Pranjal Biswas, Puranjoy Kar, Piya Roychoudhury, Sankar Basu, Souradipta Ganguly, Sanjay Ghosh, Kaustab Panda, Ruma Pal, Anjan Kr. Dasgupta*
Analytica Chemica Acta, 2017, **985**:101-113 (ISSN: 0003-2670)
DOI: https://doi.org/10.1016/j.aca.2017.07.026
PMID: 28864180
Publishers: Elsevier
Journal IF: 6.911

16. CPdock: The Complementarity Plot for Docking of Proteins: Implementing Multi-dielectric Continuum Electrostatics
Sankar Basu*
Journal of Molecular Modeling, 2018, **24**:8 (ISSN: 0948-5023)
DOI: https://doi.org/10.1007/s00894-017-3546-y
PMID: 29218430
Publishers: Springer Nature
Journal IF: 1.81

17. Salt-bridge Dynamics in Intrinsically Disordered Proteins: A trade-off between electrostatic interactions and structural flexibility
Sankar Basu and Parbati Biswas*
BBA Proteins and Proteomics, 2018, **1866** (5-6): 624-641 (ISSN: 1570-9639)
DOI: https://doi.org/10.1016/j.bbapap.2018.03.002
PMID: 29548979
Publishers: Elsevier
Journal IF: 3.036

18. Inner-view of nanomaterial incited protein conformational changes: Insights in designable interaction. (Review Article)
Arka Mukhopadhyay[$], Sankar Basu[$1], Santiswarup Singha and Hirak K Patra*
Research (Science partner Journal), 2018, 1:9712832 (ISSN: 2639-5274)
DOI: https://doi.org/10.1155/2018/9712832
PMID: 31549040
Publishers: American Association for the Advancement of Science (AAAS)
Art-work from the paper appeared as front cover in the inaugural Journal issue.

19. DelPhiPKa: Including salt in the calculations and enabling polar residues to titrate
Swagata Pahari, Lexuan Sun, Sankar Basu, Emil Alexov*
Proteins: Structure, Function and Bioinformatics, 2018, **86**(12):1277-1283 (ISSN: 1097-0134)
DOI: https://doi.org/10.1002/prot.25608
PMID: 30252159
Publishers: Wiley
Journal IF: 3.756

20. Structural perspective on revealing and altering molecular mechanisms of genetic variants linked with diseases (Review Article)
Yunhui Peng, Emil Alexov, Sankar Basu*
International Journal of Molecular Sciences, 2019, **20**(3), 548 (ISSN: 1422-0067)
DOI: https://doi.org/10.3390/ijms20030548
PMID: 32949230
Publishers: MDPI
Journal IF: 1.81

1[$] Equal Contributions

21. DelPhi suite: New developments and review of functionalities
Chuan Li*, Zhe Jia, Arghya Chakravorty, Swagata Pahari, Yunhui Peng, Sankar Basu, Mahesh Koirala, Shailesh Kumar Pandey, Marharyta Petukh, Lin Li, Emil Alexov*
Journal of Computational Chemistry, 2019, **40**(28), 2502-2508 (ISSN: 1096-987X)
DOI: https://doi.org/10.1002/jcc.26006
PMID: 31237360
Publishers: Wiley
Journal IF: 3.376

22. Graph Coloring: A Novel Heuristic Based on Trailing Path, Perspective and Applications in Structured Networks.
Abhirup Bandyopadhyay, Amit Kumar Dhar, Sankar Basu*
Soft Computing, 2019, **24**:603-625 (ISSN: 1432-7643)
DOI: https://doi.org/10.1007/s00500-019-04278-8
Publishers: Springer Nature
Journal IF: 3.732

23. A comprehensive computational study of amino acid interactions in membrane proteins
Mame Ndew MbayeY, Qingzhen HouY, Sankar Basu, Fabian Teheux, Fabrizio Pucci, Marianne Rooman*
Scientific Reports, 2019, **9**:12043 (ISSN: 2045-2322)
DOI: https://doi.org/10.1038/s41598-019-48541-2
PMID: 31427701
Publishers: *Nature*
Journal IF: 4.996

24. Criticality in the conformational phase transition among self-similar groups in intrinsically disordered proteins: probed by salt-bridge dynamics
Abhirup Bandyopadhyay, Sankar Basu*
BBA Proteins and Proteomics, 2020, **1868**(10): 140474 (ISSN: 1570-9639)
DOI: https://doi.org/10.1016/j.bbapap.2020.140474
PMID: 32579908
Publishers: Elsevier
Journal IF: 3.036

25. Plausible Blockers of Spike RBD in SARS-CoV2 – Molecular Design and Underlying Interaction Dynamics from High-Level Structural Descriptors
Sankar Basu*, Devlina Chakravarty, Pampa Saha, Dhananjay Bhattacharyya, Hirak Kumar Patra
Journal of Molecular Modeling, 2021, **27**(6):191 (ISSN: 0948-5023)
DOI: https://doi.org/10.1007/s00894-021-04779-0
PMID: 34057647
Publishers: Springer Nature
Journal IF: 1.81

26. Invited review for the article '**Phase transitions may explain why SARS-CoV-2 spreads so fast and why new variants are spreading faster'**
by authors: J. C. Phillips, Marcelo Moret, Gilney F. Zebende and Carson C. Chow.
Sankar Basu
(Biorxiv; https://www.biorxiv.org/content/10.1101/2021.02.16.431437v1)
Rapid Reviews: COVID-19 (RR:C19), March, 2021 (ISSN: 2692-4072)
https://rapidreviewscovid19.mitpress.mit.edu/pub/b4kvo7sz/release/1
(published under the Creative Commons license in "RR:C19")

27. Editorial for the "**Special Issue on 'Coronavirus: Vaccines and Other Therapeutics' (2020-21)**"
Sankar Basu*
Vaccine, 2021, **9**(10), 1083 (ISSN: 2076-393X)
DOI: https://doi.org/10.3390/vaccines9101083
Special issue on **'Coronavirus: Vaccines and other therapeutics'**;
Publishers: MDPI
Journal IF: 3.641

28. BRANEart: identify stability strength and weakness regions in membrane proteins
Sankar Basu, Simon S. Assaf, Fabian Teheux, Marianne Rooman*, Fabrizio Pucci*
Frontiers in Bioinformatics, 2021, **1**:742843 (ISSN: 2673-7647)
DOI: https://doi.org/10.3389/fbinf.2021.742843
PMID: 36303753
Publishers: Frontiers

29. Capturing a crucial 'disorder-to-order transition' at the heart of the coronavirus molecular pathology – triggered by highly persistent, interchangeable salt-bridges
Sourav Roy, Prithwi Ghosh, Abhirup Bandyapadhyay, Sankar Basu*
Vaccines, 2022, **10**:301 (ISSN: 1422-0067)
Special Issue on 'Coronavirus: Vaccines and Other Therapeutics'
DOI: 10.3390/vaccines10020301
PMID: 35214759
Publishers: MDPI
Journal IF: 3.641

30. Can the Jigsaw Puzzle Model of Protein Folding Re-assemble a Hydrophobic Core?
Gargi Biswas, Semanti Ghosh*, Sankar Basu, Dhananjay Bhattacharyya, Alok Kumar Datta, Rahul Banerjee*
Proteins: Structure, Function and Bioinformatics, 2022, **90**(7):1390-1412 (ISSN: 1097-0134)
DOI: 10.1002/prot.26321
PMID: 35157344
Publishers: Wiley
Journal IF: 3.756

31. Editorial: From the Hydrophobic Core to the Globular-Disorder Interface: New Challenges and Insights into Protein Design
Sankar Basu*, Devlina Chakravarty, Qingzhen Hou, Vladimir N. Uversky*
Frontiers in Molecular Biosciences (section: Structural Biology), 2023, vol. **10** (*ISSN: 2296-889X*)
DOI: 10.3389/fmolb.2023.1151676
Publishers: Frontiers
Journal IF: 6.113

32. On the Origin Debate and Plausible Future Endeavors of COVID-19. (Book Chapter)
Debdatta Nandy, Bijit Chatterjee, Sankar Basu* (2023).
In S. Bhattacharya, S. Mukhopadhyay & A. Kundu (Eds.). **Virus: Impacts** (pp. 25-41). Kolkata.
(*ISBN: 978-81-956797-5-1*.)
Publishers: Research Committee and Publication Cell, Asutosh College, Kolkata, India.
Pre-print at Preprints.org: https://www.preprints.org/manuscript/202310.1717/v1

33. Phosphorylcholine and KR12-containing Corneal Implants in HSV-1 infected Rabbit Corneas
Kamal Malhotra, Oleksiy Buznyk, Mohammad Mirazul Islam, Elle Edin, Sankar Basu, Marc Groleau, Delali Shana Dégué, Per Fagerholm, Adrien Fois, Sylvie Lesage, Jaganmohan R. Jangamreddy, Egidijus Šimoliūnas, Aneta Liszka, Hirak K. Patra*, May Griffith*
Pharmaceutics. 2023, **15**(6):1658. (ISSN: 1999-4923)
DOI: https://doi.org/10.3390/pharmaceutics15061658
Publishers: MDPI
Journal IF: 6.51

34. EnCPdock: a web-interface for direct conjoint comparative analyses of complementarity and binding energetics in inter-protein associations
Gargi Biswas, Debasish Mukherjee, Nalok Dutta, Prithwi Ghosh, Sankar Basu*
Journal of Molecular Modeling. 2023, **29**:239. (ISSN: 0948-5023)
DOI: https://doi.org/10.1007/s00894-023-05626-0
Publishers: Springer Nature
Journal IF: 2.172

35. Combining complementarity and binding energetics in protein interactions: EnCPdock – A practical manual (Protocol paper)
Gargi Biswas, Debasish Mukherjee, Sankar Basu*
Preprints. https://doi.org/10.20944/preprints202310.1109.v1
Journal of Computational Biology, May, 2024 (online first, volume, pp will appear in print version)
DOI: 10.1089/cmb.2024.0554

36. Plot-Tools in Protein Structure Validations: From the Ramachandran Plot to the Complementarity Plot (Book Chapter, commentary)
Sankar Basu*
Preprints, https://www.preprints.org/manuscript/202311.0741/v1
Chapter-9, in '**Critical studies in Science**' (Vol. 1), Research and Development cell & Publication cell, Asutosh College
ISBN: 978-81-966693-7-9, Date of Publication: 24th December, 2023

37. Modified Host Defence Peptide GF19 slows TNT-mediated spread of Corneal Herpes Simplex Virus Serotype I Infection
Neethi C Thathapudi, Natalia Callai Da Silva, Kamal Malhotra, Sankar Basu, Mozhgan Aghajanzadeh-Kiyaseh, Mostafa Zamani-Roudbaraki, Marc Groleau, Felix Lombard, Sylvie Lesage, May Griffith*
Scientific Reports (2024) 14:4096
DOI: https://doi.org/10.1038/s41598-024-53662-4
Publishers: Nature Portfolio
Journal IF: 4.6

38. Intrinsic disorder and other malleable arsenals of evolved protein multi-functionality (Review Article)
Asifa Aftab, Anirneya Basu, Seema Nath, Sankar Basu*
Preprints.org (2024), 2024021029.
https://doi.org/10.20944/preprints202402.1029.v3
(Accepted, In-press, **Journal of Molecular Evolution**, 2024)

39. Landscape of Intrinsically Disordered Proteins in Mental Disorder Diseases
Xinwu Zhang, Yaqing Yang, Guangchun Hu, Ruotong Liu, Na Zhou, Xixi Song, Sankar Basu*, Ming Jing*, Qingzhen Hou*
Preprints.org, (2024), 2024020573.
https://doi.org/10.20944/preprints202402.0573.v1
(under review, **Computational and Structural Biotechnology Journal**)

Software Copyrights / Patents:

1. Software for Analyzing Magnetic Images by a Fusion Imaging Approach to study Nanoscale Surface Distribution of Magnetic Force
Sankar Basu, Puja Biswas, & Anjan Dasgupta*
Indian Copyright
Diary Number. 9692/2016-CO/SW, Granted (Sept, 2017).
Registration Number. SW-9224/2017

Papers in Conference Proceedings (presented as posters):

1. Poster entitled '**Geometry of hydrophobic contact networks within proteins**', presented at the 'Physics-Biology Interface-2009' organized by Saha Institute of Nuclear Physics and Biophysical Society (December 13-16, 2009).

2. Poster entitled '**Packing motifs within protein interiors and its application in Fold recognition**', presented at the 'Conference on Informatics and Integrative Biology-2011' organized by Bose Institute (December 14-16, 2011).

3. Poster entitled '**Mapping the distribution of packing topologies within protein interiors shows predominant preference for specific packing motifs**', presented at the Recent Advances in Chemical and Physical Biology-2012 organized by Saha Institute of Nuclear Physics and the Mechanobiology Institute, Singapore (March 5-7, 2012).

4. Poster entitled '**Propagation of errors in protein crystal structures: Looking beyond the Ramachandran Plot**' presented at the International Conference on Biomolecular Forms and Functions-2013 organized by the Indian Institute of Science (January 8-11, 2013).

5. Poster entitled "**The Complementarity Plot: a novel graphical tool for protein structure validation.**" presented in the 38th Annual Symposium of Indian Biophysical Society 2014: "Molecular Architecture, Dynamics and Assembly in Living Systems"; 02/2014

6. Poster entitled '**Quality Measures and Scoring Functions for assessment of PPI models using Machine Learning and Complementarity**' presented at the **19th Annual Conference on Sbnet, Swedish Structural Biology Network (SBNET 2015)** hosted by Lund University, at Tallberg, June 12-15, 2015.

7. Poster entitled '**Proteus: A Random Forest Classifier to Predict Disorder-to-Order Transitioning Binding Regions in Intrinsically Disordered Proteins'** given in the conference 'Emerging trends in Biology' organized by department of Biochemistry, University of Calcutta, March, 2017.

◆ Oral Presentations / Invited Talks:

1. Talk entitled '**Mapping the distribution of packing topologies within protein interiors shows predominant preference for specific packing motifs**' delivered in the National Workshop 'To Predict and Model Biological Molecules and System' organized by Bioinformatics Infrastructure Facility, Department of Biochemistry & Biophysics, University of Kalyani held on March 16-18, 2011.

2. Talk entitled '**Propagation of errors in protein crystal structures: looking beyond the Ramachandran Plot**' delivered in the 'International Conference on Biomolecular Forms and Functions: Celebration of 50 years of the Ramachandran Map' organized by the Indian Institute of Science, Bangalore, 8-11 January, 2013.

3. Talk entitled '**Native deviations from ideality: its relationship to protein structural integrity – a key component to predict protein structures ab-initio, overlooked for decades.**' delivered in the 'International Conference on "Is Science able to explain the scientist?' organized by the Bhaktivedanta Institute, NJ, USA held in the Synergy Institute of Technology, Bhubaneswar, Odisha, 8 December, 2013.

4. Talk entitled "**Self Complementarity: its Applications in Probing Protein Internal Architecture, Fold Recognition and Structure Validation.**" presented in FfAME, FL, US, May 13th, 2014.

5. Talk entitled "**Self Complementarity: its Applications in Probing Protein Internal Architecture, Fold Recognition and Structure Validation.**" presented in IFM, LiU, Sweden after joining as a post doctoral fellow, Nov 4th, 2014.

6. Talk entitled "**Recent Developments in assessing the overall quality of Protein-Protein Interaction structural models: their scoring and ranking.**" presented at the **3rd** International Conference on Biotechnology and Bioinformatics, Pune, Feb 5-7, 2016, organized by International Centre for Stem Cells, Cancer and Biotechnology (ICSCCB).

7. Talk entitled "**Finding correct protein-protein docking models using ProQDock**." presented at the conference **Intelligent Systems for Molecular Biology (**ISMB-2016) Orlando, FL, US (July 8-12, 2016, organized by International Society for Computational Biology). Web-link to the talk: https://www.youtube.com/watch?v=KaBgfsog0kQ

8. Invited talk as a visiting fellow entitled "The Globular-Disordered Interface in Proteins: Addressing Molecular Evolution from Protein Design" delivered at IIIT-Alahabad, 31st October, 2017.

9. Invited talk as a visiting fellow entitled "**The Globular-Disordered Interface in Proteins: Addressing Molecular Evolution from Protein Design**" delivered at IIT-Gwuahati, 8th December, 2017.

10. Invited talk on Graph Coloring entitled '**The Trailing Path Algorithm: Resetting the solution of a classical Hard problem in Mathematics (Combinatorics): The Graph Coloring Problem; And its applications**' delivered at Ballygunge Science College, CU, Department of Biochemistry, 16th January, 2020. Web-link to the talk: https://www.youtube.com/watch?v=r33EC4DAMUA&t=2649s

11. Invited **Popular (Bilingual) talk on the COVID-19 pandemic and its therapeutic endeavors** presented for the Breakthrough Science Society, 2020. Web-link to the talk: https://www.youtube.com/watch?v=1IKm_hI1DuE&t=12s

12. Invited talk on "**Transient dynamics of salt-bridges – a key to trigger (avalanche type) transitions among disordered and ordered states in proteins**" delivered at the Birla Institute of Science & Technology (BITS, Pilani), Hyderabed campus on 22nd September, 2021. Web-link to the talk: https://www.youtube.com/watch?v=ZVRXcPVbNQ8

13. Invited talk entitled "**Transient salt-bridge dynamics – a key to trigger (avalanche type) protein disorder transitions and its extensions into latest COVID-research**" held on 04/07/2022 (Monday) at 3:00 PM. in the MBU seminar hall, Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, INDIA. Web-link to the talk: https://www.youtube.com/watch?v=9diSiaJvGg8&t=2063s

14. Invited talk entitled "**Transient salt-bridge dynamics – a key to trigger (avalanche type) protein disorder transitions and its extensions into latest COVID-research**" held on 06/07/2022 (Wednesday) at 4:00 PM. Institute of Bioinformatics and Applied Biotechnology, Biotech Park, GN Ramachandran Rd, Electronics City Phase 1, Electronic City, Bengaluru, Karnataka 560100. Web-link to the talk: https://www.youtube.com/watch?v=3PhpQ_sHLIo

Served as peer Reviewer for papers / communications:

1. Journal of Molecular Modeling (Tracking ID: JMMO-D-17-00212R1), May, 2017
2. Journal of Molecular Modeling (Tracking ID: JMMO-D-17-00447), July, 2017
3. Current Topics in Medicinal chemistry (Title: Covalent inhibition in drug discovery: filling the void in literature, Tracking ID not provided as per journal policy), January, 2018
4. Journal of Molecular Modeling (Tracking ID: JMMO-D-17-00725), March, 2018
5. Journal of Molecular Graphics and Modeling (Tracking ID: JMGM_2018_261 [180420-011890])
6. Current Computer-Aided Drug Design (Tracking ID: BMS-CCADD-2018-50), Sept, 2018
7. Journal of Molecular Modeling (Tracking ID: JMMO-D-18-00706)
8. Current Computer-Aided Drug Design (Tracking ID: BMS-CCADD-2018-95), Oct, 2018
9. Journal of Molecular Graphics and Modeling (Tracking ID: JMGM-2019-33), January, 2019
10. Computational and Structural Biotechnology Journal, (Tracking ID: CSBJ_2019_71), February, 2019
11. IEEE/ACM Transactions on Computational Biology and Bioinformatics, (Tracking ID: TCBB-2019-01-0047), March, 2019
12. Frontiers in Molecular Biosciences, section: Molecular Recognition (Tracking ID: 460353), April, 2019; "Comparative Analysis of Electrostatic Models for Ligand Docking" (Non-anonymous)
13. Peer J (Article ID: 37197), June, 2019
14. Journal of Molecular Modeling (JMMO-D-19-00321), June, 2019
15. IEEE/ACM Transactions on Computational Biology and Bioinformatics (Tracking ID: TCBB-2018-11-0517), July, 2019
16. IEEE/ACM Transactions on Computational Biology and Bioinformatics (Tracking ID: TCBB-2019-04-0175), July, 2019
17. Journal of Molecular Modeling (Tracking ID: JMMO-D-19-00547) Oct, 2019
18. Journal of Molecular Modeling (Tracking ID: JMMO-D-19-00733) Dec, 2019
19. Journal of Molecular Modeling (Tracking ID: JMMO-D-19-00804) Dec, 2019
20. IEEE/ACM Transactions on Computational Biology and Bioinformatics (Tracking ID: TCBB-2019-08-0372), December, 2019
21. Peer J Computer Science (Tracking ID: #CS-2019:04:37197:1) January, 2020
22. Engineering Reports (Tracking ID: ENG-2020-02-0313) April, 2020
23. Journal of Molecular Modeling (Tracking ID: JMMO-D-20-00383), June, 2020
24. Computational and Structural Biotechnology Journal, (Tracking ID: CSBJ-D-20-00330), September, 2020
25. Journal of Molecular Modeling (Tracking ID: JMMO-D-20-00842R1), January, 2021
26. Cancers (ISSN 2072-6694), (Manuscript ID: cancers-1067762), January, 2021
27. Rapid Reviews: COVID-19 (RR:C19) (Manuscript ID: RRC19-D-21-01305), March, 2021 (Invited review)
28. Journal of Molecular Modeling (Manuscript ID: JMMO-D-21-00035), March, 2021
29. International Journal of Molecular Science (MDPI) (Manuscript ID: ijms-1152327), April, 2021
30. Indian Journal of Science and Technology (Manuscript ID: IJST-2021-609), April, 2021
31. Computational and Structural Biotechnology Journal (Tracking ID: CSBJ-D-21-00368), April, 2021
32. Journal of Molecular Modeling (Tracking ID: JMMO-D-21-00043R2), May, 2021
33. Journal of Molecular Graphics and Modeling (Tracking ID: JMGM-D-21-00499), August, 2021
34. Viruses (Tracking ID: 1374225), August, 2021
35. Frontiers in Bioinformatics, InterPepRank: Assessment of Docked Peptide Conformations by a Deep Graph Network, (Tracking ID: 763102), September, 2021 (Non-anonymous)
36. Vaccines (Tracking ID: vaccines-1428158), October, 2021
37. Journal of Molecular Modeling (Tracking ID: JMMO-D-21-00516R1), October, 2021
38. COVID (Tracking ID: covid-1438737), October, 2021
39. Biotech, MDPI (Tracking ID: biotech-1508446), December, 2021
40. Process Biochemistry, Elsevier (Tracking ID: PRBI-D-21-01278), January, 2022
41. Scientific Reports, Nature portfolio (Ref: "Insight into the Instability in the Electrostatic Stability of Proteins" / Tracking ID not available), March, 2022 (Rejected)
42. Frontiers in Bioinformatics, Improving Peptide-Protein Docking with AlphaFold-Multimer using Forced Sampling, June, 2022 (Non-anonymous)

43. Vaccines (Tracking ID: vaccines-2167867), January, 2023
44. Security and Communication Networks (Tracking ID: 2135809), February, 2023
45. Journal of Biomolecular Structure & Dynamics (Tracking ID: TBSD-2023-0962), April, 2023

Served as the handling editor/co-editor for 'accepted and/or published' papers:

1. Neutralizing antibody response of vaccinees to SARS-CoV-2 variants. **(**Brief Report)
Maria Grazia Cusi*, Gabriele Anichini, Chiara Terrosi, Gianni Gori Savellini, Claudia Gandolfo, Federico Franchi
Vaccines 2021, *9*(5), 517; (ISSN: 2076-393X)
Special issue on **'Coronavirus: Vaccines and other therapeutics'**;
Received: 20th April, 2021; Last Revised: 16th May, 2021; Accepted: 18th May, 2021; Published: 21nd May, 2021
Academic Editor: Sankar Basu
https://www.mdpi.com/2076-393X/9/5/517
Publishers: MDPI

2. Influenza virus-like particle (VLP) vaccines expressing the SARS-CoV-2 S glycoprotein, S1, or S2 domains. (Full-length Research Paper)
Ki-Back Chu, Hae-Ji Kang, Keon-Woong Yoon, Hae Ahm Lee, Eun-Kyung Moon, Beom-Ku Han, and Fu-Shi Quan*
Vaccines 2021, *9*(8), 920; (ISSN: 2076-393X)
Special issue on '**Coronavirus: Vaccines and Other Therapeutics**'
Received: 10th May, 2021; Last Revised: 10th August, 2021; Accepted: 12th August, 2021; Published: 18th August, 2021
Academic Editor: Sankar Basu
https://doi.org/10.3390/vaccines9080920
Publishers: MDPI

3. Is It All a Conspiracy? Conspiracy Theories and People's Attitude to COVID-19 Vaccination (Article)
Zheng Yang, Xi Luo *, Hepeng Jia
Vaccines 2021, *9*(10), 1051; (ISSN: 2076-393X)
Special issue on '**Coronavirus: Vaccines and Other Therapeutics**'
Received: 31st August 2021, Last Revised: 17th September 2021, Accepted: 17th September 2021; Published: 21st September, 2021
Academic Editors: Sankar Basu and François Meurens
https://www.mdpi.com/2076-393X/9/10/1051
Publishers: MDPI

4. Parents' Decision to Vaccinate Children against COVID-19: A Scoping Review
(Scoping Review)
Fengming Pan, Hongyu Zhao, Elizabeth Maitland, Stephen Nicholas, Rugang Liu*****, Qingzhen Hou*****
Vaccines 2021, *9*(12), 1476; (ISSN: 2076-393X)
Special issue on '**Coronavirus: Vaccines and Other Therapeutics**'
Received: 17th November, 2021; Last Revised: 3rd December, 2021; Accepted: 10th December, 2021; Published: 14th December 2021
Academic Editor: Sankar Basu
https://www.mdpi.com/2076-393X/9/12/1476
Publishers: MDPI

5. How Does Severe Acute Respiratory Syndrome-Coronavirus-2 Affect the Brain and its Implications for the Vaccines Currently in Use
(Mini-Review)
Philip R. Oldfield, Jennifer Hibberd, Byram W. Bridle*
Vaccines 2022, *10*(1), 1; (ISSN: 2076-393X)
Special issue on '**Coronavirus: Vaccines and Other Therapeutics**'
Received: 8th November, 2021; Revised version received: 15th December, 2021; Accepted: 17th December, 2021; Published: 21st December, 2021
Academic Editor: Sankar Basu
Publishers: MDPI

6. Plant-based vaccines in combat against coronavirus diseases
(Review)
Benita Ortega Berlanga*, Tomasz Pniewski
Vaccines 2022, *10*(2), 138; (ISSN: 2076-393X)
Special issue on '**Coronavirus: Vaccines and Other Therapeutics**'
Received: 4th December 2021; Revised version received: 6th January 2022; Accepted: 14th January 2022; Published: 18th January 2022
Academic Editor: Sankar Basu
Publishers: MDPI

7. Effectiveness of Comirnaty® Vaccine and Correlates of Immunogenicity and Adverse Reactions: A Single-Center Prospective Case Series Study.
Fernández-Lázaro, D., Garrosa, M., Sánchez-Serrano, N., Garrosa, E., Jiménez-Callejo, E., Pardo Yanguas, M. D., et al.
Special issue on '**Coronavirus: Vaccines and Other Therapeutics**'
Vaccines 2022, 10, 1170. (ISSN: 2076-393X)
Received: 8th June 2022; Revised: 18th July 2022; Accepted: 20th July 2022; Published: 22 July 2022
10.3390/vaccines10081170
Academic Editor: Sankar Basu
Publishers: MDPI

8. Some useful ideas for multistate protein design: Effect of amino acid substitutions on the multistate proteins stability and the rate of protein structure formation.
Maria A. Majorina, Tatiana N. Melnik, Anatoly S. Glukhov, Bogdan S. Melnik*
part of the Research Topic collection: 'From the Hydrophobic Core to the Globular-Disorder Interface: New Challenges and Insights into Protein Design'
Frontiers in Molecular Bioscience, 2022 (ISSN: 1664-042X)
Sec. Structural Biology
doi: 10.3389/fmolb.2022.983009
Handling Editor: Sankar Basu
Publishers: Frontiers
https://www.frontiersin.org/articles/10.3389/fmolb.2022.983009/full

9. Prediction of Protein-Protein Interaction Sites in Intrinsically Disordered Proteins (Review Article)
Ranran Chen, Xilu Li, Yaqing Yang, Xixi Song, Cheng Wang*, Dongdong Qiao*
part of the Research Topic collection: 'From the Hydrophobic Core to the Globular-Disorder Interface: New Challenges and Insights into Protein Design'
Frontiers in Molecular Bioscience, 2022 (ISSN: 1664-042X), Section. Structural Biology
doi: 10.3389/fmolb.2022.985022
Handling Editor: Sankar Basu
Publishers: Frontiers
https://doi.org/10.3389/fmolb.2022.985022

10. Combining cysteine scanning with chemical labeling to map protein-protein interactions and infer bound structure in an intrinsically disordered region
Shahbaz Ahmed, Gopinath Chattopadhyay, Kavyashree Manjunath, Munmun Bhasin, Neelam Singh, Mubashir Rasool, Sayan Das, Varsha Rana, Neha Khan, Debarghya Mitra, Aparna Asok, Ramandeep Singh and Raghavan Varadarajan*
part of the Research Topic collection: 'From the Hydrophobic Core to the Globular-Disorder Interface: New Challenges and Insights into Protein Design'
doi: 10.3389/fmolb.2022.997653
Frontiers in Molecular Bioscience, 2022 (ISSN: 1664-042X), Section. Structural Biology
Handling Editor: Sankar Basu
Publishers: Frontiers
https://doi.org/10.3389/fmolb.2022.997653

11. Effects of a plant cyclotide on conformational dynamics and destabilization of β-amyloid fibrils through molecular dynamics simulations
Ramanathan Sowdhamini*, Neha V. Kalmankar, Bhuvaneshwari R. Gehi
Frontiers in Molecular Bioscience, 2022 (ISSN: 1664-042X), Section. Structural Biology
part of the Research Topic collection: 'From the Hydrophobic Core to the Globular-Disorder Interface: New Challenges and Insights into Protein Design'
doi: 10.3389/fmolb.2022.986704
Handling Editor: Sankar Basu
Publishers: Frontiers
https://doi.org/10.3389/fmolb.2022.986704

◆ Skills and Expertise:

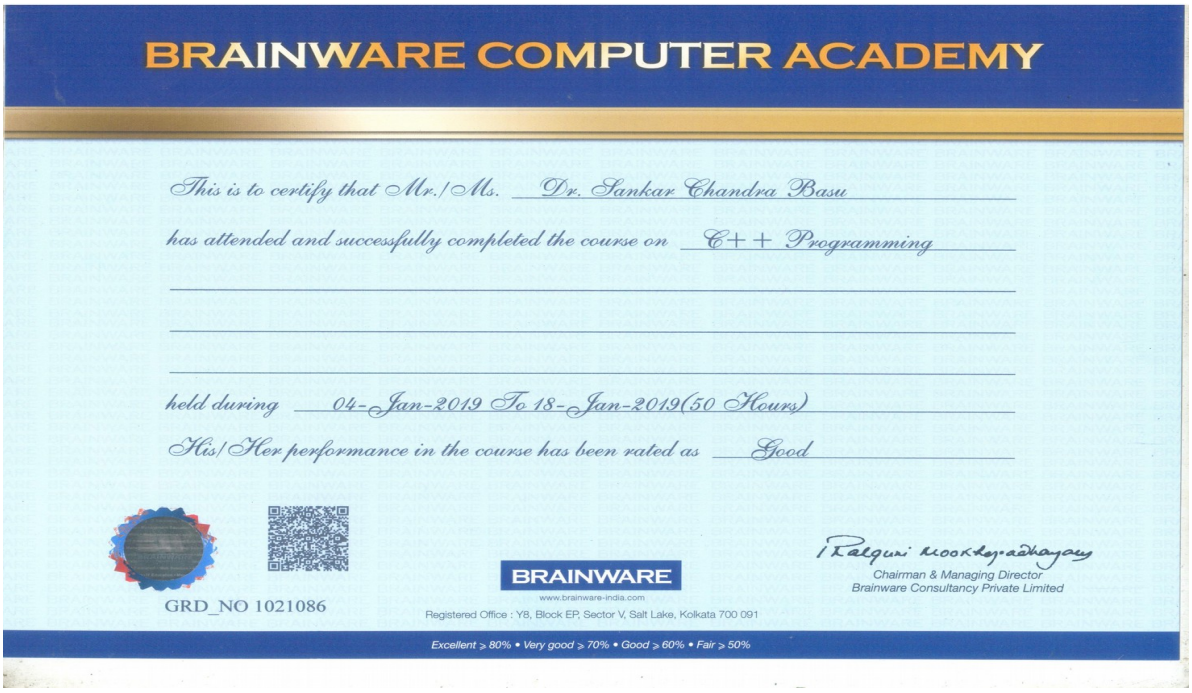
- **Sound knowledge and experience in Linear Algebra, Binary or Multibody Geometry, Eigenvalue based algebraic and geometric multiplicity, Graph Theory and Topology, Vector Analysis, Numerical and Statistical Methods, Optimization algorithms.**

- **Trained in Machine Learning: Neural Netrok, Support Vector Regression Machines, Random Forrest Classifier.**

- **Expert knowledge in construction of algorithms, design of scoring functions, ranking methods, dealing with confusion matrices, developing graphical and visualization protocols and analytical tools based on them.**

- **Experienced in writing long codes related to topology and geometry analysis, surface generation, threading, superposition, side-chain and main-chain rebuilding techniques, third and forth atom fixations, running and tinkering with available computational methods (modeling pipelines for example).**

- **Coding in FORTRAN90, PERL (with demonstrated efficiency and expertise), Python, C, C++ (with growing expertise, successfully completed a deploma course from BARINWARE, Kolkata, India).**


BRAINWARE COMPUTER ACADEMY

This is to certify that Mr./Ms. Dr. Sankar Chandra Basu

has attended and successfully completed the course on C++ Programming

held during 04-Jan-2019 To 18-Jan-2019(50 Hours)

His/Her performance in the course has been rated as Good

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- **Experienced in database studies, structural and conformational analysis, coordinate handling, large data handling.**

- **Expert knowledge in MATLAB, OCTAVE. Growing knowledge in R. Parallel computing in MATLAB, running MATLAB in the no-display mode under shell scripts, Shellscripts (Bash & Csh), Batch scripts in MS-DOS.**

- **Experienced in certain attributes of Image Processing (related to force-microscopy bioimaging and object detection).**

- **Experienced in developing web-servers (HTML, php) and development of standalone suites (shell scripts and post scripts).**

- **Hands on experience in web-interacting script writing (in PERL).**

- **Running multiple parallel jobs simultaneously using bash scripts in a multi-node environment (e.g., sbatch), parallel computing in Fortran using openMP**

- **Adaptable to any platform and language given the premise of a research problem, quick learner.**

- **Experienced in setting up Molecular Dynamic Simulations of proteins under native and denaturing conditions and the analysis of the resultant trajectories. Habituated with the standard analytical techniques like DCCM, RMSF's, multidimentional scaling, time series analysis with cross- and auto- correlations, etc. Experienced in the design and implementation of new metrics and analytical tools to analyze (both native and unfolding) simulation trajectories. Appropriate modulation of the computational protocol by incorporating parameters derived from experiments (from calorimetry, spectroscopy and other biophysical solution assays).**

- **Experienced and innovative in ideas in the computational attributes of protein design (design of hydrophobic cores, salt-bridges etc.)**

- **Molecular Architectonics of native peptides (e.g., cationic AntiMicrobial Peptides of the Cathelicidin group) in tight collaboration with experiments.**

- **Familiar with running Bioinformatic and Simulation Packages like Delphi, NAMD, CHARMM, AMBER, GROMACS, Dali Server, Reduce, SCWRL, Modeller, Stride, Rosetta and others**

- **Hands on experience in protein modeling (MODELLER), small and macromolecular docking (Autodock), applied Bioinformatic web-tools (Uniprot, SMART, Pfam, HHpred, Ali2d, BLAST, clustalx, Muscle etc.) and sequence analysis, basic knowledge of phylogeny and evolutionary biology.**

❖ **Web servers developed / participated in developing:**

PolDNAMelt: http://www.saha.ac.in/biop/www/db/local/nsdnamelt.html
(A web-server to calculate the melting thermodynamics of a contiguous polymeric ds-DNA in solution (with absolute base pairing complementarity) splitting it into sizes of preferred window & overlap by the user)

BRANEart: http://babylone.3bio.ulb.ac.be/BRANEart/index.php
(A fast and accurate method to evaluate the contribution of each amino-acid residue to the overall stability of membrane proteins and to identify interesting residues to mutate in view of modulating stability)

EnCPDock: http://scinetmol.in/EnCPDock/
(A server to compute and correlate Complementarity and Binding free energy estimates in Protein-protein complexes.)

❖ **Softwares developed / involved in the development:**

Sarama: http://www.saha.ac.in/biop/www/sarama.html
https://github.com/nemo8130/SARAMA-updated

(This is a standalone suite of programs serving as a graphical structural validation tool for globular proteins. The Complementarity Plot (CP) plots the surface and electrostatic complementarity of residues buried within proteins. Each point in the plot stands for an amino acid residue which can be located in one of the three regions : probable, less probable, improbable. CP is a sensitive indicator of the harmony or disharmony of interior residues with regard to the short and long range forces sustaining the native fold.)

SaramaInt: http://www.saha.ac.in/biop/www/db/local/sarama/SARAMAint.tar.gz
https://github.com/nemo8130/SARAMAint-updated

(This is another standalone suite of programs serving as a graphical structural validation tool (the Complementarity Plot) for protein-protein interfaces.)

DockQ: http://github.com/bjornwallner/DockQ/
https://github.com/nemo8130/DockQ-fortran-code

(This is a quality measure to assess the quality of protein-protein docking models given their experimental counterpart.)

ProQDock: https://github.com/bjornwallner/ProQDock

(This is a scoring function for protein-protein docking models built in the absence of experimental structures. The function is trained by support vector regression machines using DockQ (http://www.bioinfo.ifm.liu.se/DockQ/) as a target function on state-of-the-art databases of protein-protein docking models having experimental counterparts.)

Software's developed using Delphi (SARAMA, SARAMAint, ProQDock) can be found mentioned at (and hyperlinked from) the **Delphi tools page** (http://compbio.clemson.edu/delphi_tools)

Proteus: https://github.com/bjornwallner/proteus

(This is a random forest classifier to predict Disorder-to-Order transitioning binding regions from sequences of Intrinsically Disordered Proteins)

RNAhelix: http://www.saha.ac.in/biop/bioinformatics.html

(This is a standalone suite of programs to model Nucleic Acid Structures with Watson-Crick and Non-canonical Base pairs validated by comparing surface electrostatic potential maps of the computationally built model and the experimental structures.**)**

Chromnum: https://github.com/nemo8130/Chromnum

(This is a MATLAB & Octave code to calculate the chromatic number of a graph and return the corresponding color-map(s). The computational complexity of the problem is reduced from non-polynomial to quadratic polynomial time by adapting an unique evolutionary trailing path algorithm. This has enormous use in structured networks as well as in protein design.)

FusionImaing_mfm: https://github.com/nemo8130/FusionImaging_mfm
(This is a software for Analyzing Magnetic Images by a Fusion Imaging Approach to Study Nanoscale Surface Distribution of Magnetic Force.)

❖ Databases

1. DB2: A database of monomeric globular proteins which has been extensively used in several studies to probe protein internal architecture, fold recognition and structure validation.
https://github.com/nemo8130/DB2

2. DB3: A database of protein-protein complexes consisting of 1879 co-crystallized interacting native structures (each containing two chains) with resolution better than 2 Å, and no missing backbone atoms. https://github.com/nemo8130/DB3

➔ Experience and Employment Records:

Post Doctoral Experience:

1. Identifying stability strengths and weaknesses in membrane proteins (BRANEart: http://babylone.3bio.ulb.ac.be/BRANEart/index.php) using statistical potentials and membrane embedding (geometry). Comparative study of amino acid interactions in Membrane Proteins using statistical potentials (MuSic). Geometric embedding of membranes in membrane protein 3D atomic structures based on combining coordinates driven (knowledge-based) statistical potentials (as in: MuSic: http://dezyme.com/). (Principal Collaborator: Prof. Marianne Rooman and group, ULB Brussels). The project is still ongoing in collaboration with Prof. Rooman's group.

2. As part of the Delphi group (http://compbio.clemson.edu/delphi), Clemson University, SC, US, associated with maintaining, debugging and further advancement of the popular software Delphi (both in Fortran and C++) for numerically calculating macro-molecular electrostatics. Also associated with other software's developed in the laboratory, namely, delphipKa, SAAMBE related to probing local chemical environment of amino acids within proteins and calculation of thermodynamic parameters in the context of mutation linked with diseases.

3. Probing the role of salt-bridges in relation to flexibility of Intrinsically Disordered Proteins as revealed from their molecular dynamic simulation trajectories. This was carried out in University of Delhi, Department of Chemistry. The project is an essential component of the original DST-SERB project entitled "Building and scoring atomic models for Intrinsically Unstructured Proteins: use of machine learning algorithms and possible therapeutic applications".

4. Worked for ~10 months in University of Calcutta, Department of Biochemistry, on projects: (i) Structural modeling of Intrinsically Disordered Proteins in their bound form – potential therapeutic applications. (DST-SERB) (ii) Probing the role of Magnetic properties in biomolecular interactions with a special emphasis in proteins with intrinsic disorder, (iii) Solving classical graph theory problems (chromatic number), (iv) Deciphering the role of salt-bridges in globular and disordered proteins, (v) Performing docking and computational analyses in probing the interaction of chlorophyl-A to different molecular species of nitric oxides.

5. Worked for 1 year and 7 months in the Björn Wallner's Group, Bioinformatics Division, Department of Physics, Chemistry and Biology, Linkoping University. (http://www.bioinfo.ifm.liu.se/) on the project entitled "Probing protein-protein complexes: Design of Scoring Functions and strategies for conformational sampling". Delivered on protein-protein docking quality and scoring, structural validation of protein-protein complexes, prediction of disorder-to-order transitioning binding regions in Intrinsically Disordered Proteins (IDP's).

6. Worked temporarily for a duration of 5 months (from February to July, 2014) at the Foundation for Applied Molecular Evolution (FfAME), Gainesville, Florida in the NIH funded project entitled 'Non-conserved interactions in Orthologes.' in the group of Prof. Detliend Gerloff and Prof. David Liberles. (http://ffame.org/sbasu.php). Summary: It is a general notion that structure and function are conserved in orthologs, however for the non-classic type (protein-protein interaction) of action performed by proteins, it has been found to have more and more exceptions. Based on the web-resources already available in the public domain, we attempted to analyze chordate gene families and build a database of

non-conserved interaction in orthologs which might have implications for personalized medicine in the future. We initiated with CEACAM (Carcino Embryonic Antigen Cell Adhesion Molecule) as a case study. Learnt the art of phylogeny, meta-genomics and got exposed to personalized madicines. However, the project was not to be continued due to funding uncertainty when I got shifted to Linkoping, Sweden with my next post doc.

➔ Educational Qualification / Academic Record:

- Doctor of Philosophy (Science), Biochemistry (Specialization: Computational Biophysics) 2008-2013, Awarded on June 2, 2014, University of Calcutta
- Post Msc Associateship course, Biophysical Science, 2007-08, Saha Institute of Nuclear Physics, India (77.5%, rank: 1)
- Master of Science (M.Sc.), Biochemistry, 2005-07, Specialization: Systems Biology, Nano-Biotechnology, University of Calcutta, India (78.1%, GPA: 5.40 out of 6, rank: 3)
- Bachelor of Science (B.Sc), Microbiology (Hons), Chemistry, Mathematics, 2002-05, Bidhan Nagar College, University of Calcutta, India (68.5%)
- Higher Secondary (HS), Physics, Chemistry, Biology, Mathematics. 2000-02, Metropolitan Institution (Main), West Bengal Council of Higher Secondary Education. (81.8 %, 1st division, Distinction / Star Marks)
- Secondary (Madhyamik), Physical Science, Life Science, Mathematics, History, Geography, Bengali, English, Aditional Biology. 2000, Metropolitan Institution (Main), West Bengal Board of Secondary Education. (87.0 %, 1st devision, Distinction / Star Marks)

◆ Participation in Conference / Symposium / Schools:

1. **‘International Conference on Physics Biology Interface’,** Saha Institute of Nuclear Physics, Kolkata and Indian Biophysical Society, Kolkata on December 13-16, 2009.
2. **‘Workshop on Proteins: Structure, Function and Folding’,** the Indian Institute of Science, Bangalore on December 20 - 24, 2010.
3. **National Workshop on ‘To Predict and Model Biological Molecules and System’,** Bioinformatics Infrastructure Facility, Department of Biochemistry & Biophysics, University of Kalyani held on March 16-18, 2011.
4. **‘Conference on International and Integrative Biology-2011’,** Bose Institute on December 14-16, 2011.
5. **‘Recent Advances in Chemical and Physical Biology-2012’,** Saha Institute of Nuclear

Physics and the Mechanobiology Institute, Singapore (March 5-7, 2012).

6. **‘International Conference on Biomolecular Forms and Functions: Celebration of 50 years of the Ramachandran Map’,** the Indian Institute of Science, Bangalore, 8-11 January, 2011.

7. **International Conference on “Is Science able to explain the scientist?”** organized by the Bhaktivedanta Institute, NJ, USA held in the Synergy Institute of Technology, Bhubaneswar, Odisha, 8 December, 2013.

8. **38th Annual Symposium of Indian Biophysical Society “Molecular Architecture, Dynamics and Assembly in Living System”** jointly organized by Saha Institute of Nuclear Physics, Kolkata and Indian Biophysical Society on February 7-10, 2014.

9. **LiU Cancer Retreat** October 20 21, 2014 organized by University of Linkoping, Sweden, at Norkoping, Sweden.

10. **Solving the protein folding problem by Direct Coupling Analysis and Next Generation Sequencing, June 8-9, 2015** organized by Karolinska Institute, at Stockhome, Sweden.

11. **19th Annual Conference on SBNET, Swedish Structural Biology Network (SBNET 2015)** hosted by Lund University, at Tallberg, June 12-15, 2015.

12. **3rd International Conference on Biotechnology and Bioinformatics**, Pune, Feb 5-7, 2016, organized by International Centre for Stem Cells, Cancer and Biotechnology (ICSCCB)

13. **Intelligent Systems for Molecular Biology (**ISMB-2016) Orlando, FL, US (July 8-12, 2016, organized by International Society for Computational Biology)

14. '**Emerging trends in Biology**' organized by department of Biochemistry, University of Calcutta, March, 2017

15. **Breaking Barriers through Bioinformatics and Computational Biology-2017**, SCF-Bio, IIT Delhi, July 31st to August 1st, 2017.

16. **All Bengal Science Congress** (organized by Breakthrough Science society), Purulia, WB, India 18-19 January, 2020

◆ Organized Talks / Seminars / Webinars:

1. Webinar on Wetland and Carbon sequestration, organized by Eco-club, Asutosh College, 2nd February, 2022 (Speakers: Mr. Tapan Saha, Senior Scientist (retired), Institute of Environmental Studies and Wetland Management (IESWM), West Bengal, India; Dr. Abhirup Bandyapadhyay, Post Doctoral researcher, Cognitive and Systems Neuroscience Group, SILS, University of Amsterdam, the Netherlands); Co-ordinated the second invited talk given by Dr. Abhirup Bandyapadhyay https://www.youtube.com/watch?v=H7CIcn5h3Q4

2. Departmental student’s Seminar for semester-2 students, Department of Microbiology, Asutosh

College, affiliated to University of Calcutta, Kolkata
https://www.youtube.com/watch?v=2DAtZqJjXCo

◆ Awards, Honors, Recognition:

1. Qualified Graduate Aptitude Test in Engineering (GATE) with an All India Rank of 83; 2007.

2. Awarded UGC-Junior Research Fellowship (All India Rank: 289) in the joint CSIR-UGC National Eligibility Test (NET), June, 2009.

3. **Best Poster Award** in the International Conference on Informatics and Integrative Biology (CIIB 2011), Bose Institute, Kolkata on Decembar 14-16, 2011 for the poster entitled "**Packing motifs within protein interiors and its application in Fold recognition**".

4. '**Special mention**' at the 'International Conference on Biomolecular Forms and Functions: Celebration of 50 years of the Ramachandran Map' (ICBFF 2013), Indian Institute of Science, Bangalore, 8-11 January, 2013 for the poster entitled "**Propagation of errors in protein crystal structures: looking beyond the Ramachandran Plot**".

5. **Prof. N.N. Dasgupta Best Poster Award** in the 38th Annual Symposium of Indian Biophysical Society on "Molecular Architecture, Dynamics and Assembly in Living System" (MADALS 2014), Saha Institute of Nuclear Physics, Kolkata and Indian Biophysical Society on February 7-10, 2014 for the poster entitled "**The Complementarity Plot: A Novel Graphical Tool for Protein Structure Validation**".

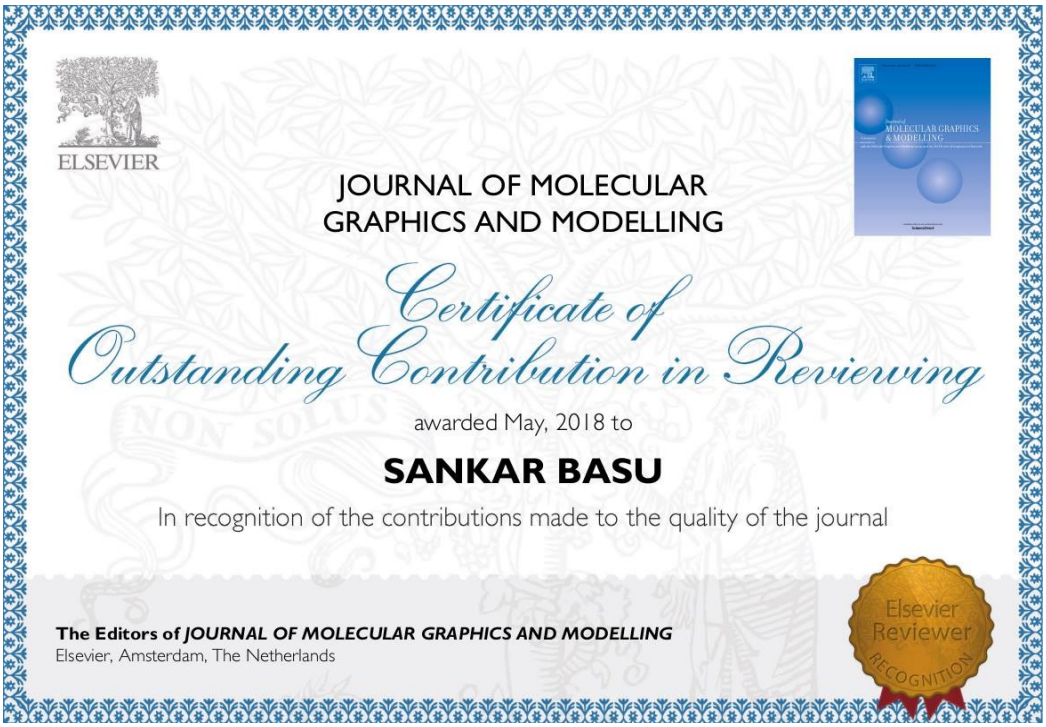
6. Invited delegate at the conference, **Intelligent Systems for Molecular Biology (**ISMB-2016: https://www.iscb.org/ismb2016) Orlando, FL, US (July 8-12, 2016, organized by International Society for Computational Biology) to present the paper '**Finding correct protein-protein docking models using ProQDock'.**

7. Awarded **National Post Doctoral Fellowship** (Science and Engineering Research Board, **Department of Science and Technology, Government of India**) for the project entitled **"Building and scoring atomic models for Intrinsically Unstructured Proteins: use of machine learning algorithms and possible therapeutic applications**" (PDF/2015/001079) for a duration of two years (2016).

8. **Travel Fellowship Award** for ISMB 2016, Orlando, USA, July 8-12, by Vale Institute of Technology, Washington State University. Travel Fellowship Committee Chairs, ISMB 2016

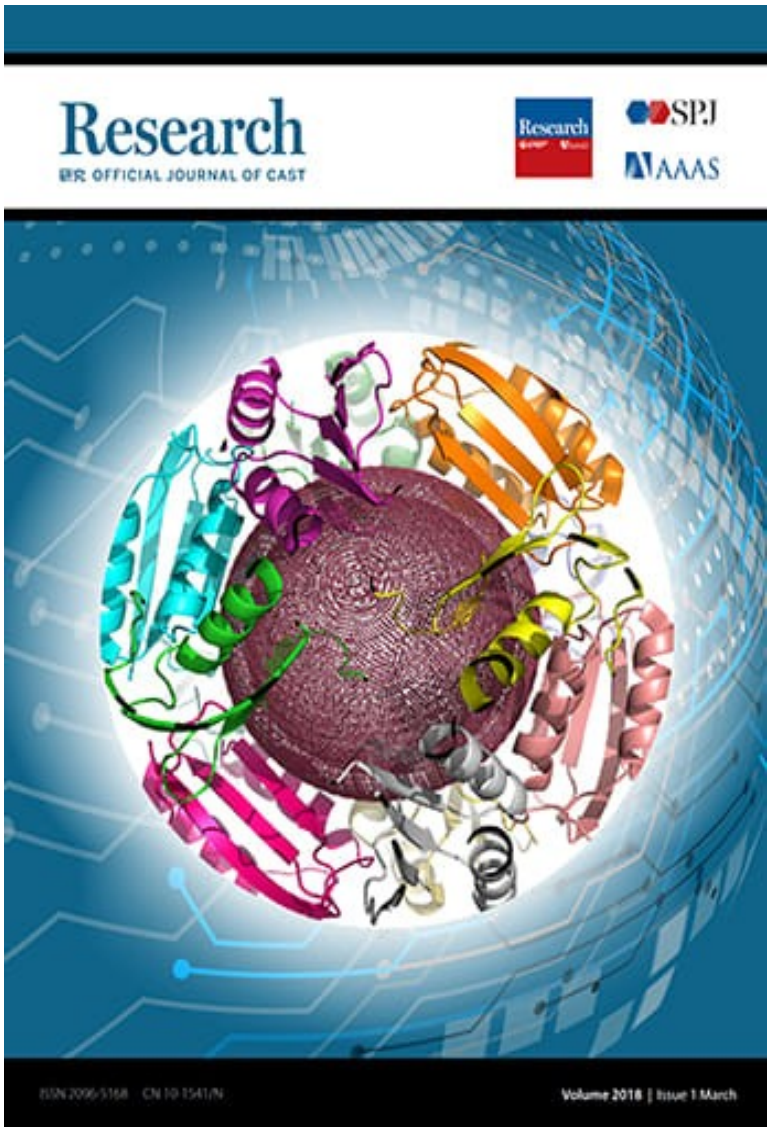
9. Awarded 'Outstanding contribution in reviewing', Journal of Molecular Graphics and

Modeling, (Elsevier) May, 2018.



10. Art-work from the review '**Inner-view of nanomaterial incited protein conformational changes: Insights in designable interaction'** appeared as front cover in the inaugural issue of

Research (Science partner Journal, AAAS), Sept, 2018.



11. Ranked – 1 in West Bengal Collage Service Commission Merit list (2018-19) in Microbiology.
https://www.wbcsconline.in/UploadDocument/Notice/159/MICRO%20BIOLOGY.pdf

12. Selected as an Editorial Board Member for the journal: 'Computational Biology and Bioinformatics', Science Publishing Group, August, 2020

(http://www.sciencepublishinggroup.com/journal/editorialboard?journalid=112)

SciencePG
Science Publishing Group

Science Publishing Group
1 Rockefeller Plaza, 11th Floors,
New York, NY 10020, U.S.A

CERTIFICATE OF EDITORIAL BOARD MEMBERSHIP

Reference: CBB **Date:** August 31, 2020

The certificate is awarded to

Dr. Sankar Chandra Basu, Department of Microbiology, Asutosh College, University of Calcutta, Kolkata, West Bengal, India

In recognition of the Editorial Board Member in

"Computational Biology and Bioinformatics(CBB);

ISSN Print: 2330-8265

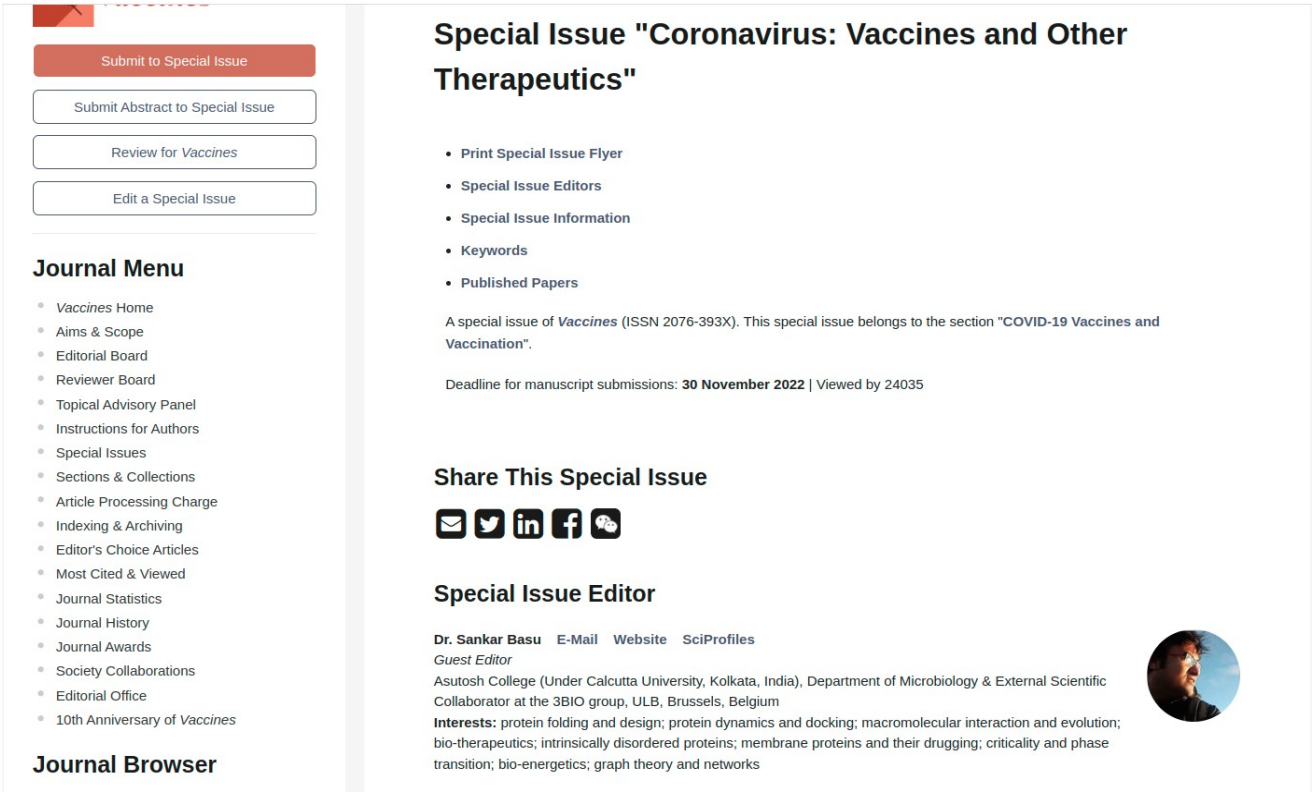
ISSN Online: 2330-8281

http://www.sciencepublishinggroup.com/j/cbb".

For and on behalf of
SCIENCE PUBLISHING GROUP INC.

Authorized Signature(s)

13. Served as a Guest Editor in the journal **Vaccines (ISSN 2076-393X)** for the Special Issue "***Coronavirus: Vaccines and Other Therapeutics***", March, 2021 – February, 2022

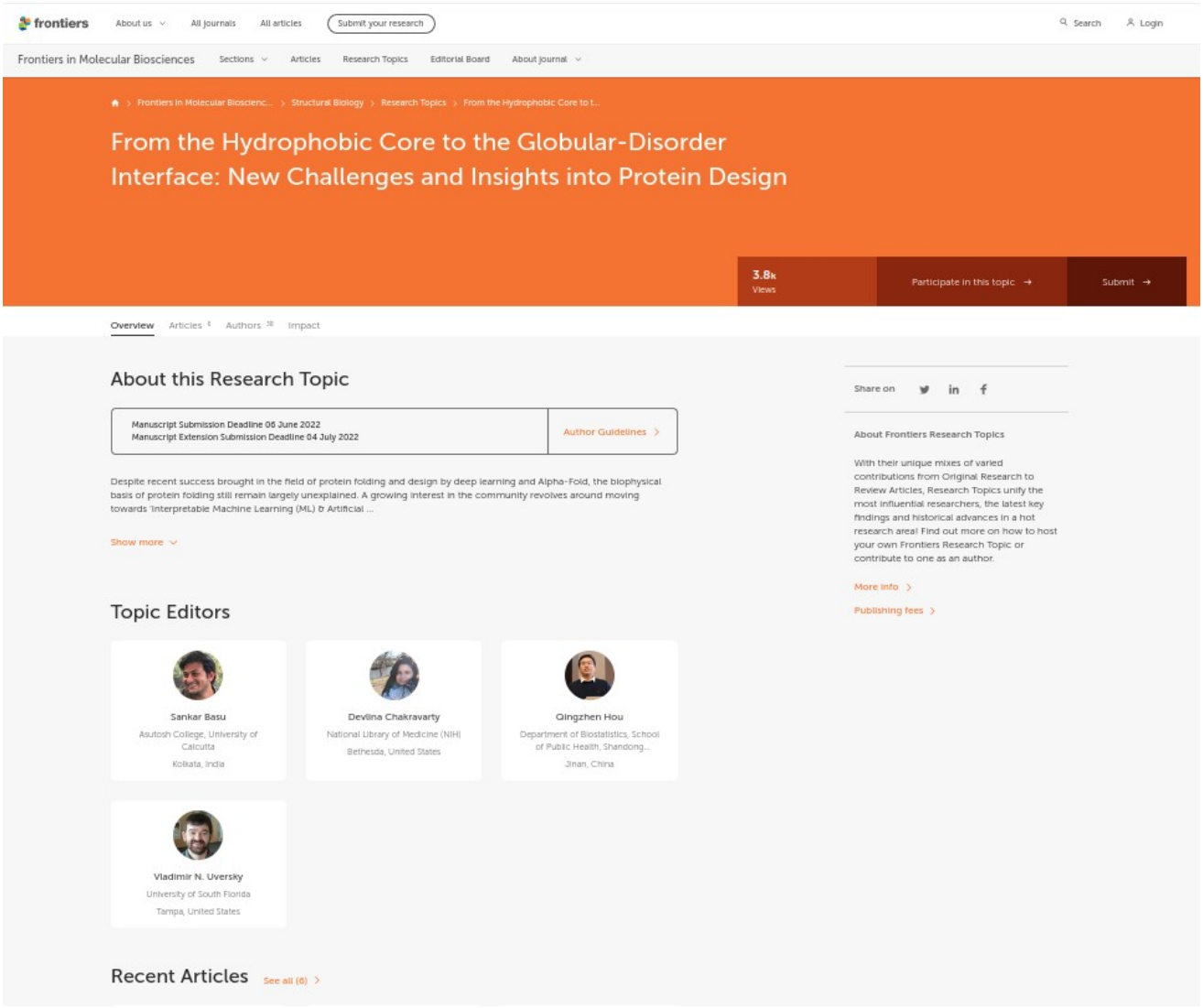


Currently in pursuit: https://www.mdpi.com/journal/vaccines/special_issues/Coronavirus_therapeutics

14. Served as a Guest Editor in the journal **Frontiers in Molecular Bio-science (ISSN 2296889X)** for the Research Topic (RT) "***From the hydrophobic core to the globular-disorder interface: New***

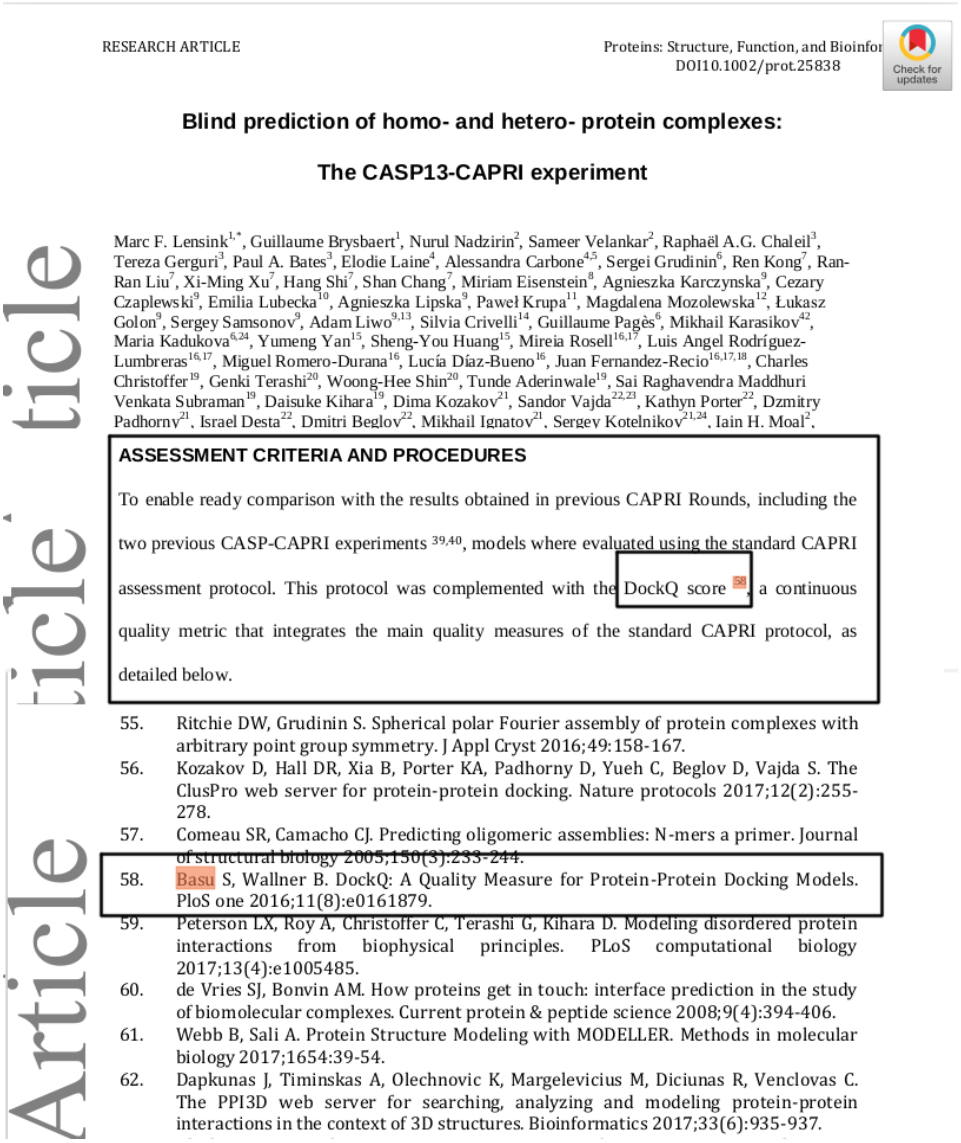
challenges and insights into protein design". June, 2021 – ongoing (extended for a second year, i.e., volume II based on the response from the related research community across the globe).

Currently in pursuit: https://www.frontiersin.org/research-topics/28437/from-the-hydrophobic-core-to-the-globular-disorder-interface-new-challenges-and-insights-into-protei?fbclid=IwAR1WSIbAxambvPz9AQYYSboSkg9owKvYgeWEoU5-fgZeGoK1-56Pik1CXoY



15. A Protein Docking Quality measure (DockQ) developed in my second post doc now-a-days (since,

2019) **serves as the quality estimate for Protein-Protein Complexes in protein Olympic (CAPRI)**



RESEARCH ARTICLE

Proteins: Structure, Function, and Bioinfor
DOI10.1002/prot.25838

Blind prediction of homo- and hetero- protein complexes:

The CASP13-CAPRI experiment

Marc F. Lensink[1,*], Guillaume Brysbaert[1], Nurul Nadzirin[2], Sameer Velankar[2], Raphaël A.G. Chaleil[3], Tereza Gerguri[3], Paul A. Bates[3], Elodie Laine[4], Alessandra Carbone[4,5], Sergei Grudinin[6], Ren Kong[7], Ran-Ran Liu[7], Xi-Ming Xu[7], Hang Shi[7], Shan Chang[7], Miriam Eisenstein[8], Agnieszka Karczynska[9], Cezary Czaplewski[9], Emilia Lubecka[10], Agnieszka Lipska[9], Paweł Krupa[11], Magdalena Mozolewska[12], Łukasz Golon[9], Sergey Samsonov[9], Adam Liwo[9,13], Silvia Crivelli[14], Guillaume Pagès[6], Mikhail Karasikov[42], Maria Kadukova[6,24], Yumeng Yan[15], Sheng-You Huang[15], Mireia Rosell[16,17], Luis Angel Rodríguez-Lumbreras[16,17], Miguel Romero-Durana[16], Lucía Díaz-Bueno[16], Juan Fernandez-Recio[16,17,18], Charles Christoffer[19], Genki Terashi[20], Woong-Hee Shin[20], Tunde Aderinwale[19], Sai Raghavendra Maddhuri Venkata Subraman[19], Daisuke Kihara[19], Dima Kozakov[21], Sandor Vajda[22,23], Kathyn Porter[22], Dzmitry Padhorny[21], Israel Desta[22], Dmitri Beglov[22], Mikhail Ignatov[21], Sergey Kotelnikov[21,24], Iain H. Moal[2],

ASSESSMENT CRITERIA AND PROCEDURES

To enable ready comparison with the results obtained in previous CAPRI Rounds, including the two previous CASP-CAPRI experiments [39,40], models where evaluated using the standard CAPRI assessment protocol. This protocol was complemented with the DockQ score [58], a continuous quality metric that integrates the main quality measures of the standard CAPRI protocol, as detailed below.

55. Ritchie DW, Grudinin S. Spherical polar Fourier assembly of protein complexes with arbitrary point group symmetry. J Appl Cryst 2016;49:158-167.
56. Kozakov D, Hall DR, Xia B, Porter KA, Padhorny D, Yueh C, Beglov D, Vajda S. The ClusPro web server for protein-protein docking. Nature protocols 2017;12(2):255-278.
57. Comeau SR, Camacho CJ. Predicting oligomeric assemblies: N-mers a primer. Journal of structural biology 2005;150(3):233-244.
58. Basu S, Wallner B. DockQ: A Quality Measure for Protein-Protein Docking Models. PloS one 2016;11(8):e0161879.
59. Peterson LX, Roy A, Christoffer C, Terashi G, Kihara D. Modeling disordered protein interactions from biophysical principles. PLoS computational biology 2017;13(4):e1005485.
60. de Vries SJ, Bonvin AM. How proteins get in touch: interface prediction in the study of biomolecular complexes. Current protein & peptide science 2008;9(4):394-406.
61. Webb B, Sali A. Protein Structure Modeling with MODELLER. Methods in molecular biology 2017;1654:39-54.
62. Dapkunas J, Timinskas A, Olechnovic K, Margelevicius M, Diciunas R, Venclovas C. The PPI3D web server for searching, analyzing and modeling protein-protein interactions in the context of 3D structures. Bioinformatics 2017;33(6):935-937.

Current number of citations for the concerned paper: 224 (https://scholar.google.co.in/citations?view_op=view_citation&hl=en&user=Q5sSUTIAAAAJ&citation_for_view=Q5sSUTIAAAAJ:iH-uZ7U-co4C)

16. Could reset the solution of one of the "Hard" problems in Mathematics and Algorithms - the **Graph Coloring Problem (GCP)**, a Combinatorial Optimization (CO) *per se*. GCP falls into the category of "NP-hard" problems in terms of computational/algorithmic complexity. It has several potential applications including that in protein design (serving as a bottleneck filter for surface contact network in designed proteins).

The paper: https://link.springer.com/article/10.1007%2Fs00500-019-04278-8
The software: https://github.com/nemo8130/Chromnum

- **Media Coverage:** Published as a popular article (in Bengali) in the most popular Bengali daily worldwide (16th October, 2019)

এষণা

কলকাতা বুধবার ১৬ অক্টোবর ২০১৯

পথিক গুহ

বাঘ, পান আর ছাগলের গল্প

গণিতশাস্ত্রে চমৎকার সাফল্য তিন বাঙালি গবেষকের

বাঘ, ছাগল আর পান। পার হবে নদী। মাঝি বেচারা ধন্দে। কারণ, তাঁর নৌকো বইতে পারে কেবল একটা জিনিস। তিনি পারাপার করবেন কোন ফর্মুলায়? পর পর বাঘ, ছাগল এবং পান? উঁহু, বাঘ খায় ছাগল। ছাগল আবার খায় পান। তাই প্রথম বার ও পারে বাঘ, ও দ্বিতীয় বারে ছাগল পৌঁছলে রক্ষে নেই। রক্ষে নেই পর পর দু'বারে ছাগল আর পান পৌঁছলেও। কী করা? বড়রা বাচ্চাদের প্রায়ই এ ধাঁধা সমাধান করতে বলেন।

তিন গবেষক ওঁদের সাফল্য ঘোষণায় সম্প্রতি এক পেপার ছেপেছেন বিখ্যাত 'সফ্‌ট কম্পিউটিং' জার্নালে।

অনেক রকম বিকল্পের মধ্যে সেরাটি খুঁজে বের করার উদাহরণ হরেক ক্ষেত্রে। যোগাযোগ, পরিবহণ, ট্রাফিক নিয়ন্ত্রণ তো সাধারণ ব্যাপার। ইন্টেরিয়র ডিজাইন বা কেমিক্যাল হাব-এর প্ল্যানিং-এর

নিয়ে পরীক্ষা করেও গাথরি দেখলেন, চারটের বেশি রং দরকার হচ্ছে না। ওটা তো পর্যবেক্ষণ। মানচিত্র যতই জটিল হোক, বাস্তব বা কাল্পনিক, তা রাঙাতে কেন মাত্র চারটের বেশি রং লাগে না? জন্ম নিল কঠিন প্রশ্ন।

কঠিনই বটে। যুক্তিতর্কে প্রশ্নের উত্তর পেতে গড়াল ১২৪ বছর। ১৯৭৬ সালে ইলিনয় বিশ্ববিদ্যালয়ের

■ **ত্রয়ী:** শঙ্কর বসু, অভিরূপ বন্দ্যোপাধ্যায় এবং অমিত কুমার ধর

গণিতজ্ঞ ফ্রান্সিস গাথরি ইংল্যান্ডের কাউন্টিগুলোর মানচিত্র আঁকতে গিয়ে এক বিচিত্র ব্যাপার লক্ষ করেন। মানচিত্রে ভিন্ন এলাকা (দেশ, রাজ্য বা জেলা) বোঝাতে আলাদা রং ব্যবহার করতে হয়। গাথরি দেখেন, মাত্র চারটে রং দিয়েই ইংল্যান্ডের সব কাউন্টি আলাদা চিহ্নিত করা যাচ্ছে। সব মানচিত্র তো ইংল্যান্ডের কাউন্টিগুলোর মতো না-ও হতে পারে। হতে পারে ঢের বেশি জটিল। সে রকম মানচিত্রে আলাদা এলাকা বোঝাতেও কি মাত্র চারটে রং যথেষ্ট? অনেক দেশ-মহাদেশের মানচিত্র

গ্রাফ হতে পারে জটিল থেকে জটিলতর। এক এক গ্রাফের ক্ষেত্রে ন্যূনতম রঙের সংখ্যা এক-এক রকম হবে। আমরা তিন বন্ধু মিলে একটা নিয়ম আবিষ্কার করেছি, যে নিয়মে নোডগুলো রং করলে সংযুক্ত দুটো নোড কখনও একই রং পাবে না। এ কাজে দরকার যে মাস্টার প্ল্যান, কম্পিউটার সায়েন্সের ভাষায় যাকে বলে অ্যালগরিদম, তা খুঁজে পেয়েছি আমরা। দরকার হয়েছে কোডিং দক্ষতা। সোজা বাংলায়, গণনা।'

কেমন সে অ্যালগরিদম? শঙ্কর জানালেন, প্রথমে ঠিক করে নিতে হবে রঙের একটি ক্রম বা অর্ডার। ক রং ফাঁকা থাকলে, তাকেই নিতে

■ বিজ্ঞান ও প্রযুক্তি বিষয়ে লেখা পাঠান। ইউনিকোড বাঞ্ছনীয়। পিডিএফ নয়, ওয়ার্ড ফাইলে পাঠান। ঠিকানা ও ফোন নম্বর থাকা জরুরি। ইমেল: eshona@abp.in

চুরি-ঠেকানো ব্যাকপ্যাক

Weblink: https://www.anandabazar.com/others/science/three-bengali-scientist-achieved-success-in-combinatorial-optimization-or-combinatorics-1.1058891?fbclid=IwAR2-c_6LXKkSToNN3FY_jZgRaS59W4qF2rr-TQhaWftdVoViQF7EOnRe1WQ

Memberships:

Member of the **International Society of Computational Biology,** 9650 Rockville Pike Bethesda, Maryland 20814, USA (https://www.iscb.org/) (2016-2018)

Annual Member of **Indian Science Congress** (June, 2017-2018) (http://www.sciencecongress.nic.in/)

Member of Breakthrough Science Society (2019 onward) (https://breakthroughindia.org/)

Editorial Board Member of 'Materials in Physics and Chemistry', EnPress Publishers (2018 onward) (http://systems.enpress-publisher.com/index.php/MPC)

Editorial Board Member of 'Computational Biology and Bioinformatics', Science Publishing Group (2020 -)
http://www.sciencepublishinggroup.com/journal/editorialboard?journalid=112

Member of Microbiological Society, WB, India (2022 -)
https://www.facebook.com/mbiosocietywb/

Member of Srijan Sujan (Education, Hopes & Dreams), WB, India (2022 -)
https://www.srijansujan.com/

Grants Awarded:

"Building and scoring atomic models for Intrinsically Unstructured Proteins: use of machine learning algorithms and possible therapeutic applications". DST-SERB National Post Doctoral Fellowship (Award Number: 2015/001079/LS). Award amount: 19,20,000/- (including fellowships, contingency and overhead) for two years (June, 2016 – March, 2018), Research carried out at Department of Biochemistry, University of Calcutta and Department of Chemistry, University of Delhi for one year each. The project directly aided in delivering four major papers (links provided below) and also contributed in three others. Apart from predicting disorder-to-order transitioning residues in Intrinsically Disordered Proteins (IDP's), we further revealed how transient dynamics of ionic-bonds is supportive of their physical flexibility and further extended to demonstrate how structural degeneracy in dynamic bio-soft matters (IDPs) may lead to fractal geometries and self organized criticality

1. https://link.springer.com/article/10.1007/s10822-017-0020-y
2. https://link.springer.com/article/10.1007/s00894-017-3376-y
3. https://www.sciencedirect.com/science/article/abs/pii/S1570963918300311
4. https://www.sciencedirect.com/science/article/abs/pii/S1570963920301217?via%3Dihub

Doctoral Thesis Title: **"Self Complementarity: its Applications in Probing Protein Internal Architecture, Fold Recognition and Structure Validation."** (Successfully defended (on May 20, 2014) and awarded (on June 2, 2014) the degree of Doctor of Philosophy (Science) in Biochemistry by University of Calcutta); Supervisor: Prof. Rahul Banerjee, Crystallography and Molecular Biology division, Saha Institute of Nuclear Physics, Kolkata, India (Duration: Sept, 2007 - Sept, 2013).

Research Summary of PhD work:

1. Our primary research involved the elucidation of side-chain packing modes within proteins. In this context, protein internal architecture was viewed as surfaces rather than point atoms and the interaction of side chain atoms was represented as a contact network based on their surface complementarity and overlap. In effect, this was the direct extension of the *jigsaw puzzle* model into protein contact networks. Some network topologies were found to be definitely preferred and they were termed 'packing motifs' (**Figure 1**), analogous to super secondary structures in proteins. Study of the distribution of these motifs revealed the ubiquitous presence of typical smaller graphs, which appear to get linked or coalesce to give larger graphs, reminiscent of the nucleation–condensation model in protein folding.

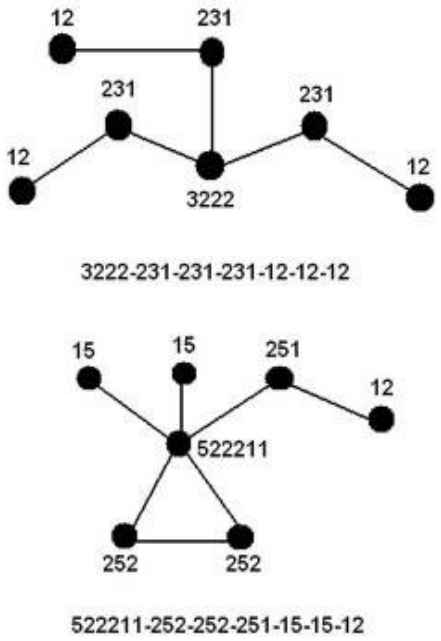


Figure 1. A novel numerical scheme to identify graphs with unique topology. Graphs (packing motifs) along with a unique number-string (motif identifier) displayed below each motif. Each node is assigned a concatenated numeric where the first digit stands for its own degree followed by degrees of its immediate neighbor sorted in a descending order.

One such frequently occurring motif, also envisaged as the unit of clustering, the three residue clique (**Figure 2**) was invariably found in regions of dense packing which exhibited distinct preference both in terms of composition and geometry.

Figure 2. A three-residue clique, embedded in the protein interior. An embedded triplet clique (from 3F67.pdb) constituted of 119-Phe (Olive), 142-Trp (Lime) and 143-Tyr (Yellow) displayed as sticks in a background of broken stretches of the backbone being displayed as cartoon (Cyan). The image was constructed using PyMol.

2. Secondly the meticulous balance of electric fields arising from different parts of the folded chain was deciphered by probing electrostatic complementarity within the native protein interior (for the first time to the best of our knowledge). Quantitative assessment or dissection of the relative contribution of different residues and atom types (side-chain or backbone) was also performed. The results showed fairly uniform and significant values for all amino acids. Interestingly, hydrophobic side chains also attain appreciable complementarity primarily due to the trajectory of the main chain (**Figure 3**).

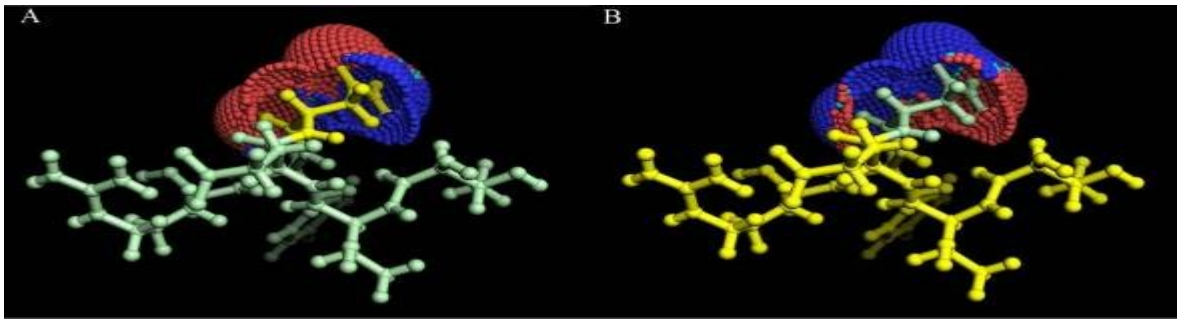


Figure 3. Molecular surface of an individual buried residue (target) exhibiting anti-correlated (complementary) electrostatic potentials. The figure shows the van der Waals surface (displayed as non-bonded spheres) of a completely buried asparagine (58-Asn from 2HAQ) along with its own atoms accompanied by a few more residues along the polypeptide chain as representative of the 'rest of the protein atoms' (sticks). Atoms (along with their interconnecting bonds) are colored by 'bright yellow' when 'charged' and by 'pale green' when 'uncharged'. Surface coloring follows standard conventions where patches of positive potentials are colored by 'blue', negative potentials by 'red' and neutral (0.0 ± 0.5 kT/e) by 'cyan'. (A) shows potentials realized due to the charged atoms of the residue itself whereas (B) shows potentials due to the rest of the charged protein atoms.

3. Thirdly, scoring functions were designed using surface and electrostatic complementarity in combination in order to detect the native fold of a protein amidst a set of decoys and also to detect a pair of sequences with low sequence identity among random sequences (the fold recognition problem) by cross-threading. The functions favorably compared with the very best available in the literature till date.

4. In order to detect local regions of suboptimal packing and electrostatics in protein structures a graphical tool for structure validation, namely, the Complementarity Plot (CP) was proposed (inspired by the famous Ramachandran Plot [1]) which performed successfully in detecting a wide range of errors. In particular, it was found to be effective in discriminating between obsolete structures and their corresponding upgraded counterparts, detection of wrong rotamer assignment (**Figure 4**) and in identifying packing anomalies. CPs were especially effective in the detection of low-intensity errors (in main-chain geometrical parameters) diffused over the entire polypeptide chain. A special feature of this validation tool is to signal unbalanced partial charges within protein interiors. Finally, the application of CP in protein homology modeling and design was demonstrated. A standalone suite of programs for CP (Sarama: http://www.saha.ac.in/biop/www/sarama.html) has been made available in the public domain.

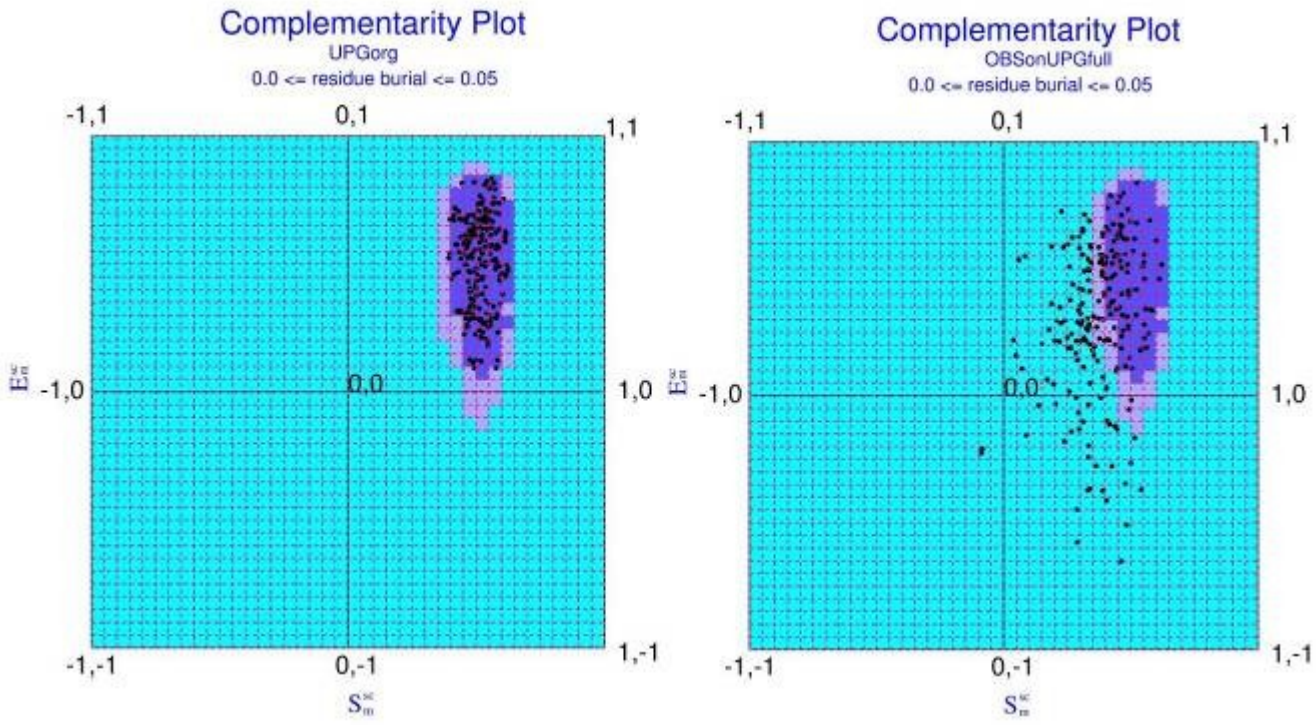


Figure 4. Distributions (in CP1) for residues with native side-chain conformers from the upgraded structures and replaced by rotamers from corresponding obsolete counterparts. Distribution of residues with native side-chains all falling into the probable regions of CP1 (Left Panel) and distribution subsequent to the replacement (Right Panel).

5. We have also probed the role of native deviations (in main-chain geometrical parameters from their corresponding ideal values) in maintaining structural integrity of globular proteins. Both unimodal [2] and Conformation Dependent Library [3] of ideal values were used for this purpose and the native deviations were found to be crucial in order to sustain the overall integrity of the native fold. Structures spanning all the four major protein class were rebuilt by reverting all main-chain bond lengths, angles and ω-torsions to their corresponding ideal values, while retaining native values for all other dihedral angles (φ, ψ, χ). This led to such large-scale distortions in the idealized structures (with respect to the original native model) that often their (C^{α}) RMSDs exceeded 10 Å **(Figure 5)**. The distortions were more pronounced for larger polypeptide chains (~100 residues or more in length) due to the accumulation of a higher number of angular idealizations. Proteins containing greater β-sheet content had more severe deformations. Also, in no case could the original structure be reconstituted by any form of energy minimization or side-chain optimization of the idealized coordinates. Idealizing bond lengths were found to cause no significant distortions while all the angular parameters played an influential causal role in giving rise to structural deformations.

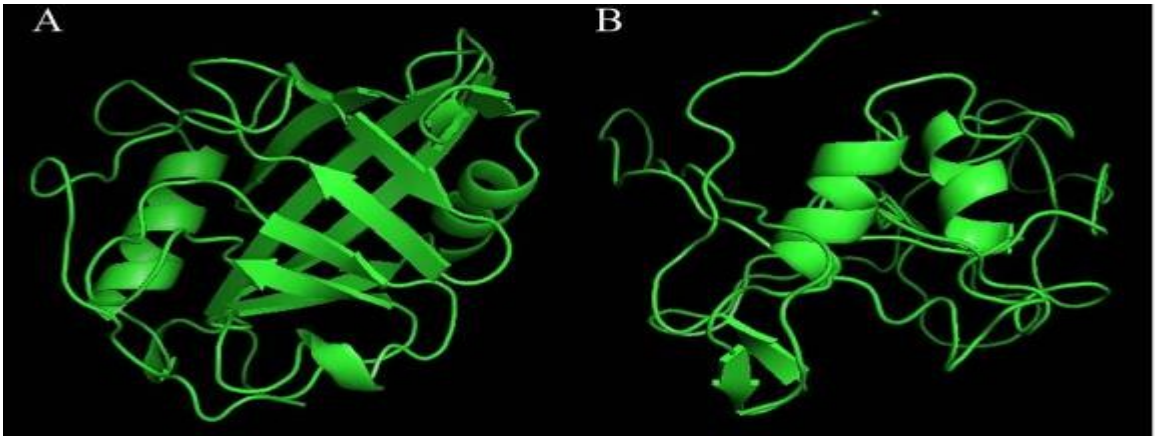


Figure 5. Distortions in the native fold due to the reversal of all main-chain bond lengths, angles and ω-torsions to their corresponding (unimodal) ideal values. (A) the native structure of cyclophilin from *L. donovani* (2HAQ) and **(B)** its corresponding idealized structure (C^{α}-RMSD: 12.86 Å, calculated at one-to-one atomic correspondence).

References:

1. Ramachandran GN, Ramakrishnan C & Sasisekharan V (1963) Stereochemistry of polypeptide chain configurations *J Mol Biol* 7, 95-99.

2. Engh RA & Huber R (2001), International Tables for Crystallography In International Tables for Crystallography, 382-392.

3. Berkholz DS, Shapovalov MV, Dunbrack RL & Karplus PA (2009) *Structure* 17, 1316-1325.

Brief Summery of post-doctoral works:

1. Worked on Biomolecular Evolution on the NIH funded project entitled 'Non-conserved interactions in Orthologes.' The major attempt was to analyze chordate gene families and build a database of non-conserved interaction in orthologs which might have implications for personalized medicine in the future. We initiated with CEACAM (Carcino Embryonic Antigen Cell Adhesion Molecule) as a case study.

2. Extending the Complementarity Plot to be applicable for protein-protein complexes for their structure validation and to work as a quality estimate for the same.

3. Developing a single and continuous quality estimate (DockQ) for protein-protein docking scoring (combining the three existing measures: Fnat, LRMS, and IRMS developed and put forwards by the CAPRI community: Critical Assessment of Protein Protein Interaction) which can be used to train machines to develop scoring functions for the same.

4. Developing ProQDock, a protein-protein docking scoring function trained on high level structural descriptors and using DockQ as a target function. ProQDock favorably compared and in fact outperformed the best existing function ZRANK2 on a large dataset of protein-protein docked complexes.

5. Developing a random forest based classifier for prediction of disorder-to-order transitioning protean segments in Intrinsically Disordered Proteins (IDPs)

6. Contributing to small molecule docking studies in the context of nitric oxide sensing of chlorophyll.

7. Characterizing and classifying the network of salt-bridges in globular, disordered proteins and protein-protein complexes. Identifying composite salt-bridge motifs and proposing new directions to salt-bridge design in proteins

8. Characterizing a meticulous mechanism by which IDPs maintain a high abundance of oppositely charged amino acid residues and simultaneously maintain their desired flexibility supporting a stochastic conformational ensemble rather than a single globular fold.

9. Contributing to the electrostatic validation of nucleic acid atomic models (both with canonical and non-canonical base pairs).

10. Extending the Complementarity Plot (CPdock) to the realm of protein-protein docking scoring (proposing it as an initial filter)

11. Reviewing nano-induced protein conformational changes, suggesting application of artificial intelligence based predictions.

12. Reviewing the role of non synonymous mutations to disease

13. Contributing to delphipKa in its extension for non-titrable residues

14. Contributing to Peptide architectonics for developing bio-therapeutics validated in a corneal transplantation system.

15. To be able to find out and reset the solution of one of the "Hard" problems in Mathematics and Algorithms - the **Graph Coloring Problem (GCP)**, a Combinatorial Optimization (CO) *per se*.

16. Contributing to the characterization of amino acid interactions in membrane proteins based on statistical potential.

17. Prediction and reclassification of amino acid residues in integral membrane proteins based on statistical potential and membrane geometry.

18. Exploring the criticality in phase transition of self-similar groups in Intrinsically Disordered Proteins. Structural demonstration of their potential multi-functionality.

Current Collaboration(s):

17. Geometric embedding of membranes in membrane protein 3D atomic coordinates based on statistical potentials (as in: MuSic: http://dezyme.com/) and their linear combination. (Principal Collaborator: Prof. Marianne Rooman and group, ULB Brussels)

18. Linking the criticality between structural degeneracy in different hierarchy of life based on self-similarity: The fractals of disorder- from proteins to brain. (Principal Collaborator: Dr. Abhirup Bandyopadhyay, PhD in Mathematics (Complex and Uncertain dynamics), Post Doc, Theoretical Neurosciences Group, Institute De Neurosciences Des Systems, Aix-Marseille University, France)

19. Prediction of protein functions from structure: Combining protein micro-environment and the Complementary Plot (Principal Collaborator: Dr. Debashree Bandyopadhyay, BITS, Pialni).

Other Interests:
Poetry and Creative writing. World Literature, Music and Spirituality, Philosophy, Cricket.

Popular Science Article on Proteins in Bengali:

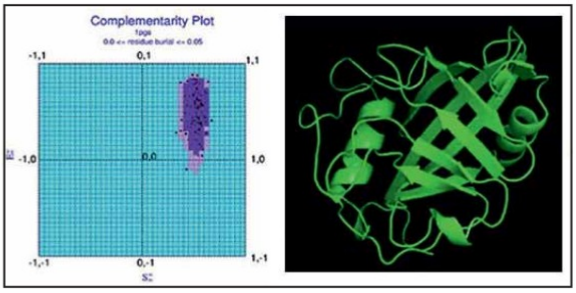
- *Protein Antohpure chyuti O Poripuran : Ekti joibo-anobik rupkatha* / Deviations and Complementarity in the Protein interior : A biomolecular fairy-tale (Sikkhyadarpon, Govt. of West Bengal, India, 2015)

প্রোটিন-অন্তঃপুরে চ্যুতি ও পরিপূরণ —
একটি জৈব-আণবিক রূপকথা

শঙ্কর বসু

উৎসর্গ : *বিশ্বপরিচয়*

রূপের রেশম যখন মাকুতে কথার বেড় দিতে দিতে পরতে পরতে পাঠক মনে গল্প-কল্পনার পুরু বুনোট তৈরি করতে থাকে, তখন তার অন্তঃপুরে রক্ত-মজ্জার জেনেসিস, তার কাঠ-পাথরের সারফেস টেনশন কিছুই আর স্বতন্ত্র থাকে না। মিলেমিশে যায় বলেই তা রসায়ন—খাঁটি রসের আড়ত। এই আপাত বস্তুবিশ্বে (যার কিনা অধিকাংশই ফাঁকা)-র মূলে যে প্রাণ-প্রশ্ন, আণবিক ডায়মেনশনে তারই ভেতর-রসায়নের নদীপথে দু-এক বাঁও নৌকা বাওয়ার সৌভাগ্য হয়েছিল একদা। সেই জলযাত্রার অনেকটাই ধুয়ে গেছে সলিলেরই স্বধর্মে, বাকি স্মৃতি উদ্ধারপর্বের থেকে উঠে আসছে এই দু'এক কলম অমৃত-মন্থন। গুরু কাণ্ডারিকে স্মরণ নিলাম, তিনি আমার মাস্টারমশাই এবং তার চেয়ে কিছু বেশি।



- A popular-science article on the Graph Coloring Problem for http://bigyan.org – An international forum for the practice and spread of Scientific awareness and literature in the Bengali language (https://bigyan.org.in/2020/04/17/trailing-the-chromatic-numbers/?fbclid=IwAR0u0_-klYJJHGHqjmCo8wqA--pEpwtribsEDAC_MJBfjnBBUX97g1mWyIA)

Outreach Activities:

Documentation on Mushroom Farming: Got intensely engaged in the documentation and advertising on Mushroom Farming, one of the prime agricultural and rural development activities taken up by a established voluntary organization called Shramajeebi Unnayan (https://www.justdial.com/Jamshedpur/Shramajivi-Unnayan-East-Singhbhum/0657PX657-X657-130515171947-C2Y4_BZDET)

The documentary is available here: https://youtu.be/S2Py2OA0ta0

Contributions to Wikipedia:
1. The Complementarity Plot: https://en.wikipedia.org/wiki/Complementarity_plot

Contributions to Scholarly Community Encyclopedia:
1. Structure-Based Approach in Drug Design: https://encyclopedia.pub/19938

Contact details of References:

(In the order of preference)

1. Dr. Hirak Kumar Patra
Professor
Department of Surgical Biotechnology,
Division of Surgery and Interventional Science,
University College London,
London, NW3 2PF, United Kingdom
+447475888637
hirak.patra@ucl.ac.uk

2. Prof. Marianne Rooman
Professor
Service 3BIO - BioControl, BioInformatics & BioMatter
Computational Biology and Bioinformatics
Office: 2.N.7.212, 3BIO group
Université libre de Bruxelles, Brussels, Belgium
+32477792286, +3226502067
mrooman@ulb.ac.be

3. Prof. Emil Alexov
Professor
Department of Physics and Astronomy
Clemson University
SC, USA
+18649084796
ealexov@g.clemson.edu

4. Prof. Raghavan Varadarajan
Professor
Molecular Biophysics Unit
Indian Institute of Science, Bangalore, India
+918022932612
varadar@iisc.ac.in

5. Prof. Anjan Dasgupta
Professor (Retired)
Department of Biochemistry
University of Calcutta, India
+919748758663
adgcal@gmail.com

6. Prof. Dhananjay Bhattacharyya
Professor (Retired)
Computational Science Division
Saha Institute of Nuclear Physics
Kolkata 700064, India
+91-9831667118
dhananjay.bhattacharyya@saha.ac.in

7. Prof. Rahul Banerjee (Ph.D supervisor)
Professor
Crystallography and Molecular Biology Division
Saha Institute of Nuclear Physics
Kolkata 700064, India
+919123994039
rahul.banerjee@saha.ac.in

8. Prof. Dhrubajyoti Chattopadhyay
Vice Chancellor,
Sister Nibedita University
West Bengal, India
+91-9831083791
dhrubajyotic@gmail.com

9. Prof. Parbati Biswas
Professor
Department of Chemistry
University of Delhi, India
+91-9818044887
pbiswas@chemistry.du.ac.in

10. Prof. Björn Wallner
Professor
IFM Bioinformatics
Linköping University
Sweden - 58183
+4613282759, +46705215665
bjornw@ifm.liu.se