



UNIVERSITY OF CALCUTTA

FACULTY ACADEMIC PROFILE/ CV

Full name of the faculty member: Dr. Soumalee Basu

Designation: Assistant Professor

Specialisation : Computational Biology and Biophysics



Contact information :

B90, Survey Park, Kolkata 700075, soumalee@gmail.com, 91-33-24168884

Academic qualifications:

College/ university from which the degree was obtained	Abbreviation of the degree
Jadavpur University	Ph.D. (Science)
University of Kalyani	MSc. (Biophysics)
University of Calcutta	BSc. (Honours in Physics)

Positions held/ holding:

...2005-2012... Assistant Professor in West Bengal University of Technology.....

...2012-till date... Assistant Professor in University of Calcutta.....

Research interests:

- Study of protein-protein and protein-ligand interaction
- Designing of molecules for therapeutics against neurodegenerative disease

Research guidance :

Number of researchers awarded M.Phil/ Ph.D degrees :1.....

Number of researchers pursuing M.Phil/ Ph.D :2+1(submitted).....

Projects :***Current projects :***

Anti-amyloidogenic effects of some antioxidant phytochemicals present in common traditional plant DST, Govt. of West Bengal ~Rs. 13.65lakhs

Identification of novel BACE - 1 inhibitors by simulating BACE1 - flavonoid interaction to identify new pharmacophore model followed by virtual screening in 3-D ligand database - a de novo drug design approach. DST, Govt. of India, ~Rs.23.90lakhs

Select list of publications:a) ***Journals:***

1. Sandipan Chakraborty, Jaya Bandyopadhyay, Sourav Chakraborty & Soumalee Basu, Multi-target screening mines hesperidin as a multi-potent inhibitor : implications in Alzheimer's Disease therapeutics. *European Journal of Medicinal Chemistry*. (2016)
2. Sandipan Chakraborty & Soumalee Basu, Structural insight into the mechanism of amyloid precursor protein recognition by β -secretase 1: A molecular dynamics study. *Biophysical Chemistry*. (2015) 202: 1-12.
3. Sucharita Das, Sandipan Chakraborty & Soumalee Basu, Fragment-based designing for the generation of novel leads against BACE1. *Central Nervous System Agents in Medicinal Chemistry*. (2015) 15:1 52-64.
4. Sandipan Chakraborty, Balaji Ramachandran & Soumalee Basu, Encompassing receptor flexibility in virtual screening using ensemble docking-based hybrid QSAR model: discovery of novel phytochemicals for BACE1 inhibition. *Molecular Biosystems* (2014) 10:2684-2692.
5. Sandipan Chakraborty & Soumalee Basu, Mechanistic insight into the radical scavenging activity of polyphenols and its application in virtual screening of phytochemical library: an in silico approach. *European Food Research Technology* (2014) DOI 10.1007/s00217-014-2285-x
6. Sandipan Chakraborty & Soumalee Basu, Insight into the anti-amyloidogenic activity of polyphenols and its application in virtual screening of phytochemical database. *Medicinal Chemistry Research* (2014) DOI 10.1007/s00044-014-1081-2.
7. Sandipan Chakraborty, Soumalee Basu & Soumen Basak, *Effect of β -cyclodextrin on the molecular properties of myrecetin upon nano-encapsulation: Insight from optical spectroscopy and quantum chemical studies*. *Carbohydrate Polymers* (2014) 99(2) 116-125.
8. Sandipan Chakraborty, Barnali Chatterjee & Soumalee Basu, Pinpointing proline substitution to be responsible for the loss of amyloidogenesis in IAPP. *Chemical Biology & Drug Design* (2013) 82(4) 446-452.
9. Aditi Maulik & Soumalee Basu, Study of Q224K, V152G double mutation in bean PGIP2, an LRR protein for plant defence- an in silico approach. *PROTEINS: Structure Function & Bioinformatics* 2013 81(5) 852-862.
10. Sandipan Chaktaborty, Barnali Chatterjee & Soumalee Basu, A mechanistic insight into the amyloidogenic structure of hIAPP peptide revealed from sequence analysis and molecular dynamics simulations. *Biophysical Chemistry* (2012) 168-169:1.

11. Aditi Maulik, Asif Sarkar, Suneeta Devi & Soumalee Basu, Study of polygalacturonase-inhibiting proteins (PGIP) – a leucine-rich repeat (LRR) protein in plant defense. *Plant Biology* (2012) 14(1) :22{Special Issue on plant pathogen interaction of February}
12. Sandipan Chakraborty. Sanjay Kumar and Soumalee Basu, Conformational transition in the substrate binding domain of β -secretase exploited by NMA and its implication in inhibitor recognition: BACE1-myricetin a case study. *Neurochemistry International* 58(8):914 (2011).
13. Sumana Banerjee, Soumalee Basu and Srimonti Sarkar, Comparative genomics reveals preferential distribution and domain organization of FYVE and PX domain proteins across eukaryotic lineages. *BMC Genomics* 11:83 (2010).
14. Sandipan Chakraborty, Soumalee Basu, Ansuman Lahiri and Soumen Basak, Inclusion of chrysin in β -cyclodextrin nanocavity and its effect on antioxidant potential of chrysin: A spectroscopic and molecular modeling approach. *Journal of Molecular Structure* 977:180 (2010).
15. Aditi Maulik, Hiren Ghosh and Soumalee Basu, Comparative study of protein-protein interaction observed in PolyGalacturonase-Inhibiting Proteins from *Phaseolus vulgaris* and *Glycine max* and PolyGalacturonase from *Fusarium moniliforme*. *BMC Genomics*, 10: S19 (2009).

Membership of Learned Societies:

.....Indian Biophysical Society.....

Patents :

PROCGR:A software for Chaos Game Representation of protein sequences CSIR, Govt. of India, New Delhi (**Registration no. L-16425/97**), 1996

Invited lectures delivered :

On “Sequence analysis-treasure or trash?” in the workshop on Computational Biology and Protein Structure Prediction” in Haldia Institute of Technology, Kolkata from 23-27 September, 2013

On “Role of a plant leucine-rich repeat (LRR) protein in host-pathogen interaction– an in silico study” in the 81st Annual Meeting of the Society for Biological Chemists held in Kolkata from November 8-11, 2012

On “Sequence Analysis and its application to Comparative Genomics” in the Workshop on Bioinformatics in Genomics & Proteomics, October 9-10, 2009 at Indian Institute of Technology, Kharagpur

On “Leucine-rich Repeat Proteins -Sequence, Structure and Evolution” in the Workshop on Current Trends in Evolutionary Biology, February 17-20, 2009 at University of Kalyani

On “Sequence Analysis and its application to Comparative Genomics” in the Workshop on Bioinformatics in Genomics & Proteomics, September 26-27, 2008 at Indian Institute of Technology, Kharagpur

On “Sequence Analysis of Nucleic Acids and Proteins - a treasure trove or a trivial pursuit?!” In the workshop on Computational Biology, January 14-15, 2008 at Department of Microbiology, Vidyasagar University

On “Basic Tools for Bioinformatics” in the Workshop on Genomics & Proteomics, September 21-22, 2007 at Indian Institute of Technology, Kharagpur

On “Basics of Bioinformatics” in the Seminar on Bioinformatics, June, 2007 at Haldia Institute of Technology

On “Bioinformatics” in the Workshop on Bioinformatics, Department of Computer Science & Informatics at Sreerampore Institute of Technology, from March 20-21, 2007

On “How important is Internet to the Medical Practitioners?” in a Conference organized by Medical Association of Calcutta in March, 2007

Awards :

- ... Overseas Fellowship-Wenner Gren Fellowship, Stockholm, Sweden 1999.....
- ... Foreign Travel Grant –DBT, Govt. of India 2009.....