Present Address
Dr. Shuchi Nagar
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Dutt Mandir Road,
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Permanent Address

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Career Objective:

To focus on developing new strategies for prognosis, diagnosis and treatment of various diseases that would help ease the life of people.

Experience Summary

- **Associate Professor (February, 2020 till date)**

Subjects Taught: Protein Modeling, Molecular Modeling and Chemoinformatics, Genomics and Proteomics, Metabolic Engineering (Focus on System Biology)
Organization: Dr. D. Y. Patil Biotechnology and Bioinformatics Institute

- **Assistant Professor (August, 2011 – February 2020)**

Subject Taught: Molecular Modeling & Chemoinformatics, Bioinfoirmatics, Chemistry
Organization: Dr. D. Y. Patil Biotechnology and Bioinformatics Institute, Pune

Research Trust Areas:

1. Target prediction for diseases – Alzheimers', Parkinsons', cancer
2. Biomarker prediction through systems biology approach
3. Small molecule designing

Awards and Fellowships:

1. DPU Innovative Teaching Recognition
2. DST Travel Grant to attend Conference, February 2010
3. CSIR-SRF 2009-2011.
4. Senior Science Fellow, Lady Tata Memorial Trust, 2007-2009.
5. Research Fellow, UGC funded project, 2007
6. First Position in Seminar Presentation in M.Sc (2005)- (*Use of Bio-Informatic Techniques to Analyze, Predict and Provide innovative measures to eradicate Huntington's disease.*)

Membership

Life Membership: World Scientific and Engineering Academic Society (WSEAS)

Anonymous Reviewer International Journals

- Letters in Drug Design related to 4D QSAR
- Journal of Biomolecular Structure and Dynamics
- Scientific reports
- Journal of Molecular Modeling and Graphics
- Molecular Diversity
- Insilico pharmacology innovation
- Computers in Medicine and Biology

Certificate Course and Workshops

1. Introduction to Systems Biology
2. Image Processing
3. Certificate course in Machine Learning & Artificial Intelligence
4. Certificate course in C/C++

No. of B. Tech/M. Tech /M.Sc. Project students Guided:

1. Ph. D. : 3 Students
2. B. Tech Biotechnology: 18 Students
3. M. Sc. : 7 Students

Education Qualification

2011 **Ph. D. (Tech.)** from Department of Chemical Technology, University of Calcutta

2005 **M.Sc** in Bio-informatics from Sikkim Manipal University with 77.68% marks.
2002 **B.Sc** in Microbiology from Mumbai University with 60% marks.

Books:

1. Khetmalas M, Pandey A, Gunasekaran P, Nawani N, Nagar S. International Conference on Advances in Biotechnology and Bioinformatics, DPU Publications, 2013.
2. Shuchi Nagar, Saurabh Dey, Aishik Das and Soumya Basu. Flavonoids: Recent Advances and Applications in Crop Breeding. 2022, Intechopen
3. Isha Zafar, Vishal K. Sahu, Bommana Kavya, Shuchi Nagar, Jyotirmoi Aich, Soumya Basu. In Vivo Testing of Biomaterials in Animal Models: Smart Ways of Biomaterial Designing Synthesis and Characterization. 1st edition, CRC Press, 2025
4. Samiksha Garse, Khadija Shahab Turabi, Jyotirmoi Aich, Amit Ranjan, Shuchi Nagar, Soumya Basu, Shine Devarajan. Cancer Diagnosis Using Artificial Intelligence (AI) and Internet of Things (IoT)
5. IGI Scientific Publishing. 2023
6. Vishal Kumar Sahu, Amit Ranjan, Manash K. Paul, Shuchi Nagar, Shine Devarajan, Jyotirmoi Aich, Soumya Basu. AI Techniques and IoT Applications Transforming the Future of Healthcare. IGI Scientific Publishing. 2023

Abstracts published

Prachi Bhole, Kiran Bharat Lokhande, Shuchi Nagar and K. Venkateswara Swamy, Molecular Docking and Molecular Dynamics Simulation studies of DHFR inhibitors in Plasmodium falciparum, Canadian Journal of Biotechnology, Volume 1, Special Issue, Page 23, 2017.

Research paper published

[1] MS Tambe, SR Shinde, AM Baheti, S Nagar, AT Pawar. (2025) Network pharmacology and in-silico studies for molecular mechanisms of analgesic, anti-inflammatory and anti-arthritic effects of Withania somnifera (L.) Dunal phytoconstituents. Journal of Ayurveda and Integrative Medicine 16 (4), 101088

[2] S Sur, D Davray, S Basu, S Kheur, JK Pal, S Nagar, A Sanap, BM Rudagi, (2025) Novel insights on oral squamous cell carcinoma management using long non-coding RNAs Oncology Research 32 (10), 1589

[3] Doiphode, S., Lokhande, K. B., Ghosh, P., Swamy, K. V., Nagar, S. (2023) Dual inhibition of cyclooxygenase-2 (COX-2) and 5-lipoxygenase (5-LOX) by resveratrol derivatives in cancer therapy: in silico approach. Journal of biomolecular structure & dynamics, 1-16.

[4] Ram, S., More-Adate, P., Tagalpallewar, A. A., Pawar, A. T., Nagar, S., & Baheti, A. M. (2023). An in-silico investigation and network pharmacology based approach to explore the anti-breast-cancer potential of Tecteria coadunata (Wall.) C. Chr. Journal of Biomolecular Structure & Dynamics, 1-12.

[5] Pandey, K., Lokhande, K. B., Saha, A., Goja, A., Swamy, K. V., & Nagar, S. (2023). Exploring Potential Non-steroidal Aromatase Inhibitors for Therapeutic Application against Estrogen-dependent Breast Cancer. Current Computer-Aided Drug Design, 19(4), 243.

[6] More-Adate, P., Lokhande, K. B., Shrivastava, A., Doiphode, S., Nagar, S., Singh, A., & Baheti, A. (2023) Pharmacoinformatics approach for the screening of Kovidra (Bauhinia variegata) phytoconstituents against tumor suppressor protein in triple negative breast cancer. Journal of biomolecular structure & dynamics, 1-20.

[7] Pallavi More-Adate, Kiran Bharat Lokhande, K. Venkateswara Swamy, Shuchi Nagar, Akshay Baheti. GC-MS profiling of Bauhinia variegata major phytoconstituents with computational identification of potential lead inhibitors of SARS-CoV-2 Mpro. Computers in Biology and Medicine. 147, 1 – 13, 2022.

[8] Kiran Bharat Lokhande, Payel Ghosh, Shuchi Nagar, K Venkateswara Swamy. Novel B, C-ring truncated deguelin derivatives reveals as potential inhibitors of cyclin D1 and cyclin E using molecular docking and molecular dynamic simulation. *Molecular diversity,* 1 – 15, 2021

[9] Khushboo Pandey, Kiran Bharat Lokhande, K. Venkateswara Swamy, Shuchi Nagar, Manjusha Dake. *In Silico* Exploration of Phytoconstituents From Phyllanthus emblica and Aegle marmelos as Potential Therapeutics Against SARS-CoV-2 RdRp. *Bioinformatics and Biology Insights*. 15, 1–13, 2021 doi:10.1177/11779322211027403

[10] Anshul Shakya, Rupesh V. Chikhale, Hans Raj Bhat, Fatmah Ali Alasmary, Tahani Mazyad Almutairi, Surajit Kumar Ghosh, Hassna Mohammed Alhajri, Siham A. Alissa, Shuchi Nagar & Md Ataul Islam. Pharmacoinformatics-based identification of transmembrane protease serine-2 inhibitors from *Morus Alba* as SARS-CoV-2 cell entry inhibitors. *Mol Divers* (2021). doi: /10.1007/s11030-021-10209-3

[11] Kiran Bharat Lokhande, Shuchi Nagar, K. Venkateswara Swamy. Molecular interaction studies of Deguelin and its derivatives with Cyclin D1 and Cyclin E in cancer cell signaling pathway: The computational approach *Scientific Reports,* 9, 1778, 2019.

[12] Saloni Shah, Swapnil Gaikwad, Shuchi Nagar, Shatavari Kulshrestha, Viniti Vaidya, Neelu Nawani and Sarika Pawar, Biofilm inhibition and anti quorum sensing activity

of phytosynthesized silver nanoparticles against nosocomial pathogen Pseudomonas aeruginosa *Biofoulin,* 35, 34-49, 2019

[13] Reddy PS, Lokhande KB, Nagar S, Reddy VD, Murthy PS, Swamy KV, Molecular Modeling, Docking, Dynamics and simulation of Gefitinib and its derivatives with EGFR in Non-Small Cell Lung Cancer *Current Computer-Aided Drug Design,* 14, 246 – 252 *2018*

[14] Shuchi Nagar and Achintya Saha, Exploring Benzocyclo Derivatives as Potent Aromatase Inhibitors using Ligand Based Modeling Studies *Euro. J. Med. Chem.*, Vol. 45, 2010, 4307-4315.

[15] Shuchi Nagar and Achintya Saha, Designing of Aromatase Inhibitors from Isoflavone Derivatives *Int. J. Pharm. Pharmaceu.* Vol 2, 2010, 126-131.

[16] Shuchi Nagar and Achintya Saha. Pharmacophore Searching of Benzofuran Derivatives for Selective CYP19 Aromatase Inhibition *J. Comp. Chem.* Vol. 31, 2010, 2342-2353.

[17] Shuchi Nagar, Md Ataul Islam, Suvadra Das, Arup Mukherjee and Achintya Saha: Pharmacophore Searching of Benzofuran Derivatives for Selective CYP19 Aromatase Inhibition *Lett. Drug Design Discov.* Vol. 6, 2009*,* 38–45.

[18] Md Ataul Islam, Sudipta Ghosh, Shuchi Nagar, Suvadra Das, Arup Mukherjee, Achintya Saha: Selectivity Requirement of Estrogen Receptor Binding Affinity of Cyclofenil Derivatives *Int. J. Appl. Comp.*, Vol. 2, 2009, 11-18.

[19] Shuchi Nagar, Md Ataul Islam, Suvadra Das, Arup Mukherjee, Achintya Saha: Pharmacophore Mapping of Flavones as Potent Aromatase Inhibitor *J. Mol. Diver.* Vol. 12(1), 2008, 65–76.

[20] Md Ataul Islam, Shuchi Nagar, Suvadra Das, Arup Mukherjee, Achintya Saha: Molecular Designed Based on Receptor-Independent Pharmacophore: Application to Estrogen Receptor Ligands *Biol. & Pharm. Bull*. Vol-31(7), 2008, 1453 –1460.

[21] Sk. Mahasin Alam, Ria Pal, Shuchi Nagar, Md. Ataul Islam and Achintya Saha: Pharmacophore Search for Anti-Fertility and Estrogenic Potencies of Estrogen Analogs *J. Mol. Mod.* Vol. 14, 2008, 1071–1082.

[22] Subhendu Mukherjee, Shuchi Nagar, Sanchita Malick, Arup Mukherjee, Achintya Saha: Pharmacophore Mapping of Arylbenzothiophene Derivatives for MCF Cell Inhibition using Classical and 3D Space Modeling Approaches *J. Mol. Graphics Model.*, Vol. 26, 2008, 884–892.

[23] Subhendu Mukherjee, Shuchi Nagar, Sanchita Malick, Arup Mukherjee, Achintya Saha: Pharmacophore Mapping of Selective Binding Affinity of Estrogen Modulators through Classical and Space Modeling Approaches: Exploration of Bridged-Cyclic Compounds with Diarylethylene Linkage J. Chem. Inform. Model., Vol. 47, 2007, 475–487.

International Conference Research Paper presentation

1. Shuchi Nagar, Md Ataul Islam, Arup Mukherjee and Achintya Saha. Pharmacophore Mapping of Flavone Derivatives for Aromatase Inhibition. Select Science, Medchem India, ITC Hotel Kakatiya Sheraton & Tower, Hyderabad, India. 12-13 April 2007.
2. Shuchi Nagar, Sanchita Mallick, Subhendu Mukherjee, Arup Mukherjee and Achintya Saha. Pharmacophore Mapping for MCF Cell Inhibition of Arylbenzothiopene Derivatives. Select Science, Recomb 2007, Sanfransisco bay, Oakland, USA. 21-25 April 2007.

3. Shuchi Nagar and Achintya Saha.Pharmacophore Modeling of Diarylalky Imidazole and Trazole Derivatives as Potent Aromatase Inhibitors. 4th International Symposium on Current Trends in Drug Design and Discovery (CTDDR-2010), CDRI, Lucknow. 17-21 February, 2010.
4. Shuchi Nagar and Achintya Saha. Exploring Pharmacophore of Isoflavone Derivatives for Aromatase Inhibition. 7th WSEAS International Conference on Advances in Biomedical Research (MABE'10), University of Cambridge, Cambridge, UK. 23-25 February, 2010.

National Conference Research Paper presentation

1. "*In silico* and *In vitro* approach to identify novel non-steroidal aromatase Inhibitors" NGBT conference, Mumbai, 30th September – 2nd October, 2019.
2. "QSAR studies on Non-Steroidal Aromatase Inhibitors." Emerging trends in Disease Model Systems, NCCS Pune, 25th – 26th March, 2019.
3. "From Sequence to Structure: Modelling Polyketide Synthase of Fusarium solani." Recent Advances in Modern Biology and Biotechnology 2019., DYPBBI, 14th – 16th March.
4. "Identifying Novel Aromatase Inhibitors from Piper Betel using Molecular Docking Studies" Recent Advances in Modern Biology and Biotechnology 2019., DYPBBI, 14th – 16th March.
5. "Selection of Novel Aromatase Inhibitors using Molecular Docking Studies." Accelerating biology 2019, C-DAC, Pune, 5th-7th February, 2019, at IISER Pune
6. "Chemometric modelling of PPAR agonists for the treatment of Type 2 diabetes" International Conference on Advances in Biotechnology & Bioinformatics 2013 & X Convention of The Biotech Research Society, Nov.25-27, 2013.
7. "Chemometric studies on potent inhibitors of Hexokinase II for the Cancer therapy" International Conference on Advances in Biotechnology & Bioinformatics 2013 & X Convention of The Biotech Research Society, Nov.25-27, 2013.
8. "Virtual screening and Molecular modeling of Hexokinase II inhibitors for Cancer therapy", 2nd UK-India MedChem Congress, 22 – 23 March, 2013.
9. "Molecular modeling of Phenyl propanoic acid derivatives for treatment of type 2 diabetes", 2nd UK-India MedChem Congress, 22 – 23 March, 2013.
10. "Dynamics, Virtual screening and Docking studies on Tau protein and its inhibitors", 2nd UK-India MedChem Congress, 22 – 23 March, 2013.
11. "Homology Modeling of PFK1: A probable target for cancer therapy", Symposium on Accelerating Biology…the Next Wave, 20-22 February, 2013.
12. "Molecular Modeling and Screening of Promising Aromatase Inhibitors" Indian Chemical Society, 1st – 2nd August 2011
13. "Exploring Pharmacophore of Isoflavone Derivatives for Aromatase Inhibition", 7th WSEAS International Conference on Advances in Biomedical Research (MABE'10), University of Cambridge, Cambridge, UK., 23-25 February, 2010
14. "Pharmacophore Modeling of Diarylalky Imidazole and Trazole Derivatives as Potent Aromatase Inhibitors", 4th International Symposium on Current Trends in Drug Design and Discovery (CTDDR-2010), CDRI, Lucknow, 17-21 February, 2010
15. "3D-QSAR Study of Benzofuran Derivatives: CoMFA And CoMSIA Using PLS Analysis" –National seminar on Recent Advances in Chemical Research, Osmania University, Hyderabad, 6th February 2009, p. 104.
16. "Three-dimensional pharmacophore sar of hydroxysteroid dehydrogenase inhibitor for the treatment of breast cancer" Indian Chemical Society, 1st – 2nd August 2008

17. “Molecular Modeling of Benzofuran Derivatives for CYP19 Aromatase Inhibition” 95th Indian Science Congress, Vishakapattnam, 3rd - 7th January 2008
18. “Exploring Pharmacophores of Sulphoanilide Derivatives for Suppressing Aromatase Expression and Activity in Breast Cancer Cell” Indian Chemical Society, 2nd – 3rd August 2007
19. “Pharmacophore Mapping for MCF Cell Inhibition of Arylbenzothiopene Derivatives”, Recomb 2007, Sanfransisco bay, Oakland, USA, 21-25 April 2007.
20. “Pharmacophore Mapping of Flavone Derivatives for Aromatase Inhibition”, Select Science, Medchem India, ITC Hotel Kakatiya Sheraton & Tower, Hyderabad, India. 12-13 April 2007.
21. "Pharmacophore Mapping of Bridged Cyclic Scaffolds for Binding Affinities to the Estrogen Receptor Subtypes using Classical and Space Modeling Approaches" College of pharmaceutical Sciences, Behrampur, Orissa, Pg.48
22. "Pharmacophore Modeling of Raloxifene Analogs for Breast Cancer Cell Line Inhibition" College of pharmaceutical Sciences, Behrampur, Orissa, Pg.49
23. "Computer-Aided Biophore Recognition (CABR): A Case Study on Apprehending Tissue Selectivity of SERMs" Indian Institute of Chemical Engineers, Pg.31-40

Conferences attended:

1. Symposium on "Streamlining Drug Design and Discovery" Royal Orchid Central Grazia, Navi Mumbai on January 24, 2019.
2. Seminar cum Hands-on Training on Bioinformatics, Resource Person, 19th – 20thJanuary, 2018
3. Stem Teacher Training Workshop to Develop Research Pedagogical Tools, 26th February to 1st March, 2017, IISER Pune
4. International Conference on Advances in Biotechnology & Bioinformatics 2013 & X Convention of The Biotech Research Society, Nov.25-27, 2013, Le Merdian, Pune.

IT Environment Proficiency

Operating System:
Windows-98, WIN 2K, Windows XP, Unix (Red Hat, Enterprise Edition).
Language: C/C++ (Certified)
Multimedia: Photoshop, Flash.

Technical Proficiency:
Microarray Data Analysis: GEO2R, Cytoscape, Pathway databases
Visualization Tools: Rasmol, SwissPdv Viewer, Cn3D
QSAR Tool : Statistica, TSAR, CoMFA, CoMSIA & HQSAR (Tripos)
Pharmacophore Desiging Tool: Catalyst
Docking: Discovery Studio, Autodock, FlexX
Dynamics & Simulation: Maestro, Gromacs

Academic Project

Project 1: Done during Second Semester in M.Sc.
Topic: "To write a program that generates random protein sequences of at least 100 amino acid length and store it in a database. Another was to write a program that back-translates the generated protein sequences into gene sequences and store it in the database."
Tools used: Visual basic, MS-Access.
Project Category: Internal.

Project 2: Done during final Semester in M.Sc.
Topic: "Organization, Structure and Comparative Analysis of KEGG and NCBI databases."
Project Category: External.
Done at the Indian Statistical Institute (ISI), in Kolkata under Dr. Rajat K. De (Machine Intelligence Unit).

Hobbies : Reading, Playing, Listening to Music