

Dr. Shuchi Nagar



Designation : Associate Professor

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Contact Number : +91 20 67919444 (ext. 9459)

Research Interest :

Drug designing for various diseases, gene expression analysis

Academic Qualification:

1. **Ph.D.** (Drug Designing) (2011) Department of Chemical Technology, University of Calcutta
Thesis Title: "Pharmacophore Search and Design of a Group of Potent Aromatase Inhibitors for Cancer Therapy"
2. **M.Sc.** (Bioinformatics) (2005) Sikkim Manipal University
3. **B. Sc.** (Microbiology) (2002) Department of Microbiology, Wilson College, Mumbai University

Teaching Experience:

1. **Associate Professor** (2020–Present): Dr. D. Y. Patil Biotechnology and Bioinformatics Institute, Dr. D. Y. Patil Vidyapeeth, Tathawade, Pune
2. **Assistant Professor** (2011–2020): Dr. D. Y. Patil Biotechnology and Bioinformatics Institute, Dr. D. Y. Patil Vidyapeeth, Tathawade, Pune

Professional Experience

1. Recognized Ph. D. guide, Dr. D. Y. Patil Biotechnology & Bioinformatics Institute, Pune
2. Senior Research Fellow (CSIR), 2009 – 2010, Department of Chemical Technology, University of Calcutta
3. Senior Science, Lady Tata Memorial Trust, 2007- 2009, Department of Chemical Technology, University of Calcutta
4. Project Fellow, UGC, 2007
5. Teacher, Sai Holy Faith, Koparkhairne, Navi Mumbai, 2002-2003

Research Grants:

1. **Dr. D. Y. Patil Vidyapeeth, Pune**, 2018–2020, *In silico* and *in vivo* studies to look for Aromatase inhibitors for cancer therapy **Rs. 10.8.0 lakhs (As PI)**
2. **Dr. D. Y. Patil Vidyapeeth, Pune**, 2018–2020, Virtual screening for novel quorum sensing inhibitors: Anti-virulence therapy against *Pseudomonas aeruginosa*. **Rs. 6.0 lakhs (As Co-PI)**

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

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

Certificate Course and Workshops

1. Image Processing
2. Certificate course in Machine Learning & Artificial Intelligence
3. Certificate course in C/C++

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

1. B. Tech Biotechnology : 18
2. M. Sc. : 7 (Other Universities)

Publications

1. Pandey K, Lokhande KB, Swamy KV, Nagar S, Dake M. 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
2. Shakya A, Chikhale RV, Bhat HR, *et al.* 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
3. Kiran Bharat Lokhande, Utkarsh Prashant Joshi, Trishna Kushwaha, Venkateswara Swamy, Shuchi Nagar, Identification of anti-cancer compounds as Hexokinase-II inhibitors through *in silico* studies, 2020 (Communicated to Medical Journal of Dr. D.Y. Patil Vidyapeeth).
4. Girish R. Apte, Khushboo Pandey, Kiran Bharat Lokhande, Shiva Bharadwaj, K. Venkateswara Swamy, Shuchi Nagar, Arvind Goja, Jayanta K. Pal and Rajesh Kumar Gupta Potentials of Pectic Polysaccharides in the inhibition of Galectins for Cancer Therapy (2020). (Communicated to Medical Journal of Dr. D.Y. Patil Vidyapeeth).
5. Lokhande KB, Nagar S, Swamy KV, 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.
6. Saloni Shah, Swapnil Gaikwad, Shuchi Nagar, Shatavari Kulshrestha, Vinita Vaidya, Neelu Nawani and Sarika Pawar, Biofilm inhibition and anti quorum sensing activity of phytosynthesized silver nanoparticles against nosocomial pathogen *Pseudomonas aeruginosa* *Biofouling*, 35, 34-49, 2019
7. 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
8. 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.
9. Shuchi Nagar and Achintya Saha, Designing of Aromatase Inhibitors from Isoflavone Derivatives *Int. J. Pharm. Pharmaceu.* Vol 2, 2010, 126-131.
10. Shuchi Nagar and Achintya Saha. Pharmacophore Searching of Benzofuran Derivatives for Selective CYP19 Aromatase Inhibition *J. Comp. Chem.* Vol. 31, 2010, 2342-2353.
11. 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.

12. 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.
13. 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.
14. 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.
15. 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.
16. 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.
17. 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.

Book/Book Chapter

Khetmalas M, Pandey A, Gunasekaran P, Nawani N, Nagar S. International Conference on Advances in Biotechnology and Bioinformatics, DPU Publications, 2013.

Abstracts published

1. 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.

Abstracts Presented in National and International Conferences

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 Diarylalkyl 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 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, Vishakapatnam, 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 Arylbenzothiopeptide 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 – 20th January, 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 Meridian, Pune.