Sagar S. Bhayye (Ph.D, M.S. Pharm, B. Pharm)

Assistant Professor, Department of Bioinformatics, Rajiv Gandhi Institute of I.T and Biotechnology, Bharati Vidyapeeth (Deemed to be University), Pune, Maharashtra, India - 411 046

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👨‍💼 Work/Research Experience

- **Assistant Professor** (July, 2023 –Present)
  Rajiv Gandhi Institute of Information Technology and Biotechnology, Bharati Vidyapeeth, Pune, Maharashtra, India
  |*Structural biology & molecular modeling*| |*Drug designing*| |*Cheminformatics*|
- **Research Scientist** (2022 – 2023)
  R&D Center, PharmCADD India Pvt. Ltd, Hyderabad, Telangana, India.
  |*Carrying out ongoing small molecule drug discovery projects with an emphasis on targeted cancer therapy*|
- **Post-doctoral Research Associate** (2019 - 2022)
  Department of Chemistry and Center for Informatics, Shiv Nadar University, Gautam Buddha Nagar, Uttar Pradesh, India
  |*Exploring the application of chemical space networks in molecular library design and drug design*| (SERB, Ref. No. : EMR/2016/002141)
- **Project Fellow** (2016 - 2018)
  Department of Chemical Technology, University of Calcutta, Kolkata, India
  |*Chemometric modeling on drug design and development of selective LRRK2 inhibitors for therapeutic application of Parkinson's disease*| (UPE-II, Ref. No. : UGC/493/UPE-II/Fellow)
- **Junior Research Fellow** (2012 - 2015)
  Department of Chemical Technology, University of Calcutta, Kolkata, India
  |*Molecular modeling studies on selective enzymes inhibitors for therapeutic application of mutagenic disease*| (UGC Major-Research Project, Ref. No. : F.41.374/2012)
- **Mentor/Consultant (Freelance)**
  Makeintern & LearnToUpgrade, New Delhi, India.

👨‍🎓 Education

- **Ph.D** (**Pharmaceutical and Fine Chemical Technology,** 2013 – 2019)
  Department of Chemical Technology, University of Calcutta, India
  |*Design and optimization of some protein modulators as anti-parkinson's agents using advanced cheminformatics techniques*|
- **M. S. Pharm** (**Pharmacoinformatics,** 2010 – 2012)
  Department of Pharmacoinformatics, NIPER, S. A. S. Nagar (Mohali), India
  |*Comparative QSAR study on Aldose reductase inhibitors*|
- **B. Pharm** (2005 – 2009)
  Dr. D. Y Patil Institute of Pharmaceutical Education and Research, University of Pune, India
  |*Antioxidant and free radical scavenging activity of Randia dumetarum (family: Rubiaceae)*|

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Skills & Activities

Skills	***Programming***	Basics of Python
	Operating System	Windows, Linux, Unix
	Bio/Cheminformatics Software	VMD, AutoDock, Accelrys Discovery Studio, Tripos Sybyl, ChemBioOffice, Modeller, Schrodinger Maestro, Desmond, Gromacs, LigBuilder, Matplotlib, NetworkX, Igraph
	Molecular Modeling	Molecular Docking, Pharmacophore Modeling, Molecular Dynamics, Homology Modeling, Virtual Screening, Structure and Ligand-Based Drug Design, Protein Modeling, 2D & 3D-QSAR
Interests	Cheminformatics, Bioinformatics, Computer aided drug design, Small molecule drug discovery, Protein modeling and dynamics, Data analysis	

Awards/Grants/Achievement

- *"Advancing Drug Discovery: In Silico Modeling of Pharmacological Targets for Tailored Anti-Cancer Agents with Emphasis on Protein and Enzyme Specificity"*(**Research grant: ₹ 1,00,000 /-, 2024-2025**, **Minor research Project, Ref. No.: BVDU/A10/2023-2024/5691**)
- *"Molecular Dynamic Simulation of Leucine Rich Repeat Kinase II (LRRK2): Probing the Effect of Pathogenic Mutations on DYG Loop dynamics"* (**Travel grant: ₹ 10,000/-, 2017, Ref. No.: UGC/544/UPE Fellow Travel)** at International Conference on Drug Design, organized by Schrodinger Inc. USA Jawaharlal Nehru University, New Delhi, India.
- "Design and Optimization of Enzyme Inhibitors associated with Parkinson's Disease : Chemoinformatics Approaches" (**Research grant: ₹ 50,000/-, 2013-2014**, **TEQIP Phase-II, Ref. No.: TEQIP-II/R&D/13/105(27))**
- Secured All India Rank **437** and fellowship for post graduate studies in **NIPER-JEE-2010** conducted by NIPER, Mohali, India.
- Secured All India Rank **267** and fellowship for post graduate studies in **GPAT 2010** conducted by M. S. University of Baroda, Vadodara, India.
- Qualified **GATE 2009** with **87.45** percentile conducted by IIT Roorkee, India.

Publication Highlights

Google Scholar Profile

Journal Publications

- Diksha Kumari, Parampreet Kour, Chetan Paul Singh, Rinku Choudhary, Syed Mudassir Ali, **Sagar S. Bhayye**, Yogesh P. Bharitkar, Kuljit Singh *"Anhydroparthenin as a dual-target inhibitor against Sterol C-24 methyltransferase and Sterol 14-α demethylase of Leishmania donovani: A comprehensive in vitro and in silico study"*, International Journal of Biological Macromolecules (2024); 269 (1), DOI: https://doi.org/10.1016/j.ijbiomac.2024.132034.
- Nalli, Yedukondalu, Sahil Bharti, Tanzeeva Amin, Rohit Singh, Jayaprakash Behera, **Sagar S. Bhayye**, Yogesh P. Bharitkar, Anindya Goswami, and Mahendra Kumar Verma *"Bioassay-guided fractionations of Cannabis sativa extract and HPLC-assisted purifications of anti-proliferative active fractions lead to the isolation of 16 known and one new phytomolecule and their in-silico analysis"*, Medicinal Chemistry Research (2024); 1-16. DOI: https://doi.org/10.1007/s00044-024-03199-y
- Chunarkar-Patil, Pritee, Mohammed Kaleem, Richa Mishra, Subhasree Ray, Aftab Ahmad, Devvret Verma, **Sagar S. Bhayye**, Rajni Dubey, Himanshu Narayan Singh, and Sanjay Kumar "Anticancer Drug

Discovery Based on Natural Products: From Computational Approaches to Clinical Studies" Biomedicines (2024); 12 (1), 201. DOI: https://doi.org/10.3390/biomedicines12010201

- Priyanka De, **Sagar S. Bhayye**, Vinay Kumar, Kunal Roy "*In silico Modeling For Quick Prediction of Inhibitory Activity Against 3CL Enzyme in SARS CoV Diseases*" Journal of Biomolecular Structure & Dynamics (2020); 1-27. DOI: 10.1080/07391102.2020.1821779
- Aalok Basu, Sonia Kundu, Aatrayee Das, Chitra Basu, **Sagar S. Bhayye**, Suvadra Das, Arup Mukherjee "*Polyphenol Capping On a Gold Nanosurface Modulates Human Serum Albumin Fibrillation*" RSC Materials Advances (2020); 1(5):1142-1150. DOI: 10.1039/d0ma00274g
- Rima Saha, **Sagar S. Bhayye**, Shuvam Ghosh, Achintya Saha, and Kishor Sarkar **"***Supramolecular Assembly Of Amino Acid Based Cationic Polymer For Efficient Gene Transfection Efficiency In Triple Negative Breast Cancer"* ACS Applied Bio Materials (2019); 2(12):1415-1424. DOI: 10.1021/acsabm.9b00639
- **Sagar S. Bhayye**, Goutam Brahmachari, Nayana Nayek, Sujata Roy and Kunal Roy "*Target Prioritization of Novel Substituted 5-aryl-2-oxo-/thioxo-2,3-dihydro-1Hbenzo[6,7]chromeno[2,3-d]pyrimidine-4,6,11(5H)- triones As Anti-cancer Agents Using In-silico Approach*" Journal of Biomolecular Structure & Dynamics (2019); 28(5):1415-1424. DOI: 10.1080/07391102.2019.1606735
- Aalok Basu, **Sagar S. Bhayye**, Sonia Kundu, Aatryee Das and Arup Mukherjee "*Andrographolide Inhibits Human Serum Albumin Fibril Formations Through Site-specific Molecular Interactions*" RSC Advances (2018); 8, 30717-30724. DOI:10.1039/c8ra04637a
- **Sagar S. Bhayye**, Achintya Saha *"QSAR and QAAR Studies on Mixtures of 3-(Benzylidene)Indolin-2-One Isomers as Leads to Develop PET Radiotracers for Detection of Parkinson's Disease"* International Journal of Quantitative Structure-Property Relationships (2018); 3, 95-114. DOI:10.4018/IJQSPR.2018070107
- **Sagar S. Bhayye**, Kunal Roy, Achintya Saha *"Molecular Dynamics Simulation Study Reveals Polar Nature of Pathogenic Mutations Responsible For Stabilizing Active Conformation of Kinase Domain in Leucine-rich repeat kinase II"* Structural Chemistry (2018); 29, 657–666. DOI:10.1007/s11224-017-1059-z
- Md Ataul Islam, **Sagar S. Bhayye**, Adebayo A Adeniyi, Mahmoud E.S. Soliman, Tahir S Pillay *"Diabetes Mellitus Caused by Mutations in Human Insulin: Analysis of Impaired Receptor Binding of Insulins Wakayama, Los Angeles and Chicago Using Pharmacoinformatics"* Journal of Biomolecular Structure & Dynamics (2016); 35(4):1-30. DOI:10.1080/07391102.2016.1160258
- **Sagar S. Bhayye**, Kunal Roy, Achintya Saha *"Pharmacophore Generation, Atom-based 3D-QSAR, HQSAR and Activity Cliff Analyses of Benzothiazine and Deazaxanthine Derivatives as Dual A_{2A} Antagonists/MAO-B Inhibitors"* SAR and QSAR in Environmental Research (2016); 27(3):1-20., DOI:10.1080/1062936X.2015.1136840
- Yogesh P Bharitkar, Mohua Das, Neha Kumari, M Padma Kumari, Abhijit Hazra, **Sagar S. Bhayye**, Ramalingam Natarajan, Siddharth Shah, Sourav Chatterjee, Nirup B Mondal *"Synthesis of Bis-pyrrolizidine-Fused Dispiro-oxindole Analogues of Curcumin via One-Pot Azomethine Ylide Cycloaddition: Experimental and Computational Approach toward Regio- and Diastereoselection"* ACS Organic Letters (2015); 17(18). DOI:10.1021/acs.orglett.5b02085
- **Sagar S. Bhayye**, Kunal Roy, Achintya Saha *"Development of Energy-Based Pharmacophore Model and Stepwise Virtual Screening of LRRK2 Inhibitors Through Molecular Dynamics and Mechanics"* Letters in Drug Design & Discovery (2015); 12, 24-32. DOI:10.2174/1570180812666150611185331
- **Sagar S. Bhayye**, Kunal Roy, Achintya Saha *"Exploring Structural Requirement, Pharmacophore Modeling, and De novo Design of LRRK2 Inhibitors Using Homology Modeling Approach"* Medicinal Chemistry Research (2014); 23(8), 3705–3713. DOI:10.1007/s00044-014-0955-7
- Swapnil Chavan, **Sagar S. Bhayye**, M Elizabeth Sobhia *"Molecular Dynamics Directed CoMFA Studies on Carbocyclic Neuraminidase Inhibitors"* Molecular Diversity (2011); 15(4), 979-87. DOI:10.1007/s11030-011-9332-3

Book Chapter

- Achintya Saha, **Sagar S. Bhayye**, Tabassum Hossain *"Design and Development of Some Selective Enzyme Inhibitors for Parkinson's and Alzheimer's Diseases Based on Molecular Modeling and Dynamics Studies"* Advances in Studies on Enzyme Inhibitors as Drugs, Vol 2 Miscellaneous Drugs, Edited by Satya P. Gupta, (2017): chapter 3: pages 51-89; Nova Science Publishers, Inc., ISBN: 978-1-53610-505-6

Conference Proceedings

Talk Poster

Sagar S. Bhayye, Achintya Saha *"Importance of Protein Crystallographic Structure for Advanced Drug Design"* at the National conference of Bangladesh Crystallographic Association organized by University of Dhaka, Bangladesh, 2013.

Sagar S. Bhayye, Kunal Roy, Achintya Saha *"Effect of Pathogenic mutations on Binding of ATP in LRRK2 using MD and MM-GBSA"* at 3rd Indo-US Conference on Molecular Modeling & Informatics in Drug Design, organized by National Institute of Pharmaceutical Education and Research (NIPER), Mohali, Punjab, India, 2014.

Sagar S. Bhayye, Kunal Roy, Achintya Saha *"Exploring pharmacophores of benzothiazine and deazaxanthine derivatives to provide dual A_{2A} antagonists/MAO-B inhibitors using multi-chemometric techniques"* at 6th International Symposium on Current trends in Drug Discovery and Research, organized by CSIR – Central Drug Research Institute, Lucknow, India, 2016.

Sagar S. Bhayye, Kunal Roy, Achintya Saha *"Molecular Dynamic Simulation of Leucine Rich Repeat Kinase II (LRRK2): Probing the Effect of Pathogenic Mutations on DYG Loop dynamics"* at International Conference on Drug Design, organized by Schrodinger Inc. USA Jawaharlal Nehru University, New Delhi, India, 2017.

Sagar S. Bhayye, Udit Raj, and N. Sukumar *"Chemical Space Network Analysis of Protein-Ligand Binding Sites"* at 3rd National Post Doc Symposium, organized by IISER, Pune, India, 2019.

Sagar S. Bhayye, Udit Raj, and N. Sukumar, *"Networking Protein-Ligand Binding Sites"* at International Conference on Drug Discovery (ICDD), organized by Schrodinger Inc. USA and BITS Hyderabad, India, 2020.