Dr. SAGAR SHIVAJI BARALE
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Objective:

To discover and disseminate knowledge about infectious diseases and disorders by utilizing my knowledge, skills, and learning, as well as to develop new technologies for human welfare.

Education:

Year of passing	Institution/ University
2015-2022	Ph. D Microbiology, Shivaji University, Kolhapur.
2016	P.G Diploma in Bioinformatics, Shivaji University, Kolhapur.
2011	M.Sc. Microbiology, Shivaji University, Kolhapur.
2009	B.Sc. Microbiology, Shivaji University, Kolhapur.

DISSERTATION: "*Studies on antibiotic resistance and inhibition of aggregation of amyloid beta peptides using antimicrobial peptides*".

Supervisor: Prof. K. D. Sonawane (Bioinformatics/Computational Biology).

This study mainly focuses on isolation of AMPs producing bacteria, extraction, purification and characterization of AMPs (surfactin), investigated antimicrobial efficacy of surfactin against antibiotic resistant bacteria and mechanism of action (membrane permeability) and amyloid beta aggregation inhibition by surfactin and arginine containing peptide using molecular modeling techniques (Most of dissertation part published as journal articles, listed in publication).

Fellowships and awards:

September 2019-June 2021	**Award of CM-SRF 2019 Chief Minister Special Research Fellowship, SARTHI, Maharashtra, India** at Department of Microbiology, Kolhapur.
December 2018- September 2019	**Research Assistant**, **DST-PURSE-II**, at Department of Microbiology, Kolhapur.
2013	Qualified **GATE** examination with 99.59% tile AIR-52
2014	Qualified **CSIR NET(National Eligibility Test) LS** rank 038/2661
2013	Qualified **CSIR NET LS** rank 047/1055
2013	Qualified Maharashtra **State Eligibility Test (SET)**

Professional Experience:

2015-2022 Doctoral research:

- Isolation of AMPs producing bacteria and microbiological identification resulted in isolation of surfactin producing *B. velezensis* SK.
- Extraction, purification, and characterization of surfactin (AMPs) were carried out using TLC, RP-HPLC, and LC-MS/MS analysis, and structural characterization using UV-Spectroscopy, FTIR, and Circular Dichroism (CD).
- Antimicrobial potential of surfactin was evaluated against drug-resistant bacteria using Diffusion assay, MIC, Killing kinetic studies, biofilm inhibition activity, along with the effect of metal ions, while membrane permeability assay was used to elucidate the mechanism of killing.
- Aβ peptides aggregation inhibition by surfactin peptides from *B. velezensis* SK was investigated using Tricine SDS-PAGE.
- Computational techniques, Molecular Docking, Molecular Dynamic simulation, free energy calculation (MM-PBSA), and Principle component analysis (PCA) were fully utilized to elucidate the mechanism of action of aggregation inhibition by surfactin and arginine containing peptide.

2014 **Project Research Fellow, National Centre for Cell Science (NCCS), Ganeshkhind, Pune.**

Supervisor: Prof. Arvind Sahu (Pathogenesis and Cellular Response).

Project Title: *"**Studies on species specificity in Pox viral complement regulators**"*.

This project aimed to produce mutant constructs of plasmid and their expression.

- Worked on the isolation of plasmid DNA and restriction digestion.
- Cloning of viral complement regulatory mutant genes, transformation in *E. coli*.
- Expression of complement regulatory protein in *E. coli* and subsequent purification.

2011-2012 **Microbiologist, R&D Hi Tech Bioscience, Sutarwadi, Tal- Mulashi, Pune.**

Role: Performing experiments related to media optimization of probiotic bacteria for maximum biomass production. Biomass and viability evaluation by O.D, total biomass, Dry Wt. and Total viable count (TVC).

Teaching Experience:

2016-2019 **Teaching Assistant, Shivaji University, Kolhapur**.

Taught Molecular Biology, Conducted postgraduate students' practical's.

2014-2015 **Assistant professor,** V.G. Shivdare College of Arts, Commerce and Science, Solapur.

Contributory Teacher, M.Sc., Pharmaceutical Microbiology (2016-2020), Post Graduate Diploma in Bioinformatics (2016-2019).

Technical Experience:

1. **Microbiological culture:** Basic handling of microorganisms (pathogens), Culturing of industrially important microorganisms (Bacteria and Fungi), and bacterial identification through phylogenetic analysis.
2. **Microbial fermentation.** Probiotic fermentation, media optimization (factorial design).
3. **Antimicrobial Bioassays:** Well, disc diffusion assay, MIC, microbial killing kinetics assay, and Biofilm inhibition assay.
4. **Protein and peptides biochemistry:** Bioactive peptides and small compound extraction by solvent and resin**,** Protein and peptides precipitation (Ammonium/acid precipitation), Chromatographic purification of peptides (RP-HPLC), Tricine-SDS-PAGE of peptides, peptides characterization **(**TLC, LC-MS/MS analysis, and CD spectroscopy).
5. **Membrane permeability assays:** Fluorescence-based propidium iodide assay and ONPG assay.
6. **Computer proficiency: OS-** Linux, Windows, Familiar with various Bioinformatics Software: AutoDock, GROMACS, Discovery Studio Visualizer, ChemDraw, MEGA, Bioedit, ClustalX, Jalview, PyRx, UCSF Chimera, PyMOL, VMD, MEGA, UGENE.
7. **Computational biology skills:** Homology modeling, Molecular Docking (Autodock), Molecular dynamic simulation (GROMACS), Free energy calculations (MM-PBSA).
8. **Drug-Discovery and Chemoinformatics:** *In-silico* methods of Ligand base and Structure-based virtual screening, ADME profiling of small molecules (Toxicity analysis), QSAR, and pharmacophore modeling using various software and online tools.
9. **Molecular biology:** Plasmid DNA isolation and quantification, restriction digestion, Agarose gel electrophoresis, DNA Ligation reaction, Transformation, Protein expression, and purification.

10. **Statistical analysis and software:** Experience in basic statistical analysis using MS Excel, Sigma Plot, MiniTab, and GraphPad Prism to interpret the significance.

Professional training:

1. One-day workshop on "Intellectual Property Awareness/Training program" under National Intellectual Property Awareness Mission, organized by Intellectual Property Office, India. 5th April 2022.
2. Online Course on "Basics of High Performance Computing" conducted jointly by IIT Kharagpur, IIT Madras, IIT Goa, and IIT Palakkad under the aegis of National Supercomputing Mission, India Nov 2020 to Feb 2021.
3. One-day workshop on, "Student-centric Teaching-learning Methods", organized by the Department of Education and IQAC of Shivaji University, 22nd June 2018.

Publications:

Research articles published:

1. **Sagar S. Barale**, Savaliram G Ghane, Kailas D. Sonawane. (2022) Purification and characterization of antibacterial surfactin isoforms produced by *B. velezensis* SK**. AMB Expr,** 12, 7. (**IF: 4.126**).
2. **Sagar S. Barale**, Rishikesh S. Parulekar, Prayagraj M. Fandilolu, Maruti J. Dhanavade and Kailas D. Sonawane. (2019) Molecular Insights into Destabilization of Alzheimer's Aβ Protofibril by Arginine Containing Short Peptides: A Molecular Modeling Approach. **ACS Omega**, 892-903. (**IF: 3.7**).
3. Sagar U. Jadhav, Rushikesh P. Dhavale, Rakesh P. Dhavale, Manish S. Bhatia, Maruti J. Dhanavade, **Sagar S. Barale**, Sachin Pathak, Vinayak G. Parale ,Kailas D. Sonawane. (2023) Exploring anticancer potential of nintedanib conjugated magnetic nanoparticles: In-vitro and in-silico studies. **Journal of Drug Delivery Science and Technology**, 81, 104213 (**IF: 5.062**).
4. Abhijeet P. Herwade, **Sagar S. Barale**, Kailas D. Sonawane, and Pankaj K. Pawar. (2022) *In vivo* developmental studies of *Helicoverpa armigera* and in silico molecular interactions with trypsin reveal the bio-insecticidal potential of

trypsin inhibitor (SSTI) isolated from *Solanum surattense*. **Int. J. Biol. Macromol**, 223, 335-345. **(IF 8.2)**.

5. Manoj Thakur, Rishikesh S. Parulekar, **Sagar S. Barale**, Kailas D. Sonawane, Kalappa Muniyappa. (2022) Interrogating the substrate specificity landscape of UvrC reveals novel insights into its non-canonical function. **Biophys J**. 121, 3103-3125. (**IF: 3.699**).
6. Navanath Kumbhar, Snehal Nimal, **Sagar Barale**, Subodh Kamble, Rohit Bavi, Kailas Sonawane, Rajesh Gacche. (2022) Identification of novel leads as potent inhibitors of HDAC3 using ligand-based pharmacophore modeling and MD simulation. **Scientific Reports,** 12, 1712. (**IF: 4.996**).
7. Subodh Kamble, **Sagar Barale**, Maruti Dhanavade, Kailas Sonawane. (2021) Structural significance of Neprylysin from *Streptococcus suis* GZ1 in the degradation of Aβ peptides a causative agent in Alzheimer's disease. **Computers in Biology and medicine**, 136, 104691. (**IF 7.7**).
8. Kailas D. Sonawane, **Sagar S. Barale**, et al. (2021) Structural insights and inhibition mechanism of TMPRSS2 by experimentally known inhibitors Camostat mesylate, Nafamostat and Bromhexine hydrochloride to control SARS-Coronavirus-2: A molecular modeling approach. **Informatics in Medicine Unlocked**, 24, 100597.
9. Kailas D. Sonawane, **Sagar S. Barale**, et.al. (2020) Homology Modeling and Docking Studies of TMPRSS2 with Experimentally Known Inhibitors Camostat Mesylate, Nafamostat and Bromhexine Hydrochloride to Control SARS-Coronavirus-2. **ChemRxiv. Preprint**).
10. Rishikesh S. Parulekar, **Sagar S. Barale,** Sonawane, D. Kailas. (2019) Antibiotic resistance mechanism of novel aminoglycoside phosphotransferase APH (5) from *B. subtilis* subsp subtilis strain RK: A combined in-vitro and in-silico approach. **Brazilian Journal of Microbiology**, 50, 887–898. (**IF: 2.214**).
11. Prakash Bansode, R. Anantacharya, Maruti Dhanavade, Subodh Kamble, **Sagar Barale**, Kailas Sonawane, Nayak D. Satyanarayan, Gajanan Rashinkar (2019) Evaluation of drug candidature: In silico ADMET, binding interactions with CDK7 and normal cell line studies of potentially anti-breast cancer enamidines. **Computational Biology and Chemistry**, 83, 107124. (**IF: 3.737**).

12. Sneha B. Paymal, **Sagar S. Barale**, Shirishkumar V. Supanekar, Kailas D. Sonawan**e. (**2023**)** Structure based virtual screening, molecular dynamic simulation to identify the oxadiazole derivatives as inhibitors of Enterococcus D-Ala-D-Ser ligase for combating vancomycin resistance. **Computers in Biology and Medicine,** 159, 106965. **(IF: 7.7)**
13. Ali A. M, **Sagar S. Barale**, Kamble S. A, Sneha B. Paymal, Kailas D. Sonawan**e.** (2023) Molecular insights into the inhibition of early stages of Aβ peptide aggregation and destabilization of Alzheimer's Aβ protofibril by dipeptide D-Trp-Aib: a molecular modelling approach. Int J Biol Macromol 242(3):124880 (**IF: 8.2**).
14. V. S. Patil, S. N. Labade, **Sagar S. Barale**, A. S. Salunkhe, N. S. Gaikwad, S. S. Sawant and R. K. Jadhav. (2023) Spectroscopic and Docking Studies on Binding of Bovine Serum Albumin with Antipsychotic Fluphenazine Drug Eur. Chem. Bull.12(12), 1826-1840.
15. Kamble, S.A., **Sagar S. Barale**, Mohammed, A.A. et al. (2024) Structural insights into the potential binding sites of Cathepsin D using molecular modelling techniques. Amino Acids 56, 33. (**IF: 3.0**)
16. Vidya Patil, **Sagar Barale**, Pratibha Patil, Smita Deore, Kishor Kakde, Ranjana Jadhav. (2024) Spectroscopic Investigations of Conformational Change in Bovine Serum Albumin (BSA) with Rising Concentration of a Mood Stabilizing Drug: Lamotrigine. Afr.J.Bio.Sc. 6(15).
17. Sneha B. Paymal, **Sagar S. Barale**, Shirishkumar V. Supanekar, Kailas D. Sonawan**e.** Kiran D. Pawar. (2025) Overexpression, Purification, and Biochemical Characterization of the vanC2 d-Ala-d-Ser Ligase from Enterococcus casseliflavus SSK and Its Inhibition by an Oxadiazole Derivative. ACS Omega. 3;10(14):14390-14402.(**IF:3.7**).
18. Mohammed AA, **Barale SS**, Dhotare PS, Sonawane KD. Polymyxin-B as a novel inhibitor of amyloid beta aggregation: computational insights and experimental validation. J Mol Struct. 2025; 1349:3.
19. Ahmed, S., **Barale, S.S.,** Kamble, R.S. et al. Mechanistic insights into amyloid β fibril disruption by ginsenosides through molecular dynamics simulations. Netw Model Anal Health Inform Bioinforma.2026;15, 45.

Book Chapters:

1. Navanath M. Kumbhar, M.A. Aparna, Snehal K. Nimal, Pallavi Shewale, **Sagar Barale,** Rajesh Gacche, Chapter 17 - New targets for old drugs: drug repurposing approach for accelerating the drug discovery engine with minimum financial inputs, Editor(s): Surya Nandan Meena, Vinod Nandre, Kisan Kodam, Ram Swaroop Meena, In Progress in Biochemistry and Biotechnology, New Horizons in Natural Compound Research, Academic Press, 2023, Pages 315-349, ISBN 9780443152320.

Conferences/Symposium:

1. **Sagar S. Barale**, Savaliram G. Ghane and Kailas D. Sonawane. Purification and characterization of surfactin and iturin produced by *B. velezensis* SK. International Conference on Infectious Diseases and Immunopathology (IDIP-2021), Organized by Department of Biotechnology, Savitribai Phule Pune University 22nd to 24th April 2021.
2. **Sagar S. Barale**, Rishikesh S. Parulekar, Prayagraj M. Fandilolu & Kailas D. Sonawane. "Molecular insights into destabilization of Aβ protofibril by short peptide containing arginine: A molecular modeling approach " in "Symposium on Accelerating Biology 2019 Towards Thinking Machines", organized by Bioinformatics group, Center for Development of Advanced Computing C-DAC Pune, India 5-7th Feb 2019.
3. **Sagar S. Barale**, Rishikesh S. Parulekar, Prayagraj M. Fandilolu & Kailas D. Sonawane. "Molecular insights into destabilization of Aβ protofibril by short peptide containing arginine" in "Symposium on Accelerating Biology 2018 Digitizing life", organized by Bioinformatics group, Center for Development of Advanced Computing C-DAC Pune, India 9-11th January 2018.
4. National conference -2019: Research and innovations in healthcare & Buisiness Management Organised by Rashtriya Shikshan Mandal's CDGIM, Pune, 5-6 November 2019.