

Name : Dr. P. Chandra Sekar
Staff ID : RCAS05012
Designation : Assistant Professor (Research)
Department : Department of Biotechnology
Experience : 3 years
Qualification : MSc., PhD., PDF (IIT-Madras)
Specialization : Bioinformatics and Computational Biology
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ACADEMICS

Degree	Branch	Institution / University	Year of Completion
Ph.D.	Biomedical Informatics	Quantitative Biology Lab, SBST, Vellore Institute of Technology, Vellore	2022
M.Sc.	Computational Biology	Center of Excellence in Bioinformatics, SBT, Madurai Kamaraj University, Madurai	2013
B.Tech.	Bioinformatics	Center for Plant Molecular Biology, Tamil Nadu Agricultural University, Coimbatore	2011

RESEARCH AND PUBLICATIONS

GRANTS

Title	Agency	Amount	Year	Status
Leveraging Generative Artificial Intelligence with Traditional Tiger and Sheep Game for Enhanced Cognitive Learning (Co-PI)	DST- NCSTC	Rs. 5,08,850	2025	Shortlisted

SEED MONEY

Title	Institution	Amount	Year	Status
Rapid Detection of Bacterial LPS in contaminated food using Janus nanomotors affinity peptide conjugates (PI)	RCAS	Rs.75,000	2024	Completed

Journal Publications

Vijay, S., Roy, S., Ponnusamy, C., Thomas, J., Husin, M. N., & Fathi, A. (2025). Efficient generation of specific counting polynomials and their subsequent indices of complex boric acid structure. *Current Organic Synthesis*, 22. Advance online publication. <https://doi.org/10.2174/0115701794366590250414051549>

Devika, V., Rajan, M. S. M., Veni, S. S., & **Ponnusamy, C.**, (2025). Photonic crystal fiber sensor with molecular docking analysis to evaluate silica efficacy for SARS-CoV-2 spike protein detection in COVID-19. *Sensing and Imaging*, 26(1), 5. <https://doi.org/10.1007/s11220-024-00534-w>

Sujatha, V. A., Gopalakrishnan, C., Anbarasu, A., & **Ponnusamy, C. S.**, 2024). Beyond the venom: Exploring the antimicrobial peptides from *Androctonus* species of scorpion. *Journal of Peptide Science*, 30(11), e3613. <https://doi.org/10.1002/psc.3613>

Nirmala, M. J., **Ponnusamy, C. S.**, Johnson, A., & Nagarajan, R. (2023). A comprehensive review of nanoadditives in plant-based biodiesels with a special emphasis on essential oils. *Fuel*, 351, 128934. <https://doi.org/10.1016/j.fuel.2023.128934>

Paul, D. M., Srinivasan, E., **Ponnusamy, C. S.**, Lavinya, B., & Rajasekaran, R. (2023). LSDBB: Lysosomal Storage Disorder Database for lysosomal proteins and their single amino-acid substitutions. *Journal of Computational Biophysics and Chemistry*, 22. <https://doi.org/10.1142/S273741652350028X>

Meshach, P. D., Gopalakrishnan, C., **Ponnusamy, C. S.**, Lavinya, B., & Rajasekaran, R. (2023). Therapeutic role of DGJ (1-deoxygalactonojirimycin) in Fabry disease: Theoretical insights. *Chemistry Select*, 8. <https://doi.org/10.1002/slct.202204457>

Ponnusamy, C. S., Srinivasan, E., Gopalakrishnan, C., Paul, M. D., Sanjay, G., Surya, S., Kumar, A. N. S., & Rajasekaran, R. (2022). Probing the competitive inhibitor efficacy of frog-skin alpha helical AMPs identified against ACE2 binding to SARS-CoV-2 S1 spike protein as therapeutic scaffold to prevent COVID-19. *Journal of Molecular Modeling*, 28(5), 128. <https://doi.org/10.1007/s00894-022-05117-8>

Chandrasekhar, G., **Ponnusamy, C. S.**, Srinivasan, E., Amarnath, A., Pengyong, H., & Rajasekaran, R. (2022). Molecular simulation unravels the amyloidogenic misfolding of nascent ApoA1 protein, driven by deleterious point mutations occurring in the 170–178 hotspot region. *Journal of Biomolecular Structure and Dynamics*, 40(23), 13278–13290. <https://doi.org/10.1080/07391102.2021.1986134>

Chandrasekhar, G., Srinivasan, E., **Ponnusamy, C. S.**, Venkataraman, S., & Rajasekaran, R. (2022). Molecular simulation probes the potency of resveratrol in regulating the toxic aggregation of mutant V30M TTR fibrils in transthyretin-mediated amyloidosis. *Journal of Molecular Graphics and Modelling*, 110, 108055. <https://doi.org/10.1016/j.jmgm.2021.108055>

Ponnusamy, C. S., Paul, M. D., Srinivasan, E., & Rajasekaran, R. (2021). Unravelling the molecular effect of Ocellatin-1, F1, K1 and S1, the frog-skin antimicrobial peptides to enhance its therapeutics – Quantum and molecular mechanical approaches. *Journal of Molecular Modeling*, 27(1), 10.

Ponnusamy, C. S., & Rajasekaran, R. (2021). Could Dermaseptin analogue be a competitive inhibitor for ACE2 towards binding with viral spike protein causing COVID-19?: Computational investigation. *International Journal of Peptide Research and Therapeutics*, 27, 1043–1056. <https://doi.org/10.1007/s10989-020-10149-w>

Ponnusamy, C. S., Chandrasekhar, G., & Rajasekaran, R. (2021). Hydrophobic residues confer the helicity and membrane permeability of Ocellatin-1 antimicrobial peptide scaffold towards therapeutics. *International Journal of Peptide Research and Therapeutics*, 27, 2459–2470.

Ponnusamy, C. S., & Rajasekaran, R. (2021). Therapeutic efficacy of antibacterial Ocellatin peptides – A comprehensive review. *Biointerface Research in Applied Chemistry*, 12(5), 6804–6814.

Srinivasan, E., Chandrasekhar, G., **Ponnusamy, C. S.,** Anbarasu, K., Vickram, A., Karunakaran, R., & Rajasekaran, R. (2021). Alpha-Synuclein aggregation in Parkinson's disease. *Frontiers in Medicine*, 8, 1704.

Srinivasan, E., Chandrasekhar, G., **Ponnusamy, C. S.,** Anbarasu, K., Vickram, S., Tayubi, I., Rajasekaran, R., & Rohini, K. (2021). Decoding conformational imprint of convoluted molecular interactions between prenylflavonoids and aggregated amyloid- β 42 peptide causing Alzheimer's disease. *Frontiers in Chemistry*, 9, 753146. <https://doi.org/10.3389/fchem.2021.753146>

Ramamoorthy, S., Sankara, N., Nagarajan, T., Punitha, S., **Ponnusamy, C. S.,** & Jebasingh, T. (2021). Novel approaches on identification of conserved miRNAs for broad-spectrum Potyvirus control measures. *Molecular Biology Reports*, 48, 1–12. <https://doi.org/10.1007/s11033-021-06271-7>

Book Chapters

Chandrasekhar, G., Caixia, X., Yanran, L., Vinutha, A., Sanjay, G., Paul, M., Sekar, C. P., Rajasekaran, R., Pengyong, H., & Zhengwei, L. (2022). Elucidating quantum semi-empirical based QSAR for predicting tannins' antioxidant activity with the help of artificial neural network. In *Intelligent computing theories and application (ICIC 2022, Lecture Notes in Computer Science, Vol. 13394)*. Springer, Cham. https://doi.org/10.1007/978-3-031-13829-4_24

Proceedings

Devika, V., & Chandrasekar, P. (2024). Computational analysis of the stability and membrane permeability of Mellitin-Lasioglossin3: A bee-venom derived anticancer hybrid peptide. *Proceedings of ICRTMRI Conference*, A.V.P. College of Arts and Science, Tirupur, Tamil Nadu, India.

PRESENTATIONS

	State Level	National	International
Conference	1	2	1
Seminar	0	2	0

PARTICIPATION

	State Level	National	International
Conference	2	4	3
Seminar	1	2	1
Workshop	0	3	1
Orientation	1	0	0

Invited Speaker / Session Chair- Conference / Seminar / Workshop

Honourable speaker in the online hands-on workshop on “*Advanced Molecular Modelling & Drug Designing by AI/ML Approach*” organized by the BIRAC-BioNEST Laboratory, Technology Business Incubator, Vellore Institute of Technology

Tutor in 15-day Pre-Research Virtual Internship entitled “Computer Aided Drug Design.” Organized by NyBerMan Bioinformatics, Europe

Eminent Resource person in National Seminar on Artificial Intelligence in Drug Discovery and Healthcare Organized by Department of Pharmaceutical Chemistry, Rathinam College of Pharmacy

Members in BoS/ Editorials/ Professional Bodies

Reviewer in Computational and Structural Biotechnology Journal

Reviewer in Journal of Biomolecular Structure and Dynamics

AWARDS, HONORS AND RECOGNITION

Awards / Honors /Recognition	Agency / Institution	Year of Award
Qualified in GATE- 2018 Biotechnology (BT)	Indian Institute of Technology, Madras	2018
Qualified in DBT Government of India Entrance Exam for Master’s degree	Department of Biotechnology, New Delhi	2013
Research Intern of Summer Research Fellowship	Indian National Science Academy	2011