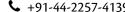
# Karthik Raman

BT 221, Block II, Bhupat and Jyoti Mehta School of Biosciences Department of Biotechnology Indian Institute of Technology Madras Chennai - 600 036, INDIA

















Born: 1981—Chennai, INDIA

Nationality: Indian

## **Current Positions**

- Professor, Department of Data Science and AI, Wadhwani School of Data Science and AI, Indian Institute of 2024-Technology (IIT) Madras
- Co-ordinator, Centre for Integrative Biology and Systems mEdicine (IBSE), IIT Madras 2015-
- Advisor, International Secretariat, Office of Global Engagement, IIT Madras 2020-
- Core Faculty, Robert Bosch Centre for Data Sciences and Artificial Intelligence (RBCDSAI), IIT Madras 2017-
- 2018-Co-founder & Director, qBiome Research Private Limited, Chennai

## Research Interests

Algorithm development for systems biology • In silico Metabolic engineering • Design Principles of Biological Networks • Integrated analysis of massive biological datasets • High-performance computing (GPGPU) for systems biology

### Research Skills

Formal education in bio-informatics and computational/systems biology, high-performance computing, data structures and algorithms, computational methods, pattern recognition

Number of publications: 73, plus posters/talks at scientific meetings.

Fluent in MATLAB, Python, scripting languages such as awk, sed. Working knowledge of C/C++.

## **Past Positions**

- Professor, Department of Biotechnology, Bhupat and Jyoti Mehta School of Biosciences, Indian Institute of 2022-24 Technology (IIT) Madras
- Associate Professor, Department of Biotechnology, Bhupat and Jyoti Mehta School of Biosciences, Indian 2018-22 Institute of Technology (IIT) Madras
- 2011-18 Assistant Professor, Department of Biotechnology, Bhupat and Jyoti Mehta School of Biosciences, Indian
- 2016 Jun-Jul Institute of Technology (IIT) Madras Visiting Research Scientist, Vantage Research, Chennai
- 2012 Jun-Jul Visiting Research Scientist, Samsung Advanced Institute of Technology (SAIT), Bangalore
- 2008-11 Post-doctoral researcher, Andreas Wagner Lab, Department of Biochemistry/Department of Evolutionary Biology and Environmental Studies, University of Zürich, Switzerland

#### **Professional Affiliations**

2022-	Society for Applied Microbiology, UK
2021-	The Society of Biological Chemists (SBC), India
2021-	Sigma Xi, The Scientific Research Honor Society
2018-	Biological Engineering Society of India
2011-	International Society for Computational Biology (ISCB)
2018	American Institute of Chemical Engineers (AIChE)
2018	Society for Biological Engineering (SBE)

### Education

2009 PHD in Systems Biology, Supercomputer Education and Research Centre/Bioinformatics Centre, Indian Institute of Science, Bangalore, India

THESIS: Systems-level Modelling and Simulation of Mycobacterium tuberculosis: Insights for Drug Discovery

Advisers: Nagasuma Chandra and Saraswathi Vishveshwara

AWARDED the Sir Vithal N. Chandavarkar Memorial Medal for the best Ph. D. thesis of the year in the Supercomputer Education and Research Centre, Indian Institute of Science

Awarded a transfer to the PhD programme, from an MTECH in *Computational Science*, at the Supercomputer Education and Research Centre, Indian Institute of Science, Bangalore, India. Graduate courses GPA: 7.3/8.0.

BTECH in Chemical Technology (First class with distinction), Institute of Chemical Technology, University of Mumbai, India

### Peer-reviewed Publications

### Pre-prints and manuscripts under review

- Shobhan Karthick Muthamilselvi Sivabalan, Varsha Vijayakumar, Pratyay Sengupta, Siddhakam Palmal, Srinivasan Krishnamurthi, Nitin Kumar Singh, Nikos Kyrpides, **Karthik Raman**\*, Kasthuri Venkateswaran\* "Unveiling Hidden Microbial Diversity in Mars 2020 Mission Assembly Cleanrooms with Molecular Insights into the Persistent and Perseverance of Novel Species Defying Metagenome Sequencing" bioRxiv Manuscript preprint:  $R\chi$
- Shuvechha Chakraborty, Indumathi Palanikumar, Yash Gune, K.V. Venkatesh, **Karthik Raman\***, Susan Idicula-Thomas\* "An integrated systems biology approach establishes arginine biosynthesis as a metabolic weakness in Candida albicans during host infection" *bioRxiv* Manuscript preprint: RX
- Shayantan Banerjee, Vijay K. Tiwari, **Karthik Raman**\*, Mohammad Inayatullah\* "Tumor-Infiltrating Lymphocytes Display Prognostic Signatures Associated with Chemotherapy Response in TNBC Patients" *bioRxiv* Manuscript preprint: Rx 📵
- Lavanya Raajaraam and **Karthik Raman\*** "COSMOS: COmmunity and Single Microbe Optimisation System" bioRxiv Manuscript preprint: RX 🚭
- Karthik Raman, Miroslav Kratochvíl, Brett G. Olivier, Matthias König, Pratyay Sengupta, ..., Andreas Dräger, Rahuman S Malik-Sheriff\* "FROG Analysis Ensures the Reproducibility of Genome Scale Metabolic Models" bioRxiv Manuscript preprint: Rx 📵
- Venkatesh Kamaraj, Ayam Gupta, **Karthik Raman**, Manikandan Narayanan, Himanshu Sinha "Unveiling Genomic Complexity: A Framework for Genome Graph Structural Analysis and Optimised Variant Calling Workflows" *bioRxiv* Manuscript preprint: RX 🚳
- Prem Jagadeesan, **Karthik Raman\*** and Arun K. Tangirala\* "A generalised method for experiment design and model selection in the Bayesian framework" *bioRxiv* Manuscript preprint: RX
- Divyang Deep Tiwari, Nils Hoffmann, Kieran Didi, Sumukh Deshpande, Sucheta Ghosh, Tung V. N. Nguyen, Karthik Raman, Henning Hermjakob\*, Rahuman Sheriff\* "BioModelsML: Building a FAIR and reproducible collection of machine learning models in life sciences and medicine for easy reuse" Manuscript preprint: RX
- 2022 Gayathri Sambamoorthy and Karthik Raman\* "Deciphering the evolution of microbial interactions: in silico

studies of two-member microbial communities" Manuscript preprint: Rx 🚳

Aarthi Ravikrishnan and **Karthik Raman\*** "Unraveling microbial interactions in the gut microbiome" Manuscript preprint: RX

- Vimaladhasan Senthamizhan, Sunanda Subramaniam, Arjun Raghavan and **Karthik Raman\*** "CASTLE: A database of synthetic lethal sets predicted from genome-scale metabolic networks" Manuscript preprint: RX
- Anand A Rajasekar, **Karthik Raman** and Balaraman Ravindran\* "Goal directed molecule generation using Monte Carlo Tree Search" Manuscript preprint:

### Articles in international journals (73)

- Karthik Raman\*, Rukmini Kumar, Cynthia J. Musante, Subha Madhavan "Integrating Model-Informed Drug Development With Al: A Synergistic Approach to Accelerating Pharmaceutical Innovation" Clinical and Translational Science 18:e70124
- Sowmya Manojna Narasimha†, Tanisha Malpani†, Omkar S. Mohite, J. Saketha Nath, **Karthik Raman\***"Understanding flux switching in metabolic networks through an analysis of synthetic lethals" npj Systems
  Biology and Applications 10:104 439289347 •
- Lavanya Raajaraam and **Karthik Raman\*** "Modeling Microbial Communities: Perspective and Challenges" ACS Synthetic Biology **13**:2260 39148432
- Indumathi Palanikumar, Himanshu Sinha, **Karthik Raman**\* "Panera: A novel framework for surmounting uncertainty in microbial community modelling using Pan-genera metabolic models" iScience **27**:110358
- Priyan Bhattacharya, **Karthik Raman\*** and Arun K. Tangirala\* "Design Principles for Perfect Adaptation in Biological Networks with Nonlinear Dynamics" *Bulletin of Mathematical Biology* **86**:100 Manuscript preprint: Rx 📵
- Pratyay Sengupta, Shobhan Karthick Muthamilselvi Sivabalan, Nitin Kumar Singh, **Karthik Raman\*** and Kasthuri Venkateswaran\* "Genomic, Functional, and Metabolic Enhancements in Multidrug-Resistant *Enter-obacter bugandensis* Facilitating its Persistence and Succession in the International Space Station" *Microbiome* 12:62 38521963 5 EB Business Standard Finhe Hindu Finhe Finhe Finhe Business World
- Georgios Miliotis, Pratyay Sengupta, Asif Hameed, Maria Chuvochina, Francesca McDonagh, Anna Simpson, Ceth Parker, Nitin Singh, Punchappady Rekha, Dearbháile Morris, **Karthik Raman**, Nikos Kyrpides, Philip Hugenholz, and Kasthuri Venkateswaran\* "Novel spore forming species exhibiting intrinsic resistance to third and fourth generation cephalosporins and description of *Tigheibacillus jepli* sp. nov" mBio
- Jonathan L. Golob\*, Tomiko T. Oskotsky\*, ..., **The Preterm Birth DREAM Community**, ..., James C. Costello and Marina Sirota\* "Microbiome preterm birth DREAM challenge: Crowdsourcing machine learning approaches to advance preterm birth research" *Cell Reports Medicine* **5**:101350
- Anna C. Simpson<sup>†</sup>, Pratyay Sengupta<sup>†</sup>, Flora Zhang, Asif Hameed, Ceth W. Parker, Nitin K. Singh, Georgios Miliotis, Punchappady D. Rekha, **Karthik Raman**, Christopher E. Mason\* and Kasthuri Venkateswaran\* "Phylogenomics, phenotypic, and functional traits of five novel (Earth-derived) bacterial species isolated from the International Space Station and their prevalence in metagenomes" *Scientific Reports* 13:19207 37932283
- Sarayu Murali, Maziya Ibrahim, Hemalatha Rajendran, Shagun Shagun, Shyam Kumar Masakapalli, **Karthik Raman** and Smita Srivastava\* "Genome-scale metabolic model led engineering of *Nothapodytes nimmoniana*plant cells for high camptothecin production" *Frontiers in Plant Science* 14:1207218
- Ludwig Geistlinger, Chloe Mirzayi, Fatima Zohra, Rimsha Azhar, Shaimaa Elsafoury, Clare Grieve, Jennifer Wokaty, Samuel David Gamboa-Tuz, Pratyay Sengupta, Issac Hecht, Aarthi Ravikrishnan, Rafael S. Gonçalves, Eric Franzosa, **Karthik Raman**, Vincent Carey, Jennifer B. Dowd, Heidi E. Jones, Sean Davis, Nicola Segata, Curtis Huttenhower and Levi Waldron\*"BugSigDB captures patterns of differential abundance across a broad range of host-associated microbial signatures" *Nature Biotechnology* Manuscript preprint: Rx
- Melpakkam Pradeep and **Karthik Raman\*** "COWAVE: A Labelled COVID-19 Wave Dataset for Building Predictive Models" *PLoS ONE* **18**:e0284076 437490468

2023	Dinesh Kumar Kuppa Baskaran, Shreyansh Umale, Zhichao Zhou, Karthik Raman*, Karthik Anantharaman*
	"Metagenome-based metabolic modelling predicts unique microbial interactions in deep-sea hydrothermal
	plume microbiomes" ISME Communications 3:42 37120693

- Pratyay Sengupta, Pratyay Sengupta, Shobhan Karthick Muthamilselvi Sivabalan, Amrita Mahesh, Indumathi Palanikumar, Dinesh Kumar Kuppa Baskaran and **Karthik Raman\*** "Big Data for a Small World: A Review on Databases and Resources for Studying Microbiomes" *Journal of the Indian Institute of Science* 37362854
- Prem Jagadeesan, **Karthik Raman\*** and Arun K. Tangirala\* "Sloppiness: fundamental study, new formalism and quantification" *PLoS ONE* **18**:e0282609 36888634
- Priyan Bhattacharya, **Karthik Raman\*** and Arun K. Tangirala\* "On biological networks capable of robust adaptation in the presence of uncertainties: A linear systems-theoretic approach" *Mathematical Biosciences* **358**:108984 436804384 Manuscript preprint: RX
- Prem Jagadeesan, **Karthik Raman\*** and Arun K. Tangirala\* "Bayesian Optimal Experiment Design for Sloppy Systems" *IFAC-PapersOnLine* **55**:121–126
  - (Part of Special Issue: 9th IFAC Conference on Foundations of Systems Biology in Engineering (FOSBE) 2022)
- Sankalpa Venkatraghavan<sup>†</sup>, Sathvik Anantakrishnan<sup>†</sup> and **Karthik Raman\*** "Probing patterning in microbial consortia with a cellular automaton for spatial organisation" *Scientific Reports* **12**:17159 436229548
- Anjana Anilkumar Sithara, Devi Priyanka Maripuri, Keerthika Moorthy, Sai Sruthi Amirtha Ganesh, Philge Philip, Shayantan Banerjee, Malvika Sudhakar and **Karthik Raman\*** "iCOMIC: a graphical interface-driven bioinformatics pipeline for analyzing cancer omics data" *Nucleic Acids Research: Genomics and Bioinformatics* 3:lgac053 N35899080
- Priyan Bhattacharya, **Karthik Raman\*** and Arun K. Tangirala\*, "Discovering design principles for biological functionalities: perspectives from systems biology" *Journal of Biosciences* **47**:56 436222149
- Sai Saranga Das and Karthik Raman "Effect of Dormant Spare Capacity on the Attack Tolerance of Complex Networks" *Physica A* **598**:127419 Manuscript preprint: Live Mint The Hindu BusinessLine Hindustan Times The Print Deccan Herald
- Rachita K Kumar, Nitin Singh, Sanjaay Balakrishnan, Ceth W. Parker, **Karthik Raman\*** and Kasthuri Venkateswaran\*, "Metabolic modeling of the International Space Station microbiome reveals key microbial interactions" *Microbiome* **10**:102 35791019 The Hindu BusinessLine New Indian Express Amar Ujala Dina Malar Dinakaran Times of India The Hindu Telegraph India Press Trust of India Prasar Bharati News Services Press Information Bureau, Government of India News 18 Hindustan Times
- Malvika Sudhakar, Raghunathan Rengaswamy\* and Karthik Raman\* "Multi-omic data helps improve prediction of personalised tumor suppressors and oncogenes" Frontiers in Genetics 13:854190 35620468 Prasar Bharati News Services © Nature India © Financial Express Analytics India Magazine The Print Indian Express Manalytics India Magazine The Hindu
- Debomita Chakraborty, Raghunathan Rengaswamy and **Karthik Raman\*** "Designing biological circuits: from principles to applications" ACS Synthetic Biology 11:1377–1388 435320676 4 Manuscript preprint:
- Priyan Bhattacharya, **Karthik Raman\*** and Arun K. Tangirala\*, "Discovering adaptation-capable biological network structures using control-theoretic approaches" *PLoS Computational Biology* **18**:e1009769 35061660
- 2022 Malvika Sudhakar, Raghunathan Rengaswamy\* and **Karthik Raman\*** "Novel ratio-metric features enable the identification of new driver genes across cancer types" *Scientific Reports* **12**:5 N34997044
- Lavanya Raajaraam and **Karthik Raman\*** "A computational framework to identify metabolic engineering strategies for the co-production of metabolites" *Frontiers in Bioengineering and Biotechnology* **9**:779405
- 2021 Maziya Ibrahim and **Karthik Raman\*** "Two-species community design of Lactic Acid Bacteria for optimal production of Lactate" *Computational and Structural Biotechnology Journal* **19**:6039–6049 34849207
- Vimaladhasan Senthamizhan, Balaraman Ravindran and **Karthik Raman\*** "NetGenes: A database of essential genes predicted using features from interaction networks" *Frontiers in Genetics* **12**:722198 434630517
- Maziya Ibrahim<sup>†</sup>, Lavanya Raajaram<sup>†</sup> and **Karthik Raman\*** "Modelling microbial communities: harnessing consortia for biotechnological applications" *Computational and Structural Biotechnology Journal* **19**:3892–3907 [434584635]
- Attila Gabor<sup>†</sup>, Marco Tognetti<sup>†</sup>, Alice Driessen, Jovan Tanevski, Baosen Guo, Wencai Cao, He Shen, Thomas

Yu, Verena Chung, Single Cell Signaling in Breast Cancer DREAM Consortium members, Bernd Bodenmiller\* and Julio Saez-Rodriguez\* "Cell-to-cell and type-to-type heterogeneity of signaling networks: insights from the crowd" Molecular Systems Biology 17:e10402

- Sahana Gangadharan and Karthik Raman\* "The art of molecular computing: whence and whither" *BioEssays* 43:202100051 434101866 Manuscript preprint:
- Sarah M. Keating\*, Dagmar Waltemath\*, ..., Karthik Raman, ..., Henning Hermjakob, John C. Doyle, Michael Hucka\*, and SBML Community members "SBML Level 3: an extensible format for the exchange and reuse of biological models" Molecular Systems Biology 16:e91110 32845085
- 2020 Ulf Liebal\*, Thuy An Phan Nguyen, Malvika Sudhakar, **Karthik Raman** and Lars M. Blank, "Machine learning applications for mass spectrometry-based metabolomics" *Metabolites* **10**:243 432545768
- Kern Rei Chng, Tarini Shankar Ghosh, Yi Han Tan, Tannistha Nandi, Ivor Russel Lee, Amanda Hui Qi Ng, Chenhao Li, Aarthi Ravikrishnan, Kar Mun Lim, David Lye, Timothy Barkham, Karthik Raman, Swaine Chen, Louis Chai, Barnaby Young\*, Yunn-Hwen Gan\* and Niranjan Nagarajan\* "Metagenome-wide association analysis identifies microbial determinants of post-antibiotic ecological recovery in the gut" Nature Ecology and Evolution 4:1256–1267 [32632261] Image: The Hindu BusinessLine
- Kuldeep Sachdeva, Manisha Goel, Malvika Sudhakar, Mansi Mehta, Rajmani Raju, **Karthik Raman**, Amit Singh and Varadharajan Sundaramurthy\* "Mycobacterium tuberculosis (Mtb) lipid-mediated lysosomal rewiring in infected macrophages modulates intracellular Mtb trafficking and survival" Journal of Biological Chemistry **295**:9192-9210 432424041
- Gayathri Sambamoorthy and **Karthik Raman\*** "MINREACT: an efficient algorithm for identifying minimal metabolic networks" *Bioinformatics* **36**:4309–4315 32407533
- Devika N T and **Karthik Raman\*** "Deciphering the metabolic capabilities of Bifidobacteria using genome-scale metabolic models" *Scientific Reports* **9**:18222 31796826
- Sarvenaz Choobdar, ..., The DREAM Module Identification Challenge Consortium, ..., Sven Bergmann\*, Daniel Marbach\* "Open Community Challenge Reveals Molecular Network Modules with Key Roles in Diseases" Nature Methods 16:843 31471613
- Aparajitha Srinivasan, Vijayakumar S, **Karthik Raman** and Smita Srivastava\* "Rational engineering of vitamin E metabolism for enhanced alpha-tocopherol production in *Helianthus annuus* cell culture" *Biochemical Engineering Journal* **151**:107256 Imagination Indian Express Imagination Indian Ind
- Abinaya Badri, **Karthik Raman\*** and Guhan Jayaraman\* "Uncovering novel pathways for enhancing hyaluronan synthesis in recombinant *Lactococcus lactis*: Genome-scale metabolic modelling and experimental validation" *Processes* **7**:343
- Gayathri Sambamoorthy, Himanshu Sinha\* and **Karthik Raman**\* "Evolutionary Design Principles in Metabolism" *Proc Biol Sci* **286**:20190098 30836874
- 2018 Karthik Azhagesan, Balaraman Ravindran\* and **Karthik Raman**\* "Network-based Features Enable Prediction of Essential Genes Across Diverse Organisms" *PLoS ONE* **13**: e0208722 430543651

Gayathri Sambamoorthy and **Karthik Raman\*** "Understanding the evolution of functional redundancy in metabolic networks" *Bioinformatics* **34**:i981–i987 30423058 (Part of Special Supplement: Proceedings of the 17<sup>th</sup> European Conference on Computational Biology (ECCB) 2018)

- Aarthi Ravikrishnan, Meghana Nasre and **Karthik Raman\*** "Enumerating all possible biosynthetic pathways in metabolic networks", *Scientific Reports* **8**:9932 29967471 Software available from RamanLab/MetQuest/
- Priyan Bhattacharya, **Karthik Raman** and Arun K. Tangirala\*, "A systems-theoretic approach towards designing biological networks that can achieve adaptation", *IFAC-PapersOnLine* **51**:307–312 (Part of Special Issue: Advances in Control & Optimization of Dynamical Systems (ACODS) 2018)
- Purva Bhatter, **Karthik Raman\***, and Vani Janakiraman\* "Elucidating the biosynthetic pathways of volatile organic compounds in *Mycobacterium tuberculosis* through a computational approach" *Molecular BioSystems*13:750–755 \*\*\quad \quad \
- Nandakumar Rajasekaran, Swaathiratna Suresh, Soundhararajan Gopi, **Karthik Raman**, and Athi N. Naganathan\* "A General Mechanism for the Propagation of Mutational Effects in Proteins" *Biochemistry* **56**:294–305 27958720
- Aditya Pratapa, Shankar Balachandran and **Karthik Raman\***, "FAST-SL: An efficient algorithm to identify synthetic lethal sets in metabolic networks", *Bioinformatics* **31**:3299–3305 26085504
- Aarthi Ravikrishnan and **Karthik Raman\***, "Critical Assessment of Genome-Scale Metabolic Networks: The Need for a Unified Standard" *Briefings in Bioinformatics* **16**:1057–1068 \$\sqrt{2}5725218 \$\sqrt{9}\$\$
- Raghavendran Partha and **Karthik Raman\*** "Revisiting robustness and evolvability: evolution in weighted genotype spaces" *PLoS ONE* **9**:e112792 25390641
- Karthik Raman\*, Nandita Damaraju and Govind Krishna Joshi "The organisational structure of protein networks: revisiting the centrality–lethality hypothesis" Systems and Synthetic Biology 8:73–81 424592293
- Anuja Kulkarni, Laxmi Ananthanarayanan\* and **Karthik Raman** "Identification of putative and cross-reactive chickpea (*Cicer arietinum*) allergens through an *in silico* approach" *Computational Biology & Chemistry* **47**:149–155 424099701
- Karthik Raman and Andreas Wagner "Evolvability and robustness in a complex signalling circuit" Molecular BioSystems 7:1081–1092 21225054
- Karthik Raman and Andreas Wagner "The evolvability of programmable hardware" *Journal of the Royal Society Interface* 8:269–281 20534598
- Karthik Raman, Ashwini Gurudas Bhat and Nagasuma Chandra "A systems perspective of host–pathogen interactions: prediction of tuberculosis disease outcome" *Molecular BioSystems* **6**:516–530 420174680 4
- Karthik Raman\* "Construction and analysis of protein–protein interaction networks" Automated Experimentation 2:2 (invited review) 420334628
- 2010 Karthik Raman and Nagasuma Chandra "Systems Biology" Resonance 15:131–153 (invited review) 💩
- Karthik Raman, Rohit Vashisht and Nagasuma Chandra "Strategies for efficient disruption of metabolism in Mycobacterium tuberculosis from network analysis" Molecular BioSystems 5:1740–1751 19593474
- Karthik Raman and Nagasuma Chandra "Flux balance analysis of biological systems: applications and challenges" Briefings in Bioinformatics 10:435–449 (invited review) 19287049
- Karthik Raman, Yeturu Kalidas and Nagasuma Chandra "targetTB: A target identification pipeline for Mycobacterium tuberculosis through an interactome, reactome and genome-scale structural analysis" BMC Systems Biology 2:109 19099550
- Karthik Raman and Nagasuma Chandra "Mycobacterium tuberculosis interactome analysis unravels potential pathways to drug resistance" BMC Microbiology 8:234 19105810
- Ketki Verkhedkar, **Karthik Raman**, Nagasuma Chandra and Saraswathi Vishveshwara "Metabolome based reaction graphs of *M. tuberculosis* and *M. leprae*: A comparative network analysis" *PLoS ONE* 2:e881 17849010
- Karthik Raman, Preethi Rajagopalan and Nagasuma Chandra "Hallmarks of Mycolic Acid Biosynthesis: A Comparative Genomics Study" *Proteins: Structure, Function and Bioinformatics* **69**: 358–368 17600834
- 2006 Karthik Raman, Preethi Rajagopalan and Nagasuma Chandra "Principles and Practices of Pathway Modelling"

Current Bioinformatics 1:147–160 🚭

Karthik Raman, Preethi Rajagopalan and Nagasuma Chandra "Flux Balance Analysis of Mycobacterium tuberculosis: targets for anti-tubercular drugs" PLoS Computational Biology 1:e46 416261191

### Books (4)

- Karthik Raman "An Introduction to Computational Systems Biology: Systems-Level Modelling of Cellular Networks" CRC Press/Taylor & Francis, Boca Raton ISBN 978-1138597327
- Aarthi Ravikrishnan and **Karthik Raman** "Systems-Level Modelling of Microbial Communities: Theory and Practice" CRC Press/Taylor & Francis, Boca Raton ISBN 978-1138596719
- Vishwesh Kulkarni, Guy-Bart Stan and **Karthik Raman** "A Systems Theoretic Approach to Systems and Synthetic Biology I: Models and System Characterizations" Springer Verlag (London) 

  ☐ ISBN 978-9401790406
- Vishwesh Kulkarni, Guy-Bart Stan and **Karthik Raman** "A Systems Theoretic Approach to Systems and Synthetic Biology II: Analysis and Design of Cellular Systems" Springer Verlag (London) 

  □ ISBN 978-9401790468

## Book chapters (5)

- Priyan Bhattacharya, **Karthik Raman\*** and Arun Tangirala "Systems-theoretic approaches to design biological networks with desired functionalities", *Methods Mol Biol* **2189**:133–155 [433180299]
- Karthik Raman\*, Aditya Pratapa, Omkar Mohite and Shankar Balachandran "Computational Prediction of Synthetic Lethals in Genome-Scale Metabolic Models Using Fast-SL", Methods Mol Biol 1716:315–336 2222760
- Abinaya Badri, Aparajitha Srinivasan and **Karthik Raman\*** "In Silico Approaches to Metabolic Engineering" In: P. Gunasekaran, S. Noronha and A. Pandey (editors), Current Developments in Biotechnology and Bioengineering, Elsevier ISBN 978-0444636676
- Karthik Raman and Nagasuma Chandra "Systems Biology of Tuberculosis: Insights for drug discovery" In: W. Dubitzky, J. Southgate and H. Fuss (editors), Understanding the Dynamics of Biological Systems: Lessons Learned from Integrative Systems Biology, Springer & ISBN 978-1441979636
- 2007 **Karthik Raman**, Yeturu Kalidas and Nagasuma Chandra "Model Driven Drug Discovery: Principles and Practices", *In*: J. Chen, A. S. Sidhu (editors), *Biological Database Modeling*, Artech House ISBN 978-1596932586

## Special Issue Editorials (2)

- Karthik Raman, Himanshu Sinha, Claudia E Vickers and Pablo Ivan Nikel "Synthetic biology beyond borders"

  Microbial Biotechnology 14:2254 434792854
- 2019 **Karthik Raman**, A Kalyanaraman "Special issue on theory and application of network algorithms in biology" Int J Adv Eng Sci Appl Math 11:89–90

### Software Tools

- Sankalpa Venkatraghavan<sup>†</sup>, Sathvik Anantakrishnan<sup>†</sup> and **Karthik Raman\*** "Probing Patterning in Microbial Consortia with picCASO: a Cellular Automaton for Spatial Organisation" Software available from ?[RamanLab/picCASO/
- Anjana Anilkumar Sithara, Devi Priyanka Maripuri, Keerthika Moorthy, Sai Sruthi Amirtha Ganesh, Philge Philip, Shayantan Banerjee, Malvika Sudhakar and **Karthik Raman\*** "iCOMIC: a graphical interface-driven bioinformatics pipeline for analyzing cancer omics data" Software available from RamanLab/iCOMIC/
- Malvika Sudhakar, Raghunathan Rengaswamy\* and **Karthik Raman\*** "Novel ratio-metric features enable the identification of new driver genes across cancer types" o Software available from RamanLab/cTaG/

- Gayathri Sambamoorthy and **Karthik Raman\*** "MINREACT: an efficient algorithm for identifying minimal metabolic networks" 

  Software available from 

  RamanLab/MinReact/
- Aarthi Ravikrishnan, Meghana Nasre and **Karthik Raman\*** "MetQuest: A tool for enumerating all possible biosynthetic pathways in metabolic networks" Software available from RamanLab/MetQuest/
- Aravind Sankar, Sayan Ranu\* and **Karthik Raman**\*, "ReactionMiner: Predicting Novel Metabolic Pathways through Subgraph Mining" Software available from MRamanLab/ReactionMiner/
- Aditya Pratapa, Shankar Balachandran and **Karthik Raman\***, "FAST-SL: An efficient algorithm to identify synthetic lethal sets in metabolic networks" Software available from RamanLab/FastSL/

# Conference Presentations, Invited Talks $\mathcal{E}$ Posters

## International Conferences (selected, \*denotes presenting author)

- Dinesh Kumar Kuppa Baskaran\* and **Karthik Raman** "A protocol for studying metabolic interactions in a microbial community using graph-based approaches" at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Madison, USA, [In-person]
- Aswathy Raghu\* and **Karthik Raman** "A constraint-based method to identify function-specific minimal microbiomes from large microbial communities" at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Madison, USA, [In-person]
- Rachita Kumar\* and **Karthik Raman** "Systems Modelling of the Skin Microbiome" at the 2<sup>nd</sup> International Conference on Microbiome Engineering (ICME), Boston, USA, (In-person)
- Aravind Sankar, Sayan Ranu and **Karthik Raman\*** "Predicting Novel Metabolic Pathways through Subgraph Mining" at the NetBIO COSI, 25<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB)/16<sup>th</sup> European Conference on Computational Biology (ECCB), Prague, Czech Republic
- Aditya Pratapa, Shankar Balachandran and **Karthik Raman\*** "FAST-SL: An efficient algorithm to identify synthetic lethal reaction sets in metabolic networks" at the 2014 RECOMB/ISCB Conference on Regulatory and Systems Genomics, San Diego, USA
- 2009 **Karthik Raman\*** "Systems-level modelling of pathogenic organisms for drug target identification", *Emerging Modelling Methodologies in Medicine and Biology*, Edinburgh, United Kingdom

### Seminars $\mathcal{E}$ Invited talks (selected)

- "UNFOLDing Biological Paradoxes: Insights into Robustness, Plasticity, and Multifunctionality of Gene Regulatory Networks", invited talk at *NetSciX* 2025, Indore, India
- "Algorithmic Adventures in Microbial Ecosystems: Disentangling Complexities with Metabolic Modelling", invited talk at Contemporary Perspectives in Computational Biology, held at the Institute of Mathematical Sciences, Chennai
- "Panera: A novel framework for surmounting uncertainty in microbial community modelling using pan-genera metabolic models", invited talk at ICBGDEES: International Conference on Biodiversity and Geochemistry of Deep and Extreme Earth Systems, held at IIT Kharagpur (online)
- "Surmounting uncertainty in microbial community modelling using Pan-genera metabolic models", invited talk at Modelling and Tackling Complex Biological Systems, held at the Institute of Mathematical Sciences, Chennai
- "Social networking in microbes: from deep sea to outer space", at CSI-IITM Symposium, IIT Madras (October 4, 2023)
- Led a session on "Utilizing Data Science to Transform Medicine, Drug Discovery and Development", at the inaugural *Chennai Al/ML symposium* co-organised by IITM and Pfizer R&D, Chennai
- "Learning on, using and from networks in Biology", invited talk at *Network Biology Day*, held at the Institute of Mathematical Sciences, Chennai
- "Computational approaches for metabolic engineering", at the Workshop on Fermentation assisted Biomanufacturing, IIT Madras

"Computational approaches to decoding microbial interactions in microbiomes", Institute of Mathematical Sciences, Chennai

- "Decoding driver genes in cancer genomes: from pan-cancer to personalised predictions", at International Online CME on Awareness on Genetic Diseases in Paediatrics & Cancer Genetics held at AIIMS, Madurai (online)
- "Decoding driver genes in cancer genomes: from pan-cancer to personalised predictions", at Symposium on Big Data Algorithms for Biology 2023 held at the Indian Institute of Science (IISc), Bengaluru
- "Decoding driver genes in cancer genomes: from pan-cancer to personalised predictions", at Workshop on Data Science in Drug Discovery held at NCCS, Pune (online)
- "Decoding driver genes in cancer genomes: from pan-cancer to personalised predictions", at the International Institute of Information Technology (IIITH), Hyderabad
- "Unravelling microbial interactions in the gut microbiome through computational approaches", at the 90th annual meeting of The Society of Biological Chemists (SBC), India
- "Computational insights into biological networks", at the *Health Informatics Summit* 2021, organized by The Department of Computational Biology at Indraprastha Institute of Information Technology Delhi (IIIT-D), alongside the Asia Pacific Bioinformatics Interaction & Networking Society (APbians)
- "Introduction and application of synthetic biology in everyday life", at iGEM Community Experts Talk (via video-conferencing)
- "Learning on, using and from networks in biology", at International Workshop on Networks & Dynamical Systems, Centre for Complex Systems and Dynamics at the Indian Institute of Technology Madras, Chennai (virtual)
- "Unravelling microbial interactions in the gut microbiome through computational approaches", at 7th BSSE Annual Research Symposium, Centre for BioSystems Science and Engineering (BSSE) at the Indian Institute of Science (IISc), Bengaluru
- "Computational Approaches to Understand Biological Networks", at The Centre for Predictive Human Model Systems (CPHMS), Atal Incubation Centre Centre for Cellular and Molecular Biology (AIC CCMB) (via video-conferencing)
- "Learning on, using and from networks in biology", at 1st Joint 4EU+/HGS MathComp Annual Colloquium hosted by the Heidelberg Graduate School of Mathematical and Computational Methods in the Sciences (via video-conferencing)
- "Computational Approaches to Understanding Microbial Interactions in Communities", at 6th Annual Metagenomics and Metadesign of Subways and Urban Biomes (MetaSUB) Conference (via video-conferencing)
- "Constraint-based models: standards, best practices & challenges for curation", at HARMONY 2020, Cambridge UK (via video-conferencing)
- "Computational insights into metabolic interactions in microbial communities", at India | EMBO Symposium |
  Engineering meets evolution: Designing biological systems, IIT Madras
- "Learning on, using and from networks in biology", at Accelerating Biology 2020: SNiPs to SPiNs, IISER Pune
- "Unravelling Molecular Mechanisms in Traditional Medicine: Systems Approaches to Understanding Diseases", at Ved-Vigyan Sammelan (VVS) 2019: A Dialogue between Vedic and Modern Sciences, IIT-BHU Varanasi
- "Unraveling microbial interactions in the gut microbiome associated with antibiotic recovery", at International Centre for Theoretical Studies (ICTS) Discussion Meeting on Mathematical and statistical explorations in disease modeling and public health
- "Computational Approaches to Understanding Complex Biological Networks", at Big Data Research Allahabad Summer School 2019, jointly organised by Allahabad University and Interdisciplinary Center for Scientific Computing (IWR) of Heidelberg University
- "Novel ratio-metric features enable the identification of new driver genes across cancer types", at the 3<sup>rd</sup> Pan-IIT Biotech Meet, IIT Madras
- 2018 "Learning and Predicting Novel Metabolic Pathways through Subgraph Mining", at IISc Bengaluru
- "A Graph-Theoretic Approach to Understand Metabolic Interactions in Microbial Communities", at the Annual meeting of Biological Engineering Society of India (BESCON) 2018, IIT Bombay, Mumbai
- "Exploiting alternate optima in linear programming to enumerate minimal cut sets in biochemical reaction networks", at the 33<sup>rd</sup> Annual Conference of the Ramanujan Mathematical Society (ACRMS-2018), New Delhi
- "Computational Approaches to Understand and Manipulate Metabolic Networks", at National Centre for Biological Sciences, Bengaluru

2017 "Learning and Predicting Novel Metabolic Pathways through Subgraph Mining", at the 4<sup>th</sup> IITM-Tokyo Tech Symposium, IIT Madras

- "Predicting Novel Metabolic Pathways through Subgraph Mining", as part of the Summer School on "Dynamics of Complex Systems", at the International Centre for Theoretical Studies (ICTS) Bengaluru, (Week 3: May 23–25, 2017)
- "Towards Understanding the Design Principles of Circadian Oscillators", at Aspects of Gene and Cellular Regulation, Institute of Mathematical Sciences, Chennai
- "Metabolic Engineering of vitamin E Biosynthesis in Sunflower Cell Cultures" at 85<sup>th</sup> Annual meeting of the Society of Biological Chemists, India (SBCI), CFTRI, Mysore
- "Revisiting robustness and evolvability: evolution on weighted genotype networks", at Network Theory: Conceptual Advances and Practical Applications, Institute of Mathematical Sciences, Chennai
- 2015 "FAST-SL: An efficient algorithm to identify synthetic lethals in metabolic networks", at the 2015 Annual Meeting of the National Network of Mathematical and Computational Biology (NNMCB), Pune
- 2015 "In Silico Modelling Of Metabolic Networks: Insights for Metabolic Engineering", at BioProcessing India 2015, Chennai
- "Modelling Metabolic Networks: From Biofuels to Better Therapies", at the 2<sup>nd</sup> Sankara Nethralaya Genetics Convention, Chennai
- "In Silico Identification of Drug Targets for Combinatorial Therapy", at the XVII ADNAT symposium, Thiruvananthapuram
- "Representation and Modelling of Metabolic Networks", at the Workshop on Analysis of Biological Networks, IIT Guwahati
- 2012 "Robustness and evolvability of biological networks", at the *International Conference on Mathematical and Theoretical Biology*, Pune

### Posters (selected, \*denotes presenting author)

- Lavanya Raajaraam and Karthik Raman\* Microbial communities vs monoculture: model-driven decision making for bioprocessing at the 9<sup>th</sup>th Metabolic Pathway Analysis (MPA), Seoul, South Korea
- 2023 Indumathi Palanikumar, Himanshu Sinha and Karthik Raman\* PAGER: Curtailing the uncertainties in analysing microbial communities using genome-scale metabolic models at the 31<sup>st</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Lyon, France
- Sarayu M, Maziya Ibrahima, Hemalatha Rajendran, Shagun Shagun, Shyam Kumar Masakapalli, **Karthik** Raman, Smita Srivastava\* CamGEM a rational metabolic engineering approach for enhancing camptothecin production in *Nothapodytes nimmoniana* at the 8<sup>th</sup> Conference on Constraint-Based Reconstruction and Analysis (COBRA 2022), Galway, Ireland
- Malvika Sudhakar\*, Raghunathan Rengaswamy and Karthik Raman PIVOT: a machine learning approach to identify personalised driver genes using multi-omic data at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) (Virtual)
- Lavanya Raajaraam\* and Karthik Raman Co-FSEOF: a computational framework to study the co-production of metabolites at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) (Virtual)
- Dinesh Kumar Kuppa Baskaran\* and Karthik Raman A protocol for studying metabolic interactions in a microbial community using graph-based approaches at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Madison, USA (In-person)
- Aswathy Raghu\* and Karthik Raman A constraint-based method to identify function-specific minimal microbiomes from large microbial communities at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Madison, USA (In-person)
- 2022 <u>Indumathi Palanikumar</u>\*, **Karthik Raman** and Himanshu Sinha Machine-learning based identification of discriminatory microbial features for the classification of a diarrheal gut microbiota at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) (Virtual)
- 2022 Sowmya Manojna Narasimha\*, Omkar Mohite S, Saketha Nath J and **Karthik Raman** Understanding flux rerouting in metabolic networks through an analysis of synthetic lethal pairs at the 30<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) (Virtual)

- Gayathri Sambamoorthy\* and **Karthik Raman** "Understanding the evolutionary dynamics of microbial communities through *in silico* studies" at the 28<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) (Virtual)
- 2020 <u>Rachita Kumar</u>\* and **Karthik Raman** "Systems Modelling of the Skin Microbiome" at the 28<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) (Virtual)
- 2020 <u>Malvika Sudhakar</u>\*, **Karthik Raman** and Raghunathan Rengaswamy "BinOpt: An algorithm to optimally assign feature importance to classes" at the 28<sup>th</sup> Annual International Conference on Intelligent Systems for
- Molecular Biology (ISMB) (Virtual) Malvika Sudhakar\*, Karthik Raman and Raghunathan Rengaswamy "Novel ratio-metric features enable the identification of new driver genes across cancer types" at the 17<sup>th</sup> European Conference on Computational Biology (ECCB), Athens, Greece
- 2018 Gayathri Sambamoorthy\* and **Karthik Raman** "Understanding the evolution of functional redundancy in metabolic networks" at the 17<sup>th</sup> European Conference on Computational Biology (ECCB), Athens, Greece
- Aarthi Ravikrishnan\*, Meghana Nasre and **Karthik Raman** "ComPass A graph-based algorithm for pathway analysis in microbial communities" at the 25<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB)/16<sup>th</sup> European Conference on Computational Biology (ECCB), Prague, Czech Republic
- 2016 <u>Srikiran Chandrasekaran</u>\* and **Karthik Raman** "An Analysis of Stochastic Algorithms for Parameter Estimation in Biological Systems", at the Asia-Pacific Bioinformatics Conference 2016, San Francisco, USA
- Aparajitha Srinivasan\*, **Karthik Raman** and Smita Srivastava "Metabolic Engineering Of  $\alpha$ -tocopherol in Helianthus annuus L.", at the 2<sup>nd</sup> International Conference on Natural Products Utilization: From Plants to Pharmacy Shelf, Plovdiv, Bulgaria
- Abinaya Badri\*, **Karthik Raman** and Guhan Jayaraman "A genome scale metabolic model for studying hyaluronan synthesis in recombinant *Lactococcus lactis*", at the 5<sup>th</sup> International Conference on Biomolecular Engineering, Austin, USA
- Nandita Damaraju\* and Karthik Raman "Design Principles of Circadian Systems", at the 2014 RECOMB/ISCB Conference on Regulatory and Systems Genomics, San Diego, USA
- 2013 Karthik Azhagesan and Karthik Raman\* "Joint' phylogenetic profiling of protein pairs reveals novel unique protein-protein associations and evolutionarily conserved protein interactions", at the NetBIO SIG meeting preceding ISMB-ECCB 2013, Berlin, Germany
- Karthik Raman, Aditya Barve and Andreas Wagner "Metabolite pairs are predominantly decoupled in genome-scale metabolic networks", at the Swiss Institute of Bioinformatics Days 2011, Bienne, Switzerland 
  □
- Karthik Raman and Andreas Wagner "Novel phenotypes and robustness in a complex signalling circuit", at the workshop on Emerging Modelling Methodologies in Medicine and Biology, Edinburgh, United Kingdom
- Kalidas Yeturu\*, **Karthik Raman** and Nagasuma Chandra "Drug Targetability Estimation through Comparative 'Pocket-omics' of Host and Pathogen: A Case Study in *Mycobacterium tuberculosis*" at the 9<sup>th</sup> International Conference on Systems Biology, Gothenburg, Sweden
- Karthik Raman and Nagasuma Chandra, "Protein-protein influences in Saccharomyces cerevisiae" at the 7<sup>th</sup>
  International Conference on Systems Biology, Yokohama, Japan

# Grants $\mathcal{S}$ funding

### **Extra-mural Funding**

- Co-investigator on a project "Rational Metabolic Engineering Strategies for Enhanced Production of Camptothecin in *Nothapodytes nimmoniana* Plant Cells" for a period of three years (₹23 lakhs), with Dr. Smita Srivastava (PI)
- Co-Principal investigator on a project "INCENTIVE Indo-European Consortium for Next-Generation Influenza Vaccine Innovation" (funded by Department of Biotechnology, GoI) for a period of five years (₹265 lakhs), with Dr. Himanshu Sinha (PI), Manikandan Narayanan (co-PI), Nirav Bhatt (co-PI), Ravindran B (co-PI)
- Principal investigator on a project "Understanding microbial interactions in microbiomes through metabolic modelling" (funded by Science and Engineering Board, GoI) for a period of three years (₹6.6 lakhs)
- 2020 Co-investigator on a project "GenomeIndia 10K: Cataloguing the genetic variation in Indians" (funded by

Department of Biotechnology, GoI) for a period of five years (₹140 lakhs), with Dr. Himanshu Sinha (IITM, PI) and Dr. Manikandan Narayanan (IITM, co-PI)

- Principal investigator on a project "A Computational Pipeline for Identifying the Context of Key Mutations in Cancer Genomes" (funded by the Department of Biotechnology, Government of India) for a period of three years (₹52.8 lakhs), with Dr. Raghunathan Rengaswamy (IITM, co-PI) and Dr. B. Ravindran (IITM, co-PI)
- 2017 nVidia Hardware Grant, of Titan X graphics processing unit for research
- Principal investigator on a project "Metabolic network analysis of pathogenic organisms for designing novel therapeutic intervention strategies" (funded by the Department of Biotechnology, Government of India) for a period of three years (₹24.4 lakhs), with Dr. Manoj N (IITM, co-PI)
- Co-investigator on a project "Control of *in vivo* polymerisation by synthetic biology approaches" (funded by the Department of Biotechnology, Government of India) for a period of four years (₹136 lakhs), with Prof. Guhan Jayaraman (IITM, PI)
- 2013 CUDA Research Centre grant from nVidia, including gift of nVidia Tesla K20 graphics processing unit for research
- Co-investigator on a project "Enhanced production of α-tocopherol by genetically transformed cell culture of *Helianthus annuus L.*" (funded by the Department of Biotechnology, Government of India) for a period of three years (₹29 lakhs), with Dr. Srivastava S (IITM, PI), Dr. Baskar R (IITM, co-PI)
- 2011 CUDA Research Centre grant from nVidia, including gift of nVidia Tesla C2070 graphics processing unit for research

### **Intra-mural Funding**

- Co-investigator on a project "Centre for Integrative Biology and Systems medicinE (IBSE)" (pCoE grant under the IoE scheme) for a period of two years (₹73 lakhs), along with Dr. Himanshu Sinha (PI, IITM) and Dr. Manikandan Narayanan (Co-PI, IITM)
- Co-investigator on a project "Deployable Artificial Intelligence (DAI)" (pCoE grant under the IoE scheme) for a period of two years, along with Dr. Arun Rajkumar (PI, IITM), Prof. B. Ravindran (Co-PI, IITM), Dr. Gitakrishnan Ramadurai (Co-PI, IITM), Dr. Nandan Sudarsanam (Co-PI, IITM) and Prof. Raghunathan Rengaswamy (Co-PI, IITM)
- Co-investigator on a project "Cancer Genomics & Molecular Therapeutics" (pCoE grant under the IoE scheme) for a period of two years (₹130 lakhs), along with Prof. Mahalingam S (PI, IITM) and Dr. Himanshu Sinha (Co-PI, IITM)
- Principal investigator on a project "Bio-surveillance of Antimicrobial Resistance (AMR) and COVID-19 prevalence in Chennai: A MetaSUB approach using metagenomics" (exploratory research project funded by RBCDSAI) for a period of two years (₹40.845 lakhs), along with Dr. Himanshu Sinha (Co-PI, IITM)
- Principal investigator on a project "Reconstruction and Modelling of a Lactobacillus Co-culture for Metabolic Engineering of Lactic Acid" for a period of one year (₹8 lakhs)
- 2015–17 Co-investigator on a large team project "Interdisciplinary Laboratory for Data Sciences", along with Dr. Ravindran Balaraman (PI, IITM) and several others
- Principal investigator on a project "Engineering a consortium of microbes for production of Bio-ethanol" (exploratory research project funded by IIT Madras) for a period of one year (₹5 lakhs), with Dr. Smita Srivastava (IITM, co-PI)
- Principal investigator on a project "MetREC: A Database of Systematically Annotated Genome-Scale Metabolic Reconstructions" (new faculty seed grant funded by IIT Madras) for a period of three years (₹5.23 lakhs)

## **Industrial Consultancy**

- Principal investigator on a project "Methods for construction and use of network models from RNA-seq data" funded by Aganitha Cognitive Solutions (₹2.35 lakhs)
- Principal investigator on a project "AI Samarth: AI Literacy Curriculum" funded by Central Square Foundation (₹94.40 lakhs)
- Principal investigator on a project "Scientific Knowledge Graph Analytics Development" funded by Pfizer Inc. (₹20.22 lakhs)
- 2023 Principal investigator on a project "Genome-scale Metabolic Modelling of Microalgae and Other Organisms"

funded by Yokogawa Technology Solutions India (₹4.60 lakhs)

- 2023–25 Principal investigator on a project "Microbiome Systems Biology: Understanding Microbial Interactions and Identifying Optimal Intervention Strategies in Home Microbiomes" funded by Hindustan Unilever Limited (₹70.99 lakhs)
- Principal investigator on a project "Skin Microbiome Systems Biology: Unravelling Metabolic Capabilities of Microbes in Communities" funded by Hindustan Unilever Limited (₹45.54 lakhs)
- 2022-25 Co-investigator on "MOOCs on Biological Big Data Analysis" funded by Excelra Knowledge Solutions Private Limited (₹96.8 lakhs)
- 2017–22 Co-investigator on "Robert Bosch Centre for Data Science and Artificial Intelligence (RBC-DSAI)" funded by Robert Bosch Engineering and Business Solutions Private Limited (₹2000.5 lakhs)
- Principal investigator on a project "Systems-level modelling approaches for quantitative systems pharmacology" funded by Vantage Research Private Limited, Chennai (₹3.59 lakhs)

# Honours $\mathcal{E}$ awards (selected)

- 2021 Institute Research and Development Award (Early Career) (IIT Madras), for outstanding achievements in teaching, scholarship and creative research work
- 2015 Young Faculty Recognition Award (IIT Madras), for excellence in teaching and research
- Sir Vithal N. Chandavarkar Memorial Medal for the best Ph. D. thesis of the year in the Supercomputer Education and Research Centre, Indian Institute of Science

# **Teaching**

## Graduate and undergraduate courses

- BT 1010 Module on "Big Data in Biology" (Jul-Nov 2017)
- BT 2020 Numerical Methods for Biology (Jan-May 2018, 2019)
- BT 3051 Data Structures and Algorithms for Biology (Jul-Nov 2014-2019, 2021-22)
- BT 3240 Metabolic Regulation (Jul-Nov 2011-2013)
- BT 4110 Computational Biology Lab (Jul-Nov 2015-2017)
- BT 4310 Current Topics in Synthetic Biology (Jul–Nov 2014, 2019)
- BT 5240 Computational Systems Biology (Jan–May 2013–2025, Winter 2017) DA 1300 Programming and Data Structures (Jul–Nov 2024)
- DA 1301 Programming Lab (Jul-Nov 2024)

### Workshops $\mathcal{E}$ Schools

- Lectured (online) on "Biological Networks", "Structure of Networks", "Network Models" and "Applications of Networks Biology" Statistical Genomics Workshop at NCBS (August 16–19, 2023)
- 2022 Co-taught a course "BE506 Biological Modelling and Simulation Course" at IIT Mandi (May 2022)
- Co-organised IITM-EMBL-EBI Winter School 2021 on reproducibility and modelling in systems biology, with Dr. Rahuman Sheriff, EMBL-EBI, at *IIT Madras* (December 6–9, 2021)
- 2021 ISCB Academy tutorial on "Metabolic modelling of microbial interactions in microbiomes" (October 22, 2021)
- "Introduction to Constraint-Based Modelling of Metabolic Networks" at the AICTE ATAL Online FDP on Computational Synthetic and Systems Biology, *IIT Guwahati* (July 28, 2021)
- Lectures on Computational Systems Biology at The MS University of Baroda (April 2021)
- NPTEL Lab Workshop for faculty and PhD scholars from across the country (August 24–27, 2020)
- 2019 Co-organised IITM-EBI modelling workshop, with Dr. Rahuman Sheriff, EMBL-EBI at *IIT Madras* (December 2–5, 2019)
- Lecture and Lab sessions on "Introduction to Network Biology" at the "A National Workshop on Scientific computations using MATLAB", at *Banasthali Vidyapeeth*, Rajasthan (January 19, 2019)
- 2018 "Introduction to Constraint-Based Modelling of Metabolic Networks", at the IFCAM Summer School, IISc

	Bengaluru (July 23, 2018)
2018	Co-taught at the "Training Workshop on Systems Biology", at the National Institute of Biomedical Genomics (NIBMG), Kalyani, West Bengal (July 21, 2018)
2017	Co-taught a summer school on "Dynamics of Complex Systems", at the <i>International Centre for Theoretical Studies (ICTS)</i> , Bengaluru (Week 3: May 23–25, 2017)
2017	Organised an AICTE-approved short-term training programme on "Computational Systems Biology" for faculty from colleges in India, at <i>IIT Madras</i> (Feb 6–11, 2017)
2016	Lecture on "Genome-Scale Modelling of Metabolic Networks: Insights for Metabolic Engineering" as part of the Global Initiative on Academic Networks Course on Metabolic Engineering at <i>IIT Madras</i> (July 9, 2016)
2016	"Introduction to Constraint-Based Modelling of Metabolic Networks" at NNMCB Second Instructional School on Mathematical and Computational Biology, IISc Bengaluru
2016	Taught a pre-school on computational biology preceding the NNMCB Second Instructional School on Mathematical and Computational Biology, at <i>IISc Bengaluru</i> (May 18–21, 2016)
2015	Taught employees from <i>Cognizant Technology Solutions</i> a module on "Basics of Biology/Computation for Biology" in a "Short Term Certification Programme on Bioinformatics"
	Other instruction-related activities
2019	Mentored two schoolchildren from Chennai on a project related to DNA Computing, as part of the RSI-Chennai 2019
2018	Mentored four schoolchildren from Chennai on projects related to DNA Computing and Network Biology, as part of the Research Science Initiative Chennai (RSI-Chennai) 2018
2017	Mentored two schoolchildren from Chennai on a project related to DNA Computing, as part of the RSI- Chennai 2017
2016	Mentored two schoolchildren from Chennai on a project related to DNA Computing, as part of the RSI- Chennai 2016
2015	Mentored two schoolchildren from Chennai on a project related to Network Biology, as part of the RSI- Chennai 2015
	Academic Mentorship
	PhD (major advisor/co-advisor)
2013–2019	Aarthi Ravikrishnan "Understanding microbial interactions in communities through an integrated computational and experimental framework" (co-advised by Dr. Smita Srivastava; recipient of award for "Best PhD thesis in Data Science (2020)" and DAAD-UGC Fellowship)
2014–2021	Gayathri S "Understanding the design principles of metabolic networks", recipient of "Institute Research Award (2018-19)"
2015–2023	Malvika Sudhakar "Machine learning on multi-omic data for identifying driver genes in cancer" (co-advised by Prof. Raghunathan Rengaswamy, Chemical Engineering)
2016–2023	Priyan Bhattacharya "Systems-Theoretic Approaches to Discover Adaption-capable Biological Networks" (coadvised by Prof. Arun Tangirala, Chemical Engineering)
2016–2024	Prem Jagadeesh "System Identification of Biological Processes" (co-advised by Prof. Arun Tangirala, Chemical Engineering)
2017–	Lavanya Raajaraam
2018–	Debomita Chakraborty (co-advised by Prof. Raghunathan Rengaswamy, Chemical Engineering)
2019–	Indumathi P (PMRF, co-advised by Dr. Himanshu Sinha)
2020–	Pratyay Sengupta (PMRF)
2022-	Shradha Sharma
2024–	Sandhya Vasudevan

# PhD (minor advisor)

2012–2020 Aparajitha Srinivasan "Strategies for enhanced production of alpha-tocopherol in cell culture of Helianthus

annuus L." (co-advised by Dr. Smita Srivastava; recipient of NAMASTE India-EU Fellowship)

M5 (	major	advisor	/co-advisor)

- Aditya Pratapa, "Design of efficient algorithms for synthetic lethality analysis" (co-advised by Dr. Shankar Balachandran, Computer Science)
- 2015–19 Beethika Tripathi, "Applications of Community Detection and Link Prediction on Multi-relational Networks" (coadvised by Prof. B. Ravindran, Computer Science
- 2015–18 Karthik Azhagesan, "Machine Learning Approaches to Predict Essential Genes Across Organisms" (co-advised by Prof. B. Ravindran, Computer Science)
- Shayantan Banerjee "Sequence neighborhoods enable reliable prediction of pathogenic mutations in cancer genomes" (co-advised by Prof. B. Ravindran, Computer Science)
- 2020–23 Dinesh Kumar K B "A protocol for studying metabolic interactions in microbial communities using graph-based approaches"
- 2023- Srikrishnan B
- 2024– Yuvaram Singh

#### MS (minor advisor)

Abinaya Badri, "Investigation of metabolic capabilities of recombinant Lactococcus lactis for hyaluronan production using a genome-scale metabolic model" (co-advised by Prof. Guhan Jayaraman)

#### **Post-doctoral Fellows**

2023-	Dr. Aarti Ravindran
2023-24	Dr. Chaitranjali Yadla
2016–19	Dr. Devika N.T.
2017–	Dr. Maziya Ibrahim
2021	Dr. Aswathy Raghu

### MTech projects

2024	Varsha V
2024–	varsna v

- 2024– Aryamitra Srinivasan
- 2023–24 Muthu Arunachalam "Understanding the Microbial differences between Urban and Rural built-environment"
- 2020–21 Sanjaay Balakrishnan "A toolbox for the analysis of microbiomes: Applications to ocular and ISS microbiomes"

## MTech (Dual Degree thesis projects)

- Jacqueline Elsa Binu
   Pradeep Melpakkam
   Rajagopalan Subramaniam
   Aswin Balamurugan
- 2023–24 Shobhan Karthick "Exploring Microbial Dark Matter: A Deep Dive into Genomics of Space-associated Cleanroom Microorganisms"
- 2023–24 Prashanth Joseph Ramanathan "Leveraging generative AI to learn from and disrupt protein–protein interfaces"
- 2022–23 Amrita Mahesh "Systematic analysis of Indian pancreatic cancer genomes"
- Hemanth Ram (with Prof. B. Ravindran, Computer Science) "Structure-based Drug Design using Distance Prediction with Graph Neural Networks"
- Sreeharsha Peesapati S S (with Prof. Arun Tangirala, Chemical Engineering) "Quantifying adaptation and mapping it to the parameter space in bio-chemical networks using systems theory"
- 2021–22 Prashant Govindarajan (with Prof. B. Ravindran, Computer Science) "Graph generative models for binding sitespecific molecule generation"
- 2020-21 Ninad Rajandekar "A computational study of microbial community formation upon evolution"
- 2020–21 Rohan Jebin Anbiah "Identification of Strain Optimization Strategies for Single Organisms and Communities in

	Metabolic Engineering"
2020–21	Raghav Moar "Phylogenetic analysis of Metabolic Pathways: An On-line Tool"
2020–21	Vishnu Harshit "Machine learning approach to study protein–ligand interactions"
2019–20	Rohini J S "Comparing Circadian Oscillators Across Organisms"
2019–20	Shreya Swaminathan "Efficient Enumeration of Synthetic Lethal Reactions for Pan Cancer Lethality Analysis"
2019–20	Anand A R "Goal-directed Molecule Generation using Reinforcement Learning" (with Prof. B. Ravindran, Com-
2010 10	puter Science) Secretar C (with Prof. Arun Tangirala Chamical Engineering)
2018–19	Soorya G (with Prof. Arun Tangirala, Chemical Engineering) Sachin Agrawal, "Deep Learning for Network Chemistry and Network Biology" (with Prof. B. Ravindran,
2018–19	Computer Science)
2018–19	Vishnu Narayan, "Parallelisation of Dynamic Model Simulations"
2018–19	Abhijeet Mavi, "Topological Sensitivity Analyses of Target-of-Rapamycin pathway in Saccharomyces cerevisiae"
2016–13	Saransh Umale (with Prof. Raghunathan Rengaswamy, Chemical Engineering), "Design Principles of Modular
2010-10	Gene Oscillators: An ODE-based approach"
2016–18	Muthukumarasamy Saravanan, "Learning and Predicting Reactions from Metabolic Networks"
2017–18	Pradeep Natarajan, (with Prof. Raghunathan Rengaswamy, Chemical Engineering), "Design Principles for the
2017 10	Synthesis of Modular Genetic Oscillators"
2016–17	Omkar Mohite, "Understanding redundancy in metabolic networks through analysis of Synthetic Lethals"
2015–16	Aravind Sankar (with Dr. Sayan Ranu, Computer Science), "Predicting Chemical Reactions through Graph
	Mining"
2015–16	Pallavi Gudipati (with Prof. B. Ravindran, Computer Science), "Neighborhood Analysis of Genomic Data"
2015–16	Abhishek Sivaram (with Prof. Raghunathan Rengaswamy, Chemical Engineering), "Application of Variants of
	Principal Component Analysis to Biological Systems — A Source Separation Framework"
2015–16	Aparnna Suresh, "Identifying Network Topologies That Can Exhibit Switch-Like Behaviour"
2015–16	Dileep Kishore, "Discovering the Design Principles of Circadian Rhythms using GPGPUs"
2014–15	Pankaj Kumar (with Dr. Sayan Ranu, Computer Science), "Identifying novel reaction routes to synthetic
	metabolites"
2014–15	Parthasarathy Gopavarapu (with Prof. B. Ravindran, Computer Science), "Predicting Essential Genes in Mi-
	crobes"
2013–14	Govind Krishna Joshi, "Multi-timescale multi-algorithm simulation of a cell"
2013–14	Raghavendran Partha, "Revisiting robustness and evolvability: evolution on weighted genotype networks"
2012–13	Sagar Laygude, "GPU-based massively parallel in silico phenotyping"
2012–13	Namrata Kamat, "Microbial community modelling"
	BTech (Undergraduate thesis projects)
2014–15	Narasimhan Balakrishnan (with Prof. Arun Tangirala, Chemical Engineering)
2014–15	Adarsh Chavakula (with Prof. Shankar Narasimhan, Chemical Engineering)
2014–15	Balaji Kumar
2014–15	Srikiran Chandrasekaran
2014–15	Sanjan T P
2014–15	Aravindabharathi Ramakrishnan
2013–14	Nandita Damaraju
2012–13	Aditya Sriganesh
2012–13	Shashank Garlapati
	Junior Research Fellows/Project Associates/Post-baccalaureate fellows
2024–	Hari Priya Narahari (NPTEL Post-baccalaureate Fellow)
2024–	Prithvi Prabhu (IBSE Post-baccalaureate Fellow)
2024–	Sounak Mukherjee (IBSE Post-baccalaureate Fellow)
2023-	Tanisha Malpani (IBSE Post-baccalaureate Fellow)
2023–24	Anirudh Rao (Young Research Fellow)
2023–24	Aditya Ray (Young Research Fellow)

2022–23	Rajagopal Subramaniam C (Young Research Fellow)
2021–22	Harish Manoharan (Young Research Fellow)
2019–22	Keerthika Moorthy (Project Associate)
2020–21	Amrita Mahesh (Young Research Fellow)
2020–21	Sai Sruthi A (Junior Research Fellow)
2020–21	Shreyansh Umale (IBSE post-baccalaureate Fellow)
2020–21	Rachita Kumar (IBSE post-baccalaureate Fellow)
2019–21	Senthamizhan V (IBSE post-baccalaureate Fellow)
2018–20	Anjana A S (Project Associate)
2017–19	Priyanka Maripuri (Project Associate)
2015–16	Smrithi Krishnan (Project Associate)
2017–18	Likith Reddy (Junior Research Fellow)
2015–16	Sivaratna Kumari Narisetti (Project Associate)
2014–15	Murali Karthikeyan (Project Associate)
2013–15	Priyanka Barman (Project Associate)

## **Outreach Activities**

### Science Outreach/Media

**RBCDSAI** blog

Lab website blog

Our work featured in the press

Times of India: Why is Big data on Biology so big

BioSpectrum India: IITs make giant strides in precision onco research

DataQuest India 'DeepTech' podcast: Biotechnology 2.0: IIT Madras Prof on the era of biology, math and programming combined

#### **International Outreach Activities**

Represented IIT Madras at the *Graduate Program India–Heidelberg* meeting organised by *University of Heidelberg*, Jun 21–23, Heidelberg; also gave a talk on "Computational Approaches to Understand and Manipulate Metabolic Networks"

Represented IIT Madras at the Seminar on Synthetic Biology organised by the Academy of Finland, Nov 21–22, Helsinki

#### **National Outreach Activities**

Drug Discovery Hackathon 2020 (DDH2020) platform was an open source drug discovery Hackathon against COVID-19, and a joint initiative of AICTE, CSIR and supported by Office of Principal Scientific Advisor, Govt. of India, NIC and MyGov. I was part of an expert panel that put out problem statements, reviewed submissions and mentored successful teams. My challenge, to "Develop a reinforcement learning-based algorithm to identify lead molecules by emulating ligand-protein interactions" can be viewed at https://innovateindia.mygov.in/drug\_ps/ddt2-01/.

### Lectures at Industries

- Lecture on "Al Meets Biology: A Powerful Partnership for Understanding Life" at Zydus Research, Ahmedabad (December 14, 2023)
- Lecture on "Social networking in microbes: from deep sea to outer space" at Hindustan Unilever Research Centre, Bengaluru (June 21, 2023)
- Lecture on "Robustness and Evolvability in Complex Systems" at Culture Machine, Mumbai (January 4, 2017)
- Lectures on "Introduction to Mathematical Modelling and Systems Biology" at Vantage Research Private Limited, Chennai (June 2016)

Lecture on "Engineering Metabolic Networks using *in silico* approaches" at Hindustan Petroleum Corporation Limited, Bangalore (January 30, 2014)

Lecture on "Metabolic Engineering" at Samsung India Software Operations, Bangalore (April 20, 2012)

### **Professional Service**

### Institutional Service — IIT Madras

BS Curriculum Committee, IITM Zanzibar (2023)

Advisor, Office of Global Engagement (2020-)

Research Committee (2021–23)

Course allotment committee (2014 Aug—2020)

Department Faculty Meeting Secretary (2011)

Ph. D/M. S. admission committee (2011 Dec-2015 Dec)

Faculty applications screening committee (2013, 2015)

### **Grant Referee**

Department of Biotechnology , Biotechnology Industry Research Assistance Council (BIRAC) Breast Cancer Now , Indian Council for Medical Research , Science and Engineering Board , European Research Council , Dutch Research Council (NWO)

### **Editorial Responsibilities**

- 2023– PLoS Complex Systems, Editorial Board Member
- 2023– Responsibilities: Assess whether manuscripts should be sent for peer review, manage npj Systems Biology and Applications, Editorial Board Member
- 2022– Microbial Biotechnology, Editorial Board Member
- 2022- PLoS ONE, Editorial Board Member
- 2021– Responsibilities: Assess whether manuscripts should be sent for peer review, manage ACS Synthetic Biology, **Editorial Advisory Board** peer review of manuscripts, make final editorial decisions
- 2019– Scientific Reports, Editorial Board Member

Responsibilities: Assess whether manuscripts should be sent for peer review, manage peer review of manuscripts, make final editorial decisions

## **Conference Committees**

- 5th IBSE International Symposium Microbiomes in Environment, Space and in Human Health, at IIT Madras, February 19–25 2024 (Co-organiser)
- 4th IBSE International Symposium Microbiomes in Environment, Space and in Human Health, at IIT Madras, October 31–November 2 2022 (Co-organiser)
- 2022 RBCDSAI-IBSE HPC Symposium, at IIT Madras (online), January 4–7, 2022 (Co-organiser)
- 2022 Advances in Control & Optimization of Dynamical Systems (ACODS) 2022 (Associate Editor)
- 2020 ISMB 2020 (Programme Committee Member of NetBio COSI: Network Biology)
- 2020 2nd IBSE International Symposium EMBO | India Symposium | Engineering meets Evolution: Designing biological systems, at IIT Madras, January 30–February 1 2020 (Co-organiser)
- 2020 Advances in Control & Optimization of Dynamical Systems (ACODS) 2020 (Associate Editor)
- 2019 ISMB/ECCB 2019 (Programme Committee Member of NetBio COSI: Network Biology)
- 2018 ISMB 2018 (Programme Committee Member of NetBio COSI: Network Biology)
- 2018 Advances in Control & Optimization of Dynamical Systems (ACODS) 2018 (Associate Editor)
- 2018 1st IBSE International Symposium From Genotype to Phenotype: Computational Approaches to Understand Biological Systems, at IIT Madras, January 22–24 2018 (Co-organiser)

### Journal Referee

Archives of Medical Research, ACS Synthetic Biology, Applied Mathematical Modelling, BBA Molecular Basis of Disease, Biochemical Society Transactions, Bioinformatics, Bioresource Technology, BMC Bioinformatics, BMC Genomics, BMC Systems Biology, Cells Tissues Organs, Computational and Structural Biotechnology, Computational Biology and Chemistry, Computers in Biology and Medicine, Critical Reviews in Biotechnology, Frontiers in Bioengineering and Biotechnology, Gigascience, IEEE Access, IEEE/ACM Transactions on Computational Biology and Bioinformatics, iScience, ISME Journal, Journal of Applied Microbiology, Journal of Biosciences, Journal of Theoretical Biology, Journal of the Indian Institute of Science, Journal of the Royal Society: Interface, Life Sciences in Space Research, Mathematical Biosciences, Metabolic Engineering Communications, Microbial Biotechnology, Microbial Cell Factories, Molecular Ecology, Molecular Microbiology, Molecular Nutrition and Food Research, Molecular Omics, mSystems, Nature Microbiology, Nature Chemical Biology, Nature Communications, npj Systems Biology and Applications, Nucleic Acids Research: Cancer, Nucleic Acids Research: Genomics & Bioinformatics, Nucleic Acids Research, Pathogens and Disease, Physica A, PLoS Computational Biology, PLoS ONE, Review Commons, Scientific Data, Tuberculosis