Dr. Sahaya Vijay Jeyaraj, Ph.D.

Postdoctoral Researcher, National Institute for Materials Science (NIMS), Tsukuba, Japan.
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Research Profile

I am a computational researcher with a Ph.D. in Mathematics on molecular graph theory and cheminformatics. I have postdoctoral experience in dynamical system analysis such as the mathematical modelling of biochemical reaction networks of proto-metabolism at RIKEN, and of electrochemical reaction networks at the National Institute for Materials Science (NIMS). I have published Quantitative Structure-Property Relationship (QSPR) and machine-learning studies on drug-like molecules, including Central Nervous System (CNS) drugs and anticancer agents. I am a developer of the Molecular Property and Topological Indices Evaluator (MolTIE), a desktop Graphical User Interface (GUI) with a JavaScript interface for molecular descriptor computation, built using agentic Artificial Intelligence (AI). I am strong in numerical simulation, numerical methods, graph algorithms, applied mathematics and quantitative model building. I have 14 peer-reviewed publications, 2 preprints and 2 under review. I am seeking to apply machine learning to drug discovery, molecular simulation and biophysics.

Core Technical Skills

- **Programming:** Python (primary, for scientific software development), JavaScript (graphical user interfaces), C++, Java, MATLAB, Mathematica
- **Agentic AI development:** Direct Artificial Intelligence (AI) coding agents to design, build and test scientific software, including the Molecular Property and Topological Indices Evaluator (MolTIE) desktop Graphical User Interface (GUI). I define the algorithms and specifications and validate the outputs.
- **Machine learning:** Descriptor-based machine learning for molecular and materials property prediction. Online certificate in Python Programming for Machine Learning
- **Cheminformatics and molecular modelling:** Molecular graph descriptors and topological indices, QSPR and QSAR modelling, molecular entropy measures, Hückel MO analysis, DFT and molecular docking (collaborative studies)
- **Mathematical and numerical methods:** Graph theory, linear algebra, chemical kinetics and reaction network modelling, stability and timescale analysis, impedance spectra modelling
- **Tools:** Git and GitHub, LaTeX, VS code, Claude AI (Licensed)

Research Experience

NIMS Postdoctoral Researcher **Apr 2026 - Present**

Mathematical Catalysis Research Team, GREEN Center, NIMS, Tsukuba (PI: Dr. Hideshi Ooka)

- Work on the FOREST project, building analytical microkinetic models of electrochemical impedance for multi-step catalytic reactions.
- Derived a new mathematical equation to fit electrochemical impedance spectroscopy (EIS) data.

Postdoctoral Researcher **Jan 2025 - Mar 2026**

CSRS Biofunctional Catalyst Research Team, RIKEN, Wako (PI: Prof. Ryuhei Nakamura)

- Worked on the "Chemistry of the CO world" project, modelling proto-metabolism occur in an open system with biochemical reaction networks.
- Obtained the amplification rate of autocatalysis and used it to analyse the growth rate of catalytic reaction networks to sustain the life.
- Developed methods to compute the lifetime of autocatalytic networks and the timescale decomposition of linear networks. Reported in a ChemRxiv preprint, three RIKEN research achievement registrations and talks at the Asian Conference on Mathematical Biology 2025.

Ph.D. Researcher and Assistant Professor Fellow **Sep 2020 - Feb 2024**

Vellore Institute of Technology (VIT), India (Supervisor: Dr. Roy Santiago)

- Computed degree-based, distance-based and entropy descriptors for molecular, crystalline and nanostructured systems, and developed efficient algorithms for their generation.

- Carried out QSPR modelling of CNS drugs and anticancer drugs, and descriptor-based machine learning for graphene nanoribbons.

SELECTED SOFTWARE AND RESEARCH PROJECTS

- **PyTIE (Python, 2025).** Software for evaluating degree-based topological descriptors and molecular entropy from molecular graphs. Four packages (PyTIE_D, PyTIE_DS, PyTIE_SMS_DE, PyTIE_SMS_DSE). Described in arXiv:2510.26813. Code at github.com/sahayavijay/PyTIE-0.0.1.
- **MolTIE (Python desktop GUI, manuscript in preparation).** Designed and built a standalone JavaScript HTML file that computes molecular topological indices and performs Hückel MO analysis through a graphical interface, so users need no programming. Feature-compared with Mordred, RDKit and ChemGraphX.
- **QSPR and machine learning on drug-like molecules.** CNS drug activity modelling, anticancer drug property and entropy analysis, and piperidin-4-one analogs as ALK inhibitors (DFT, topological descriptors, docking and pharmacological profiling, in collaboration).
- **Reaction network theory.** Amplification rate, lifetime and timescale decomposition for autocatalytic and linear chemical reaction networks.

EDUCATIONAL DETAILS

1. **Sep 2020 - Apr 2024: Ph.D.** in Mathematics, School of Advanced Sciences, Vellore Institute of Technology, India. Thesis: *A Study on Molecular Topology of Certain Bipartite Chemical Structures.*
2. **Jul 2016 - Sep 2017: M.Phil.** (Mathematics), St. Joseph's College, India. Thesis: *Minimum Metric Dimension of Certain Networks.*
3. **Jun 2014 - Apr 2016: M.Sc.** (Mathematics), St. Joseph's College, India. Thesis: *Vector space of graph.*
4. **Jun 2011 - Apr 2014: B.Sc.** (Mathematics), Arul Anandar College, Madurai, India.

PUBLICATIONS

Machine learning, QSPR and drug-related cheminformatics

1. **Sahaya Vijay Jeyaraj**, R. Santiago, M. Azeem, Tony Augustine, M. N. Husin, Quantitative Structure-Property Relationship (QSPR) Modeling of Central Nervous System (CNS) Drug Activity Using Molecular Descriptors, *Current Organic Synthesis*, 22(7), 2024, 799-810. **DOI:** 10.2174/0115701794349717241024100059.
2. K. Jyothish, Roy Santiago, P. Chandra Sekar, K. B. Gayathri, **Sahaya Vijay Jeyaraj**, Tony Augustine, Machine Learning Approach on Topological Features of Bottom-up Synthesized Graphene Nanoribbons using Valency Based Descriptors, *Frontiers in Chemistry*, 14, 2026. **DOI:** 10.3389/fchem.2026.1750413.
3. Gayathri K. B., Roy Santiago, **Sahaya Vijay Jeyaraj**, Chandra Sekar P., Tony Augustine, Machine Learning Approach on Degree-Sum Based Topological Indices of Bottom-up-Synthesized Graphene Nanoribbons, *Nano*, 2025, 2650008. **DOI:** 10.1142/S1793292026500086.
4. Tony Augustine, Roy Santiago, **Sahaya Vijay Jeyaraj**, Mohamad Azeem, Exploring Neighborhood Topological Descriptors for Quantitative Structure-Property Relationship (QSPR) Analysis and Entropy Measures of Some Anti-cancer Drugs, *Current Organic Synthesis*, 22(8), 2025, 934-943. **DOI:** 10.2174/0115701794349166241217085334.
5. Sonadevi S., Rajaraman D., Periyasamy D., **Sahaya Vijay Jeyaraj**, Tony Augustine, Roy Santiago, Saritha M., Athishu Anthony L., In Silico Rationalization of Piperidin-4-One Analogs as Anaplastic Lymphoma Kinase Inhibitors: Integration of Density Functional Theory, Topological Descriptor, Molecular Docking and Pharmacological Feature Profiling, *Journal of Molecular Structure*, 1311, 2024, 138356. **DOI:** 10.1016/j.molstruc.2024.138356.

Cheminformatics software and algorithms

6. **Sahaya Vijay Jeyaraj**, K. Jyothish, Jyothish K, Govardhan Sriramulu, Tony Augustine, Roy Santiago, and Noah Antony Daniel Renai P., MolTIE: A Single-File Graphical Interface for Topological Indices, Graph Entropy, and Spectral Graph Descriptors of Molecular Graphs, *MATCH Commun. Math. Comput. Chem.*, 2026. **Under review**
7. **Sahaya Vijay Jeyaraj**, Roy Santiago, Govardhan S., Tony Augustine, Jyothish K., PyTIE: A Python Program for the Evaluation of Degree-Based Topological Descriptors and Molecular Entropy, *arXiv*, 2025. **DOI:** 10.48550/arXiv.2510.26813.
8. **Sahaya Vijay Jeyaraj**, Roy Santiago, Chandra Sekar Ponnusamy, Jain Maria Thomas, Mohamad Husin, Abdelli Fathi, Efficient Generation of Specific Counting Polynomials and Its Subsequent Indices of Complex Boric Acid Structure, *Current Organic Synthesis*, 22(7), 2025, 821-828. **DOI:** 10.2174/0115701794366590250414051549.

9. **Sahaya Vijay Jeyaraj**, Roy Santiago, A Study on Efficient Technique for Generating Vertex-based Topological Characterization of Boric Acid 2D Structure, *ACS Omega*, 8(25), 2023, 23089-23097. **DOI:** 10.1021/acsomega.3c02477.

Molecular topology and computational chemistry

10. S. Prabhu, **Sahaya Vijay Jeyaraj**, V. Manimozhi, Micheal Arockiaraj, Roy Santiago, J. Celin Fiona, Krishna Balasubramanian, Topological, Graph-Spectral Properties, NMR and ESR Spectral Patterns of Hydrogen-Bonded Nanosheets of Boric Acid, *Journal of Cluster Science*, 37(48), 2026. **DOI:** 10.1007/s10876-026-02996-2.
11. Abdelli Fathi, Tony Augustine, Mohamad Nazri Husin, **Sahaya Vijay Jeyaraj**, Jain Maria Thomas, Roy Santiago, Graph Theoretical Approach to Topological Features of Zeolitic Tetrahedral Imidazolate Framework-3, *Malaysian Journal of Fundamental and Applied Sciences (MJFAS)*, 21(2), 2025. **DOI:** 10.11113/mjfas.v21n2.4127.
12. A. Fathi, **Sahaya Vijay Jeyaraj**, M. N. Husin, Tony Augustine, Valency-Based Molecular Descriptor on Structural Property Relationship of Ni Tetrathiafulvalene Tetrathionate, *Malaysian Journal of Fundamental and Applied Sciences (MJFAS)*, 20(6), 2024. **DOI:** 10.11113/mjfas.v20n6.3831.
13. **Sahaya Vijay Jeyaraj**, Roy Santiago, Charles Beromeo Bheeter, Mohamad Nazri Husin, Tony Augustine, Rudrusamy U. Gobithaasan, Easuraja Michael, Topological Properties and Entropy Calculations of Aluminophosphates, *Mathematics*, 11(11), 2023, 2443. **DOI:** 10.3390/math11112443.
14. **Sahaya Vijay Jeyaraj**, Roy Santiago, Computation of Wiener Descriptor for Melamine Cyanuric Acid Structure, *Polycyclic Aromatic Compounds*, 44(2), 2023, 1057–1071. **DOI:** 10.1080/10406638.2023.2186441.
15. Tony Augustine, Roy Santiago, **Sahaya Vijay Jeyaraj**, Jain Maria Thomas, Shanmugam Palanisamy, Topological study on degree based molecular descriptors of fullerene cages, *Molecular Physics*, 121(4), 2023, e2179858. **DOI:** 10.1080/00268976.2023.2179858.

Reaction networks and other

16. **Sahaya Vijay Jeyaraj**, Hirokazu Komatsu, Tomoharu Suda, Ryuhei Nakamura, Hideshi Ooka, Kinetic Boundary between Autocatalysis and Diffusion in the Origin of Life, *ChemRxiv*, 2026. **DOI:** 10.26434/chemrxiv.15004763/v. (**Under review at *Physical Review E***)
17. F. Sherin Rebecca, R. Sharmila, **Sahaya Vijay Jeyaraj**, Fikadu Tesgera Tolasa, Rajamanickam Pon Nivedha, Janani Ezhilan, Tony Augustine, Anticancer Activity with Physical Property Analysis of Mollugo Cerviana (L). Ser Whole Plant Extract on Hepatocellular Carcinomic Cell Lines -HEPG2, *Scientific Reports*, 2026. **DOI:** 10.1038/s41598-026-58687-5.

AWARDS AND RESEARCH ACHIEVEMENTS

1. **Raman Research Award**, April 2023, June 2023 and August 2023.
2. **RARS Application R25007251** (March 2026). Calculating the lifetime of Autocatalytic Chemical Reaction Networks. Authors: **Jeyaraj Sahaya Vijay**, Nakamura Ryuhei, Ooka Hideshi, Kawasaki Mayu.
3. **RARS Application R25007252** (March 2026). Timescale Decomposition of Linear Chemical Reaction network. Authors: Ooka Hideshi, **Jeyaraj Sahaya Vijay**, Nakamura Ryuhei, Kawasaki Mayu.
4. **RARS Application R25007253** (March 2026). Stability Analysis of chemical reaction networks based on the amplification rate of autocatalysis. Authors: Ooka Hideshi, **Jeyaraj Sahaya Vijay**, Nakamura Ryuhei, Kawasaki Mayu.

INVITED TALKS AND SELECTED PRESENTATIONS

1. **Resource Person**, "Mathematical Tools and Modern Techniques for Research, Thesis Writing and Scholarly Publication", Dhanalakshmi Srinivasan University, Tiruchirappalli, India, **September 8, 2026**.
2. **International invited speaker**, "Enhancing Research Capacity: Publication, Grants and Research Impact" (FDP), Dhanalakshmi Srinivasan University, Tiruchirappalli, India, **August 27, 2026**.
3. **Keynote speaker**, "3rd International Conference on Recent Trends in Data Science (ICRTDS-2026)", St. Xavier's College (Autonomous), Palayamkottai, India, **March 5-6, 2026**.
4. **Keynote international speaker**, "3rd International Conference on Innovation in Science and Humanities (ICISH-2025)", Saveetha Engineering College, Chennai, India, **August 19-20, 2025**.
5. **Sahaya Vijay Jeyaraj**, Hirokazu Komatsu, Hideshi Ooka, Ryuhei Nakamura, *Calculating the lifetime of autocatalytic networks*, Joint conference of the Asian Conference on Mathematical Biology and the Annual Meeting of the Japanese Society for Mathematical Biology, Kyoto TERRSA, Japan, **July 11-17, 2025**.

6. Hideshi Ooka, **Sahaya Vijay Jeyaraj**, Ryuhei Nakamura, *Analyzing the Stability of Autocatalytic Chemical Reaction Networks Based on their Amplification Rate*, Japan Geoscience Union Meeting 2025, Makuhari Messe, Chiba, Japan, **May 29, 2025**.
7. **Sahaya Vijay Jeyaraj**, *A Cut Method Technique Used on Topological Descriptors of Melamine Cyanuric Acid*, International Conference on Mathematics and Its Applications (ICMA-2024), Sacred Heart College (Autonomous), Tirupattur, India, **February 15-16, 2024**.
8. **Sahaya Vijay Jeyaraj**, *Quantitative-Structure Activity Relationship Based Drug Designing*, BIRAC-BioNEST Laboratory, VIT-TBI, VIT University, Vellore, India, **March 11, 2023**.
9. **Sahaya Vijay Jeyaraj** and Roy Santiago, *Topological Properties and Entropy Calculations of Aluminophosphates*, International Conference on Modelling, Simulation and Optimization of Energy Systems (MSOES-2023), Canadian University Dubai, UAE, **June 17-18, 2023**.

ACADEMIC APPOINTMENTS

1. **Apr 2021 - Feb 2024: Assistant Professor Fellowship**, VIT University, Vellore, India.
2. **Aug 2019 - Sep 2020: Assistant Professor**, Department of Science and Humanities, Vaigai College of Engineering, Anna University, India.
3. **Jul 2017 - Dec 2018: Assistant Professor**, St. Joseph University, Nagaland, India.

RESEARCHER IDS

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REFERENCES

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