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Research Area: Organic Chemistry, Natural Product Synthesis, Chiral Catalysis, Photophysical Studies, and Sustainable Resources

Personal Details

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Academic Background

Education

2015	:	Ph.D. (Synthetic Organic Chemistry) Mahatma Gandhi University
2002	:	M.Sc. Chemistry Mahatma Gandhi University
1999	:	B. Sc Chemistrty Kerala University

Professional Profile

2016- present	:	Assistant Professor, Department of Chemistry, TKM College of Arts and Science, Kollam
2014-2016	:	Research and Teaching Assistant, IIRBS, Mahatma Gandhi University

Distinctive Achievements

1. Conference Coordination

- Co-convened the **InternationalConference** on Tropical Plants and Molecular Design in February 2017, organized by the Post Graduate and Research Department of Chemistry, TKM College of Arts and Science.
- Convened an international level **Distinguished Chemistry Lecture** on “Separation Techniques in Chemistry “on 2018 organized by the Post Graduate and Research Department of Chemistry, TKM College of Arts and Science

2. Innovative Research

Secured one **Indian Patent** during research at T. K. M. College of Arts and Science.

Publications

- **Hydrogen Bond-Assisted Excited State Switching and Fluoride Responsive Behavior of Orthogonal spiroborate Ester Derived from Naturally Occurring α -Mangostin.**

Swathy Unnikrishnapillai Saraswathy, Lekshmi Chandranpillai Lalithabai, Sandip Giri, Safa Ayoob, **Simimole Haleema***, Anakuthil Anoop* and Sumalekshmy Sarojiniamma*, *Eur. J. Org. Chem.* **2025**, e202401411, 1-7
DOI: [10.1002/ejoc.202401411](https://doi.org/10.1002/ejoc.202401411)

- **Medicinally Significant Enantiopure Compounds from Garcinia Acid Isolated from *Garcinia gummi-gutta***

Simimole Haleema*, Chithra Gopinath, Zabeera Kallingathodi, Grace Thomas and Prasad L. Polavarapu*, *Symmetry* **2024**, 16(10), 1331.
DOI: [10.3390/sym16101331](https://doi.org/10.3390/sym16101331) (Invited Article)

- **Graphene Quantum Dots Derived from Honey and Mangostin as Sustainable Materials to Construct Fluorescence Turn-On Molecular Switches for Pesticide Detection**

Chandranpillai Lalithabai Lekshmi, Unnikrishnapillai Saraswathy Swathy, Keerthi Vijayan, **Haleema Simimole**, and Sarojiniamma Sumalekshmy*, *ChemistrySelect*, **2023**, 8, e202204869 1-5
DOI: [10.1002/slct.202204869](https://doi.org/10.1002/slct.202204869)

- **Review on Synthetic and Pharmacological Potential of Compounds Isolated from *Garcinia mangostana* Linn**

Swathy Unnikrishna Pillai Saraswathy, Lekshmi Chandran Pillai Lalitha, Sherifa Rahim, Chithra Gopinath, **Simimole Haleema***, Sumalekshmy Sarojini Amma*, Hassan Y. Aboul-Enein*, *Phytomedicine Plus*, **2022**, 2, 100253.
DOI: [10.1016/j.phyplu.2022.100253](https://doi.org/10.1016/j.phyplu.2022.100253)

- **How important are the intermolecular hydrogen bonding interactions in methanol solvent for interpreting the chiroptical properties?**

Prasad L. Polavarapu, Ernesto Santoro, Cody L. Covington, Jordan L. Johnson, Andrew R. Puente, Nathan D. Schley, Zabeera Kallingathodi, Prasanth C. Prakasan, **Simimole Haleema**, Annu Anna Thomas, Ibrahim Ibnusaud, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 247, 119094.
DOI: [10.1016/j.saa.2020.119094](https://doi.org/10.1016/j.saa.2020.119094)

- **Natural Product-Derived Chiral Pyrrolidine-2,5-diones, Their Molecular Structures and Conversion to Pharmacologically Important Skeletons**

DeenammaHabel, Divya S. Nair, ZabeeraKallingathodi, Chithra Mohan, Sarath M. Pillai, Rani R. Nair, Grace Thomas, **Simimole Haleema**, ChithraGopinath, Rinshad V., Abdul,Matthew Fritz, Andrew R. Puente, Jordan L. Johnson, Prasad L. Polavarapu, and Ibrahim Ibnusaud, *Journal of Natural Products (ACS)*, **2020**, 83, 2178.

DOI: [10.1021/acs.jnatprod.0c00211](https://doi.org/10.1021/acs.jnatprod.0c00211)

- **A highly sensitive GC–MS method for simultaneous determination of anacardic acids in cashew (Anacardiumoccidentale) nut shell oil in the presence of other phenolic lipid derivatives.**

Osman, S. M., Abdel-Megied, A. M., Zain Eldain, M. H., **Simimole, H.**, Gopinath, C., Sumalekshmy, S., and Aboul-Enein, H. Y., *Biomedical Chromatography*, **2019**, 33, e4659

DOI: [10.1002/bmc.4659](https://doi.org/10.1002/bmc.4659)

- **Capillary zone electrophoresis for the analysis of naturally occurring 2-hydroxycitric acids and their lactones**

Abhijith, B. L., Moolya Mohan, David Joseph, **Simimole Haleema**, Hassan Y. Aboul-Enein, Ibrahim Ibnusaud, *Journal of Separation Science*, **2017**, 40, 3351.

DOI: [10.1002/jssc.201700192](https://doi.org/10.1002/jssc.201700192)

- **Enantiomerically pure compounds related to chiral hydroxy acids derived from renewable resources**

Simimole H., Sasi, P. V.,Ibnusaud, I.,Polavarapu, P. L., Kagan, H. B. *RSC Advances*. **2012**, 2, 9257.

DOI: [10.1039/c2ra21205f](https://doi.org/10.1039/c2ra21205f)

- **Importance of solvation in understanding the chiroptical spectra of natural products in solution phase: Garcinia acid dimethyl ester**

Prasad L. Polavarapu, Giovanni Scalmani, Edward K. Hawkins, Carnelo Rizzo, Neha Jeirath, Ibrahim Ibnusaud. DeenammaHabel,DivyaSadasivan Nair, and **Simimole H.**, *Journal of Natural Products (ACS)*. **2011**, 74, 321.

DOI: [10.1021/np100512w](https://doi.org/10.1021/np100512w)

- **Synthesis of enantiopure concave(+)-avenaciolide and (-)- canadensolide skeletons**

Susan Varghese, Salini Thomas, **Simimole H.**,Tom Thomas Puthiarambil, and Ibrahim Ibnusaud, *Tetrahedron Letters*, **2007**, 48, 8209.

DOI: [10.1016/j.tetlet.2007.09.081](https://doi.org/10.1016/j.tetlet.2007.09.081)

Patents

- **An Improved Method for The Large-Scale Isolation of Garcinia Acid**
Simimole Haleema, Grace Thomas, Chithra Gopinath, Rani R. Nair
Patent No: 202441059956
Filed 08/08/2024
Published on 09/05/2025

Meetings/Workshops/Seminars Organized

1. Co-convener of the International Seminar on Tropical Plants and Molecular Design, held in February 2017, organized by the Post Graduate and Research Department of Chemistry, TKM College of Arts and Science.
2. Convened an international level Distinguished Chemistry Lecture on “Separation Techniques in Chemistry “on 2018 organized by the Post Graduate and Research Department of Chemistry, TKM College of Arts and Science
3. Resource Person for SASTHRA PADHAM, a science promotion program for high school students, organized in January 2019 by Samagra Shiksha Kerala, the Directorate of Collegiate Education, and the Department of Higher Secondary Education hosted at TKM College of Arts and Science.
4. Resource Person for SASTHRA JAALAKAM, a science promotion program for high school students, conducted by the Government of Kerala (Higher Secondary Education) hosted at TKM College of Arts and Science.

Awards/Recognition/Fellowship from State/National/Government-Recognized Body

- Received the Best Poster Award presented by the Royal Society of Chemistry at the International Seminar on ‘Tropical Plants and Molecular Design’, organized by T.K.M. College of Arts and Science on 14th and 15th February 2017

Guideship

- Research Guide: University of Kerala, Centre-T. K. M. College of Arts and Science, Kollam

Dissertations guided

- M. Sc- 10
- B. Sc- 33

Mentor of Funded Student Project

Title of the Project	Funding Agency	Amount	Period
Synthetic modification and photophysical studies of water soluble xanthone based fluorescent molecules derived from naturally occurring α -mangostin	KSCSTE(Student Project Completed)	Rs.10,000/-	2018