Faculty Profile

Dr. P. Kumaradhas, M.Sc., M.Phil., Ph.D.
Professor & Associate Dean of Research
Department of Physics

HIGHLIGHTS:

- Number of Journal Publications: **140**
- H-Index: **25**
- i10 index: 70

PROFESSIONAL LINKS:

- Scopus ID: 6602140501
- Scopus Link: https://www.scopus.com/authid/detail.uri?authorId=6602140501&source=sd-apx&adobe_mc=MCMID%3D27827389968727922241500758856585675114%7CMCORGID%3D4D6368F454EC41940A4C98A6%2540AdobeOrg%7CTS%3D1780128414
- Google Scholar ID: https://scholar.google.com/citations?user=LOMJJaoAAAAJ&hl=en
- ORCID No: 0000-0001-6322-1909 (https://orcid.org/0000-0001-6322-1909)
- AICTE Faculty ID: 1-44967536332

PROFESSIONAL BACKGROUND:

- Teaching Experience till date : 21 years 7 months
- Research Experience : 23 years 5 months
- No. of Ph.D produced: 17
- No. of M.Phil projects Guided: 45
- No. of M.Sc Projects Guided : 60

AREA OF SPECIALIZATION:

- X-ray and Quantum Crystallography
- Charge Density
- Quantum Chemical Calculations
- Molecular Modelling and Molecular dynamics simulation

ACHIEVEMENTS AND AWARDS:

Fellowships

- Post-Doctoral Research at University of Texas, Houston, **USA**, 2002.
- Post-Doctoral Research at University of Toledo, Ohio, **USA**, 2000-2002.
- Post-Doctoral Research at University of Witwatersrand, Johannesburg, **SOUTH AFRICA** 1999-2000.
- Post-Doctoral Research at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, **INDIA**, 1997-1999.

Received Awards:

- International Union of Crystallography (IUCR), Travel Grant Young Scientist award for the year 1998.
- Prestigious Post-Doctoral Fellowship, University of Witwatersrand, South Africa, 1999.
- Life time Achievement Award by Indian Spectroscopic Association (ISPA), 2022.

LIST OF INSTRUMENT/COMPUTERS HANDLING

- Bruker-Single Crystal X-ray Diffratometer
- Low-temperature Cooling system
- High-performance Cluster Computing (HPC)

PROFESSIONAL MEMBERSHIPS:

- Member in International Union of Crystallography
- Member of Indian Crystallographic Association
- Member of High energy materials society

CONFERENCES/SEMINARS/WORKSHOPS ORGANIZED:

No. of Programme Organized: 30

SELECTED PUBLICATIONS

1. Exploring the interplay of electron density distribution and electrostatic potential in the interaction of nilutamide and flutamide with androgen receptor using quantum crystallography, Hemalatha Balasubramanian, **Kumaradhas Poomani*** Saravanan Kandasamy, Venkatesha R Hatwar and Rajesh G. Gonnade. *RSC Adv.*, (2026), 16, 3830-3849.

2. Topological Electron Density Analysis and Electrostatic Properties of Aspirin: An Experimental and Theoretical Study, A. David Stephen, Venkatesha R. Hathwar, Tayur N. Guru Row and **P. Kumaradhas*,** *Cryst. Growth. Des, 12, 4357-4366,(2012).*

   (Appeared in Cover Page)

3. Iruthayaraj, A, Kalaiarasi. C,, Kunal Kumar. J, Parthapratim. M, Pavan. M.S, & Kumaradhas. P. Topology of electron density and electrostatic potential of HIV reverse transcriptase inhibitor zidovudine from high resolution X-ray diffraction and charge density analysis. *J. Mol. Struct.* 1180, 683–697, (2019).

4. Rajalakshmi, G., Hathwar, V. R. & Kumaradhas, P. Topological analysis of electron density and the electrostatic properties of isoniazid: An experimental and theoretical study. *Acta Crystallogr.* B70, 331–341, (2014). (**Appeared in Cover Page**)

5. Zhurova, E. A., Zhurov, V. V., Kumaradhas, P., Cenedese, S. & Alan Pinkerton, A. Charge Density and Electrostatic Potential Study of 16α,17β-Estriol and the Binding of Estrogen Molecules to the Estrogen Receptors ERα and ERβ. *Journal of Physical Chemistry B* 120, 8882–8891, (2016).

6. Understanding the N-N bond cleavage and the electrostatic properties of isoniazid drug molecule via theoretical charge density study. Gnanasekaran Rajalakshmi, Balu Devipriya, Azhagesan Renuga Parameshwari, Arputharaj David Stephen, **Poomani Kumaradhas**. *Comput. and Theo. Chem. 966, 259-264, (2011).*

7. Identification of novel flavonoid inhibitor of Catechol-O-Methyltransferase enzyme by molecular screening, quantum mechanics/molecular mechanics and molecular dynamics simulations. Hunday Govindasamy, Sivanandam Magudeeswaran and **Kumaradhas Poomani,** Journal of Biomolecular structure and Dynamics. 38, 5307-5319, (2020).

8. Design and Molecular dynamic Investigations of 7, 8-Dihydroxyflavone Derivatives as Potential Neuroprotective Agents Against Alpha-synuclein, Thangavel Mohankumar, Vivek Chandramohan, Haralur Shankaraiah Lalithamba, Richard L Jayaraj, **Poomani Kumaradhas**, Magudeeswaran Sivanandam, Govindasamy Hunday, Rajendran Vijayakumar, Rangasamy Balakrishnan, Dharmar Manimaran, Namasivayam Elangovan, ***Scientific reports, 599, (2020). (Nature's)***

9. Combined quantum mechanics/molecular mechanics (QM/MM) methods to understand the charge density distribution of estrogens in the active site of estrogen receptors C Kalaiarasi, S Manjula, **P Kumaradhas*,** *RSC Advances 9 (69), 40758-40771, (2019).*

10. Investigation of bond topological and electrostatic properties of plumbagin molecule: An experimental and theoretical charge density study, C Kalaiarasi, M Sivanandam, S Suganya, G Christy, RG Gonnade, Venkatesha R Hathwar, **Poomani Kumaradhas*,** *Journal of Molecular Structure 1220, 128714, (2020).*

Invited Lectures:

On invitation delivered several lectures in seminars, conferences and workshops (some of them are listed here)

1. International High energy material conference and Exhibit, TBRL, Chandigarh, India.
2. National conference on Biomolecular structure and Function, Department of Science and Humanities, V. V college of Engineering, Tisaiyanvilai.
3. International conference on Biological Inorganic Chemistry, ICBIC, Department of Chemistry, Periyar University, Salem.
4. Seminar on materials for Advanced Technology, Department of Physics, Periyar University, Salem- 11.
5. Inaguaration of Physics association, Department of Physics, Adhiyaman arts and Science College for Women, Uthengarai.
6. UGC Sponsored National Seminar On Recent trends in X-ray Crystallography, Seethalakshmi Ramaswamy College. Tiruchirapalli.
7. Workshop on Development in X-ray Crystallography, MG University, Kottayam, Kerala.
8. National Seminar on Current trends in Chemistry, APC Mahalaxmi College for Women, Thoothukudi.
9. Young Student Scientist Programme (YSSP)-MAY2015, Kandaswami Kandar's College, Velur, Nammakkal. C-DAC GARUDA NKN Partners Meet, held at NIAS Auditorium, IISc Campus, Bangalore.
10. Workshop on Advanced Materials for Societal Applications, held at Periyar University Centre for Post Graduate and Research Studies, Dharmapuri.

(Many more lectures delivered)

Projects:

Received projects from the funding agencies **UGC, DRDO and TANSCHE: Rs. 68 Lakhs**

DST-FIST2018: Rs.1.63 Crore

Total Amount mobilized: **Rs. 2.31 Crore**

University Projects:

Establishment of Electrical Power: ~ **1 Crore**
Solar Power Plant (300KVA) : ~ **2 Crore**
Establishment of Centre for Instrumentation & Maintenance Facility (CIMF) in Periyar University: **32.5 Lakhs**
Establishment of Instrumentation Facility from RUSA fund in CIMF of Periyar University: **3 Crore**