



## Dr. Mahendra M., Ph.D., UGC Raman Fellow

### Personal Information

**Name** : Mahendra Madegowda

**Official Address** : Professor, Department of Studies in Physics,  
Manasagangotri, University of Mysore, Mysuru, Karnataka,  
570 006, India.

**Telephone** : +91-821-2419603 (office)  
+91-9964330328 (Mob.)

**E-mail** : mahendra@physics.uni-mysore.ac.in  
mahendrashiri@gmail.com

### Academic Profile

Bachelor of Science (1997) - University of Mysore, Mysuru, India.  
Master of Science in Physics (1999) - University of Mysore, Mysuru, India.  
PG Diploma in Software Development (2002) - University of Mysore, Mysuru, India.  
Ph.D. in Physics (2005) - University of Mysore, Mysuru, India

### Work Experience Details

Position	Institute	Duration
Director and Professor	University-Industry Interaction Centre, University of Mysore, Manasagangotri	2025 to Present
Professor	DoS in Physics, University of Mysore, Manasagangotri	2022 to Present
Associate Professor	DoS in Physics, University of Mysore, Manasagangotri	2019 to 2022
Assistant Professor	DoS in Physics, University of Mysore, Manasagangotri	2007 to 2019
UGC Raman Post-Doctoral Fellow	Department of Cellular Biology and Pharmacology, Herbert Wertheim College of Medicine, Florida International University, Miami, USA	2014 to 2015
Post-Doctoral Research Associate	Biology Department, Brookhaven National Laboratory, Upton, New York, USA	2005 to 2007

CSIR Senior Research Fellow	DoS in Physics, University of Mysore, Manasagangotri	2004 to 2005
Ph.D. Research Scholar	DoS in Physics, University of Mysore, Manasagangotri	2000 to 2004
Research Assistant	JNCASR, Theoretical Sciences Unit, Bangalore	2000

#### Academic Affiliations/Awards

- **CSIR Senior Research Fellow Award**, Government of India (2004)
- **Post-Doctoral Fellow**, Brookhaven National Laboratory , Upton, NY, USA (2005-07)
- **UGC Raman Post-Doctoral Fellow**, Florida International University, Miami, FL, USA (2014-2015)
- **Life member**, Indian Crystallographic Association
- **Life member**, Indian Science Congress Association
- **Member**, American Crystallographic Association
- **Member**, New York Structural Genomics Consortium (NYSGXRC)
- **Member**, International Structural Genomics Organization (ISGO)

#### Research Projects:

Sl. No.	Title of the project	Principal/Co-Investigator	Funding Agency	Amount	Year (From-To)
1.	Organic Chromophores with Nonlinear Optical Properties for Opto-electronic and Sensing Applications	Principal Investigator	K-FIST-L2, VGST	30 Lakhs	2024-Present
2.	Synthesis, growth and characterization of Chalcone based nonlinear optical materials	Principal Investigator	Minor Research Project, University of Mysore	75,000/-	2018-2019
3.	Structural studies of storage protein from the tuber of <i>amorphophalluspaeoniifolius</i> (Letter No. F. No. 41-920/2012(SR), Dated: 25-07-2012)	Principal Investigator	UGC, New Delhi	13,23,800/-	2012-2015
4.	Molecular Docking and Crystallographic studies of Aminoglycoside N-acetyl transferases	Principal Investigator	Start Up Grant, University of Mysore	1 Lakh	2009-2011

#### Ph. D Candidates Currently Working/Finished:

Sl.No	Name of candidate	Subject	Thesis work	Status
1.	Mr. Chandra	Physics	Structure and Molecular Docking Studies of Some Biologically Important Compounds	Completed
2.	Mr. Nasseem Ahamad muhsen el-khatatneh	Physics	Crystal and Molecular Structure Studies of Some Medicinally Heterocyclic Compounds.	Completed
3.	Ms. Vishalakshi G. J.	Biophysics	Exploring the Toxic Effects of Selected Phenolics on Platelets and Erythrocytes	Completed
4	Mr. Hussien Ahmed Hussien Khamees	Physics	Structural analysis and DFT studies of some biologically important compounds	Completed
5.	Mr. Ananda S.	Physics	Studies on the Growth and Characterization of Some Nonlinear Optical Materials	Completed
6.	Ms. Bhavya N.R.	Physics	Computational and Experimental Investigations on Some Fluorescent Materials	Completed
7.	Mr. Omantheswara N.	Physics	Structural Investigations and Computational Studies of Therapeutically Important Compounds	Pursuing
8.	Mr. Keerthikumara V.	Physics	Experimental and Computational Investigations of Technologically Important Nonlinear Optical Materials	Pursuing
9.	Mr. Keshav Kumar H.	Physics	Structural and Computational Insights of Biologically Significant Ligands	Pursuing
10.	Mr. Chethan V.	Physics	First Principles Investigation on Physical and Chemical Properties of Some Technologically Important Nano Materials	Pursuing
11.	Mr. Bhanu Prakash M.	Physics	-	Enrolled

12.	Ms. Kavya B.R.	Physics	-	Enrolled
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#### Protein Structures Repository:

- Crystal structure of the human phosphatase (DUSP9). **PDB CODE: 2HXP**
- Crystal structure of Hemolysin binding component from *Bacillus cereus*. **PDB CODE: 2NRJ**
- Crystal structure of a putative HTH-type transcriptional regulator ytcD. **PDB CODE: 2HZT**
- Crystal structure of hypothetical protein TM1727 from *Thermatogamaritima*. **PDB CODE: 2I76**
- Crystal structure of YokD protein from *Bacillus subtilis*. **PDB CODE: 2NYG**
- Crystal structure of T110839 protein from *Synechococcus elongatus*. **PDB CODE: 2PLG**
- Crystal structure of CDP-diacylglycerolpyrophosphatase. **PDB CODE: 2POF**
- Crystal structure of mandelate racemase/muconatelactonizing enzyme-like protein from *Rubrobacter xylophilus* DSM 9941. **PDB CODE: 2QQ6**
- Crystal structure of the Mn (II)-bound glyoxalase from *Novosphingobium aromaticivorans*. **PDB CODE: 3B59**
- Crystal structure of an uncharacterized protein from *Listeria monocytogenes*, trigonal form. **PDB CODE: 3BQS**
- Crystal structure of a protein of unknown function from *Listeria monocytogenes*, tetragonal form. **PDB CODE: 3BQT**
- Crystal structure of a protein of unknown function from *Listeria monocytogenes*, triclinic form. **PDB CODE: 3BQS**
- Crystal structure of a putative lactoylglutathionelyase from *Bdellovibrio bacteriovorus*. **PDB CODE: 3G12**
- Crystal Structure of the complex formed between group II phospholipase A2 and a plant alkaloid ajmaline at 2.0 Å resolution. **PDB CODE: 1ZR8**

#### PUBLICATIONS

##### 2025

1. Development of novel pyrimidine-thio-triazoles targeting EGFR in breast Cancer cells via one-pot copper-catalyzed 1,3-dipolar cycloaddition Bhanuprakash C. N., Akshay R, Baburajeev C. P., Narasimha M. B., Shreeja B, Divakar V., Rangappa K. S., Omantheswara N., Mahendra M., Chandrashekara P. G. and Basappa. *Results in Chemistry*, (2025), 14, 102150

2. In-silico studies of 3-tert-butyl-7-[2-phenyl ethenyl]-4H-[1,3,4]thiadiazolo [2,3-c][1,2,4] triazin-4-one as a Potential SARS-CoV-2 Inhibitor: Insights from an experimental and computational approach: Chandra, Lohith T. N., Shamantha Kumar., Gayathri B. H., Divya K., Sridhar M. A., Mehran Feizi-Dehnayebi, Mahendra M., Karthik V., and Ghodsi Mohammadi Ziarani. *Journal of Molecular Structure*. (2025), 1330, 141356.
3. Crystal structure, hirshfeld surface and computational nonlinear optical studies of isonicotinohydrazide derivative: Keerthikumara V., Ananda S., Prashanth K N., and Mahendra M. *AIP Conference Proceedings*, (2025), 3198, 020072.
4. Exploration of electronic and optical properties of chalcogenide perovskite materials AHfS3 (A= Ba, Sr) for light-emitting semiconductors: First-principles study: Chethan V., Sujith C P., and Mahendra M. *AIP Conference Proceedings*, (2025), 3198, 020070.
5. Optimizing Adamantane Derivatives for Enhanced EGFR Inhibition in MCF-7 Breast Cancer Cells: Pradeep M., Keshav Kumar H., Narasimha M B., Zhang Xi, Chaithanya S., Mahendra M., Mamatha S K., Sindhu M P., Peter E Lobie, Rangappa K S., Vijay P., Basappa. *Journal of Molecular Structure*, (2025), 1331, 141554.
6. The pivotal role of the carbonyl group in methoxy chalcones: comprehensive analyses of the structure and computational insights into binding affinity towards monoamine oxidase enzymes: Keshav Kumar H., Hussien A. K., Keerthikumara V., Omantheswara N., and Mahendra M. *Molecular Systems Design & Engineering* (2025).
7. Physicochemical properties of thiazole-based NLO crystal: An efficient material for optoelectronic applications: Keerthikumara V., Sheela K., Mahesh S. S., Ananda S., Mahendra M., Tejaswi Ashok Hegde., and Sadashiva M. P. *Journal of Molecular Structure*, (2025), 1319, 139459.

## 2024

8. Probing the hybridized triazole-chalcones: an in-depth investigations of molecular structure journey towards antibacterial potential against DNA gyrase: Keshav Kumar H., K., Vinutha K., Omantheswara N., Bhavya N. R., Rajeena C. A., and Mahendra M. *Journal of Biomolecular Structure and Dynamics*, (2024), 1-30.
9. Eco-Friendly Mercury Ion Detection and Removal in Water Using Anthocyanins: Mechanistic Insights through DFT Methods: Mane P. V., Mahishi A., Bhat M. P., Lee K. H., Ananda S., Mahendra M., and Mahaveer K. *Journal of Environmental Chemical Engineering*, (2024), 115288.

10. Synthesis of Tetrahydrocarbazole-Tethered Triazoles as Compounds Targeting Telomerase in Human Breast Cancer Cells: Uppar P. M., Ravish A., Xi Z., Keshav Kumar H, Kumar A. M., Poonacha L. K., and Mahendra M. *Catalysts*, (2024), 14, 726.
11. Isoxazole based nucleosides induce autophagy through the production of ROS and the suppression of the  $\beta$ -catenin pathway in human colorectal carcinoma cells: Kim N. Y., Vishwanath D., Basappa, Keshav Kumar Harish H, Mahendra M, Rangappa K. S., and Ahn K. S. *Chemico-Biological Interactions*, (2024), 111285.
12. Optical limiting and third-order nonlinear optical properties of thiazole-based chalcone derivative: Insights from experimental and theoretical approaches: Keerthikumara V., Mahesh S. S., Ananda S., Mahendra M., Ravi Singh K., Tejaswi A. H., and Sadashiva M. P. *Optical materials*, (2024), 157, 116068.
13. Pyrimidine–triazole-tethered tert-butyl-piperazinecarboxylate suppresses breast cancer by targeting estrogen receptor signaling and  $\beta$ -catenin activation: Jie Y., Li Yang, Zhi L., Zhang H., Qun W., Wang B., Arunachalam C., Chandramohan G., Shreeja B., Omantheswara N., Mahendra M., Narasimha M. B., Vladimir N. N., Minghua W., Wang G., Rangappa K. S., and Basappa. *IUBMB life*, (2024), 39275910.
14. Oxazine drug-seed induces paraptosis and apoptosis through reactive oxygen species/JNK pathway in human breast cancer cells: Na Young Kim, Dukany D., Gautam S., Swamy S. G., Omantheswara N., Ananda S., Divakar V., Keerthikumara V., Shreeja B., Arunachalam C., Mahendra M., Alexey S., Vijay P., Kwang S. A., and Basappa. *Translational Oncology*, (2024), 49, 1-20.
15. Ab initio Investigation of quasi-one-dimensional ternary chalcogenides  $\text{Sr}_2\text{ZnX}_3$  (X = S, Se, Te) for efficient photovoltaic and thermoelectric applications: Chethan V., and Mahendra M. *Journal of Physics and Chemistry of Solids*, (2024), 194, 112222.
16. Discovery of oxazine-linked pyridine as an inhibitor of breast cancer growth and metastasis by abrogating NF-KB activation: Jie Yuan, Bhanuprakash C. N., Akshay R., Li Yang, Hua Zhang, Qun Wang, Zhi Li, Keshav Kumar H., Arunachalam C., Chandramohan G., Mahendra M., and Basappa. *Oncology*, (2024), 14, 1-13.
17. A novel drug prejudice scaffold-imidazopyridine-conjugate can promote cell death in a colorectal cancer model by binding to  $\beta$ -catenin and suppressing the Wnt signaling pathway: Min Hee Yang, Basappa, Suresha N. D., Akshay R., Arunkumar M., Omantheswara N., Mahendra M., Rangappa K. S., Amudha D., and Vijay P. *Journal of Advanced Research* (2024), 1232(24), 39067696.

18. A new thiadiazole-triazine derivative: structural investigation, DFT studies, ADME-T analysis and SARS-CoV-2 activity by docking simulation: Lohith T. N., Gayathri B. H., Shamantha Kumar, Shivaprasad C. M., Divya K., Sridhar M. A., and Mahendra M. *Journal of Molecular Structure*, (2024), 1317, 139133.
19. Development of Novel Pyridine and Pyrimidine Clubbed Bisindoles as Inhibitors of AKT Pathway: Lisha K. P., Prashant K. M., Akshay R., Omantheswara N., Arun M. Kumar, Nanjunda S. S., Mahendra M., Peter E. L., and Vijay Pandey. *ChemistrySelect*, (2024), **9**(27), 1-11.
20. Thiouracil and triazole conjugate induces autophagy through the downregulation of Wnt/ $\beta$ -catenin signaling pathway in human breast cancer cells: Bada Yoon, Basappa, Shreeja B., Omantheswara N., Mahendra M., Rangappa K. S., Gautam S., and Kwang S. A. *IUBMB Life*, (2024), 76, 1-15.
21. Synthesis, crystal structure, Hirshfeld, DFT, molecular docking, dynamics studies, and anti-cancer activity of 1-substituted-2-(4-(diethylamino)-2-hydroxyphenyl)-1H-benzo[d]imidazole-5-ethyl carboxylates: Ganavi D., Vasantha Kumar, Akhileshwari P., Ashwini Prabhu, Omantheswara N., Mahendra M., and Boja Poojary. *Journal of Molecular Structure*, (2024), 1314, 138657.
22. A simple fluorescent "Turn-Off" Schiff base sensor for Cu<sup>2+</sup> and Fe<sup>2+</sup> ions and its applications in real water sample analysis and logic gate construction: Jyothi Priya M, Revanasiddappa H.D., Jayalakshmi B., Ananda S., Mahendra M., Muzaffar Iqbal, Chandan S, and Shiva Prasad K. *Polyhedron*, (2024), 260, 117110.
23. Emphasized DFT, DNA binding, and electrochemical studies of hybrid 1, 3, 4-thiadiazole-linked chalcone confined via a sulfur bridge: Kamat V., Bhavya N. R., Poojary B., Patil V. B., Ramesh G., and Mahendra M. *Journal of Chemical Sciences*, (2024), 136(2), 1-11.
24. Crystal structure, molecular mechanics and *In silico* analyses of piperazine derivative against human mammary carcinoma cells inhibition: Keshav Kumar H., Ananda S., Dukanya, Keerthikumara V, Basappa, Mahendra M. *IOP Conf. Ser.: Mater. Sci. Eng.*, (2024), 1300, 012007.
25. Imidazole-centred cupric ions sensor: Experimental validation, theoretical understanding, and zebrafish bioimaging: Keshav Kumar H., Aravind R.N., Naveen Kumar K., Praveen Naik, Mahendra M., Anup P., Kholood A.D., Saikh Mohammad, Shivarudrappa H.P., Sharanakumar T.M., Guddappa H. *Journal of Photochemistry and Photobiology A: Chemistry*, (2024), 452, 115565.

26. Molecular and Biomolecular Spectroscopy Chalcone-based Turn-Off Chemosensor for Selective and Susceptible Detection of Fe<sup>2+</sup> ions: Spectroscopic and DFT Investigations: Bhavya N.R., Ananda S., Keshav Kumar H., Keerthikumara V. and Mahendra M. *Journal of Fluorescence*, (2024), 1-15.
27. Computational and experimental studies of nonlinear optical properties of acetohydrazide derivative: Ananda S., Keerthikumara V., Bhavya N.R., Harshitha H.N., Pooja S., Rudresh K., Rajendra Kumar and Mahendra M. *AIP Conference Proceedings*, (2024), 2995, 020098.
28. Structural, DFT and nonlinear optical studies of hemihydrate thiadiazole derivative: Ananda S., Keerthikumara V., Keshav Kumar H., Chethan V., Pooja S., Rudresh K., Rajendra Kumar, Mahendra M. *AIP Conference Proceedings*, (2024), 2995, 020061.

## 2023

29. The quest for optimal photovoltaics: A theoretical exploration of quasi-one-dimensional tin-based chalcogenides XSnS<sub>3</sub> (X= Ba, Sr): Chethan V., Sujith C.P., Thomas Mathew, and Mahendra M. *Materials Today Communications*, (2023), 37, 107501.
30. Highly selective and sensitive fluorescent “TURN-ON” furan-based Schiff base for zinc (ii) ion probing: chemical synthesis, DFT studies, and X-ray crystal structure: Divyashree N.R., Revanasiddappa H.D., Yathirajan H.S., Bhavya N.R., Mahendra M., Iqbal M., Shivamallu C., Amachawadi R.G. and Kollur S.P. *New Journal of Chemistry*, (2023), 37, 17420-17433.
31. Methyl-Thiol-Bridged Oxadiazole and Triazole Heterocycles as Inhibitors of NF-κB in Chronic Myelogenous Leukemia Cells: Basappa, Young Y. J., Akshay R., Zhang Xi, Ananda S., Mahendra M., Vijay P., Peter E L., Gautam S., Kwang S. A. *Biomedicines*, (2023), 11, 1662.
32. Third-order nonlinear response of a novel organic acetohydrazide derivative: Experimental and theoretical approach: Ananda S., Keerthikumara V., Keshav Kumar H., Bhavya N. R., Chethan V., Mahendra M., and Tejaswi Ashok Hegde. *Optical Materials*, (2023), 139, 113826.
33. Discovery of Pyrimidine- and Coumarin-Linked Hybrid Molecules as Inducers of JNK Phosphorylation through ROS Generation in Breast Cancer Cells: Kim, Na Young, Divakar V., Zhang Xi, Omantheswara N., Ananda S., Keshav Kumar H., Shreeja B., Mahendra M.,

- Vijay Pandey, Gautam Sethi, Peter E. Lobie, Kwang Seok Ahn, and Basappa. *Molecules*, (2023), 28(8), 3450.
34. Azaneylylidene-based Tetradentate Schiff base as a new "ON-OFF" Fluorescent Probe for the Detection of Cu (II) Ion: Synthesis, Characterization and Real Sample Analysis: Divyashree N.R., Revanasiddappa H.D., Bhavya N.R., Mahendra M., Jayalakshmi B., Shivamallu C., and Kollur S.P. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, (2023), 292.
  35. De Novo Design of Imidazopyridine-Tethered Pyrazolines That Target Phosphorylation of STAT3 in Human Breast Cancer Cells: Akshay R., Rashmi S., Zhang Xi, Min H. Y., Ji-Rui Y., Ananda S., Omantheswara N., Mahendra M., Arunachalam C., Sulaiman A. A., Vijay P., Gautam S., Kwang S. A., Peter E. L., and Basappa. *Bioengineering*, (2023), 10(2).
  36. Nano-ZrO<sub>2</sub>-Catalyzed Biginelli Reaction and the Synthesis of Bioactive Dihydropyrimidinones That Targets PPAR-γ in Human Breast Cancer Cells: Suresha N. D., Ji-Rui Yang, Zhang Xi, Omantheswara N., Kashifa F. R., Bhanuprakash C. N., Gautam S., Ganga P., Mahendra M., Shobith R., Vijay P., Peter E. L., Basappa. *Catalysts*, (2023), 13(8), 228, 1-17.
  37. Nano-Zirconium Dioxide Catalyzed Multicomponent Synthesis of Bioactive Pyranopyrazoles That Target Cyclin Dependent Kinase 1 in Human Breast Cancer Cells: Basappa, Lisha K. P., Zhang Xi, Divakar V., Ji-Rui Yang, Omantheswara N., Ananda S., Mahendra M., Arunachalam C., Sulaiman Ali A., Doddahosuru M. G., Vijay Pandey, Nanjundaswamy S., Kwang S. A., Gautam S., Peter E. L., and Priya B. S. *Biomedicines*, (2023), 11(1), 172.
  38. One-pot reproducible Sonosynthesis of trans-[Br(NNN')Cu(μBr)<sub>2</sub>Cu(NNN')Br] dimer: [H....BrS (9)] synthons, spectral, DFT/XRD/HSA, thermal, docking and novel LOX/COX enzyme inhibition: AlAli, Anas, Hussien Ahmed Khamees, Mahendra M., Abdelkader Z., Karthik K., Nasseem El-khatatneh, Ismail Warad, and Shaukath Ara Khanum. *Journal of Molecular Structure*, (2023), 1275.
  39. Studies on New Imidazo[2,1-b][1,3,4] thiadiazole Derivatives: Molecular Structure, Quantum Chemical Computational, and In silico Study of Inhibitory Activity Against Pim-1 Protein by Using Molecular Modelling Methods and ADMET Profiling: Hussien Ahmed Khameesa. Mahesh S.S., Omantheswara N., Mahendra M., Vindu Vahini M., Kumara C.,

Jagadeesh Prasad D. and Ismail Warade. *Journal of Molecular Structure*, (2022), 1272, 134161

## 2022

40. Third-order nonlinear optical studies of Bis (4-methylbenzylammonium) tetrachloridocuprate metal-organic crystal with optical limiting behaviour: Experimental and Theoretical Investigations: Ananda S., Mahesh S. S., Vindu Vahini, Hussien Ahmed Khamees, Mahendra M., Vinayakprasanna N Hegde, Tejaswi Ashok Hegde, Vinitha G. *Journal of Molecular Structure*, (2022), 1269, 133827
41. Development of 1-(4-(Substituted)piperazin-1-yl)-2-((2-((4-methoxybenzyl)thio)pyrimidin-4-yl)oxy)ethanones That Target Poly (ADP-Ribose) Polymerase in Human Breast Cancer Cells: Suresha N.D., Prashant K.M., Rashmi S., Ji-Rui Y., Shobith R., Ananda S., Muthu K.S., Omantheswara N., Mahendra M., Priya B.S., Arunachalam C., Sulaiman A.A., Vijay P., Kwang S.A., Peter E.L. and Basappa. *Molecules*, (2022), 27, 1-19
42. A Novel Schiff Base Derivative as a Fluorescent Probe for Selective Detection of Cu<sup>2+</sup> ions in buffered solution at pH 7.5: Experimental and Quantum Chemical Calculations: Bhavya N. R., Mahendra M., Javarappa R. and Nagaraja Naik. *Journal of Molecular Structure*, (2022), 1254, 132327

## 2021

43. Dithiane Based Boronic Acid as a Carbohydrate Sensor in an Aqueous Solution at pH 7.5: Theoretical and Experimental Approach: Bhavya N.R. and Mahendra M. *Journal of Fluorescence*, (2021), 31, 1683-1703
44. Investigation of NPB Analogs That Target Phosphorylation of BAD-Ser99 in Human Mammary Carcinoma Cells: Swamy S.G., Dukanya, Ananda S., Divya M.G., Mahendra M., Ganga P., Rangappa K.S., Vijay P., Peter E. L. and Basappa. *International Journal of Molecular Sciences*, (2021), 22, 1-16
45. Synthesis, Molecular Structure, DFT Studies, *In silico* Docking and Molecular Dynamics Simulations of 2, 6 dimethoxychalcone Derivatives as BRD4 Inhibitors: Hussien A. K., Mahendra M., Ananda S., Sangappa Y., Fares H. Al-Ostoot and Nadeem Abad. *Journal of Molecular Structure*, (2021), 1245, 131032

46. Synthesis, crystal structure, DFT calculations, Hirshfeld surface analysis, energy frameworks, molecular dynamics and docking studies of novel isoxazolequinoxaline derivative (IZQ) as anti-cancer drug: Nadeem A., Hamdi H. S., Fares H. Al-Ostoot, Hussien A. K., Sultan A. Al-horaibi, Shaukath A. K., Mahendra M., Mohamed El H., Joel T. M., El Mokhtar E. and Youssef R. *Journal of Molecular Structure*, (2021), 1232, 130004
  
47. Structural, thermal, dielectric, nonlinear optical properties and DFT investigations of a novel material 2-(6-chloropyridin-3-yl)-N'-(2, 3-dihydro-1, 4-benzodioxin-6-ylmethylidene) acetohydrazide for optoelectronic applications: Ananda S., Hussien A. K., Mahendra M., Kumara C., Jagadeesh Prasad D., Tejaswi A. H. and Vinitha G. *Journal of Materials Science: Materials in Electronics*, (2021), 32, 1-26
  
48. Design, synthesis, docking, Hirshfeld surface analysis and DFT calculations of 2-methylxanthen-9-with the FtsZ protein from Staphylococcus aureus: Ranganatha V. L., Mallikarjunaswamy C., Jagadeep Chandra S., Ramith R., Prithvi S. S., Naveen Kumar, Sowmya B. P., Hussien A. K., Mahendra M. and Shaukath Ara K. *Bio information*, (2021), 17 (3), 393-403

## 2020

49. Pyridine based boronic acid as carbohydrate sensor: DFT and spectroscopic investigations: Bhavya N. R., Ananda S., Khamees H. A. and Mahendra M. *AIP Conference Proceedings*, (2020), 2265 (1), 030360
  
50. Growth, crystal structure, Hirshfeld surface analysis, DFT and nonlinear optical studies of bis (4-methoxybenzylammonium) tetrachloridocadmate (II): Ananda S, Khamees H. A., Bhavya N. R. and Mahendra M. *AIP Conference Proceedings*, (2020), 2265 (1), 030408
  
51. Facile fabrication of silk fibroin microparticles: their characterization and potential adsorption study: Parushuram N., Ranjana R., Narayana B., Mahendra M. and Sangappa Y. *Journal of Dispersion Science and Technology*, (2020), 1-19.
  
52. Structural, Quantum Chemical and Spectroscopic Investigations on Photophysical Properties of Fluorescent Saccharide Sensor: Theoretical and Experimental Studies: Hussien A. Khamees, Bhavya N. R, Mahendra M, Jeyaseelan Sebastian, Doreswamy B. Haruvegowda and Shamantha Kumar. *ChemistrySelect*, (2020), 5, 5227-5238.

53. Molecular Structure and Antioxidant Activity of Phenoxy Thiazole Derivative: Experimental and Computational Studies: : Lakshmi R. S., Hussien Ahmed Khamees, Madhu Ambat, Mohammed Faizal, Keshav Kumar H., Shivani S Rane and Mahendra M. *Proceedings of International Conference on Drug Discovery (ICDD)*, (2020), SSRN
54. Structural Properties and Anti-Inflammatory Activity of Acetamide Thiazole Derivatives: Density Functional Theory and Schrödinger Suites: Hussien Ahmed Khamees, Lakshmi R. S., Madhu Ambat, Mohammed Faizal, Keshav Kumar H., Shivani S Rane and Mahendra M. *Proceedings of International Conference on Drug Discovery (ICDD)*, (2020), SSRN
55. Fabrication and characterization of conductive silk fibroin–gold nanocomposite films: Ranjana R., Parushuram N., Harisha K. S., Asha S., Narayana B., Mahendra M., Sangappa Y. *Journal of Materials Science: Materials in Electronics*, (2020), 31(1), 249-264
56. Effect of o-difluoro and p-methyl substituents on the structure, optical properties and anti-inflammatory activity of phenoxy thiazole acetamide derivatives: Theoretical and experimental studies: Hussien Ahmed Khamees, Yasser Hussein Eissa Mohammed, Ananda S, Fares Hezam Al-Ostoot, Sangappa Y, Saad Alghamdi, Shaukath Ara Khanum, Mahendra M. *Journal of Molecular Structure*, (2020), 1199, 127024.

## 2019

57. Crystal structure, DFT calculation, Hirshfeld surface analysis and energy framework study of 6-bromo-2-(4-bromo-phen-yl)imidazo[1,2-a]pyridine: Hussien A. Khamees, Kumara C., Nasseem A. El-khatatneh, Ananda S., Kwong H. Chong, Jagadeesh Prasad D., and Mahendra Madegowda. *Acta Cryst.*, (2019), E75, 1620-1626.
58. Synthesis, crystal structure and studies of physical parameters of novel compound N-(2,6-dichlorophenyl)-4-(naphthalen-2-yl)-1,3-thiazol-2-amine: Gayathri B.H., Ravindra R.K., Jagadeesh Prasad D., Bhavya N.R., Lokanath N.K., Mahendra M., Laxmana K., Karegoudar Prakash. *Chemical Data Collections*, (2019), 24, 100286
59. Computational and spectroscopic investigations on boronic acid based fluorescent carbohydrate sensor in aqueous solution at physiological pH 7.5: N.R. Bhavya, M. Mahendra, H. B. Doreswamy, Shamantha Kumar, Maryam Gilandoust and Nasseem Ahmad El-khatatneh. *Journal of Molecular Structure*, (2019), 1197, 305-319.

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165. Synthesis and crystal structure of 1-methyl-3-(4-nitrophenyl)-1,2,3 triazolium perchlorate: Doreswamy B.H., Mahendra M., Sridhar M.A., Shashidhara Prasad J., Mantelingu K., Basappa S. and Rangappa K.S., *Mol. Cryst. Liq. Cryst.*, (2003), 403, 67.
166. Structural studies on praseodymium malonate hydrate: Doreswamy B.H., Mahendra M., Sridhar M.A., Shashidhara Prasad J., Varughese P.A., Saban K.V. and George Varghese, *J. Mol. Str.*, (2003), 659, 81.

### Meetings/Conferences/Workshops Attended

1. Presented a paper entitled “Exploring structural, DFT, and nonlinear optical properties of a novel organic thiazole derivative for optoelectronics applications: A combined experimental and theoretical approach” at the “IEMDST-2024” conference held at Department of Physics, National Institute of Technology, Warangal, Telangana, India, from July 4<sup>th</sup> to 5<sup>th</sup>, 2024.
2. Presented a paper entitled “Towards sustainable energy: A first-principles study of quaternary chalcogenide BaScAgTe<sub>3</sub> material for photovoltaic application” at the “IEMDST-2024” conference held at Department of Physics, National Institute of Technology, Warangal, Telangana, India, from July 4<sup>th</sup> to 5<sup>th</sup>, 2024
3. Presented a paper entitled “Exploration of Electronic and Optical Properties of Chalcogenide Pervskite Materials AHfS<sub>3</sub> (A = Ba, Sr) for Light-Emitting Semiconductor: First Principles Study” at the “DAE-SSPS” conference held at Gandhi Institute of Technology and Management (GITAM) Visakhapatnam, Andhra Pradesh, India, from December 20<sup>th</sup> to 24<sup>th</sup>, 2023.
4. Presented a paper entitled “Crystal Structure, Hirshfeld Surface and Computational Nonlinear Optical Studies of Isonicotinohydrazide Derivative” at the “DAE-SSPS” conference held at Gandhi Institute of Technology and Management (GITAM) Visakhapatnam, Andhra Pradesh, India, from December 20<sup>th</sup> to 24<sup>th</sup>, 2023.
5. Presented a paper entitled “Crystal structure, molecular mechanics, and In silico analyses of piperazine derivative against human mammary carcinoma cells inhibition” at the “ICPN 2023” conference held at Department of Physics, Mangalore University, Karnataka, India, from September 21- 23, 2023.
6. Presented a paper entitled “Synthesis, Crystal structure, Hirshfeld Surface Analysis, DFT and NLO Studies of Thiazole derivative” at the “ICPN 2023” conference held at Department of Physics, Mangalore University from September 21- 23, 2023.
7. Presented a paper entitled “Computational and Experimental Study of Optoelectronic and Nonlinear Optical Properties of Acetohydrazide Derivative” at the “DAE-SSPS” conference held at Birla Institute of Technology Mesra, Ranchi, Jharkhand, from December 18<sup>th</sup> to 27<sup>th</sup>, 2022.

8. Presented a paper entitled "Structural, DFT and Nonlinear Optical Studies of Hemihydrate Thiadiazole Derivative" at the "DAE-SSPS" conference held at Birla Institute of Technology Mesra, Ranchi, Jharkhand, from December 18<sup>th</sup> to 27<sup>th</sup>, 2022.
9. Participated in the 48<sup>th</sup> National Seminar on Crystallography held at Indian Institute of Technology, Roorkee, from 25<sup>th</sup> to 27<sup>th</sup> November 2021.
10. Presented a paper entitled "Experimental and Theoretical Studies of Organic Nonlinear Optical Material: Acetohydrazide Derivative" at the four days DAE-BRNS National Laser Symposium (NLS-28) Conference will be held at Vellore Institute of Technology, Chennai, Tamilnadu, from 08<sup>th</sup> to 11<sup>th</sup> January 2020.
11. Presented a paper entitled "Pyridine based boronic acid as carbohydrate sensor: DFT and spectroscopic investigations" at the five days 64<sup>th</sup> DAE Solid State Physics Symposium will be held at Indian Institute of Technology Jodhpur, Rajasthan, from 16<sup>th</sup> to 24<sup>th</sup> December 2019.
12. Presented a paper entitled "Synthesis, Crystal structure, Hirshfeld surface analysis, DFT and Nonlinear optical studies: Acetohydrazide Derivative" at the "Current Application in Material Science" held at SJB Institute of Technology Kengeri, Bengaluru on May 4<sup>th</sup>, 2019.
13. Presented a paper entitled "Synthesis, Crystal structure, Hirshfeld surface analysis, DFT and Nonlinear optical studies of 2-(6-chloropyridin-3-yl)-N'-(2,3-dihydro-1,4-benzodioxin-6-ylmethylidene)acetohydrazide" at the "Advanced Functional Materials for Energy, Environment and Health Care (AFMEEHC)" held at Vijnan Bhavan, University of Mysore, Mysuru on March 18<sup>th</sup> to 20<sup>th</sup>, 2019.
14. Participated in the three day lecture workshop on "Quantum Statistics-Theory & Experiments" organised by the Department of Physics, St. Philomena's College (Autonomous), Mysuru, in association with science Academies of India from February 15<sup>th</sup> to 17<sup>th</sup> 2019.
15. Participated in the three day refresher course organised by Committee for the Development of Science in Schools, in Vijnan Bhavan, University of Mysore, Mysuru from September 18<sup>th</sup> to 20<sup>th</sup> 2019.
16. Presented a paper entitled "Synthesis, Crystal structure, Hirshfeld surface analysis, DFT and Nonlinear optical studies of Bis(4-methylbenzylammonium) Tetrachloridocuprate(II)" at the "46<sup>th</sup> National Seminar on Crystallography 2018" held at NIMHANS, Bengaluru on June 27<sup>th</sup> to 29<sup>th</sup>, 2018.

17. Participated in the three day lecture workshop on “Quantum Information and Computation” organised by the Department of Physics, St. Philomena’s College (Autonomous), Mysuru, in association with science Academies of India from August 18<sup>th</sup> to 20<sup>th</sup> 2018.
18. Participated in the “Twenty-ninth Mid-Year Meeting of the Indian Academy of Science” held in Infosys Training Centre, Mysuru from June 29<sup>th</sup> to 30<sup>th</sup> 2018.
19. Presented a paper entitled “Crystal Structure and DFT Studies on Bio-sensing Material: 2-ethoxy-4-fluorophenylboronic acid” at the “Current application in Material Science” held at SJB Institute of Technology Kengeri, Bengaluru on May 9<sup>th</sup>, 2018.
20. Participated in the “Special Lecture Series in Environmental science”, sponsored by University with Potential for Excellence held from March 16<sup>th</sup> to 19<sup>th</sup> 2018 at the Department of studies in Environmental Science, Manasagangotri, Mysuru-06
21. Participated in the three day lecture workshop on “Frontiers in Astronomy” organised by the Department of Physics, St. Philomena’s College (Autonomous), Mysuru, in association with science Academies of India from February 17<sup>th</sup> to 19<sup>th</sup> 2018.
22. Participated in the National Conference on “Geometric Function Theory and its Application” organized by University of Mysore (UPE) held at Department of Studies in Physics, Manasagangotri, Mysuru from January 29<sup>th</sup> to 30<sup>th</sup> 2018.
23. Presented a paper entitled “Synthesis, Single Crystal X-ray and Computational studies of (4-chlorophenyl) (2-(methylthio) thiophen-3-yl) methanone” at the “Recent Advances in Materials Science and Biophysics (RAMSB)” held at Mangalore University, Mangaluru on January 23<sup>rd</sup> to 25<sup>th</sup>, 2018.
24. Participated in the “10<sup>th</sup> Annual Conference of Karnataka Science and Technology Academy 2018” jointly organized by Karnataka Science and Technology Academy and REVA University held during January 18<sup>th</sup> to 19<sup>th</sup> 2018.
25. Participated in the Eight Days National Training on “Application and Trouble Shooting of Scientific Equipment” organized by Institution of Excellence in association with UPE, University of Mysore, Vijnana Bhavana, Mysuru from December 01<sup>st</sup> to 08<sup>th</sup> 2017.
26. Presented a paper entitled “Crystal structure of N-(2, 6-dichlorobenzylidene)-3,5-dichlorobenzenamine” at the “Recent Trends in Material Science and Environmental Issues” held at SJB Institute of Technology Kengeri, Bengaluru on May 10<sup>th</sup>, 2017.

27. Participated in the Science Academies 84<sup>th</sup> 16 day Refresher Course “ In Experimental Physics” organized by the Department of Physics, St. Philomena’s College (Autonomous), Mysuru from February 14<sup>th</sup> to march 1<sup>st</sup> 2017.
28. Participated as a delegate in the “XL Indian Social Science Congress” jointly organized by Indian Academy of Social Sciences and University of Mysore, held at DOS in Physics, University of Mysore, Mysuru from December 19<sup>th</sup> to 23<sup>rd</sup> 2016.
29. Participated in the “103<sup>rd</sup> Indian Science Congress” held at University of Mysore, Mysuru from January 3<sup>rd</sup> to 7<sup>th</sup> 2016.
30. Presented a paper entitled “Crystal structure of a putative NADP dependent oxidoreductase TM1727 from *Thermotoga maritima*” at the “5<sup>th</sup> Winter School Soft X-rays in Macromolecular Crystallography”, University of Georgia, Athens, USA held on March 1<sup>st</sup> to 4<sup>th</sup>, 2015.
31. Participated as a delegate in the one-day seminar on “Radioactivity- Natural and Manmade”, organized by Indian Nuclear Society, Mysore and Vidya Vikas Institute of Engineering and Technology at VVIET Campus, Mysore held on March 15<sup>th</sup>, 2014.
32. Presented a paper entitled “Synthesis and Structural Studies of Ethyl 2-methyl-4-phenyl-1-(4-(trifluoromethyl)benzyl)-1H-pyrrole-3-carboxylate” at the UGC sponsored two days National Seminar on “Material Science and Engineering (NSMSE)”, held at JSS College of Arts, Commerce and Science, Mysore during March 21-22<sup>nd</sup>, 2014.
33. Presented a paper entitled “Synthesis and characterization of novel Ethyl 5-oxo-4-phenyl-5,6-dihydro-4H-1,3,4-oxadiazine-2-carboxylate” at the International Symposium on Chemical Biology- Drug Discovery Programme, held at University of Mysore, Mysore during January 9-10<sup>th</sup>, 2014.
34. Presented a paper entitled “Structure of conserved hypothetical protein TM1727 from *Thermatoga maritime*: a probable NADP dependent-dehydrogenase” at the International Symposium on Chemical Biology- Drug Discovery Programme, held at University of Mysore, Mysore during January 9-10<sup>th</sup>, 2014.
35. Presented a paper entitled “ Synthesis and crystal structure studies of Ethyl 4-methyl-1, 3-diphenyl-1H- pyrazole-5-carboxylate” at the 58<sup>th</sup> DAE Solid State Physics Symposium, held at Thapar University, Patiala, Punjab during December 17-21, 2013.
36. Presented a paper entitled “Synthesis and crystal structure studies of Ethyl 5-methyl-1, 3-diphenyl-1H- pyrazole-4-carboxylate” at the 42<sup>nd</sup> National Seminar on Crystallography

and International Workshop on Application of X-ray Diffraction for Drug Discovery, held at Jawaharlal Nehru University, New Delhi during November 21-23, 2013.

37. Presented a paper entitled "Hydrothermal synthesis, crystal structure and characterization of  $\text{LiSrHP}_2\text{O}_7$ " at the National seminar on Current Trends of Research in Precambrian Geology and Vision 2020, held at Department of Studies in Earth Science, University of Mysore, Manasagangotri, Mysore during March 20-21, 2013.
38. Participated as a delegate in the Four-day National workshop on "Basic techniques in molecular biology and bioinformatics", organized by postgraduate department of Biotechnology, JSS College for Arts, Commerce and Science, Ooty road, Mysore, in association with association of Microbiologists of India (AMI) (Mysore chapter) and BIORAD, held from 15<sup>th</sup> to 18<sup>th</sup> March 2013.
39. Presented a paper entitled "Structure of putative aminoglycoside N-Acetyl transferase from *Bacillus subtilis*" at the International Conference on Biomolecular Forms and Functions, held at J. N. Tata Auditorium, Indian Institute of Science, Bangalore during January 8-11, 2013.
40. Presented a paper entitled "Growth and Characterization of a Semi-organic NLO Material: L-Serine Potassium Nitrate" at the 24<sup>th</sup> National Seminar on Crystal Growth, held at Anna University, Chennai, India during December 20-22, 2012.
41. Participated as a delegate in the one-day technical seminar on "Nuclear Energy-Environment and Safety" (NEEDS-2012), Jointly organized by Indian Nuclear Society, Mysore and Department of Studies in Physics, University of Mysore on 3<sup>rd</sup> March 2012 at DOS in Physics, University of Mysore, Mysore.
42. Presented a paper entitled "Crystal structure studies of Diethyl-(6-chloro-2-carbazolyl)methyl malonate an intermediate in the synthesis of anti-inflammatory drug Carprofen" at the 40<sup>th</sup> International Seminar on Crystallography, held at Osmania University, Hyderabad, India during November 26-28, 2011.
43. Presented a paper entitled "Synthesis and Crystal Structure of stable nitrenium ion complex: 1-Hydroxy-3-methyl benzotriazoliumtrifluoromethane sulfonate" at the National Conference on "Recent trends in Material Chemistry and Engineering (RTMCE- 2011), held at Department of Chemistry, RNS Institute of technology, Bangalore, India during September 29-30, 2011.

44. Participated 'UGC Sponsored Refresher Course in Physics, Batch -XVII' held from September 8<sup>th</sup> to 28<sup>th</sup> 2011, at Academic Staff College, University of Madras, Chennai.
45. Participated 'UGC Sponsored National Conference on Applications of Mathematics and Statistics' held at Yuvaraja's College, Mysore during March 25-26, 2011.
46. Presented a paper entitled "X-ray Structure of Aminoglycoside 3-n-acetyl transferase (YokD) from *Bacillus Subtilis*" at the International Symposium on Challenges in Drug Discovery Programme- 2011 (ISCDDP-2011) held at KSOU, Manasagangotri, Mysore, India during February 16-17, 2011.
47. Presented a paper entitled "Synthesis and Crystal structure of a novel antibacterial durg: 1,2-Bis(N-methylbenzimidazolyl)benzene" at the International Symposium on Challenges in Drug Discovery Programme- 2011 (ISCDDP-2011) held at KSOU, Manasagangotri, Mysore, India during February 16-17, 2011.
48. Presented a paper entitled " Structure and Docking studies of Aminoglycoside 3-N-acetyltransferase from *Bacillus subtilis*" at the 6<sup>th</sup> International Structural Biology and Functional Genomics Conference, Dec 6-8, 2010, National University of Singapore, Singapore.
49. Participated 'Science Academies' Lecture Workshop on some topics in "Biophysics" at Department of Studies in Physics, University of Mysore, Mysore, India, Sep 16-17, 2010.
50. Participated the State Inter University meeting of Vision Group on Science and Technology in Physics, Chemistry and Material Science subjects at Department of Studies in Physics, University of Mysore, Mysore, India, March 08-09, 2010.
51. Presented a paper entitled "Crystal structure of yokD protein form *Bacillus subtilis*" at the 8<sup>th</sup> Asia Pacific Bioinformatics Conference, Bangalore, India, Jan18-21, 2010.
52. Participated UGC sponsored 84<sup>th</sup> Orientation course at Academic Staff College, University of Mysore, Mysore, Oct 7<sup>th</sup> to 3<sup>rd</sup> November 2009.
53. Presented a paper entitled "Crystal Structure of Dual Specificity Human Phosphatase DUSP9" at the 38<sup>th</sup> National Seminar on Crystallography, University of Mysore, Mysore, Feb 11-13, 2009.

54. Presented a paper entitled "Synthesis and X-ray Structure of 1,2-bis(N-methylbenzimidazolyl)Benzene" at the 38<sup>th</sup> National Seminar on Crystallography, University of Mysore, Mysore, Feb 11-13,2009.
55. Presented a paper "Crystal structure of hypothetical protein TM1727 from *Thermatogamaritima*" at the American Crystallographic Association, Honalulu, Hawaii, USA, July 21-26,2006.
56. Presented a paper entitled "Crystal Structure of Novel 2-butyl-4-chloro-1H-Imidazolyl-5-Carboxaldehyde", at the XXXIII National Seminar on Crystallography, National Chemical Laboratory, Pune, January 8-10, 2004.
57. Presented a paper entitled "Synthesis and X-ray Structure of 1,2-bis(N-methylbenzimidazolyl)benzene", at the XXXIII National Seminar on Crystallography, National Chemical Laboratory, Pune, January 8-10, 2004.
58. Presented a paper entitled "Crystal Structure of 1-methyl-3-(4-nitrophenyl)-1,2,3triazolium perchlorate", at the XXXIII National Seminar on Crystallography, National Chemical Laboratory, Pune, January 8-10, 2004.
59. Presented a paper entitled "Hydrothermal Synthesis and Structure of New Condensed Hydrated Lithium Cobalt Pentaphosphate", at the DAE-Solid State Physics Symposium, Jiwaji University,Gwalior, India, December 26-30, 2003.
60. Presented a paper entitled "Structural studies of Samarium malonatehexahydrate", at the DAE-Solid State Physics Symposium, Jiwaji University, Gwalior, India, December 26-30, 2003.
61. Participated in Indo-German school on Synchrotron Radiation Sources and their Applications at Centre for Advanced Technology,Indore,India,November 11-22-2002.
62. Presented a paper entitled "Crystalline structural studies of solid electrolyte compounds like  $M^+NiP_2O_7$  [ $M^+=Na, Cs$ ]", at the XXXII National Seminar on Crystallography held at University of Jammu, Jammu Tawi, India, October 24–26, 2002.

63. Presented a paper entitled "Synthesis and structural characterization of solid electrolyte compound  $\text{CsCoP}_2\text{O}_7$ ", at the XXXII National Seminar on Crystallography held at University of Jammu, Jammu Tawi, India, October 24–26, 2002.
64. Presented a paper entitled "Structure analysis of tetra thiourea copper(II) chloride complex", at the XXXII National Seminar on Crystallography held at University of Jammu, Jammu Tawi, India, October 24–26, 2002.
65. Participated in the International Conference on "Problems and Prospect of IT Professionals in the New Millenium" and National Seminar on "World Wide Web Education", University of Mysore, Mysore, January 13-16, 2002.
66. Presented a paper entitled "Crystal and Molecular structure studies of LignocainiumOctochloroBis ( $\mu$ -Dichloro) Dibismathate(III)", at the DAE-Solid State Physics Symposium, Bhabha Atomic Research Centre, Mumbai, December 26-30, 2001.
67. Attended the meeting of International symposium on Crystallography and Bioinformatics in Structural Biology, at IISc and National centre for Biological Sciences, Bangalore, November 22-25, 2001.
68. Attended the IV meeting of Asian Crystallographic Association held at Indian Institute of Science. Bangalore, India, November 18-21, 2001.