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Notice for the PhD Viva Voce Examination

Ms Athira Maria John (Registration Number: 2071404), PhD Scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore will defend her PhD thesis at the public viva-voce examination on Wednesday, 19 March 2025 at 10.00 am in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru-560029, Karnataka, India.

Title of the Thesis	:	**Heteroaryl Azo Based Molecular Switches: Theoretical Design with Experimental Validation**
Discipline	:	**Chemistry**
External Examiner - I	:	**Dr Puneet Gupta** Associate Professor Department of Chemistry Indian Institute of Technology Roorkee, Uttarakhand-247667
External Examiner - II	:	**Dr M R Prathapachandra Kurup** Professor (Retired) Department of Chemistry Central University of Kerala Periye, Kasaragod-671320 Kerala
Supervisor	:	**Dr Sreeja P B** Associate Professor Department of Chemistry School of Sciences CHRIST (Deemed to be University) Bengaluru-560029 Karnataka

The members of the Research Advisory Committee of the Scholar, the faculty members of the Department and the School, interested experts and research scholars of all the branches of research are cordially invited to attend this open viva-voce examination.

Registrar (Academics)

Place: Bengaluru
Date: 04 March 2025

ABSTRACT

Azobenzene derivatives are renowned as robust molecular switches due to their reversible *trans-cis* photoisomerization, finding wide application in contemporary chemistry, material science, and biology. However, heteroaryl azo derivatives, which could offer enhanced properties, have been relatively underexplored. This thesis presents a comprehensive study of heteroaryl azo derivatives, specifically azopyridine, azoimidazole, and azopyrimidine, encompassing both theoretical modeling using Gaussian 16W and eco-friendly synthesis of select compounds. A detailed analysis of the switching mechanisms revealed that all three derivatives undergo an inversion pathway for isomerization, supported by close alignment between theoretical and experimental results.

Each derivative demonstrated promising Non-Linear Optical activity, with the azopyridine derivative standing out for its efficient switching capabilities, suggesting potential for use in optical-limiting applications. Additionally, the azopyridine derivative's biological relevance was assessed through Density Functional Theory, molecular docking, molecular dynamics simulations, and *in-vitro* assays, indicating strong anti-trypsin activity. This highlights its promise in photodynamic therapy, where photoswitchable biological agents are increasingly valuable. In conclusion, this study demonstrates that heteroaryl substitution can enhance azobenzene derivatives, producing compounds with superior NLO properties and bioactivity, broadening their potential applications in photonic and therapeutic technologies.

Keywords: *Molecular Photoswitch, Photoisomerization, Heteroaryl azo derivatives, Density Functional Theory, Optical Limiters, Photodynamic Therapy*

Select Publications:

1. **Athira Maria John,** Sharanya C Suresh, Anjana Baby, Saranya Jayaram, Suma Sarojini, Renjith Thomas, Sreeja Puthanveetil Balakrishnan, Unveiling the therapeutic potential of azopyridine derivatives for trypsin inhibition: a DFT and *In-Vitro* approach, *Molecular Physics*, **2024**, e2415951, DOI: 10.1080/00268976.2024.2415951
2. **Athira Maria John**, Sebin Sebastian Xavier, Cyril Benny, Reji Philip, Sreeja Puthanveetil Balakrishnan, Photoisomerization dynamics of 2-[(*E*)-(4-fluorophenyl)diazenyl]-1*H*-imidazole: A Theoretical and Experimental Insight, *Journal of Computational Biophysics and Chemistry,* **2024**, DOI: 10.1142/S2737416524500698
3. **Athira Maria John**, Cyril Benny, Reji Philip, Sreeja P Balakrishnan, Experimental and Theoretical Investigation of 3-[(2-chlorophenyl) diazenyl] pyridine-2, 6-diamine as Optical Limiter, *ChemistrySelect*, **2023**, 8 (48), e202303348, DOI: 10.1002/slct.202303348.
4. **Athira Maria John**, Anjana Baby, Sreeja P Balakrishnan, Fluorescent Photosensitizers: A Promising Tool for Biomedicine, Photosensitizers and Their Applications, **2022**, 1, 91-107, Nova Science Publishers, DOI: 10.52305/KWAV1221.
5. **Athira M John**, Renjith Thomas, Sreeja P Balakrishnan, Nabil Al-Zaqri, Ali Alsalme, Ismail Warad, Diazo-pyrazole analogues as photosensitizers in dye sensitised solar cells: tuning for a better photovoltaic efficiency using a new modelling strategy using experimental and computational data, *Zeitschrift für Physikalische Chemie*, **2021**, 235 (9), 1227-1245, DOI: 10.1515/zpch-2020-1722