

## Notice for the PhD Viva-Voce Examination

Mr Polina Sai Babu (Registration Number: 1981405), PhD scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore will defend his PhD thesis at the public viva-voce examination on Tuesday, 21 November 2023 at 11.00 am in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029.

Title of the Thesis Synthesis of Thiazines, Thiazinones and :

N-Cycloalkyl Azoles via Novel Synthetic

Routes

Discipline : Chemistry

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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.

Place: Bengaluru

Date: 07 November 2023

Registrar

## **ABSTRACT**

Heterocyclic building blocks have gained utmost importance in recent past on the account of their significance in biological and pharmaceutical fields. Among these heterocyclic building blocks thiazines, thiazinones and N-cyclo alkyl heterocyclic motifs hold an important role in medicinal chemistry. These cores were used for the treatment of various life threating diseases like cancer, cardiovascular, Parkinson, Alzheimer's and various nuero degenerative diseases. As per the literature review, Synthesis of these motifs was done using multi steps and harsh conditions which limited the substrate scope. In this thesis we described our studies on development of one pot, mild condition for synthesis of thiazine and thiazinone cores using P(NMe<sub>2</sub>)<sub>3</sub> (HMPT). We had developed HMPT [P(NMe<sub>2</sub>)<sub>3</sub>] mediated reactions towards synthesis of Carbon-Nitrogen/Carbon-Sulphur bond. Molecular docking studies were conducted for the synthesized compounds considering MOA-B inhibitors as target and showed good binding affinity. MOA-B inhibitor motifs were approved for the treatment of Parkinson illness. We had developed a new mild synthetic strategy using T3P mediated synthetic protocol for the synthesis of N-cyclo alkyl azoles.

In this developed synthetic methodology various regioselective N-cyclo alkyl heterocycles were synthesized. The molecular docking studies of these synthesised molecules are conducted against EGFR inhibitors, which are used for various cancer treatments. The synthesized molecules well resided with in binding region and maintained key interactions.

Keywords: Aza-Michael addition; Benzothiazin-4-ones; Cascade reaction; Cyclic enones; HMPT; N,S-heterocycles; N-cyclo alkyl heterocycles; P(NMe<sub>2</sub>)<sub>3</sub>; Spiro compounds; T3P-mediated; 1,2-diazoles

## **Publications:**

- 1. Saibabu Polina, VPRK Putta, R Gujjarappa, V Singh, PP Pujar, CC Malakar. P(III)-Mediated Cascade C-N/C-S Bond Formation: A Protocol towards the Synthesis of N,S-Heterocycles and Spiro Compounds. Advanced Synthesis & Catalysis 363 (2), 431-445. 20-Nov-2020, https://doi.org/10.1002/adsc.202001149
- 2. Saibabu Polina, VPRK Putta, R Gujjarappa, PP Pujar, CC Malakar. Aza-Michael addition of 1, 2-diazoles to structurally diverse enones: Efficient methods towards β-amino ketones. *Journal of Heterocyclic Chemistry 58 (4), 1029-103*, 31-Dec-2020, <a href="https://doi.org/10.1002/jhet.4221">https://doi.org/10.1002/jhet.4221</a>.