INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: *Unlocking the Multi-Faceted Reactivity of 4-Hydroxythiocoumarin: Sustainable Synthesis of Novel Hybrid Heterocyclic Scaffolds with Therapeutic Potential*

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SHORT ABSTRACT

The contents of this thesis are organized into five chapters encompassing a systematic exploration of the synthetic versatility and reactivity of 4-hydroxythiocoumarin, aimed at developing sustainable methodologies for the construction of novel sulfur-containing heterocyclic hybrids with potential therapeutic relevance.

Chapter 1 is divided into two parts. **Part A** provides a comprehensive overview of the structural and electronic features, reactivity, and medicinal relevance of 4-hydroxycoumarins and their thio analogs, outlining their reactivity as well as their synthetic applications in the design and development of novel molecules. It also includes a brief introduction to hybrid heterocyclic compounds, emphasizing their biological importance and highlighting key synthetic transformations leading to hybrid scaffolds. **Part B** describes synthetic approaches to 4-hydroxythiocoumarin derivatives, including a revised methodology, reaction optimization, and compound characterization.

Chapter 2 presents a solvent- and catalyst-free pseudo-three-component reaction yielding previously unreported pentacyclic-dione derivatives *via* a sequential Knoevenagel condensation, Michael addition, and cyclization pathway, demonstrating high atom economy and alignment with green chemistry principles.

Chapter 3 describes the regioselective *S*-allylation/propargylation and subsequent thio-Claisen rearrangement of 4-hydroxythiocoumarins, leading to chromone-fused thiopyran and thiophene scaffolds. Mechanistic insights were supported by Density Functional Theory (DFT) studies, explaining solvent-dependent rearrangement behavior.

Chapter 4 introduces a mild, one-pot three-component synthesis of thieno[2,3-*b*]chromen-4-one derivatives featuring pendant imine functionalities from 4-hydroxythiocoumarin, *trans*-β-nitrostyrene, and salicylaldehyde (or aryl aldehydes). The reaction proceeds through the reaction of 4-hydroxythiocoumarin and *trans*-β-nitrostyrene *via* tandem Michael addition and intramolecular cyclization, followed by an unusual oxime-to-amine transformation through a disproportionation pathway, and finally, Schiff base formation with the aryl aldehyde component.

Chapter 5 summarizes the key findings, places them in the context of current research, and outlines prospective directions such as pharmacological evaluation, structural modification, post-synthetic diversification, and assessment of scale-up potential.

Overall, the work establishes 4-hydroxythiocoumarin as a valuable building block for accessing diverse hybrid heterocyclic frameworks *via* efficient, selective, and sustainable synthetic routes.