CU-CATALYZED DOMINO SYNTHESIS OF THIOAURONE AND THIOINDIRUBIN FROM ODORLESS XANTHATE AS SULFUR SURROGATE

IITM Technology Available for Licensing

Problem Statement

- Conventionally, thioindirubin derivatives are prepared by radical intramolecular cyclization of triethylammonium thiolates utilizing **expensive starting materials**
- Further, **multistep process is required** to prepare the starting material

Intellectual Property

- **IITM IDF Ref. 2218**
- **IN 402159-Granted**

Technology Category/ Market

Category –Chemistry & Chemical Analysis
Applications –Chemicals,Drugs and pharmaceuticals, manufacturing
Industry –Chemicals, Pharmaceuticals, Textiles
Market - Organic Chemicals Market Size was valued at USD 11.3 Billion in 2022 and is projected to grow from 12.15 Billion in 2023 to USD 21.66 Billion by 2032, exhibiting a compound annual growth rate (CAGR) of 7.50% during the said forecasting period

Key Features / Value Proposition

Technical perspective

- ✓ **Environmentally benign and cost-effective copper catalyst** to perform the domino reaction that furnished **thioaurone and thioindirubin derivatives** in **excellent yields with pure form**
- ✓ The process resulted in **(Z)-2-(4- methylbenzylidene) benzo[b]thiophen-3(2H)-one** in **92% yield after 24h** and**(E)-1-benzyl-5-methyl-3-(3-oxobenzo[b]thiophen -2(3H)-ylldene) indolin-2-one** in **83% yield after 28 h**

User perspective

- ✓ **Odourless,** and **avoids use of hazardous solvents** and inert atmosphere to carry out the reaction.
- ✓ **Easy handling** of starting materials, air atmosphere, **energy efficient** process**, applied in industrial scale**
- ✓ Shows **cytotoxicity to cancer cells and fat affinity**, possess a wide range application, also **used in dyes**

Technology

- The present invention describes the copper iodide (**VII**) catalyzed synthesis of thioaurone (**I**) and thioindirubin (**II**) from the 2-iodochalcones (**III**, **IV**).
- **Potassium ethyl xanthate (V)**(sulfur source) used along with **iodine as additive (VI**) in **1,4-Dioxane** (**VIII**) at reflux temperature of **120 ºC.(Fig.1)**
- The reaction proceeds via sulfur insertion and simultaneous region-selective cyclization **Two C-S σ–bonds, one C-C σ-bond and one C=C π-bonds were formed in this single step.**
- The same protocol is applied for attaining synthetically important several thioindirubin derivatives
- Period of the time may vary depends on the substitution of the starting materials all reactions are monitored by **thin layer chromatography** and the product is extracted , further **purified by silica gel column chromatography**

Image

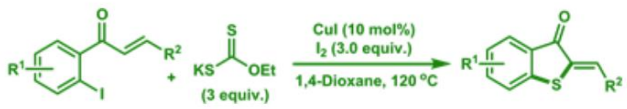

Fig. 1 Reaction scheme for performing the process

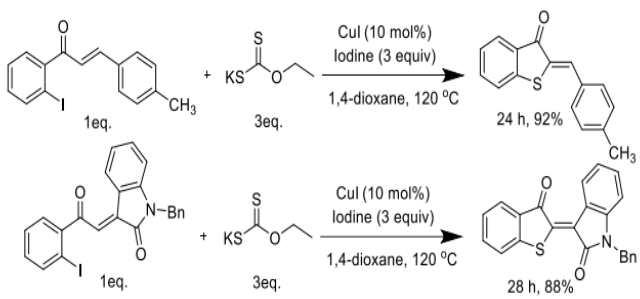

Fig. 2 Reaction schemes for process for preparing thio-aurone and thioindirubin

TRL (Technology Readiness Level)

TRL-3, **Experimental proof of concept**

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