Drug Discovery & Development

Photochemical Preparation of Fluorinated Aryl Ethers for Agrochemicals and Pharmaceuticals

WiSys: T230006US02

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WiSys is seeking a strategic partner in the agrochemical industry who can provide a route to market for the commercialization, scale-up, and use of this novel method for synthesis of aryl fluorinated ethers for pharmaceuticals and agrochemicals.

Overview

The element fluorine has acquired an ever-increasing prevalence in synthetic drugs and agrochemicals due to its positive impact on the metabolism, chemical stability, and modulating lipophilicity of agrochemicals, thereby increasing the activity of the active ingredients. In agriculture, fluorine-containing functional groups are appealing in potential herbicides, pesticides, and fungicides. Over the past two decades, more than half of newly registered agrochemical actives have contained at least one fluorine atom. However, there are challenges to introducing fluorine into pharmaceutical and agrochemical structures, particularly via modification of an existing active ingredient. Fluorination can require harsh reaction conditions, high temperatures, expensive reagents, toxic reagents, or transition metal catalysts. There is a need to improve the functionality of existing drugs and agrochemicals and to develop new techniques for introducing fluorinated functional groups into molecules.

The Invention

Researchers from the University of Wisconsin-Platteville have recently developed a novel photochemical method for the synthesis of aryl fluorinated ethers. The method relies on milligram quantities of a photocatalyst, blue LED lights, and a simple sodium bicarbonate base to couple abundant, inexpensive aryl chloride starting materials with a readily available fluorinated alcohol. The resulting aryl fluorinated ethers are produced without the need for high reaction temperatures or harsh reagents. This method has a clear advantage for the production of fluorinated starting materials for agrochemical synthesis and also is applicable for late-stage functionalization of bioactive ingredients. This reaction has been tested on existing fungicides with up to a 77% yield of the fluorinated ether derivative of known potent pharmaceutical fungicides. Testing on existing pharmaceutical and agrochemical fungicides is ongoing.

Key Benefits

- Produces more active agrochemicals that will require less volume of application
- Uses readily available and inexpensive starting materials
- Allows for production of fluorinated starting materials as well as late-stage functionalization of bioactive ingredients
- Removes the need for high reaction temperatures or harsh reagents
- Applies to existing and well-known fungicides and pesticides

Stage of Development

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Tech Fields

- Animals, Agriculture & Food : Plant health

- Drug Discovery & Development : Drug production & design
- Materials & Chemicals : Synthesis

For current licensing status, please contact Allee Marti at amarti@wisys.org or 608-316-4037