Benzoxaborole Protecting Groups

Lead Inventor

John W. Tomsho, PhD. Associate Professor. Director, Graduate Programs in Chemistry and Biochemistry; Director, Chemistry Core Facility; Director, NMR Spectrometer Laboratory.

Unmet Need

Fungal pathogens are a threat to the agriculture industry and the greater global food supply. The Food and Agriculture Organization of the United Nations (FAO) estimates that plant disease costs the global economy around $220 billion per year.[1] Collectively, pathogenic fungi are responsible for the destruction of roughly 125 million tons of crop annually, where the global damage caused by fungi to rice, wheat, maize, potatoes, and soybeans alone costs $60 billion per year.[2]

Fungicides are essential to address this threat. The agrichemical sector most recently has been focusing on the use of benzoxaborole compounds to create novel fungicides, however, due to their sensitivity to certain reactions, chemically synthesizing benzoxaboroles can be challenging, costly, and possibly compromising for the environment.

Opportunity

Fortune Business Insights reports that the global fungicide market size was valued at $17.1 billion in 2020 and is expected to grow at a compound annual growth rate (CAGR) of 4.93% to $25.81 billion by 2028.[3] With the expansion of the global fungicide market, which includes manufacturing benzoxaboroles in large quantities, Dr. Tomsho's protecting group invention will enable more efficient syntheses in this market.

The versatile benzoxaborole protecting groups discovered at St. Joseph's University (formerly the University of the Sciences in Philadelphia) can mask undesired reactivity and reduce the limitations imposed by current modes of synthesis which require late-stage incorporation of boron.

The Tomsho team has reported the design, synthesis, and evaluation of two families of compounds that form divalent, zwitterionic complexes with benzoxaboroles. These compounds efficiently and reversibly protect the benzoxaborole functionality through one or more chemical steps that are incompatible with the unprotected benzoxaborole. The chemical robustness of these protecting groups has been characterized, and investigators determined that these protecting groups offered improved reaction scope diversity when compared with the previous state of the art. Additionally, compound solubility in organic solvents is generally improved thus facilitating reactions where the unprotected substrate was not soluble.

---

[1] *Food system consequences of a fungal disease epidemic in a major crop*. National Library of Medicine, December 2016.
[2] *Tackle fungal forces to save crops, forests, and endangered animals, say scientists*. Imperial College London, April 2012.
[3] *Fungicides Market Size…Forecasts, 2021 – 2028*. Fortune Business Insights, January 2022.

Unique Attributes

- Rigidified and semi-conjugated system that exhibits enhanced stability to reaction conditions and to common synthetic manipulations (i.e., extractions, flash chromatography).
- Protected benzoxaboroles have significantly enhanced stability under both oxidative and reductive conditions.
- Protecting groups shield boron from nucleophilic attack.
- Ability to introduce boron earlier in the chemical synthesis process, enabling access to a greater range of benzoxaborole compounds.
- Enhanced synthesis efficiency of any product containing benzoxaborole.

Applications

Chemists or industry manufacturers pursuing benzoxaborole in their design studies will benefit from more efficient syntheses of benzoxaborole-containing products. During synthesis, boron may be introduced earlier in the chemical synthesis process, which enables the use of more environmentally friendly chemical synthesis methods. Reagents can be commercialized through a chemical supply company, making them available for purchase by labs and / or manufacturers.

Stage of Development

In laboratory use.

Intellectual Property

US Patent 11,427,603 B2.

References and Publications

Gamrat, J. M.; Mancini, G.; Burke, S. J.; Colandrea, R. C.; Sadowski, N. R.; Figula, B. C.; Tomsho, J. W. Protection of the Benzoxaborole Functionality: Synthesis and Functionalization of Zwitterionic Benzoxaborole Complexes. Submitted March 16, 2018.

Licensing Opportunity

Actively seeking licensee for commercialization.

Institutional Contact

Jean-Francois "JF" Jasmin PhD
+1 215.596.8512
jjasmin@sju.edu

L2C Partners Contacts

Merle Gilmore, MBA
+1 610.662.0940
gilmore@l2cpartners.com

Alex Toglia, MS
+1 610.937.1067
toglia@l2cpartners.com