



Boron Heterocyclic Compounds with Antimicrobial Activity

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HIGHLIGHTS

- Chemoselective synthetic and purification procedures to access diverse libraries of functionalized analogs of naphthoid boroheterocycles.
- Benzoxaborine and benzodiazaborine compounds with promising DMPK properties and antimicrobial activity.

OPPORTUNITY

Researchers at University of Alberta identified that members of several subclasses of naphthoid boroheterocycles inspired by the successful benzoxaborole chemotype demonstrate anti-infective properties. The researchers explored the compatibility of four subclasses with a selection of common transformations used in drug discovery, such as chemoselective Suzuki–Miyaura, Chan–Lam, and amidation reactions to develop small model libraries of derivatives. Moreover, they determined the physical properties of prototypic members of four sub-classes in aqueous media including acidity, boranol (B–OH) exchange, solubility, and logP, which confirmed that critical differences in the Lewis acidity of the boron atom of these benzoborines could affect many aspects of their reactivity, synthetic chemistry, antibacterial activity, and DMPK behavior. Small model libraries of derivatives including 70-80 analogs were prepared and screened for antifungal (*C. albicans*) and antibacterial activity (MRSA, *E. coli*), unveiling promising lead compounds with low micromolar MICs. DMPK assays for representative compounds suggest promising drug-like behavior, with high metabolic stability and excellent membrane permeability.

COMPETITIVE ADVANTAGE

- Structurally novel small model libraries of benzoxaborine and benzodiazaborine derivatives with excellent bench/storage stability.
- New derivatives demonstrated potent antifungal (*C. albicans*) and antibacterial activity (MRSA) with MICs around or below 1 micromol/L, with one analog being superior to tavaborole (CA) and one other nearly as good as vancomycin (MRSA).
- ADME studies of prototypic members of each of the four subclasses studied show promising druggability with excellent transport and metabolic stability.

STATUS

- Patent Pending

INVENTORS

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MORE INFORMATION

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