Medicinal Chemistry Functionalization of Brexazine, a Chiral Tricyclic Diamine Mimetic from the GDB Chemical Space

Leon Rebhan[1], Jean-Louis Reymond[1]

[1]University of Berne

University of Bern, Department of Chemistry, Biochemistry and Pharmaceutical Sciences, Freiestrasse 3, 3012 Bern, CH

leon.rebhan@unibe.ch

The generated databases (GDBs) are a collection of possible molecules up to a certain size which are filtered by rules of synthetic feasibility and chemical stability. A large number of these molecules are novel, intrinsically chiral, 3D-shaped and have never been synthesized[1]. As such, they are a great source for new building blocks for medicinal chemistry.[2] A recent example for such a building block is brexazine (see Figure 1) which we synthesized from a commercially available norbornene. Brexazine is a tricyclic diamine that we envision to be used as a diamine mimetic with novel topology and exit vectors. [3] We have worked on various applications for this building block which we will present here.

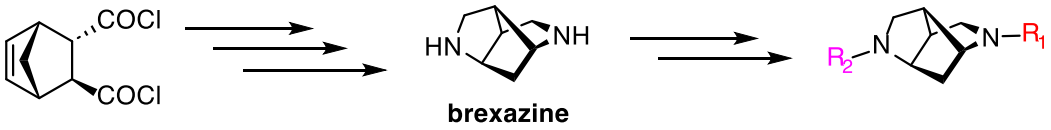

Figure 1: Synthesis and functionalization of brexazine.

References

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[3] L. Rebhan, Y. Buehler, J. Reymond, 'Diamonds in Chemical Space: The Synthesis of Brexazine', *Helvetica Chimica Acta* **2025**, *108*, e202400175.