Synthesis of novel bicyclic diamine scaffolds derived from tropinone

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The generated databases (GDBs) are a large collection of generated chemical scaffolds which adhere to principles of synthetic feasibility and chemical stability. Interestingly, most of the compounds in the database are novel which make the GDB an important resource for discovering novel chemical targets and allows us to explore previously unknown chemical space.

From the GDB we have found an interesting novel family of tricyclic and bicyclic chemical scaffolds which can be accessed synthetically from tropinone.
In this poster we describe a simple synthesis to obtain novel bi-cyclic diamine scaffolds from tropinone which can be easily functionalized to explore novel medicinal chemistry space.

Small molecule drugs often consist of rigid scaffolds equipped with reactive handles, typically amino groups which can be functionalized. To explore previously unknown chemical space, we can use generated databases (GDBs), which are a large collection of generated chemical scaffolds adhering to principles of synthetic feasibility and chemical stability. Comparing the generated databases (GDB) with biologically active small molecules in ChEMBL reveals that many scaffolds, even structurally simple ones, have never been synthesized (1).

Here we discuss the synthesis of a novel family of tricyclic and bicyclic amino containing chemical scaffolds which can be accessed synthetically from tropinone and can be easily functionalized to explore differentiated medicinal chemistry space.

[1] Ye Buehler and Jean-Louis Reymond**,** *J. Chem. Inf. Model.* **2023**, 63, 20, 6239–6248.