Synthesis of novel polycyclic diamine scaffolds derived from tropinone

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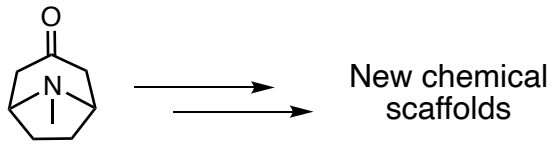
Small molecule drugs often consist of rigid scaffolds equipped with reactive handles, typically amino groups functionalized with pharmacophores. To explore previously unknown chemical space, we can use generated databases (GDBs), which are a large collection of generated chemical scaffolds adhering to 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).



Tropinone

Figure 1. Readily available tropinone can be used as a starting point for synthesis of novel chemical scaffolds.

From the GDB we have found interesting families of tricyclic and bicyclic chemical scaffolds which can be accessed synthetically from tropinone (Fig 1).
In this poster we describe the simple synthesis to obtain these novel poly-cyclic diamine scaffolds from tropinone which 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.
[2] Leon Rebhan, Ye Buehler and Jean-Louis Reymond, *Helvetica*. **2024**, 108, 1522-2675.
[3] Aline Carrel, Adonis Yiannakas, Jaap-Jan RoukensInes, Reynoso-Moreno, Markus Orsi, Amol Thakkar, Josep Arus-Pous, Daniele Pellegata, Jürg Gertsch and Jean-Louis Reymond. *J. Med. Chem*. **2025**, 68, 9, 9176–9201