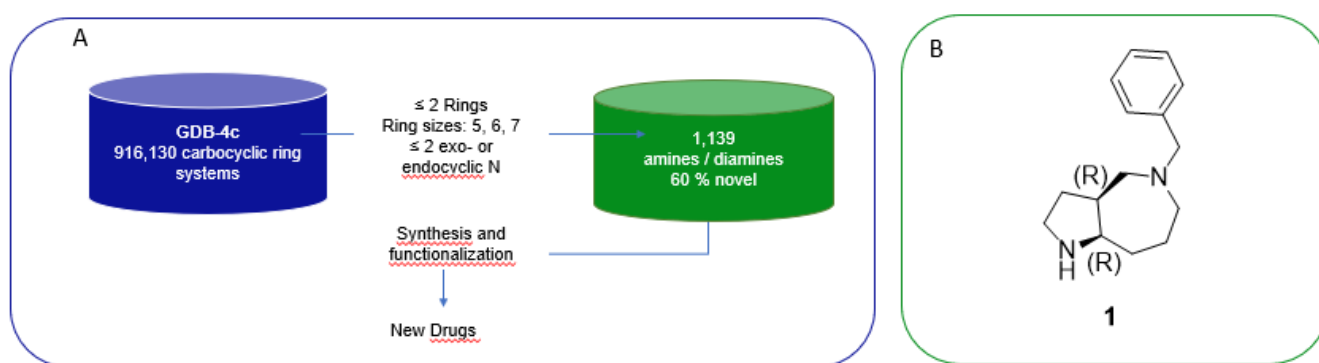


Synthesis of GDB Derived Bicyclic Diamines as Scaffolds for Medicinal Chemistry

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The Generated Data Base (GDB), curated by the Reymond group, offers stable, feasible, 3D-shaped chiral molecules, enabling exploration a vast chemical space, providing promising scaffolds for Medicinal Chemistry. (1) These molecules are innovative due to their polycyclic system, high sp^3 -hybridized carbon fraction and the presence of many quaternary carbons. (2)(3) This project exploits a subset of the GDB, listing 1139 mono- and bicyclic saturated diamine scaffolds containing 5, 6 or 7 membered rings, including 680 novel accessible scaffolds (Figure A). Herein I discuss initial synthetic steps for preparing a target subset of these diamines based on Diels-Alder and ring expansion reactions. As a proof-of-concept molecule **1** (Figure B) was recently synthesised in the group, showing potent inhibition of monoamine transporter, with selectivity to norepinephrine and dopamine transporter ($IC_{50} < 100$ nM).(4) Moreover, the amine functional group within the cyclic scaffolds grants straightforward functionalisation with desired moieties.



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