

POSTER PRESENTATION

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Go with the flow: de-orphaning focused combinatorial libraries

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The fast pace of drug discovery programs, aided by high-throughput screening campaigns, often relies on the generation of combinatorial libraries to identify new chemical entities. The Ugi 4- and 3-component reactions in particular [1], have proven to be robust in producing both tool compounds and drugs [2,3]. Here we report a high-throughput entry into the imidazopyridine scaffold, using a microfluidic-assisted synthesis setup, coupled to a target prediction tool to de-orphan a focused compound library with high success rate, and identify an innovative GPCR-inhibiting chemotype. Combinatorial compounds were correctly identified as ligand-efficient adenosine $A_{1/2B}$, and adrenergic $\alpha_{1A/B}$ inhibitors with K_i values in the low micromolar range.

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