Polyfunctional heterocycles in drug discovery: diversity-oriented synthesis and chemico-physical analysis

Summary
Diversity-oriented synthesis is emerging as a powerful tool in drug discovery due to its ability to generate a large number of compounds with high structural diversity in few steps. In this context, we developed a Ti(IV)-promoted three-component reaction of aromatic heterocycles, aldehydes, and active methylene compounds to afford polyfunctionalized heterocycles of biological interest [1]. The experimental procedure was optimized by studying the reaction mechanism [2]. The stereochemical stability of the products was also investigated by HPLC and NMR spectroscopy in view of their use as fragments in a fragment-based drug discovery approach [3].

References