HTE as a Tool in Reaction Discovery

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Our efforts within late-stage functionalization have been diverse and we are agnostic when it comes to the choice of mechanistic manifold and transition metal. Herein, I will focus on the HTE (high throughput experimentation) development of, among other reactions, a cobalt-catalyzed C–H methylation reaction, that takes advantage of functional groups, which are inherently present in modern drug molecules, to allow selective and predictable late-stage functionalization. The lack of literature precedence and complexity of the transformation necessitated the use of carefully planned HTE during the reaction optimization, to finally realize an efficient and robust procedure suitable for medicinal chemistry purposes.

With this chemistry we not only save valuable time during the synthesis of methylated drug analogues, but also enable easy access to novel high-value compounds in a sustainable manner. Finally, HTE is not a magical solution I will, discuss hurdles and opportunities of this approach.