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A Photoredox (C)sp³-(C)sp² Coupling Method Comparison Study

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Abstract : Drug discovery and delivery involve drug targeting, an approach that helps find a drug against a chosen target through high throughput screening and other methods by way of identifying the physical properties of the potential lead compound. Physical properties of potential drug candidates have been an imperative focus since the unveiling of Lipinski's Rule of 5 for oral drugs. Throughout a compound's journey from discovery, clinical phase trials, then becoming a classified drug on the market, the desirable properties are optimized while minimizing/eliminating toxicity and undesirable properties. In the pharmaceutical industry, the ability to generate molecules in parallel with maximum efficiency is a substantial factor achieved through sp^2-sp^2 carbon coupling reactions, e.g., Suzuki Coupling reactions. These reaction types allow for the increase of aromatic fragments onto a compound. More recent literature has found benefits to decreasing aromaticity, calling for more sp^3-sp^2 carbon coupling reactions instead. The objective of this project is to provide a comparison between various sp^3-sp^2 carbon coupling methods and reaction conditions, collecting data on production of the desired product. There were four different coupling methods being tested amongst three cores and 4-5 installation groups per method; each method ran under three distinct reaction conditions. The tested methods include the Photoredox Decarboxylative Coupling, the Photoredox Potassium Alkyl Trifluoroborate (BF3K) Coupling, the Photoredox Cross-Electrophile (PCE) Coupling, and the Weix Cross-Electrophile (WCE) Coupling. The results concluded that the Decarboxylative method was very difficult in yielding product despite the several literature conditions chosen. The BF3K and PCE methods produced competitive results. Amongst the two Cross-Electrophile coupling methods, the Photoredox method surpassed the Weix method on numerous accounts. The results will be used to build future libraries.

Keywords : drug discovery, high throughput chemistry, photoredox chemistry, sp^3-sp^2 carbon coupling methods
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