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Enantioselective and Diastereoselective Synthesis of Quinolines Using Reissert Compounds JAEUN SHIN, RICHARD KYUNG, CRG-NJ — The Reissert reaction is a chemical reaction that transforms quinoline to quinaldic acid. Quinolines react with acid chlorides and potassium cyanide to produce Reissert compounds and the quinaldic acid is obtained by hydrolysis. In this project, we assessed the thermodynamic and stereochemical analysis for the intermediate and final products obtained in the Reissert reaction to figure out the spontaneous behavior and dynamics of the reaction. Molecular editing program was used to model, optimize, and quantify the chemical and physical properties of the molecular compounds obtained in the process. Alkylation of a Reissert compounds to produce isoquinolines was analyzed: For example, a computational simulation on the stereoselective asymmetric allylic alkylation of Reissert compounds yielding functionalized 1,2-dihydroisoquinolines bearing adjacent stereocenters was performed. The molecular editing program equipped with an auto-optimization feature determined the theoretical values of all the structures atomic and molecular properties of the intermediate and final products through the Density Functional Theory (DFT). This process allows users to build virtually any molecule and optimize its geometry according to various force field options.

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