

Reduction of Chiral Molecule Tert-butyl (5(-cyanobenzoyl)-2-fluorophenyl) Carbamate with Reductase Enzyme and Optimization for its Scale Up †

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Abstract: The chiral selectivity of active pharmaceutical ingredient (API) intermediate is important, which can be achieved using keto-reductases. Here, tert-butyl (5(-3cyanophenyl)hydroxy methyl)-2-fluorophenyl carbamate was synthesised by reduction of tert-butyl (5(-cyanobenzoyl)-2-fluorophenyl) carbamate using keto-reductase. To get a higher conversion and chiral selectivity, the commercial enzymes (Codexis and Syncozyme) were screened. The high performer enzyme was taken for process optimization. It was observed that the maximum chiral selectivity (99%) and yield (100%) were seen at 40°C, 10% enzyme loading, and pH 7. Further, the optimized condition was tested for the gram scale studies, which was found to be feasible with the highly chiral selective product. The synthesized API intermediate was characterized by using Fourier transform infrared (FTIR) spectroscopy, High-performance liquid chromatography (HPLC) chromatogram, NMR, and liquid chromatogram mass spectroscopy (LC-MS). This article will open up a new avenue in the field of API intermediate synthesis by the enzymatic green route.

Keywords: reductase; scale up; chiral; Codexis; insecticide.

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Conflicts of Interest

The authors declare no conflict of interest.