Experimental determination of thermodynamic equilibrium in biocatalytic transamination

The equilibrium constant is a critical parameter for making rational design choices in biocatalytic transamination for the synthesis of chiral amines. However, very few reports are available in the scientific literature determining the equilibrium constant (K) for the transamination of ketones. Various methods for determining (or estimating) equilibrium have previously been suggested, both experimental as well as computational (based on group contribution methods). However, none of these were found suitable for determining the equilibrium constant for the transamination of ketones. Therefore, in this communication we suggest a simple experimental methodology which we hope will stimulate more accurate determination of thermodynamic equilibria when reporting the results of transaminase-catalyzed reactions in order to increase understanding of the relationship between substrate and product molecular structure on reaction thermodynamics.

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