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Deslauriers, Maria Gundersen; Lloyd, Richard C; Woodley, John

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Selections of minimal conditions for a simple intensification and scale up of ω -transaminase reactions

Maria T Gundersen¹, Richard C Lloyd² and John M Woodley¹

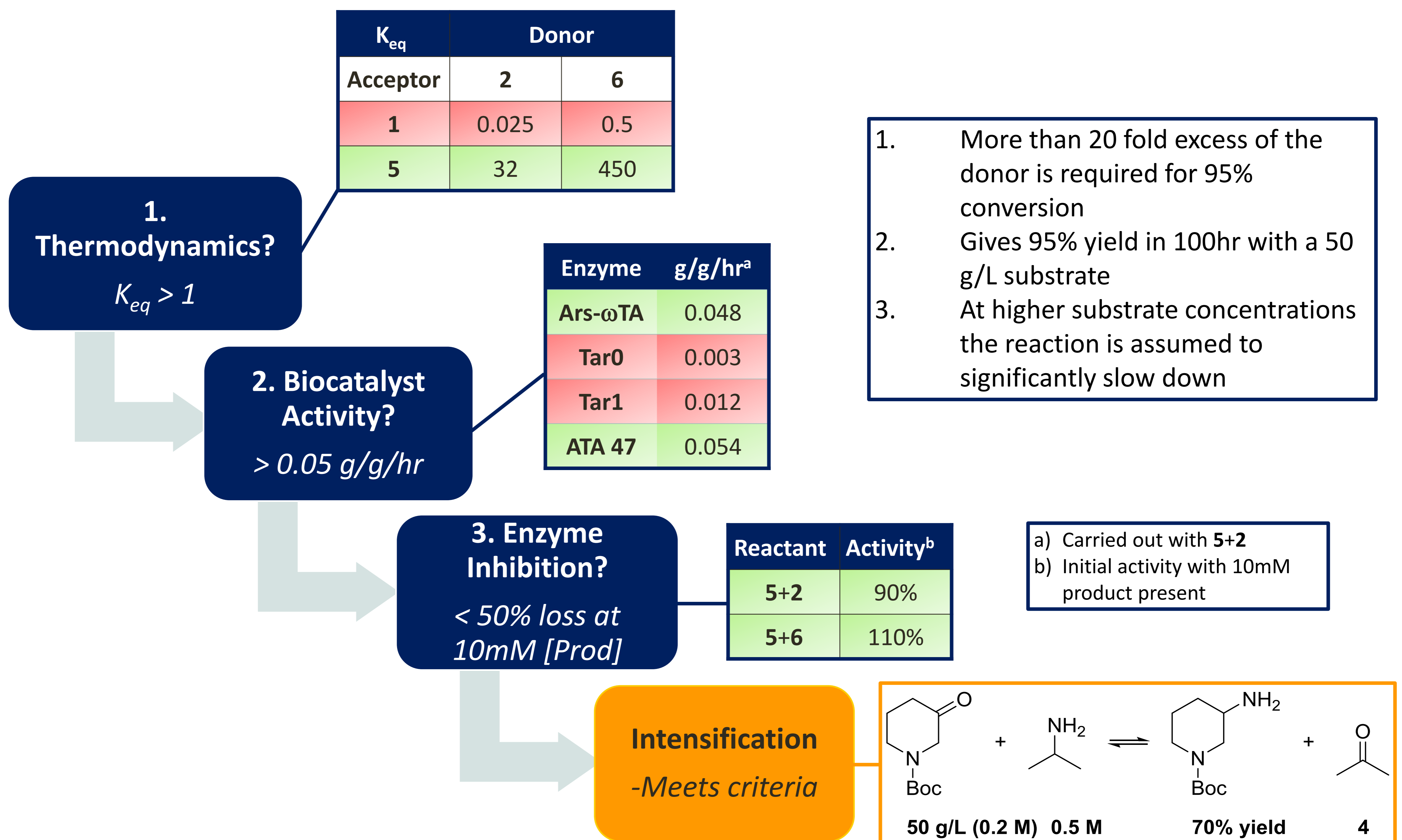
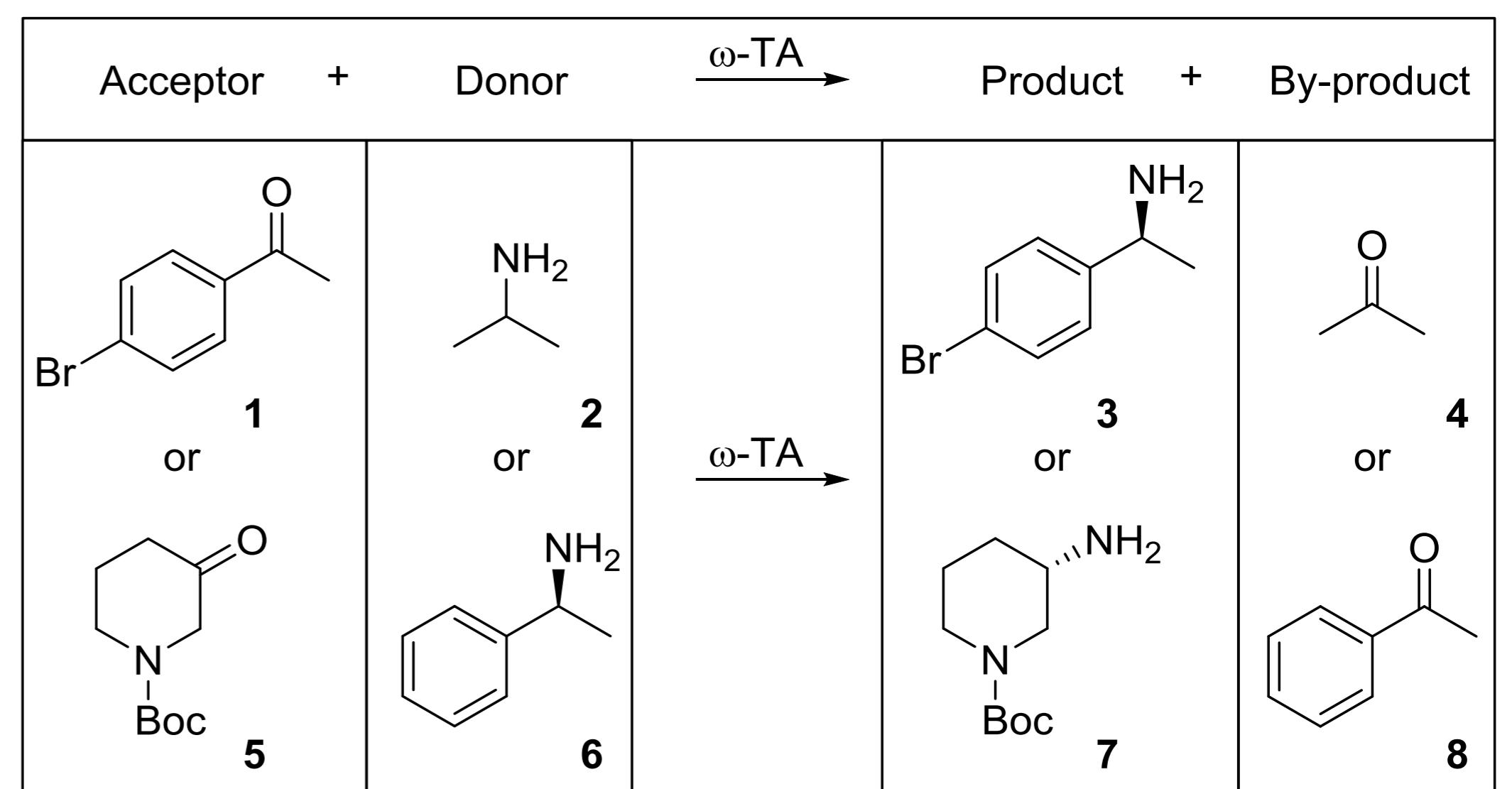
1) Department of Chemical and Biochemical Engineering, DTU, DK

2) Dr. Reddy's Chirotech Technology Centre, Cambridge, UK

INTRODUCTION

A step wise decision matrix is presented to quickly evaluate ω -transaminase for a 'simple scale up' in the synthetic direction. Here a 'simple scale up' is defined as a system without specialized equipment or process development, thus a rapid implementation. The three step method consists of: 1. thermodynamic evaluation, 2. biocatalyst screen and 3. inhibition characterization. Each step of the method has a cut off value for easy implementation. Demonstrated by a case study which eliminated reaction pair candidates based on the cut off criteria. Finally, the most promising candidate was intensified.

CASE STUDY



CONCLUSION

We have here outlined and successfully demonstrated a simple method for selecting reaction candidates suitable for a simple and rapid intensification and scale up. This can be valuable in processes where time is of the essence, such as small singular batches and pharmaceutical applications. Although, the ω -transaminase reaction is used here, we nonetheless argue that this method can be applied for other biocatalytic reactions, for well developed enzymes, where the limitations of the implementation is known.

INTENSIFICATION

The best reaction candidate pair 1-Boc-3-piperidone and isopropylamine was successfully and intensified up to 75 g/L and ran at a 25 mL scale. The best isolated product yields were obtained with the 50 g/L reaction where 70% (S)-(+)-3-amino-1-Boc-piperidine was isolated.