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From renewable raw materials to recyclable materials: Bio-Capa - Biobased Epsilon-Caprolactone

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PURPOSE OF THE ABSTRACT

Epsilon-Caprolactone is the building block of the biodegradable polyester polycaprolactone and is required on a multi-10.000 ton scale. Addressing the raw material change from petrochemical towards renewable resources the development of a sustainable, efficient and economically attractive bio-based production process for the bulk chemical Epsilon-Caprolactone is targeted.
In this project different synthetic routes based on various renewable raw materials will be evaluated for the production of Epsilon-Caprolactone.[1] All routes include chemoenzymatic key steps. The prioritized route will be further upscaled and the so produced Epsilon-Caprolactone will then be evaluated at the BYK company in application tests (Scheme 1).[1]
One production process for the bulk chemical polycaprolactone based on phenol was described in 2017.[2] There, a combination of chemocatalysis and biocatalysis was implemented for the hydrogenation of phenol to cyclohexanol and the subsequent enzymatic cascade oxidation towards Epsilon-Caprolactone (Scheme 2). This cascade reaction combines the double oxidation of cyclohexanol catalyzed by an alcohol dehydrogenase (ADH) and a Baeyer-Villiger monooxygenase (BVMO) with in situ cofactor recycling.
In this work the hydrogenation of phenol was further investigated to implement this step in an industrial applicable process. Therefore, different commercial and synthesized catalysts were screened and evaluated. These catalysts were studied considering the space time yield and conditions needed for the hydrogenation. Mild conditions as low temperature and pressure, fast reaction times, low catalyst loading and low costs should be achieved.

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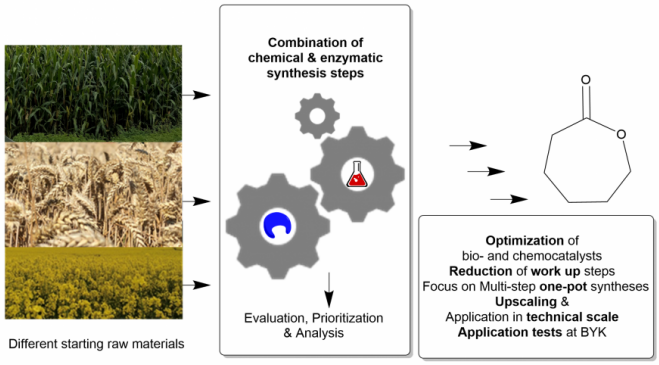
FIGURES



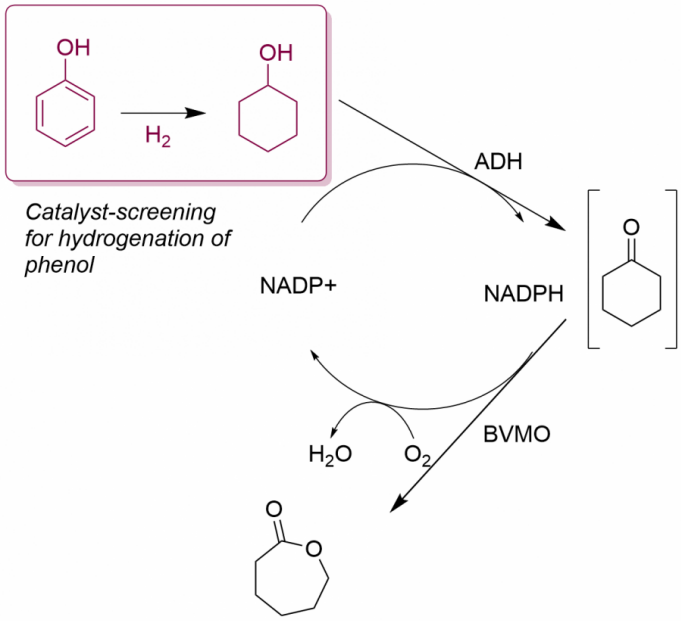


FIGURE 1

Schematic overview of the project.
Combination of chemical & enzymatic synthesis steps for the production of Epsilon-Caprolactone.

FIGURE 2

Chemoenzymatic synthesis of Epsilon-Caprolactone.[2]
Alcohol dehydrogenase (ADH), Baeyer-Villiger monooxygenase (BVMO).

KEYWORDS

Hydrogenation | Biobased Caprolactone | Renewable Raw Materials

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