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Toward the synthesis of platform molecules by enzymatic catalysis

Alexis Bolac,[1] Adrien Debard,[1] Jean-Louis Petit,[1] Camille Baland,[1] Pierre Loïc Saiidi,[1] Louis Mouterde,[2] Anne Zaparucha,[1] Carine Vergne-Vaxelaire[1]

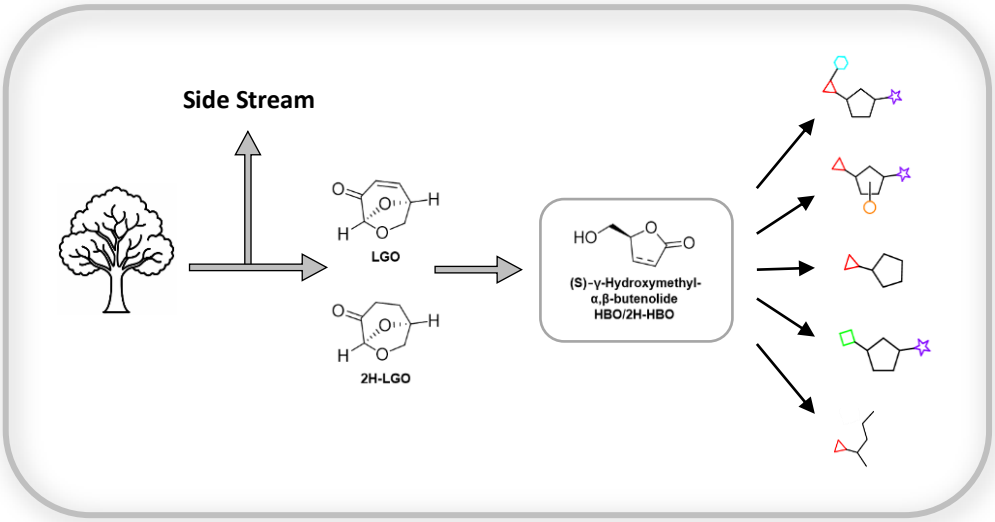
[1]Génomique Métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, 91057 Evry, France

[2]URD ABI, Ecole AgroParisTech, 51110 Pomacle

abolac@genoscope.cns.fr

Over the past two decades, the interest for biomass-derived compounds has grown rapidly, arising from the need to find sustainable alternatives to petro-based resources for our chemical industry.[1] The growing demand for sustainable molecules, along with the need for more efficient and selective synthetic route design, is strongly driving industrial implementation. Enzymes are powerful catalysts due to their high selectivity and their suitability for one-pot cascade reactions, providing sustainable and efficient reactions. Two interesting bio-based molecules, (S)-δ-Hydroxymethyl-α-β-butenolide (**HBO**) and its reduced form **2H-HBO**, stand out due to their multifunctionality and stereochemistry, which provide a wide range of potential applications such as drugs, flavours and antiviral agents' synthesis [2]. Currently, there is no enzymatic synthesis pathway to exploit these platform molecules. The aim of the project is to identify enzymes that catalyse the transformation of the chemical groups present in (2H-)HBO, to reach primary building blocks for the synthesis of more complex organic molecules (*Scheme 1*).

Alcohol Dehydrogenase family (ADH) has been particularly studied to catalyse oxidative and reductive transformations on small to large non-aromatic ring molecules [3]. We will present the preliminary results on the identification of ADH from biodiversity, obtained using a genome-mining approach, showing activity toward HBO/2H-HBO in the oxidation of the primary alcohol and the reduction of the lactone moieties.



Scheme 1. Exploration of a biomass valorisation pathway using (S)-γ-Hydroxymethyl-α,β-butenolide as key component to access building blocks

References :

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[2] Flourat A. L.; Peru A. A .M. ; Green Chem. **2015**, *17*, 404-412.

[3] De Miranda A. S.; Milagre C. D. F. Front. Catal. **2022**, *2*