GreenSolRes

Deliverable 2.1

Report on optimized catalyst in batch mode

Demonstration of solvent and resin production from lignocellulosic biomass via the platform chemical levulinic acid

The project leading to this application has received funding from the Bio Based Industries Joint Undertaking under the European Union's Horizon 2020 research and innovation programme under grant agreement No 720695

Bio-based Industries Consortium

BIO-BASED INDUSTRIES Public-Private Partnership

Horizon 2020 European Union Funding for Research & Innovation

About GreenSolRes

The need to establish economic and sustainable large-scale operations for the conversion of renewable resources to chemical building blocks is becoming increasingly urgent in the context of climate change and depleting fossil fuel reservoirs. Pathways for manufacturing of bio-based fuels and chemicals have been developed but most of them rely on sugar and starch crops for feedstock. GreenSolRes aims at a sustainable and competitive industrial production of the platform chemical levulinic acid (LVA) from lignocellulosic wastes and residues originating from forestry and agricultural sector. Further, the conversion of LVA into industry relevant building blocks γ-valerolactone (GVL), 1-methyl-1,4-butanediol (MeBDO) and 2-methyltetrahydrofuran (2-MTHF) will take place by new catalytic methods developed during the course of this project. Finally, these chemicals will be upgraded to solvents and resin monomers for the production of high added value adhesives and consumer products. This project was started in September 2016 and has a duration of four years.

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Hybrid Catalysis Custom Synthesis & Screening

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About this document

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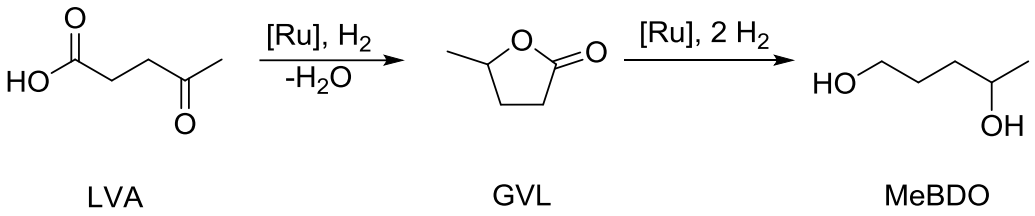
Publishable Summary

Within the first year of the GreenSolRes project, a tailored molecular catalyst should be developed, providing the envisaged activity, selectivity and stability in the consecutive hydrogenation of levulinic acid (LVA) to γ-valerolactone (GVL) and 1-methyl-1,4-butanediol (MeBDO) (Scheme 1).



Scheme 1: Conversion of LVA to GVL and MeBDO.

In the comprehensive scientific approach, a collection of potential catalyst structures was initially established and the selected organometallic compounds were synthesized in lab scale quantities. The novel catalyst structures were subsequently purified and fully characterized according to established criteria. Afterwards, the molecular catalysts were comprehensibly tested in dedicated high pressure autoclaves in the homogenous hydrogenation of LVA and GVL. Gratifyingly, a selection of the developed catalysts disclosed the envisaged key-performance indicators, paving the way to capable candidates for the considered large scale application. Consequently, the tailored molecular catalyst systems enabled a selective hydrogenation with a turnover number (TON) ≥ 250 000 and a space time yield (STY) of ≥ 1000 kg/l·h.

Abbreviations

acac	Acetylacetonato
BP	Boiling point [°C]
COD	Cyclooctadiene
DCM	Dichloromethane
DIBAL-H	Diisobutylaluminium hydride
eq	Equivalents
Et	Ethyl
GC	Gas chromatography
GVL	γ-Valerolactone
LVA	Levulinic acid
MeBDO	1-Methyl-1,4-butanediol
m%	Mass fraction
min	Minutes
mL	Milliliters
MTHF	Methyltetrahydrofuran
NMR	Nuclear magnetic resonance
p	Pressure [bar]
pKa	Acid dissociation constant
ppm	Parts per million
R	Organic moiety
S	Selectivity [%]
STY	Space time yield [kg/l·h]
T	Reaction time [min]
THF	Tetrahydrofuran
TMM	Trimethylenemethane
TON	Turnover number
Triphos	1,1,1-Tris(diphenylphosphinomethyl)ethane
T_{sol}	Temperature of complete solubility [°C]
X	Conversion [%]
Xyl / Xylyl	3,5-Dimethylphenyl
Y	Yield [%]
δ	Chemical shift [ppm]