GreenSolRes

Deliverable 4.7

STATUS REPORT ON THE SAFETY ASSESSMENT OF THE BIOMASS DERIVATIVES (2-MTHF, GVL AND MEBDO; INCLUDING DATA FOR IUCLID-REACH) AND CONCLUSIONS ON THE BENCHMARKING TO FOSSIL DERIVATIVES

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

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BBI JU

Bio-based Industries Consortium

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 often rely on sugar and starch crops for feedstock. The European Demonstration project - GreenSolRes aims at a sustainable and competitive industrial production of the platform chemical levulinic acid (LVA) from non-food lignocellulosic biomass. Further, the conversion of LVA and LVA esters 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 to produce high added value adhesives and consumer products.

Project Coordinator

RWTH AACHEN UNIVERSITY

Project Office

SYNCOM

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Catalysis LIKAT Leibniz-Institut für Katalyse e.V.

SYNCOM

Hybrid Catalysis Custom Synthesis & Screening

vito

BASF We create chemistry

Lenzing Innovative by nature

About this document

Deliverable №:	4.7	
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PU	Public	x
CO	Confidential, only for members of the consortium (including the Commission Services)	

Executive Summary

This report reflects the results of the safety assessment of the biomass-derived chemicals 2-methyl-tetrahydrofuran (2-MTHF), γ-valerolactone (GVL) and 1-methyl-1,4-butanediol (MeBDO) and of the benchmarking against fossil-based derivatives gamma-butyrolactone (GBL), 1,3-butanediol (1,3-BDO) and tetrahydrofuran (THF) respectively. The assessment included also the examination of potential influence of impurities resulting from feedstock sources or production processes in GreenSolRes samples on the toxicity, compared to commercial molecules.

Safety assessment was based on human and environmental hazard assessment and limit values for exposure on the one hand, and on expected exposure concentrations during manufacture and use of the chemicals.

For MeBDO, a number of human toxicity tests for REACH registration were performed with GLP certificate, which are usable for REACH registration. For human toxicity endpoints including *in vitro* skin and eye irritation, bacterial genotoxicity, human *in vitro* genotoxicity, acute oral toxicity and preliminary assessment of oral repeated dose toxicity for 14 days up to 2000 mg/kg bw no harmful effects were observed.

Test results indicated no toxicity for MeBDO and no impact of impurities on the toxicity of GreenSolRes-batches of MeBDO, GVL, 2-MTHF and levulinic acid.

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Comparison of environmental and human health toxicity profiles for the biobased substances and their fossil-fuel based benchmarks showed a less toxic profile for

1. GVL with lower human acute toxicity (GVL classified as not harmful, GBL as harmful), and GBL being on the regulatory list of drug precursors while GVL is not, and
2. 2-MTHF with expected lower risk from chronic exposure as the benchmark THF is classified as suspected carcinogen while the European Chemicals Agency (ECHA) did not request a carcinogenicity study for 2-MTHF.
3. For MeBDO the toxicity profile was similar to the benchmark.

Exposure modelling of MeBDO showed similar exposure levels and similar, low risk for humans and the environment as the benchmark. The same low risk is expected for GVL as for the benchmark. For 2-MTHF a lower risk from chronic exposure is expected than for the benchmark (THF) which is classified as suspected carcinogen.

Data confidentiality

VITO is not able to share more information in this report as VITO has the intention to write a peer-reviewed publication which includes the test results. Only data that have not been published elsewhere are acceptable for publication in a scientific journal, therefore VITO would prefer to keep the data confidential for now.
Since a new test is to be performed by VITO for inclusion in the manuscript and a multiple peer review process of journals also takes a long time, the envisaged timing for the first submission is 31/12/2022, and for manuscript acceptance with final publication 31/12/2023. It will be an open access publication.
Optional envisaged journals are (non-exhaustive list):

- Green Chemistry
- ChemSusChem
- Process Safety and Environmental Protection

More information on the results is available in the periodic report covering 01/09/2020 to 31/12/2021 (not publicly available) and in the confidential annex of the review report.

The GLP test reports will be made available via EU platform (e.g. Zenodo) after publication of the manuscript.