

Abstract PADDL-2

Polymer additives from lignin building blocks II, full cSBO with a proposed starting date on 1 December 2021 and a proposed duration of 30 months, with research partners UAntwerpen, KU Leuven, Centexbel and VITO. Follow-up project of the currently running Moonshot sprint cSBO project PADDL (<https://moonshotflanders.be/mot1-paddl/>).

The overarching goal of the cSBO PADDL project is to develop new polymer additives from lignin-derived platform molecules via the lignin-first biorefinery technology, employing reductive catalytic fractionation (RCF) on lignocellulose feedstock such as wood. These new polymer additives will hereby contribute to the reduction of CO₂ emissions by using renewable carbon. Additionally, they need to provide safer alternatives for current petrochemical additives of which many have been included in the REACH Authorization List or placed on the Candidate List in recent years.

The PADDL project will follow a 'safe by design' approach for the discovery of new plastic additives to avoid regrettable substitutions of petrochemical additives. Based on market size, plasticizers and flame retardants have been selected as targets for PADDL-2. In addition, the potential to combine two properties in one additive molecule will be evaluated. The designed and synthesized candidate molecules will undergo a rapid preliminary performance tests and those with promising properties become "hit compounds". Hit compounds are selected for the acute ecotoxicity screening and those which fulfil both the initial performance and acute ecotoxicity screening criteria become "lead compounds". Lead compounds undergo advanced ecotoxicity studies (assessment of potential chronic and behavioural ecotoxicity as well as mode of action tests when appropriate), as well as more advanced standardized performance testing. For the latter, a limited number of polymer matrices is chosen (PP and PLA for flame retardants, PVC and PLA for plasticizers). Subsequently, on those lead compounds which successfully passed all these studies preliminary human toxicity tests will be performed. Finally, compatibility of the new plastic additives with the recycling process (mechanical recycling of polymer with additive and/or extractive removal of the additive to facilitate the recycling) will be evaluated as well as the feasibility of production from real-life feedstock. This approach will lead to the identification of at least one New Molecular Entity (NME) in each of the two targeted application areas: flame retardants and plasticizers.

Further development of these NMEs towards the market is not a part of PADDL-2 and will be the subject of further R&D in collaboration with interested companies. This will involve various other aspects such as the optimization of the synthesis suitable for scale up, optimization of dosing in function of the application, long-term performance studies taking into account stability of the material (both the additive and the polymer itself) under various conditions, full profiling of (eco)toxicity towards REACH registration, pilot production and finally, commercial scale production.

For substantive questions about this project proposal, please contact MOT1 representative Isabelle Monnaie (imonnaie@catalisti.be; +32 471 506 833).