Development of PFAS-free coatings in a safe and sustainable by design (SSbD) approach- the PROPLANET project

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Poly- and perfluoroalkyl substances (PFAS) are widely used in diverse production sectors, including constructions, food packaging and textiles, for their water- and oil-repellence properties, high thermal stability, and durability. Despite these advantageous properties, PFAS have been heavily debated due to their high persistency in the environment and potential adverse health outcomes. Some PFAS species are subject to restrictions, and the European Chemicals Agency (ECHA) issued a full ban proposal in February 2023.

In this context, the EC Horizon Europe project PROPLANET aims to develop novel PFAS-free coating materials, to overcome the barriers for environmental and human safety, chemical improvements, and circular value chains. The main goal of PROPLANET is to design and optimise three innovative coatings for the industrial sectors textile, food-packaging, and glass, by applying Safety and Sustainability by design (SSbD) principles.

The PROPLANET approach for the safety of the new coatings is based on risk assessment and management requirements, and builds on previous experience and knowledge on hazard assessment, methods standardization, computational models and safe-by-design tools developed within H2020 projects such as RiskGONE, NanoSolveIT and SABYDOMA. A stage-gate approach for safety evaluation along the development process should ensure safer products by a cost- and time efficient manner. Starting from the early development phase of the materials, existing information and data on the toxicological properties of the individual chemicals have been collected, and data gaps identified. New approach methodologies (NAMs), both *in vitro* and *in silico* methods, have been reviewed and selected for gap filling studies, using a tiered approach consistent with the development and life-stage of the materials. In this respect, the development of Quantitative Structure-Activity Relationship (QSAR) models can contribute to the identification of safer PFAS-alternative substances. In this work, the Ames test for Mutagenicity endpoint was investigated using *in silico* in-house QSAR models.

In addition, the formulations developed (the chemical mixtures) are tested using *in vitro* methods for human hazard assessment. A tiered approach is applied in the project, where the traditional cellular models (or 2D models) and screening assays are used for hazard assessment in the earlier development phases of the project, and advanced (3D) models and assays will be used to test the final products. The testing strategy addresses

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main toxicological endpoints according to regulatory requirements and takes into consideration Adverse Outcome Pathways (AOPs) addressing key events linked to the potential toxicity of the new materials.

To conclude, the coatings are evaluated based on their technical performance while ensuring the safety and sustainability throughout their life cycle. This work also supports the international effort towards the acceptance of NAMs for regulatory use in view of next generation risk assessment (NGRA).