ASSESSING THE APPLICABILITY OF THE SAFE AND SUSTAINABLE BY DESIGN TOOLBOX: INSIGHTS FROM THE BISPHENOL A CASE

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ABSTRACT

The Safe and Sustainable by Design (SSbD) framework described by the EC JRC^{[1], [2]} aims to guide the innovation process towards the development and assessment of new and existing chemicals based on circular economy principles while mitigating any adverse effects on human health and the environment. Within the PARC project, an SSbD toolbox for the operationalization of the SSbD framework is being developed. The PARC SSbD toolbox will include and develop tools, as well as automated pipelines with model connections covering all the five steps of the framework through the innovation process. To test the applicability of the pilot version of the toolbox, we carried out a case study on Bisphenol-A and two alternative substances, Bisphenol AP and Isosorbide. The chosen substances were evaluated in two different applications: BPA replacement in polycarbonate bottles and BPA replacement in epoxy resin paints. The case study was implemented in both early and late innovation stages to evaluate if the toolbox could be utilized to its full potential in all stages and to investigate potential differences in the results obtained. In both cases, a range of tools was employed, including INTEGRA, ECETOC TRA and MERLIN-Expo. In terms of environmental sustainability assessment, a type of screening/prospective Life Cycle Assessment (LCA) was performed using the GaBi LCA software. In the early innovation stage, where data availability was limited, the application of Quantitative Structure-Activity Relationship (QSAR) models and tools, such as VEGA, was of significant importance in hazard predictions. Given that, the SSbD scores for Steps 1-3 exhibit variation based on the selection of QSARs. The incorporation of New Approach Methodologies (NAMs) alongside QSARs is highly important in addressing hazard potency. Furthermore, it is imperative to focus on the integration of reliable predictive models for toxicity, as well as tools for prospective LCA and socioeconomic assessment. In conclusion, the pilot run of the SSbD toolbox led valuable insights. These findings are significant in refining its functional and modeling framework, facilitating the development of an integrative toolbox consolidating numerous policies and strategies.

KEYWORDS: Safe and Sustainable by Design, Innovation, Toolbox, Safety, Sustainability

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