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Design of bio-based solvents

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The European consumption of solvents is significant, with about 6 million metric tons out of the 28 million tons worldwide consumed in 2012.[1] They are used in many applications such as the formulations of pesticides, inks, and paints, or for industrial cleaning, extraction / separation processes and syntheses. The depletion of fossil resources, stricter regulations and collective awareness for the environmental protection incite the development of alternatives to the use of petrochemical solvents. Therefore, the chemical industry shows a growing interest in designing bio-based solvents made from renewable raw materials and supposed to prevent hazards in the field of health, safety and environment.
Two methodologies different from the trial and error approach, were developed to design these novel bioproducts. The first methodology, predictive, is based on the properties prediction thanks to various models [2] before the synthesis of the molecules. The reverse design is, in turn, an innovative methodology to design molecules of biosolvents through a virtual laboratory. Stages of generation of molecular structures and properties prediction are integrated in a computer-aided molecular design tool (CAMD) providing solutions that meet the outlined specifications. This tool is able to help the chemist to find out the optimal structures in agreement with defined specifications in terms of physico-chemical properties (Hansen solubility parameters, boiling point, melting point, vapor pressure, and flash point), toxicity and ecotoxicity. [3]
These methodologies lead to identify a pool of candidate molecules derived from a bio-based building block that may act as a solvent for the target applications. Then, the relevance of these best candidates is checked with respect to their ability to be synthesized according to the green chemistry principles and their real performance in the target application. The feasibility of their syntheses is studied by retrosynthetic analyses.
The reverse design approach is more rational and efficient to find the best molecules suitable for the application: it presents the advantages to generate time, energy and cost-savings. Only potentially interesting molecules (with predicted properties meeting the specifications) are synthesized and validated in application.

References
[1] IHS Chemical Global Solvents Report: Opportunities for Greener Solvents
[2] M. Bergez-Lacoste, S. Thiebaud-Roux, P. De Caro, J.F. Fabre, V.Gerbaud, Z. Mouloungui, “From chemical platform molecules to new biosolvents: Design engineering as substitution methodology”, Biofuels, Bioproducts & Biorefining 2014, 8, 438-451.
[3] J. Heintz, J.P. Belaud, N. Pandyaa, M. Teles Dos Santosa, V. Gerbaud, Computer aided product design tool for sustainable product development, Computers and Chemical Engineering 2014, 71, 362–37

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