Solvents and solvo-surfactants : *Conception with GRASS, Modelling with COSMO-RS, Physicochemical and Functional Properties, Stability*

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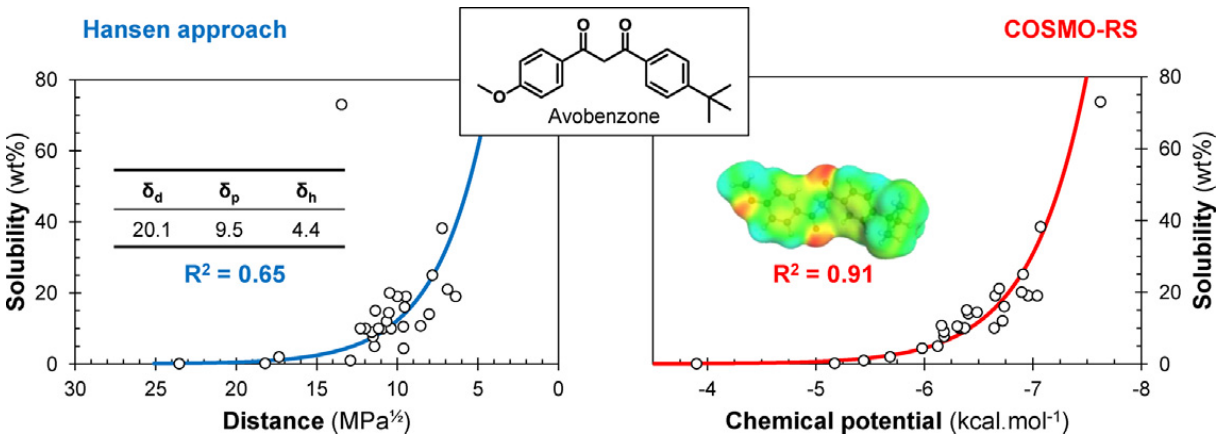
A number of tools have been developed in the laboratory to design virtual bio-based solvents meeting predefined specifications. The most promising candidates are then synthesized and their physicochemical and functional properties are measured and compared with predicted values.

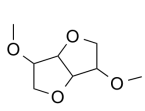
GRASS (GeneratoR of Agro-based Sustainable Solvents) is a computer-assisted organic synthesis program helping in the design of sustainable solvents from biomass feedstock. The method will be exemplified starting from itaconic acid, a multifunctional bio-based building block.

The solvent properties of virtual and actual solvents may be described through the traditional **Hansen solubility parameters** approach. Alternatively, the quantum chemical prediction model **COSMO-RS** allows the estimation of a wide range of solvent properties from the mere knowledge of the molecular structure.

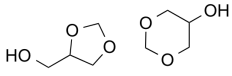
The performances of both methods will be compared by investigating the solubilisation of the UV-filter, avobenzone, in a series of cosmetic solvents.



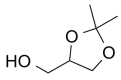
Finally the experimental properties (B.p., Flash Point, ΔH_{vap}) of bio-based solvents are assessed as well as their stability towards hydrolysis and autoxidation by oxygen. The methodology will be illustrated on new solvents derived from isosorbide (dimethylisosorbide) or glycerol (monoglyceryl ether and glycerol acetals and ketals).



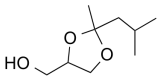
Dimethyl Isosorbide



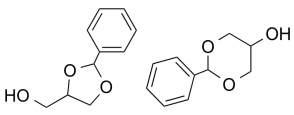
Glycerol formal



Solketal



1-2-Methylisobutylidene glycerol



Benzaldehyde glycerol acetal