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TOPIC(s) : Alternative solvents

Designing ionic liquids and deep eutectic solvents for enhancing the solubility of water-insoluble natural dyes

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PURPOSE OF THE ABSTRACT

Dyes and pigments have been used for dyeing materials, textiles and paper, in applied arts, in cosmetics and in food production for many thousands of years. Natural dyes are obtained from plants, animals or minerals but their usage is often limited by their low water solubility. Rational solvent design aiming at increasing their solubility can contribute to the improvement of dying processes and broaden their usage.
Herein, ionic solvents were designed by means of COSMO calculations [1,2] predictions and experimental solubility measurements in order to enhance the solubility of natural dyes.
The ionic solvents were designed using a two-step procedure. First, the most promising ion pairs for the dissolution of an active were selected in silico using COSMO predictions. [2] For example, Fig. 1 shows the results of the most promising ion pair for indigo solubilization. The same procedure was realized with carboxylic acids, organic bases or other molecular species in order to screen potential hydrogen bond donors for deep eutectic solvent formation. The second step consisted in the synthesis of the selected ionic liquids (ILs) or deep eutectic solvent (DES) prior to measure the experimental solubility of the natural dyes.

Once the best ILs and DES were selected the effect of water and surfactant on the experimental solubility of the natural dyes was assessed. For some natural dyes, the addition of small quantities of water can enhance their solubility in the ionic solvent (Fig. 2).[3] The use of ionic solvents such as ILs and DES for the dissolution of natural dyes, as well as their mixtures with water and surfactant will be discussed.

The molecular mechanism of solubility enhancement in the presence of water was studied by means of molecular dynamics simulations. Although the selected IL and DES are both ionic solvents, their local structure analysis revealed two different solvation patterns.[4]

By using these in silico methodologies and based on the selection of natural origin starting materials and eco-respectful processes, new promising green ionic liquids and natural deep eutectic solvents compliant with the green chemistry principles could be further proposed for the solubilization and formulation of water-insoluble natural actives.

FIGURES

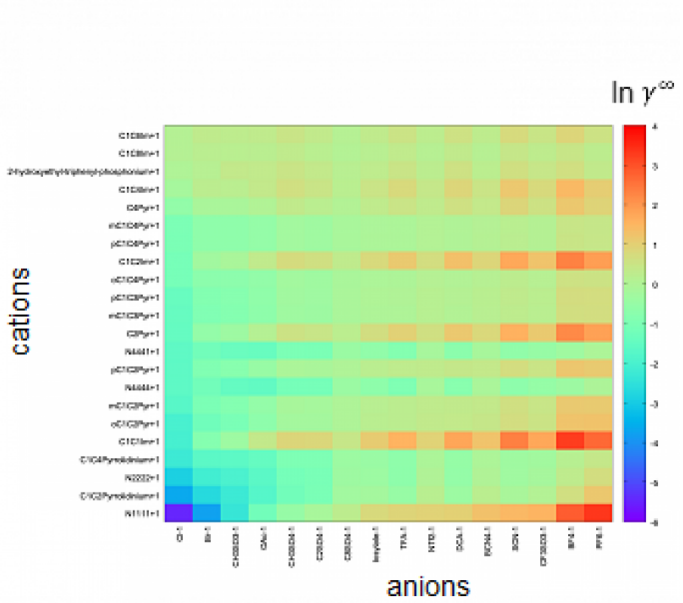

FIGURE 1

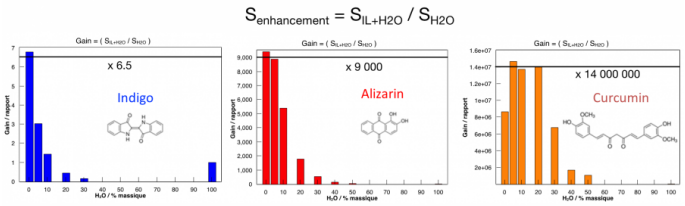

FIGURE 2

Fig 2. Indigo, alizarin and curcumin solubility enhancement as a function of water percentage in IL/H2O mixtures at 25°C in a designed IL.

KEYWORDS

ionic liquids | deep eutectic solvent | solubilization of pigments | COSMO calculation and molecular dynamics simulatio

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