

# The magic of aqueous solutions of ionic liquids: ionic liquids as a powerful class of hydrotropes

Ana Filipa M. Cláudio<sup>1</sup>, Márcia C. Neves<sup>1</sup>, Karina Shimizu<sup>2</sup>, José N. Canongia Lopes<sup>2</sup>, Mara G. Freire<sup>1</sup>, João A. P. Coutinho<sup>1</sup>

Advances in the dissolution of poorly soluble compounds in aqueous media play an important role in the formulation of more effective drugs, cleaning agents and personal care products. Hydrotropes are compounds typically used in these formulations to increase the concentration of hydrophobic solutes in aqueous solutions.

Recently, we demonstrated that ionic liquids are a new class of powerful hydrotropes, where both the cation and the anion synergistically contribute to increase the solubility of poorly water-soluble compounds in water.<sup>1</sup> The effects of the ionic liquid chemical structures, their concentration and the temperature on the solubility of two model solutes/antioxidants (vanillin and gallic acid) were evaluated and compared with the performance of conventional hydrotropes. The solubility of these two solutes was studied in the entire composition range, from pure water to pure ionic liquids, and an increase in the solubility of up to 40-fold was observed in aqueous solutions of ionic liquids. Using dynamic light scattering, nuclear magnetic resonance spectroscopy and molecular dynamics simulations, it was demonstrated that the remarkable enhanced solubility observed in aqueous solutions is related to the formation of ionic-liquid-solute aggregates, and that ionic liquids act as hydrotropes, as depicted in Figure 1.

Finally, we demonstrated that the hydrotropy phenomenon induced by ionic liquids can be used to recover value-added solutes from aqueous media by precipitation, simply by using water as an anti-solvent (the greenest solvent overall). The results obtained have a significant impact on the understanding of the promising role of ionic liquid aqueous solutions in the extraction of value-added compounds from biomass<sup>2</sup> as well as in the design of novel processes for their recovery from aqueous media. We are now actively engaged on the application of ionic liquids (hydrotropes) aqueous solutions to the extraction and recovery of value-added compounds with therapeutic properties from biomass.

<sup>1</sup> — Department of Chemistry & CICECO, University of Aveiro  
<sup>2</sup> — Centro de Química Estrutural, Instituto Superior Técnico, Lisboa

**FIGURE 1**

Simulation snapshots and discrete probability distribution functions of aggregate sizes,  $P(n_a)$  for different types of system and aggregate type. (a-b) Ionic liquid aqueous solutions; (c) water-vanillin mixture; (d-e) vanillin in ionic liquid aqueous solutions. (green graphs): ionic liquid polar aggregates (strands); (blue graphs): anion-water network; (red graphs) vanillin clusters.

