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BOOK OF ABSTRACTS

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Faculty of Science, University of Porto, Portugal

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POSTER COMMUNICATIONS (P)

Solubility of olive oil phenolic compounds in green solvents

POSTER_P3.20 - Phase Equilibria and Fluid Properties

Mariana Vale[1], Aline Zambom[1,2], Felipe Krüger[1], Mónia A. R. Martins[1], João A. P. Coutinho[2], Simão P. Pinho[1], António M. Peres[1], Olga Ferreira[1,*]

[1]*CIMO, LA SusTEC, Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal*
[2]*CICECO, Aveiro Institute of Materials, Complexo de Laboratórios Tecnológicos, Universidade de Aveiro, Campus Universitário de Santiago, Aveiro, Portugal*

**oferreira@ipb.pt*

The production of olive oil generates various by-products that are rich in phenyl alcohols, secoiridoids, phenolic acids and aldehydes, flavonoids, and other bioactive compounds. Due to their diverse biological activities, these compounds have promising potential as functional additives in the food, pharmaceutical, and cosmetics industries.[1] However, data on their solubility in water and common volatile organic solvents, as well as partitioning behavior—critical for optimizing extraction, purification, and formulation processes—remains very limited.[2]

In this study, the solubility of tyrosol (a phenyl alcohol) was experimentally determined in ten pure solvents and five aqueous binary solvent mixtures, using acetone, ethanol, 2-propanol, 1,3-butanediol, and 1,3-propanediol as co-solvents. Measurements were performed at 298 K using the analytical isothermal shake-flask method. Additionally, the COnductor-like Screening MOdel for Real Solvents (COSMO-RS)[3] using the default conformer distribution was employed to predict the solubility of tyrosol, hydroxytyrosol, and oleuropein in a wide range of pure organic solvents varying in polarity and functional groups, as well as in aqueous binary solvent mixtures. For tyrosol, the influence of solvent conformers and their apolar, hydrogen-bond donor, and acceptor characteristics on COSMO-RS predictions was analyzed, as illustrated in Figure 1 for water–ethanol mixtures. Overall, the model effectively captures general solubility trends, though with reduced quantitative accuracy in polar aprotic solvents, indicating its utility for preliminary solvent selection.

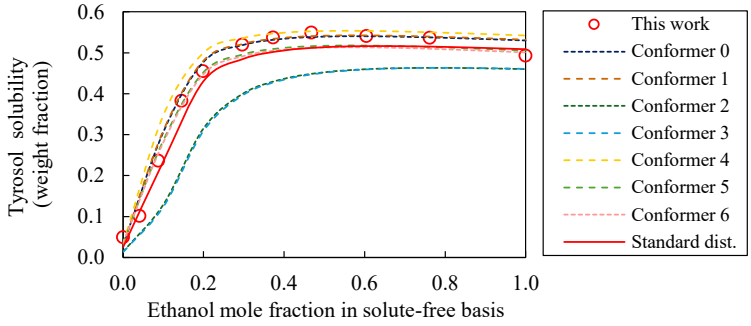

Figure 1: Solubility of tyrosol (in weight fraction) in binary mixtures of water and ethanol, at 298 K: experimental data (○, this work) and COSMO-RS predictions for different conformers of Tyrosol (C0 – C6).

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