

# ICCT 25

27<sup>th</sup> IUPAC International  
Conference on Chemical  
Thermodynamics

July 20 to 24<sup>th</sup>, 2025  
Faculty of Sciences  
University of Porto

## BOOK OF ABSTRACTS

Editor: José C. S. Costa  
Faculty of Science, University of Porto, Portugal

U. PORTO



27<sup>th</sup> IUPAC International  
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**Book of Abstracts of the 27th IUPAC International Conference on Chemical Thermodynamics**

**ICCT2025**

27th IUPAC International Conference on Chemical Thermodynamics - 20<sup>th</sup> to 24<sup>th</sup> July 2025

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José C. S. Costa

University of Porto, Faculty of Science

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## Solubility of olive oil phenolic compounds in green solvents

### POSTER\_P3.20 - Phase Equilibria and Fluid Properties

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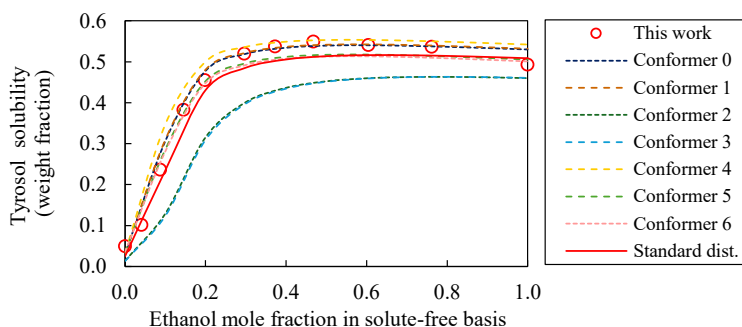
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The production of olive oil generates various by-products that are rich in phenyl alcohols, secoiridoids, phenolic acids and aldehydes, flavonoids, and other bioactive compounds. Due to their diverse biological activities, these compounds have promising potential as functional additives in the food, pharmaceutical, and cosmetics industries.<sup>1</sup> 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.<sup>2</sup>

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)<sup>3</sup> 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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