

Solubility of olive oil compounds in green solvents

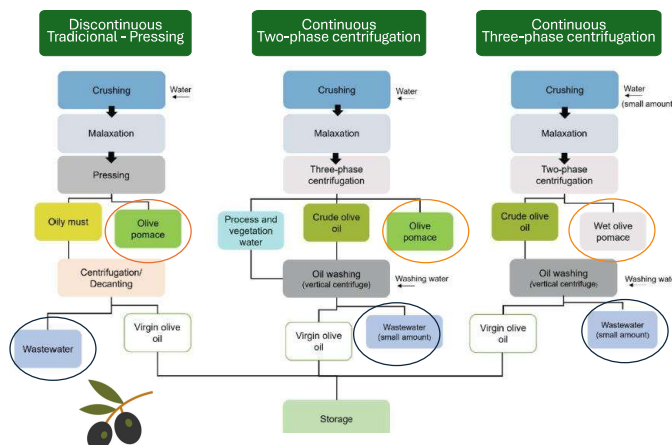
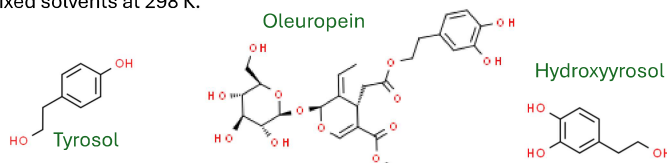
Mariana Vale¹, Aline Zambom^{1,2}, Felipe Krüger¹, Mónia A. R. Martins¹, João A. P. Coutinho², Simão P. Pinho¹, António Peres¹, Olga Ferreira^{1,*}

¹CIMO, LA SusTEC, Bragança Polytechnic University, Campus de Santa Apolónia, 5300-253 Bragança, Portugal.

²CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

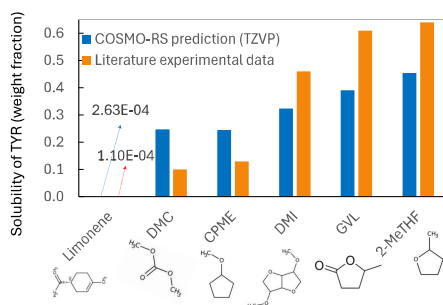
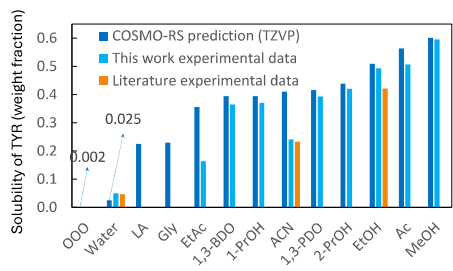
*oferreira@ipb.pt

- Olive oil production yields by-products rich in **bioactive phenolics** (tyrosol, hydroxytyrosol, and oleuropein) with potential uses in several types of industries. However, data on their **solubility** in water or organic solvents and **partition behavior**, essential for extraction and formulation, remain **limited**.
- COSMO-RS was used to **predict** their solubility of tyrosol, hydroxytyrosol, and oleuropein in a wide range of **pure** and **aqueous mixed solvents**. **Tyrosol solubility was also experimentally measured** in ten pure and five aqueous mixed solvents at 298 K.

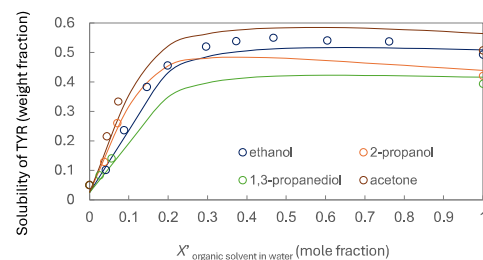


Results

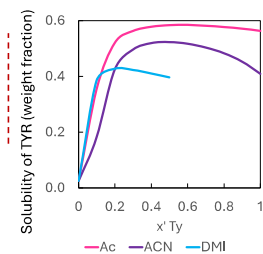
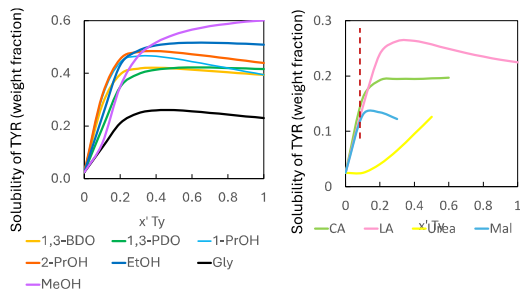
Tyrosol solubility in pure solvents



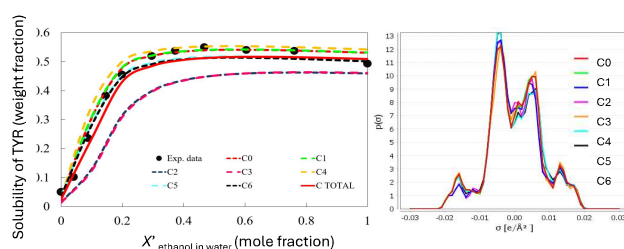
Solubility enhancement in mixed solvents



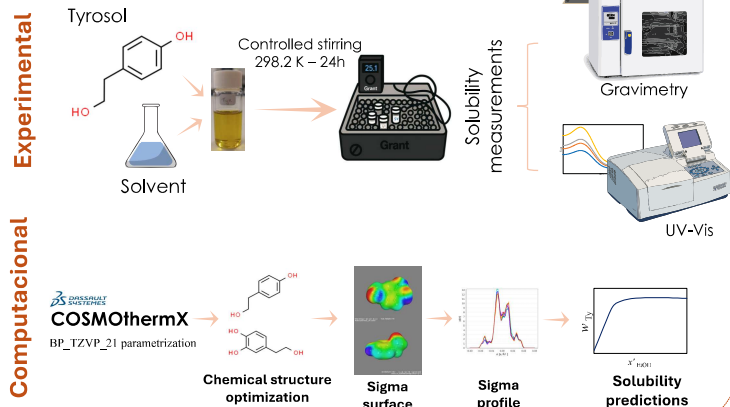
Solubility enhancement in mixed solvents



Tyrosol solubility with different conformers



Methods



Take-home message

- COSMO-RS showed good accuracy for protic solvents (e.g., methanol and ethanol) but was less precise for aprotic solvents (e.g., acetonitrile and ethyl acetate), suggesting further refinement.
- A consistent correlation was observed between the experimental data and COSMO's predictions, considering different conformers and sigma-profile interactions. For Ty, conformers C2 and C3 showed the least interaction with hydrogen bonding, leading to underestimated solubility values.
- DMI emerged as the most effective green co-solvent, while lower solubilities were predicted in glycerol, gamma-valerolactone, lactic acid, limonene, and triolein.
- TYR generally demonstrated greater solubility across solvents with less co-solvent needed compared to HTYR.
- Further experimental data using a broader range of solvents at different temperatures, and solutes (HTYR and oleuropein) are needed.

Acknowledgements

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