There is no "away": The CO₂ invoice when using non-conventional media or water in biocatalysis.

Pablo Domínguez de María

Sustainable Momentum, SL. Av. Ansite 3, 4-6. 35011 Las Palmas de Gran Canaria. Canary Is. Spain. E-mail: <u>dominguez@sustainable-momentum.net</u>

Biocatalysis has emerged as a sustainable alternative for many synthetic processes.^[1] To sustain the greenness of enzymatic procedures the simple qualitative use of the Green Chemistry Principles is oftentimes employed. This has created the misleading perception that biocatalysis is green *per se*, regardless of other important aspects of the reaction (e.g. substrate loadings, the downstream unit, etc.). To validate the greenness of the reactions, the need of incorporating quantitative green chemistry metrics appears mandatory.^[2]

This is particularly relevant when the reaction media is considered. Biocatalytic processes can be performed in water or in non-conventional media. Once the synthesis is terminated, two main waste streams are generated: i) a wastewater effluent if reactions are performed in water as reaction system; ii) and an organic fraction, coming from enzymatic reactions in non-aqueous media, and from the downstream processing. The fate of the wastewater treatment can be the Wastewater Treatment Plant (WWTP), whereas incineration is commonly applied for the organic fractions and water-based recalcitrant effluents. Both approaches generate CO₂, what can be used as the common metric to compare (bio)catalytic reactions (kg CO₂ \cdot kg product⁻¹).^[3,4]

This presentation will discuss how biocatalysis can become a green and efficient alternative for chemical processes when environmental metrics – in particular, the CO_2 production –, are measured in relation to the fates of the wastewater and the organic fraction. Several scenarios will be presented, emphasizing the need of setting recycling loops and intensified processes to reach decent sustainable metrics. In particular, a forward-discussion on the fate of Deep Eutectic Solvents (DES) and their environmental impact will be provided.^[5]

References.

[1] Alcántara, A.R.; Domínguez de María, P.; Littlechild, J.; Schürmann, M.; Sheldon, R.; Wohlgemuth, R. Biocatalysis as Key to Sustainable Industrial Chemistry. *ChemSusChem* **2022**, *15*, e202102709.

[2] Domínguez de María, P. Biocatalysis, sustainability and industrial applications: Show me the metrics. *Curr. Op. Green Sust. Chem.*, **2021**, *31*, 100514.

[3] Onken, U.; Koettgen, A.; Scheidat, H.; Schueepp, P; Gallou, F. Environmental metrics to drive a cultural change: Our Green Eco-Label. *Chimia* **2019**, 73, 730.

[4] Biocatalysis in water or in non-conventional media? Adding the CO_2 production for the debate. *Molecules* **2023**, 28, 6452.

[5] Domínguez de María, P.; Kara, S. On the fate of Deep Eutectic Solvents after their use as reaction media: The CO₂ production during downstream and ultimate disposal. *RSC Sustainability* **2024**, *2*, 608-615.