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Deep Eutectic Solvents for the Enzymatic Synthesis of Sugar Esters: A Generalizable Strategy?

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PURPOSE OF THE ABSTRACT

Sugar Fatty Acid Esters (SFAEs) (or just “sugar esters”) are non-ionic surfactants with excellent emulsifying, stabilizing, and detergent properties. Moreover, they are tasteless, odourless, non-toxic, benign to the environment, fully biodegradable, and can be derived from renewable sources.

The preparation of these industrially relevant compounds is cumbersome due to the opposite solubility profile of the substrates, i.e. the polar head (sugar) and the hydrophobic tail (fatty acid), which forces the use of environmentally unfriendly reaction media and harsh operational conditions. As a result, high energy consumption, formation of byproducts, and low regioselectivity are encountered. [1,2] In this context, using nonconventional (benign) media and an enzyme-based synthesis can overcome the above-mentioned drawbacks.

Whereas glucose and saccharose esters have been widely studied in this frame, lactose has been underinvestigated despite its large availability, being the most abundant component of cheese whey, the main waste stream of the dairy industry.

Herein, [3] deep eutectic solvents (DESs) were considered as promising reaction media, starting from the evidence that glucose-based esters can be obtained by lipase-based (trans)esterification of this monosaccharide with different acyl donors in classic DESs like choline chloride/urea (ChCl/U) as well as in hydrophobic DESs. [4,5] However, when lactose is used, enzymes cannot efficiently perform (trans)esterifications in a number of DESs (ChCl/U, ChCl/Lac.H2O, lidocaine/palmitic acid), while the same reactions can proceed in “conventional” mixtures like pyridine/tetrahydrofuran (Py/THF).

Computational solubility studies and molecular dynamics simulations (Figure 1) [3] of both ChCl/U and Py/THF systems played a pivotal role to rationalize this output, highlighting two effects: (i) on the one hand, large acyl donors (more than C10) display poor solubility in DESs and (ii) on the other hand, lactose interacts with DES components. Thus, the DES affects the conformation of lactose (compared to that observed in the Py/THF mixture), in such a way that the enzymatic reaction results impaired.

Despite that classic DESs (e.g., ChCl/U) may not be useful for generalizing their use in saccharide ester synthesis, we hope that the theoretical understanding of the reaction here achieved will pave the way for designing novel DESs that can broaden the use of these solvents in sugar chemistry.

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FIGURES

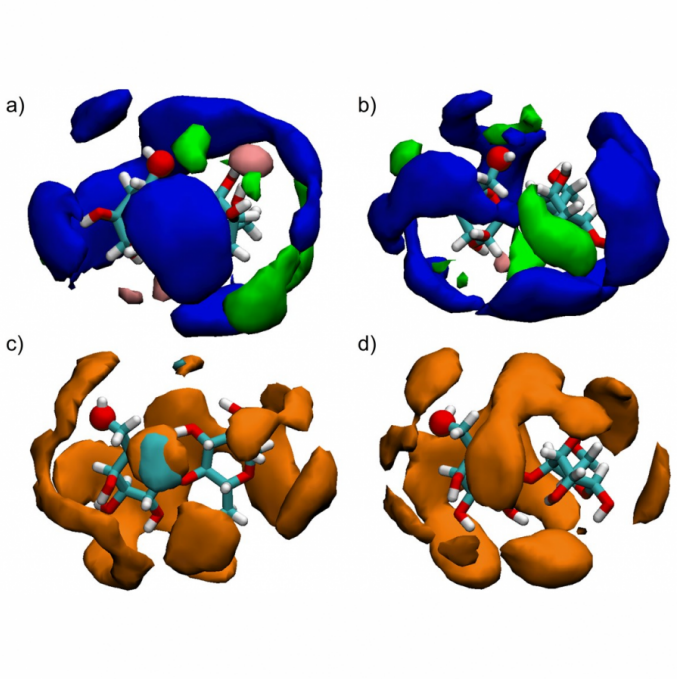

FIGURE 1

Figure 1

FIGURE 2

KEYWORDS

deep eutectic solvents | lactose esters | molecular dynamics simulation | COSMO-RS

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