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Supporting information (SI)

Lipase-catalysed esterification in a reactive natural deep eutectic solvent leads to lauroylcholine chloride rather than glucose ester

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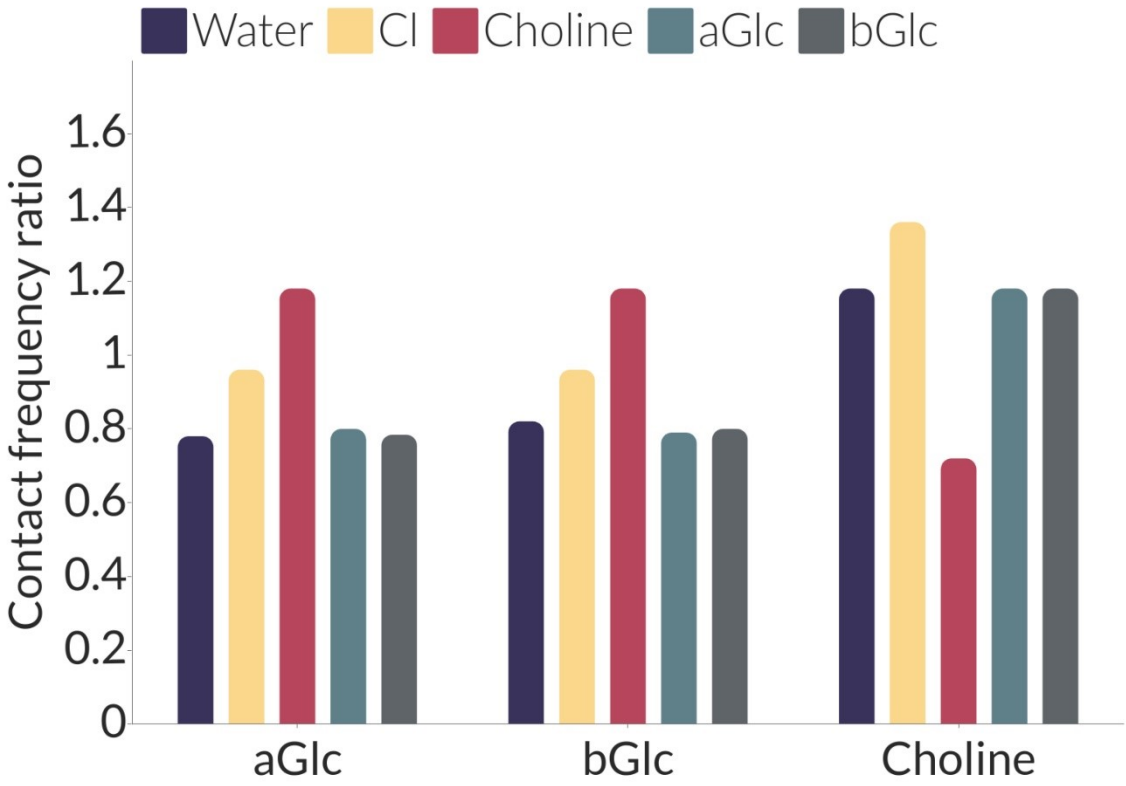

Figure S1. Contact frequency ratio of α- and β-glucose and choline with all the components of the NADES in the proportion ChCl:Glucose:water (2:1:1) obtained from MD trajectories.

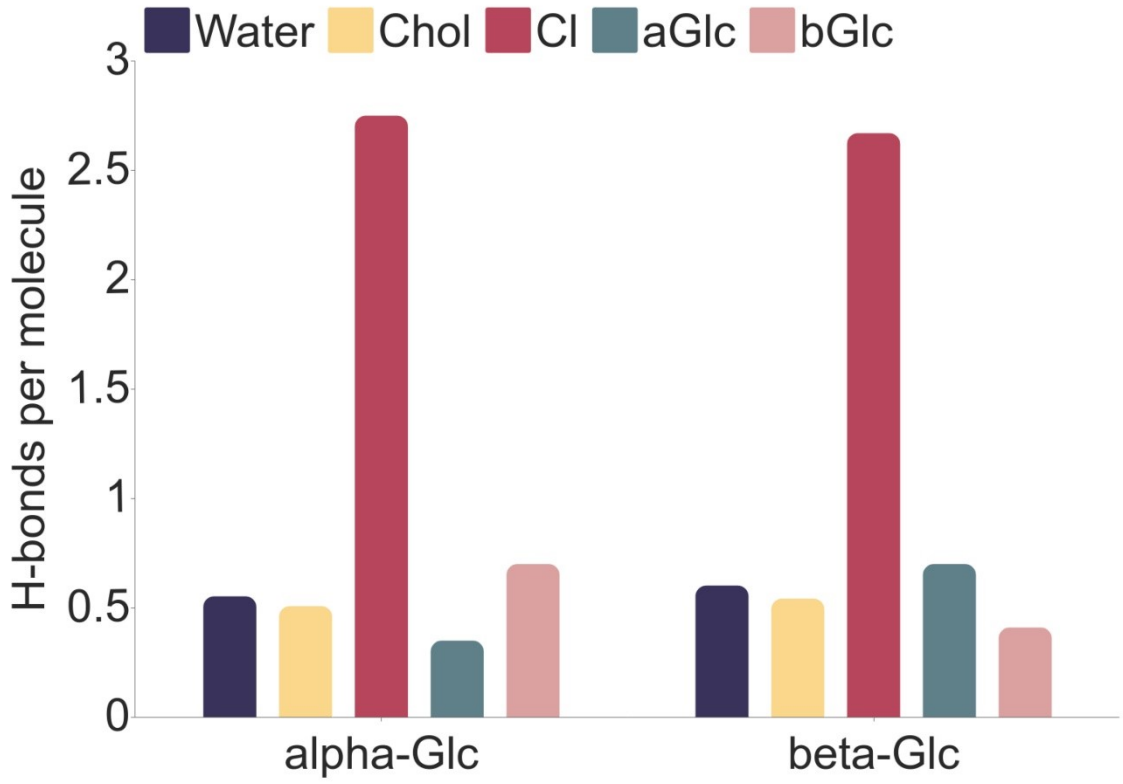

Figure S2. H-bond analysis of α- and β-glucose with all the components of the NADES in the proportion ChCl:Glucose:water (2:1:1) obtained from MD trajectories.

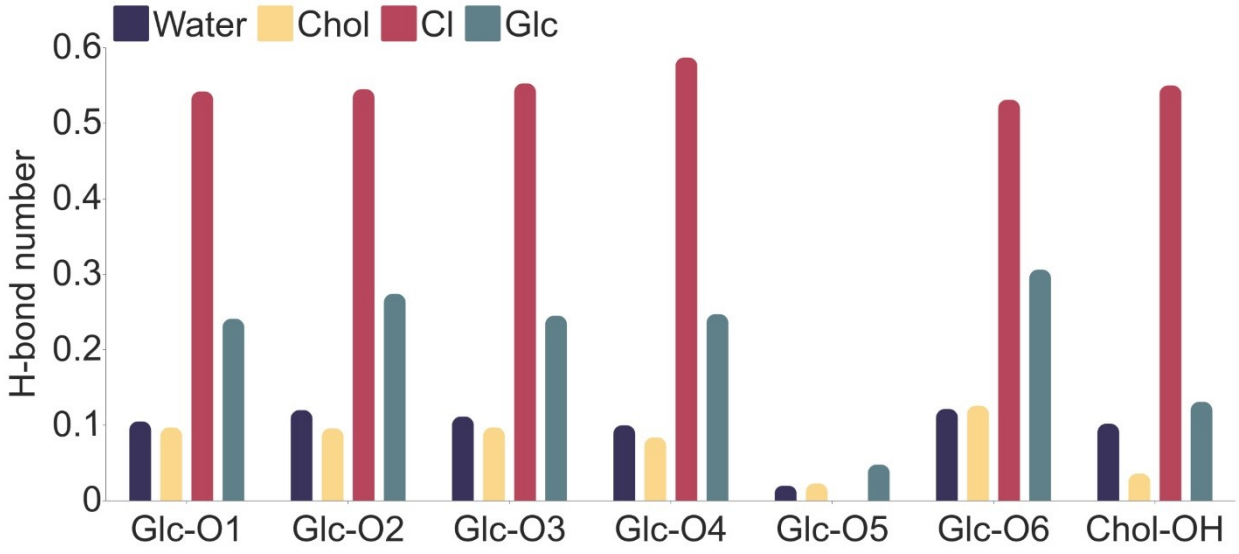

Figure S3. H-bond analysis of each hydroxyl group of glucose and choline with all the components of the NADES in the proportion ChCl:Glucose:water (2:1:1) obtained from MD trajectories.

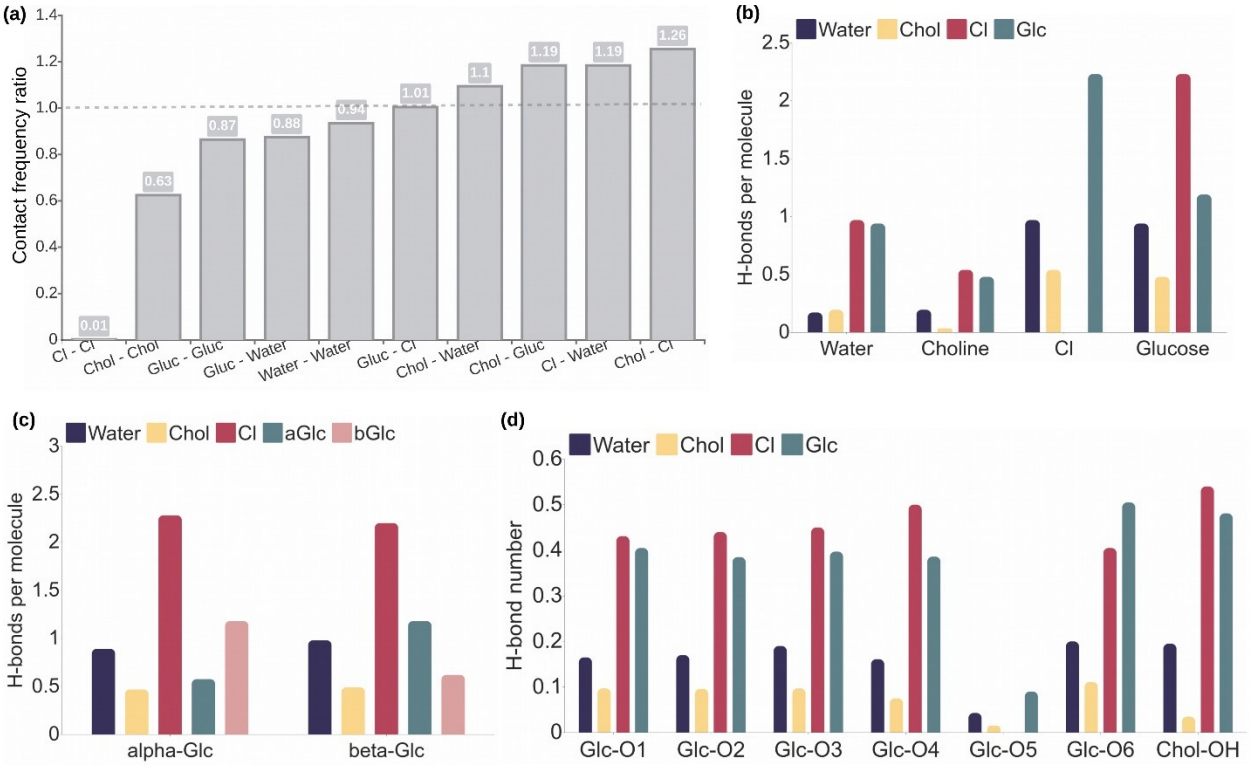

Figure S4. Computational structural analysis of CalB in glucose-based NADES (1:1:1). (a) Contact frequency ratio, (b) H-bond analysis between the different components in the NADES ChCl:glucose:water (1:1:1) obtained from MD trajectories. (c) H-bond analysis of α- and β-glucose with all the components of the mixture. (d) H-bond analysis of each hydroxyl group of glucose and choline with all the components of the NADES.

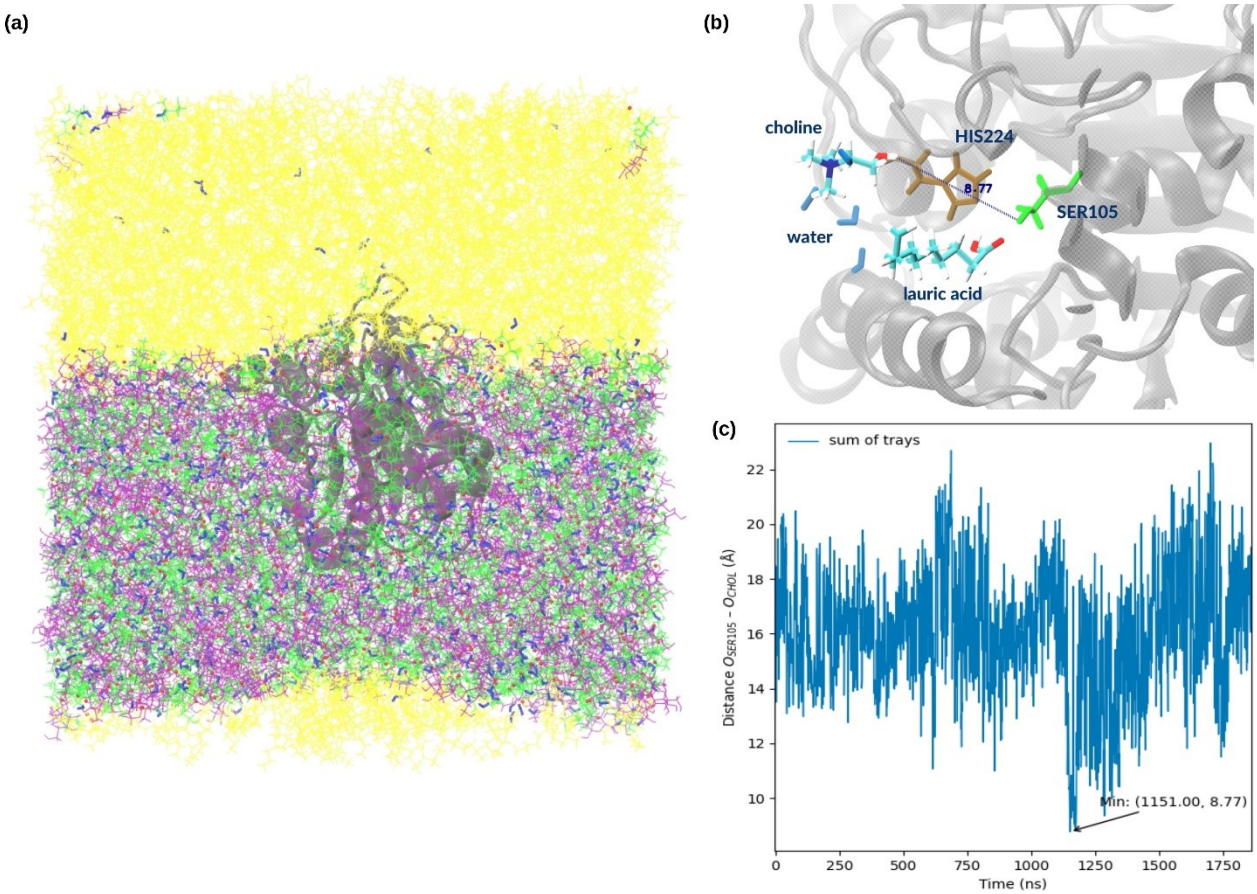

Figure S5. Computational structural analysis of CalB in glucose-based NADES and lauric acid (1:1:1:1). (a) Representative snapshot of the bibasic equilibrated system. The components are colour-coded for clarity: lauric acid (yellow), glucose (purple), choline (green), water (blue) and chloride ions (red). (b) Representative snapshot of the CalB catalytic pocket from MD trajectories, focusing on the binding between lauric acid molecule and Ser105 and the closest location of a choline molecule to the catalytic residue. (c) Evolution of the atomic distance between the hydroxyl oxygens of Ser105 and the choline molecule at the entrance of the pocket in the same MD trajectories.

Table S1. Number of molecules used in the different systems for the MD simulations**.**

	Simulation box				
	R-NADES		R-NADES + CalB	R-NADES+CalB+LA	
R-NADES proportion	*(1:1:1)*	*(2:1:1)*	*(2:1:1)*	*(1:1:1)*	*(2:1:1)*
Choline molecules	500	2000	2001	1001	2001
Chloride molecules	500	2000	2000	1000	2000
α-D-glucose molecules	250	500	500	500	500
β-D-glucose molecules	250	500	500	500	500
Water molecules	500	1000	1000	1000	1000
Lauric acid molecules	-	-	-	1000	1000

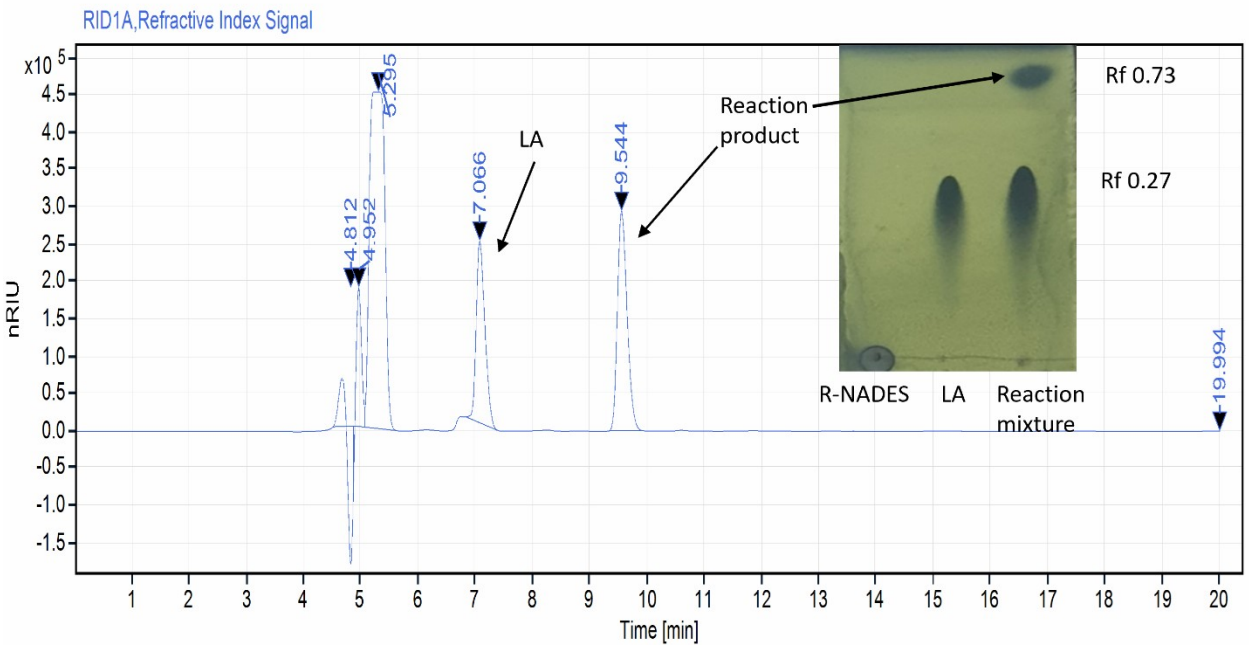

Figure S6. HPLC of a reaction mixture at 24 h, showing the unreacted lauric acid (LA) at 7.066 min, and the reaction product, eluted at 9.544 min. The insert is the TLC of the same reaction mixture, that clearly shows the reaction product (R_f 0.73).

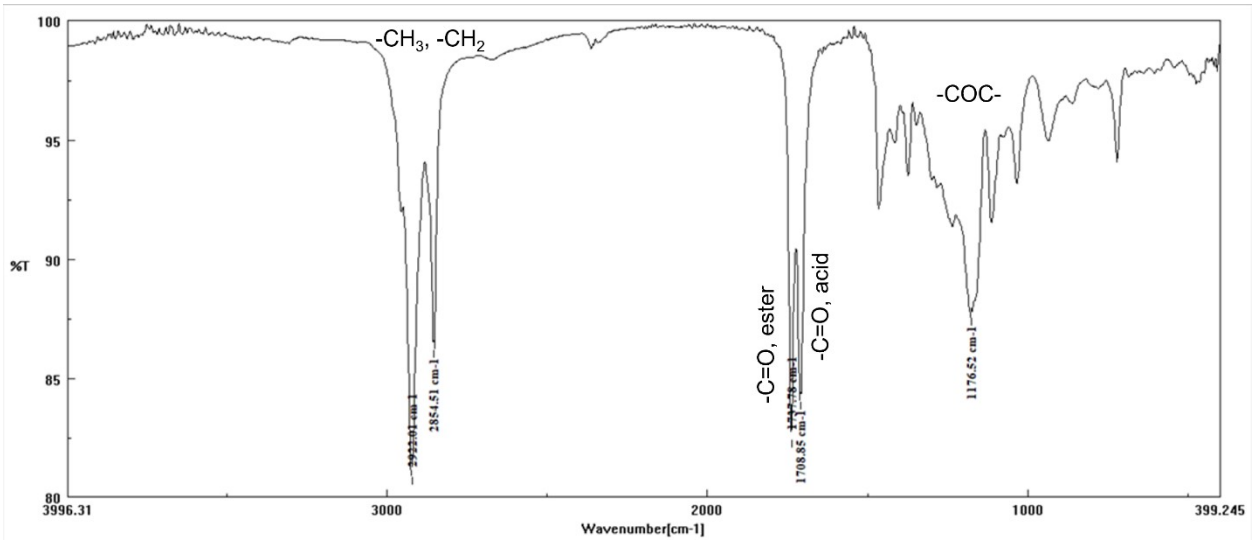

Figure S7. FTIR spectrum of hexane extract, showing the ester and free lauric acid.