Synthesis of cholesterol-reducing sterol esters by enzymatic catalysis in biobased solvents or solvent-free

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Figure S1. Kinetic screening of the esterification of β-sitosterol using different lipase enzymes. The control experiment contained no enzyme. CR= Candida rugosa, CALA= Candida antarctica lipase A, CALB= Candida antarctica lipase B.



Figure S2: Plot of the natural logarithm of the initial reaction rate in different solvents versus their polarity. No correlation is seen.



Figure S3: Plot of the natural logarithm of the initial reaction rate in different solvents versus their basicity. No correlation is seen.



Figure S4: Plot of the natural logarithm of the initial reaction rate in different solvents versus their molar volume. No correlation is seen.



Figure S5: Plot of the natural logarithm of the initial reaction rate in different solvents versus

their partitioning coefficient. A correlation is seen with an R2= 0.86. The solvents that follow the trend are shown in red. The three outliers are shown in blue.



Figure S6. Kinetic study of the esterification of β -sitosterol at different reaction temperatures.



Figure S7. Kinetic study of the esterification of β-sitosterol with different acyl donors. Butyric acid (C4:0); Caprylic acid (C8:0); Lauric acid (C12:0); Stearic acid (C16:0) and Behenic acid (C22:0).



Figure S8. ¹H NMR spectrum of ß-sitosterol.



Figure S9. ¹³C NMR spectrum of ß-sitosterol.



Figure S10. ¹H NMR spectrum of Stearic acid.



Figure S11. ¹³C NMR spectrum of Stearic acid.



Figure S12. ¹H NMR spectrum of ß-sitosterol ester. Characteristic peaks assigned to protons by A-F.



Figure S13. ¹³C NMR spectrum ß-sitosterol ester. Characteristic peaks assigned to carbons by A-D.