SUPPLEMENTARY MATERIAL FOR:

Transesterification of soybean oil using a switchable-hydrophilicity solvent, 2-(dibutylamino)ethanol

Kelsey J. Viner, Hannah M. Roy, Roland Lee, Ouwen He, Pascale Champagne,^{*} and Philip G. Jessop^{*}

Analysis of the FAME mixture

A standard SupelcoTM 37 component FAME mixture (with known concentrations) obtained from Sigma-Aldrich Co. was used to determine the concentration of FAMEs in our unknown samples. Linear calibration curves for each of the FAMEs with known concentrations were created on graphs with the peak area as a function of concentration and then based on the peak areas obtained for each of the FAMEs in our unknown samples, the concentrations of FAMEs were determined by plugging in the peak area values in the linear calibration curve (y=mx+b) associated with each of the FAMEs. Then, each of the FAME concentrations were converted to a percentage based on the total composition of FAMEs.

NMR spectra



Figure S1. The ¹H NMR spectrum of crude (not esterified) soybean oil.



Figure S2. The ¹H NMR spectrum of 2-DBAE.



Figure S3. The ¹H NMR spectrum of the FAME product mixture after initial washing with carbonated water. Peaks of 2-DBAE are visible at 2.6 and 3.5 ppm. The large singlet at 3.68 ppm is the methyl group of the methyl esters.



Figure S4. The ¹H NMR spectrum of the FAME product mixture after repeated washing with carbonated water. Peaks of 2-DBAE are no longer visible at 2.6 and 3.5 ppm. Note also that peaks at 3.86, 3.95 and 5.10 which would indicate¹ the presence of 2-monoacylglyceride, 1-monoacylglyceride, or 1,2-diacylglyceride are either absent or very small.

References

 Nieva-Echevarría, B., Goicoechea, E., Manzanos, M.J., Guillén, M.D., 2014. A method based on ¹H NMR spectral data useful to evaluate the hydrolysis level in complex lipid mixtures. *Food Res. Int.* (2014) *66*, 379-387. https://doi.org/10.1016/j.foodres.2014.09.031