Electronic Supplementary Material (ESI) for Food & Function. This journal is © The Royal Society of Chemistry 2019

Supporting Information

Lipid digestion of oil-in-water emulsions stabilized with low molecular weight surfactants

Natalie Ng¹, Peter X. Chen^{1,2}, Saeed M. Ghazani¹, Alejandro Marangoni¹, H. Douglas Goff¹, Iris J. Joye¹, and Michael A. Rogers^{1*}

Corresponding Author

*Email: mroger09@uoguelph.ca

¹Department of Food Science, University of Guelph, Guelph, Ontario, Canada, N1G 2W1 ²School of Pharmacy, University of Waterloo, Waterloo, Ontario, Canada, N2L 3G1

Proton NMR

The ¹H NMR spectrum was collected on a Bruker AVANCE III 600 MHz spectrometer (Bruker, Milton, ON, Canada) equipped with a 5 mm TCI cryoprobe (Bruker, Milton, ON, Canada). A 20 uL sample of purified sn-2 glycerol monooleate (2-GMO) was dissolved in 600 uL CDCl₃ (99.9%, Cambridge Isotype Laboratories, Tewksbury, MA, USA) and temperature was regulated at 298 ± 1 K. The spectrum was referenced to residual internal CHCl₃ (δ 7.26). Purified 2-GMO: ¹H NMR (CDCl₃, 600 MHz): δ 5.34 (m, 2H), 4.92 (quint, 1H, J = 4.7 Hz), 3.83 (m, 4H), 2.37 (t, 2H, J = 7.6 Hz), 2.01 (m, 4H), 1.64 (quint, 2H, J = 7.4 Hz), 1.28 (m, 36.6H), 0.88 (t, 12.6H, J = 7.0 Hz). The inflated integrations of 36.6H and 12.6H are due to residual heptane in the sample (Figure S1). These assignments are consistent with those reported for sn-2 monoglycerides from soybean oil ⁸³.

The region from 5.25 to 3.5 ppm of the ¹H NMR spectrum (Figure S2) included intense peaks attributed to glycerol backbone protons of 2-GMO and low intensity peaks corresponding to the glycerol backbone protons of diolein and *sn*-1/3 glycerol monooleate. Other low intensity peaks in this region included a multiplet corresponding to a CH₂ group from the ethyl oleate byproduct at 4.11 ppm and a peak at 4.02 ppm attributed to an unknown impurity, which was also present in the ¹H NMR of the pure triolein starting material (data not shown). By integrating all the peaks in this region, the purity of 2-GMO was calculated relative to all the glycerol-containing compounds and found to be ~97 mol %.

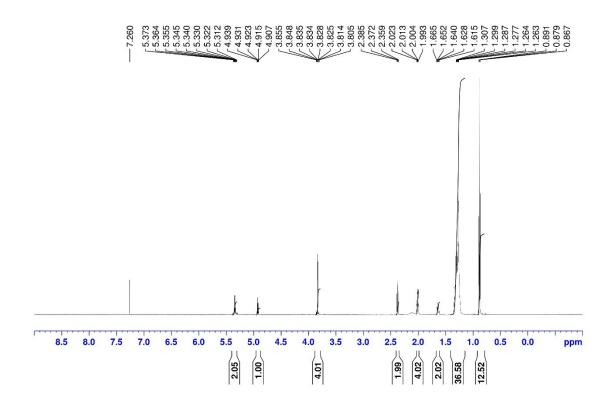


Figure S1. ¹H NMR spectrum (CDCl₃, 600 MHz) of 2-GMO.

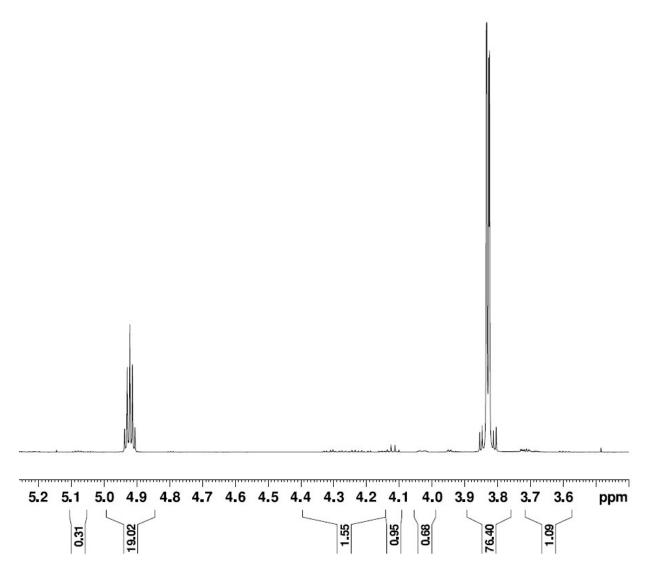


Figure S2. ¹H NMR spectrum (CDCl₃, 600 MHz) of the glycerol backbone region of 2-GMO.

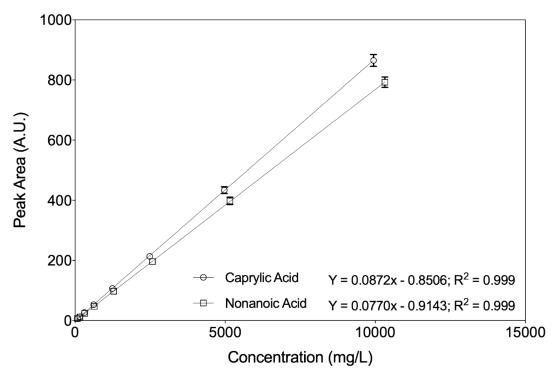


Figure S3. Calibration curves for nonanoic acid and caprylic acid in acetonitrile-water (60:40) over a concentration range of 78-10000 mg/L using HPLC-DAD with absorbance set to 210nm.

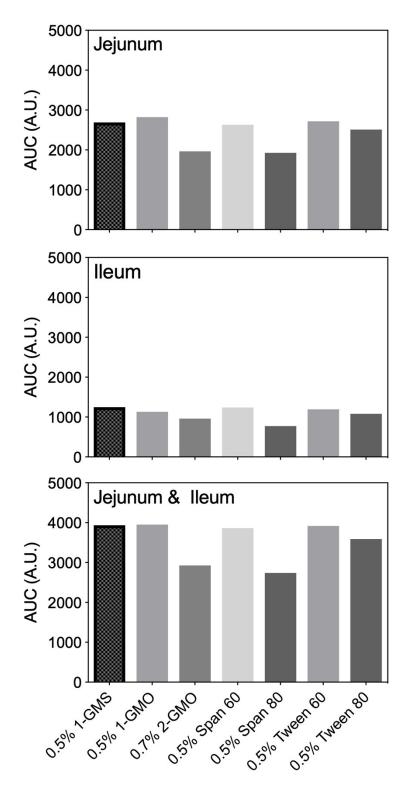


Figure S4. Area under the curve (AUC, expressed in A.U.) calculated from the absolute bioaccessibility values of caprylic acid over the 5 h digestion period using the trapezoid method.