

SUPPORTING INFORMATION

Sophorolipid butyl ester: an antimicrobial stabilizer of essential oil-based emulsions and interactions with chitosan and γ -poly(glutamic acid)

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Natural sophorolipids (SLs) production via fermentation

SLs were prepared by fermentation of *Starmerella bombicola* using 40 g of high oleic acid sunflower oil, 100 g of glucose, 10 g of yeast extract, and 1 g of urea for 1 L of water following a literature procedure.¹ The crude SLs were extracted with ethyl acetate from the fermentation broth and the solvent was removed by rotary-evaporation under vacuum. The crude product, a mixture of oil and SLs, was dissolved in ethyl acetate at 77 °C and then an equal volume of hexane was added. The hexane/ethyl acetate solution was kept at -20°C for overnight until lactonic SLs (white precipitates) were obtained. The precipitate was then filtered and dried. This was repeated until all oil had been removed. Analysis of the final mixture by LC–MS following a literature procedure showed that the major component (approx. 95 mol%) is di-acetylated LSL.²

Synthesis of SLBE

The synthesis of SLBE was performed via ring-opening transesterification under alkaline conditions. LSLs (10 g) was dissolved in 15 mL 1-butanol at 100 °C. Sodium (0.15 g) was reacted with 5 mL 1-butanol for 1 h to prepare sodium butyrate. The LSLs/butanol solution was treated with sodium butyrate at 100 °C for 4 h under N₂ atmosphere. Reaction progress was tracked by silica thin layer chromatography using CHCl₃/CH₃OH (8:2 v/v) as the eluent. Upon completion, the reaction mixture was acidified to pH 4 with 3M HCl and solvent was removed by rotary-evaporation under vacuum. The crude product (brown solid) was dissolved in of boiling ethanol (15 mL) to which 100 mL iced water was added. The ethanol/water solution was kept at -20 °C overnight until a white precipitate was obtained. The precipitate was then filtered and lyophilized. Further purification was performed by flash chromatography with an automated Biotage SP system (Charlotte, NC, USA) fitted with a 100 g Biotage silica SNAP column. The eluent was CHCl₃/CH₃OH with a gradient from 95% to 60% CHCl₃ over 2376 mL total volume. The final purified SLBE product was obtained in 60% yield as a white solid (melting point 140 °C). Structure analysis of SLBE was performed by LC-MS, ¹H NMR, and ¹³C NMR. Results of these analyses when compared to spectra of closely related SL-esters confirmed that SLBE was obtained in high purity (> 98%).^{3,4}

Lipid phase viscosity

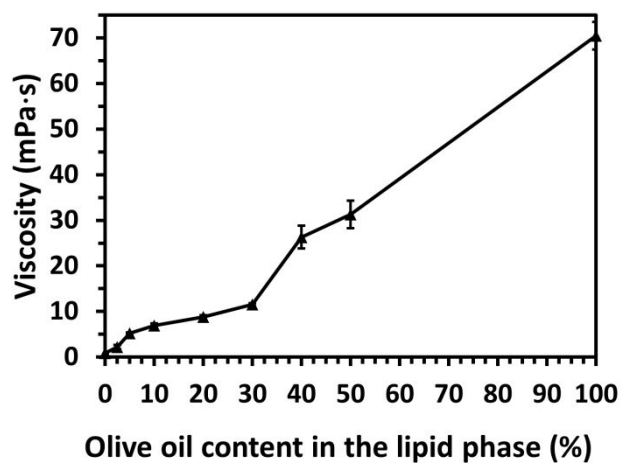


Figure S1. Lipid phase viscosity at different olive oil content. At 0%, the lipid phase contains pure oregano oil, whereas, at 100%, the lipid phase consists of pure olive oil.

Table S1. Values of lipid phase viscosity at different olive oil content

Olive oil content	Viscosity (mPa·s)
0 %	0.9 ± 0.2
2.5 %	2.2 ± 0.5
5 %	5.2 ± 0.2
10 %	6.9 ± 0.5
20 %	8.8 ± 0.38
30 %	11.5 ± 0.37
40 %	26.3 ± 2.5

50 %	31.3 ± 3
100 %	70.5 ± 3

Viscosity of γ -PGA/CH emulsions

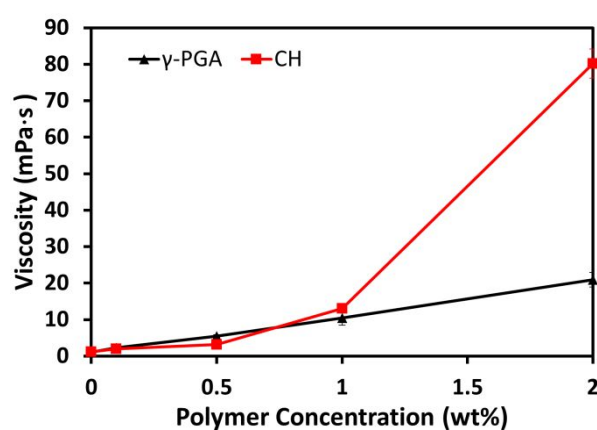


Figure S2. Emulsion viscosity as a function of polymer concentration. Emulsions were prepared with acetate buffer (10 mM for γ -PGA emulsions and 100 mM for CH emulsions, pH 3.6) at 0.5 wt% SLBE and 5wt% oregano/olive oil (4:1 w/w). All measurements were taken at 25 °C.

References

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