

Supporting data for

Lipophilic arginine esters: The gateway to preservatives without side effects

Authors: Iram Shahzadi^a, Aamir Jalil^a, Mulazim Hussain Asim^{a,b}, Andrea Hupfauf^c, Ronald Gust^c, Philipp Alexander Nelles^d, Ludwig Knabl^d, Andreas Bernkop-Schnürch^{a,*}

^aCenter for Chemistry and Biomedicine, Department of Pharmaceutical Technology, Institute of Pharmacy, University of Innsbruck, Innrain 80-82, A-6020 Innsbruck, Austria.

^bDepartment of Pharmaceutics, Faculty of Pharmacy, University of Sargodha, 40100 Sargodha, Pakistan.

^cCenter for Chemistry and Biomedicine, Department of Pharmaceutical Chemistry, Institute of Pharmacy, University of Innsbruck, Innrain 80-82, A-6020 Innsbruck, Austria.

^dInstitute of Hygiene and Medical Microbiology, Department of Hygiene, Microbiology and Public Health, Medical University of Innsbruck, Schöpfstrasse 41, A-6020 Innsbruck, Austria.

*Corresponding author:

Andreas Bernkop-Schnürch, e-mail address: andreas.bernkop@uibk.ac.at;

Tel: +43 512 507 58601, Fax: +43 512 507 58699

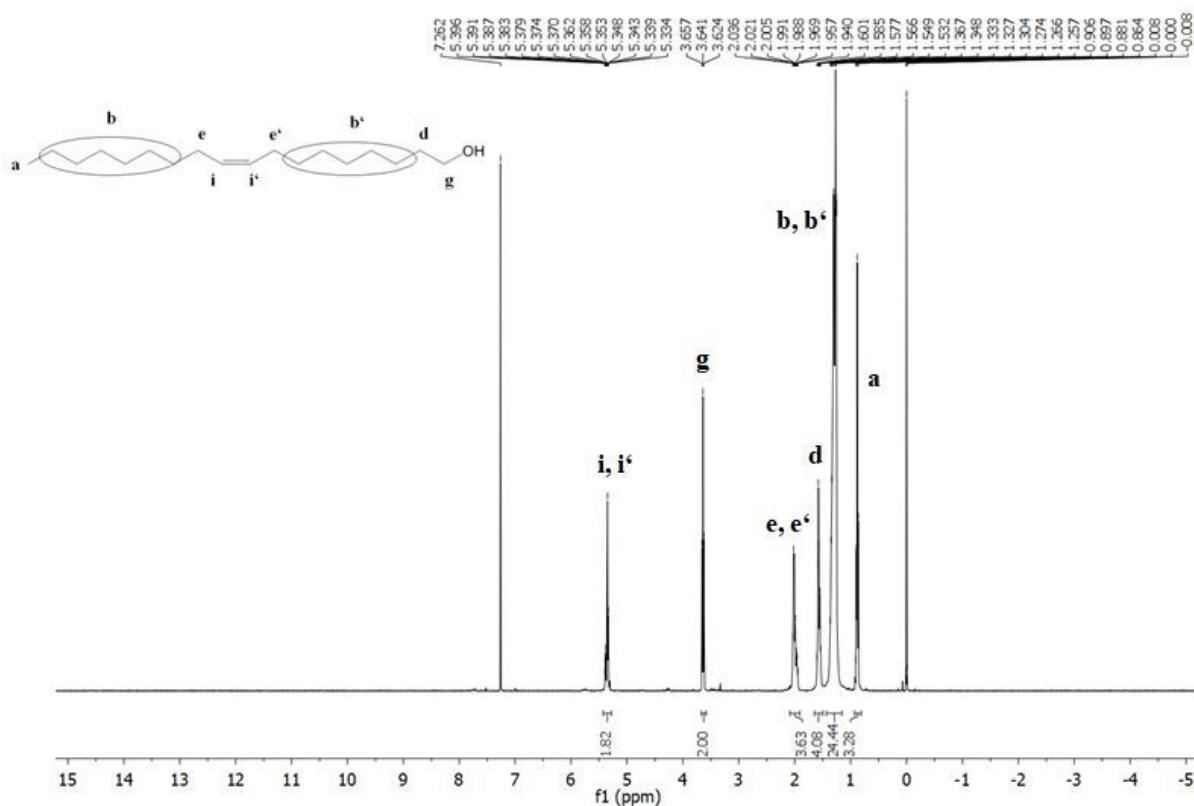


Figure S-1: ^1H -NMR spectrum of OL (oleyl alcohol) in deuterated chloroform.

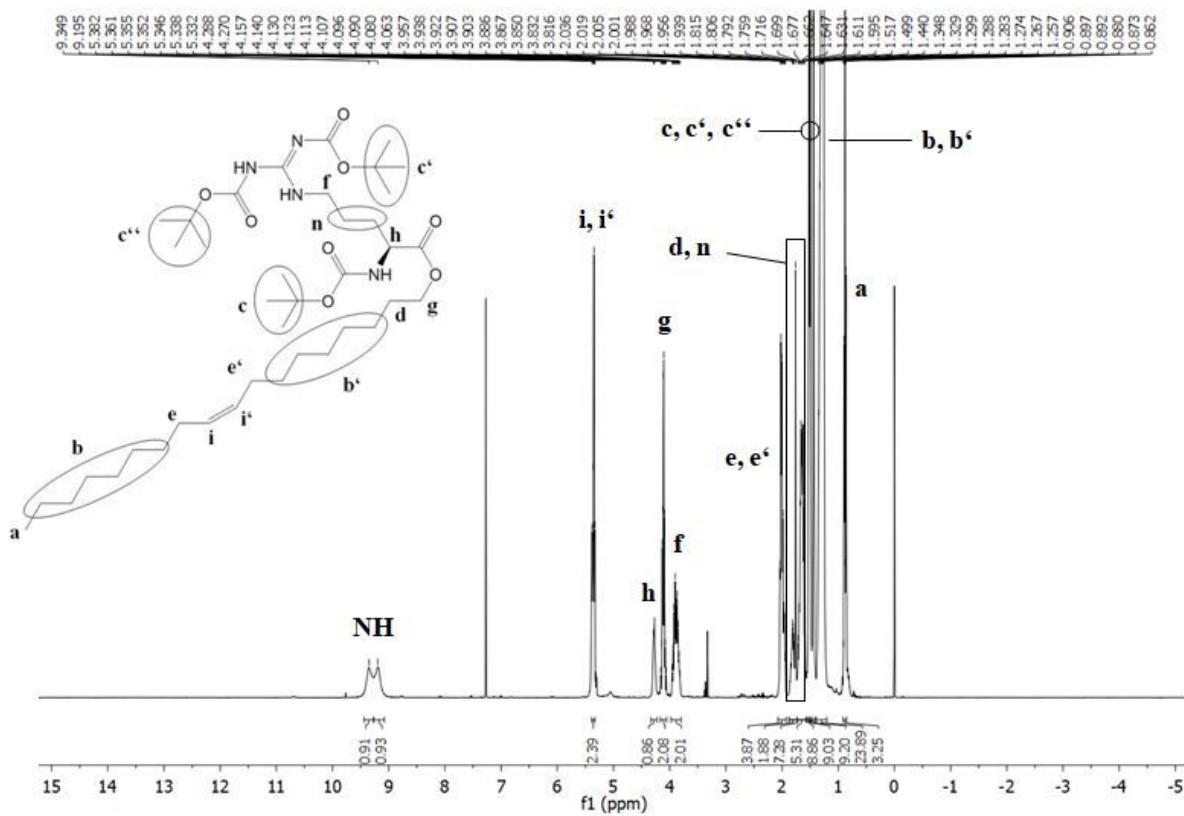


Figure S-2: ^1H -NMR spectrum of Boc-Arg-OL (Boc-protected octadec-9-en-1-yl arginate) in deuterated chloroform.

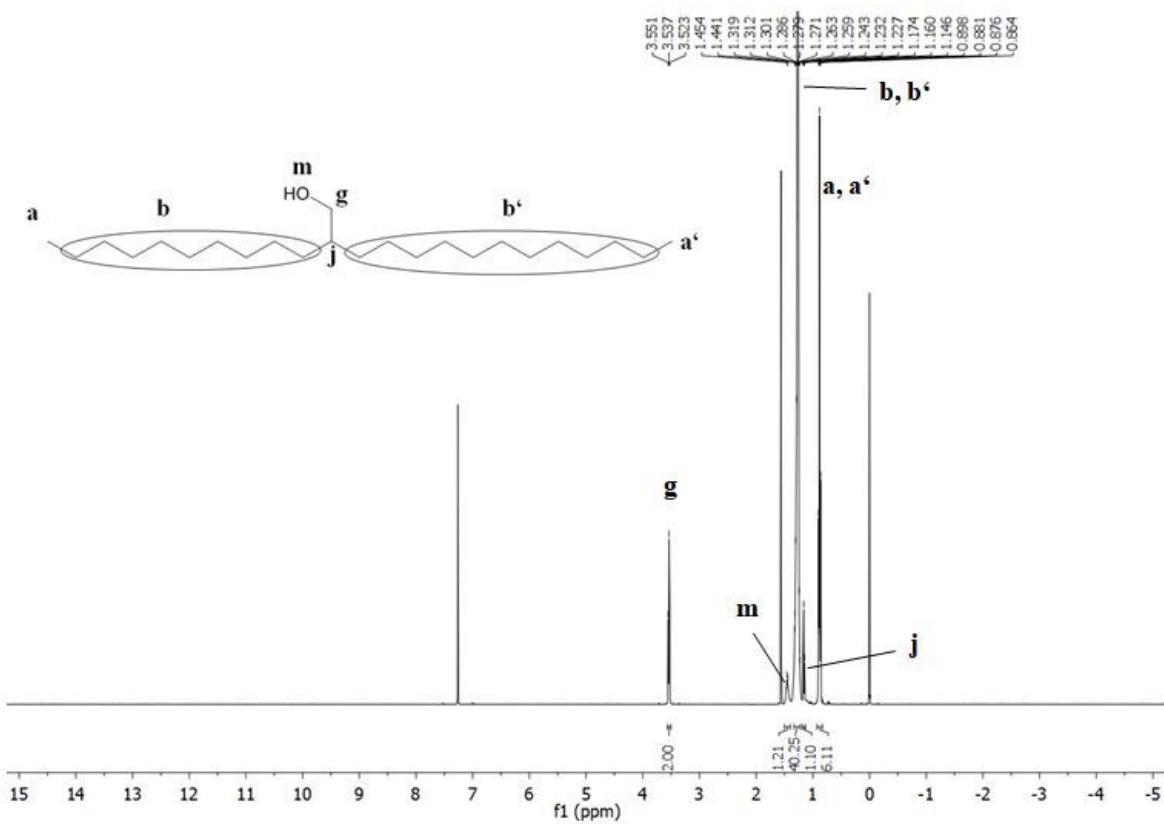


Figure S-3: ^1H -NMR spectrum of DT (2-decyldtetradecyl) in deuterated chloroform.

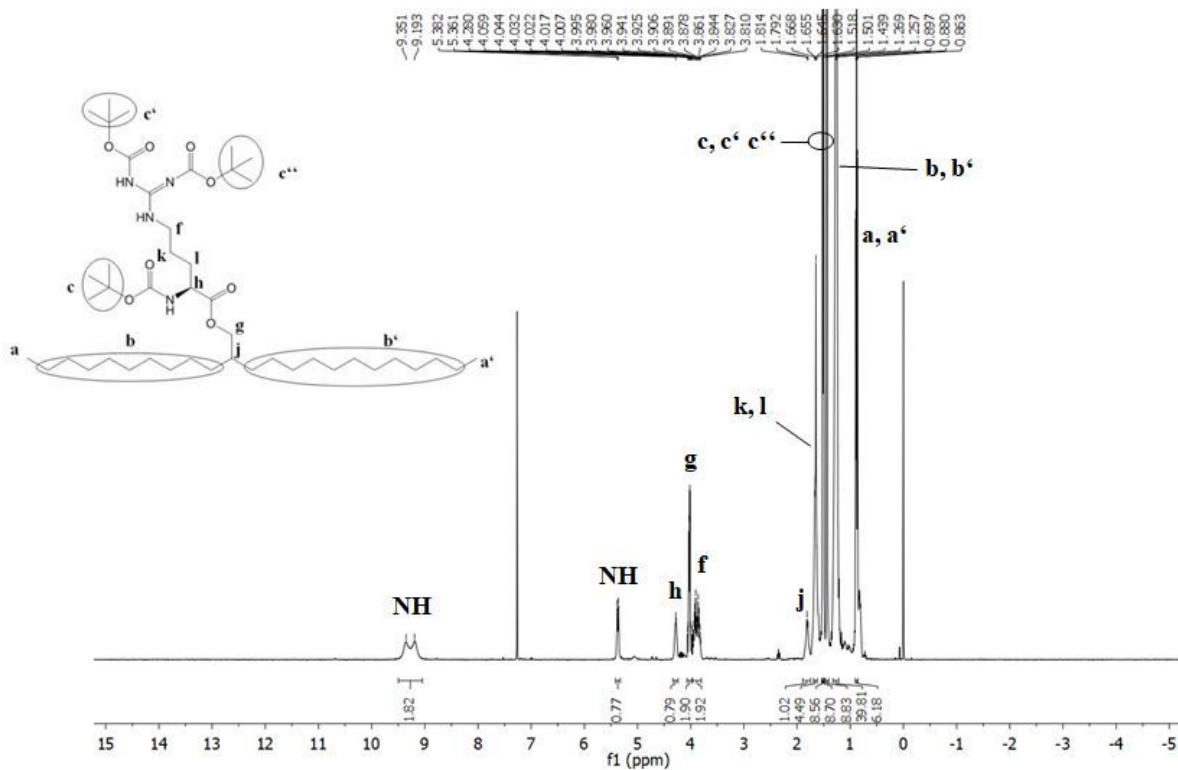


Figure S-4: ^1H -NMR spectrum of Boc-Arg-DT (Boc-protected 2-decyldodecyl arginate) in deuterated chloroform.

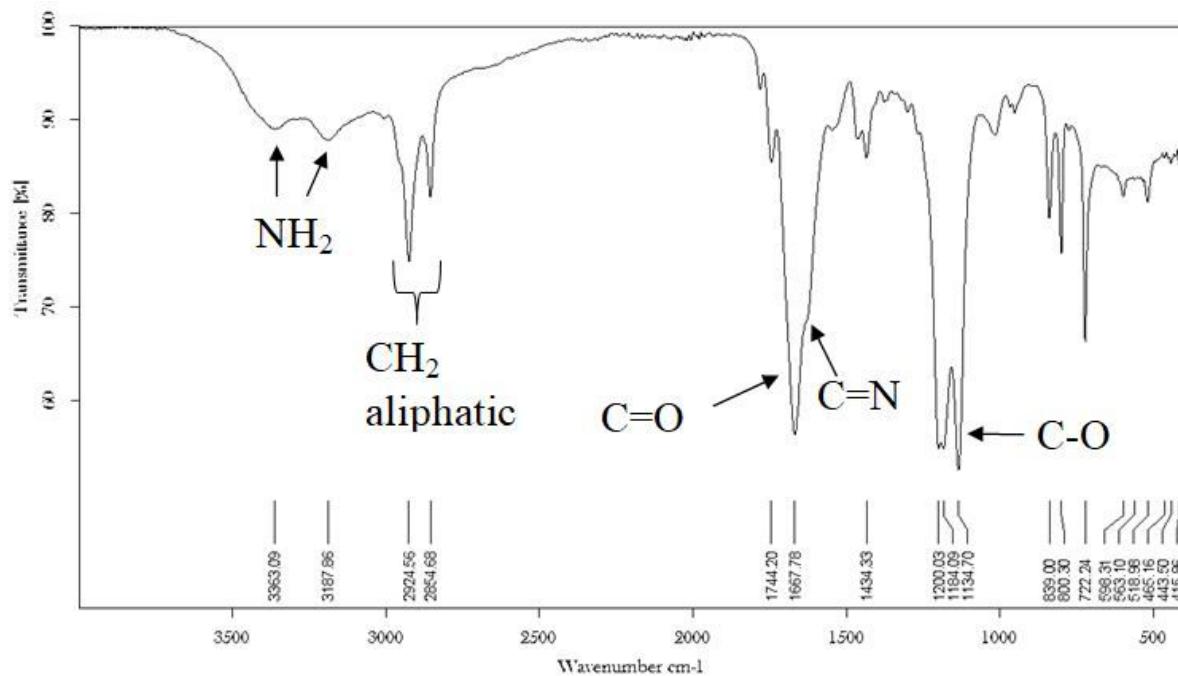


Figure S-5: IR spectrum of Arg-OL (octadec-9-en-1-yl argininate).

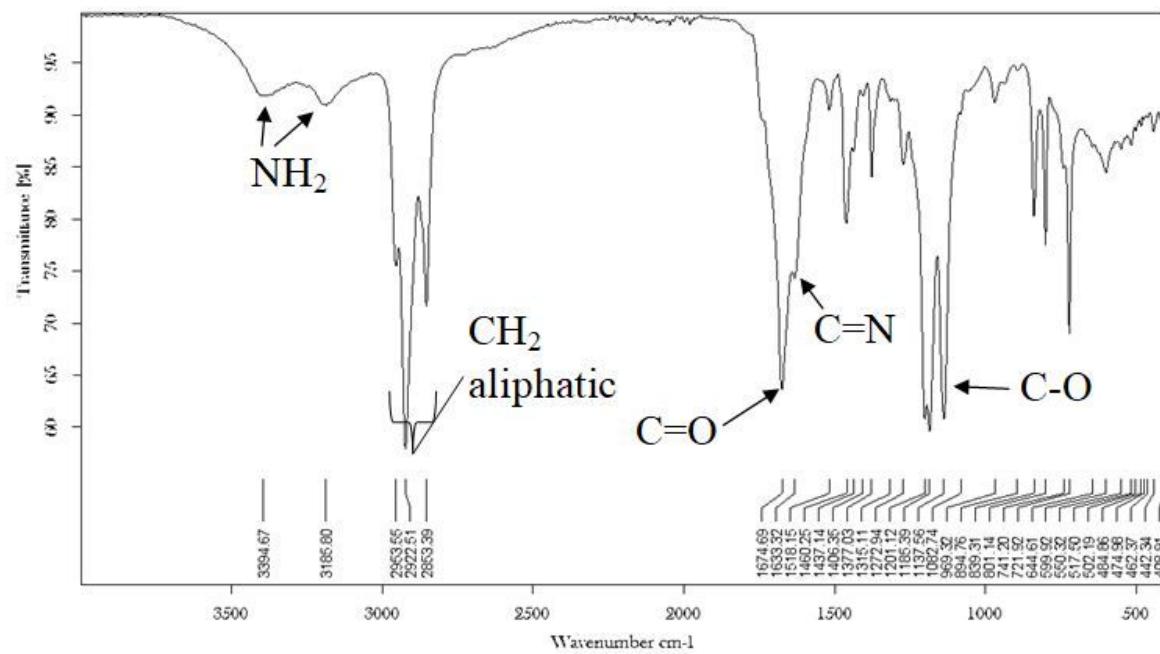


Figure S-6: IR-spectrum of Arg-DT (2-decyldodecyl argininate).

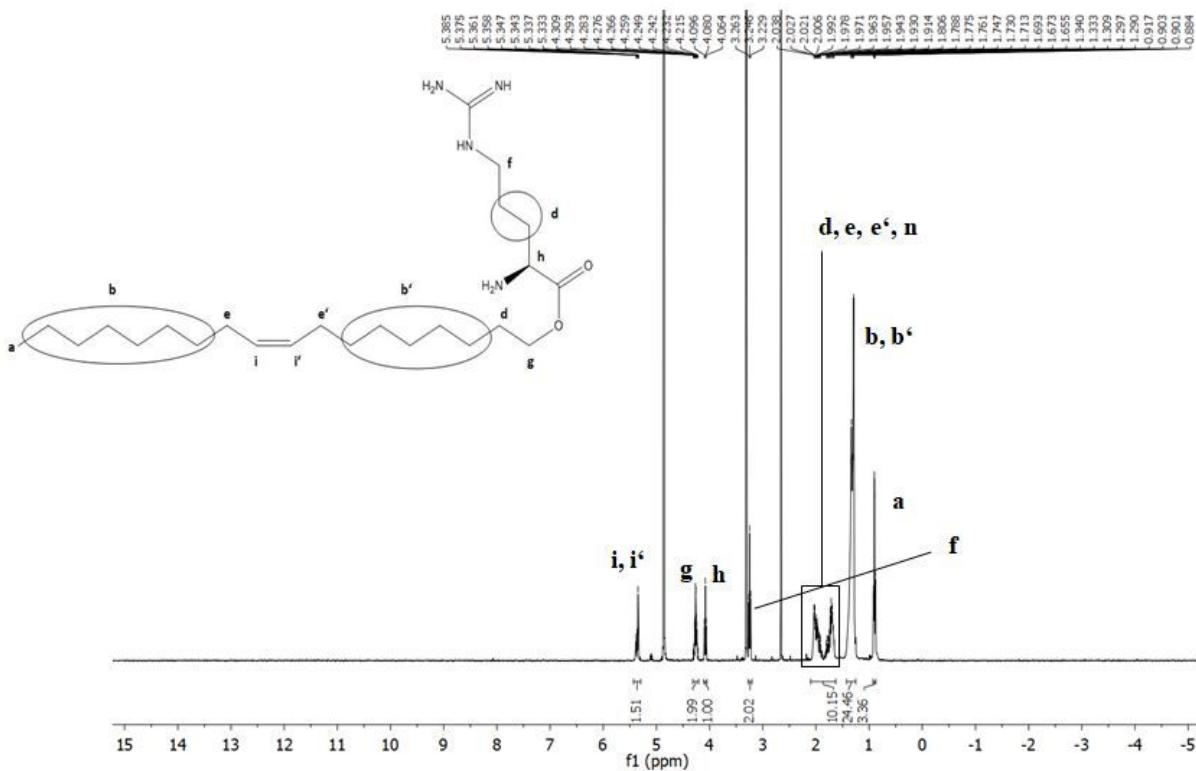


Figure S-7: ^1H -NMR spectrum of Arg-OL (octadec-9-en-1-yl arginate) in deuterated methanol.

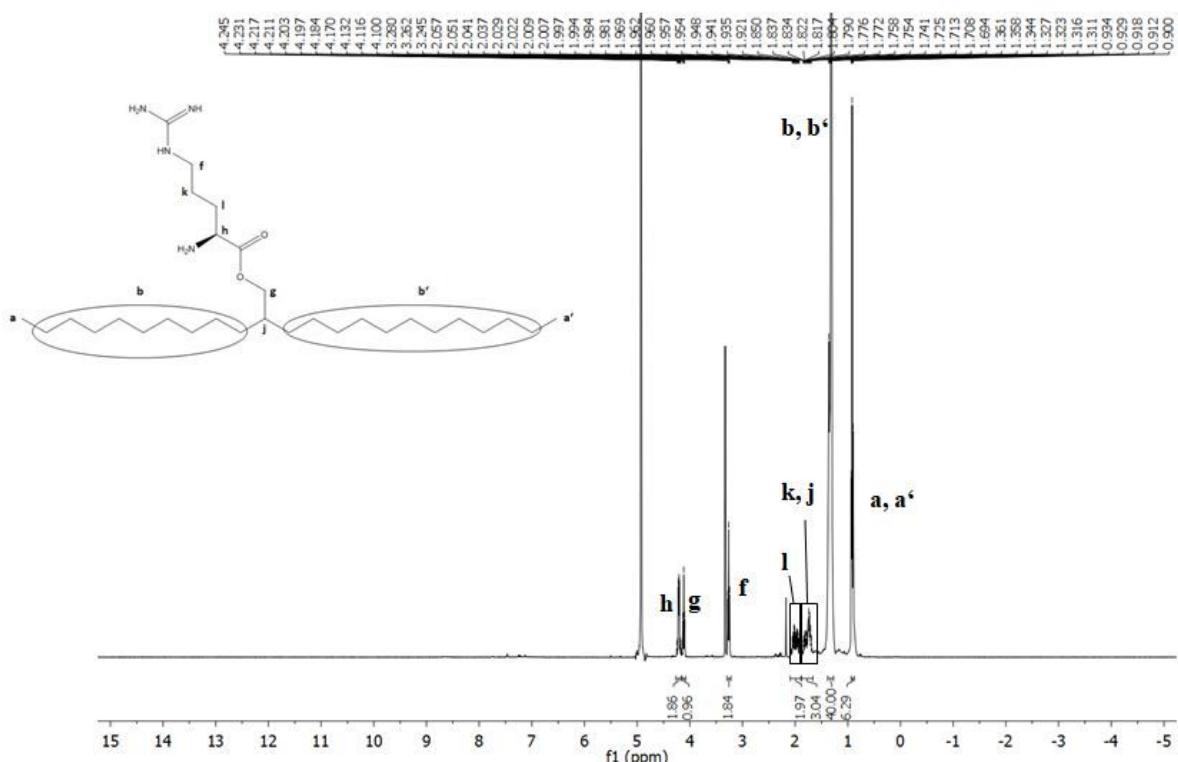


Figure S-8: ^1H -NMR spectrum of Arg-DT (2-decyldodecyl arginate) in deuterated methanol.

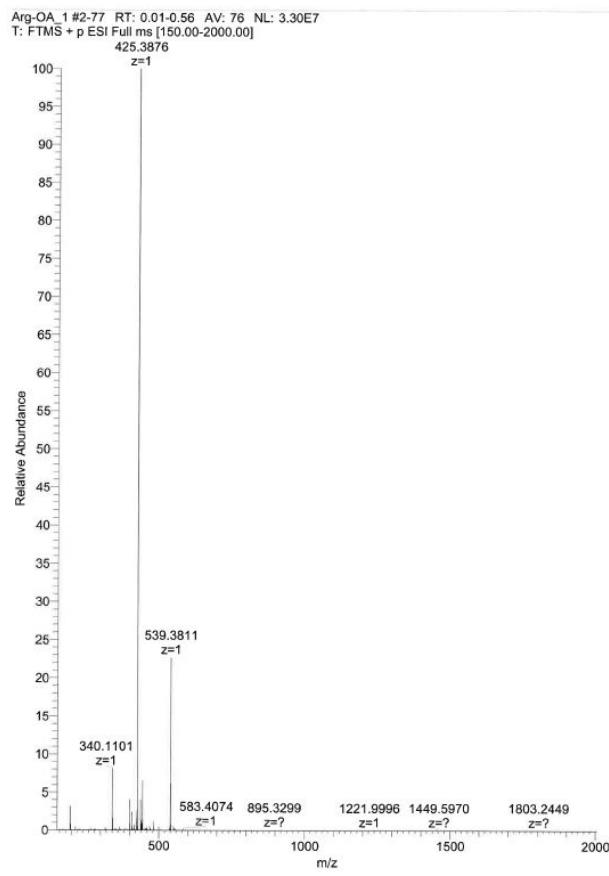


Figure S-9: Mass spectrum of Arg-OL (octadec-9-en-1-yl argininate).

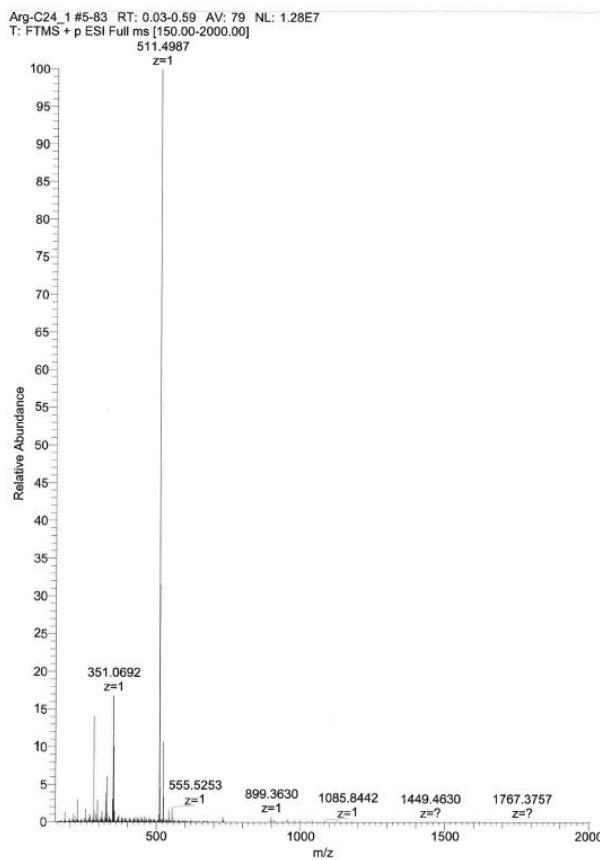


Figure S-10: Mass spectrum of Arg-DT (2-decyldodecyl arginate).

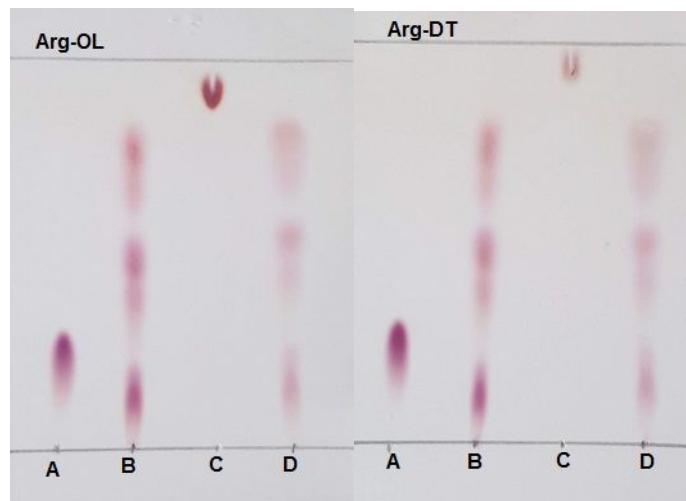
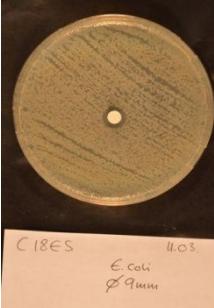
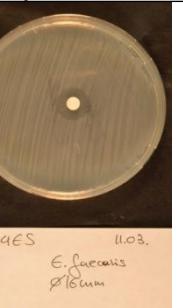
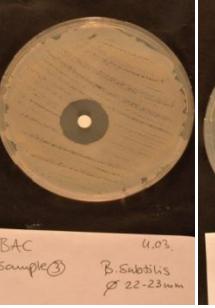
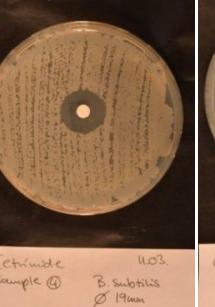
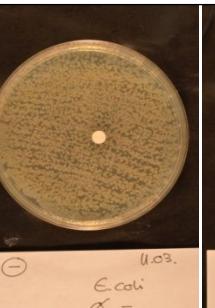


Figure S-11. Biodegradation of Arg-esters by lipase. On each TLC: A=L-arginine, B=lipase, C= Arg-ester before lipase addition and D= Arg-ester after incubation with lipase for 3 h. As shown by TLC, there is no ester spot after 3 h and only lipase spots are visible.

Table S-1. Zones of inhibition against indicated bacteria

Test compound	Observed zones of inhibition			
Arg-OL (10 mg mL⁻¹)	 C18ES 10.03. <i>E. coli</i> Ø 9mm	 C18ES 10.03. <i>S. aureus</i> Ø 19mm	 C18ES 10.03. <i>B. subtilis</i> Ø 16mm	 C18ES 10.03. <i>E. faecalis</i> Ø 18mm
Arg-DT (10 mg mL⁻¹)	 C24ES 10.03. <i>E. coli</i> Ø 9mm	 C24ES 10.03. <i>S. aureus</i> Ø 16mm	 C24ES 10.03. <i>B. subtilis</i> Ø 18mm	 C24ES 10.03. <i>E. faecalis</i> Ø 16mm
BAC (10 mg mL⁻¹)	 BAC Sample ③ 10.03. <i>E. coli</i> Ø 14mm	 BAC Sample ③ 10.03. <i>S. aureus</i> Ø 21mm	 BAC Sample ③ 10.03. <i>B. subtilis</i> Ø 22-23mm	 BAC Sample ③ 10.03. <i>E. faecalis</i> Ø 20mm
Cetrimide (10 mg mL⁻¹)	 Cetrimide sample ④ 10.03. <i>E. coli</i> Ø 12mm	 Cetrimide sample ④ 10.03. <i>S. aureus</i> Ø 19mm	 Cetrimide sample ④ 10.03. <i>B. subtilis</i> Ø 19mm	 Cetrimide sample ④ 10.03. <i>E. faecalis</i> Ø 19mm
Negative control (water with 10% v/v DMSO)	 ⊖ 10.03. <i>S. aureus</i> Ø -	 ⊖ 10.03. <i>E. faecalis</i> Ø -	 ⊖ 10.03. <i>E. coli</i> Ø -	 ⊖ 10.03. <i>B. subtilis</i> Ø -