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Supplementary materials: Quaternary Ammonium Leucine-Based Surfactants: The Effect of a Benzyl Group on Physicochemical Properties and Antimicrobial Activity

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Table S1. Chemical structures and H^1-NMR interpretation for benzyl quaternary ammonium leucine-based surfactants.

C10 LEU BENZ	^{1}H NMR (DMSO) δ 7.68-7.50 (m, 5H, ArH); 4.83-4.60 (dd, 2H, CH_2); 4.39-4.20 (m, 3H, CH and CH_2); 3.03-3.01 (m, 8H, CH_3 and CH_2); 2.15-1.95 (m, 2H, CH_2); 1.66-1.60 (m, 2H, CH_2); 1.50-1.44 (m, 1H, CH); 1.36-1.20 (m, 12H, CH_2); 1.02-0.94 (m, 6H, CH_3); 0.85 (t, 3H, CH_3).
C12 LEU BENZ	^{1}H NMR (DMSO) δ 7.68-7.50 (m, 5H, ArH); 4.83-4.56 (dd, 2H, CH_2); 4.39-4.20 (m, 3H, CH and CH_2); 3.18 (s, 6H, CH_3); 3.06-3.01 (m, 2H, CH_2); 1.90-1.81 (m, 2H, CH_2); 1.66-1.60 (m, 2H, CH_2); 1.48-1.44 (m, 1H, CH); 1.28-1.20 (m, 16H, CH_2); 1.02-0.94 (m, 6H, CH_3); 0.85 (t, 3H, CH_3).
C14 LEU BENZ	^{1}H NMR (DMSO) δ 7.68-7.50 (m, 5H, ArH); 4.83-4.56 (dd, 2H, CH_2); 4.38-4.29 (m, 3H, CH and CH_2); 3.18 (s, 6H, CH_3); 3.06-2.97 (m, 2H, CH_2); 1.89-1.81 (m, 2H, CH_2); 1.70-1.59 (m, 2H, CH_2); 1.48-1.40 (m, 1H, CH); 1.38-1.12 (m, 20H, CH_2); 1.04-0.83 (m, 9H, CH_3).

Table S2. Selectivity index (EC50/MIC) for the synthesized leucine-based quaternary ammonium surfactants in comparison to BAC. EC50 values are from MTS assay.

	Selectivity index EC_{50}/MIC				
	Caco-2				
	S. aureus	***E. faecalis***	***E. coli***	***P. aeruginosa***	***C. albicans***
BAC	11.5	11.5	2.9	0.4	2.9
C10 LEU BENZ	42.1	28.1	1.3	0.6	1.3
C12 LEU BENZ	1.5	1.5	0.3	0.07	0.5
C14 LEU BENZ	5	3.7	0.5	0.06	0.9
	Calu-3				
BAC	7.7	7.7	1.9	0.2	1.9
C10 LEU BENZ	30.8	15.2	0.9	0.5	0.9
C12 LEU BENZ	1.0	1.0	0.2	0.05	0.4
C14 LEU BENZ	5.4	4.0	0.5	0.06	1.0