

Supporting Information

Table S1. Phospholipid constituents of the model *Staphylococcus Aureus* (left column) together with their assigned 4-letter codes (right column).¹

Lipids	Lipid code
PG (a15:0/a15:0)	FFPG
PG (i15:0/a15:0)	IFPG
PG (16:0/a15:0)	PFPG
PG (i17:0/a15:0)	JFPG
PG (a17:0/a15:0)	ZFPG
PG (i17:0/i15:0)	JIPG
PG (a17:0/i15:0)	ZIPG
PG (18:0/a15:0)	SFPG
PG (i19:0/a15:0)	VFPG
PG (a19:0/a15:0)	TFPG
PG (a19:0/i15:0)	TIPG
PG (20:0/a15:0)	XFPG
PG (18:1/i15:0)	OIPG
PG (18:1/a15:0)	OFPG
LPG (i17:0/a15:0)	JFGK
LPG (a17:0/a15:0)	ZFGK
LPG (18:0/a15:0)	SFGK
LPG (a19:0/a15:0)	TFGK
CL (a17:0/a15:0)	ZFCL

Table S2. Letter Codes representing Fatty Acyl Tails which are not present in CHARMM-GUI Membrane Builder module.¹

Lipid tail	Code	Explanation
a15:0	F	anteisopentadecanoyl, F ifteen for pentadecane
i15:0	I	I sopentadecanoyl
a17:0	Z	anteisomargaroyl, Z for g
i17:0	J	isomargaroyl, J for g
a19:0	T	an T eisononadecanoyl
i19:0	V	isononadecanoyl, V is after T and resembles an iso branch
20:0	X	arachidoyl, X for ch

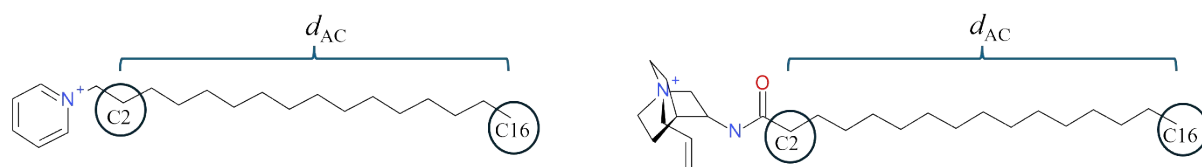
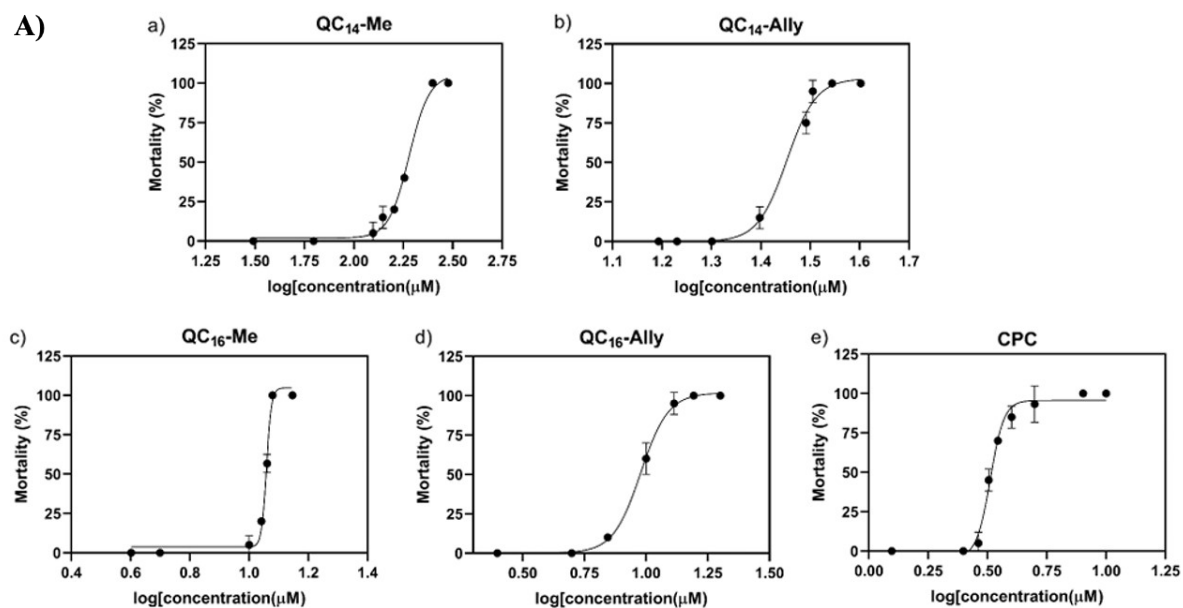


Figure S1. CPC (left) and QC₁₆-Allyl molecules. Atoms used to define the distance d_{AC} (distance between the C2 and C16 atoms in the aliphatic chain) are denoted with the blue ellipses.



B)

Sample	LC ₅₀ , μM	Confidence interval, CI (95%)	Hill Slope
QC ₁₄ -Me	190.1	183.0-200.1	8.481
QC ₁₄ -Allyl	28.37	27.46-29.30	14.75
QC ₁₆ -Me	11.45	11.38-11.52	51.81
QC ₁₆ -Allyl	9.516	9.082-9.895	7.756
CPC	3.250	3.150-3.360	14.97

Figure S2. A) Concentration-response curves used for the calculation of the *Danio rerio* mortality after 120 hours of exposure to: a) QC₁₄-Me, b) QC₁₄-Allyl, c) QC₁₆-Me, d) QC₁₆-Allyl and e) CPC. **B)** Dose-inhibition results obtained after 120 hours of *Danio rerio* exposure to tested samples.