Supporting Information

A Synthetic Antimicrobial Peptidomimetic (LTX 109) – the Stereochemical Impact on Membrane Disruption

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S1. 1D superimposition of LTX109, LTX109-F₃ and RTbtR
S2. NOESY: RTbtR + DOPC
S3. NOESY: LTX 109 + DOPC
S4. NOESY: LTX 109 + DOPC
S5. NOESY: LTX 109 + DOPC
S6. NOESY: LTX 109 + POPE:DMPC, 8:2
Figure S1. Superimposition of the aromatic region of the 1D proton spectra for LTX109 (1) (A, red), LTX109-F5 (B, blue) and RTbtR (C, green) inserted into DOPC liposome membranes at 37 °C. The difference between A and B shows the location of the phenyl protons and the difference between B and C reveals the HN10.
Figure S2. NOESY spectrum of R-Tbt-R in DOPC showing the aromatic-aliphatic region, giving the tert-butyl groups assignments.
Figure S3. NOESY spectrum of LTX 109-F₅ in DOPC showing the aromatic-aliphatic region, giving the beta- and gamma protons assignments of the C-terminal arginine.
Figure S4. NOESY spectrum of 1 showing the aromatic-aliphatic region.
Figure S5. NOESY spectrum of 1 in DOPC showing the aromatic-aromatic region.
Figure 6. NOESY spectra of the L-L-L peptide (1) (A, 100 ms; C, 300 ms mixing time) and the L-L-D peptide (7) (B, 100 ms; D, 300 ms mixing time) in POPE:DMPC 8:2 liposomes. Both peptides show contacts between the phenyl moiety (denoted 38, 39 and 40) and the Tbt methyls (denoted 30, 32 and 34) when inserted into the membrane, despite that peptide 4 lacks this contact in aqueous solution.