Supporting Information

Melittin adsorption and lipid monolayer disruption at liquid–liquid interfaces

The calculation of the charge vs. pH curve for the peptide was carried out, in a very first approximation, by summing up the charge contributions from the various groups according to the Henderson-Hasselbalch equation¹. The peptide structure presented in this figure was drawn using the software VMD^2 and the PDB file of the X-ray structure with a resolution of 2 Å.³



Fig. S1. Calculated charge versus pH curve for melittin (H_2N –QQRKRKIWSILAPLGTTLVKLVAGIG) where arginine (R) and lysine (K) residues have been appear in yellow in the graphical representation of the peptide obtained with VMD.

Melittin has a maximum net charge of +6, four of which are consecutive and located in the basic N-terminal region (R-K-R-K), and the remaining positively charged, K- 20, close to the C-terminal region (G-26). This asymmetric distribution of polar and non–polar residues makes of melittin an amphipathic peptide that adopts an α -helical conformation. The peptide helix has also been confirmed to bend because of the presence of a proline (P-13) in its sequence.³



Fig. S2. Video snapshots at different galvanic potentials of an aqueous droplet containing melittin ($x = 20 \mu$ M) and DCE in absence of DPPC.



Fig. S3. Four phase junction boundary angle dependence on the galvanic potential across the interface formed between DCE in absence of DPPC and an aqueous solution containing melittin (x = 20 μ M) obtained for the forward (red) and backward (blue) scan at 10 mV·s⁻¹.

References:

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- (2) Humphrey, W.; Dalke, A.; Schulten, K. J. Molec. Graph. 1996, 14, 33-38.
- (3) Terwilliger, T. C.; Elisenberg, D. J. Biol. Chem. 1982, 257, (11), 6010-6015.