Supporting Material for:

Cardiolipin models for molecular simulations of bacterial and mitochondrial membranes

Thomas Lemmin[*], Christophe Bovigny[*],
Diane Lançon, and Matteo Dal Peraro[†]

Laboratory for Biomolecular Modeling, Institute of Bioengineering,

School of Life Sciences, Ecole Polytechnique Fédérale de Lausanne (EPFL),

CH-1015 Switzerland

* These authors contributed equally to this work

[†] Corresponding author: matteo.dalperaro@epfl.ch

Address: EPFL SV IBI LBM, AAB 010

Station 19, CH-1015 Lausanne

Phone: +41 21 693 1861

Supporting Figures, Tables and Files

In the mixed patch simulation using the AMBER-based models, intra-molecular interactions were observed for the cardiolipin bilayers. The tighter packing of the lipids in the AMBER simulation significantly favors the direct interaction of Mg^{2+}, where nearly 74% of the Mg^{2+} within 4 Å of the cardiolipins have a direct coordination site with a phosphate group. These interactions correspond to the first peak in the radial distribution function (Fig. S1).

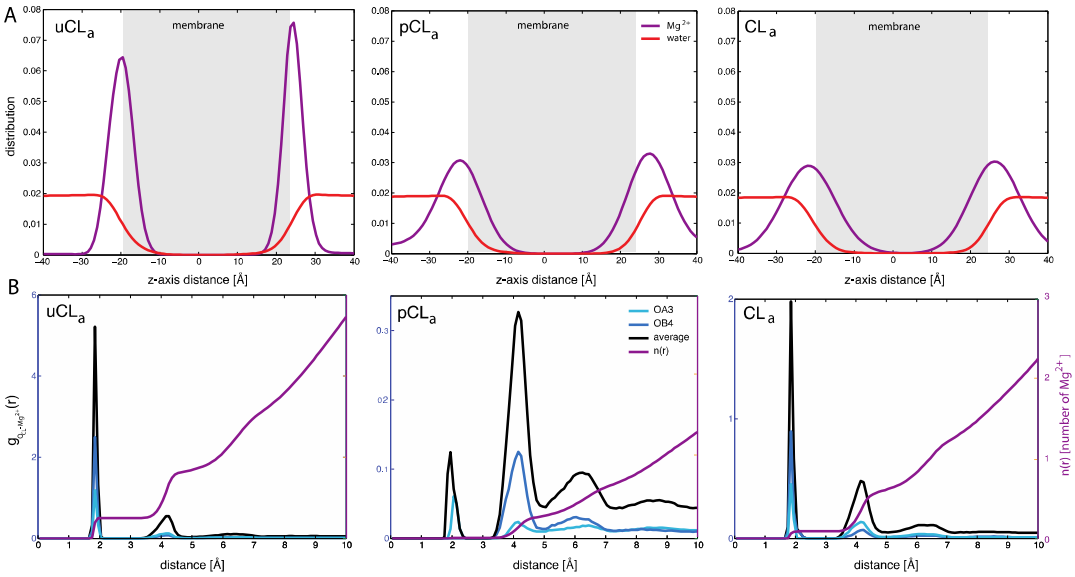

Figure S1 Cardiolipin interactions with divalent cations for CL models compatible with the AMBER force field. (A) Distribution of Mg^{2+} (in purple) and water molecules (in red) along the z-axis normal to the membrane surface. From left to right, data for the uCL, pCL and CL (mixed uCL/pCL) systems are reported when using the CHARMM force field. (B) Radial distribution function g(r) and coordination number n(r) (in orange) of Mg^{2+} around phosphate oxygen atoms for simulations carried out with AMBER force field.

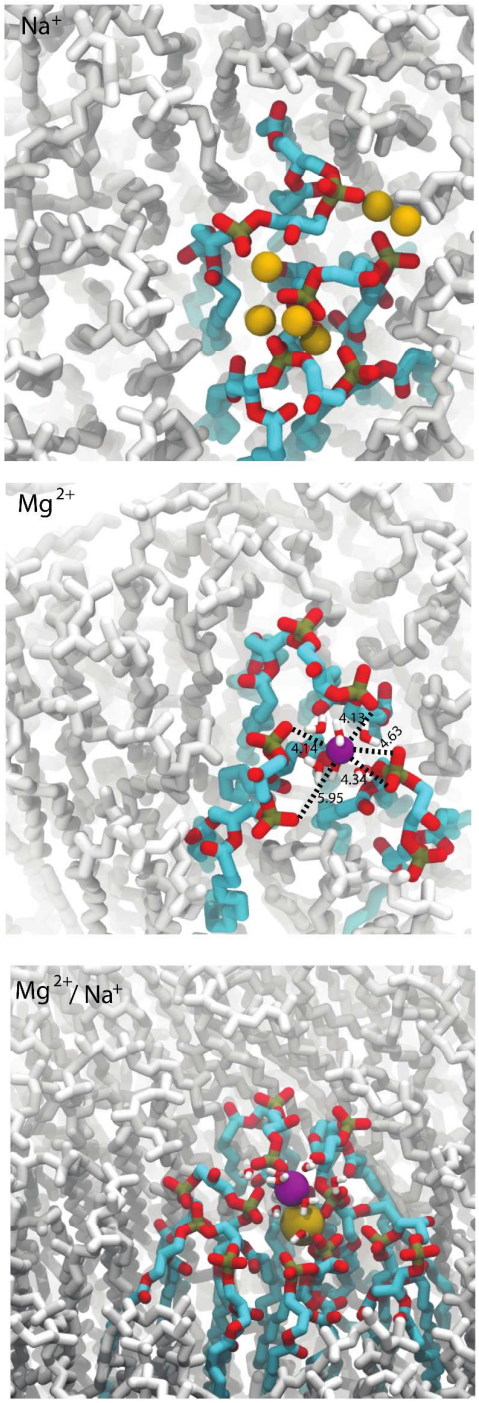

Figure S2 Coordination of cations around CL molecules. (Top) A single cardiolipin molecule interacts with up to three Na^+ cations (orange). The cation interacts directly with the phosphate group (see Figures 4 and 6 of the main text). (Middle) Four cardiolipins (in cyan) trap a Mg^{2+} cation (purple) with its first solvation shell. The phosphate groups interact directly with the solvation shell are localized at ~4 Å from the cation, whereas the second phosphate group is localized at ~6 Å. (see Figures 5 and 6 of the main text).

(Bottom) Na^+ cations bring the CL head group closer allowing it to trap a Mg^{2+} cation.

Table 1. PDB id used for data mining. PDB codes are reported below.

1E14, 1JGW, 1JGY, 1JGZ, 1K6L, 1K6N, 1KB9, 1KBY, 1KQF, 1KQG, 1M3X, 1NEK, 1NEN, 1OGV, 1OKC, 1P84, 1PP9, 1PPJ, 1QOV, 1RG5, 1RQK, 1RVJ, 1RY5, 1RZH, 1SQP, 1V54, 1V55, 1YF6, 2A06, 2ACZ, 2C3E, 2DYR, 2DYS, 2EIJ, 2EIK, 2EIL, 2EIM, 2EIN, 2GNU, 2HG3, 2HG9, 2HH1, 2HHK, 2HIT, 2HJ6, 2J8C, 2J8D, 2JIY, 2JJ0, 2UWU, 2UWW, 2UX3, 2UX4, 2UX5, 2UXJ, 2UXK, 2WX5, 2YBB, 2YL4, 2ZXW, 3ABK, 3ABL, 3ABM, 3AG1, 3AG2, 3AG3, 3AG4, 3ASN, 3ASO, 3CWB, 3CX5, 3DSY, 3DTA, 3DTR, 3DTS, 3DU2, 3DU3, 3DUQ, 3H1H, 3H1I, 3H1J, 3H1K, 3H1L, 3I4D, 3L70, 3L71, 3L72, 3L73, 3L74, 3L75, 3MA7

Additional files:

Formatted parameter and topology files for uCL and pCL models for the CHARMM and AMBER force fields are attached as supporting material in a separate archive.