Molecular Dynamics Protocol

A computational protocol similar to our previous work was used [15]. For the ions, we used the parameters of Amber force field ff03 (corresponding to the library of 1994). Namely, Na$^+$ $\sigma = 3.32840e^{-01}$ and $\varepsilon = 1.17152e^{-02}$, Cl$^-$ $\sigma = 4.40104e^{-01}$ and $\varepsilon = 4.18400e^{-01}$. [29] For the galactose, RESP [56] charges were calculated fitting an electrostatic potential calculated using the 6-31G* basis set and B3LYP [57, 58] functional and the Gaussian03 [59] program. The simulations were performed in periodic boundary conditions at 310 K using the Nose-Hoover thermostat [60] and Parrinello-Rahman barostat [61, 62] with a semisotropic pressure coupling type and a time step of 2 fs.

The BE-META calculations were conducted in the NVT ensemble.

During all the simulations, we took care in particular that important parameters of the membrane, such as the Area Per Lipid (APL) and thickness, were in agreement with experimental values [63].

References