

# **Amyloid- $\beta$ tetramers and divalent cations at the membrane/water interface: Simple models support a functional role.**

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## **Supplementary data**

- Figure S1 - Minimal distance between addressed cation and any of the atoms in DMPC measured in cMD along with time.
- Figure S2 - Radial distribution function ( $g(r)$ ) of M-OX pairs, with OX any oxygen atom in DMPC, measured in cMD.
- Figure S3 - Distribution of SASA<sub>PM</sub> and SASA<sub>P</sub> measured for models **1-3**/DMPC, in the differ-ent cMD trajectories (1-5).
- The frequency of values of  $R \geq 0.05$  is also reported for each separated trajectory (right) in Fig. 3.

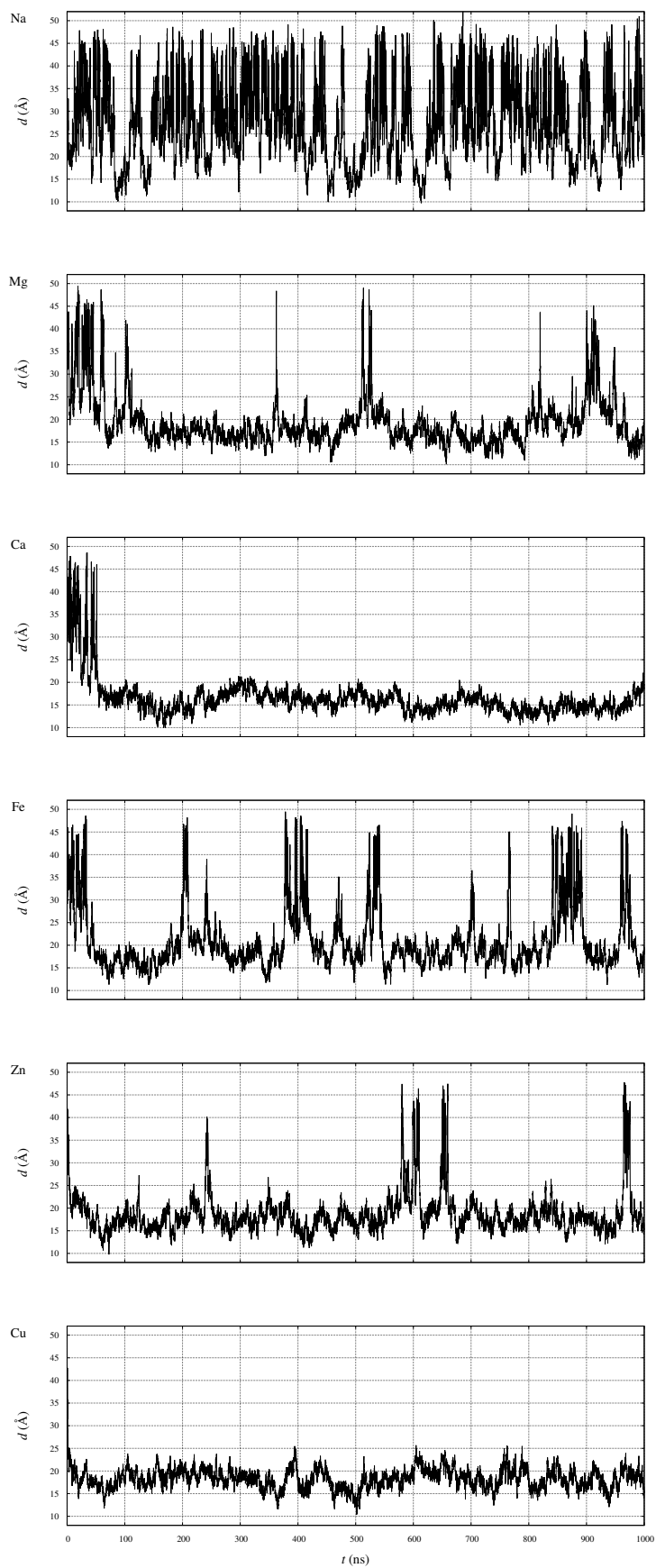


Figure S1: Minimal distance ( $d$ ) between addressed cation M and any of the atoms in DMPC as measured in cMD simulations along with time  $t$ .

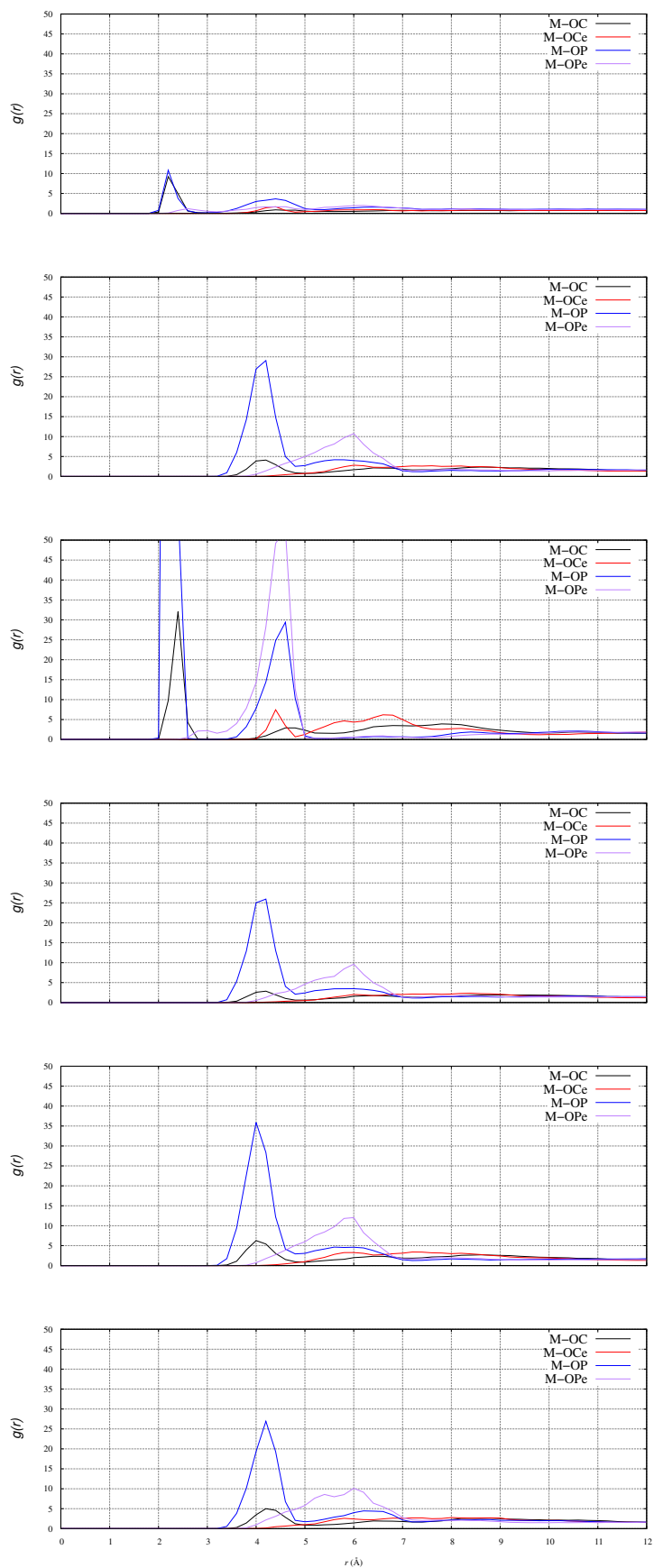


Figure S2: Radial distribution function ( $g(r)$ ) of M-OX pairs, with M the addressed cation and OX the O atoms in DMPC, measured in cMD simulations. M-OC (black); M-OCe (red); M-OP (blue); M-OPe (purple). OC is the carbonyl oxygen; OCe is the ester oxygen; OP is the terminal phosphodiester oxygen; OPe is the bridging phosphodiester oxygen.

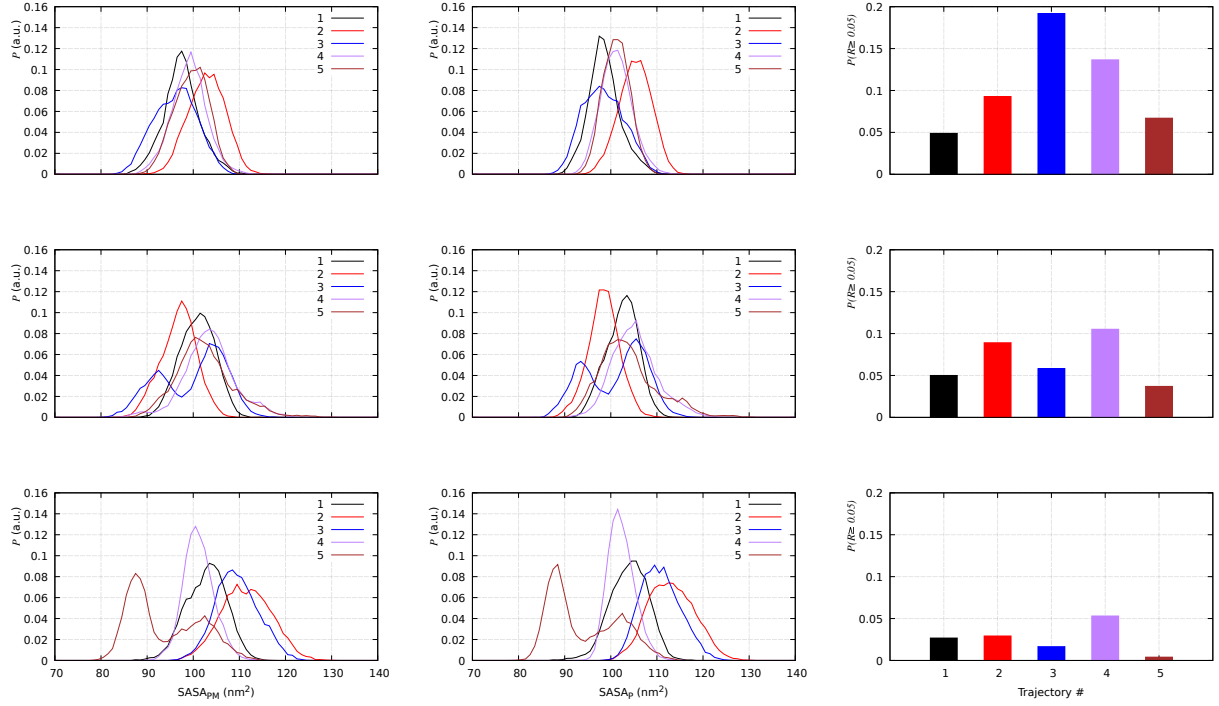


Figure S3: Distribution of SASAP<sub>M</sub> (left) and SASAP (middle) (see Methods) of A 42 tetramers in the different models exposed to DMPC. Right - Frequency of samples with  $R \geq 0.05$  for each trajectory ( $x$ -axis). The different curves (1-5) are obtained by the different independent cMD trajectories (see Table 2 in the main text). Top - model 1/DMPC; middle - 2/DMPC; bottom - 3/DMPC.