Electronic Supplementary Material (ESI) for Soft Matter

Supporting Information for

Interactions of PEO-PPO-PEO block copolymers with membranes: a computational and experimental study linking membrane lysis with polymer structure

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Figure 1S. Mass density profile for Pluronic L64 and DPPC atoms. Left: initial configuration with the polymer in the water phase. Right: final configuration after 300 ns after the polymer has translocated inside the DPPC membrane. The distributions have been averaged over 10 ns.

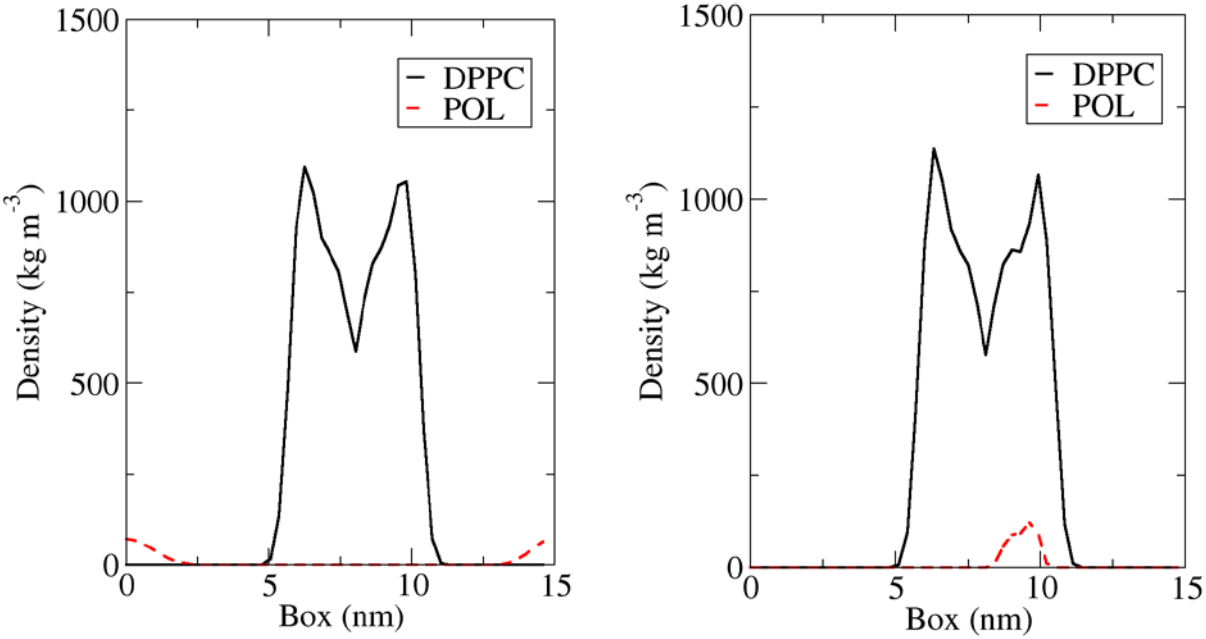


Figure 2S. Two different conformations of the Pluronic L61(EO_3-PO_{31}-EO_3) adopted after 200ns starting from the same initial configuration. Top: initial arrangement of L61 immersed in a coiled configuration placed centrally in the membranes hydrophobic region. Large beads represent the PEO blocks connected either side of a central PPO block. Bottom left: the Pluronic is spread across the bilayer spanning both monolayers with the PEO block interacting with adjacent monolayers of the bilayer membrane. Bottom right: the Pluronic adopts a U-shaped configuration where both PEO block interact with the same monolayer.

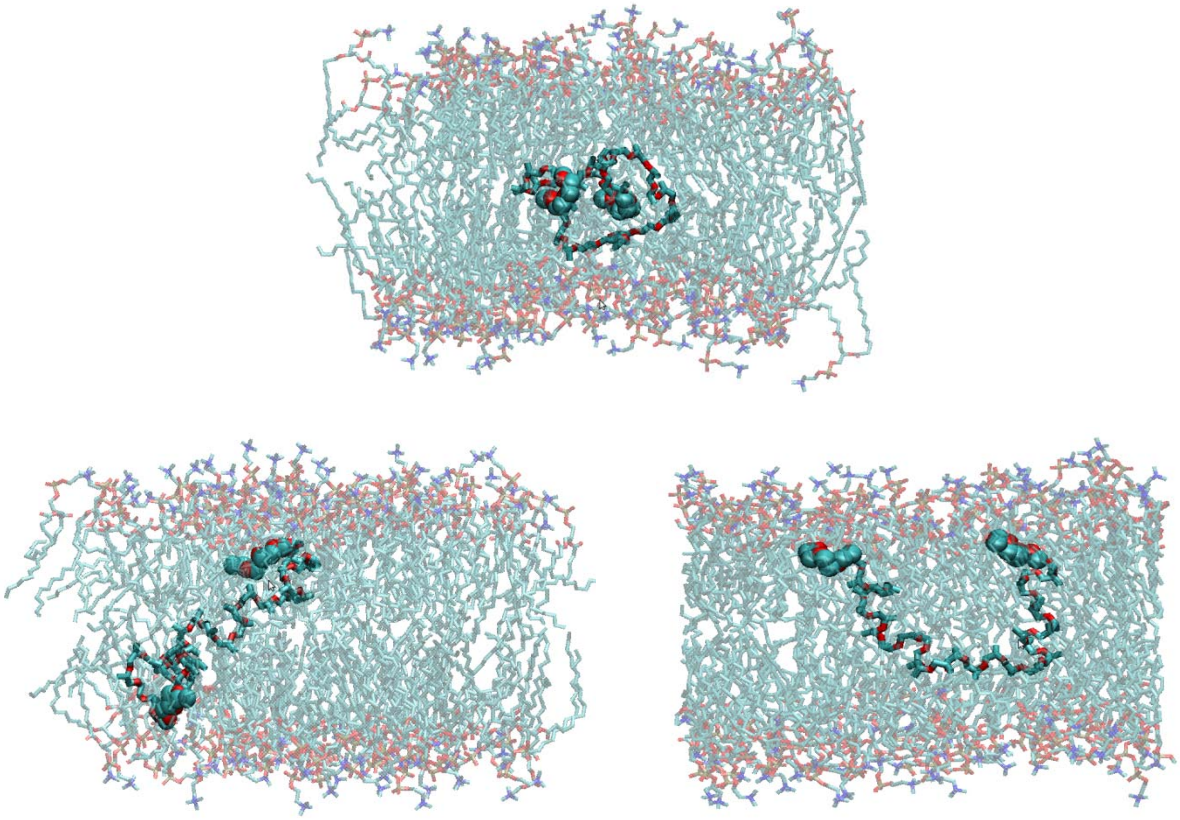


Figure 3S. Two different conformations of the Pluronic L62(EO_6-PO_{31}-EO_6) adopted after 200ns starting from the same initial configuration. Top: initial arrangement of L62 immersed in a coiled configuration placed centrally in the membranes hydrophobic region. Large beads represent the PEO blocks connected either side of a central PPO block. Bottom left: the Pluronic is spread across the bilayer spanning both monolayers with the PEO block interacting with adjacent monolayers of the bilayer membrane. Bottom right: the Pluronic adopts a U-shaped configuration where both PEO block interact with the same monolayer.

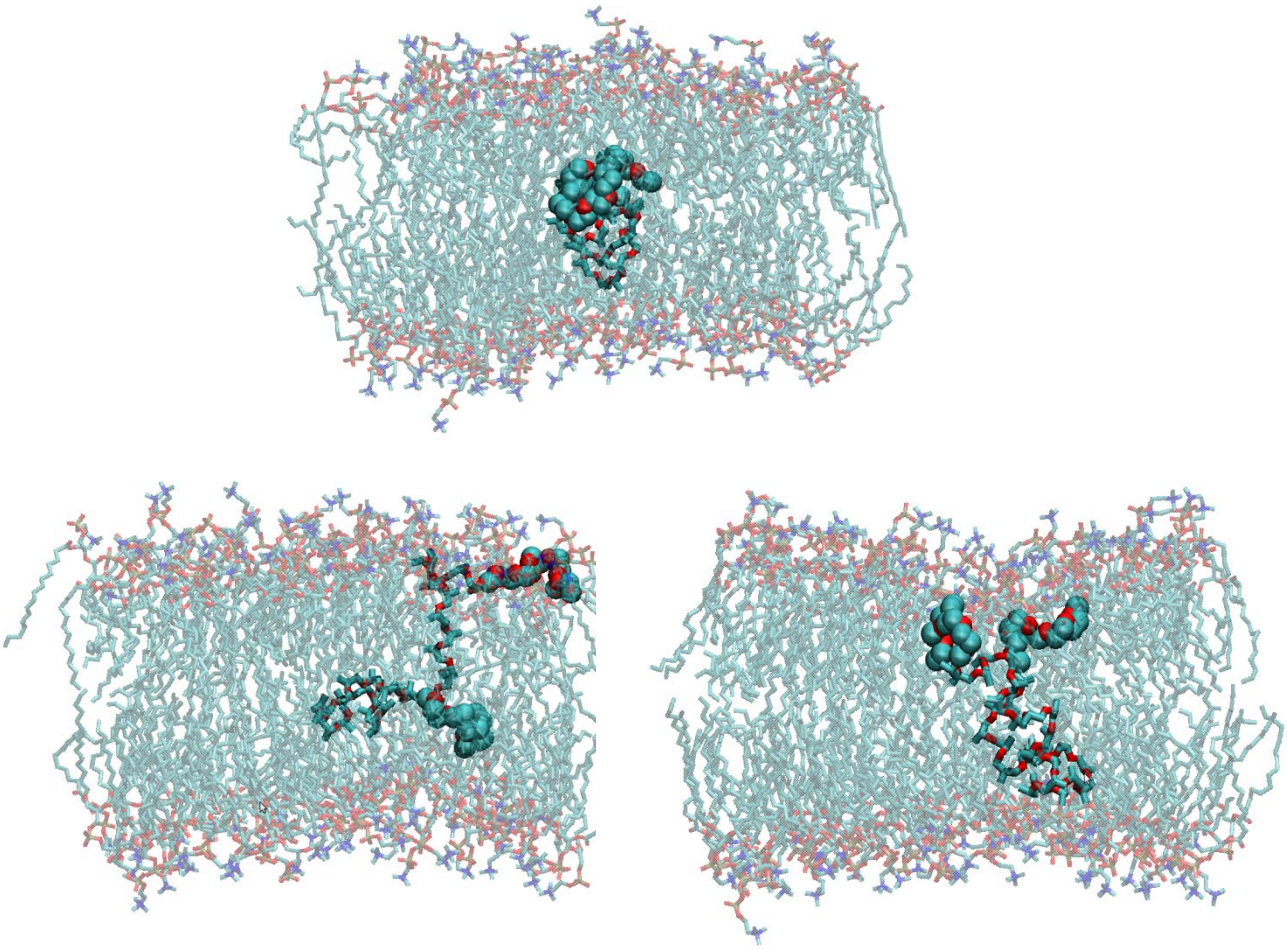
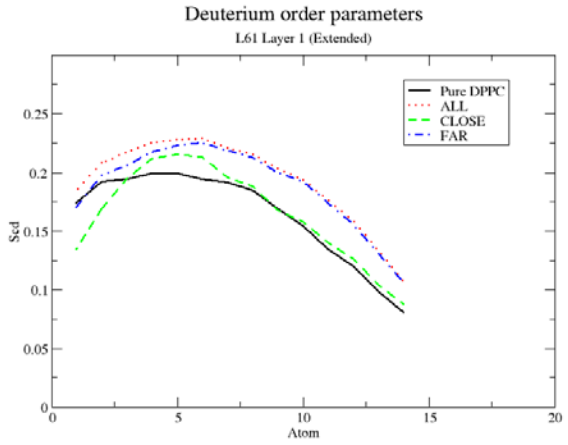
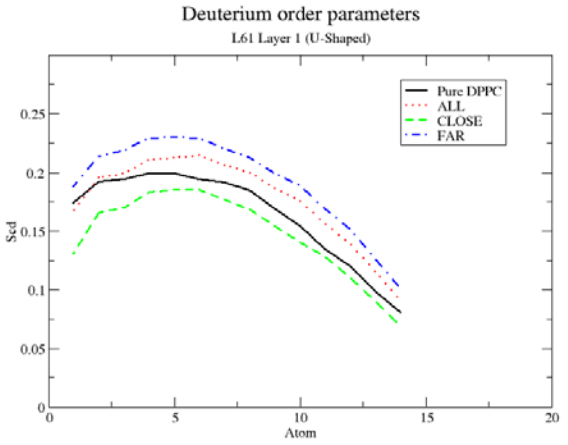
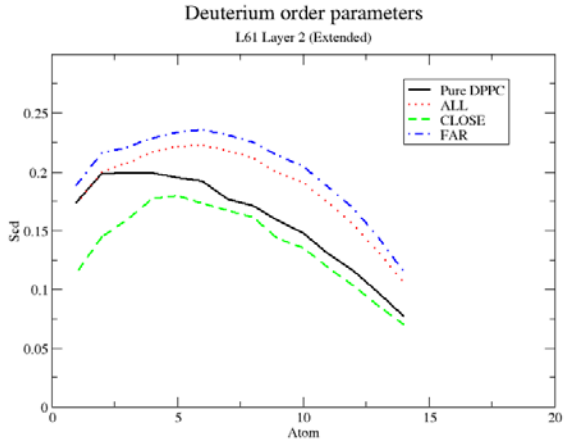


Figure 4S. Deuterium order parameter calculated per monolayer using the last 10ns of a 200ns simulation for the Pluronic L61(EO_3-PO_{31}-EO_3) adopting both the U-shaped and spanned configuration. Layer 1 corresponds to the top layer of the membrane from figure 2S and layer 2 corresponds to the bottom layer.







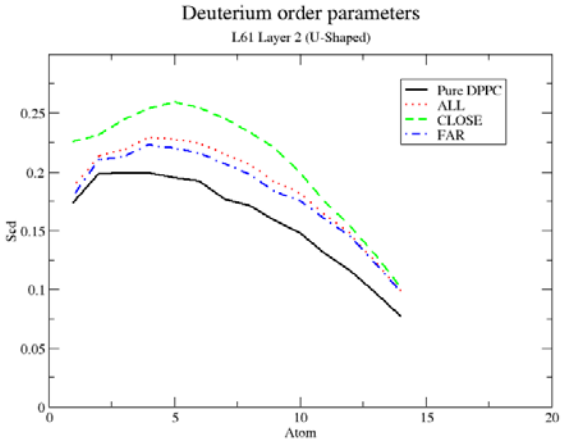


Figure 5S. Deuterium order parameter calculated per monolayer using the last 10ns of a 200ns simulation for the Pluronic L62(EO_6-PO_{31}-EO_6) adopting both the U-shaped and spanned configuration. Layer 1 corresponds to the top layer of the membrane from figure 3S and layer 2 corresponds to the bottom layer.