Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Structural behavior of amphiphilic polyion complexes interacting with saturated lipid membranes investigated by coarse-grained molecular dynamic simulations

Daniel G. Angelescu

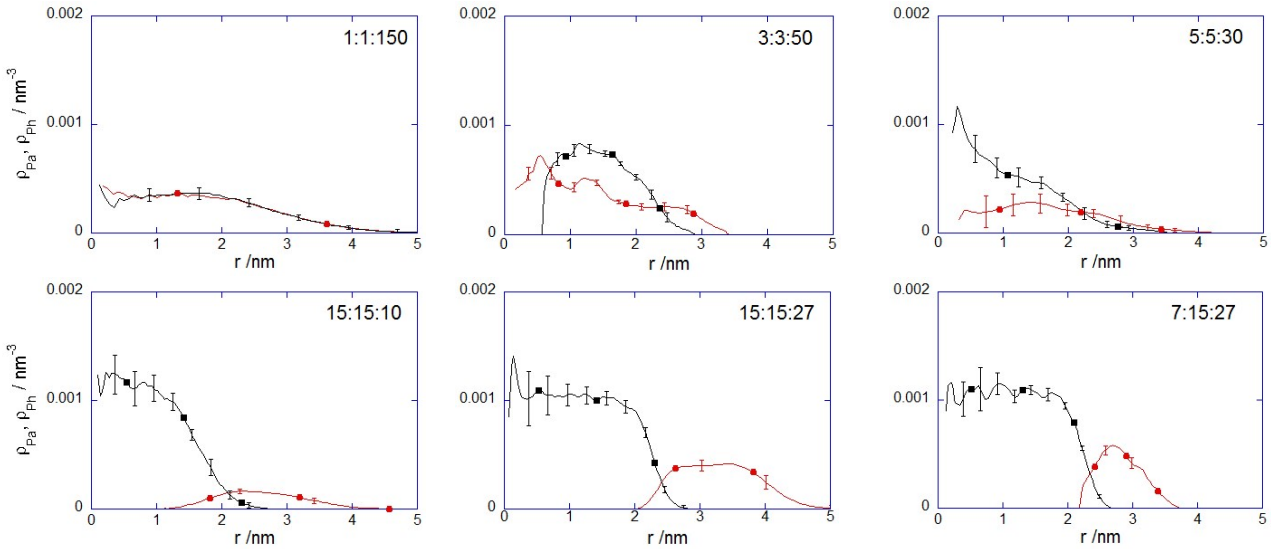
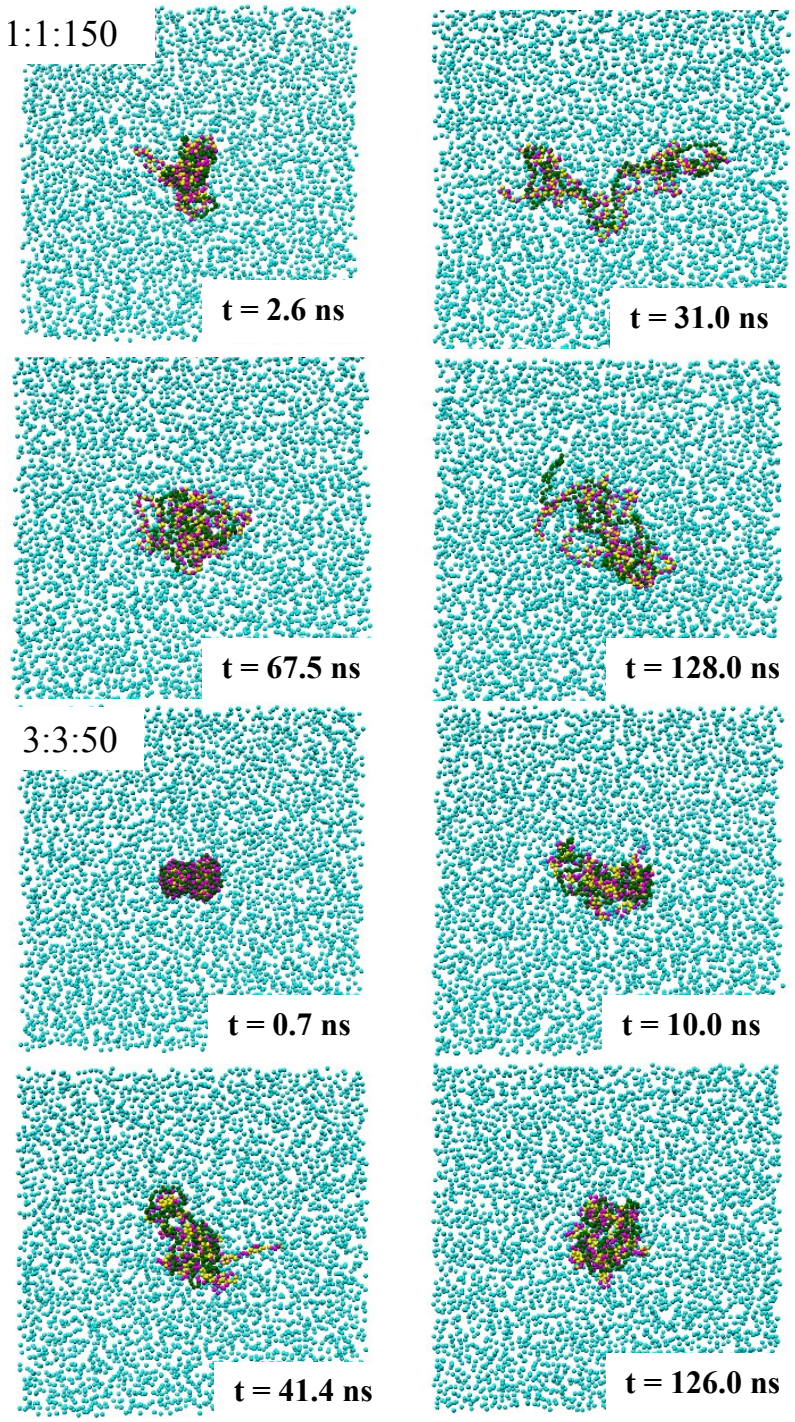
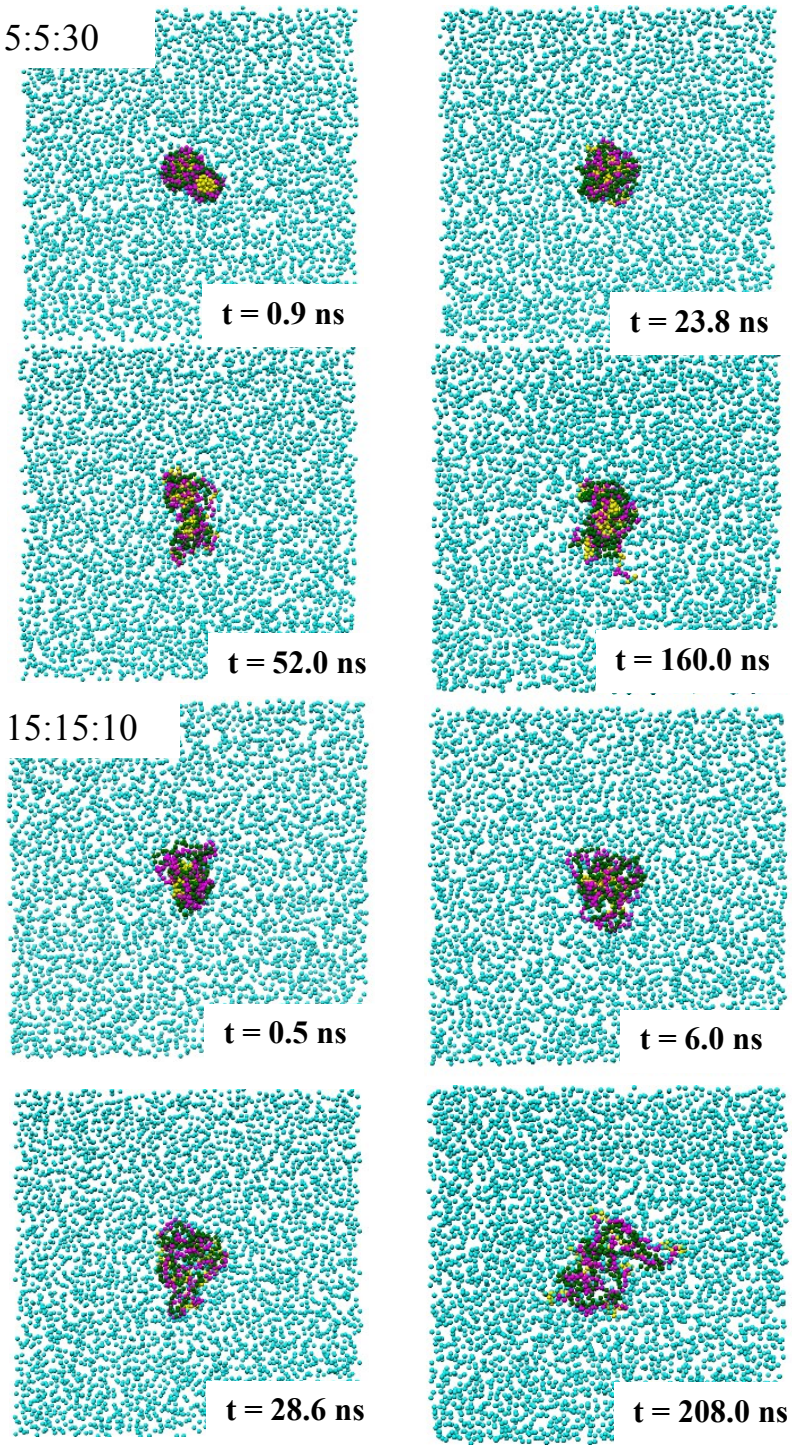


Figure S1. Bead number densities of the anionic (circles) ρ_{Pa} and hydrophobic beads (squares) ρ_{Ph} of the amphiphilic block copolymer as a function of the center of mass of complex for the indicated free PECs.


1:1:150
t = 2.6 ns
t = 31.0 ns
t = 67.5 ns
t = 128.0 ns
3:3:50
t = 0.7 ns
t = 10.0 ns
t = 41.4 ns
t = 126.0 ns


5:5:30
t = 0.9 ns
t = 23.8 ns
t = 52.0 ns
t = 160.0 ns
15:15:10
t = 0.5 ns
t = 6.0 ns
t = 28.6 ns
t = 208.0 ns

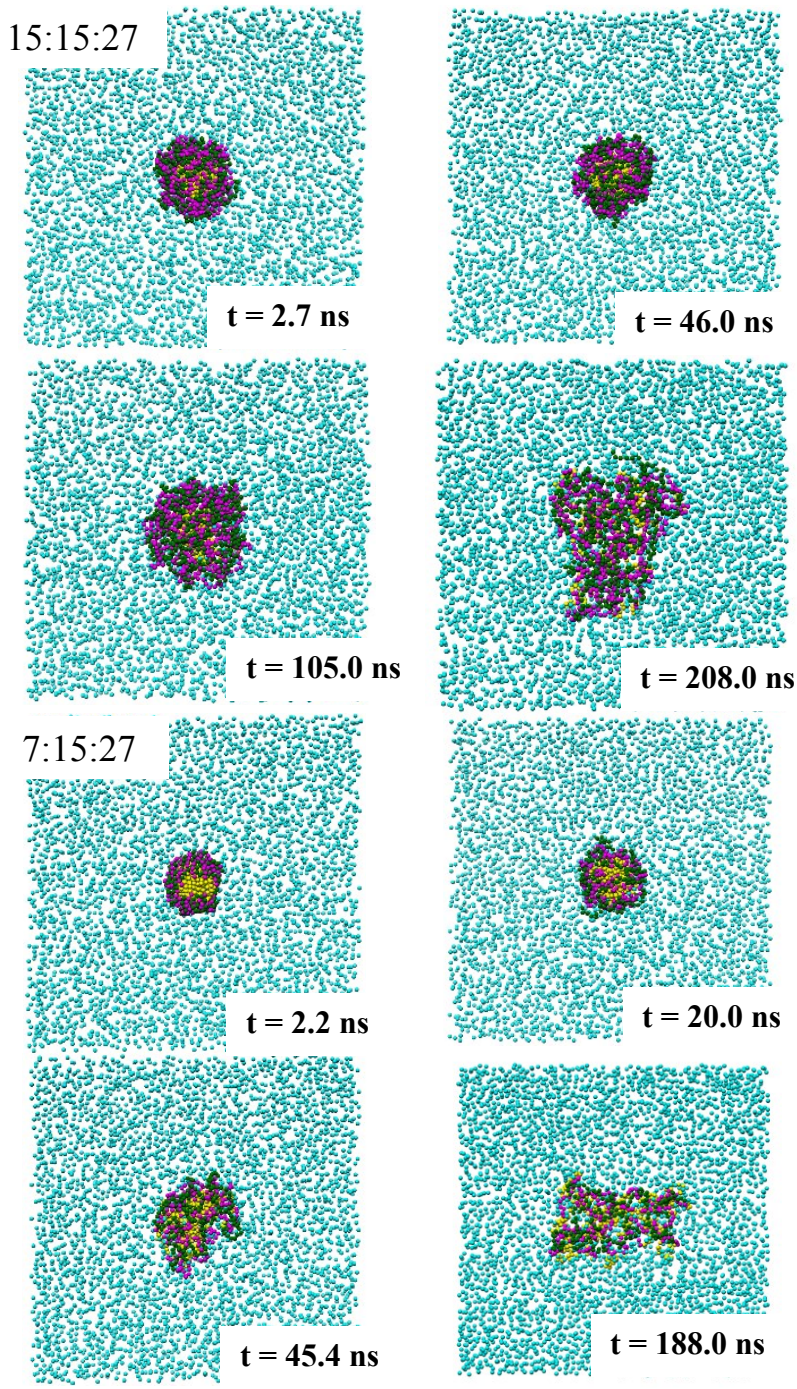


Figure S2. Time sequence of representative morphologies (top view) of indicated PECs binding to and internalized into the DPPC bilayer; the color code is the same as in Figure 1, with the choline beads of DPPC displayed only for sake of clarity; the side views are given in Figs. 2 and 3.

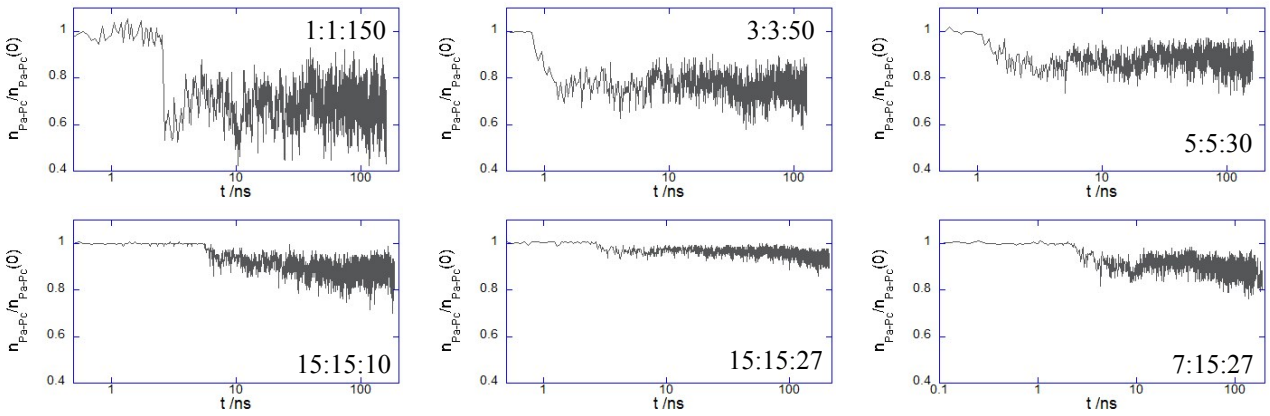


Figure S3. The time-evolution of the normalised number of contacts between the anionic and cationic beads $n_{Pa\text{-}Pc}/ n_{Pa\text{-}Pc}(0)$ for the indicated PEC.

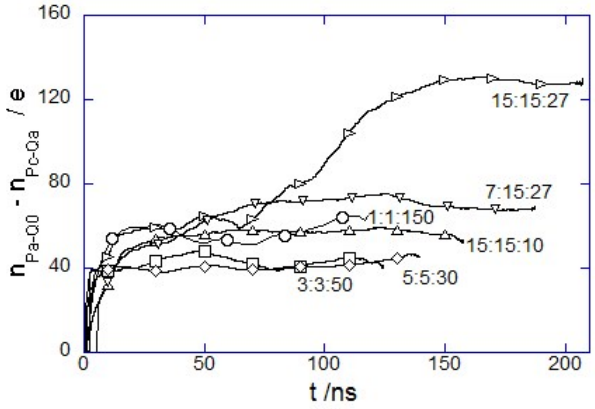


Figure S4. Net charge at the PEC-bilayer interface $n_{Pa\text{-}Q0}$ - $n_{Pc\text{-}Qa}$ for the indicated PECs.

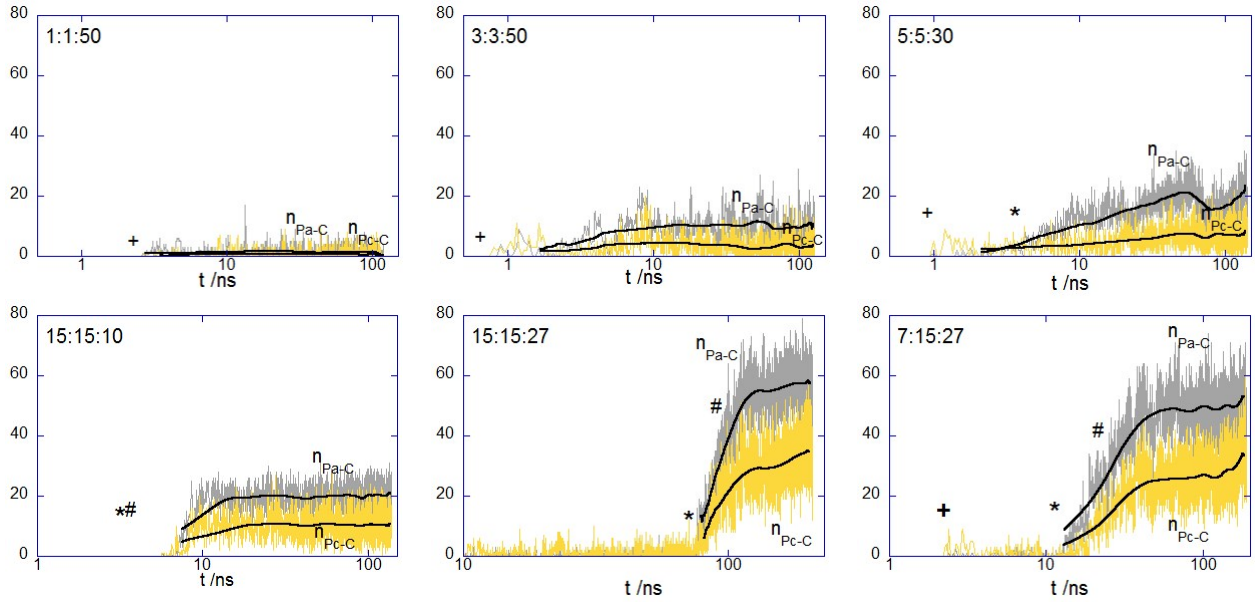


Figure S5. Number of contacts between charged beads of the complex and alkyl chains $n_{Pa\text{-}C}$ and $n_{Pc\text{-}C}$ for the indicated PECs; cross, star and hash symbols indicate the onset for the binding, internalization in the membrane core and binding to the distal layer.

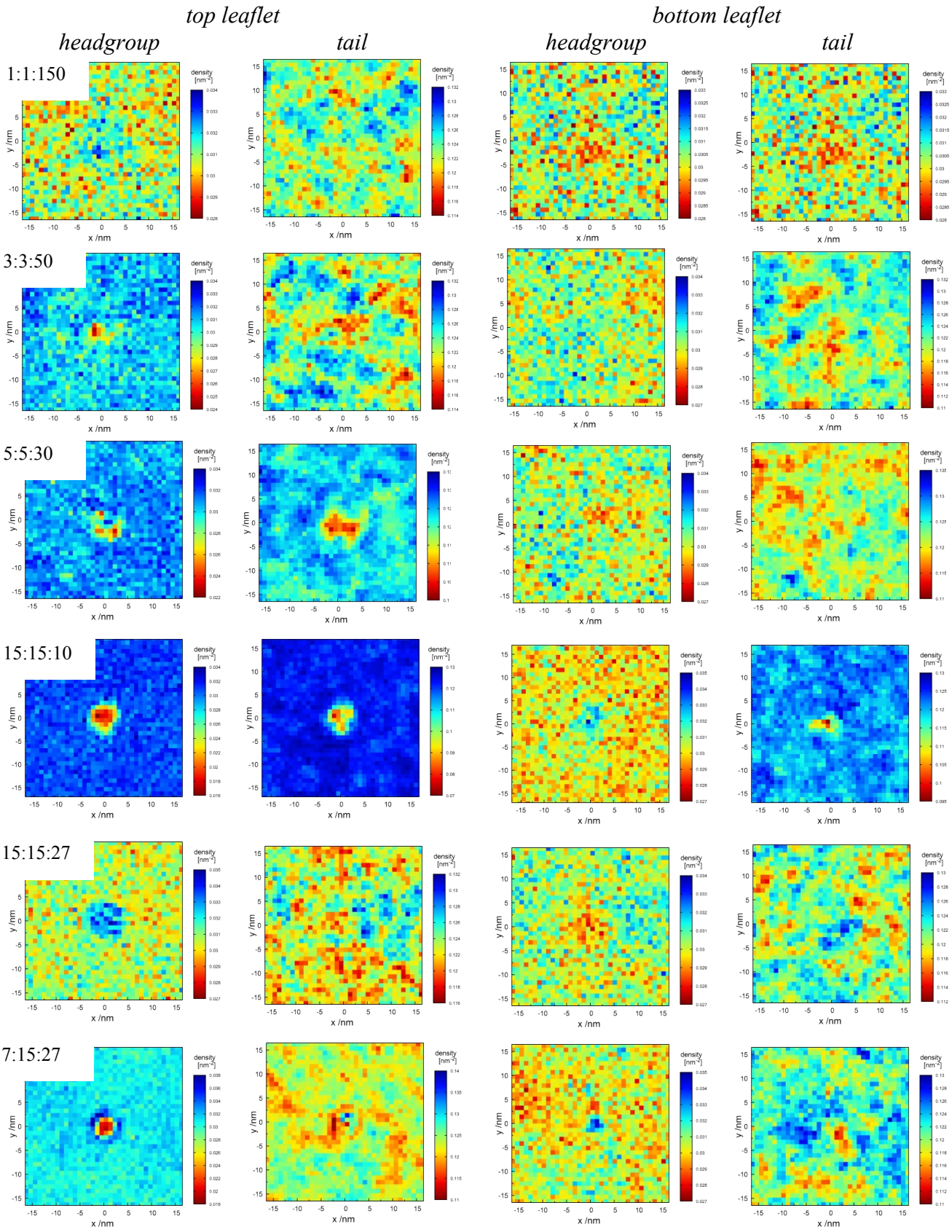
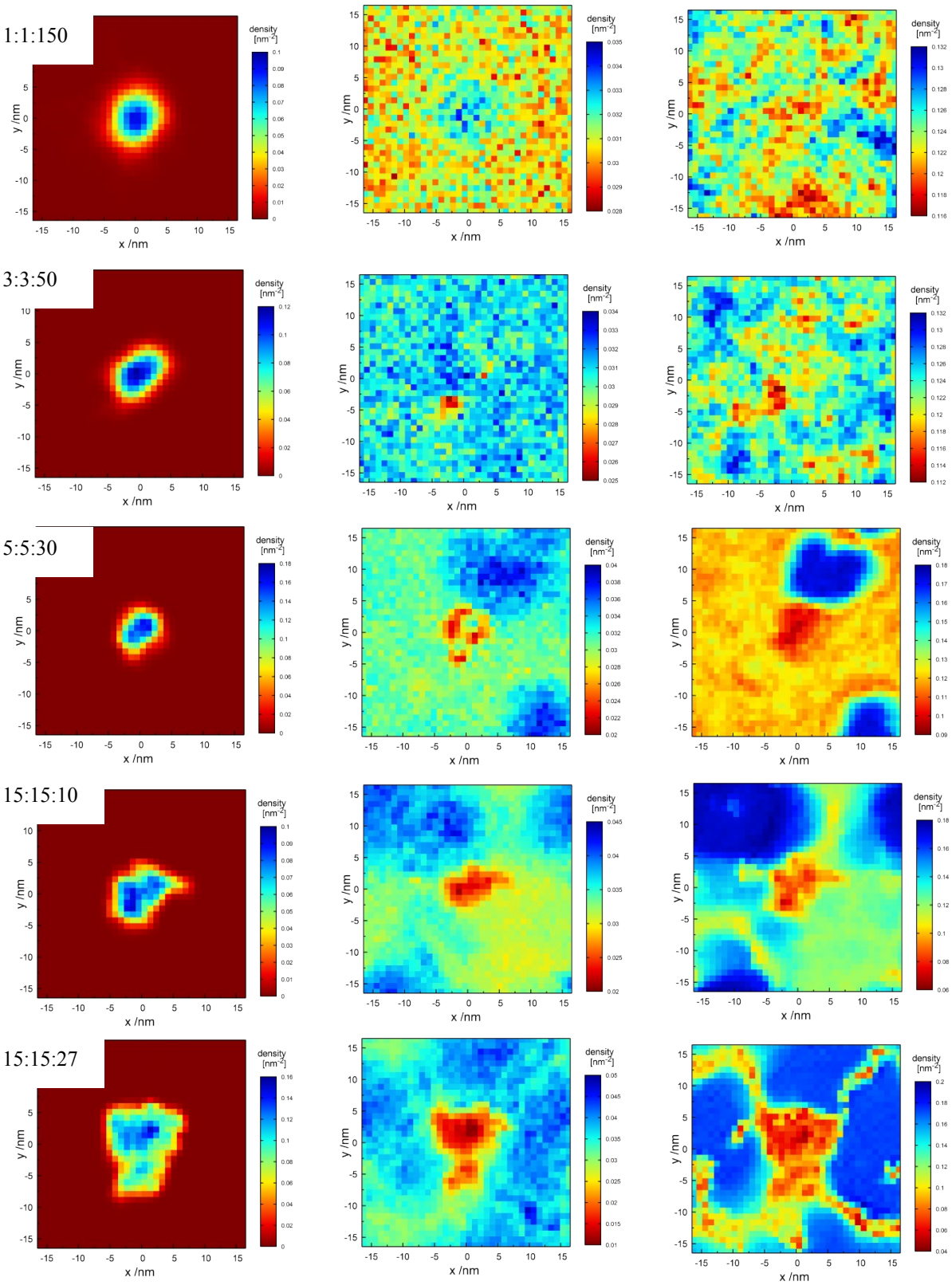


Figure S6. 2D representation of the number densities of the lipid heads and tails in both leaflets at indicated PECs; densities were obtained from the first 20 ns simulation trajectories.


1:1:150
3:3:50
5:5:30
15:15:10
15:15:27
density [nm^{-2}]
x /nm
y /nm

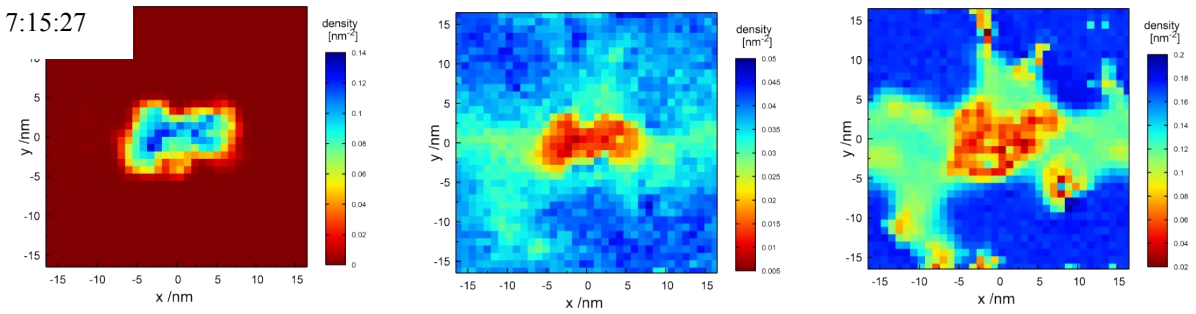


Figure S7. 2D representation of the number densities of the PEC beads(left), the lipid heads (middle) and tails (right) in the entrance layer at indicated PECs; densities were calculated from the last 20 ns simulation trajectories.

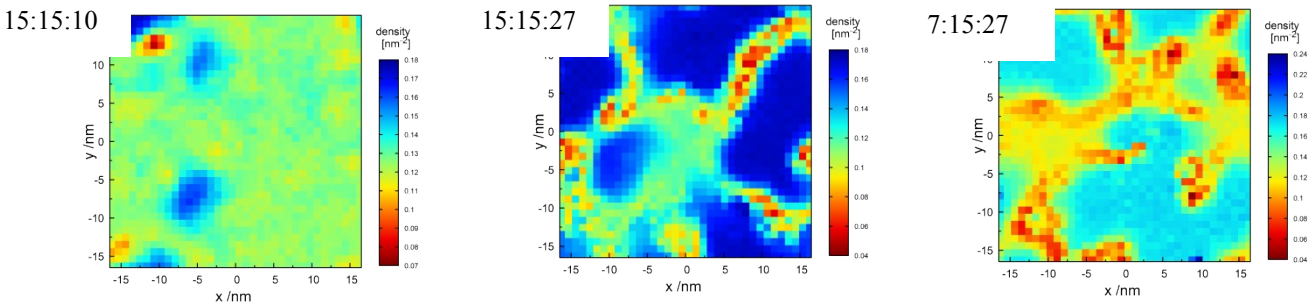


Figure 8. 2D representation of the number densities of lipid tails in the distal layer at indicated PECs; densities were calculated from the last 20 ns simulation trajectories.