Supporting information for

Behaviour of NBD-headgroup labelled phosphatidylethanolamines in POPC bilayers: A molecular dynamics study

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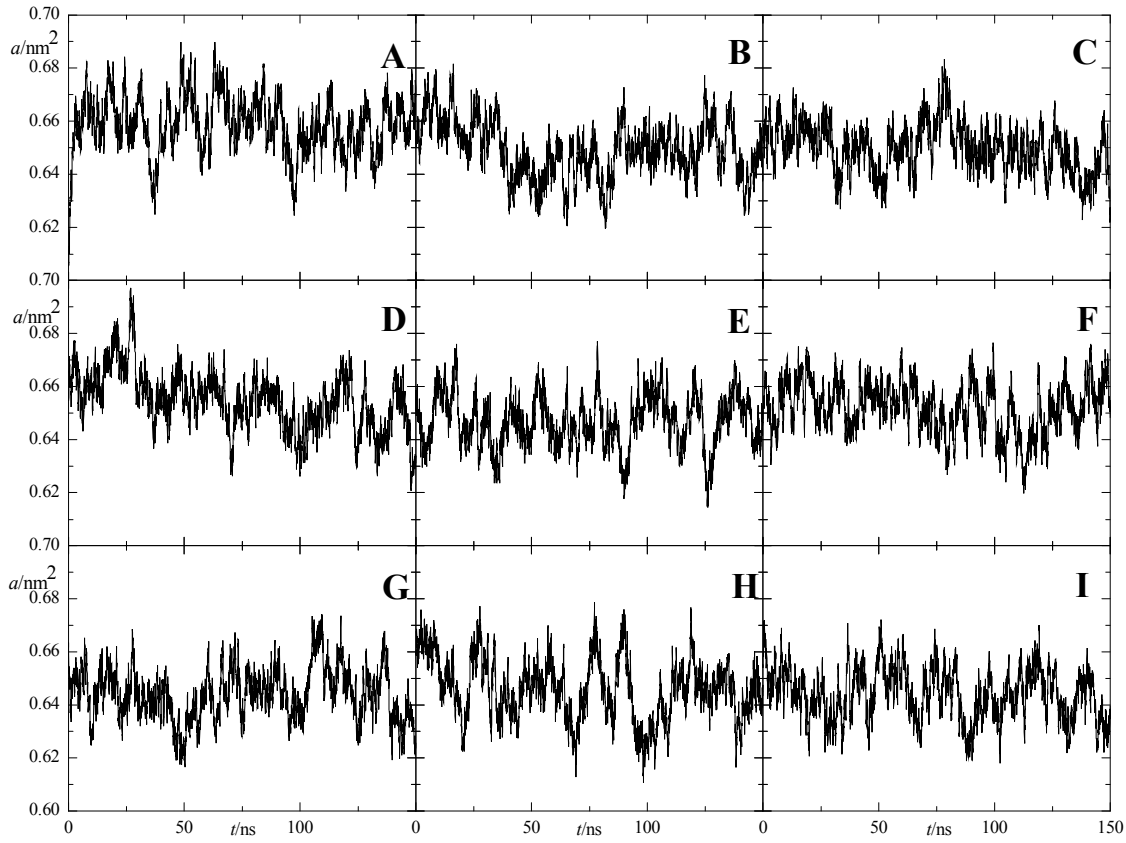

Figure S1. Time evolution of the molecular areas (a) for all systems (from A to I: pure POPC, POPC + NBD-diC_4PE, POPC + NBD-diC_6PE, POPC + NBD-diC_8PE, POPC + NBD-diC_{10}PE, POPC + NBD-diC_{12}PE, POPC + NBD-diC_{14}PE, POPC + NBD-diC_{16}PE, POPC + NBD-diC_{18}PE).

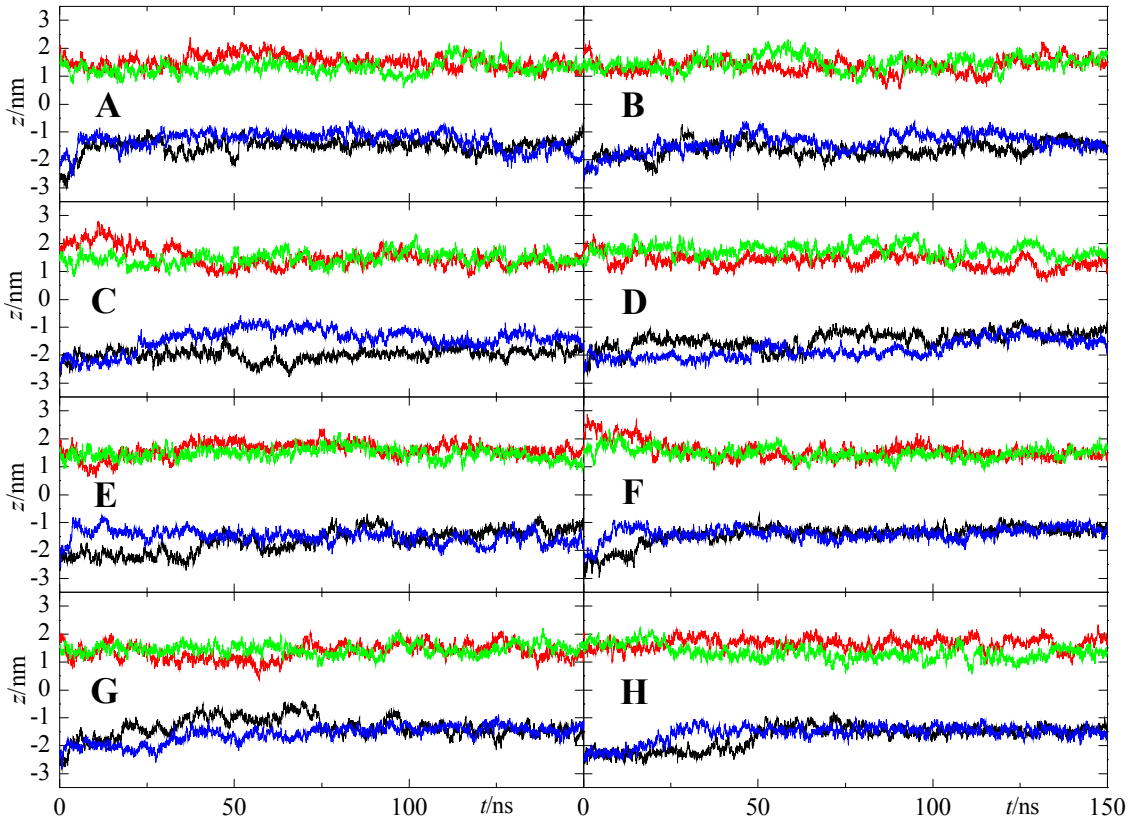

Figure S2. Time evolution of the transverse position z of the fluorophore center of mass, for the 4 individual NBD-diC_nPE molecules of each system (from A to H: NBD-diC_4PE, NBD-diC_6PE, NBD-diC_8PE, NBD-diC_{10}PE, NBD-diC_{12}PE, NBD-diC_{14}PE, NBD-diC_{16}PE, NBD-diC_{18}PE).

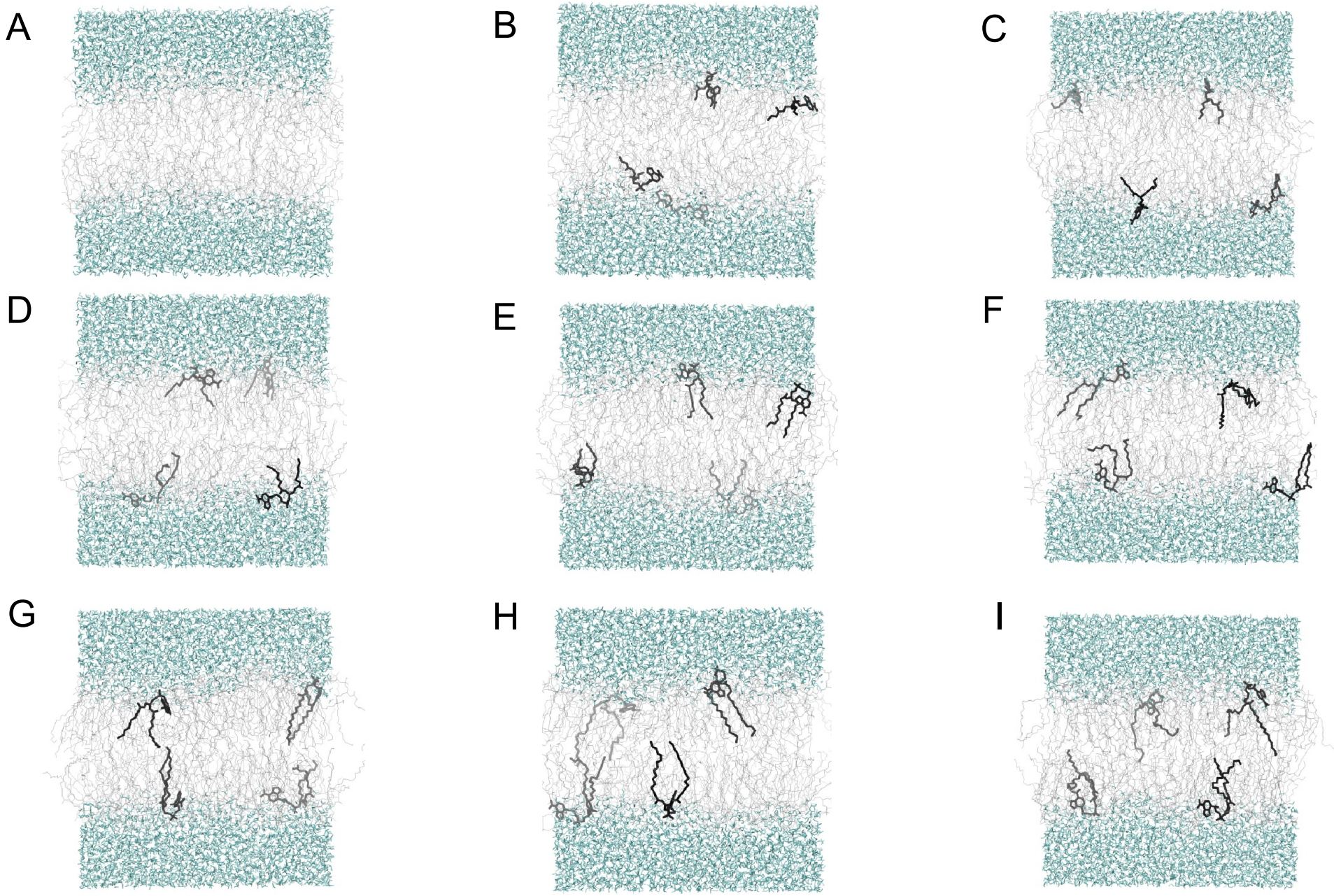

Figure S3. Final structures of all systems (from A to I: pure POPC, POPC + NBD-diC_4PE, POPC + NBD-diC_6PE, POPC + NBD-diC_8PE, POPC + NBD-diC_{10}PE, POPC + NBD-diC_{12}PE, POPC + NBD-diC_{14}PE, POPC + NBD-diC_{16}PE, POPC + NBD-diC_{18}PE).

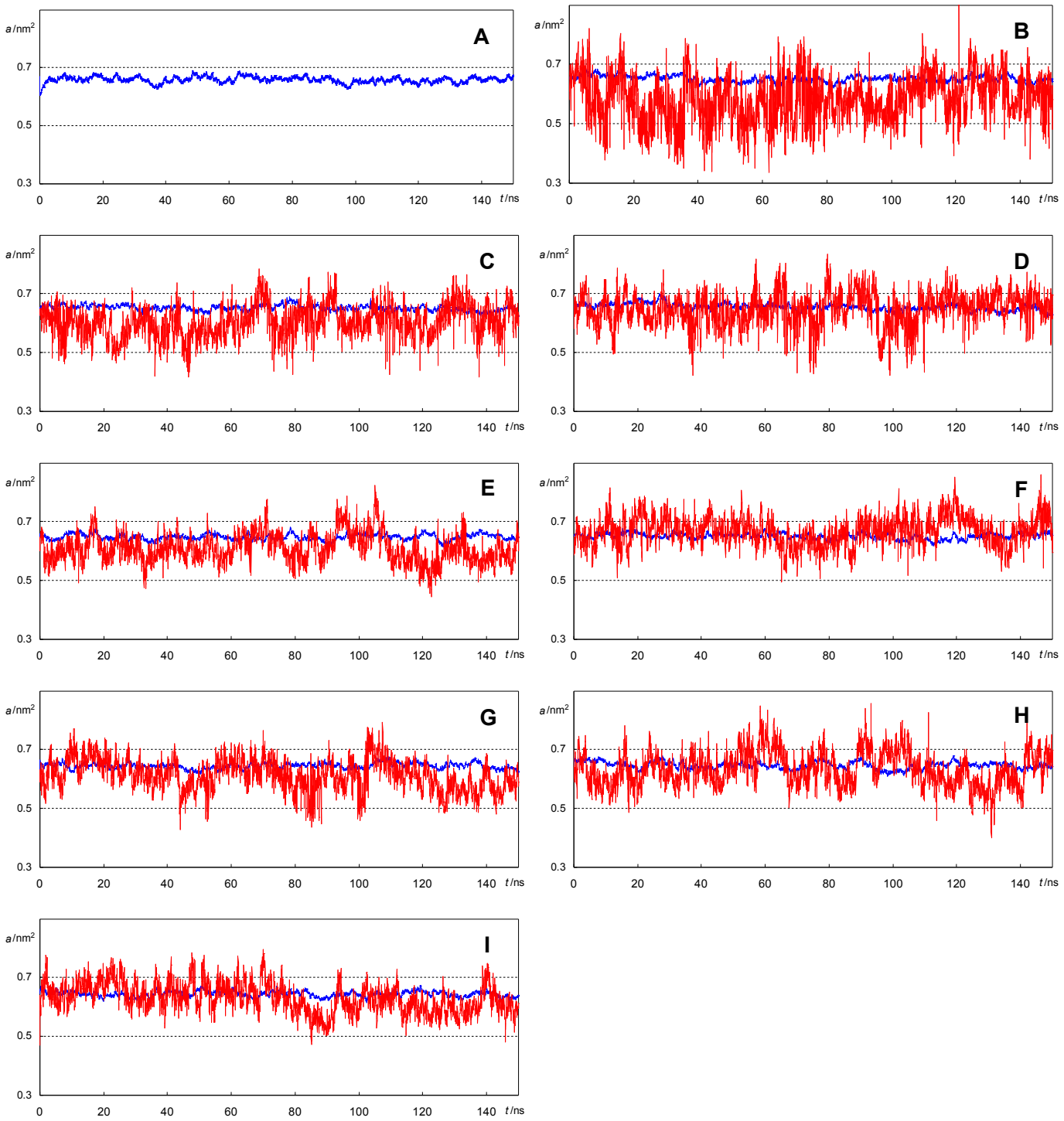

Figure S4. Time variations of average areas per POPC (blue) and NBD-diC_nPE (red) obtained by Voronoi tessellation (using APL@Voro, http://www.aplvoro.org) for all systems (from A to I: pure POPC, POPC + NBD-diC_4PE, POPC + NBD-diC_6PE, POPC + NBD-diC_8PE, POPC + NBD-diC_{10}PE, POPC + NBD-diC_{12}PE, POPC + NBD-diC_{14}PE, POPC + NBD-diC_{16}PE, POPC + NBD-diC_{18}PE).

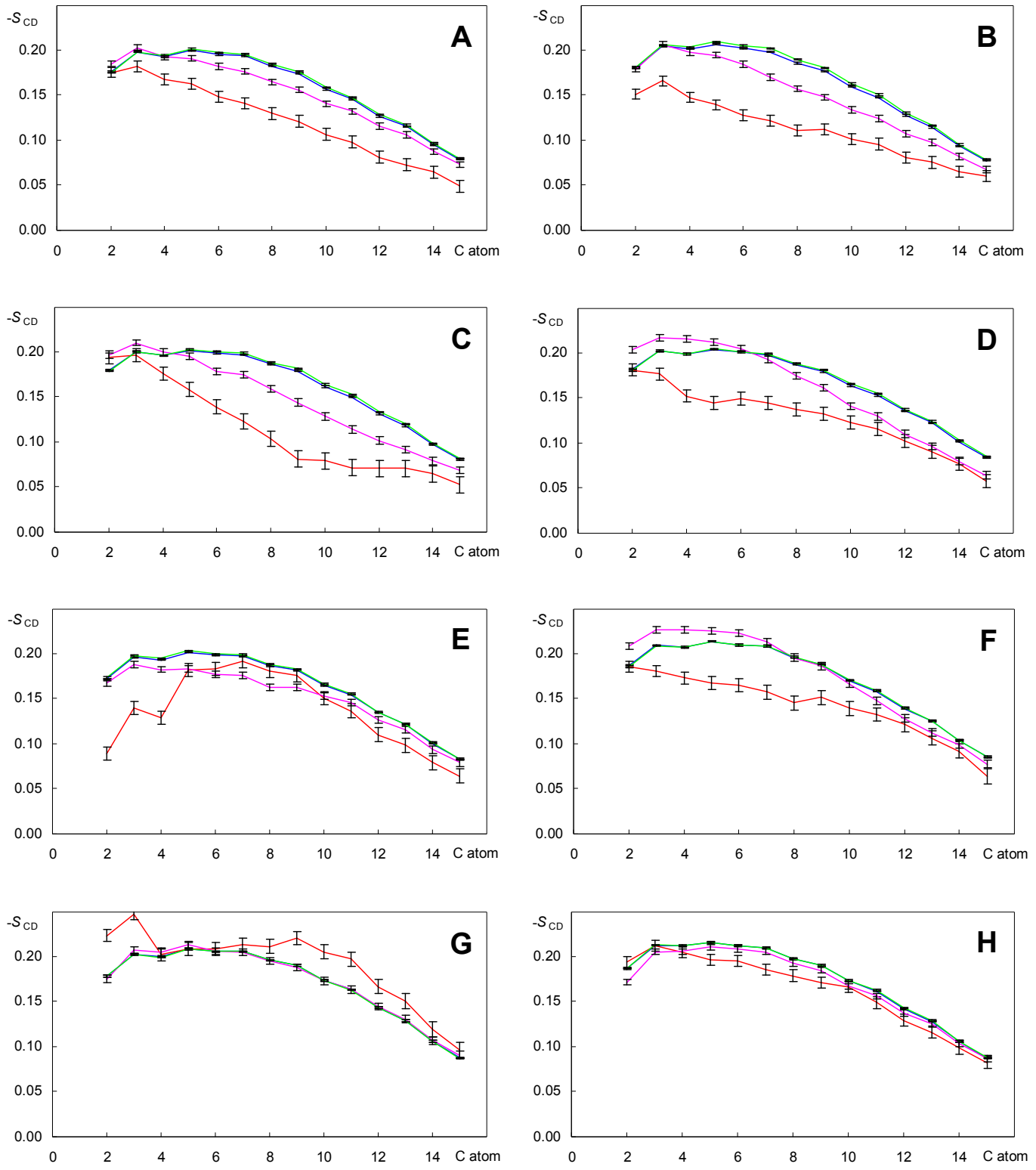

Figure S5. Deuterium order parameter of POPC *sn*-1 acyl chains located at lateral distance $R < 0.4$ nm (red), 0.4 nm $< R < 0.8$ nm (magenta), and $R > 0.8$ nm (green) to the closest NBD-diC_nPE in the same bilayer leaflet. The overall profile is depicted in blue for each system (from A to H: NBD-diC_4PE, NBD-diC_6PE, NBD-diC_8PE, NBD-diC_{10}PE, NBD-diC_{12}PE, NBD-diC_{14}PE, NBD-diC_{16}PE, NBD-diC_{18}PE).

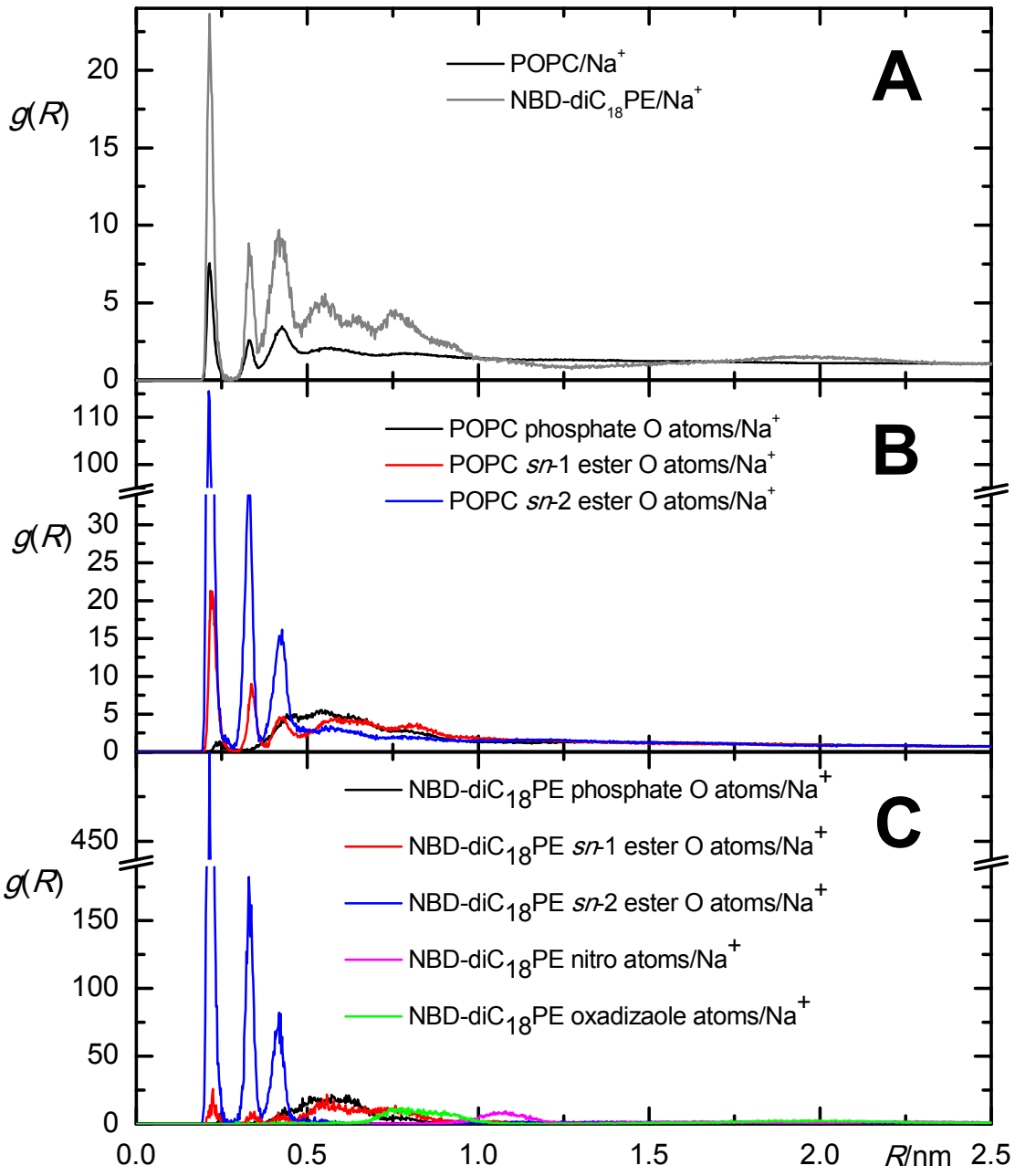

Figure S6. Radial distribution functions $g(R)$ of sodium ions around electronegative lipid and probe atoms. Both overall (A) and discriminated (B and C for POPC and NBD-diC$_{18}$PE atoms, respectively) $g(R)$ functions are depicted.

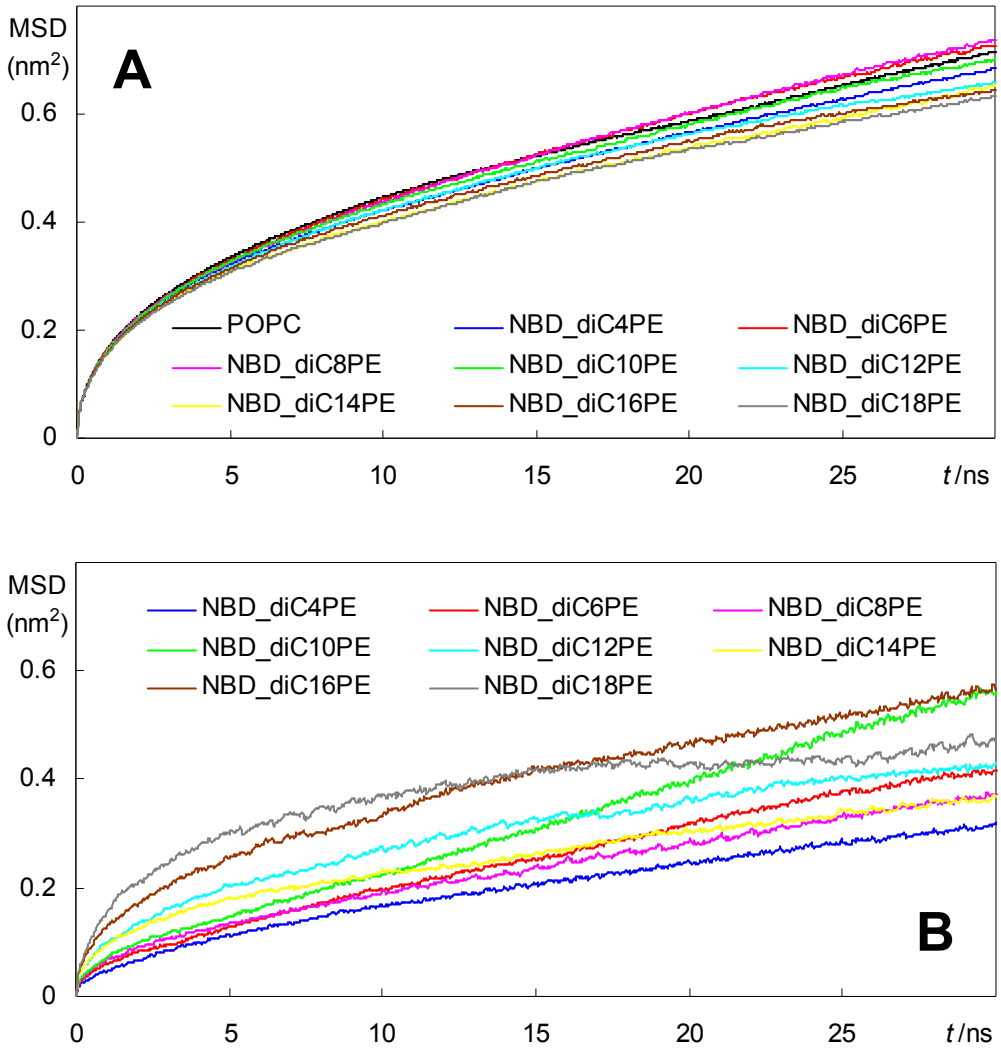

Figure S7. Lateral mean square displacements of POPC (A) and NBD-diC_nPE (B).

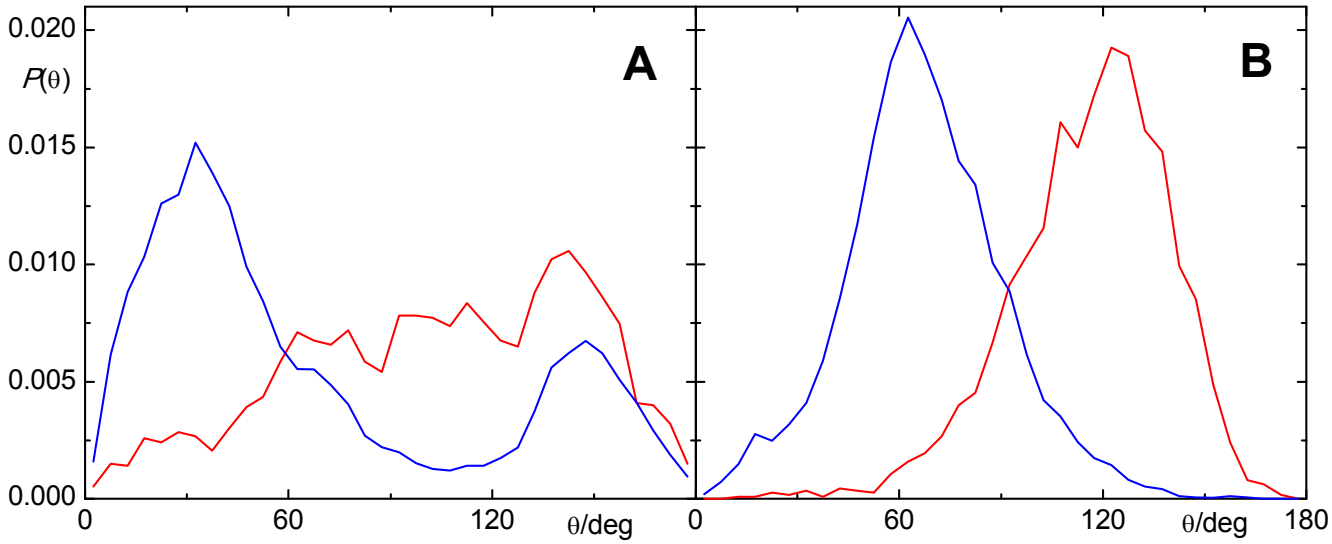

Figure S8. Angular orientation distributions for the long (A) and short (B) axes of the NBD fluorophore (see Fig. 1 for definition) in C6-NBD-PC/DPPC (red; data taken from L. M. S. Loura and J. P. Prates Ramalho, *Biochim. Biophys. Acta*, 2007, **1768**, 467-478) and NBD-diC_{16}PE/POPC (blue).