Membranes are an indispensable constituent of biological cells, providing a unique hydrophilic and hydrophobic platform for adsorption and anchoring of a wide range of biomolecules. Molecular dynamics (MD) simulations has been proven to be a powerful tool for the study of structural and dynamical properties of lipid membranes, in atomic detail. However, even with the numerous works employing MD to characterize membrane structural properties, only a few studies had been dedicated to analyze mixtures of different phospholipids assembled into a single membrane. In this context, the current work intends to construct and validate models of some of the most common human membrane phospholipids, 1,2-dipalmitoyl-sn-glycero-3-sphingomyelin (DPSM), 1-palmitoyl-2-oleoyl-sn-glycero-3-sphingomyelin (POSM), 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoserin (POPS), 1,2-dipalmitoyl-sn-glycero-3-phosphoserine (DPPS), 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine (POPE) and 1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine (DPPE), not previously studied by MD, employing GROMOS96 53a6 united atom force field and GROMACS simulation suite. The so obtained membranes will allow the building of an endoplasmatic reticulum membrane with a mixture of these majority phospholipids as a support structure for cellular glycosylation machinery.

Key words: GROMOS96 53a6 force field, lipid model, membrane simulation
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