Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Support Information Material

Understanding the Stability of Polypeptide Membranes in Ionic Liquid: A Theoretical Molecular Dynamics Study

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ABSTRACT

In this work, we have observed the structural and energetic stability of a polypeptide nanosheet formed by a polypeptide skeleton of six alanines (ALA) or leucines (LEU) and a polar head composed of aspartic acid (ASP), lysine (LYS) or arginine (ARG). The six membrane structures, A_6D; A_6K; A_6R; L_6D; L_6K; and L_6R were subjected to molecular dynamics simulations in ionic liquid formed by the cholinium-glycine pair [CHO][GLY]. Our results show how the hydrogen bonds between the polypeptides and the ionic liquid are structured, the energetic behavior, mobility, surface topology of the membrane besides the stiffness of the structure when subjected to the extraction of a polypeptide from the macro structure. Different structural combinations were considered in order to verify the difference due to the electrostatic behavior in the systems. Our analysis aims to contribute information that can increase the use of these organic and biodegradable materials in other environments.

Keywords: Molecular dynamics; polypeptide; nanosheet; Ionic Liquids.

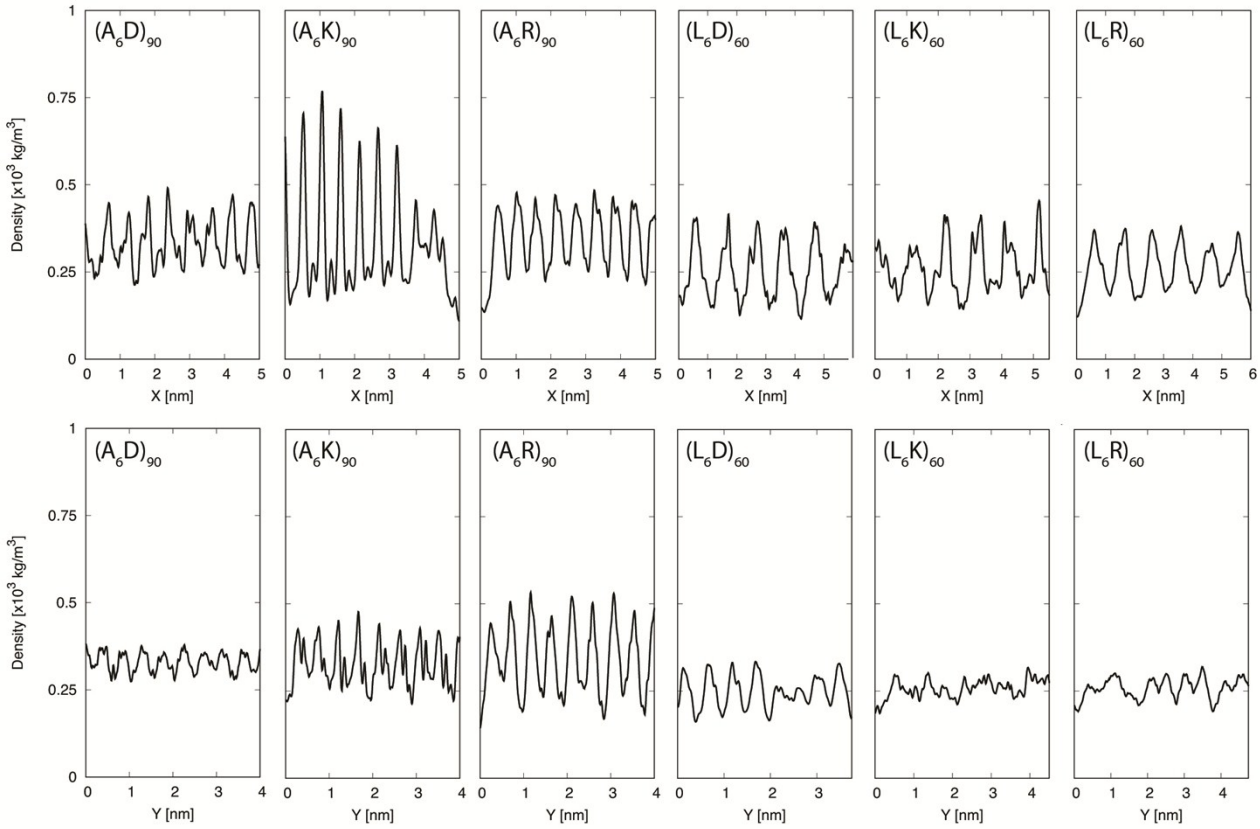


Figure S1: Density profile of the six equilibrated nanosheet simulated in this work in the X and Y directions.

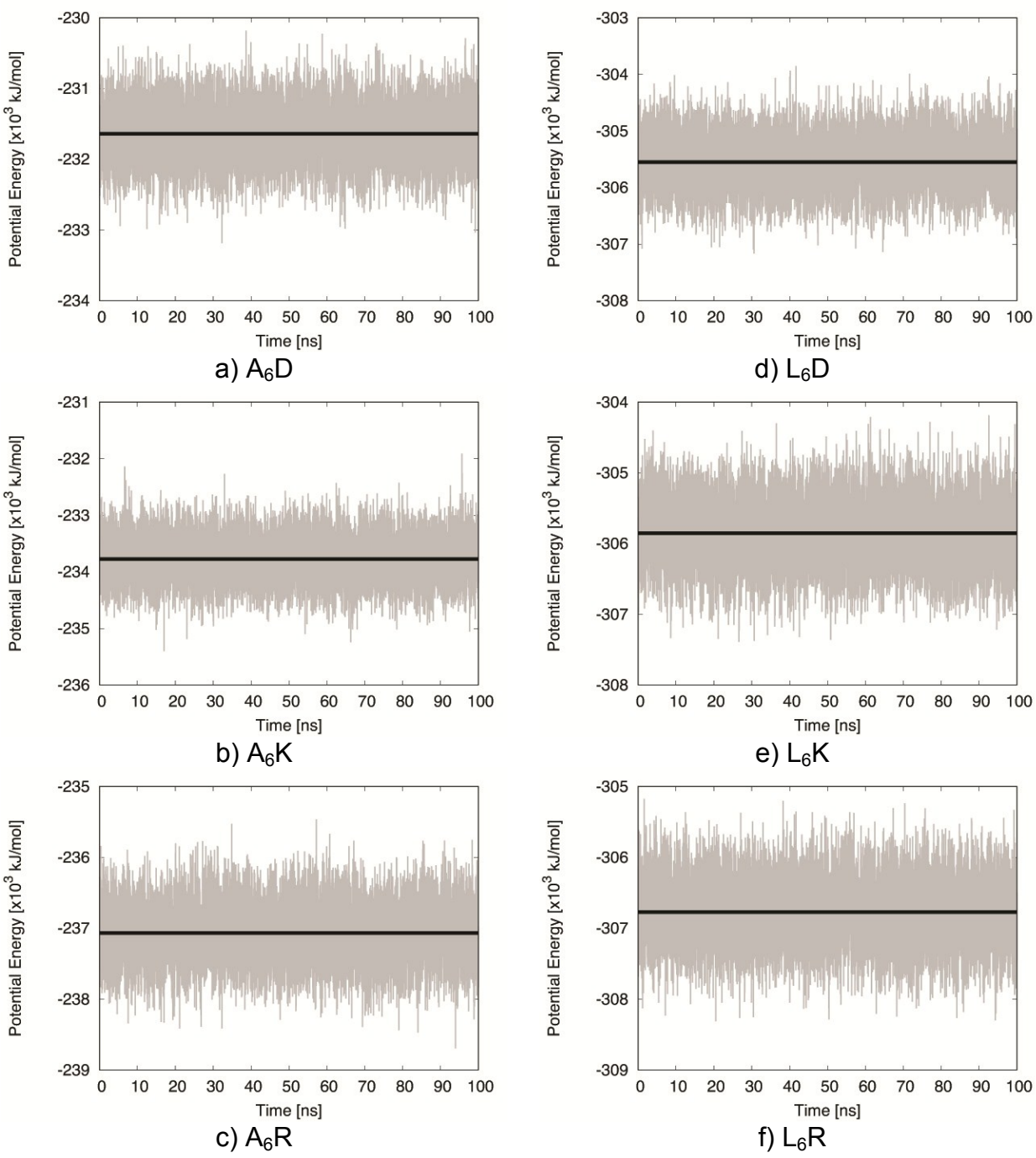


Figure S2: Potential energy profile of the six equilibrated monomers simulated in this work.

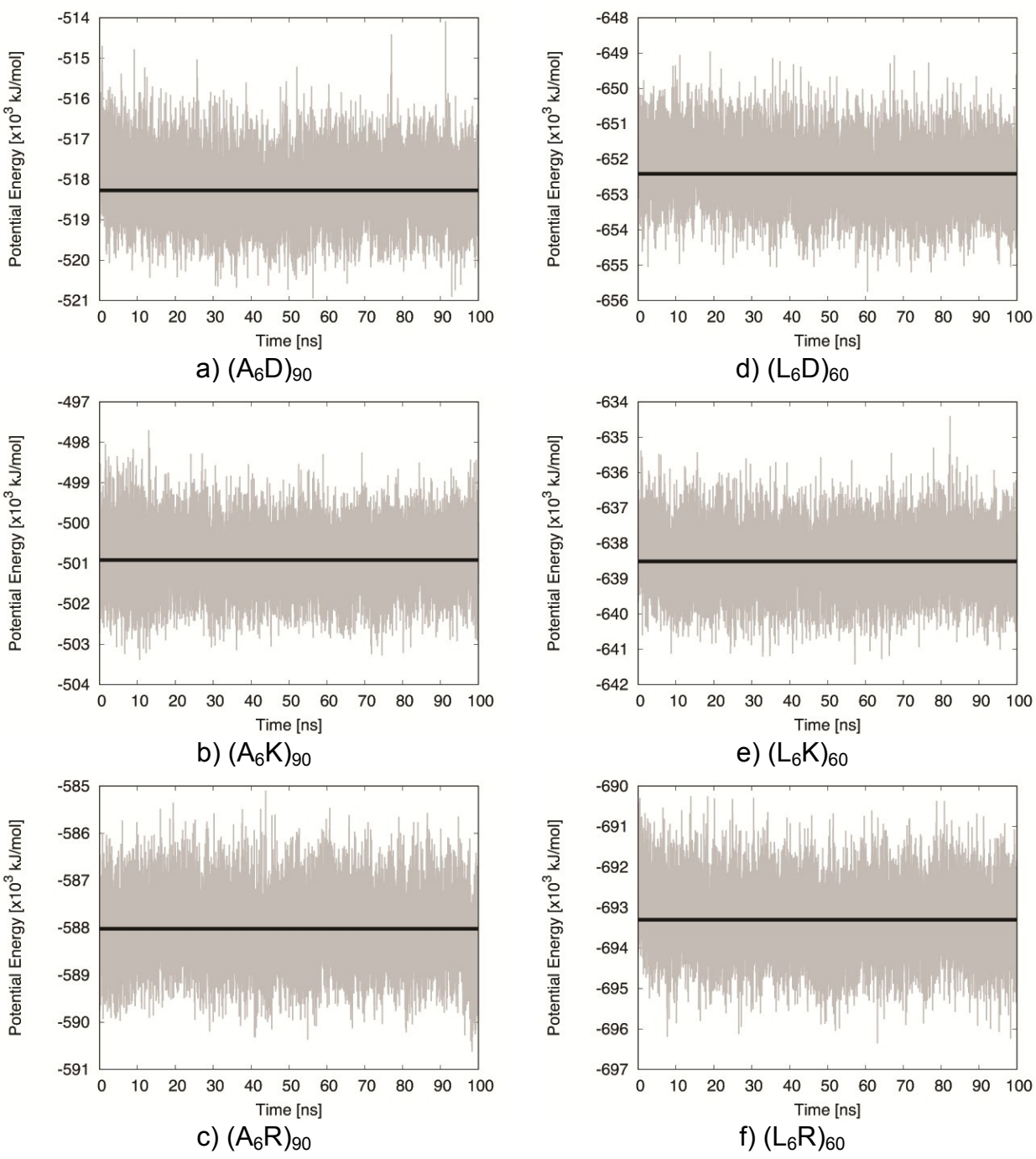


Figure S3: Potential energy profile of the six equilibrated membranes simulated in this work.

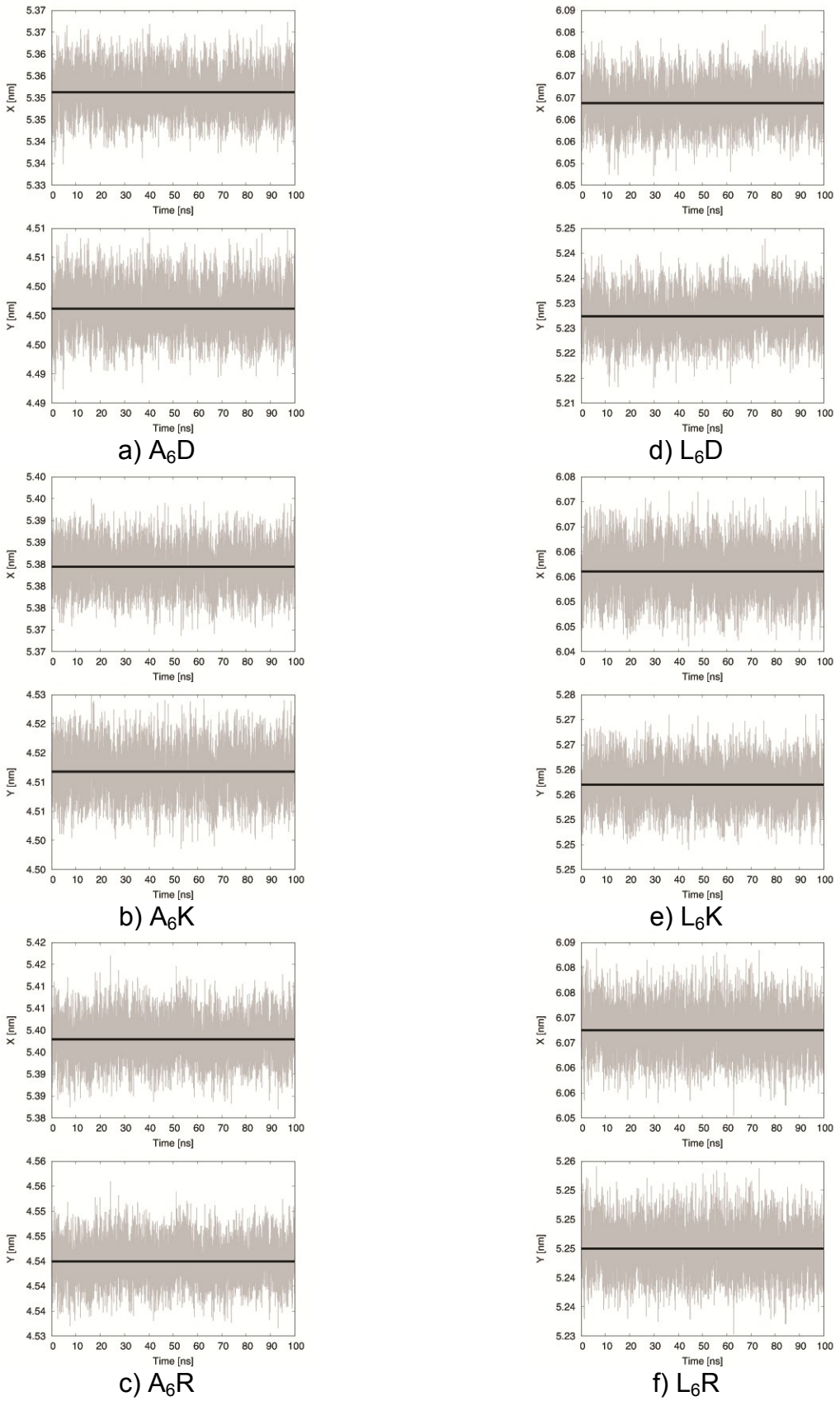
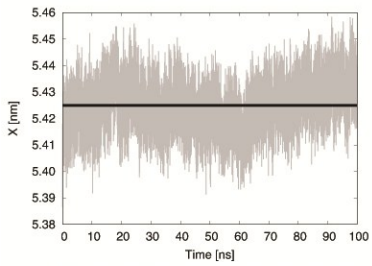
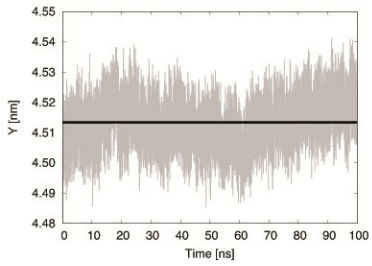
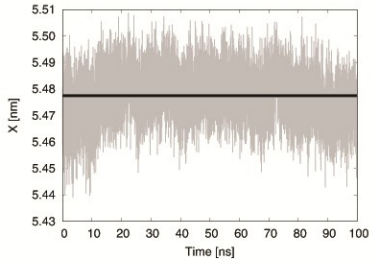


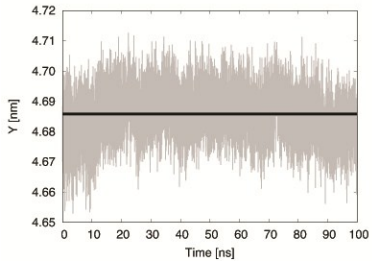
Figure S4: Box length variation, in (nm), of the six equilibrated monomers simulated in this work.



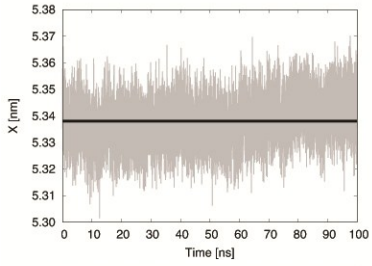


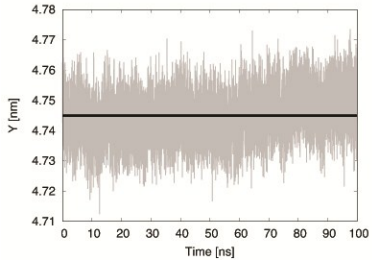
a) $(A_6D)_{90}$



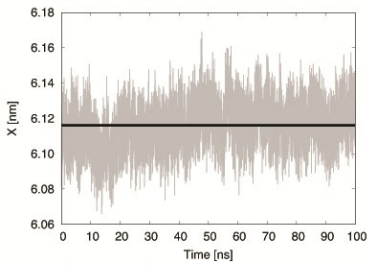


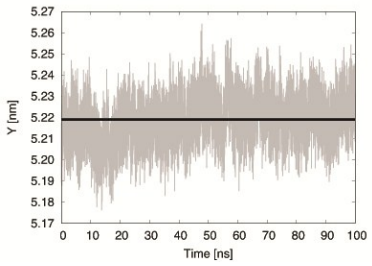
b) $(A_6K)_{90}$



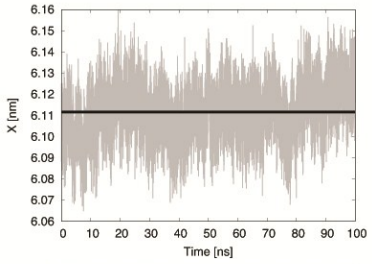


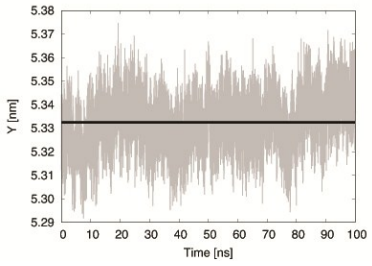
c) $(A_6R)_{90}$



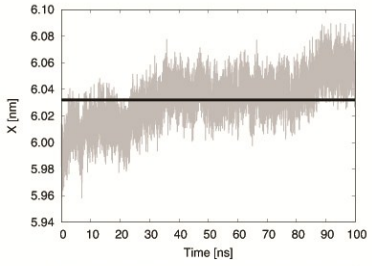


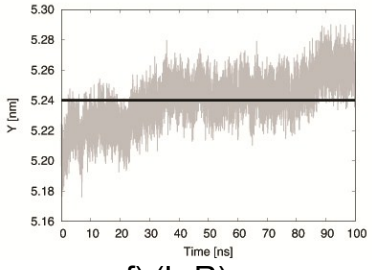
d) $(L_6D)_{60}$





e) $(L_6K)_{60}$





f) $(L_6R)_{60}$

Figure S5: Box length variation, in (nm), of the six equilibrated membranes simulated in this work.