Contribution ID: **42** Type: **Poster**

Structure and elasticity of mitochondrial membranes from molecular dynamics simulations

Mitochondria are crucial for energy metabolism. In living cells, they undergo continuous shape transformations in order to perform various biological functions such as fission and fusion rearrangement. The shape of the membrane is determined by the bulk mechanical parameters of the membrane such as lateral tension, bending modulus and spontaneous curvature. These parameters, in turns, depend substantially on the molecular interaction between membrane lipids, especially between cardiolipins, the specific phospholipid of mitochondrial membranes, which plays an important role in the structural organization and the function of mitochondrial membranes. Alterations in cardiolipin concentration have been associated with mitochondrial dysfunction in multiple tissues in several physiopathological conditions and aging. To understand the molecular mechanism caused mitochondrial dysfunction, in this work, we perform all-atom molecular dynamics simulations of various mitochondrial membrane models to study how the structure and elastic moduli of the membrane depend on the cardiolipin concentration. We show that the variation in the cardiolipin from 0% - 15% does not induce significant changes in the membrane thickness, lipid area, and lipid order parameters. However, the bending modulus increases from 13.62x10-20 J at 0% cardiolipin to 16.75x10-20 J at 15% cardiolipin. This suggests that too high cardiolipin concentration may lead to stiffening of the mitochondrial membranes, thus limiting their functions.

Acknowledgement:
This research is supported by The Grant agreement No. 101034407 of the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska Curie actions: "FP-DYNAMO-PARIS FELLOWSHIP PROGRAMME-Regulation of Mitochondrial Function/Dysfunction by Focused Ultrasound"

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Session

Structural biology

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Session Classification: Clip Session