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Editorial: Biomolecular function and activity modulated by membranes

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Editorial on the Research Topic

Biomolecular function and activity modulated by membranes

Our knowledge of cellular membranes and their components' critical role is recent and so far, unfinished. Bilayers of lipids were proposed less than 100 years ago (Gorter and Grendel, 1925). "Fluid mosaic model", which explains fundamental issues like membrane organization, is just 50 years old (Singer and Nicolson, 1972). Many other core aspects are still a heated source of debate and discovery (Nicolson, 2014; Nieto-Garai et al., 2022). Today, we know that biological membranes are much more complex than any catch-all model, and almost every new investigation confirms this idea. In light of this, it is clear that more advanced experimental methods and more complex computational models, as well as finding ways to integrate the former two, are essential for the future of biological membrane research. This short Research Topic showcases four studies that use various methods to investigate membrane-related phenomena. Polasa et al. use an extensive set of equilibrium and non-equilibrium molecular dynamics simulations to describe the conformational changes in the YidC during membrane insertion (Polasa et al.). Similarly, Li et al. consider the effect of cholesterol and membrane composition on C99 dimerization with ramifications in Alzheimer's disease (Li et al.). Be it atomistic or coarse-grained, molecular dynamics uses a physics-based approach to explicitly describe the interaction between molecular moieties of interest with an outstanding resolution. Aslam and Alvi present a different computational approach based on systems biology. Their mathematical modeling allowed the complete exploration of a novel postsynaptic channel for glutamatergic synaptic transmission and its effector molecules composed of ions, diacylglycerides, and protein kinases (Aslam and Alvi). Unlike molecular dynamics, systems biology works at much larger scales and aims to characterize emergent phenomena from complex and interdependent processes and interactions in biological systems. Advancing our knowledge of membrane-related processes depends on experimental methods as well. The Research Topic includes the purely experimental work by Kurakin et al., who studied lipid vesicle and divalent ion interactions (Kurakin et al.). This process is of paramount importance in signaling and membrane structure. Overall, we show that advancement in membrane research requires synergies from widespread techniques.

Author contributions

GE wrote the first draft of the editorial. JL and HM-S edited.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

References

Gorter, E., and Grendel, F. (1925). On bimolecular layers of lipoids on the chromocytes of the blood. *J. Exp. Med.* 41 (4), 439–443. doi:10.1084/jem.41.4.439

Nicolson, G. L. (2014). The fluid—mosaic model of membrane structure: Still relevant to understanding the structure, function and dynamics of biological membranes after more than 40years. *Biochimica Biophysica Acta (BBA) - Biomembr.* 1838 (6), 1451–1466. doi:10.1016/j.bbamem.2013.10.019

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Nieto-Garai, J. A., Lorizate, M., and Contreras, F.-X. (2022). Shedding light on membrane rafts structure and dynamics in living cells. *Biochimica Biophysica Acta (BBA) - Biomembr.* 1864 (1), 183813. doi:10.1016/j.bbamem.2021.183813

Singer, S. J., and Nicolson, G. L. (1972). The fluid mosaic model of the structure of cell membranes. *Science* 175 (4023), 720–731. doi:10.1126/science.175.4023.720