Neuronal Plasma Membrane: A Computational Investigation

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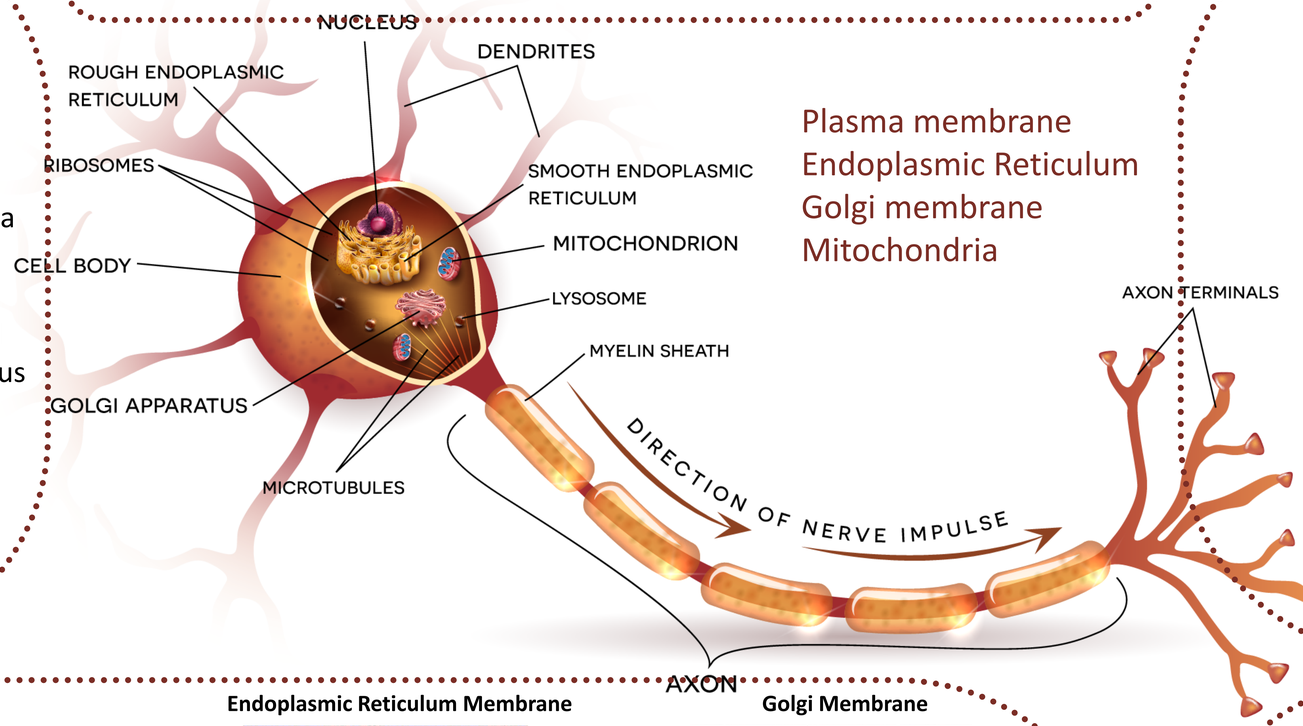
Introduction

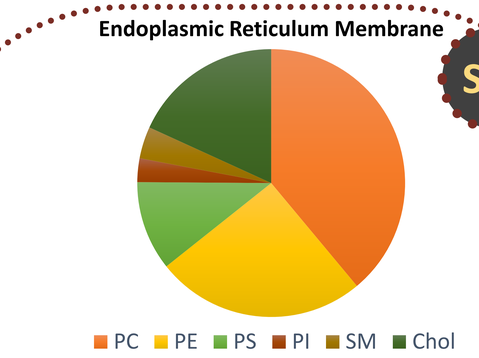
- Lipid membranes protect and regulate traffic through their semipermeable walls
- A typical membrane is an asymmetric bilayer, composed of hundreds of lipid types
- Lipid composition of a membrane varies within a cell's organelles
- A **neuronal cell membrane** composition is influenced by several factors including diet, and defects in lipid regulation can be linked to various neurological diseases.
- The complexity of the membrane is crucial; changes in composition affects overall bilayer properties, dynamics, and lipid organization of cellular membranes.

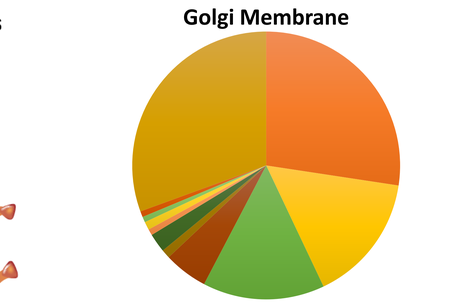
Neuron and cellular compartments



Plasma membrane
Endoplasmic Reticulum
Golgi membrane
Mitochondria

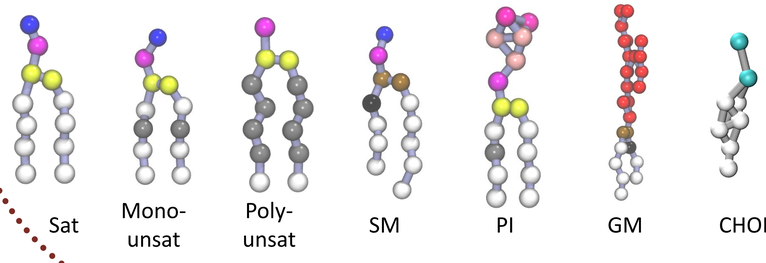
System



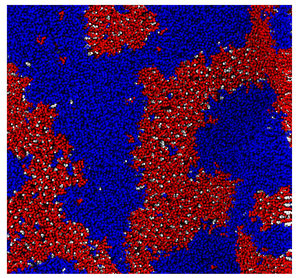


Results

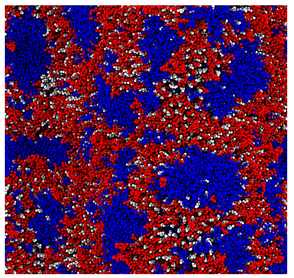
- Diversity in lipid composition, both in head groups and tail saturation levels, were obtained from lipidomics data
- Molecular dynamics simulations were performed at a coarse-grain level using Martini force-field
- The simulations are set to run for 5µs
- The systems were both visually examined and analyses performed to study and compare membrane properties



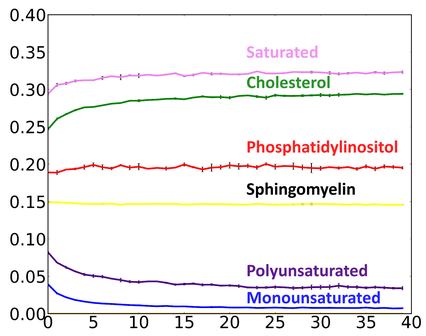
Endoplasmic Reticulum Membrane

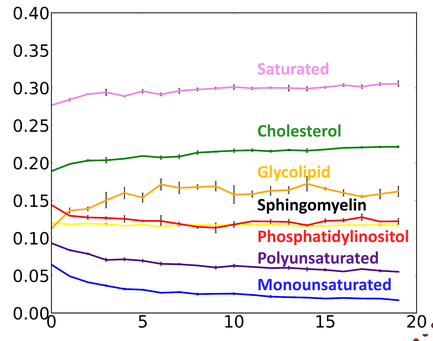


Golgi Membrane



Unsaturated Lipids Saturated Lipids Cholesterol





time =0.5 µs

Conclusions

- Domain formation–saturated lipids and cholesterol assemble together, while unsaturated lipids form separate domains
- Lipid mixing parameter for saturated lipid confirms the preferential association of saturated lipids with itself, followed by cholesterol.
- Change in lipid composition and increase in lipid diversity shows difference in lipid mixing even within 2µs of simulation length
- Further investigation of membrane properties such as hydrophobic thickness, lipid order parameter, will provide additional comparative points to study membrane diversity

References

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Acknowledgments

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