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Molecular Simulations of Glycolipids: Towards Mammalian Cell Membrane Models

David Shorthouse, George Hedger, Heidi Koldsø, Mark S.P. Sansom

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Glycolipids are key components of mammalian cell membranes, influencing a diverse range of cellular functions. For example, a number of receptor tyrosine kinases, including the epidermal growth factor receptor (EGFR), are allosterically regulated by the glycolipid monosialodihexosylganglioside (GM3). Recent advances in molecular dynamics methods, especially the development of coarse-grained models, have enabled simulations of increasingly complex models of cell membranes. We demonstrate these methodological developments *via* a case study of a coarse-grained model for the ganglioside GM3. This glycolipid is included in simulations of a mixed lipid bilayer model reflecting the compositional complexity of a mammalian cell membrane. The resultant membrane model is used to simulate the interactions of GM3 with the transmembrane domain of the EGFR.

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