Designing Transmembrane Signaling Systems in Artificial Cells using DNA Structures

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Building an artificial cell is an essential step to creating artificial life-like systems and a critical step in this endeavour is to design molecular systems which enable the communication of an artificial cell with its environment. Such artificial life-like systems hold great promise for biomedical engineering. In biomedical applications, such nanoscopic artificial life-like system will be able to, e.g., shape artificial tissues, as part of entirely novel therapeutic strategies. By mimicking biological mechanisms to enable the transmission of information from the exterior of artificial cells across membranes to their interior [1], we will contribute to creating new artificial life-like systems and gain insights to essential biological information processing mechanisms [2] and advance simulation method development [3]. In this work, we will design novel DNA-based transmembrane signaling systems using multi-scale simulations [1], [4]. DNA structures can be synthesized to function as receptors in artificial life-like systems. These DNA structures transmit signals across the membrane which mark the external boundary of artificial cellular systems. Using an atomistic molecular dynamics simulation approach, we study DNA attached to molecule of Cholesterol Tetraethylene glycol (CholTEG) in lipid membranes. In the simulations we investigate how CholTEG interacts with the membranes and how DNA-CholTEG changes local membrane structure.

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