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StatMech Insights on Na+/I– Symporter transport cycle

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The intrinsic transmembrane protein known as sodium iodide symporter (NIS) facilitates the active transport of iodide across the basolateral membrane of thyroid follicular cells. Iodine is an essential molecule that is used to produce the classical thyroid hormones.
To perform a molecular dynamics (MD) simulation, we used structures of apo-NIS and NIS with I– and an oxyanion (ReO4–) bound to it.
The goal of our computational study was to explore the conformational space of NIS and gain insights into the conformations it assumes over the course of its transport cycle.
We prepared a realistic simulation system that included NIS Na+ + I– / Na+ + ReO4– complexes embedded in a central membrane with the mammalian lipid composition, with two half-membrane leaflets on either side. We simulated the membrane potential by applying a constant external electrical field to the system, thereby bringing about the equivalent of a membrane potential. We are using this system to conduct unbiased and enhanced dynamics (metadynamics, Deep-Tica), a NPT statistical ensemble, with the program GROMACS (2023.3) and a modified CHARMM36 force-field, to include non-bonded interactions between I– and the oxyanion ReO4–. In order to determine the effects of the potential on the outwardly open NIS events, simulations were conducted with three different membrane potentials (0, −70, and −140 mV) using the wild-type NIS with the anion and oxyanion bound to it, and using a double mutant with interesting transport characteristics.
The resulting MD trajectories are currently being analyzed using a Python 3.11 script and some public libraries such as mdtraj (v1.9), MDanalysis (v2.7), Pyemma (v2.5.12), mlcolvs and pytorch for deep-learning analysis. Metadynamics calculations of the transport of I–/ReO4– free energy along the transport path are currently being done for the different membrane potentials, using funnel bias metadynamics.

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