Intense nanosecond-scale electric field effect on kinesin: molecular dynamics study

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Proteins are the fundamental nanoscopic machines which execute life processes. Therefore, having effective means to affect protein function would be beneficial both for novel potential biomedical therapies as well as applications in bionanotechnology. Intense nanosecond electric field seems to be an effective tool to manipulate protein conformation [1]–[3]. However, effect of intense electric field on soluble proteins in water are poorly explored so far. In our current project [4], we focused on a protein kinesin. Kinesin is a protein nanomotor which converts chemical energy into mechanical work. It is important for intracellular transport of cargo and in cell division. Since electrostatic forces are crucial for kinesin function, we propose that intense nanosecond scale pulsed electric field could affect the function of kinesin.

To explore this hypothesis, we performed molecular dynamics simulation of a kinesin head docked on a subunit of its microtubule track - single tubulin heterodimer. In the simulation, we exposed the kinesin head to 100 MV/m electric field for 50 ns. We found that while the structure and dynamics of the functionally important kinesin segments, including microtubule binding motifs as well as nucleotide hydrolysis site which power the nanomotor was affected only slightly, the electric field effect is strong enough to affect non-covalent interaction between kinesin and tubulin. Additionally, we found indication that kinesin head can be detached from its microtubule track and effectivity of this process depends not only on electric field strength but also on the electric field direction with respect to kinesin-microtubule axis.

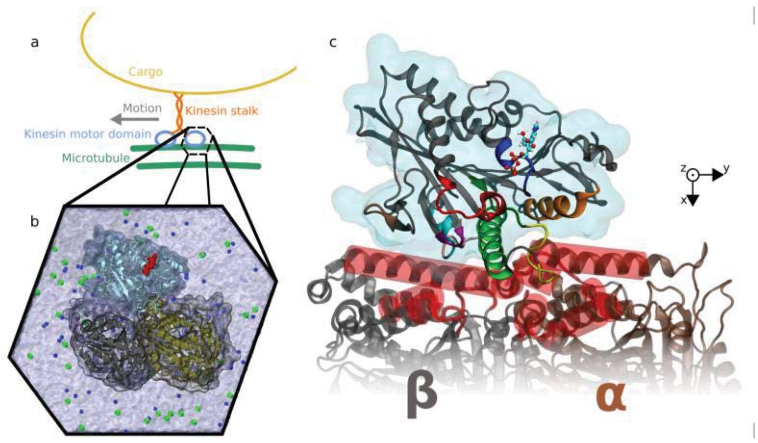

Figure 1. **a** – schematics kinesin as cargo carrier in cells, **b**,**c** – close up on the molecular simulation system of kinesin on a tubulin heterodimer. Image adopted from [4].

These findings indicate that external intense nanosecond-scale electric field can affect kinesin function. Our results contribute to developing novel electromagnetic methods for modulating function of biomolecular matter at the nanoscale.

Authors acknowledge support from the Czech Science Foundation p.no. GA18-23597S, and participate in COST CA15211, and exchange project, no. SAV-18-11.

References

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