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Molecular dynamics simulation study of intense electric field effect on tubulin

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Functions of proteins and interactions between them are primarily based on electric and electrodynamic forces. Charge distribution and fluctuations of the individual atomic groups on proteins generates local electric field that ultimately determines how proteins bind and interact. Possibility of modifying and possibly controlling protein function by external electric field lends itself as a tool for both understanding and controlling biological processes. Here we demonstrate, using molecular dynamics, that intense, yet experimentally attainable, electric field affects tubulin dimer conformation within several nanoseconds. We focused on the effects of electric field on the structure and dynamics of C-terminus of beta tubulin. The tail of C-terminus (i) is important for interactions with other proteins such as motor proteins and microtubule severing proteins, (ii) is a major site for mutations and post-translational modifications, (iii) possesses a significant fraction of tubulin electric charge hence it is a natural target of electric field effects.

We found that a field with intensity equal to or greater than 20 MV/m (200 V / 10 um) causes straightening of beta tubulin C-terminus as quantified by change of the protein dipole moment. The dynamics of the straightening was shown to be intensity dependent. Tubulin starts to unfold (unzip) from the C-terminus for intensities larger than 50 MV/m.

Based on our results we believe that electric field can be used to modify tubulin function by acting on C-terminus tail.

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