

How Electric Fields May Shape Inhibition: A Molecular Dynamics Study of GABA-A Receptors

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Transcranial direct current stimulation (tDCS) is a non-invasive technique used to treat psychiatric and neurological disorders by modulating brain activity using electrical currents. Although effective, the mechanisms by which tDCS alters brain function, particularly its effect on proteins such as GABA-A receptors, are still unclear. GABA-A receptors regulate neuronal excitability by allowing chloride ions to enter the cells, leading to inhibitory effects. It is assumed that tDCS alters the conformation and dynamics of these receptors and thus impairs their function.

To investigate these changes, molecular dynamics simulations could be used to model how electric fields affect GABA-A receptors embedded in a bilipid membrane. The hypothesis is that tDCS causes rapid, transient conformational changes that influence the duration of ion channel opening and thus modulate chloride entry. The bilipid membrane also plays a crucial role, as its interaction with the receptor can enhance or attenuate the tDCS effects.

Due to the complexity of the system, high-performance computing resources are essential to capture dynamic changes at atomic resolution over biologically relevant timescales.

Although the results are not yet available at the time of this submission, this work-in-progress poster will present the simulation strategy, system setup, and computational protocols employed. By sharing our methodological approach, we aim to foster discussion and receive early feedback from the scientific community, which will inform subsequent data analysis and interpretation.

Keywords: tDCS, GABA-A Receptor, Molecular Dynamics