Title: **Molecular dynamics simulation of the protein mobility under the influence of an external electric field.**

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Proteins and macromolecules generally have a surface charge that confers stability in aqueous solution. In the presence of ions, however, this can substantially alter the electrical properties of the surface of the molecule, altering its electrophoretic mobility and hydrodynamic properties.

In this TFG we study by simulation the behavior of a peptide in the presence of an electric field. The results of the molecular dynamics allows to quantify the electrophoretic mobility depending on the ionic conditions of the medium. Subsequently, the behavior of a protein in the presence of an electric field.

To learn to use the Gromacs simulation program the following strategy was followed. First, I carried out simulations of a model peptide without electric field. Then, I applied the electric field and measured the mobility. Finally, I applied the procedure to study the electrophoretic mobility of a selected protein.

In the case of the model peptide, polylysine, the obtained results indicates that the simulated electrophoretic mobility of the peptide decreases with increasing the ionic strength following the Kohlrausch law.

The obtained value of the electrophoretic mobility of the Venom toxin, the protein studied, indicates that the same applied electric field used in the simulations of the peptide is also applicable in case of proteins.

Keywords: Molecular dynamics, electrophoretic mobility