

The aim of this thesis was to probe the effect of the subTHz electric field on a key protein - tubulin dimer, which is crucial for the cell's stability, motility and division. This study was done *in silico*, which means that we studied the system through the simulations. We worked in the framework of classical molecular dynamics with force-fields. We used the GROMACS package together with our own Python and bash scripts. We were dealing with nonequilibrium molecular dynamics simulations since the external electric field (EEF) was applied. To study the effect EEF on the structure and stability of tubulin dimer, root mean square deviations, root mean square fluctuations and dipole moment analysis were performed. Additionally, we also analyzed the rotational motion caused by EEF. We probed 15 different frequencies of EEF - 10, 20, 30, . . . , 150 GHz in 6 different directions. For statistics, all calculations were done three times, each time with different initial velocities assigned before equilibrations, to probe different parts of the phase space. For better results, much larger statistics needs to be done in the future. Unfortunately, this was not possible since the simulations had already been very computationally expensive. Still, we were able to learn a lot from our results, such as that the electric field of 10 - 40 GHz had a strong rotational effect on the tubulin dimer, where it rotated in such a way that its longitudinal axis became parallel to the electric field oscillation direction. Regarding the conformational changes, they are evident for all frequencies and directions, but yet again, more statistics is needed. Additionally, we saw some changes in rigidity of the parts of the tubulin that are important for binding the anti-tubulin drugs, such as vinca alkaloids, colchicine and a small effect on paclitaxel binding site. Furthermore, the effect on the  $\beta$ :M-loop and  $\alpha$ :H1-B2 loop, which are important in lateral interactions of tubulin in microtubules, was observed. Since our tubulin also has two unstructured C-terminal ends (which are crucial for many tubulin functions, such as binding the microtubule-associated proteins), we were able to study their switching between different conformational ensembles under the effects of EEF. These C-terminal ends are very sensitive to the effect of EEF since they are negatively charged and intrinsically disordered.