

Αγγλική Περίληψη

The use of microwaves technology in everyday activities renders the study of effects of microwaves on biological matter necessary. Molecular dynamics simulations in conjunction with Linear Response Theory have been previously shown to be a reliable theoretical tool for the calculation of the dielectric properties of biomolecular systems. In this work a software has been developed using a combination of MVC and microservices architectures in order to simplify and speed up the above task. It combines the C++, Tcl and GNU plot languages. The software has been tested in the case of a lysozyme solution (Clys = 128.33 mg/mL) at 300K. In addition it has been also applied in the case of an ectoine solution (Cect = 198.87 mg/mL) at 300K.