

**P029** Understanding electromagnetic (e/m) field effects on proteins: a molecular dynamics case study of field and charge interactions in Hen Egg White Lysozyme (HEWL)

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A recent Molecular Dynamics (MD) study of non-thermal electromagnetic radiation effects, carried out in collaboration with this group, observed that exposure of a protein to e/m fields induced partial protein unfolding comparable to the initial stages of temperature induced unfolding. To further probe these effects we carry out MD simulations of several HEWL variants and observe the effects of altering the net charge of the protein. A variety of HEWL variants are constructed to modify the overall charge of the protein. These modifications consist of a combination of mutations of charged residues (i.e. alanine substitutions) as well as altering the residue protonation state. The alanine substitutions are done using the WHAT\_IF homology modelling tool MUTATE. MD simulations are performed using the GROMACS 3.3.1 molecular simulations package, modified to include an external electromagnetic field. Changes at the secondary structure level of the wild-type and mutant HEWL during the simulations are monitored using the DSSP program. As a preliminary result we report results of two simulations (one MD simulation of wild type HEWL and one of a HEWL variant) and based on the differences of these simulations we discuss further the interaction and influence of an electromagnetic field on a charged protein