PREDICTING TERTIARY STRUCTURES OF GLYCINE-RICH PEPTIDES WITH DISORDER REGIONS BY USING MOLECULAR DYNAMICS.

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Some peptides have been shown a real challenge, once that were impossible to model by homology or threading methods due to the presence of unclear disorder regions. These regions show one or more tandem sequences of glycine or proline residues, which give great mobility and instability. These dominions correspond to approximately 40%, being remaining residues having lower homology to proteins deposited to data bank, reducing the feasibility of a conventional molecular model. Indeed, we propose the use of molecular dynamics (MD) for peptide structure prediction. By using Gromos force field and GROMACS packages a water box was constructed as a solvent environment for the 55 residues of *Psidium guajava* antimicrobial peptide (*Pg*-AMP1). *Pg*-AMP1 is a glicine rich peptide, showed a dimeric form with no homology to known protein structures. After 60ns of simulation in a temperature of 300 ^{o}K, six final models were evaluated using VADAR web server. The best structure was used to construct a dimeric model, using HEX docking software, repeating stability checking. As result, the final model consisted in two charged α-helices compacting a high hydrophobic core. This is an alternative method for molecular modeling of peptides with disorder regions.

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