CONFORMATIONAL VARIABILITY OF THE ANTICOCCIDIAN PEPTIDE PW2 IN SOLUTION STUDIED BY NMR AND MOLECULAR DYNAMICS

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PW2 is a cationic peptide selected from phage display libraries that shows anticoccidial activity. The comparison between the structure of PW2 interacting with SDS and DPC micelles showed similarities mainly in the aromatic region that contains the motif WWR, probably responsible for anchoring the peptide to the interface. In this work we will describe the NMR studies of paramagnetic spin-labeled PW2. We used TOAC, an amino acid containing a nitroxide. The paramagnetic effect in the relaxation parameters R1 and R2 is dependent on the distance between the spin-label and the studied hydrogen. Measuring these parameters we were able to calculate the distances between the N-terminal and amide hydrogens. The distances were compatible with a curvature around WWR, similar to the conformation in micelles. This structural tendency of the peptide in solution resulted probably from fluctuation among pre-existent structure families. To assess these pre-existent structures a 10 ns unrestrained molecular dynamics simulation was performed in a water shell and the order parameter of the calculated structures corroborate the paramagnetic data. All these data can give more information for the development of new drugs against coccidiosis.

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