COMBINING SIMULATIONAL AND EXPERIMENTAL METHODS: A NEW APPROACH FOR PROTEIN STRUCTURAL PREDICTION THROUGH COMPUTATIONAL TOOLS  
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Computational tools play an important role to explore biological systems, since several processes and mechanisms may not be fully tracked experimentally. Therefore, computational approaches require experimental support, becoming genuine the combination of both techniques. On this work we applied experimental data obtained from Small Angle X-ray Scattering (SAXS) and Monte Carlo Simulations to predict the protein structural arrangement in solution. This choice was well thought because of the many advantages of this technique such as, the simplicity on the sample preparation, seeing that it remains in solution, and the expense of each analysis in comparison to other similar techniques. Since the thermodynamic hypothesis proposed by Anfinsen, it is known about the accessibility of proteins to its functional state, stability and that all necessary information for the folding of globular proteins is available on its amino acids sequence, i.e., on its primary structure. Considering that, the purpose is to use the primary structure information and SAXS profiles to run Monte Carlo simulations and estimate a tertiary structure.  
The developed software uses the protein’s primary structure and estimate a theoretical SAXS profile that is compared with the experimental one and a discrepancy value called, chi, is calculated and used to analyze the nonconformity between a random conformation envelope, calculated through Monte Carlo simulations with intrinsic system constrains, and the one experimentally obtained. The smaller the value of chi the closer the theoretical envelope is from the experimental profile. The software results were compared with similar software, already known in the scientific community, and the experimental profile itself. Both approaches were optimistic. The use of SAXS profiles combined to Monte Carlo simulations is a different way of approaching the complicated problem of protein structure prediction and it may help many others lines of research.  

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**Key words: Protein Structure Prediction, Computational simulations, SAXS**