Although the main function of the prion protein (PrP) remains controversial, a number of ligands this cell surface protein have been well characterized. Recent studies suggest that PrP serves as an interaction platform for other proteins, modulating various cell signaling processes whose effects can be translated into different functional consequences. Proteins that interact with more than one ligand can undergo conformational changes upon binding to a first ligand, increasing or decreasing their affinity for a second ligand. Such allosteric effects can be evidenced by the order and/or stoichiometry of interaction of ligands with PrP. Among the PrP ligands previously described we can mention the co-chaperone hop/STI1, laminin receptor precursor (LRP), a cell adhesion molecule N-CAM, and non-protein ligands, such as nucleic acids and copper ions. Our study is directed to protein ligands, and each of these has mapped domains for the interaction with PrP, which in turn also has mapped their regions of interaction with its ligands. Our goal is to determine the conformational changes undergone by PrP (human and murine) when linked to one or more of its ligands by computational simulation and spectroscopic techniques. Previous results of molecular docking using the server CLUS-PRO from Boston University-USA, which uses an optimization algorithm for protein-protein interaction, provided us models of interaction between PrP and the listed ligands, providing information about the stoichiometry and affinity of the interactions. The models generated are actually being refined by molecular dynamics using the GROMACS softwares package from Groningen University, Netherlands.

**Word Keys:** prion, allosteric effect, computational simulations, spectroscopy  
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