To be or not to be (bound):
Impact of ligand binding on galectin-1 structure and thermal stability

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The stability of proteins involves a critical balance between interactions of different order of magnitude. Based on previous experimental evidence of an increased thermal stability gained in galectin-1 (a β-galactosyl terminal binding lectin involved in the immune response) upon binding to the lactose disaccharide, in this work we analyze the structural changes occurring upon binding, and thermal denaturation of the protein and the complex. Using an approach that provides insight into the molecular determinants of the observed phenomenum, molecular dynamics simulations were carried out followed by a detailed computation of thermodynamic properties: internal energy, solvation free energy, and conformational entropy. The energetic profile of the binding process is also presented.

Our results show that while the ligand (lactose) binding do not alter galectin-1 structure significantly, changes in the flexibility of different regions and internal energy of the protein can be attributed to the binding, conferring the protein an increased thermal stability. A discussion of the main factors involved in the increased stability of the protein is presented.