

## AN INVESTIGATION OF THE PROTONATION STATES OF HUMAN LACTOFERRIN IRON-BINDING PROTEIN

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**Abstract.** In this study, the protonation states of ionizable groups of human lactoferrin in various conformations were investigated theoretically, at physiological pH (7.365). These calculations show that the transition of the protein from a conformation to another one is accompanied by changes in the protonation state of specific amino acid residues. Analysis of the  $pK_a$  calculations underlined the importance of participation of two arginines and one lysine in the opening / closing of the protein. In addition, it was found that the mechanism of iron release depends on the protonation state of TYR-192. Protonated state of this residue in the closed form of lactoferrin will trigger the opening of protein and release of iron ions.

**Keywords:** lactoferrin, ionizable residues, protonation, continuum electrostatics.

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