PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

REVISITING THE CONFORMATIONAL TRANSITION MODEL FOR THE PH DEPENDENCE OF BSA STRUCTURE USING PHOTOLUMINESCENCE, CIRCULAR DICHROISM, AND ELLIPSOMETRIC RAMAN SPECTROSCOPY

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Changes in pH affect metabolic pathways primarily by modulating enzyme conformations; therefore, a detailed analysis of pH-driven conformational transitions is required to understand the underlying biochemistry of diseases and biological organisms. In this work, we examined the pH-driven conformational dynamics of Bovine Serum Albumin (BSA) within the framework of the Foster Model. Circular Dichroism and Raman Optical Activity showed the conversion of helical into beta-rich structures in the acidic and basic regions, while an opening of the BSA tertiary structure was evidenced by the upsurge in accessibility of ANS-BSA binding sites and the increase of random contributions in regions F and B. We could then revisit the Foster Model by introducing two additional intermediate conformational states and structural reorganization at

extreme pH values. The revisited model shows two new conformational populations. [1] These are responsible for further transitions involving the exposure of a reactive surface that promotes structural reorganization of BSA (conversion of alpha-helices into beta-rich structures) at extreme pH values, such as 2 and 12, solely by changing one physicochemical parameter: pH. The existence of two intermediate species, sufficiently stable to promote the conversion of helical into beta-rich structures, and the fact that the regular structure is maintained at these extreme pH levels, are likely to have an impact on protein folding studies and theories, especially regarding globular proteins.Studying protein-substrate interactions at different pH levels can indicate further specificities; indeed, new molecules may emerge as better candidates for substrates, which is highly relevant for drug design. Furthermore, a new range of possibilities for the preparation of protein-based biomaterials will be opened as the known pH range for conformational stability has increased. This expanded model opens up new possibilities concerning protein-molecule interactions, promising far-reaching implications for fields such as drug delivery and biomaterials.

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[1] L.F.T. de Resende et al. International Journal of Biological Macromolecules 259 (2024) 129142.

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