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CENTRO DE CIÊNCIAS EXATAS E TECNOLÓGICAS
DEPARTAMENTO DE TECNOLOGIA DE ALIMENTOS
Secretaria da Pós-Graduação em Ciência e Tecnologia de Alimentos

Campus Universitário – Viçosa, MG – 36570-900 – Telefone (31)3612-6705/6760 – E-mail: tc a@ufv.br

TAL 797 – Seminário

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Exploring the Thermodynamics and Kinetics of Complexes between Proteins and Bioactive Compounds

Pós-graduando: Gláucia Valéria Fonseca Leonel
Orientador: Ana Clarissa dos Santos Pires (Departamento de tecnologia de alimentos)
Nível: ( ) MS (x) DS

The consumption of bioactive compounds has gained prominence in recent years, driven by changes in consumer dietary patterns aimed at prioritizing health and well-being. However, these compounds exhibit limitations in their use, such as low water solubility, light instability, and susceptibility to oxygen. In this context, the formation of complexes between proteins and bioactive compounds is a promising strategy to overcome these limitations. The study of intermolecular interactions between proteins and bioactive compounds provides the understanding of molecular recognition mechanisms and the quantification of thermodynamic parameters that govern the interaction between these molecules. During the process of intermolecular interaction, the involved energy can result from electrostatic interactions, hydrogen bonding, van der Waals interactions, and hydrophobic interactions. Energy variation allows for the determination of the driving forces that guide the process of intermolecular interaction and thermodynamic variables, such as the standard Gibbs free energy change (ΔG^0), standard entropy change (ΔS^0), and standard enthalpy change (ΔH^0). Additionally, understanding the rate of formation (k_a) and dissociation (k_d) of thermodynamically stable protein-molecule complexes, along with energetic parameters (activation energy ($E^{\ddagger}$), Gibbs free energy change of activation ($\Delta G^{\ddagger}$), entropy change of activation ($\Delta S^{\ddagger}$), and enthalpy change of activation ($\Delta H^{\ddagger}$)) associated with the transition complexes that mediate the formation of these stable complexes, is indispensable for the knowledge of the molecular dynamics of protein-bioactive compounds interactions. The determination of these parameters will provide insights into molecular recognition mechanisms, which are key components in the development of more specific, optimized, and functional nanocarriers to be incorporated into food matrices.

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