**Molecular interactions between soybean glycinin (11S), genistin and genistein** **using spectroscopic and in silico analyses**

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Consumption of plant based proteins has grown significantly in recent years due to an increased awareness of their health benefits and a consumer shift towards a more plant based diet. Soybean (*Glycine max*) dominates the current market for plant based protein choice and is a source of all 9 essential amino acids. Soy protein can be further divided into its main constituents, glycinin (11S) and beta conglycinin (7S) which contribute approximately 40% and 30% of their total protein content respectively, and are easily digested by the human body[1]. In addition, soybeans are a rich source of the phenolic compounds genistein and genistin, which have been associated with decreased oxidative stress, antioxidant properties as well as chemoprotective abilities[2].

There is presently very little research published on the interactions between soy protein fractions and soy derived phenolic compounds. Knowledge of the interactions between these compounds will assist in the development of functional foods and other applications in the food industry. This work utilises molecular docking studies to assist in demonstrating and predicting the different binding sites between genistein and genistin and glycinin. With more in-depth molecular dynamics simulations offering an insight into changes to solvent accessible surface area, intramolecular hydrogen bonding and alterations to secondary structure, induced by binding interactions[3]. Fluorescence quenching analysis and circular dichroism yield binding constants and secondary structure changes respectively, which are in broad agreement *with in-silico* analysis.

The binding affinity and location of phenolic compounds on the glycinin molecule is dependent on the structure of the phenolic compounds, and the presence or absence of a glycosidically linked sugar moiety. Further investigation is needed regarding the changes to the techno- and bio-functionality of the phenolic and glycinin molecules that may be induced by their interaction at ambient and high temperature treatments.

**References**

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