An Investigative Study of Reactions Involving Glucosinolates and Isothiocyanates

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Abstract: Glucosinolates (GSL) are thioglucosides normally found in Brassica vegetables and most are known to have health promoting properties. Some of their degradation products such as isothiocyanates have been shown to exhibit chemopreventive action. The availability, accessibility and properties of glucosinolates and their hydrolysis products may however be affected if they react with other cellular components such as metal ions. In this study reaction mixtures consisting of a glucosinolate (sinigrin) and a metal ion (Fe³⁺, Fe²⁺, Cu²⁺, Zn²⁺, Mg²⁺, and Ni²⁺) and an isothiocyanate (allyl isothiocyanate) with a metal ion were analyzed by UV-Vis Spectrophotometry to determine possible interactions under physiological conditions. Both sinigrin and allyl isothiocyanate exhibited apparent interactions with aqueous solutions of FeCl₃, Cu(NO₃)₂ and Zn(NO₃)₂. Based on the difference spectra generated, no significant interactions were found between the standards and Fe²⁺, Mg²⁺and Ni²⁺ salts. These findings show that glucosinolates and isothiocyanates have promising anti – Fenton activity. Further investigation on the interactions with Fe³⁺ was made by analysis of the reaction mixtures by high performance liquid chromatography (HPLC) using a refractive index detector and by liquid chromatography – mass spectrometry (LC-MS). Results from HPLC analysis revealed no significant covalent interactions between Fe³⁺ and either sinigrin or allyl isothiocyanate. However, LC-MS analysis showed a prominent ion at m/z 413 with the formula [C₁₀H₁₀KOS₂Fe]⁺, the probable product formed between Fe³⁺ and sinigrin. Analysis of the Fe³⁺ - allyl isothiocyanate reaction mixture also indicated the formation of a possible product with the formula [(C₄H₆NS)₃Fe + H]⁺ at m/z 353.

KEYWORDS: glucosinolate; sinigrin; allyl isothiocyanate; LC-MS (liquid chromatography – mass spectrometry)