



An Investigative Study of Reactions Involving Glucosinolates and Isothiocyanates

Alzea Chrisel H. Alea¹, Diane Elaine T. Co² and Marissa G Noel^{3*}

^{1,2,3}Chemistry Department, De La Salle University, 2401 Taft Ave., Manila

*Corresponding Author: marissa.noel@dlsu.edu.ph

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 (Fe^{3+} , Fe^{2+} , Cu^{2+} , Zn^{2+} , Mg^{2+} , and Ni^{2+}) 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 FeCl_3 , $\text{Cu}(\text{NO}_3)_2$ and $\text{Zn}(\text{NO}_3)_2$. Based on the difference spectra generated, no significant interactions were found between the standards and Fe^{2+} , Mg^{2+} and Ni^{2+} salts. These findings show that glucosinolates and isothiocyanates have promising anti-Fenton activity. Further investigation on the interactions with Fe^{3+} 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 Fe^{3+} and either sinigrin or allyl isothiocyanate. However, LC-MS analysis showed a prominent ion at m/z 413 with the formula $[\text{C}_{10}\text{H}_{16}\text{KO}_9\text{S}_2\text{Fe}]^+$, the probable product formed between Fe^{3+} and sinigrin. Analysis of the Fe^{3+} - allyl isothiocyanate reaction mixture also indicated the formation of a possible product with the formula $[(\text{C}_4\text{H}_5\text{NS})_3\text{Fe} + \text{H}]^+$ at m/z 353.

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