

CHAPTER 1

INTRODUCTION

1.1 Background

Coffee is being consumed almost all the time worldwide, and is also one of the most frequently consumed beverages. In a year around 400 billion cups of coffee are consumed or around 2.25 billion cups daily, making it the most popular beverage in the world. There are two types of coffee beans that are consumed worldwide, Arabica (*Coffea arabica*) and Robusta (*Coffea canephora*). Coffee is mostly sought and consumed by people for its caffeine, a well known chemical found in coffee beans. Bioactive compounds are extra nutritional constituents that usually occur in small amounts in foods. Bioactive compounds are mostly found in plants and their byproducts naturally, and these compounds are studied extensively in order to understand and evaluate any possible impacts on health. Categorized, few examples of bioactive compounds are carotenoids, flavonoids, carnitine, choline, phytosterols and many more. This includes vitamins and minerals since they have certain pharmacological properties in them. Within a coffee bean, several examples of bioactive compounds are caffeine, caffeic acid, chlorogenic acids, trigonelline, diterpenes, and melanoidins which some have been discovered for their properties and benefits for the human body, while others are not so popular. As stated before, coffee has its beneficial properties as well as health risks, and coffee has a very strong relation with the cardiovascular system, which may promote diseases including stroke, other common side effects of coffee consumption are insomnia, restlessness, an upset stomach, nausea, and an increased heart rate. The world of bioactive compounds is heavily related to

Proteomics A study of omics that is highly focused on large groups of proteins and their functions.

Stroke is responsible for many deaths and disabilities around the world, including Indonesia, where it is considered common. The burden of stroke in Indonesia is considered high. According to WHO, it is the number one cause of death, killing 328,5 thousand people (21.2% of total deaths) in 2012. The risk factors for stroke are high blood pressure, tobacco smoking, obesity, high blood cholesterol, and diabetes mellitus. However, the main risk factor is high blood pressure, which accounts for 35 - 50% of the stroke risk. Medications vary, ranging from anticoagulation drugs, surgery, and changes in dietary lifestyle. Aside from drugs in treating and preventing stroke there is also an alternative supplement that helps in reducing the risks of stroke and improving recovery. The benefits of this can be obtained from the consumption of Folic acid and vitamin B-6 and vitamin B-12. With the presence of supplements, it acts as an extra nutrient to boost medications and other health needs alike, thus opening a new window of learning and research to further improve the utilization of supplements.

There are many previous studies regarding the relationship between coffee, the cardiovascular system, and stroke. This includes meta analysis, and molecular docking studies and dynamics. However, currently there is no known research attempting to molecular dock the compounds from coffee with Beta-2 microglobulin specifically as a target that is related to stroke. With this gap, the author hopes to shed some light on the potential of the compounds within coffee compounds.

1.2 Objective

The primary objective of the current project is to explore the possibility of bioactive compounds that can be found in coffee. There are bioactive compounds present within coffee beans that might be useful in the form of supplements to help medicate stroke patients, both preventing the disease and recovering from it. The project will also give more insights into bioactive compounds other than caffeine that can be studied more and implemented further in future studies.

1.3 Significance, Scope and Definitions

The project will utilize bioactive compounds and the target from web sources. RCSB PDB and FoodChemEx are a few available online repositories where data can be obtained. The tools that will be used include online predicting software such as PASS Server's Way2Drug and Lipinski's rule of five prediction online tool from SCF BIO and other specific tools to perform certain tasks, such as software to perform docking and docking analysis and also tools for visual aid . The final results and findings will be summarized in a complete report in a simplified manner. Additionally, molecular dynamics will also be performed as well.