Computational Bioinformatics Study of Noni to Lower Cholesterol Levels (Morinda citrifolia)

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ABSTRACT

Increased cholesterol levels or also known as hypercholesterolemia is one of the risk factors for coronary heart disease. A person can be categorized as having hypercholesterolemia if the cholesterol level is declared high if in adults the cholesterol value reaches >240 mg/dl while in children and adolescents the total cholesterol value reaches 200 mg/dl or more has been declared high. To reduce hypercholesterolemia or cholesterol levels in the blood, it can be done using traditional medicine, one of which is noni fruit. Noni fruit (Morinda citrifolia) can reduce total blood cholesterol, LDL, triglycerides and increase HDL and can improve the histology structure of the aortic vessels (thickening of the tunica media) in mice given a high-fat diet.

Keywords: Cholesterol or Hypercholesterolemia, Noni

1. INTRODUCTION

Increased cholesterol levels or also known as hypercholesterolemia is one of the risk factors for coronary heart disease [1][2][21]. In Indonesia alone, there are about 36 million people or about 18% of the Indonesian population who suffer from this blood lipid disorder [3][4]. Of that number, 80% of patients died suddenly from a heart attack and 50% of them were asymptomatic [5]. Hypercholesterolemia is defined as an increase in plasma cholesterol levels above normal [6][7]. Cholesterol levels in adults are declared high if they reach a value of >240 mg/dl while in children and adolescents the total cholesterol value reaches 200 mg/dl or more has been declared high [8][9][10].

Actually cholesterol in appropriate levels is actually needed by the body in helping to build new cells so that the body can continue to function normally [11][12]. Cholesterol serves to help the body produce vitamin D, a number of hormones, and bile acids to digest fat[ 13][14]. In the blood, cholesterol is carried by proteins [15]. The combination of the two is called a lipoprotein. The two main types of lipoproteins are low-density lipoprotein (LDL) commonly referred to as bad cholesterol and high-density lipoprotein (HDL) commonly referred to as good cholesterol [16][17].

The duty of LDL is to transport cholesterol from the liver to the cells that need it [18]. However, if the amount of cholesterol exceeds the need, it can settle on the walls of the arteries.
causing disease[19][22]. Meanwhile, HDL is responsible for transporting cholesterol back into the liver as opposed to LDL. In the liver, cholesterol will be destroyed or excreted by the body through feces or feces [20][23].

To reduce hypercholesterolemia or cholesterol levels in the blood, it can be done using traditional medicine, one of which is noni fruit [24][25]. Noni fruit (Morinda citrifolia) can reduce total blood cholesterol, LDL, triglycerides and increase HDL and can improve the histological structure of the aortic vessels (thickening of the tunica media) of mice given a high-fat diet [26][27].

2. LITERATURE REVIEW

Noni (Morinda citrifolia L.) is a plant that has long been used by the community as a food ingredient as well as treatment. Noni contains scopoletin which functions to dilate narrowed blood vessels, so that the heart is not too hard to pump blood and blood pressure becomes normal. The discovery of medicinal plants that have potential as hypertension can now use the Molecular docking method [28]. Molecular docking can help in silico screening to predict whether the chemical content of the active ingredients in certain plants has the potential as antihypertensive by comparing it with a compound with known antihypertensive effect [29].

According to the results of the study, giving noni (Morinda citrifolia) capsules consisting of 90% dry extract of noni fruit and 10% filler can reduce total blood cholesterol levels. Noni (Morinda citrifolia) is also known as noni fruit. Noni is green and has black spots, and has a bitter taste. Noni is a fruit that is commonly found in Australia, India, and Southeast Asia, including in Indonesia [30].

3. EXPERIMENTAL

This research is a bioinformatics study with noni fruit samples to determine the active compounds in it by analyzing its structure and content through Phytochem https://phytochem.nal.usda.gov/, PubChem https://pubchem.ncbi.nlm.nih.gov/ , and Swiss target http://swisstargetprediction.ch/, as well as chemdraw and chem3d.

The chemical compounds found in the noni fruit, look at the content and active compounds used in phytochem, in phytochem we will use the active sentawa in the noni fruit, the active compounds that we got earlier we checked the structure, properties, and smile through pubchem, swiss target and chemdraw and chem3d aplikasi apps.
The implementation of this research aims to utilize regional plants as medicine to cure diseases. In addition, this study is an observational descriptive study conducted with an objective condition by looking back (retrospectively). The plants tested were noni fruit.

Furthermore, these plants were identified using Dr. Duke's Phytochemical and Ethnobotanical Database with the scientific name Morinda citrifolia. The search on the site aims to see the chemical compounds contained in these plants.

After that, one by one the chemical compounds were extracted in pubchem and the compound elements were taken in Isomeric SMILES then entered the compound elements in Swisstarget.
prediction to see which percentage of the compound contained a lot. The next step is to copy the IUPAC Name in Pubchem earlier, and access to Chemdraw and make optimizations with Chem3d to see a 3D structure image and how much energy is generated.

The last step is the disseminate result, which from the chemical obtained from swisstarget prediction, the result is an enzyme.

4. RESULTS AND DISCUSSION

4.1 Results

This research is viewed from the number of people who experience Diabetes Mellitus. Which is where most people do not have a healthy diet and think that DM is seen from heredity only. Whereas various factors that cause this disease are obesity, overeating, lack of exercise, and the most important supporting factor is an unhealthy lifestyle.

Based on the observations that have been made with many people living an unhealthy lifestyle and not regulating an unhealthy diet, this scientific paper was written. In order to make us more productive again in carrying out activities without experiencing disturbances, especially DM disease, where the complaint that often occurs is feeling tired quickly.

In overcoming the problem of DM among the community, the author urges to make lifestyle changes for the better. Which can be done by exercising 3-4 times a week and reducing food portions. The point here is not to reduce the food ration that should be 3 times a day to 2 times a day, but this is done by replacing carbohydrates from rice. Because we both know that rice is the food that contains the most glucose, which can cause obesity if we eat too much rice and can cause DM. To evaluate the occurrence of this problem, it is better if we replace the carbohydrates obtained from rice with purple sweet potatoes. By eating purple sweet potatoes, one of the substances contained in it is dipeptidyl peptidase which is an enzyme and binding protein found in various tissues including the liver, kidneys, pancreas, and endothelial cells that can function in maintaining blood sugar levels in the body.

<table>
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<tr>
<th>Activities Count</th>
<th>Chemical</th>
<th>Plant Part</th>
<th>Low PPM</th>
<th>High PPM</th>
<th>StdDev</th>
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<tr>
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<tr>
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<tr>
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</table>
The following is data on chemical compounds in noni that have been analyzed using pubchem, chemdraw ultra, chemdraw 3D and swisstarget prediction.

1. (Z)-6-DODECENO-GAMMA-LACTONE

![Figure 3. 5-[(Z)-oct-2-enyl]oxolan -2-one](image)
Figure 4. Prior Optimizing

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Figure 5. Cartesian table
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**Figure 6.** Internal coordinate table
Figure 7. Following optimization

2. \((Z,Z)-2,5\text{-UNDECADIEN-1-OL}\)

Figure 8. \(2\ Z\ Z\text{-undeca-2,5-dien-1-ol}\)

Figure 9. Prior Optimizing
Figure 10. Cartesian Table

<table>
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Figure 10. Cartesian Table

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Figure 11. Internal Coordinates

Figure 12. Following optimization
4.2 Discussion

Based on the data analysis, the research conducted can be said to be successful. This can be seen in the active compound contained in Chanoclavine, namely proteases which have a percentage of 33.3 %. Which is a substance dipeptidyl peptidase IV (DPP IV) is associated with diabetes, where it plays a role in inactivating a number of peptides involved in blood sugar balance. This can be used by people with diabetes mellitus, because it can maintain blood sugar levels and provide a faster feeling of fullness when consuming purple sweet potatoes. In addition, the active compounds contained are also able to prevent stress.

5. CONCLUSION

Based on the descriptive results and data analysis on purple sweet potato, 5 active compounds were obtained, namely Chanoclavine, Elymoclavine, Ergine, Ergometrine, and Isoergine. Where in Chanoclavine contains 33.3% proteases, 20% enzymes, 20% chytochrome, 6.7% ligand gated channel, 6.7% electrochemical, 6.7% kinase, and 6.7% Family AG protein coupled receptor. Elymoclavine contains 46.7% Family AG protein coupled receptors, 26.7% electrochemicals, 6.7% proteases, 6.7% enzymes, 6.7% kinases and 6.7% membrane receptors. Ergometrine contains 93.3% Family AG protein coupled receptor and 6.75 chytochrome. Meanwhile, Ergine and Isoergine only contain Family AG protein coupled receptor with a percentage of 100%.

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REFERENCES


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