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Phytochemical Screening of *Moringa oleifera* as Antioxidant and Anticancer through Chemoinformatics Approach

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Sin War Naw[1], Nur Sofiatul Aini[2,3]*, Ahmad Affan Ali Murtadlo[3,4], Muhammad Badrut Tamam[3,5], Dora Dayu Rahma Turista[3,6], Md. Emdad Ullah[7]

[1]Department of Chemistry, Myitkyina University, Myitkyina, Myanmar
[2]Faculty of Mathematics and Natural Sciences, Universitas Negeri Surabaya, Surabaya, Indonesia
[3]Generasi Biologi Indonesia Foundation, Gresik, Indonesia
[4]Faculty of Science and Technology, Universitas Airlangga, Surabaya, Indonesia
[5]Department of Biology, Faculty of Sciences and Technology, Universitas Muhammadiyah Lamongan, Lamongan, Indonesia
[6]Biology Education Department, Faculty of Teacher Training and Education, Mulawarman University, Samarinda, Indonesia
[7]Department of Chemistry, Mississippi State University, Mississippi State, United States

* Corresponding Author: nursofiatul.aini@gmail.com

ABSTRACT

Moringa oleifera, also known as kelor, this plant is better known to have benefits in the field of health including having properties as an antioxidant and anticancer. Several previous studies have revealed the potential of *Moringa oleifera* in the health sector such as anti-inflammatory, wound healing, antidiabetic, and antiviral. This study aims to obtain preliminary information on the possible bioactive activities of *Moringa oleifera*, which can be the basis for further research and development of its therapeutic potential. The in silico method used in this study consists of sample preparation of compounds from Moringa oleifera in the database, prediction of antioxidant and anticancer probabilities, and visualization of the three-dimensional structure of target compounds with positive predictions. *Moringa oleifera* has Rutin compounds that act as antioxidants and anticancer based on bioactivity tests. This can provide an illustration of future prospects that *Moringa oleifera* can be used as an alternative treatment and supplement. The higher probability of activity indicates the potential presence that results when these compounds are already used in the form of standardized drug products.

Keywords: Anticancer, Antioxidant, Chemoinformatics, *In Silico*, *Moringa oleifera*

INTRODUCTION

Moringa oleifera, also known as kelor, is widely known in the world for its medicinal benefits and traditional food sources[1,2,3]. This plant is better known to have benefits in the field of health including having properties as an antioxidant and anticancer[4,5,6]. Phytochemical compounds from *Moringa oleifera* are the focus of this research for understanding the therapeutic potential and alternative treatment solutions[7,8,9]. Several previous studies have revealed the potential of *Moringa oleifera* in the health sector such as anti-inflammatory, wound healing, antidiabetic, and antiviral[10,11,12]. A chemoinformatics approach was used to conduct phytochemical screening of *Moringa oleifera*[13,14,15]. Phytochemical screening is the process of identifying and analyzing active chemical compounds contained in plants[16,17,18]. In this case, researchers are interested in identifying compounds in *Moringa oleifera* that have potential as antioxidants and anticancer.

† Footnotes relating to the title and/or authors should appear here.
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PASSOnline is a computational method used to predict the biological activity or bioactivity of chemical compounds. PASS (Prediction of Activity Spectra for Substances) is an online program that provides bioactivity prediction services based on the chemical structure of a given molecule[19,20]. Bioactivity predictions provided by PASSOnline include various aspects such as pharmacological activity, toxic effects, and activity against specific biological systems[21,22]. The bioactivity prediction results can provide an initial insight into the potential biological activity of a compound before further research or laboratory tests are conducted[23,24]. Researchers can access bioactivity predictions quickly and efficiently, helping in new drug research, discovery of bioactive compounds, as well as early understanding of the potential biological effects of certain chemical compounds.

This study aims to obtain preliminary information on the possible bioactive activities of *Moringa oleifera*, which can be the basis for further research and development of its therapeutic potential. By using a chemoinformatics approach, this research is expected to provide new insights into the utilization of *Moringa oleifera* as a potential source for the development of antioxidant and anticancer compounds. Phytochemical screening and chemoinformatics approaches provide a preliminary approach in the study, and the findings need to be verified through further biological and clinical trials. However, this study makes an important contribution in understanding the potential of *Moringa oleifera* as a source of bioactive compounds that can be used in the development of antioxidant and anticancer therapies.

METHOD

Compounds Preparation

PubChem database (https://pubchem.ncbi.nlm.nih.gov/) was used for data retrieval of query compounds from *Moringa oleifera* consisting of CID, formula, SMILE Canonical, and molecular weight (g/mol). The 3D structures of the query compounds were downloaded with structure data format files. The compounds of the two medicinal plants consist of Quercitrin, Rutin, Ferulic acid, Gallic acid, and Vanillin. PubChem is a specific database used for storing information such as organic, synthetic, and bioassay chemical compounds, the database is also equipped with a server to draw the two-dimensional structure of the query compound[25].

Bioactivity Prediction

Bioactivity in this study refers to determining the nature of a query compound as an antioxidant and anticancer with a probability value. PASSOnline server was used for bioactivity prediction of query compounds, probabillity activation (Pa) score >0.3 to reveal the potential of *Moringa oleifera* as antioxidant and anticancer. The probabillity inhibition (Pi) score must be lower than Pa so that bioactivity is not inhibited when the query compound enters the body of *Homo sapiens*. Pa>0.3 indicates the potency of the query compound is only proven through computational or theoretical approaches[26].

3D Structural Visualization

Visualization of three-dimensional structures on query compounds from *Moringa oleifera* with antioxidant and anticancer activity was performed through PyMol v2.5 software. The structures displayed were cartoons, surfaces, ribbons, and sticks with publication standards. The coloring selection method is also performed on query compounds based on C, H, O, and N atoms[27].

RESULTS AND DISCUSSION

This study used compounds from *Moringa oleifera* consisting of Quercitrin, Rutin, Ferulic acid, Gallic acid, and Vanillin. Information from PubChem consisting of compound name, CID, molecular weight (g/mol), formula, and SMILE Canonical on compounds from *Moringa oleifera* has been obtained (Table 1). *Moringa oleifera* is identified as having antioxidant activity proven through *in vitro* studies with the mechanism of producing antioxidant chemical compounds that bind to free radicals. Apoptosis agonist activity was identified in extracts from *Moringa oleifera* leaves when used as a breast and intestinal cancer treatment[28,29]. However, based on these two scientific evidence, the compounds that act as antioxidants and anticancer from *Moringa oleifera* are still unclear and very little scientific evidence, which led to this research.

Table 1. Chemical compounds of *Moringa oleifera* from PubChem

Compound	PubChem CID	Molecular Weight (g/mol)	Formula	SMILE Canonical
Quercitrin	5280459	448.4	$C_{21}H_{20}O_{11}$	CC1C(C(C(C(O1)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)C4=CC(=C(C=C4)O)O)O)O)O
Rutin	5280805	610.5	$C_{27}H_{30}O_{16}$	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O
Ferulic acid	445858	194.18	$C_{10}H_{10}O_4$	COC1=C(C=CC(=C1)C=CC(=O)O)O
Gallic acid	370	170.12	$C_7H_6O_5$	C1=C(C=C(C(=C1O)O)O)C(=O)O
Vanillin	1183	152.15	$C_8H_8O_3$	COC1=C(C=CC(=C1)C=O)O

The identification of bioactivity aims to determine the activity of query compounds used for the treatment of certain diseases such as cancer and viral infections. It can be used to determine new drug candidates in general, the value of bioactivity refers to the probability of activation (Pa) and inhibition (Pi). The activity of a query compound is proven computationally or theoretically if it has a value of Pa>0.3 and Pa>Pi, the value of Pa must be greater than Pi to trigger the formation of the desired therapeutic activity[30,31]. The bioactivity prediction results show that compounds from *Moringa oleifera* that act as antioxidant and anticancer candidates are Rutin (Table 2). Compounds from *Moringa oleifera* (Figure 1). with positive predictions as antiviral and anticancer are displayed in the form of sticks with staining selection.

Table 2. Bioactivity prediction of compounds from *Moringa oleifera*

Compound	Antioxidant		Anticancer	
	Pa	Pi	Pa	Pi
Quercitrin	0.683	0.007	0.943	0.002
Rutin	**0.885**	**0.003**	**0.968**	**0.001**
Ferulic acid	0.540	0.005	0.616	0.012
Gallic acid	0.520	0.006	0.395	0.031
Vanillin	0.403	0.012	0.388	0.033

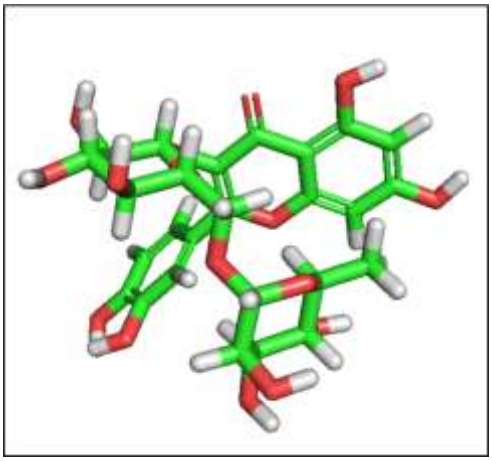

Figure 1. Visualization of three-dimensional structures of Rutin from *Moringa oleifera*.

CONCLUSION

Moringa oleifera has Rutin compounds that act as antioxidants and anticancer based on bioactivity tests. This can provide an illustration of future prospects that *Moringa oleifera* can be used as an alternative treatment and supplement. The higher probability of activity indicates the potential presence that results when these compounds are already used in the form of standardized drug products. However, the results of this study must be validated through further tests to strengthen scientific evidence.

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