SAINTEK
International Journal on Applied Science, Advanced Technology and Informatics
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Antiviral and Anticancer Activity from *Curcuma longa* L. and *Tamarindus indica* Bioactive Compounds through *In Silico* Analysis

Received 02 June 2023,
Accepted 28 June 2023

DOI: 10.24036/sainstek/vol2-iss01/21

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ABSTRACT
Various efforts are made for the discovery and development of an effective and safe treatment as a solution to the problem. One of the approaches used in this study is the development of drugs based on natural ingredients such as *Curcuma longa* L. and *Tamarindus indica* with various known health benefits. In this study, in silico analysis was conducted to evaluate the potential antiviral and anticancer activities of bioactive compounds contained in *Curcuma longa* L. and *Tamarindus indica*. The in silico method used in this study consists of the preparation of ligand samples from *Tamarindus indica* and *Curcuma longa* L. in the compound database (PubChem) and identification of the probability of potential query compounds through the PASSOnline server to determine the potential as antiviral and anticancer. *Tamarindus indica* and *Curcuma longa* L. are predicted to act as effective antiviral and anticancer candidates because the probability of bioactivity activation is higher than inhibition. Campesterol and α-Amyrin compounds are potential compounds from *Tamarindus indica*. Quercetin from *Curcuma longa* L. may have dual activity as antiviral and anticancer.

Keywords: Anticancer, Antiviral, Bioactivity, Health, *In Silico*

INTRODUCTION

A disease that occurs due to viral infections and cancer is a major challenge in the medical field that spans the globe. Various efforts are made for the discovery and development of an effective and safe treatment as a solution to the problem[1,2,3]. One of the approaches used in this study is the development of drugs based on natural ingredients such as *Curcuma longa* L. and *Tamarindus indica* with various known health benefits[4,5,6]. In this study, in silico analysis was conducted to evaluate the potential antiviral and anticancer activities of bioactive compounds contained in *Curcuma longa* L. and *Tamarindus indica*[7,8,9]. In silico analysis is a computational approach used to predict the biological activity of compounds based on their chemical

† Footnotes relating to the title and/or authors should appear here.
Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.24036/sainstek/vol2-iss01/21

structure[10,11,12]. Previous studies have identified bioactive compounds such as curcumin contained in *Curcuma longa* L. and phenolic compounds contained in *Tamarindus indica* as having potential antiviral and anticancer activities[13,14,15]. However, it is important to conduct further evaluation through in silico analysis to understand the potential mechanism of action, molecular targets, and structure-activity relationships of these compounds.

Bioactivity prediction on PASSOnline is a computational method used to predict the biological activity or bioactivity of chemical compounds[16,17,18]. 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. 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[21]. However, it is important to note that these predictions are approximate and need to be verified through experiments and further research. 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.

The in silico method in this study aims to evaluate the antiviral and anticancer potential of bioactive compounds in *Curcuma longa* L. and *Tamarindus indica*. The results of in silico analysis can provide additional insight into the potential activity of these compounds and become the basis for further research in the development of new drugs. Combining traditional knowledge about the use of *Curcuma longa* L. and *Tamarindus indica* in medicine with an in silico approach, it is hoped that this research can contribute to the potential development of more effective and safe antiviral and anticancer treatments.

METHOD

Compounds Preparation

PubChem database (https://pubchem.ncbi.nlm.nih.gov/) was used for data retrieval of query compounds from *Tamarindus indica* and *Curcuma longa* L. 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 γ-Sitosterol, Campesterol, α-Amyrin, Curcumin, Ellagic acid, and Quercetin[22,23]. 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[24,25].

Bioactivity Prediction

Bioactivity in this study refers to determining the nature of a query compound as an antiviral 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 *Tamarindus indica* and *Curcuma longa* L. as antiviral 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[25].

3D Structural Visualization

Visualization of three-dimensional structures on query compounds from *Tamarindus indica* and *Curcuma longa* L. with antiviral 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[26,27].

RESULTS AND DISCUSSION

Previous studies have revealed the potential of *Curcuma longa* L. as an antiviral through the mechanism of increasing the immune response or immunomodulator, it can effectively eliminate pathogens such as viruses. Anticancer activity in *Curcuma longa* L. is shown through apoptosis of cancer cells that occurs in in vitro research. Another mechanism as an anticancer is shown by *Tamarindus indica* through inhibition of proliferation and angiogenesis of cancer cells shown through *in vitro* studies. The antiviral activity of *Tamarindus indica* is shown through a decrease in viral replication rate after administration of the crude extract, this is proven in vitro but the detailed mechanism is not yet known. Through this research, it can be used for the discovery of new anticancer and antiviral candidate compounds

from *Tamarindus indica* and *Curcuma longa* L. *Tamarindus indica* and *Curcuma longa* L. have chemical compounds consisting of γ-Sitosterol, Campesterol, α-Amyrin, Curcumin, Ellagic acid and Quercetin. Information on ligands from PubChem in this study consists of compound name, CID, molecular weight, formula, and SMILE Canonical has been obtained (Table 1).

Table 1. Chemical compounds of *Tamarindus indica* and *Curcuma longa* L. from PubChem

Natural Source	Compound	PubChem CID	Molecular Weight (g/mol)	Formula	SMILE Canonical
Tamarindus indica	γ-Sitosterol	457801	414.7	$C_{29}H_{50}O$	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
	Campesterol	173183	400.7	$C_{28}H_{48}O$	CC(C)C(C)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
	α-Amyrin	73170	426.7	$C_{30}H_{50}O$	CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1C)C)C
Curcuma longa L.	Curcumin	969516	368.4	$C_{21}H_{20}O_6$	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O
	Ellagic acid	5281855	302.19	$C_{14}H_6O_8$	C1=C2C3=C(C(=C1O)O)OC(=O)C4=CC(=C(C(=C43)OC2=O)O)O
	Quercetin	5280343	302.23	$C_{15}H_{10}O_7$	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)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[28]. 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)[30]. 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[31,32]. The bioactivity prediction results show that compounds from Tamarindus indica that act as antiviral and anticancer candidates are α-Amyrin and Campesterol. Quercetin from *Curcuma longa* L. has a higher Pa in both potentials (antiviral and anticancer) (Table 2). Compounds from *Tamarindus indica* and *Curcuma longa* L (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 *Tamarindus indica* and *Curcuma longa* L.

Natural Source	Compound	Antiviral		Anticancer	
		Pa	Pi	Pa	Pi
Tamarindus indica	γ-Sitosterol	0.686	0.006	0.319	0.046
	Campesterol	0.664	0.008	**0.336**	0.038
	α-Amyrin	**0.793**	0.003	0.309	0.055
Curcuma longa L.	Curcumin	0.471	0.028	0.611	0.012
	Ellagic acid	0.481	0.005	0.396	0.031
	Quercetin	**0.498**	0.005	**0.757**	0.007

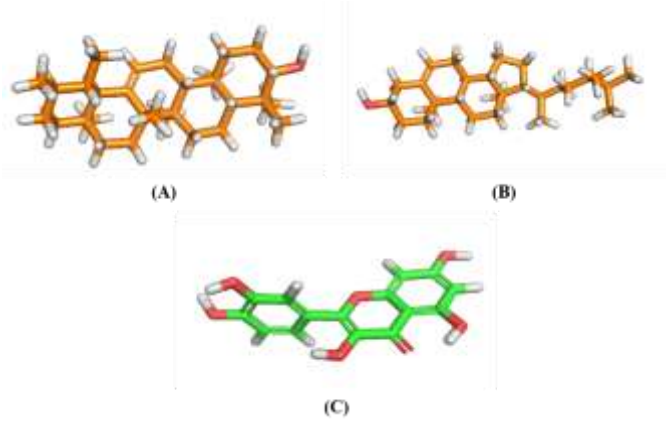

Figure 1. Visualization of three-dimensional structures of bioactive compounds from T*amarindus indica* and *Curcuma longa* L. (A) Campesterol (B) α-Amyrin (C) Quercetin.

CONCLUSION

Tamarindus indica and *Curcuma longa* L. are predicted to act as effective antiviral and anticancer candidates because the probability of bioactivity activation is higher than inhibition. Campesterol and α-Amyrin compounds are potential compounds from *Tamarindus indica*. Quercetin from *Curcuma longa* L. may have dual activity as antiviral and anticancer. However, these findings must be tested through further research for the validation process of scientific evidence.

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