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Elastichalcone A: A Potent Antioxidant Chalcone Derivative Compound Isolated from the Ethyl Acetate Extract of Breadfruit (*Artocarpus communis*) Leaves

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ABSTRACT

This research aims to isolate and determine the structure of isolated compounds from ethyl acetate extract of *Artocarpus communis* leaves and the antioxidant activity using a DPPH assay. *A. communis* leaves were macerated with ethyl acetate, and several chromatography techniques were used for separation and purification. One chalcone derivative compound, Elastichalcone A, was successfully isolated, ~~and~~ its structure was determined based on UV-Vis, FTIR, and NMR spectroscopy data analysis—the antioxidant test of Elastichalcone A, which showed high antioxidant activity with an IC_{50} value of 82.7 ppm.

Keywords: antioxidant, *Artocarpus communis*, Elastichalcone A, ethyl acetate extract

INTRODUCTION

Artocarpus communis (breadfruit) is a plant from the genus *Artocarpus* in the Moraceae family. This breadfruit plant can grow to around 30 meters and typically produces fruit and flowers every two years [1]. *A. communis* is often compared to *Artocarpus altilis*, also known as the breadfruit tree. According to research by Akinloye in 2015, the characteristics of *A. communis* and *A. altilis*' fruits, such as their size, shape, surface texture, and seeds, are different. However, the distinctions between these two breadfruit species are not limited to their fruits alone but extend to their leaves, stems, and roots. Breadfruit leaves are vast, single, alternate, elongated, rough-haired, pointed at the tip, 50–70 cm long, and 25–30 cm wide [2]. Breadfruit plants grow scattered in the regions of South Asia, Southeast Asia, Papua, and the South Pacific and have been extensively cultivated by communities as a food source, building material, or herbal medicine to address various ailments such as liver cirrhosis, hypertension, diabetes, skin diseases, and tapeworm infections [3]. Traditionally, burning breadfruit flowers is believed to alleviate toothache, boiled breadfruit roots are used to treat dysentery, breadfruit leaves are utilized to manage diabetes and cardiovascular issues, and the bark of the breadfruit tree is consumed as a remedy for headaches [4].

Phytochemical studies in different parts of the *Artocarpus communis* plant, such as the leaves, roots, bark, and wood, revealed that this species contained flavonoids [5-8), terpenoids [1], and stilbenes [3] derivatives. Some isolated compounds showed interesting biological activities such as antimicrobial [4], antibacterial [1], antioxidant [1, 9], antidiabetic [10], antifungal [11], and cytotoxicity against various cells [5, 8,12, 13].

Thus, Chalcones are a class of naturally occurring compounds known for their diverse pharmacological activities, including antioxidant, anti-inflammatory, antimicrobial, and anticancer properties [14]. The study introduces a bioactive molecule from the ethyl acetate fraction of the leaves of the *A. communis* species by isolating and evaluating the antioxidant properties of Elastichalcone A, a chalcone derivative compound. This study adds to the list of bioactive compounds found in *Artocarpus* plants and makes it possible to look into their medical or industrial uses.

EXPERIMENTAL SECTION

Material and Instrumental

The leaves of *A. communis* (1.2 kg) were collected from Sukabumi, West Java, Indonesia, in 2019. The herbarium staff at the Biology laboratory at Universitas Negeri Jakarta confirmed the plant, and a voucher specimen (no. 20211104) was stored. The General experiment procedures: UV spectra measured with SHIMADZU, UVmini-1240, while ^{1}H NMR data was recorded with a JEOL ECA 500 spectrometer operating at 500 (^{1}H) and 125 (^{13}C) MHz, using residual and deuterated solvent peaks as reference standards, and infrared spectra measured with CARY 670. Vacuum Liquid Chromatography (VLC), centrifugal chromatography, and column chromatography were carried out on silica gel PF254, silica gel GF254, and Sephadex LH-20. Precoated silica gel plates (Merck 60) were used for TLC analysis.

Methods

The sample of the powdered leaves of *Artocarpus communis* (1.2 kg) was macerated with ethyl acetate for 24 hours (3x) and evaporated to yield ethyl acetate extract (60.1 g). The ethyl acetate extract was fractionated using VLC (Silica gel, using the increasing polarity of the eluents *n*-hexane: ethyl acetate, into eleven significant fractions, A-K. The H fraction (13 g) was separated using VLC (*n*-hexane: ethyl acetate 8:2) to produce 12 fractions, H1-H12. The H10 (4.38 g) fractions were separated using VLC (*n*-hexane: ethyl acetate 8:2) to yield 11 fractions, H101-H1011. The H1010 (3.42 g) was then separated and purified by repeated centrifugal chromatography (*n*-hexane: acetone 8:2), resulting in 10 fractions. The H1010.2 fraction was obtained as an isolated compound.

Antioxidant Activity Assay

The DPPH scavenging activity was assessed using a previously adapted technique (15). The IC_{50} values, which represent the concentration of isolated compounds needed to scavenge 50% of the DPPH radical, were determined by analyzing a graph that plotted the percentage of inhibitions against the concentration of the isolates. Ascorbic acid and BHT were used as reference standards.

RESULTS AND DISCUSSION

The isolated compound obtained appears as a yellow gum (30 mg), displaying maximum UV spectra absorption of band I at a wavelength of 314 nm, indicating the presence of cinnamoyl groups originating from the conjugated B ring with carbonyl groups. Maximum absorption of band II appears at 275 nm, indicating the presence of benzoyl groups on the A ring and hydroxyl substituents (16). The FTIR spectrum displayed absorption at 3,627 $cm^{-1,}$ indicating the presence of hydroxyl groups (-OH.), 1,594 cm^{-1} for carbonyl groups (C=O), 1,236 cm^{-1} for ether groups (C-O), 3,029 cm^{-1} for aromatic (C-H) groups, and 1,475 cm^{-1} for aromatic groups, indicating absorption for the main functional groups of a compound belonging to the chalcone group.

The ^{1}H-NMR spectrum showed the highly deshielded signal at δ12.79 ppm), evidence of the chelated hydroxyl moiety. The α and β protons appeared as triplets at δ 3.10 and 2.90 ppm with a typical coupling constant of 7.9 Hz, suggesting a dihydrochalcone skeleton structure. Furthermore, the ^{1}H-NMR spectrum exhibited two sets of *ortho*-coupled aromatic protons at δH 6.67 (2H, *d*, *J* = 8.7 Hz) and δH 7.64 (2H, *d*, *J* = 8.4 Hz), which assigned to H-3/H-5 protons and H-2/H-6 which indicated the aromatic ring is 1,4-disubstituted. The second aromatic ring is *penta*substituted with a prominent sharp singlet at δ 7.18 assigned to H-6. The appearance of six protons singlet at δ 1.39 (3H, s) and 1.35 (3H,s) and a set of doublets at δ 6.55 and δ 5.62 with typical coupling constant (*J* = 10.1 Hz) are typical characteristics of 2,2-dimethyl chromene ring. The rest of the signals are due to the prenyl side-chain characterized by the chemical shifts at δ 3.22 (1H., *d, J*=7.2 Hz); δH 5.08 (2H, *t, J*=7.2 Hz); δ H 1.62 (3H, *s*), and δ H 1.72 (3H, *s*) ppm. Twenty-five carbon signals were visible in the ^{13}C-NMR spectrum, including signals for the carbonyl group, the sp^3 carbon group, the carbon group involved in hydroxyl bonds, and the sp^2 carbon group. Based on the above evidence, the isolated compound was identified as 20,4-dihydroxy-40,50-(2,2-dimethyl chromen)-30-prenyl dihydrochalcone. Additional

evidence was acquired by comparing the ^{1}H-NMR and ^{13}C-NMR spectra of the isolated compound with those of the elastichalcone A (17) (Table 1).

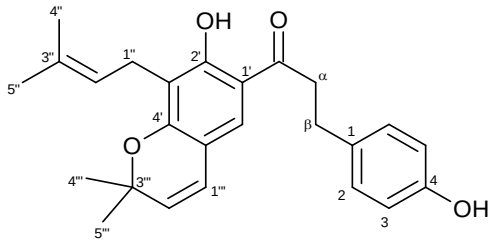

Figure 1. The Structure of elastichalcone A

Table 1. Data ^{1}H and ^{13}C NMR elastichalcone A in $CDCl_3$(500Mhz) and literature in $CDCl_3$ (400Mhz)

No. C	™$_H$ (*mult.*, *J* in Hz)		™$_C$	
	elastichalcone A	**Literature**	elastichalcone A	**Literature**
α	3.10 (*t*, 7.9)	3.15 (*t*, 7.9)	40.9	40.0
β	2.90 (*t*, 7.9)	2.95 (*t*, 7.9)	28.5	29.8
1			135.7	133.2
2	7.64 (*d*, 8.7)	7.09 (*d*, 8.4)	132.4	129.6
3	6.67 (*d*, 8.7)	6.75 (*d*, 8.4)	119.5	115.4
4			162.9	154.0
5	6.67 (*d*, 8.7)	6.75 (*d*, 8.4)	119.1	115.4
6	7.64 (*d*, 8.7)	7.09 (*d*, 8.4)	132.3	129.6
1'			111.9	113.0
2'			163.0	163.1
3'			114.6	117.0
4'			165.3	157.6
5'			113.8	113.2
6'	7.18 (*s*)	7.18 (*s*)	124.0	125.4
1"	3.22 (*d*, 7.2)	3.31 (*d*, 7.2)	21.7	21.5
2"	5.08 (*t*, 7.2)	5.17 (*t*, 7.2)	121.2	122.6
3"			130.2	131.6
4"	1.62 (*s*)	1.65 (*s*)	25.7	25.9
5"	1.72 (*s*)	1.78 (*s*)	17.7	17.9
1'''	6.55 (*d*, 10.1)	6.18 (*d*, 10.1)	121.1	121.6
2'''	5.62 (*d*, 10.1)	5.54 (*d*, 10.1)	128.0	128.6
3'''			77.6	77.6
4'''			26.6	28.5
5'''	1.39 (*s*)	1.41 (*s*)	26.2	28.5
C=O	1.35 (*s*)	1.41 (*s*)	204.0	203.7
OH	12.79	12.85		

*Reference 11.

The antioxidant activity of the isolated compound against 2,2-diphenyl-1-picrylhydrazyl (DPPH) shows its IC_{50} 82.7 ppm. The result of antioxidant activity showed that isolated compound has potential activity as an antioxidant.

CONCLUSION

One chalcone derivative compound, elastichone A, was isolated from the ethyl acetate extract of breadfruit (*Artocarpus communis*) Leaves. This isolated compound exhibited antioxidant activity against 2,2-diphenyl-1 picrylhydrazyl (DPPH) with IC_{50} values of 82.7 ppm, suggesting its potential as an antioxidant.

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