JOURNAL of THE Turkish CHEMICAL SOCIETY Section: A CHEMISTRY

TURKISH CHEMICAL SOCIETY

Study of Chromophores Potential in Binahong Leaf Extracts for Solar Cell Development

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Abstract: Solar cell material from organic chromophores is interesting to develop because it has adjustable electronic and optical properties, the material is relatively cheap, the manufacturing method is simple, environmentally friendly, and easy to recycle. This research aims to study the potential of leaf extract from binahong as a raw material for the development of organic solar cells in terms of its chromophore. The study was carried out through an analysis of leaf extracts from binahong with red stems and leaf extracts from binahong with green stems with the help of a UV-VIS spectrophotometer instrument and a Shimadzu LCMS – 8040 LC/MS instrument. The compounds identified from each extract through their LCMS chromatograms were then characterized computationally using gamess applications with the DFT method and 6.31G* basis set. The results showed that the leaf extract from binahong with red stems had a different color and band gap than the leaf extract from binahong with green stems. This is because the red-stemmed binahong leaf extract has an excess of 3 compounds, namely kaempferol-3-(6"-malonyl glucoside), prodelphinidin B1, and prodelphinidin C2. The LCMS chromatogram showed that there were 55 bioactive compounds identified in the leaf extract from binahong with red stems and 52 compounds identified in the leaf extract from binahong with green stems. Of all these compounds, the majority, namely 44 compounds in the leaf extract from binahong leaves with red stems and 42 compounds in the leaf extract from binahong with green stems, are chromophores that have the potential to be used as raw materials for developing solar cells.

Keywords: Binahong, solar cell, organic, band gap.

Submitted: December 11, 2022. **Accepted:** October 5, 2024.

Cite this: Sanjaya IGM, Setiarso P. Study of Chromophores Potential in Binahong Leaf Extracts for Solar Cell Development. JOTCSA. 2024;11(4): 1651-8.

DOI: https://doi.org/10.18596/jotcsa.1217367

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1. INTRODUCTION

The rapid increase in energy consumption due to population growth and modernization which is not matched by rapid energy production due to limited primary energy sources, has triggered a global energy crisis (1). This also causes an increase in the amount of carbon in the air which contributes greatly to air pollution and an increase in global temperatures which is the main cause of the greenhouse effect (2). To solve this, it is necessary to develop new energy sources that are oriented towards renewable and environmentally friendly energy sources or clean energy (3).

Sources of clean energy that are much looked at and are being intensively studied include solar cells (4). This is related to abundant sunlight that has not been utilized optimally yet (5). It should be noted that the average exposure to sunlight reaches 12 hours more per day (4,422 hours per year) for the tropics (6), which is equivalent to energy above 120 W/m^2 (7). The solar cell works by converting light energy or photons from the sun into electrical energy. Of course, as one of the most important sources of sustainable electricity that is fossil-free and environmentally friendly, the realization of highly efficient solar energy is urgently needed.

Silicon-based solar cells with an optimum band gap of 1.12 eV, which dominate the market and are used worldwide, can use at most about 30% of the sun's energy to be converted into electricity (8,9). This happens because of the spectral mismatch between the solar spectrum (photons) and the absorption properties of the material. For example, photons with an energy higher than the band gap that is absorbed exhibits excess energy lost due to thermalization. Meanwhile, photons with lower energy than the band gap are not absorbed and their energy is not used for the generation of charge carriers. Another limiting factor is due to the recombination of charge carriers.

Solar cells developed with silicon-based inorganic materials, apart from having high production costs and low efficiency (10), also have the potential to pollute the environment (11). Therefore, attention is diverted to solar cells made from organic materials called organic solar cells.

The use of organic materials as raw materials for solar cells has attracted a lot of attention because of their promising properties. Organic solar cells have adjustable electronic and optical properties, relatively inexpensive materials, simple manufacturing methods, low material toxicity, environmental friendliness and easy recycling (12,13). The organic materials used to develop organic solar cells are materials that can be conductors or semiconductors. These materials have chromophores in the form of functional groups which are generally in the form of conjugated bonds (alternating single and double bonds). Such bonding results in a delocalization of the electrons along the chain. The conjugated π bonds of these organic compounds have received great attention during the last three decades due to their advanced technological applications in the field of photodiodes (14,15), solar cell (16,17), and molecular electronics (18,19) in addition to its adjustable electronic devices, optical properties and stability properties (20).

Organic materials used as raw materials for making organic solar cells are generally obtained from plants that have parts such as roots, stems, leaves, flowers or fruit that are colored (21). Plants of this kind that are easy to grow and have the potential to be used as raw materials for making organic solar cells, include binahong.

Binahong, with the Latin name *Anredera cordifolia*, is really important to study as a promising potential raw material for the development of organic solar cells, because binahong, which is a vine, is very easy to grow in various locations with fruit, leaves or stems producing quite strong colors. This causes binahong to be estimated to have the potential to produce efficient solar cells because the stronger the color, the higher the efficiency of the solar cell (22).

The study of the binahong plant as a source of chromophore in the development of organic solar cells this time starts from the extract of the leaves, which besides the fruit, are also thought to contain organic compounds that have conjugated double bonds (23). Potentially important compounds in the development of organic solar cells from third generation solar cells and organic-inorganic combination solar cells from fourth generation solar cells (24).

Because the binahong plant generally grows with red stems and green stems, the chromophore potential of the leaf extract of the red-trunked binahong plant and the leaf extract of the binahong plant with green stems is currently being studied as a raw material for making organic solar cells. To ensure the possibility of each of these extracts being used as a raw material for solar cell development, the band gap is checked with a UV-VIS spectrophotometer. Furthermore, to detect the compounds contained in each binahong leaf extract, analysis is carried out using LCMS. As for predicting these compounds as potential chromophores for the development of organic solar cells, chemical computations are carried out with the B3LYP function, the DFT method, and the 6.31G* basis set where the results are then compared with the TiO_2 conduction band energy and the energy of the LUMO redox couple of I^-/I_3^-.

2. EXPERIMENTAL SECTION

2.1. Materials

The main research material was binahong leaves from the red-stemmed binahong plant and from the green-stemmed binahong plant which were harvested from the environment in East Java, besides aquadest. The instruments used are a rotary evaporator, UV-VIS spectrophotometer, Shimadzu LCMS – 8040 LC/MS, and a Zeon computer with gamess applications to perform chemical computations and Avogadro to virtualize molecules and create input files.

2.2. Method

2.2.1. Preparation of binahong leaf extract

Each binahong leaf extract was obtained by extracting the dried binahong leaves with water solvent using a rotary evaporator. Each extract obtained was divided into two. A part of the extract was measured for its spectrum with a UV-VIS spectrophotometer to determine the band gap (25). The other part of the extract was analyzed with the help of the Shimadzu LCMS – 8040 LC/MS to determine the compounds contained in each of the binahong leaf extracts (26).

2.2.2. Determination of chromophores in extracts that have potential as raw materials for solar cells

The potential of the compounds contained in binahong leaf extract as a raw material for solar cells was determined through chemical computation. Molecular models of the compounds detected in the LCMS chromatograms were made by redrawing the molecules and then optimizing their geometries using the Avogadro application. The molecular model has then degenerated into a games application input file with the B3LYP function, the DFT method, and a 6.31G* basis set using the games input generator in the Avogadro application. Furthermore, a chemical computation process was carried out using the games application to obtain information on the HOMO, LUMO, and bandgap energies of each molecular model of the compounds detected in the binahong leaf extract. The LUMO energy was then compared with the TiO_2 conduction band energy and the HOMO energy was compared with the LUMO redox couple of I^-/I_3^- energy to find the potential of the compounds in each binahong leaf extract as chromophores for the development of organic solar cells.

3. RESULTS AND DISCUSSION

3.1. Results

The binahong leaf extract produced from the red-trunked binahong plant and the green-trunked binahong plant extracted using distilled water is shown in Figure 1. Measurement of light absorption of each binahong leaf extract with a UV-VIS spectrophotometer produced spectra as shown in Figure 2. Figure 3 shows the chromatogram of the extracts of binahong leaves with red stems and binahong leaves with green stems produced using the Shimadzu LCMS – 8040 LC/MS instrument.

Figure 1: Extracts of leaves from binahong with red stems (left) and binahong with green stems (right).

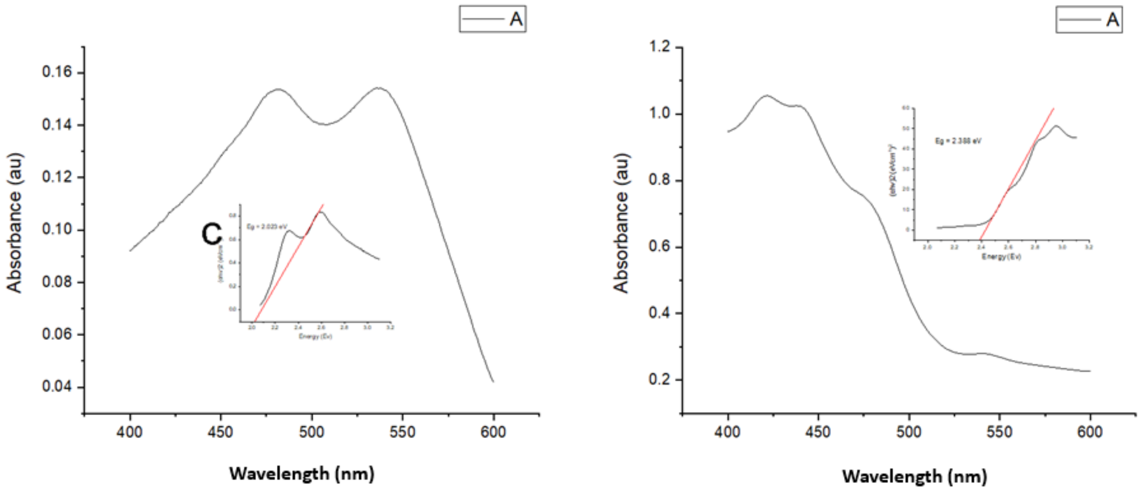


Figure 2: UV-VIS spectra of leaf extracts from binahong with red stems (left) and binahong with green stems (right).

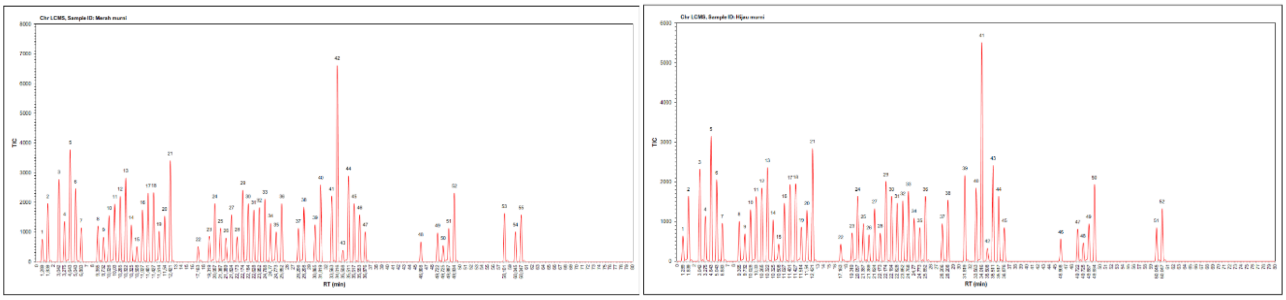


Figure 3: LCMS Chromatogram results of binahong leaf extracts with red stems (left) and green stems (right).

The details of the compounds identified through each chromatogram and the computational results of the HOMO, LUMO, and band gap energies of each molecule using the games application with the DFT method and 6.31G* basis set are shown in Table 1.

Table 1: List of compounds and computational results for each molecule contained in binahong leaf extract.

No.	Red Binahong	Green Binahong	HOMO Energy (eV)	LUMO Energy (eV)	Band Gap (eV)
1	benzoic acid	benzoic acid	-6.9906	-1.2136	5.7770
2	p-coumaric acid	p-coumaric acid	-5.8967	-1.5402	4.3565
3	gallic acid	gallic acid	-5.8967	-0.9687	4.9280
4	esculetin	esculetin	-5.7770	-1.5837	4.1933
5	caffeic acid	caffeic acid	-5.7361	-1.5211	4.2150
6	ferulic acid	ferulic acid	-5.8423	-1.5402	4.3021
7	spathulenol	spathulenol	-6.1253	0.8816	7.0069
8	apigenin	apigenin	-5.8178	-1.6000	4.2178
9	naringenin	naringenin	-5.9185	-1.3252	4.5933
10	7-O-methyl-cryptostrobin	7-O-methyl-cryptostrobin	-5.6790	-0.8980	4.7810
11	demethoxymatteucinol	demethoxymatteucinol	-5.6436	-0.8626	4.7810
12	luteolin	luteolin	-5.7661	-1.5755	4.1905
13	kaempferol	kaempferol	-5.6191	-1.2572	4.3620
14	fisetin	fisetin	-5.7416	-1.1592	4.5824
15	phytol	phytol	-6.1933	0.6993	6.8926
16	desmosflavone	desmosflavone	-5.6028	-1.7470	3.8558
17	ellagic acid	ellagic acid	-6.1525	-1.8395	4.3130
18	quercetin	quercetin	-5.6436	-1.2789	4.3647
19	myricetin	myricetin	-5.6083	-1.2436	4.3647
20	4,7-dihydroxy-5-methoxy-6-methyl-8-formylflavan	4,7-dihydroxy-5-methoxy-6-methyl-8-formylflavan	-5.7008	-1.4095	4.2912
21	chlorogenic acid	chlorogenic acid	-5.7552	-1.6490	4.1062
22	β-sitosterol	β-sitosterol	-0.8408 (α) / -6.0681(β)	0.9306 (α) /-0.8408 (β)	1.7715 (α) /5.2273 (β)
23	β-amyrin	β-amyrin	-5.7933	0.7538	6.5470
24	6-β-D-glucopyranosyl-4',5,7-trihydroxyflavone	6-β-D-glucopyranosyl-4',5,7-trihydroxyflavone	-5.6981	-1.5891	4.1089
25	vitexin	vitexin	-5.8586	-1.6272	4.2314
26	apigetrin	apigetrin	-5.9021	-1.6980	4.2041
27	larreagenin A	larreagenin A	-5.9402	0.1578	6.0981
28	astragalin	astragalin	-6.0028	-1.4612	4.5416
29	quercetin-3-O-rhamnoside	quercetin-3-O-rhamnoside	-5.8722	-1.1456	4.7266
30	fisetin-4'-glucoside	fisetin-4'-glucoside	-5.5865	-1.5592	4.0273
31	luteolin-7-glucoside	luteolin-7-glucoside	-5.9212	-1.6980	4.2232
32	diosmetin-7-O-β-Dglucopyranoside	diosmetin-7-O-β-Dglucopyranoside	-1.6925 (α) /-5.8015 (β)	-1.1565(α) /-1.6925 (β)	0.5361(α) /4.1089 (β)
33	kaempferol-3-(2''-acetylrhamnoside)	kaempferol-3-(2''-acetylrhamnoside)	-1.5075 (α) /-5.5266 (β)	-0.9769 (α) /-1.5075 (β)	0.5306 (α) /4.0191 (β)
34	kaempferol-3-(3''-acetylrhamnoside)	kaempferol-3-(3''-acetylrhamnoside)	-5.5946	-1.2789	4.3157
35	kaempferol-3-(4''-acetylrhamnoside)	kaempferol-3-(4''-acetylrhamnoside)	-1.6925 () /-5.5729 ()	-1.2898 () /-1.6925 ()	0.4027 () /3.8803 ()
36	isorhamnetin-3-O-β-Dgalactopyranoside	isorhamnetin-3-O-β-Dgalactopyranoside	-1.5919 () /-5.5620 ()	-1.3769 () /-1.5919 ()	0.2150 () /3.9701 ()
37	kaempferol-3-(2'',4''-diacetylrhamnoside)	kaempferol-3-(2'',4''-diacetylrhamnoside)	-5.3824	-1.3987	3.9837
38	kaempferol-3-(3'',4''-diacetylrhamnoside)	kaempferol-3-(3'',4''-diacetylrhamnoside)	-5.8504	-1.5102	4.3402
39	kaempferol-3-(6"-malonyl glucoside)	-	-1.5021 () /-5.5130 ()	-1.0694 () /-1.5021 ()	0.4327 () /4.0109 ()
40	quercetin-3-Omalonylglucoside	quercetin-3-Omalonylglucoside	-1.5510 () /-5.3579()	-1.1021 () /-1.5510 ()	0.4490 () /3.8069 ()
41	naringin	naringin	-6.0355	-1.2436	4.7919
42	kaempferol 3-(5''-feruloylapioside)	kaempferol 3-(5''-feruloylapioside)	-5.6627	-1.6000	4.0627
43	kaempferol 3-(6''-caffeoylglucoside)	kaempferol 3-(6''-caffeoylglucoside)	-1.6789 () /-5.5212 ()	-1.3034 () /-1.6789 ()	0.3755 () /3.8422 ()

44	quercetin-3-glucoside-7-rhamnoside	quercetin-3-glucoside-7-rhamnoside	-3.6273	-2.5960	1.0313
45	rutin	rutin	-5.8123	-1.6735	4.1388
46	prodelphinidin B1	-	-5.2926	-0.0190	5.2736
47	myricetin 3-rutinoside	myricetin 3-rutinoside	-5.8668	-1.6980	4.1688
48	momordin Ic	momordin Ic	-5.7851	-0.3646	5.4205
49	boussingoside A2	boussingoside A2	-4.8355	-2.3184	2.5170
50	momordin Ia	momordin Ia	-5.8559	0.0136	5.8695
51	boussingoside E	boussingoside E	-5.9076	-0.1388	5.7688
52	quinoasaponin 9	quinoasaponin 9	-5.8178	-0.1170	5.7008
53	prodelphinidin C2	-	-7.3090	3.2082	10.5172
54	momordin Iic	momordin Iic	-3.9164	4.2966	8.2130
55	momordin Iia	momordin Iia	-7.4483	3.9731	11.4214

3.2. Discussion

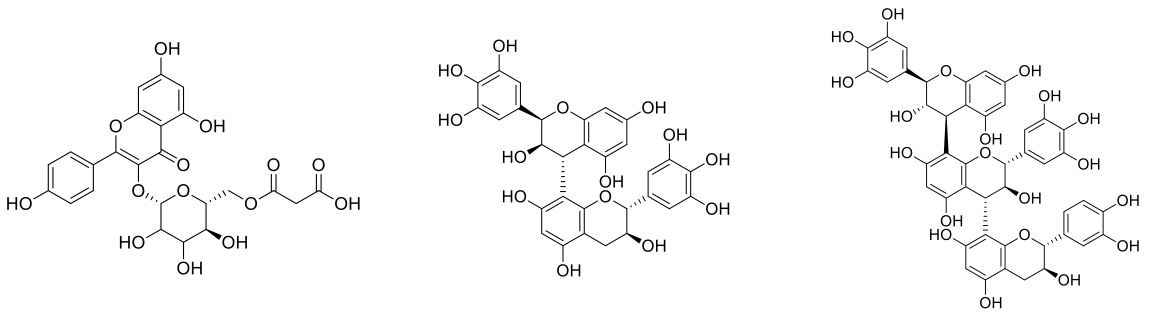
Figure 1 shows the leaf extract of the red-stemmed binahong plant which is red in color, is different from the leaf extract of the green-stemmed binahong plant which is greenish-yellow in color. In addition, there is also a difference in the band gap between the two types of extracts based on the results of the respective UV-VIS spectral measurements in Figure 2 which can be rewritten in Table 2.

Table 2: Band gap of binahong leaf extract.

No.	**Sample**	**Band Gap (eV)**
1	Leaf extract from red-stemmed binahong	2.023
2	Leaf extract from binahong has green stems	2.388

Even so, the difference in the band gap still exists in the band gap area which has efficiency in converting power from sunlight (27).

The color difference produced in the red-stemmed binahong leaf extract and the green-stemmed binahong leaf extract in Figure 1 occurs because there are differences in the content of bioactive compounds in each extract (28,29). As shown in table 1 which details the chromatogram results from Figure 2, there are 3 compounds that cause color differences in the red-stemmed binahong leaf extract from the green-stemmed binahong leaf extract, namely kaempferol-3-(6"-malonyl glucoside), prodelphinidin B1, and prodelphinidin C2.



kaempferol-3-(6"-malonyl glucoside) **prodelphinidin B1** **prodelphinidin C2**

Figure 4: Three compounds that differentiate the red-stemmed binahong leaf extract from the green-trunked binahong leaf extract.

Table 1 shows that the bioactive compounds contained in leaf extracts from red-stemmed binahong and leaf extracts from green-stemmed binahong are generally semiconductors with energy band gaps ranging from 1.0313 eV to 11.4214 eV. Semiconductors from bioactive compounds that have an energy gap above the standard silicon energy gap, namely 1.12 eV, work outdoors in bright light.

Based on an understanding of the DSSC chart (30) and an understanding of the optimal electron donor-acceptor pair that can be selected based on an understanding of the TiO_2 conduction band as a standard, namely -4.05 eV (31,32), then the LUMO energy of the chromophore in binahong leaf extract that must be sought is the one with a more positive value than the TiO_2 conduction band. This is based on the assumption that the excited state of the chromophore is in the LUMO state. This state is related to the ability of the chromophore molecule to inject electrons from its excited state into the TiO_2 conduction band. For HOMO from the chromophore of binahong leaf extract, it is necessary to find a molecule that has a HOMO energy that is more negative than the energy of the LUMO redox couple of I^-/I_3^- = -4,85 eV (33-35).

Based on the computation of the HOMO, LUMO, and band gap in Table 1, ignoring molecules that have two types of band gaps energy, there are 44 compounds in the leaf extract from the red stemmed binahong and 42 compounds in the leaf extract from the green stemmed binahong which have the possibility of being new chromophores for interest in the development of organic solar cells.

4. CONCLUSION

The leaf extract from binahong with red stems has a different color than the color of the leaf extract from binahong with green stems, as well as the band gap. The causes of these differences were the compounds kaempferol-3-(6"-malonyl glucoside), prodelphinidin B1, and prodelphinidin C2 which were only present in leaf extracts from red-trunked binahong, not found in leaf extracts from green-trunked binahong. The LCMS chromatogram showed that there were 55 bioactive compounds identified in the leaf extract from binahong with red stems and 52 compounds identified in the leaf extract from binahong with green stems. Of all these compounds, the majority, namely 44 compounds in the leaf extract from the red-stemmed binahong and 42 compounds in the leaf extract from the green-stemmed binahong, are chromophores that have the potential to be used as raw materials for the development of organic solar cells. Based on this and the results of the band gap measurements, each binahong leaf extract has the potential to be used as a raw material for solar cell development.

5. ACKNOWLEDGMENT

We are grateful to State University of Surabaya for providing research grants and facilitating the implementation of this research.

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