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Potential of Fruit Extract from Green-Stemmed Binahong (*Anredera cordifolia*) as a Natural Chromophore for Solar Cell Development

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Abstract: The increasing demand for clean and renewable energy has driven the exploration of alternative materials for solar cell development. In this context, natural chromophores derived from plants offer an eco-friendly and sustainable solution due to their availability, low toxicity, and diverse molecular structures. This study investigates the chromophoric potential of the green-stemmed binahong (*Anredera cordifolia*) fruit and evaluates natural compounds that can be efficient light-absorbing materials in solar energy applications. Extracts of the binahong fruit were analyzed using Liquid Chromatography–Mass Spectrometry (LC-MS), revealing 66 distinct molecular peaks. Each compound was subjected to quantum chemical simulations using Time-Dependent Density Functional Theory (TD-DFT) following initial geometry optimization through Density Functional Theory (DFT) calculations. The simulations were conducted using the ORCA software, with molecular input prepared via the ChemCompute and Avogadro platforms. Parameters such as HOMO–LUMO energy levels and bandgap values were determined for all detected compounds. From these, 17 compounds exhibited favorable electronic characteristics, including bandgap values ranging from 1.3 to 4.4 eV and well-delocalized frontier orbitals. Notably, betalain compounds such as betanin and indicaxanthin showed strong visible light absorption and low energy gaps, while flavonoids and phenolic acids offered structural stability and tunable electronic properties. This research presents a novel computational approach to screening plant-based chromophores from non-model species, integrating LC-MS and TD-DFT data to highlight their light-harvesting capabilities. In conclusion, green-stemmed binahong is shown to be a promising source of natural chromophores for use in environmentally friendly solar technologies. The selected chromophores, especially those with optimal electronic configurations, are expected to be applied in future organic photovoltaic materials or integrated into green chemistry education as part of renewable energy awareness.

Keywords: *Anredera cordifolia*; Natural Dye; Chromophore; HOMO-LUMO; Solar Energy.

Introduction

The increasing demand for clean and renewable energy has driven continuous innovation in solar technology development. Conventional solar cells based on inorganic materials such as silicon and perovskite dominate the market due to their high efficiency, but often raise concerns over toxicity, cost, and sustainability [1], [2]. In contrast, natural chromophores derived from plants have attracted attention as biodegradable and low-cost alternatives [3], [4].

These plant-based dyes exhibit diverse conjugated structures and donor–acceptor characteristics, enabling strong light absorption in the visible range [5], [6]. Common classes of natural dyes include flavonoids, betalains, phenolic acids, coumarins, and quinones each offering unique optical and electronic properties [7]. Betalains, for instance, have shown high molar absorptivity and strong coloration due to their conjugated systems and hydrophilic groups, making them suitable for green chemistry and energy harvesting applications [8].

Anredera cordifolia, a medicinal plant native to Southeast Asia, is known to contain various bioactive compounds such as flavonoids, phenolic acids, and betalains [9]. However, its potential as a source of chromophores has not been widely explored computationally.

Previous studies have applied similar approaches to other plant sources, such as Hibiscus sabdariffa [10], Opuntia ficus-indica [11], and pomegranate peel [12], where flavonoids and betalains were computationally evaluated using TD-DFT. However, few have investigated Anredera cordifolia—particularly the fruit from green-stemmed variants—despite its rich phytochemical content. This gap motivates the current study, which integrates LC-MS profiling with quantum chemical simulations to explore novel chromophore candidates.

This study aims to identify and evaluate potential chromophores from the green-stemmed binahong fruit using a combination of LC-MS analysis and TD-DFT simulation. The computational screening targets key electronic parameters such as HOMO–LUMO energy levels and bandgaps, which are essential indicators of light-harvesting efficiency [13], [14].

Previous studies on plant-derived chromophores have mostly focused on model species such as hibiscus, pomegranate, or dragon fruit, with betalain and flavonoid-rich profiles [4], [8]. However, the chromophoric potential of Anredera cordifolia, particularly its green-stemmed variety, has not been comprehensively explored. Furthermore, many existing works rely heavily on empirical characterization (e.g., UV-Vis spectroscopy), lacking in-depth electronic analysis.

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This study introduces a novel computational approach combining LC-MS profiling and TD-DFT simulations to evaluate the electronic properties of binahong-derived compounds. This integrative screening method allows the prediction of bandgap values, electron delocalization, and frontier orbital distributions, thus supporting the rational selection of chromophores for bio-based solar technologies.

Research Methods

Sample Preparation and LC-MS Analysis

Fresh green-stemmed binahong (Anredera cordifolia) fruits were obtained from a local e-commerce platform in Indonesia. The fruits were separated from their stems, chopped, and homogenized using a household chopper. The resulting pulp was filtered through a fine mesh to obtain a concentrated extract. Ethanol was used as the solvent for maceration, and the extract was stored in refrigeration before instrumental analysis.

The identification of compounds was performed using Liquid Chromatography–Mass Spectrometry (LC-MS), a highly sensitive technique commonly applied for profiling natural product mixtures [14], [15]. The LC component separates compounds based on polarity, while the MS detector identifies their molecular weights via mass-to-charge ratio (m/z). A total of 66 peaks were identified from the binahong fruit extract.

Molecular Structure Construction and Optimization

Each compound identified from LC-MS was structurally modeled based on its molecular formula, using ChemCompute (https://chemcompute.org), a cloud-based quantum chemistry simulation platform. Molecular geometries were constructed manually or fetched from PubChem when available, then converted into ORCA-compatible input files.

Geometry optimization was carried out using the B3LYP functional with the 6-31G* basis set in the ORCA 5.0 software. The initial input file was configured via Avogadro, an open-source molecule editor, using the following keyword block:

```
!Opt Freq B3LYP 6-31G* TightSCF
```

This step ensures that the molecular conformation used in later simulations reflects its lowest-energy geometry, which is crucial for accurate predictions of electronic properties [16].

TD-DFT Simulation for Electronic Excitations

Following structural optimization, Time-Dependent Density Functional Theory (TD-DFT) calculations were performed to simulate the electronic excitation properties of each compound. These calculations were conducted using the following configuration:

```
!B3LYP 6-31G* TightSCF

%maxcore 1000

%td-dft
        nroots 10
        maxdim t
        tda true
end

%output
        Print [p_mos] true
        Print [p_basis] 5
end
```

TD-DFT is widely recognized for its effectiveness in predicting UV-Vis absorption and transition states in organic chromophores [9], [17]. Output parameters include the energies of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), their spatial distributions, and the resulting bandgap values (ΔE). These features serve as primary criteria in evaluating chromophore potential.

Due to the computational nature of this study, simulations were performed once per compound without replicates. However, all 66 molecules were calculated under identical TD-DFT simulation parameters using ORCA software to ensure consistency and comparability of the resulting HOMO-LUMO energies and bandgap values [18].

Data Analysis and Chromophore Selection

Although no replicates were conducted for each simulation, all computational calculations were carried out using the same DFT/TD-DFT parameters and software versions to ensure comparability across all compounds. All quantum chemical simulations yielded output files containing numerical and graphical information regarding the molecular orbital distribution and excitation characteristics of each compound. These outputs were processed using Avogadro to extract key parameters including HOMO and LUMO energies, energy gap (ΔE), and spatial electron distribution. The bandgap values were calculated by subtracting the HOMO energy from the LUMO energy [19]:

$$\Delta E_{\mathrm{bandgap}} = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}$$

This value serves as a primary indicator of a compound's optical activity and light absorption potential [9].

In addition to bandgap evaluation, the spatial distribution of frontier orbitals was analyzed visually using Avogadro to assess delocalization patterns and donor–acceptor interactions. Molecules exhibiting extended delocalization and balanced charge transfer characteristics were considered favorable for chromophore function [13].

The chromophore selection process was based on three main criteria:

a) Bandgap values between approximately 1.3 and 4.5 eV, representing the optimal absorption range for visible light [9],
b) Clear evidence of π-electron delocalization between donor and acceptor regions, and
c) Structural features that support intramolecular charge transfer, such as conjugated backbones and polar functional groups [16].

From the total of 66 compounds analyzed, 17 were shortlisted based on their electronic suitability. These were further classified into five chemical groups for comparative evaluation.

Results and Discussion

Selection and Classification of Natural Chromophores

66 compounds were initially identified from green-stemmed binahong (Anredera cordifolia) fruit extract via LC-MS analysis. These compounds were computationally screened using Time-Dependent Density Functional Theory (TD-DFT) to evaluate their suitability as natural chromophores based on three key criteria:

a) a bandgap between 1.3–4.5 eV,
b) partial delocalization of the HOMO–LUMO orbitals
c) presence of donor–acceptor characteristics in their structure.

From this screening, 17 compounds met the electronic requirements and were selected for further classification into five chemical groups: betalains, flavonoids, phenolic acids, coumarins, and quinones.

Betalain Compounds

Betalains are nitrogen-containing pigments commonly found in plants of the Caryophyllales family, classified into betacyanins (red–purple) and betaxanthins (yellow–orange). Four compounds were selected based on their electronic and optical properties: betanin, indicaxanthin, tyrosine-betaxanthin, and betalamic acid. These molecules exhibited favorable bandgap values (1.3–3.5 eV), strong coloration, and conjugated systems conducive to efficient light absorption.

Four of the 17 selected compounds belonged to the betalain group: betanin, indicaxanthin, tyrosine-betaxanthin, and betalamic acid. These compounds showed relatively low bandgap values ranging from 1.32 to 3.47 eV, suggesting their ability to absorb photons in the visible region.

Table 1. Electronic properties of selected betalain compounds

Compounds	HOMO (eV)	LUMO (eV)	Bandgap (eV)	Color
Betanin	-4.691	-3.371	1.320	Red-purple
Indicaxanthin	-4.887	-3.457	1.381	Yellow-orange
Betalamic acid	-5.740	-2.888	2.852	Yellow
Tyrosine-betaxanthin	-5.492	-1.923	3.569	Orange

These results suggest that betalains are strong candidates for solar applications, not only because of their favorable electronic structures but also due to their functional –OH and –COOH groups that facilitate binding with semiconductor surfaces like TiO_2.

Betanin and indicaxanthin are known for their strong natural coloration due to extended conjugation and the presence of hydrophilic groups such as –OH and –COOH, which also facilitate binding to semiconductors [4], [8]. Their π-delocalized structure supports efficient electron excitation from HOMO to LUMO, consistent with their potential as light-harvesting materials [4].

Flavonoid Compounds

Flavonoids are phenolic compounds with a C6–C3–C6 backbone that supports broad π-conjugation and optical stability. Six flavonoids were selected due to their acceptable bandgap values (3.8–4.4 eV) and electron delocalization patterns: quercetin, fisetin, myricetin, kaempferol, isorhamnetin, and apigenin-7-glucoside-4’-trans-caffeate.

Six selected compounds were classified as flavonoids: apigenin-7-glucoside-4′-trans-caffeate, quercetin, fisetin, myricetin, kaempferol, and isorhamnetin. These molecules exhibited moderate bandgap values between 3.80 and 4.42 eV, within the optimal range for visible light absorption.

Table 2. Electronic properties of selected flavonoid compounds

Compounds	HOMO (eV)	LUMO (eV)	Bandgap (eV)	Color
Apigenin-7-glucoside-4’-trans-caffeate	-5.432	-1.634	3.798	Pale Orange
Isohamnetin	-5.427	-1.598	3.829	Pale Yellow
Fisetin	-5.488	-1.648	3.840	Yellow
Quercetin	-5.457	-1.613	3.844	Yellow
Myricetin	-5.510	-1.609	3.901	Yellow
Kaempferol	-5.519	-1.575	3.944	Yellow

Flavonoids provide structural versatility, low toxicity, and high antioxidant activity, making them suitable as natural dyes for environmentally friendly solar energy devices.

Previous computational studies have shown that quercetin and kaempferol possess suitable electronic properties for optical materials, including HOMO–LUMO distributions that support $\pi \rightarrow \pi^*$ transitions [17], [20]. Moreover, their planar structures and abundant hydroxyl groups enhance stability and electron delocalization across the aromatic system.

Phenolic Acid Compounds

Phenolic acids have simpler structures and smaller molecular weights but still show potential as chromophores due to π-conjugated aromatic systems. Four compounds, caffeic acid, ferulic acid, sinapic acid, and chlorogenic acid, were selected.

The selected phenolic compounds included caffeic, ferulic, sinapic, and chlorogenic acids. Despite having slightly higher bandgaps (~4.0–4.2 eV), their aromatic backbone and conjugated systems still allow visible light absorption.

Despite relatively higher bandgaps, phenolic acids retain potential especially when derivatized or combined with other dyes. These compounds have also been reported as redox-active dyes with moderate light absorption efficiency [21], [22]. Their carboxyl and hydroxyl groups are anchoring sites and support intramolecular charge transfer mechanisms.

Table 3. Electronic properties of selected phenolic acid compounds

Compounds	HOMO (eV)	LUMO (eV)	Bandgap (eV)	Color
Chlorogenic acid	-5.504	-1.411	4.093	Colorless
Ferulic acid	-5.629	-1.449	4.186	Pale Yellow
Sinapic acid	-5.639	-1.443	4.190	Pale Yellow
Caffeic acid	-5.721	-1.515	4.206	Pale Yellow

Coumarin Compounds

Two coumarin derivatives, esculetin and scopoletin, were chosen due to their planar aromatic structure and moderate bandgap values.

Two coumarin compounds, esculetin and scopoletin, showed bandgap values in the 4.31–4.39 eV range. Their planar aromatic systems and electron-rich structures enable absorption in the near-UV to visible region.

Table 4. Electronic properties of selected coumarin compounds

Compounds	HOMO (eV)	LUMO (eV)	Bandgap (eV)	Color
Esculetin	-5.602	-1.287	4.315	Pale Yellow
Scopoletin	-5.603	-1.241	4.362	White

Coumarins are known for their fluorescent properties, contributing to their light absorption capability in the UV–blue spectrum.

Coumarins are well known for their fluorescence and photoactive properties, making them potential candidates in organic optoelectronics and dye-sensitized applications [23], [24].

Quinone Compounds

Only one compound from this group, dopaxanthin-quinone, was retained from this class. Only one compound, dopaxanthin-quinone, fulfilled the selection criteria within the quinone group.

Table 5. Electronic properties of selected betalain compounds

Compounds	HOMO (eV)	LUMO (eV)	Bandgap (eV)	Color
Dopaxanthin-quinone	-5.231	-2.911	2.320	Yellow-orange

With a bandgap of 2.32 eV, this molecule demonstrates promising light-absorption potential in the orange region and features favorable charge-transfer pathways due to its quinonoid structure.

With a bandgap value of 2.32 eV. Quinones possess a highly conjugated and planar π-system, facilitating intramolecular charge transfer and strong absorption in the yellow–orange region of the visible spectrum [25].

Conclusion

This study successfully identified and computationally evaluated natural chromophores from the fruit extract of green-stemmed binahong (Anredera cordifolia) using LC-MS analysis and quantum chemical simulations. A total of 66 compounds were screened using Time-Dependent Density Functional Theory (TD-DFT) to determine key electronic parameters such as HOMO–LUMO energy levels, bandgap values, and electron delocalization patterns. Based on these criteria, 17 compounds were shortlisted as promising chromophore candidates and classified into five major chemical groups: betalains, flavonoids, phenolic acids, coumarins, and quinones. The shortlisted compounds, which belong to five structural classes: betalains, flavonoids, phenolic acids, coumarins, and quinones, demonstrated appropriate energy bandgaps (1.3–4.5 eV), strong light absorption potential, and molecular features favorable for intramolecular charge transfer. The findings emphasize the contribution of computational chemistry in identifying low-cost and biodegradable chromophores for solar energy applications. The combined use of LC-MS and TD-DFT provides a reliable and efficient method for screening natural compounds as light-absorbing materials. These insights can support future design and development of bio-based solar cells and serve as a teaching resource in green energy education. Experimental trials and device integration studies are recommended as the next step to further validate the results.

Author's Contribution

Ni Nyoman Triyani Damayanti: conducted the experimental work, computational modelling, data interpretation, and manuscript preparation; I Gusti Made Sanjaya: supervised the research process and provided critical guidance during the data analysis and writing phases. Both authors reviewed and approved the final version of the manuscript.

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