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Microwave-assisted extraction and computational modelling of curcumin from turmeric (*Curcuma longa*) for sunscreen applications

Ekstraksi kurkumin dari kunyit (*Curcuma longa*) menggunakan microwave-assisted extraction dan pemodelan komputasi untuk aplikasi tabir surya

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ABSTRACT

Excessive exposure to ultraviolet (UV) radiation from sunlight can cause skin damage, including premature aging, sunburn, and increased risk of skin cancer. While synthetic sunscreen agents are widely used, concerns over their long-term safety have driven interest in natural alternatives. In this study, curcumin was extracted from turmeric rhizomes (*Curcuma longa*) using microwave-assisted extraction (MAE) as a potential natural sunscreen. The highest yield was obtained using ethanol as solvent (5.5%), 100 watts of microwave power (5.7%), and solvent temperature of 50 °C (7.8%). Curcumin presence was confirmed by thin layer chromatography (TLC), with Rf values from 0.63 (methanol) to 0.82 (ethanol). Fourier transform infrared (FTIR) spectroscopy showed functional groups including O–H, C–H, C=C, C=O, and C–O, along with trans-C–H benzoate vibrations. ^{1}H-NMR spectra supported its presence, with chemical shifts at 3.80–3.92, 6.54–7.18, and 7.31–7.49 ppm. UV-Vis analysis revealed strong absorption in the UV-A region (320–420 nm), and DFT-based computational modelling showed peaks at 276 and 405 nm. These results highlight curcumin's potential as a photoprotective agent, supporting safer, plant-based sunscreen formulations and offering a sustainable alternative for the cosmetic industry.

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ABSTRAK

Paparan berlebihan terhadap radiasi ultraviolet (UV) dari sinar matahari dapat menyebabkan kerusakan kulit, termasuk penuaan dini, kulit terbakar, dan peningkatan risiko kanker kulit. Meskipun tabir surya sintetis banyak digunakan, kekhawatiran terhadap keamanan jangka panjangnya telah mendorong minat terhadap alternatif alami. Dalam studi ini, kurkumin diekstraksi dari rimpang kunyit (*Curcuma longa*) menggunakan metode ekstraksi berbantuan gelombang mikro (MAE) sebagai kandidat tabir surya alami. Hasil ekstraksi tertinggi diperoleh menggunakan etanol sebagai pelarut (5.5%), daya gelombang mikro 100 watt (5.7%), dan suhu pelarut 50 °C (7.8%). Keberadaan kurkumin dikonfirmasi melalui kromatografi lapis tipis (TLC), dengan nilai Rf antara 0.63 (metanol) hingga 0.82 (etanol). Spektroskopi FTIR menunjukkan gugus fungsi seperti O–H, C–H, C=C, C=O, dan C–O, serta vibrasi trans-C–H benzoat. Spektra ^{1}H-NMR mendukung keberadaan kurkumin dengan pergeseran kimia pada 3.80–3.92; 6.54–7.18; dan 7.31–7.49 ppm. Analisis UV-Vis menunjukkan penyerapan kuat di wilayah UV-A (320–420 nm), dan pemodelan komputasi berbasis DFT menunjukkan puncak pada 276 dan 405 nm. Temuan ini menyoroti potensi kurkumin sebagai agen fotoprotektif, mendukung formulasi tabir surya berbahan nabati yang lebih aman dan menawarkan alternatif berkelanjutan bagi industri kosmetik.

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INTRODUCTION

Sunlight contains vitamin D with various benefits, one of which is for bone health. In addition, sunlight also has negative impacts on humans, especially due to the depletion of the ozone layer, which increases the intensity of solar radiation. Combined with prolonged exposure to various air pollutants, this can cause premature aging, skin cancer, sunburn, pigmentation, and photosensitivity (Puspitasari et al., 2018). UV light is divided into three parts, namely UV-A (320–400 nm), UV-B (290–315 nm), and UV-C (100–290 nm), which have a negative impact on human skin.

Currently, various strategies are used to protect the skin from sun exposure, one of which is the use of cosmetics such as lotions, creams, and sunscreens. However, the cosmetics circulating in the market are dominated by sunscreen products containing synthetic active substances, raising concerns about potential side effects on human skin (Kanani et al., 2017). Natural ingredients for sunscreen compounds that are safer for the skin are generally rarely used, one of which is phenolic compounds that are able to protect tissues from damage caused by solar radiation and also flavonoid compounds as components to counteract ultraviolet-induced radicals (Puspitasari et al., 2018).

One of the bioactive compounds of phenolics and flavonoids as active ingredients of sunscreen and antioxidants (Furi et al., 2019) is turmeric. Turmeric contains curcumin which **is** able to absorb UV light because it has a chromophore group (conjugated double bond), so it can be used as a sunscreen compound in the manufacture of cosmetics (Salmahaminati and Fajar, 2015). The molecular structure of curcumin is presented in Figure 1, illustrating the presence of aromatic rings, α,β-unsaturated carbonyl groups, and hydroxyl groups—each contributing to its UV absorption and antioxidant activity.

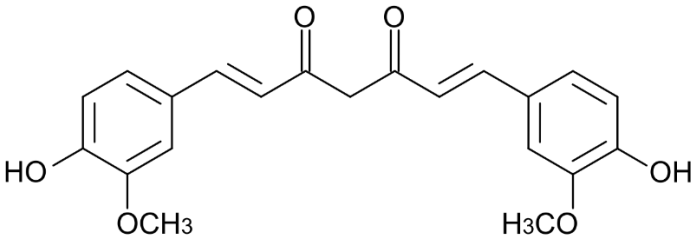


Figure 1. Molecular structure of curcumin.

Curcumin extract from turmeric rhizome is obtained by an extraction process such as soxhletation. However, soxhlet extraction has several limitations, including long processing time, inconsistent heating temperature, and the requirement for large volumes of solvent. Therefore, a more efficient curcumin extraction method is needed, such as the green extraction method known as microwave-assisted extraction (MAE) (Chemat et al., 2012). MAE is a green extraction technique currently under development in the fields of chemistry, biology, and applied technology. It is designed and used on a laboratory scale to reduce the use of harmful substances for the environment (Margaretta et al., 2011). MAE utilizes microwave energy to accelerate the extraction process efficiently (Calinescu et al., 2018).

In recent years, the MAE method has been utilized to extract curcumin from plant materials under various operating conditions. Key factors explored by researchers include microwave power, time intervals (both irradiation and cooling durations), temperature, plant material size, and the type of solvent used. In some cases, dry microwave irradiation is applied to enhance cell wall degradation and improve solvent penetration, making powdered samples more susceptible to microwave heating. These modifications can significantly improve both the extraction rate and efficiency (Mandal et al., 2009). For instance, Mandal et al. (2009) employed a Taguchi L9 orthogonal design using microwave-assisted solvent–sample duo-heating synergism to extract curcumin from *Curcuma longa* L. The optimal conditions identified were 140 W (20%) microwave power, 4 min of irradiation, plant particles screened through a sieve 20, 8 mL of methanol as a modifier,

and a solid-to-solvent (acetone) ratio of 1:20. Under these conditions, the curcumin yield reached 4.98%, surpassing the yields achieved through Soxhlet extraction, maceration, and stirring extraction.

In this study, the authors are interested in extracting curcumin from turmeric with several variations of solvents, temperatures, and power to determine the results of good curcumin yields with efficient time and affordable costs. Computational analysis is also used to strengthen and validate the laboratory results. However, only a limited number of studies have explored the integration of microwave-assisted extraction and computational modelling, particularly the use of density functional theory (DFT), to predict the ultraviolet-visible absorption characteristics of curcumin. This presents a significant research gap considering the growing demand for natural and safe sunscreen agents. Therefore, this study aims to optimize curcumin extraction conditions using MAE and to apply DFT-based modelling to evaluate its potential as a UV-A-absorbing compound for sunscreen formulations (Rowe et al., 2009).

MATERIALS & METHODS

Materials

The plant material used in this study was turmeric (*Curcuma longa*) rhizome, which was obtained from a local traditional market in Yogyakarta, Indonesia. The rhizomes were cleaned, air-dried at room temperature, then ground into powder and sieved through a 40-mesh screen before use. Solvents and reagents used for extraction and formulation included ethanol 70% (Merck, Germany), methanol (Merck, Germany), *n*-hexane (Merck, Germany), isopropanol (Merck, Germany), ethyl acetate (Merck, Germany), nipasol and nipagin (Brataco, Indonesia), cetyl alcohol (Sigma-Aldrich, USA), butylated hydroxytoluene (BHT; Sigma-Aldrich, USA), triethanolamine (TEA; Sigma-Aldrich, USA), glycerin (Brataco, Indonesia), and distilled water (Brataco, Indonesia).

Instrumentation used in this research included a microwave-assisted extractor (Electrolux EMG23K22B, Electrolux, Sweden), a UV–visible spectrophotometer (U-2900, Hitachi High-Tech Corporation, Japan), a fourier transform infrared (FTIR) spectrometer (Spectrum Two System L160000A, PerkinElmer Inc., USA), and a rotary evaporator (R-300, Buchi Labortechnik AG, Switzerland). Thin layer chromatography (TLC) was performed using silica gel 60 F254 plates (Merck, Germany), and nuclear magnetic resonance (^{1}H-NMR) analysis was conducted using a 60 MHz NMR spectrometer (Nanalysis NMR Ready 60Pro, Nanalysis Corp., Canada). Additional laboratory tools included glassware (Pyrex, Corning Inc., USA), 40-mesh sieves, filter paper, aluminum foil, a pH meter (Hanna Instruments, USA), thermometer, and analytical balance.

For computational modelling, molecular structures were constructed and pre-optimized using HyperChem 8.0 (Hypercube Inc., USA) and Avogadro 1.2 (Open Chemistry Project). Geometry optimization and UV–visible spectra prediction were carried out using Gaussian09 and GaussView 05 (Gaussian, Inc., USA) at the density functional theory (DFT) level.

Curcumin extraction using microwave-assisted extraction (MAE)

The extraction of curcumin from turmeric was carried out using the microwave-assisted extraction (MAE) method under three different sets of conditions: solvent variation, microwave power variation, and temperature variation. In the solvent variation experiment, 10 g of turmeric powder were each mixed with 50 mL of one of the following solvents: ethanol, methanol, isopropanol, and *n*-hexane. The mixtures were placed in a beaker and subjected to microwave irradiation at a power of 100 watts for 5 min. The resulting mixtures were filtered, and the filtrates were evaporated using a rotary evaporator to obtain the crude extract.

Based on the solvent that produced the highest yield in the previous step, further extractions were performed to investigate the effect of microwave power. Ten grams of turmeric powder were dissolved in 50 mL of the selected solvent, and the mixture was microwaved at 100 W, 200 W, and 300 W, respectively, for 5 min. Each extract was then filtered and

concentrated using a rotary evaporator. Next, temperature variation was investigated using the best solvent and microwave power combination. The turmeric-solvent mixtures were extracted using microwave heating at 30 °C, 40 °C, and 50 °C for 5 min. The extracts were filtered and concentrated as previously described.

Determination of maximum wavelength and SPF value

The UV absorption spectrum of curcumin was analyzed to determine its photoprotective potential. A 100 ppm solution was prepared by dissolving 2.5 mg of turmeric extract in 70% ethanol and diluting the solution in a 25 mL volumetric flask. The absorbance spectrum was recorded over the wavelength range of 200–500 nm using a UV–visible spectrophotometer. The absorbance values between 290 and 320 nm were used to calculate the sun protection factor (SPF) following the method of Mansur (1986), as cited in Mokodompit et al. (2013).

Characterization of extracted compounds

The chemical composition and functional groups present in the turmeric extract were characterized using several analytical techniques. The FTIR spectrometer was used to identify characteristic functional groups in the extract. Proton nuclear magnetic resonance (^{1}H-NMR) spectroscopy was employed to confirm the chemical structure and purity of curcumin. Thin layer chromatography (TLC) was used for compound separation and identification, and UV–Vis spectrophotometry further supported the detection of the active compound.

Computational Modelling of Curcumin

To evaluate the photophysical properties of curcumin, computational modeling was conducted. The initial molecular structure was drawn using HyperChem 8.0 and pre-optimized with the universal force field (UFF) via Avogadro 1.2. Further geometry optimization was performed using density functional theory (DFT) at the B3LYP/6-31G(d,p) level with Gaussian09. To simulate electronic excitation and absorption characteristics, time-dependent DFT (TD-DFT) calculations were also carried out. The computational analysis yielded data on dipole moment, HOMO–LUMO energy levels, atomic charges, and predicted UV–Vis spectra, as referenced in previous studies (Purnama et al., 2019; Salmahaminati et al., 2021, 2023).

RESULTS & DISCUSSION

Extraction and characterization of curcumin by MAE

The best result in the solvent variation experiment (procedure A) was identified using FTIR spectroscopy. For the temperature variation (procedure C), the extracts were characterized using ^{1}H-NMR and UV–Vis spectroscopy. The FTIR spectrum of turmeric extract (Figure 2) confirmed the presence of curcumin through characteristic absorption bands. A broad band at 3356 cm^{-1} indicated O–H stretching vibrations typical of phenolic groups. The sharp band at 1676 cm^{-1} corresponded to C=O stretching, while C=C aromatic ring stretching appeared at 1677 cm^{-1}. Additional bands were observed at 1512 cm^{-1} (aromatic C–H bending), 1445 cm^{-1} (CH_2 bending), 1030 cm^{-1} (C–O stretching), and 968 cm^{-1} (C–H deformation).

The ^{1}H-NMR spectrum (Figure 3) showed signals corresponding to different groups of metabolites extracted based on solvent polarity. The spectrum displayed three major regions: 0.5–2.75 ppm (amino acids and fatty acids), 2.75–5.75 ppm (saccharides), and 5.75–8.0 ppm (aromatic compounds). Curcumin, as an aromatic molecule, was primarily found in the range of 6.5–7.75 ppm, confirming its presence in the extract (Dwiseptianti et al., 2019). The identification of curcumin using thin layer chromatography (TLC) is shown in Table 1. Compound identification was performed by comparing Rf values of extracts to standard curcumin values. Under UV light at 245 and 366 nm, extracts obtained with ethanol, methanol, and isopropanol exhibited a yellow color indicative of curcumin, while the *n*-hexane extract showed almost no color. Across different microwave power and temperature settings, yellow coloration was consistently observed, supporting curcumin presence. According to Silverstein et al. (1981), curcumin typically exhibits Rf values ranging from 0.69 to 0.88.

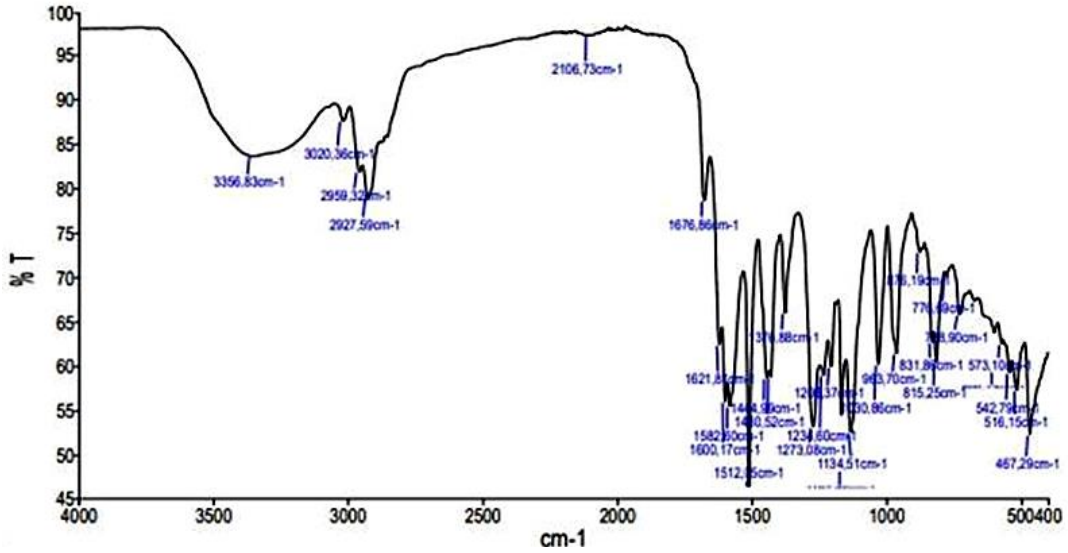


Figure 2. FTIR spectra of turmeric extract

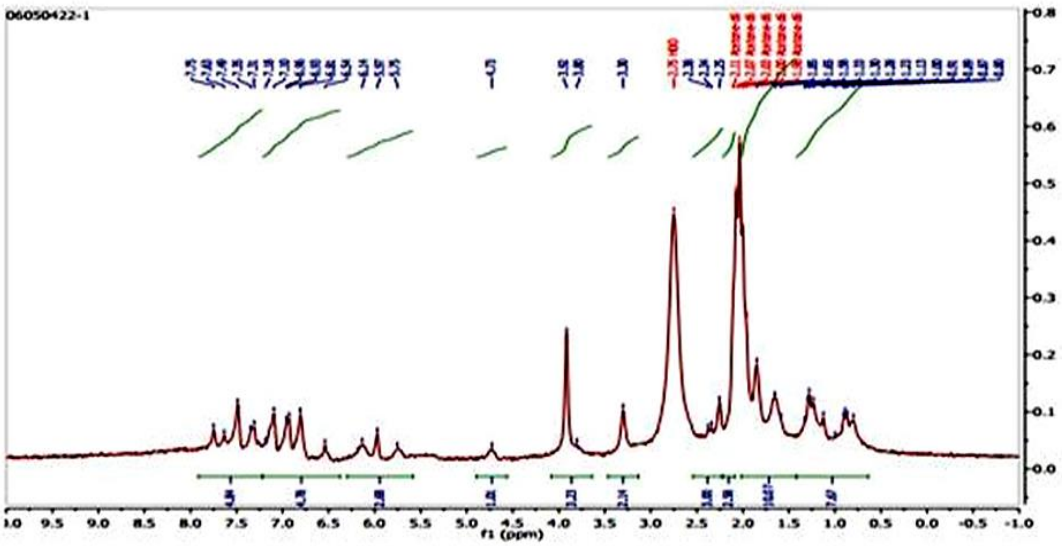
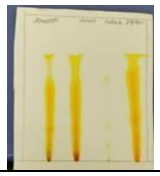
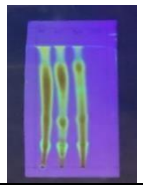
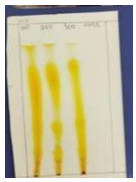
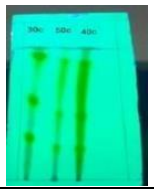
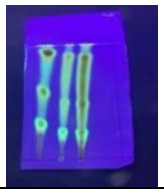


Figure 3. ^{1}H-NMR spectra of turmeric extract.

The optimal isolation conditions for curcumin were achieved using ethanol as the solvent, 100 watts of microwave power, and an extraction temperature of 50 °C. This combination resulted in the highest yield (7.8%), as shown in Table 2. Ethanol was effective due to its polarity, which closely matches that of curcumin, enhancing its solubility and extraction efficiency (Priyadarsini, 2014). Additionally, 100 watts of microwave power produced better yields than higher powers, likely due to reduced degradation at moderate energy input. This is consistent with Mandal et al. (2009), who reported 140 W as optimal. The highest extraction temperature (50 °C) further improved extraction due to enhanced solvent penetration and diffusion (Sucipto et al., 2019).

Table 1. Analysis result of curcumin using TLC

Variation/radiation	245 nm	366 nm	No radiation
Solvent (isopropyl alcohol, n-hexane, ethanol, methanol) *			
Watt (100, 200, 300) *			
Temperature (30, 40, 50°C) *			

Note. * is from left to right

Table 2. Rf value and yield of turmeric extracts under different treatments

Variation	Rf Value	Yield (%)
Ethanol	0.64	5.5
Methanol	0.63	5.2
Isopropanol	0.68	5.0
n-Hexane	0.66	3.3
100 W	0.73	5.7
200 W	0.73	3.5
300 W	0.73	0.5
30 °C	0.82	6.6
40 °C	0.77	7.2
50 °C	0.79	7.8

Sunscreen activity and UV absorption properties

To evaluate the sunscreen potential of curcumin, the absorbance of a 100-ppm solution was measured across the 200–500 nm range using UV–Vis spectrophotometry. As shown in Figure 4, the extract exhibited strong absorbance between 320–420 nm, with a maximum peak at 421 nm as similar with previous research at 419 nm (Zarate et al, 2021). This corresponds to the UV-A region, indicating that curcumin is capable of absorbing harmful UV-A rays. The SPF value, calculated using the method by Mansur (1986), was 30.42, categorizing the extract as an ultra-protection sunscreen (Mokodompit et al., 2013).

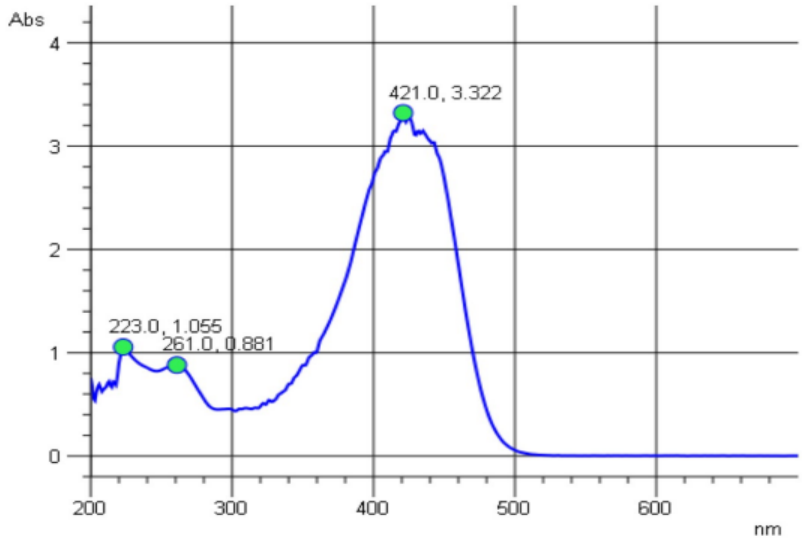


Figure 4. UV–Vis absorption spectrum of turmeric extract curcumin

Computational validation using TD-DFT

To support the spectrophotometric findings, computational modelling was conducted using geometry optimization and time-dependent density functional theory (TD-DFT). The optimized molecular structure is shown in Figure 5, while the simulated absorption spectrum is shown in Figure 6.

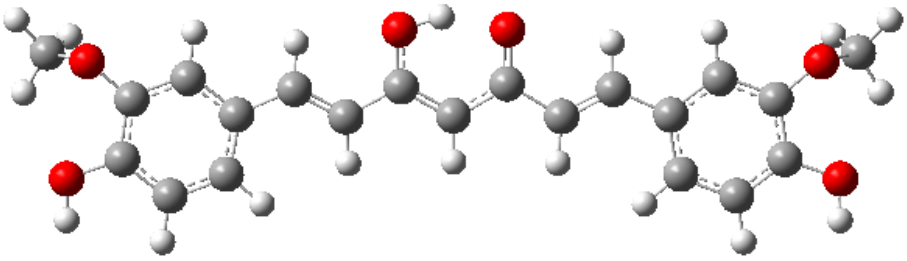


Figure 5. Optimized structure of curcumin

Table 3. HOMO–LUMO transitions of curcumin (Garino et al., 2016; Salmahaminati et al., 2023).

n.state	Energy (eV)	Wavelength (nm)	Oscillator Strength	Major Contributions
1	3.06	405	1.572	H–1 → LUMO (99%)
8	4.49	276	0.288	H–1 → L+1 (86%)

TD-DFT analysis revealed two main absorption peaks at 405 nm and 276 nm. The 405 nm peak corresponds to π→π* transitions involving the aromatic rings and β-diketone moiety, which aligns with UV-A absorption. The 276 nm peak is associated with transitions in the UV-B region, suggesting dual protection.

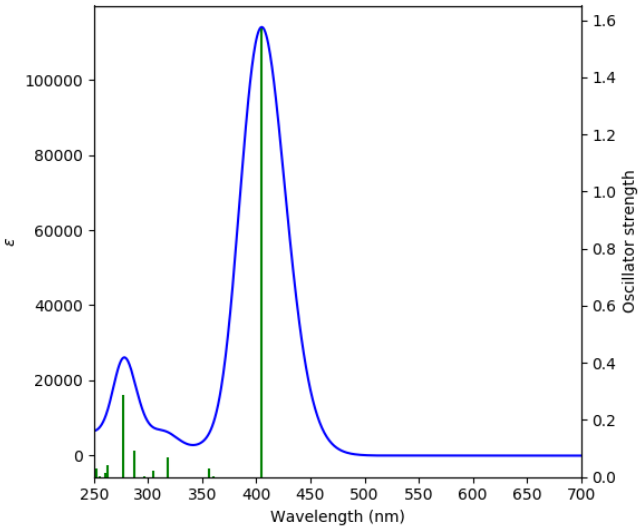


Figure 6. TD-DFT spectrum of curcumin.

These results are consistent with previous computational and experimental findings, including those by Shen and Ji (2006) and Gorman et al. (1994), which also reported strong UV-A/U-VB absorption capabilities for curcumin. From the TD-DFT analysis, it is evident that curcumin's structure contains unconjugated and conjugated chromophores, including aromatic rings, carbonyl groups, and C=C linkages, which contribute to its optical properties. The major transitions responsible for UV-A absorption were: H–1 → LUMO transition: involving benzene, C=O, and alkene π→π* transitions at 405 nm and for UV-B absorption were: H–1 → L+1 transition: benzene ring π→π* transition at approximately 276 nm (Theint et al., 2025; Van Nong et al., 2016; Wu et al., 2019).

Turmeric lotion formulation and physical properties

A lotion formulation containing the turmeric extract was developed. The product appeared orange in color, had a pH of 6.7, and a spread ability of 5 cm. These properties complied with the Indonesian National Standard SNI 16-4399-1996, which ensures safety and acceptability for topical use. The physical form of the lotion is shown in Figure 7.

Figure 7. Turmeric-based lotion formulation.

CONCLUSIONS

Curcumin extraction was successfully performed using the microwave-assisted extraction (MAE) method, which utilizes electromagnetic energy to enhance extraction efficiency. The optimal conditions were achieved using ethanol as the solvent, yielding 5.5%, due to its high polarity and compatibility with the curcumin molecule. The best microwave power was found to be 100 watts, resulting in a 5.7% yield. Higher power levels likely led to degradation of thermolabile

compounds and structural damage to plant tissues. The highest extraction yield, 7.8%, was obtained at a solvent temperature of 50 °C, where increased thermal energy enhanced cell permeability and solvent diffusion. UV–visible spectrophotometric analysis showed a maximum absorption peak at 421 nm, while computational modelling using density functional theory (DFT) predicted a similar absorption at 405 nm. These values correspond to π→π* electronic transitions in the chromophore groups of curcumin, particularly in the aromatic and conjugated carbonyl structures. These findings confirm that curcumin possesses strong UV-A-absorbing capabilities and demonstrates potential as a natural active ingredient in sunscreen formulations. However, this study has several limitations. The sunscreen efficacy was only evaluated through in vitro UV–Vis absorbance and computational modelling, without biological testing or skin compatibility assessments. The formulation was developed at the laboratory scale without long-term stability or sensory evaluations. Future research should focus on in vivo testing of curcumin-based sunscreen formulations, assessment of skin irritation potential, and incorporation of curcumin into advanced delivery systems such as nanoemulsions or liposomes to enhance bioavailability and photostability. In addition, further exploration of synergistic combinations with other natural UV-absorbing compounds may enhance the protective spectrum and formulation performance.

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