Research Article
Sciences of Phytochemistry

Phytochemical characterization of Marula (*Sclerocarya birrea*) ethanolic leaf extract: A Precursor for Green Corrosion Inhibitor Development

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Abstract: In the search for environmentally friendly corrosion inhibitors, medicinal plants rich in various phytochemicals present promising options due to their natural ability to adsorb onto metal surfaces, forming protective barriers against corrosive agents. This study examines the phytochemical profile of the ethanolic extract of *Sclerocarya birrea* using Fourier Transform Infrared Spectroscopy (FTIR), Ultraviolet-Visible (UV-Vis) spectroscopy, and Gas Chromatography-Mass Spectrometry (GC-MS). The UV-Vis spectrum displayed distinct absorption peaks characteristic of the extract's components. FTIR analysis confirmed the presence of functional groups associated with alkanes, alkenes, phenols, amines, aromatics, esters, ketones, and aldehydes. GC-MS detected 17 phytochemical compounds, including notable components such as γ-sitosterol (39.44%), l-(+)-ascorbic acid 2,6-dihexadecanoate (17.37%), pagicerine (14.66%), hexadecanoic acid derivatives (10.45%), octadecanoic acid (4.34%), and phytol (3.46%). These compounds are known for their medicinal properties and chemical structures that support effective corrosion inhibition. The phytochemicals primarily contribute to corrosion protection by adsorbing onto metal surfaces, creating protective films that impede both anodic and cathodic reactions, thus reducing metal dissolution and increasing resistance. The detailed phytochemical analysis provides a solid basis for further research into *S. birrea* as a sustainable and effective corrosion inhibitor for various metals in different corrosive environments. This work emphasizes the extract's potential as an environmentally friendly alternative to traditional synthetic inhibitors.

Introduction

In recent years, medicinal plants have gained prominence in the field of green corrosion inhibition of metallic materials in various aggressive environments. Green inhibitors are increasingly favored over synthetic alternatives due to their environmental friendliness, biodegradability, and cost-effectiveness, which mitigate issues related to the toxicity and persistence of synthetic compounds (1). Plant extracts are rich in phytochemicals containing functional groups and heteroatoms that adsorb on metal surfaces, forming protective barriers that hinder corrosion (2). The plant leaf extracts have proven to be one of the most effective components, with various studies reporting high inhibition efficiencies in a range of corrosive environments.

Leaves represent the wealthiest part of plants in organic compounds, as they are the primary site of synthesis via photosynthesis, producing a diverse array of bioactive molecules (3). They are also widely available and easily accessible, which ensures a consistent and sustainable supply for inhibitor production. Leaves dry quickly, are easily ground into a fine powder, and yield reproducible extracts with high surface-active phytochemicals. Moreover, leaves are often abundant in active constituents, including tannin, polyphenol, flavonoid, and alkaloid compounds, well recognized for their affinity to adsorb onto metal surfaces, thereby forming protective film barriers that effectively inhibit corrosion.

For a plant leaf extract to be considered a corrosion inhibitor, it must be characterized to confirm the presence of heteroatoms, polar functional groups, aromatic rings, and other relevant phytochemicals known to interact with metals (4). While the presence of these compounds suggests inhibitory potential, further research is necessary to elucidate their mechanistic roles from kinetic and thermodynamic perspectives. Medicinal plant leaf extracts have recently attracted substantial interest for their potential application as a protective coating for metallic surfaces in various settings. These recently studied plant leaves for corrosion inhibition include the following: *Arbutus unedo* (5), *Falcaria vulgaris* (6), *Terminalia arjuna* (7), *Acanthopanax senticosus* (8), *Artabotrytis odoratissimus*

(9), and *Dalbergia odorifera* (10).

The native *Sclerocarya birrea* is also referred to as the marula tree, which is a drought-resistant species widely distributed in Africa, but mostly in sub-Saharan Africa (11). It is known to be a particularly salt-tolerant tree that may exceed 18 meters in height, featuring a trunk diameter of 120 cm, grey bark, and secondary roots that potentially span 30 meters. Marula trees grow well in sandy, stony, or sandy loam soils with yearly precipitation ranging from 200 to 1370 mm (12). Marula is a versatile tree because of its nutritional value extracted from the fruit, cosmetic oil from the seed, which includes high fat, citric acid, protein, malic acid, phosphorus, and zinc, among others, and therapeutic value from the bark and leaves (13).

Numerous studies have focused on the critical components of marula trees that contribute to their therapeutic effects (14). *S. birrea* has been extensively studied for its anti-diabetic, anti-inflammatory, analgesic, antiparasitic, antibacterial, and antihypertensive effects (15). This led to the analysis of the phytochemical substances present in the various parts of the tree, depending on which portion of the tree is of interest at the time, as phytochemicals are typically thought to have therapeutic properties that can bring healing (16). There are polyphenols, tannins, flavonoids, alkaloids, anthocyanins, and substantial quantities of saponosides. Quercetin and its derivatives also contain tannins (mostly procyanidins), triterpenoids, polyphenols, phytosterols, organic acids (gallic and quinic), and other flavonoids (17), which have been reported in various literature to aid in corrosion inhibition.

Despite the documented phytochemical richness and medicinal applications of *S. birrea*, its leaf extract remains underexplored in terms of phytochemical characterization relevant to corrosion inhibition. This study addresses this gap by analyzing ethanol-extracted *S. birrea* leaves using Fourier Transform Infrared Spectroscopy (FTIR), Ultraviolet-Visible (UV-Vis) spectroscopy, and Gas Chromatography-Mass Spectrometry (GC-MS) to identify functional groups and bioactive constituents. By elucidating the phytochemical profile, this work aims to establish the potential of *S. birrea* as a sustainable and effective green corrosion inhibitor, providing a foundation for future corrosion control applications.

Experimental Section

Preparation of Plant Leaf Extract

S. birrea leaves were collected near the Department of Engineering at Botswana International University of Science and Technology (BIUST), Botswana, and authenticated by a BIUST botanist. Mature, healthy leaves were selected, washed 2–3 times to remove impurities, and shade-dried naturally at ambient temperature for 10 days to preserve heat-sensitive phytochemicals. The dried leaves were milled using a hammer mill and ground to a fine powder to enhance ethanol penetration during extraction.

Extraction was performed by maceration, with 500 g of leaf powder soaked in 2500 mL of analytical-grade (95%) ethanol (solvent-to-sample ratio 5:1) for 72 h under periodic agitation. The solvent-to-sample ratio of 5:1 (2500 mL of ethanol to 500 g of powdered leaves) was selected based on preliminary optimization trials, which indicated that this ratio ensured the efficient solubilization of phytochemicals while preventing solvent saturation. Ratios significantly lower than this led to incomplete extraction, while higher ratios did not yield additional phytochemical benefits but unnecessarily increased solvent use. This ratio was chosen based on preliminary trials and relevant literature to ensure efficient phytochemical extraction while maintaining solvent economy (18, 19). The mixture was filtered using Whatman No. 1 filter paper over 24 h to obtain a homogeneous solution. This was then concentrated via rotary evaporation at 40 °C and 100 rpm to yield a thick slurry. The extract was stored at 4 °C in an airtight container before subsequent analyses. A summary of the *S. birrea* ethanol extract preparation is displayed in **Figure 1** below.

Fourier Transform Infrared spectroscopy (FTIR) Analysis

The *S. birrea* ethanolic extract and powdered leaf samples were analyzed using a Bruker Vortex 70 V vacuum FTIR spectrometer (Bruker, China) to identify and characterize functional groups. Samples were placed directly into the FTIR sample holder, and spectra were acquired in transmittance mode over the range of 4000 to 400 cm^{-1} at room temperature (27 °C). The spectral resolution was set to 4 cm^{-1}, and each spectrum was averaged over 32 scans to

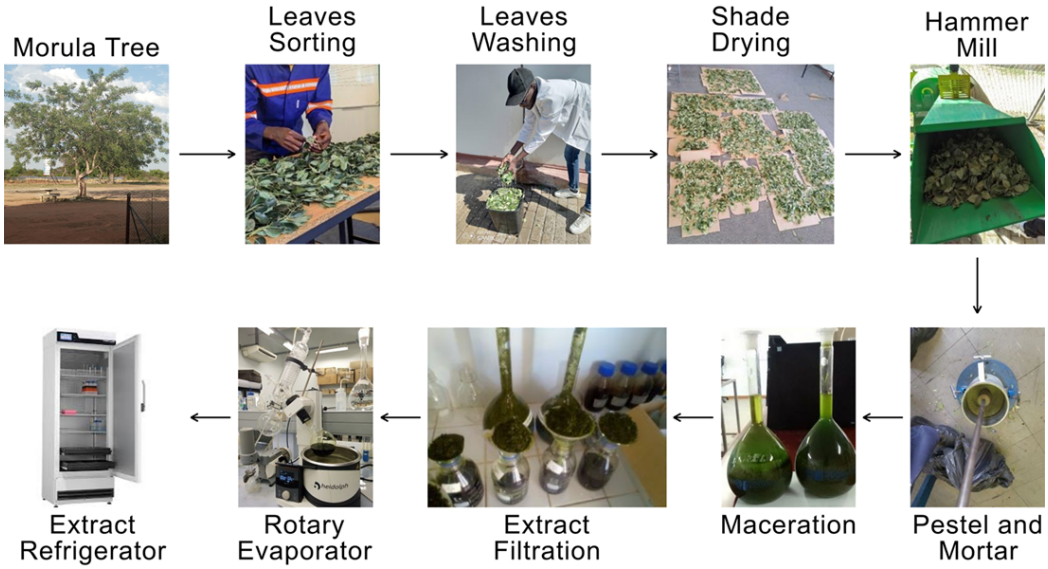

Figure 1.*Sclerocarya birrea* extract preparation.

enhance signal quality. Characteristic functional groups were assigned based on distinct absorption peaks in the recorded spectra.

Ultra-Violet Visible Spectroscopy (UV-Vis) Analysis

Ultraviolet-visible (UV-Vis) spectroscopy analysis of the *S. birrea* ethanolic extract was performed using a PerkinElmer Lambda 75 double-beam spectrophotometer (PerkinElmer, USA) to identify characteristic chromophoric groups indicative of phytochemicals. Spectra were recorded at room temperature over the wavelength range of 200 to 800 nm, using quartz cuvettes with a 1 cm path length. Ethanol was employed as a blank reference to correct for solvent absorbance. The spectral bandwidth was set at 1 nm, with a scanning speed of 400 nm/min, ensuring accurate detection of absorption peaks. Interpretation of the spectra involved examining characteristic absorption bands and comparing them against standard reference spectra and literature data to confirm the presence of functional groups such as phenols, flavonoids, and other bioactive compounds relevant to corrosion inhibition.

Gas Chromatography – Mass Spectroscopy (GC-MS) Analysis

The phytochemical profile of the *S. birrea* ethanolic extract was analyzed using a Shimadzu GC-MS-QP2010 Ultra system (Shimadzu, Japan) equipped with a fused silica capillary column (30 m × 0.25 mm internal diameter × 0.25 µm film thickness. Helium served as the carrier gas at a constant flow rate of 1.0 mL/min. A 1 µL sample was injected in splitless mode with the injector temperature set at 250 °C. The oven temperature program started at 70 °C (held for 1 minute), ramped at 10 °C/min to 200 °C (held isothermal for 1 minute), then increased at 10 °C/min to 250 °C. The interface temperature was maintained at 250 °C (20).). Mass spectra of the compounds were taken by electron ionization at 70eV. The experimental steps were examined within the 40–600 m/z range at intervals of 0.5 s. To ensure the reliability of the results, blank runs using pure ethanol were performed before sample analysis to account for any background signals or contaminants originating from the solvent or instrument. The chromatogram data were analyzed and cross-referenced with the Wiley Spectral library search engines.

Results and Discussion

The ethanolic leaf extract was analyzed using GC-MS, FTIR, and UV-Vis to determine the phytochemical compounds, organic compounds, and functional groups present that aid in inhibiting metal corrosion in corrosive media.

FTIR Analysis

The FTIR spectra analysis revealed distinct characteristic peak values of different functional groups found in ethanolic *S. birrea* leaf extract (**Figure 2**). Furthermore, the functional groups were detected at other bands and are attributed to phytochemical compounds, such as tannins, saponins, alkaloids, anthraquinones, and flavonoids, that are found in this noble tree leaf.

Meanwhile, **Table 1** below displays a range of distinct peaks at specific wavenumbers. These peaks correspond to vibrational modes associated with different functional groups, providing insight into the molecular composition of the extract. The most prominent peaks are 3851, 3748, 1693, 1044, and 673 cm^{-1}, which indicate O-H stretching vibrations and the presence of alcohols or phenols.

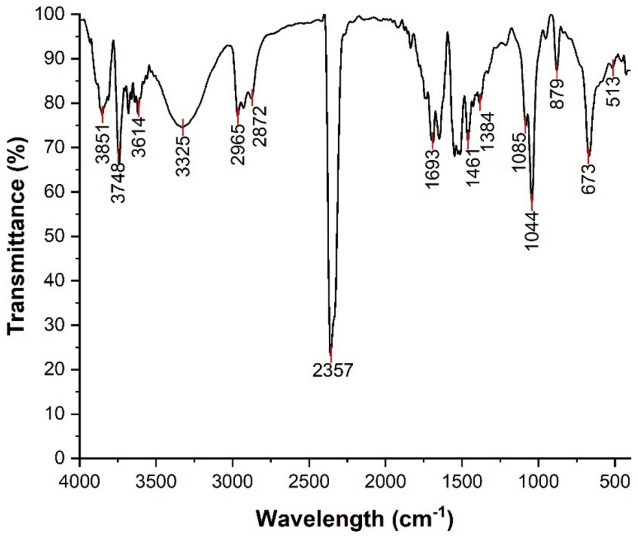

Figure 2. FTIR Spectrum for ethanolic extract of Sclerocarya birrea.

Table 1. FTIR peak values and functional groups derived from *Sclerocarya birrea* ethanolic extract.

No.	Bond	Functional Group	Peak value
1.	O-H	Alcohol	3851
2.	COOH	Carboxylic acid	3748
3.	C-H	Aromatic	3614
4.	N-H	Primary amine	3325
5.	C-H	alkane	2965
6.	C-H	aldehydes or ketones	2872
7.	C≡C	Amine	2357
8.	C=O	Ketone	1693
9.	C-H	Alkane	1461
10.	C=C	Alkene	1384
11.	C-O	Ester	1085
12.	C-H	Out-of-plane bend in aromatic compounds.	1044
13.	C-Cl	Alkyl chlorides	879
14.	C-Br	Alkyl bromides	673
15.	C-I	Alkyl iodides	513
16.	C-O	Ether	496

Prominent peaks observed at 3851 and 3748 cm^{-1} are attributed to O–H stretching vibrations, indicating the presence of alcohols and phenolic compounds, which are known for their antioxidant and corrosion-preventive properties. Aliphatic C–H stretching vibrations at 2965 and 1461 cm^{-1} suggest alkane structures within the extract. The strong carbonyl stretching peak at 1693 cm^{-1} corresponds to aldehydes, ketones, or esters, while the band at 1384 cm^{-1} indicates C=C double bonds characteristic of alkenes. The presence of amines or amides is suggested by C–N stretching vibrations near 3325 cm^{-1}, and aromatic compounds are supported by benzene ring bending at 1044 cm^{-1}.

Notably, peaks assigned to halogenated functional

groups (C–Cl at 879 cm^{-1}, C–Br at 673 cm^{-1}, and C–I at 5130 cm^{-1}) were detected. Given the natural origin of the extract and the absence of halogenated solvents during extraction, these signals likely stem from trace laboratory contamination or environmental sources rather than inherent chemical constituents.

Overall, these results reveal a diverse range of functional groups, offering a comprehensive understanding of the chemical composition of *S. birrea* leaf extract. Alcohols, phenols, alkanes, alkynes, carbonyls, alkenes, amines or amides, and aromatic chemicals have all been identified to contribute to the extract's complexity (21). Phenolic compounds are renowned for their corrosion-prevention capabilities (22) and have been discovered to be present in the *S. birrea* extract based on the O-H stretching vibrations observed in the FTIR spectrum. These compounds have the potential to absorb onto the metallic surface and generate a thin-film coating, inhibiting the oxidation-reduction process and shielding the metal, therefore impeding corrosion processes (23, 24). Furthermore, phenols contain heteroatoms (nitrogen, oxygen, sulphur, and so on) that protonate in solutions, donating lone electron pairs, double or triple bonds, and planar conjugated systems with various aromatic cycles in their structures, and that contribute to their effectiveness as corrosion inhibitors (25).

UV-Vis Analysis

UV-Vis spectroscopy was used to detect and identify the phytoconstituent profile of *S. birrea* extract, as shown in the spectrum above (**Figure 3**). This analysis was conducted to identify compounds containing σ bonds, π bonds, lone pairs of electrons, chromophores, and aromatic rings, all of which are known to contribute significantly to corrosion inhibition due to their electronic and structural properties. The presence of such features suggests the potential of the extract to adsorb onto the metal surface, thereby forming a protective barrier that mitigates the corrosive interaction between the metal and its environment (26). The spectral range was set between 200 and 800 nm to achieve distinct peak sharpness and a clear, stable baseline necessary for precise interpretation. However, the UV-Vis spectrum of the ethanolic extract of *S. birrea*, as detailed in **Table 2**, exhibits absorption within the wavelength range of 209–679 nm.

The absorption peaks observed in the 200–400 nm region indicate the presence of unsaturated moieties and

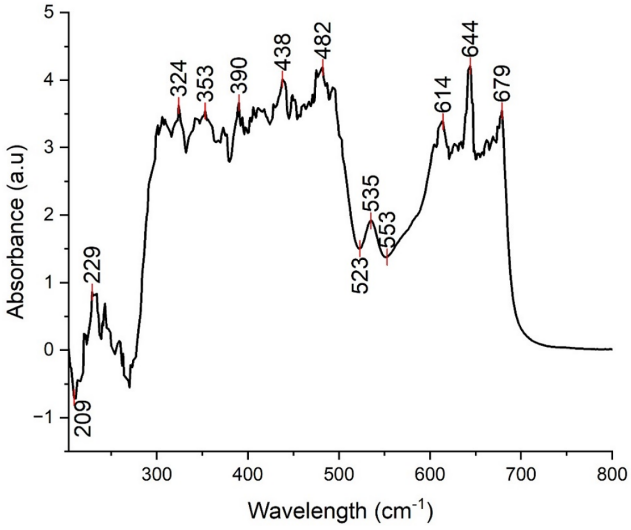

Figure 3. UV-Vis Spectrum of ethanolic extract of *Sclerocarya birrea*.

Table 2. *Sclerocarya birrea* ethanolic extract UV-Vis profile indicating the observed absorption wavelengths and corresponding peak absorbance.

No	Wavelength (nm)	Absorbance (a.u)
1.	209	0.001399654
2.	229	0.311306404
3.	239	0.180704354
4.	270	0.063772838
5.	307	0.835008062
6.	324	0.876372136
7.	353	0.864873572
8.	381	0.721332439
9.	390	0.883084852
10.	402	0.753459239
11.	425	0.833893528
12.	438	0.952784449
13.	482	0.994375441
14.	523	0.452774494
15.	535	0.531942979
16.	552	0.432929827
17.	614	0.830348781
18.	621	0.720826868
19.	644	0.995859163
20.	679	0.860618401

heteroatoms, such as sulfur, nitrogen, and oxygen, which are typically involved in π-π and n-π electronic transitions (27). Prominent bands at 229–324 nm correspond to π-π* transitions in conjugated double bonds and aromatic rings, while absorptions at 353–425 nm are attributed to n-π* transitions associated with carbonyl and hydroxyl-containing chromophores. Peaks between 239 and 679 nm in the spectrum profile indicate the presence of phenolic chemicals and alkaloids (28). The π-π* transitions facilitate electron donation from delocalized π-electron systems of aromatic rings to vacant d-orbitals of the metal surface, promoting chemisorption (29,30). Similarly, n-π* transitions reflect the role of lone-pair electrons on heteroatoms (O, N) in coordinating with metal centers, thereby strengthening surface interactions (31). Thus, the observed spectral profile not only confirms the complex phytochemical composition of the extract but also directly supports its potential to form protective films on metallic substrates through electronic transitions that enable adsorption and surface passivation.

GC-MS Analysis

The GC-MS analysis of an ethanolic extract of *S. birrea* was conducted over 60 60-minute run time, with a 5-minute delay to identify the volatile and semi-volatile phytochemical constituents (32). Mass spectrum of the phytochemical compounds detected in the leaf extract is displayed in Supplementary **Figure 1**. The components that have been found and the peak percentages that correspond to them are Dodecane (3.22 %), Nonadecane (3.09 %), Benzenaminium, 4-carboxy-N,N,N-trimethyl-, hydroxide, inner salt (1.84 %), Ethanol, 2-(octadecyloxy) (1.25 %), 3,7,11,15-Tetramethyl-2-hexadecen-1-ol (2.01 %), Lupan-3-ol, acetate (1.63 %), l-(+)-Ascorbic acid 2,6-dihexadecanoate (17.37%), Hexadecanoic

acid, ethyl ester(10.34%), 1-Cyclopenten-3-one, 1-(1-cyclohexen-1-yl)-2-[(carboxyethyl)(cyano)methyl] (1.65 %), Phytol (3.46 %), β-N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl-boronate-3,8-di(trimethylsilyl) (9.18 %), Octadecanoic acid (4.34 %), Octadecanoic acid, ethyl ester(1.84 %), γ-Sitosterol (39.44 %), Pagicerine (14.66 %), 9,19-Cyclolanostane-3,7-diol, Hexadecanoic acid (10.45 %), 1-(hydroxymethyl)-1,2-ethanediyl ester (11.76 %).

The *S. birrea* ethanolic extract yielded 17 phytochemical compounds at varied retention durations, which are given in **Supplementary Table 1**. All these compounds were adequately characterized and identified after comparing their mass spectra to those in the main library. The spectral fingerprints of the compounds were cross-referenced with those found in the National Institute of Standards and Technology (NIST) and the Wiley 9.0 databases to ensure accurate identification. Additionally included were the molecular weight, molecular structure, retention time (RT), and percentage peak area of the active phytoconstituents.

Twelve of the seventeen phytochemical compounds identified in *S. birrea* leaf extract have been previously characterized for their corrosion inhibition properties. Notably, 3,7,11,15-tetramethyl-2-hexadecen-1-ol, a significant constituent, is known to form stable protective films on metal surfaces, effectively inhibiting mild steel corrosion through mixed-type inhibition with predominant anodic effects (33). Similarly, octadecanoic acid (stearic acid) and its derivatives, found in significant amounts in the extract, are well documented to reduce corrosion rates by forming chemisorbed protective layers on various metals (34). Hexadecanoic acid ethyl ester and l-(+)-ascorbic acid 2,6-dihexadecanoate also contribute to metal surface passivation, enhancing corrosion resistance by their adsorption behavior (35, 36).

Other compounds, such as phytol and pagicerine, though less commonly studied in corrosion contexts, may play supplementary roles due to their chemical structures conducive to surface adsorption and film formation (37). These phytochemicals act synergistically by adsorbing to metal surfaces and forming protective barriers that inhibit anodic dissolution and cathodic reactions, resulting in improved corrosion resistance. A comprehensive, detailed discussion of each compound's specific literature and mechanism has been moved to the supplementary section to maintain focus and clarity in this main discussion. The biological activity of the detected compounds in *S. birrea* has also been reported in **Supplementary Table 2**.

Conclusions

This study demonstrates that *S. birrea* ethanolic leaf extract contains a diverse phytochemical profile characterized by key functional groups and bioactive compounds, such as phytol, octadecanoic acid, pagicerine, and γ-sitosterol, which collectively suggest strong potential as a green corrosion inhibitor. The abundance of oxygen- and nitrogen-containing groups, together with antioxidant and metal-coordinating compounds, underscores the extract's potential to adsorb on metal surfaces and retard both anodic and cathodic reactions. These findings highlight the promise of *S. birrea* as an eco-friendly, plant-based alternative for sustainable corrosion protection. Further research assessing its inhibition efficiency under various environmental conditions, using electrochemical and surface analysis techniques, is warranted to confirm its practical applicability.

Abbreviations

FTIR= Fourier Transform Infrared Spectroscopy; UV-Vis= Ultraviolet-visible spectroscopy; GC-MS= Gas Chromatography Mass Spectroscopy; BIUST= Botswana International University of Science and Technology.

Declarations

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Conflict of Interest

The authors declare no conflicting interest.

Data Availability

The unpublished data is available upon request to the corresponding author.

Ethics Statement

Not applicable.

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Supplemental Material

Supplementary data associated with this article can be found in the online version at https://etflin.com/file/document/20250826053009326237802.docx

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Additional Information

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