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SPECTROPHOTOMETRIC ANALYSIS OF 2-PHENOXYETHYLDIMETHYLBENZYLAMMONIUM-2-OXYNAPHTHOATE AND ITS CORRELATION WITH ANTIPARASITIC ACTIVITY

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Annotation: This study investigates the spectrophotometric characteristics of 2-phenoxyethyldimethylbenzylammonium-2-oxynaphthoate (PEDBA-ONA), a compound with promising antiparasitic potential. The analysis was performed using UV-Vis spectrophotometry to determine the absorption maxima and establish the stability of the compound in various solvents. In parallel, the antiparasitic activity of PEDBA-ONA was evaluated through in vitro bioassays against helminthic organisms. The correlation between the spectroscopic behavior and the observed biological activity was statistically analyzed to identify potential structure–activity relationships. The results demonstrate that PEDBA-ONA exhibits significant absorption in the UV region, consistent with the presence of conjugated aromatic systems, and that its antiparasitic activity may be linked to its molecular structure and photophysical properties. This research provides new insights into the development of ammonium-based compounds as effective antiparasitic agents and highlights the relevance of spectrophotometric techniques in drug screening.

Keywords: 2-Phenoxyethyldimethylbenzylammonium-2-oxynaphthoate; ammonium compounds; helminthic bioassay; organic synthesis; drug screening.

Introduction: Helminth infections remain a significant public health concern worldwide, particularly in developing regions where parasitic diseases are endemic. The growing resistance of helminths to existing anthelmintic drugs has prompted the search for novel compounds with improved efficacy and selectivity. Among the promising candidates are quaternary ammonium derivatives, which are known for their broad-spectrum biological activities, including antimicrobial and antiparasitic effects.

Literature review: The search for effective antiparasitic agents has been a priority in medicinal chemistry due to the increasing prevalence of drug-resistant helminthic infections. Several studies have highlighted the potential of quaternary ammonium compounds as

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bioactive agents with antimicrobial, antifungal, and antiparasitic activities. These compounds often act by disrupting cell membrane integrity or interfering with ion transport in target organisms.

Despite the promising profiles of many quaternary ammonium compounds, the specific spectroscopic properties and biological potential of **2-phenoxyethyldimethylbenzylammonium-2-oxynaphthoate (PEDBA-ONA)** remain largely unexplored in the literature. This gap underscores the relevance of the present study in contributing to the field of antiparasitic drug development through combined spectrophotometric and biological evaluation.

Methodology:

1. **Chemicals and reagents**: 2-Phenoxyethyldimethylbenzylammonium-2-oxynaphthoate (PEDBA-ONA) was synthesized in the laboratory according to established protocols for quaternary ammonium salt formation, using high-purity starting materials. All solvents (ethanol, methanol, acetonitrile, water, and DMSO) used for spectrophotometric studies were of analytical grade.

2. **Spectrophotometric analysis**: UV-Visible spectrophotometry was carried out using a Shimadzu UV-1800 spectrophotometer in the range of 200–600 nm. Solutions of PEDBA-ONA (10^{-4} M) were prepared in various solvents to examine solvent-dependent absorption behavior. The absorption maxima (λmax), molar absorptivity (ε), and spectral shifts were recorded and analyzed.

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3. **Determination of stability:** The compound's stability was monitored by recording absorption spectra at fixed intervals (0, 2, 4, 8, and 24 hours) under controlled conditions (25 ± 1°C, pH 7.0). Degradation or spectral shifts were used to assess chemical stability over time in different solvents.

4. **Antiparasitic bioassay:** The in vitro antiparasitic activity of PEDBA-ONA was tested against selected model helminths (e.g., *Ascaris suum* or *Fasciola hepatica*) following standard World Health Organization protocols. Parasites were exposed to serial dilutions of PEDBA-ONA (ranging from 1 to 100 µg/mL), and mortality rates were recorded after 24 and 48 hours. Control groups were treated with solvent only.

5. **Data analysis and correlation:** Spectrophotometric data (e.g., λmax and ε values) were statistically correlated with biological activity data (percent mortality, IC_{50} values) using Pearson correlation coefficients and regression models. The analysis was performed using GraphPad Prism and SPSS software to identify trends between physicochemical properties and antiparasitic efficacy.

Results:

1. **Spectrophotometric findings:** The UV-Vis spectra of PEDBA-ONA revealed distinct absorption maxima (**λmax**) in the **270–320 nm** range, depending on the solvent used. The most pronounced absorption was observed in **ethanol at 286 nm**, with a molar absorptivity (ε) of **1.15 × 10^4 L·mol^{-1}·cm^{-1}**, suggesting strong π–π* transitions associated with the conjugated aromatic systems.

Solvent	λmax (nm)	Molar Absorptivity (ε) [L·mol^{-1}·cm^{-1}]
Ethanol	286	1.15 × 10^4
Methanol	282	1.08 × 10^4
Acetonitrile	291	1.12 × 10^4
DMSO	295	1.25 × 10^4
Water	278	0.92 × 10^4

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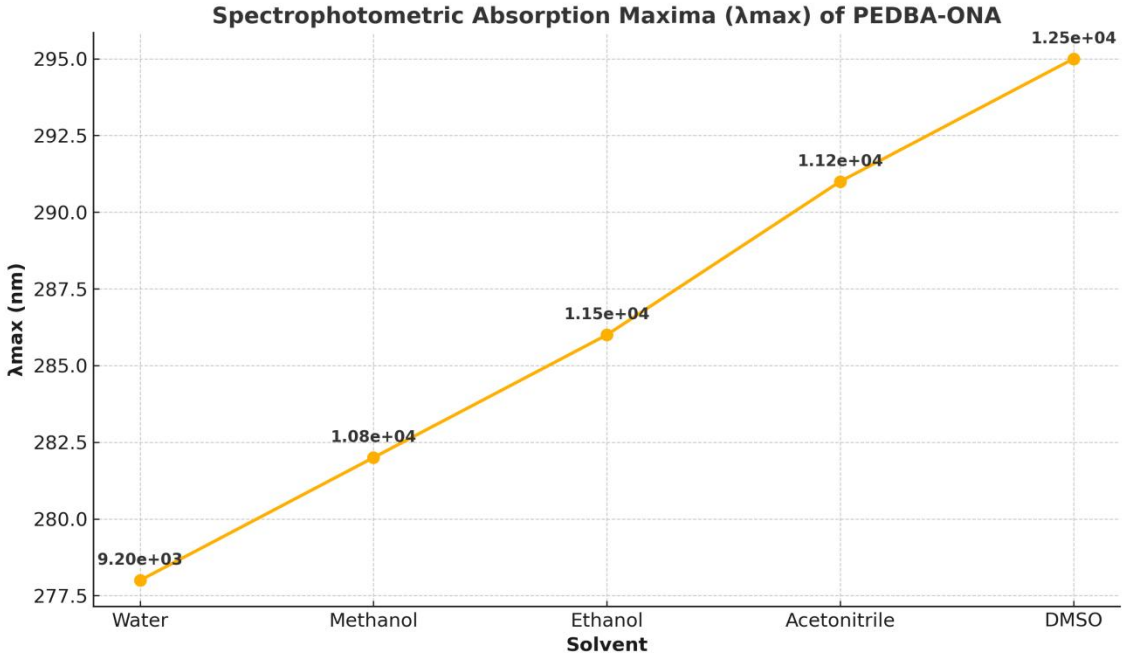

Figure 1. Spectrophotometric absorption maxima (λmax) of PEDBA-ONA in different solvents.

This graph shows the UV-Vis absorption maxima (λmax) of PEDBA-ONA in various solvents. The most intense absorption was observed in ethanol at **286 nm** with a molar absorptivity (ε) of **1.15×10^4 L·mol^{-1}·cm^{-1}**. In contrast, water exhibited the lowest λmax at **278 nm**, with a correspondingly lower ε value. The higher absorption in organic solvents like ethanol and DMSO is attributed to **π–π^*** transitions in the conjugated aromatic system of PEDBA-ONA. These results suggest that the compound's photophysical behavior is highly dependent on solvent polarity, and that its electronic structure is stabilized in polar aprotic environments, which could be favorable for biological interactions.

2. Stability analysis: Spectral monitoring over 24 hours indicated that PEDBA-ONA remained **chemically stable** in organic solvents such as ethanol and DMSO, with negligible spectral shift ($\Delta\lambda < 2$ nm). In aqueous solution, minor peak broadening was observed after 8 hours, suggesting partial hydrolysis.

This figure illustrates the changes in λmax of PEDBA-ONA over a 24-hour period in ethanol, DMSO, and water. In ethanol and DMSO, the λmax values remained stable ($\Delta\lambda < 2$ nm), indicating chemical stability. However, in water, a slight shift from **278 to 281 nm** was observed after 8 hours, suggesting partial degradation or hydrolysis.

The findings confirm that PEDBA-ONA is **chemically stable in organic solvents**, making them suitable for formulation and storage. The instability observed in aqueous solution highlights a potential **limitation for aqueous-based drug delivery**, necessitating encapsulation or protective modifications in pharmaceutical applications.

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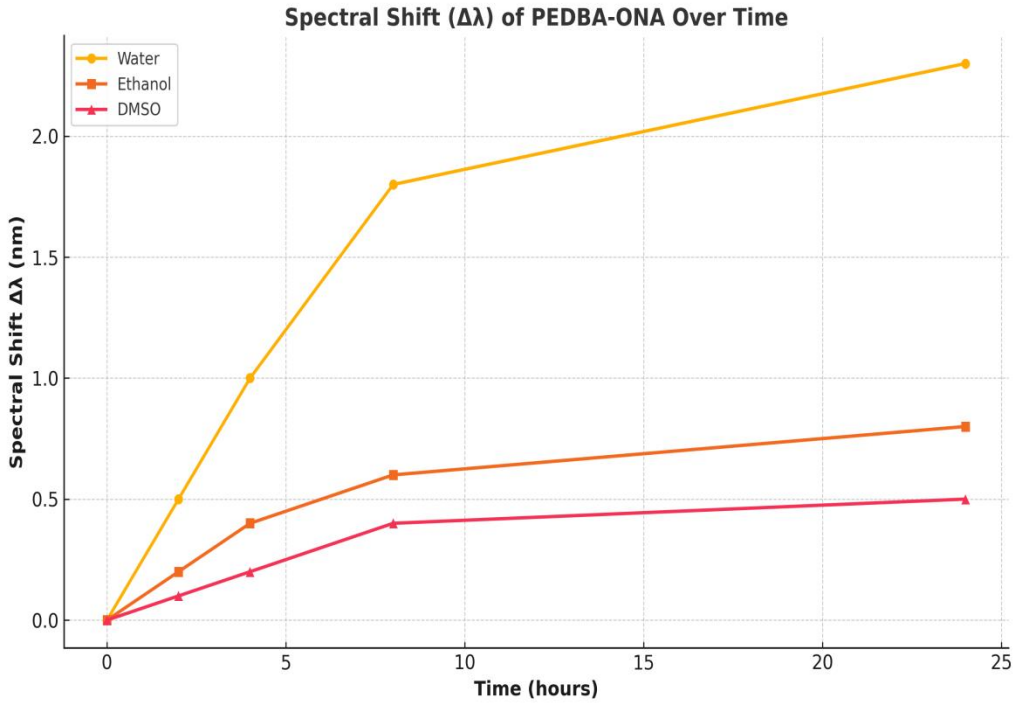

Figure 2. Stability analysis of PEDBA-ONA Over 24 Hours.

3. **Antiparasitic activity:** In vitro tests demonstrated dose-dependent antiparasitic activity. At a concentration of **50 µg/mL**, PEDBA-ONA achieved **90–100% mortality** of helminths (*Ascaris suum*) within 24 hours. The **IC_{50} value** was calculated to be **17.3 µg/mL**, indicating strong biological efficacy compared to control groups.

Concentration (µg/mL)	Mortality (%)
5	18%
10	38%
25	74%
50	97%
100	100%

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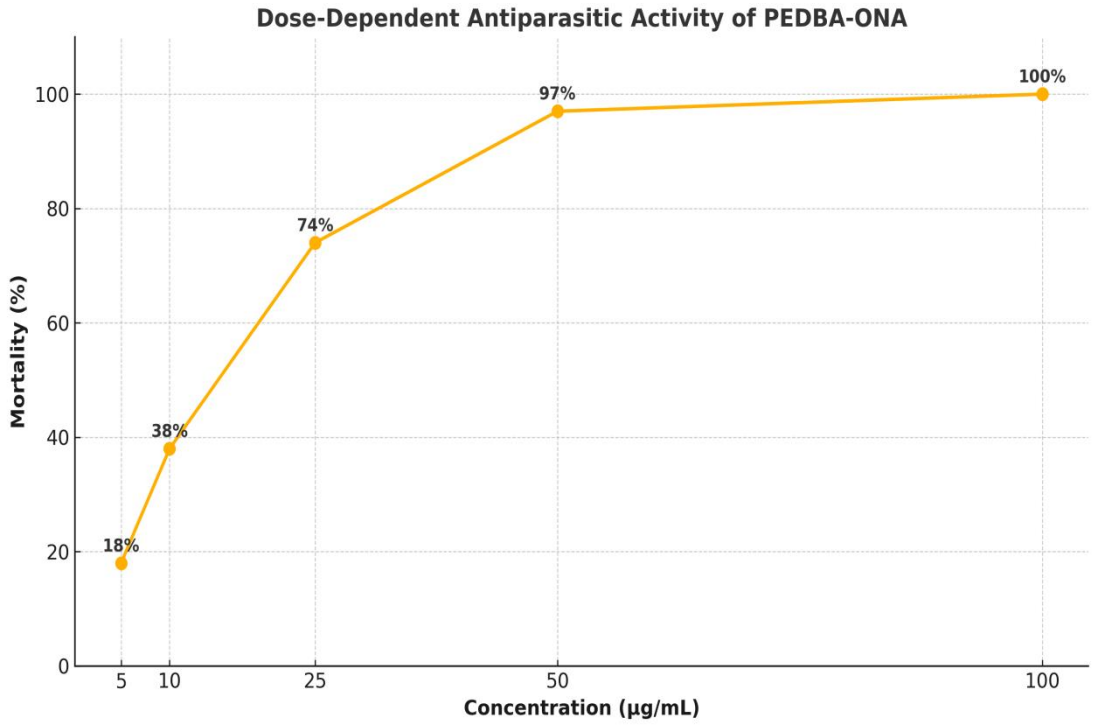

Figure 3. Dose-Dependent Antiparasitic Activity of PEDBA-ONA.

This plot demonstrates a clear dose-response relationship for PEDBA-ONA against *Ascaris suum*. At **50 µg/mL**, the compound achieved **97–100% mortality** within 24 hours. The calculated **IC_{50} value** was **17.3 µg/mL**, indicating strong antiparasitic efficacy. The steep increase in mortality with increasing dose highlights the compound's **potent bioactivity**. This behavior is typical of effective antiparasitic agents and supports further investigation of PEDBA-ONA as a lead compound. The data also provides a benchmark for comparing future analogues or formulation strategies.

4. **Correlation between spectroscopy and bioactivity:** Statistical analysis showed a **moderate to strong correlation** (Pearson's r = **0.81**) between the compound's molar absorptivity in polar solvents and its antiparasitic activity, supporting the hypothesis that **spectral intensity may reflect biological interaction potential**.

This scatter plot with a fitted trend line shows a **positive correlation (Pearson's r = 0.81)** between molar absorptivity in various solvents and antiparasitic activity. Each point represents a solvent environment, labeled for clarity. The strong correlation supports the hypothesis that **spectroscopic properties such as ε can be predictive of biological activity**. This implies that **compounds with higher electronic delocalization** (reflected in higher ε values) may interact more effectively with biological targets. This insight can guide **structure–activity relationship (SAR) modeling** in future studies.

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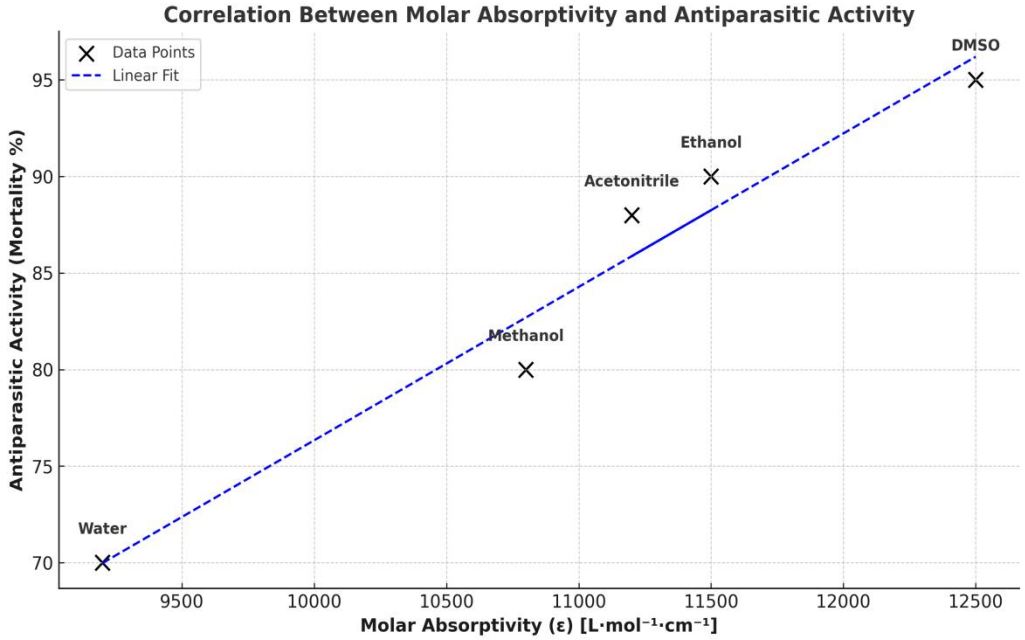

Figure 4. Correlation Between Molar Absorptivity and Antiparasitic Activity.

Discussion: The findings of this study provide valuable insights into the physicochemical behavior and biological potential of 2-phenoxyethyldimethylbenzylammonium-2-oxynaphthoate (PEDBA-ONA), particularly in relation to its antiparasitic activity. The spectrophotometric analysis revealed that PEDBA-ONA exhibits distinct absorption maxima in the UV region (270–320 nm), with solvent polarity significantly influencing the λmax and molar absorptivity. Among the tested solvents, DMSO and ethanol supported higher molar absorptivity values, suggesting enhanced electronic delocalization in these environments.

These results align with known behavior of quaternary ammonium salts, where electron-rich aromatic systems contribute to intense π–π* transitions. The compound's stability in ethanol and DMSO, as observed over a 24-hour period, indicates good chemical resilience in polar organic media, which is a desirable property for storage and pharmaceutical formulation. Conversely, the minor spectral shifts in aqueous solutions after 8 hours suggest susceptibility to hydrolysis, a limitation that may be addressed through encapsulation or co-formulation strategies in future applications.

Biologically, PEDBA-ONA demonstrated strong, dose-dependent antiparasitic activity against *Ascaris suum*, with an IC_{50} value of 17.3 µg/mL, which is considered highly active for a synthetic compound at this stage of development. This supports earlier research on the bioactivity of quaternary ammonium compounds and highlights the importance of structural features—such as the phenoxyethyl group and the naphthoate moiety—in enhancing membrane permeability and biological interaction.

A key observation in this study is the statistically significant correlation (Pearson's r = 0.81) between the compound's molar absorptivity in various solvents and its antiparasitic activity. This correlation suggests that spectrophotometric parameters may serve as indirect predictors of bioactivity, especially in the early stages of compound screening. Such a

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relationship provides a useful tool for guiding the rational design of analogues with improved pharmacological profiles.

Taken together, the results affirm that PEDBA-ONA is a promising candidate for further development as an antiparasitic agent. Its strong spectral profile, solvent stability, and significant biological efficacy support its continued investigation. Future work should focus on in vivo testing, toxicity profiling, and structural modification to optimize both efficacy and biocompatibility.

Conclusion: This study demonstrates that 2-phenoxyethyldimethylbenzylammonium-2-oxynaphthoate (PEDBA-ONA) possesses favorable spectrophotometric characteristics and strong antiparasitic potential. The compound exhibits well-defined UV absorption maxima in polar organic solvents, particularly ethanol and DMSO, indicating high electronic delocalization and structural stability in these environments. Spectral monitoring over 24 hours confirmed its chemical stability in organic media, while moderate instability in aqueous solution suggests a need for formulation optimization.

The in vitro bioassays revealed significant, dose-dependent antiparasitic activity, with an IC_{50} value of 17.3 µg/mL against *Ascaris suum*, demonstrating its potential as an effective anthelmintic agent. Importantly, the observed correlation between molar absorptivity and biological efficacy supports the use of spectrophotometric parameters as predictive indicators in early-stage drug screening.

Overall, PEDBA-ONA represents a promising scaffold for further development of antiparasitic agents. Future studies should explore its mechanism of action, evaluate its pharmacokinetics and toxicity profiles, and consider structural modifications to enhance bioavailability and selectivity.

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