



Synthesis, Spectral Characterization, and Photocatalytic Application of Metallo-phthalocyanines Bearing Schiff Base Moieties for Dye-Contaminated Wastewater Remediation and ADMET-Based Evaluation of Their Potential as Therapeutic Agents

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Abstract

Background: Industrial dyes are persistent pollutants that resist conventional treatment and pose environmental risks. ADMET analysis is a valuable computational approach for predicting the pharmacokinetic and safety profiles of newly synthesized compounds. **Objective:** The purpose of the present study was to synthesize and characterize novel metal-free and Metallo phthalocyanine complexes containing Schiff base moieties, evaluate their visible-light photocatalytic activity, and predict their ADMET properties. **Methodology:** This experimental study was conducted at the Department of Chemistry at College of Science, University of Babylon, Iraq from September 2025 to May 2026. Phthalocyanine complexes were prepared for medical purposes. The synthesized compounds were characterized by FT-IR, UV-Vis, ¹H-NMR, and ¹³C-NMR. Their photocatalytic activity was evaluated using Congo Red and Methylene Blue dyes, while ADMET analysis was used to predict their pharmacokinetic and toxicity profiles. **Results:** The synthesized complexes exhibited characteristic phthalocyanine absorption bands with optical band gaps of 1.63 to 1.69 eV. The Fe (II) complex showed the highest photocatalytic activity, achieving 70.6% Congo Red degradation within 60 min. Catalyst dosage enhanced degradation efficiency, whereas higher dye concentration reduced it. ADMET analysis indicated favorable pharmacokinetic behavior and predicted safety, supporting the pharmaceutical potential of the synthesized compounds. **Conclusion:** The synthesized metallophthalocyanine complexes demonstrated promising visible-light photocatalytic performance, particularly the Fe (II) complex, together with encouraging predicted ADMET properties, highlighting their potential for both wastewater treatment and future pharmaceutical applications. [Bangladesh Journal of Infectious Diseases, June 2026;13(1):235-244]

Keywords: Metallo phthalocyanines; Schiff base; photocatalytic oxidation; Congo Red degradation; water remediation

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Introduction

Synthetic dyes from industries such as textiles, plastics, and printing contaminate water and represent a global environmental disaster^{1,2}.

Synthetic dyes, particularly azo dyes such as Congo Red, are quite stable in the environment, are bioaccumulative, and are highly toxic or carcinogenic to aquatic organisms^{3,4}. Conventional

methods of treatment such as coagulation, sedimentation, and simple filtration are often not effective as they lead to secondary sludge or do not destroy the stable aromatic configuration of the pollutants^{5,6}. To overcome these limitations, Heterogeneous Photocatalysis, a subdivision of Advanced Oxidation Processes (AOPs), has emerged as a promising, cost-effective, and eco-friendly technology that is able to completely mineralize pollutants into harmless end-products such as CO₂ and H₂O under exposure to light^{7,8}.

Phthalocyanines (Pcs) and metallophthalocyanines (MPcs) are a remarkable class of structural macrocycle configurations that have attracted great scientific attention in environmental engineering and solar energy conversion^{9,10}. Due to their planar 18 π -electron aromatic systems, these materials exhibit excellent thermal and chemical stability and great architectural tunability by changing the central metal core or modifying the peripheral architecture^{11,12}. Most importantly, phthalocyanines have strong absorption cross sections in the visible region (Q-band at 600 to 800 nm), which allows them to effectively utilize solar spectra, overcoming the structural limitations of wide bandgap metal oxide catalysts such as TiO₂ or ZnO^{13,14}.

However, the major drawback of pristine phthalocyanines is their poor processability and high tendency to aggregate due to strong intermolecular interactions¹⁵. The functional insertion of active organic bridges, such as imine linkages or Schiff base moieties, into the macrocyclic core offers a viable pathway to tune their structural properties, modulate solubility behavior, and improve electronic transfer during photocatalysis^{16,17}. Comprehensive structural optimization via diverse synthesis strategies, including peripheral tuning^{18,19} and central metal ion adaptation^{20,21} has been established to dramatically improve their solar excitation features.

Consequently, this study reports the synthesis and full structural and optical characterization of a novel group of metallophthalocyanine complexes²⁻⁸ and their metal-free alternative derived from an orange Schiff base intermediate¹. The main emphasis of this work is to explore the visible-light-driven photocatalytic oxidation performance of these macrocycles against two contrasting organic models: anionic Congo Red and cationic Methylene Blue, building on established macromolecular degradation frameworks^{22,23}. This study aimed to develop novel metallophthalocyanine complexes incorporating Schiff base moieties, investigate their

structural and optical properties, evaluate their efficiency as visible-light photocatalysts for wastewater remediation through the degradation of Congo Red and Methylene Blue dyes, and explore their pharmaceutical potential using comprehensive ADMET analysis.

Methodology

Study Design: This experimental study was conducted at the Department of Chemistry, College of Science, University of Babylon, Iraq, from September 2025 to May 2026. Phthalocyanine complexes were prepared for medical purposes.

Synthesis of Schiff Base Ligand Precursor¹: The Schiff base ligand had been synthesized by (3.306g, 0.012mol) of 4-aminophthalonitrile in (2.90) ml of aldehyde and (20) ml of ethanol, with the addition of (2-3) drops of glacial acetic acid. The mixture was then refluxed for (5) hours, left to dry, and then recrystallized using ethanol (Figure I).

General Synthesis of Metallo phthalocyanine Complexes²⁻³: The target Metallo phthalocyanine complexes bearing the Schiff base outer-ring units were prepared through a high-temperature chemical melt procedure. In a typical reaction, the prepared Schiff base precursor (1) (0.5 g) was combined and thoroughly ground into a fine homogeneous powder with ammonium molybdate catalyst (0.01 g) and urea (2.33 g), alongside the stoichiometric amounts of the corresponding anhydrous transition metal chlorides: cobalt (II) chloride (0.063 g), zinc (II) chloride (0.066 g), or iron (II) chloride (0.062 g). The solid reaction mixture was transferred into a sealed glass tube and carefully heated in a sand bath

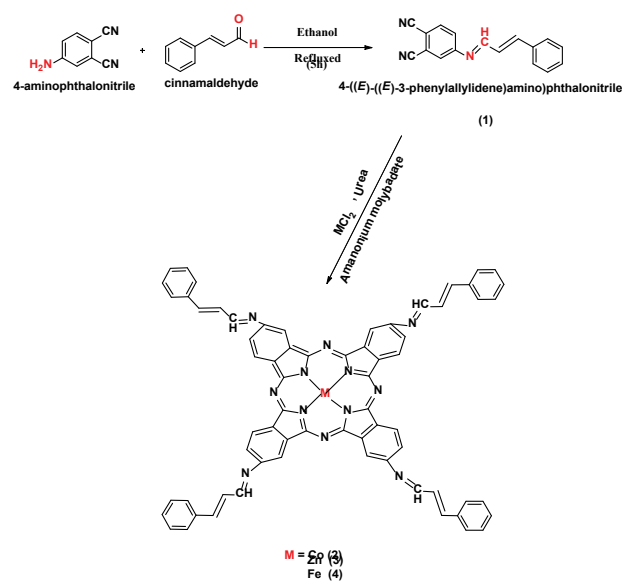


Figure I: Synthesis of Compounds²⁻⁴

until complete fusion occurred. The melt was maintained at a constant elevated temperature to complete the macrocyclic cyclotetramerization. After cooling, the resulting deeply colored solids were thoroughly washed with water and common organic non-solvents to remove unreacted urea and salt residues. The crude green and olive macrocyclic complexes were then isolated and fully purified by recrystallization from hot *N,N*-dimethylformamide (DMF) to yield the pure coordinated products (Figure I).

Preparation of Dye Stock Solutions: Stock solutions of the target pollutants, namely anionic Congo Red ($C_{32}H_{22}N_6Na_2O_6S_2$, $\lambda_{max} = 497$ nm) and cationic Methylene Blue ($C_{16}H_{18}ClN_3S$, $\lambda_{max} = 664$ nm), were prepared at a concentration of 25 ppm. Typically, the required mass of each pure dye powder was thoroughly dissolved in distilled water and quantitatively transferred into a volumetric flask to reach the designated volume. The residual concentration of each dye at different stages of the process was precisely monitored by recording the absorbance at their respective maximum absorption wavelengths (λ_{max}) using the UV-Vis spectrophotometer.

Effect of Contact Time on Photocatalytic Efficiency: To evaluate the impact of irradiation time, a 100 mL aliquot of the dye solution (25 ppm) was treated with 0.1 g of the synthesized phthalocyanine catalyst. The resulting heterogeneous suspension was subjected to continuous visible light irradiation inside a mechanical shaker operating at a constant shaking speed of 145 rpm to maintain uniform catalyst dispersion. At sequential time intervals (2, 15, 30, 45, and 60), sample aliquots were extracted from the reactor and immediately centrifuged to isolate the solid catalyst residue from the supernatant. The clear supernatant was collected, and its residual absorbance was measured at the λ_{max} of the corresponding dye using the UV-Vis spectrophotometer. The photocatalytic degradation efficiency (PDE%) was quantified using the following expression:

$$\text{Dye Removal Efficiency (\%)} = \left(\frac{C_0 - C_t}{C_0} \right) \times 100$$

Where C_0 is the initial concentration of the dye (mg/L or ppm) prior to light exposure, and C_t represents the residual dye concentration (mg/L or ppm) at a specific irradiation time t .

Effect of Photocatalyst Dosage: The influence of catalyst loading on the degradation kinetics was systematically optimized using the most active derivative, Fe (II)-Phthalocyanine. Variations in

catalyst weight (0.01, 0.02, 0.10, 0.15, and 0.20 g) were individually introduced into separate 100 mL volumes of the dye solution (25 ppm). The reaction mixtures were irradiated continuously under constant agitation at 145 rpm in the mechanical shaker. Aliquots were sampled at the designated time horizons (2, 15, 30, 45, and 60 min), centrifuged to remove the solid particles, and analyzed spectrophotometrically to establish the relationship between catalyst mass and target dye remediation kinetics.

Effect of Initial Dye Concentration: To study site-saturation phenomena, the initial concentration of the target dye was varied across a range of 5, 10, 15, 20, and 25 ppm. For these runs, a fixed dosage of 0.20 g of Pc-Fe was suspended in 100 mL of each respective dye solution. The configurations were exposed to visible light under continuous shaking at 145 rpm. Analytical samples were drawn at intervals of 2, 15, 30, 45, and 60 min, isolated via centrifugation, and measured using the UV-Vis spectrophotometer to assess the performance of the macrocyclic system under different initial pollution loads.

Statistical Analysis: The Statistical Package for the Social Sciences (SPSS) application V 21.0 (2019) was utilized to assess the impact of various groups on study parameters. The T-test and Least Significant Difference (LSD) were employed to compare means significantly. The Chi-Square test was employed to compare percentages significantly. Estimation of the correlation coefficient among various factors in patient groups within this study.

Ethics Approval: The study was conducted in accordance with the ethical standards of the institutional research committee. Ethical approval was obtained from the relevant institutional ethics committee (approval code: CSEC/1025/0148 October 27, 2025). Written informed consent was obtained from all participants prior to inclusion in the study.

Results

Physical and Solubility: The synthesized compounds exhibited good yields, thermal stability, and satisfactory solubility in common organic solvents.

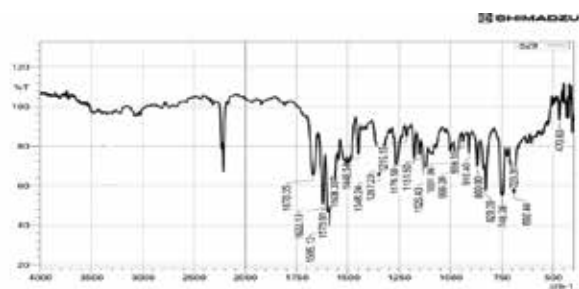
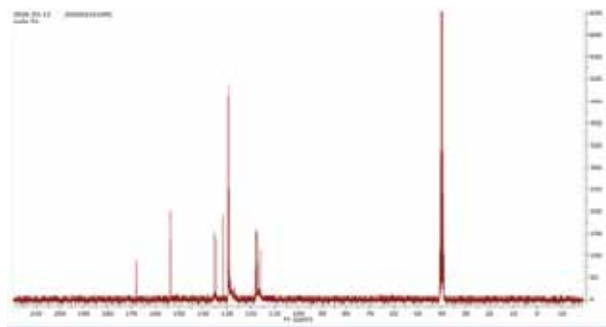
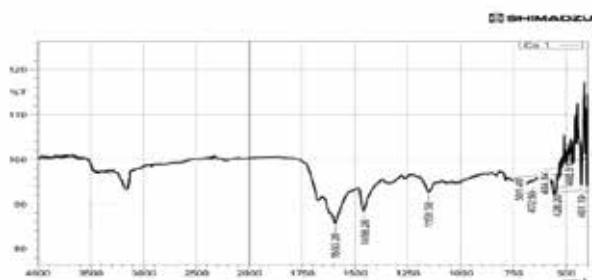
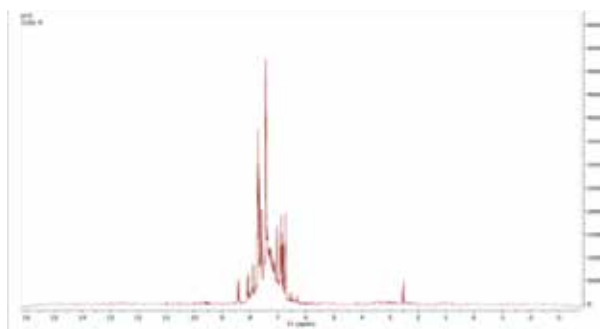
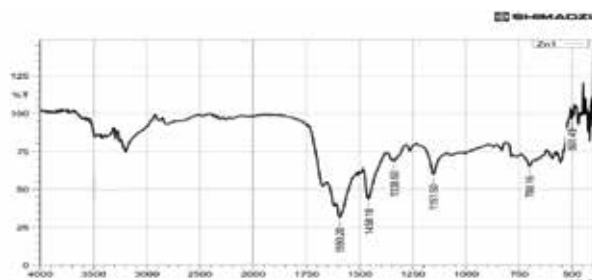
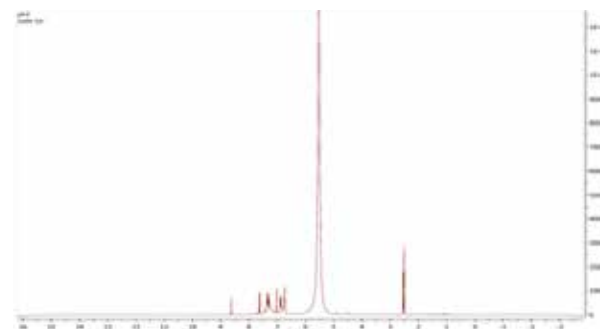
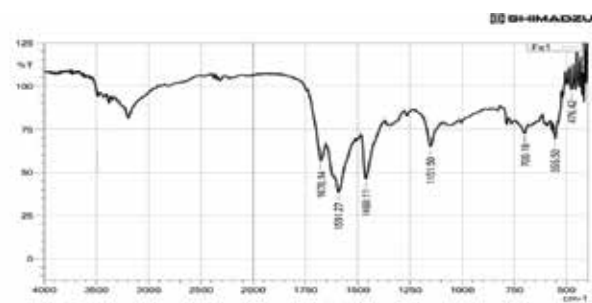
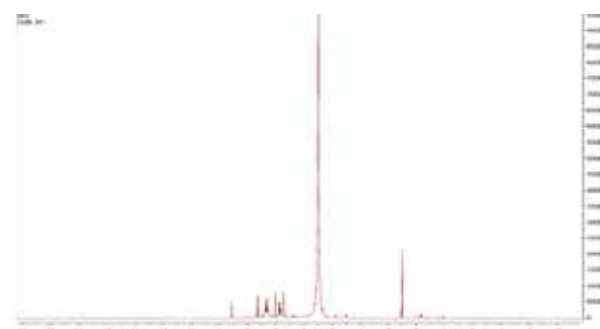
FT-IR Characterization: FT-IR spectra confirmed the successful formation of the synthesized compounds through the characteristic absorption bands.

NMR Spectral Observations: The ^1H and ^{13}C NMR spectra were consistent with the proposed structures of the synthesized compounds.

Table 1: Physical Properties and Solubility Features of the Synthesized Compounds

Compd.	M.P (°C)	Color	Yield (%)	Solubility					
				H ₂ O	Hot-H ₂ O	C ₂ H ₆ O	DMSO	CH ₃ OH	(CH ₃) ₂ CO
1	214 to 217	Orange	78.0%	-	+	P	+	P	P
2	293 to 295	Dark Green	65.0%	-	P	P	+	P	P
3	291 to 295	Green	68.0%	-	P	P	+	P	P
4	296 to 298	Olive	68.0%	-	P	P	+	P	P

Note: (-) Insoluble, (+) Completely soluble, (P) Partially soluble.

**Figure II: FTIR spectrum for compound (1)****Figure 5: ¹³C NMR Spectrum Compound****Figure 4: FTIR spectrum for compound (2)****Figure 6: ¹H NMR Spectrum Compound (1)****Figure 5: FTIR Spectrum for Compound (3)****Figure 8: ¹H NMR Spectrum Compound (3)****Figure 9. FTIR spectrum for compound (4)****UV-Visible Electronic Profiles and Optical Band**

Gap Energies: The UV–Vis spectra confirmed the characteristic electronic transitions, and the optical band gap energies were successfully determined.

Table 2: Electronic Absorption Bands, Edge Wavelengths (λ_{edge}), and Optical Band Gap Energies (E_g)

Compound	Absorption Edge Wavelength, λ_{edge} (nm)	Optical Band Gap Energy, E_g (eV) [$E_g = 1240/\lambda_{\text{edge}}$ (nm)]
Sch (1)	745	1.66
Co (2)	735	1.69
Zn (3)	760	1.63
Fe (4)	738	1.68

Table 3: Comparative Photocatalytic Degradation Efficiency (%) of Compounds for Congo Red Versus Methylene Blue At 60 Minutes

Target Pollutant Dye	Co (2)	Zn (3)	Fe (4)
Congo Red (CR) Removal %	17.73%	47.90%	70.60%
Methylene Blue (MB) Removal %	11.60%	3.10%	12.20%

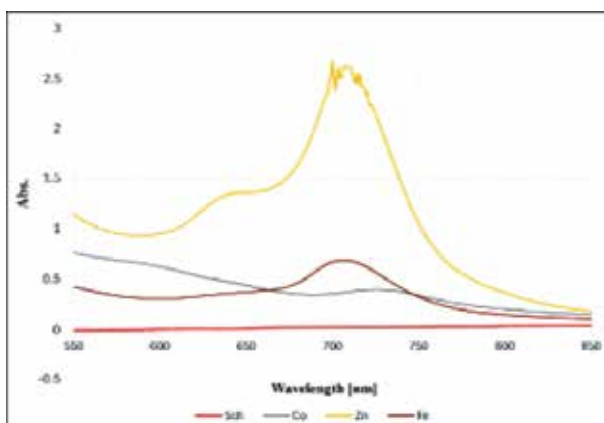


Figure 10: UV-Vis spectra of compounds (1,2,3,4)

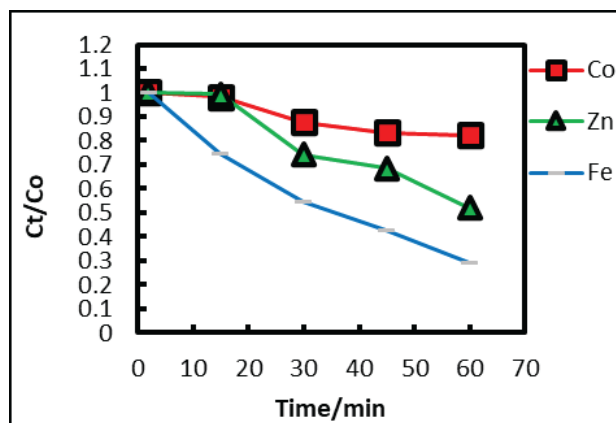


Figure 11: Photocatalytic Oxidation Efficiency of Congo Red Dye Using Metal Complexes Under Light for compounds (2,3,4)

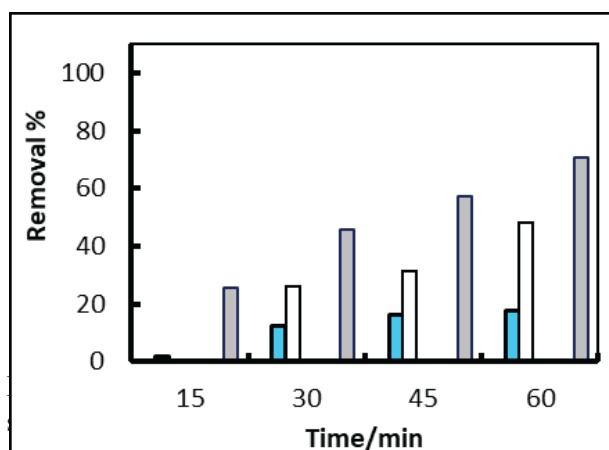


Figure 12: Effect of Contact Time on the Removal Efficiency of Congo Red Dye Using Metal Complexes Under Light for compounds (2,3,4)

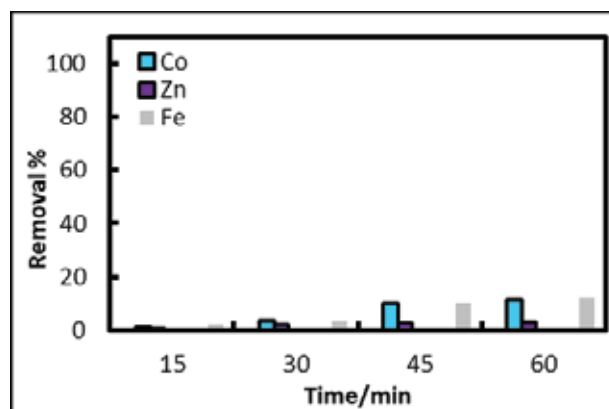


Figure 13: Photocatalytic oxidation Efficiency of Methylene Blue Dye Using Metal Complexes (2,3,4) Under Light

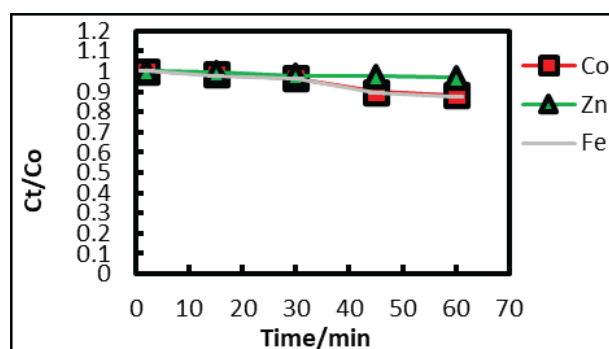
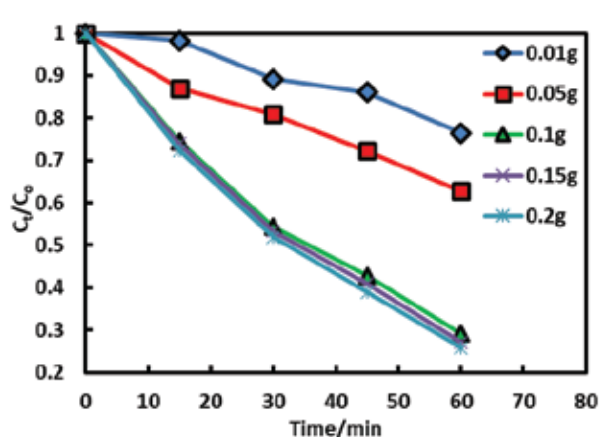
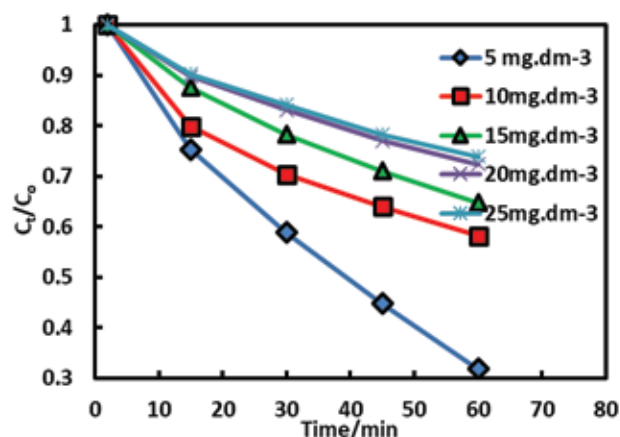
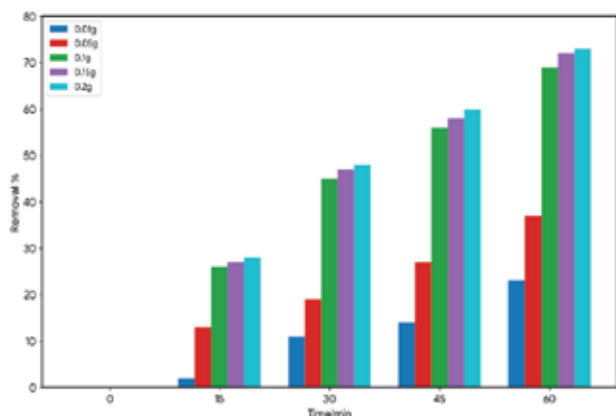
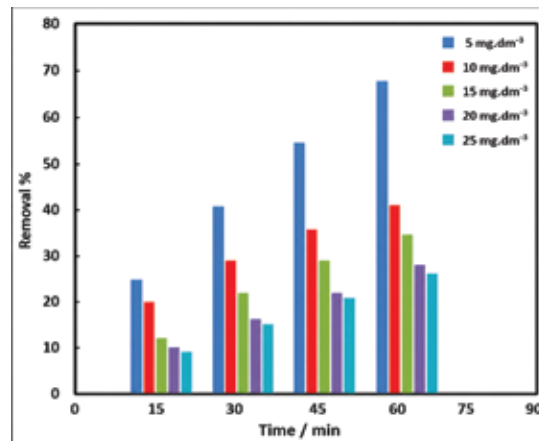


Figure 14: Effect of Contact Time on the Removal Efficiency of Methylene Blue Dye Using Metal Complexes (2,3,4) Under Light

Table 4: Variation of Photocatalytic Degradation Efficiency (%) as a function of Fe(II)-Pc catalyst dosage for Congo Red (25 ppm)

Time (min)	0.01 g	0.02 g	0.10 g	0.15 g	0.20 g
0	0.0%	0.0%	0.0%	0.0%	0.0%
15	1.72%	12.96%	25.48%	26.04%	27.59%
30	10.74%	19.05%	45.67%	46.68%	48.10%
45	13.96%	27.69%	57.21%	58.97%	61.01%
60	23.52%	37.21%	70.91%	72.97%	74.18%

**Figure 15: Effect of Fe (II) Photocatalytic Oxidation of a 25 mg L-1 Dye Solution Under Visible-Light-Irradiation Effect of Phthalocyanine Dosage (0.01-0.20g)****Figure 17: Effect of Initial Dye Concentration (5-25 mg L-1) on the Normalized Dye Concentration (Ct/C0) during Photocatalytic Oxidation with Fe(II) Phthalocyanine (0.2 g)****Figure 16: Effect of Fe(II) Influence of Phthalocyanine Dose (0.01–0.20 g) on Photocatalytic Oxidation Efficiency of a 25 mg L-1 Dye Solution****Figure 18: Effect of Initial Dye Concentration (5–25 mg L-1) on the Efficiency of Photocatalytic Oxidation of Fe(II) Phthalocyanine****Table 5: Effect of initial Congo Red dye concentration on the Degradation Efficiency (%) using 0.2 g of Fe(II)-Pc**

Time (min)	5 mg L ⁻¹	10 mg L ⁻¹	15 mg L ⁻¹	20 mg L ⁻¹	25 mg L ⁻¹
0	0.0%	0.0%	0.0%	0.0%	0.0%
15	24.71%	20.11%	12.44%	10.17%	9.72%
30	41.18%	29.63%	21.76%	16.86%	15.86%
45	55.29%	35.98%	29.02%	22.97%	21.74%
60	68.24%	41.80%	35.23%	27.62%	26.09%

3.6. ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) Analysis of the Synthesized Compounds (2, 3, 4):

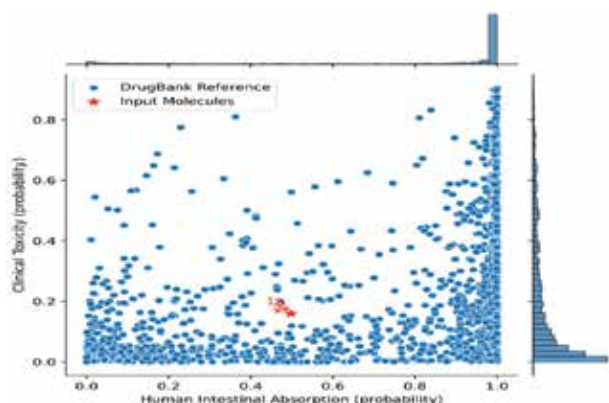


Figure 19: Showing ADMET predictions for Co (II) (2), Zn (II) (3) and Fe (II) (4), metal-complexes compared to the Drug Bank reference set

Discussion

Physical properties of the synthesized Schiff base intermediate (1) and macrocyclic phthalocyanines (2, 3, 4) are shown in Table 2. The cyclotetramerization process resulted in a remarkable change in color and thermal profile, in agreement with the conventional symmetrical and unsymmetrical phthalocyanine architectures [24]. The orange Schiff base intermediate (1) had melting point 214 to 217°C. The macrocyclic configurations of the metal-free and Metallo phthalocyanine derivatives appeared as dark green, green and olive. A significant increase in thermal stability was observed, showing high melting points above 280°C. Yields were good, ranging from 62.0% to 78.0%.

The FT-IR spectral profiles offered clear evidence of the chemical conversions. The stretching vibration frequencies of all the synthesized targets were important in the 1668 to 1672 cm^{-1} (1) and 1620 to 163 cm^{-1} regions, corresponding to the C=N (imine) stretching and aromatic (C=C) bands, respectively, in line with the patterns established for imine bridges²⁵⁻²⁶. This confirms that the imine skeleton introduced by the Schiff base was not damaged during macrocycle synthesis. Most importantly, the characteristic stretching band of nitrile groups (C≡N) that usually appears at 2220 to 2240 cm^{-1} in 4-aminophthalonitrile vanished totally in the macrocyclic spectra. The lack of nitrile absorption indicates that the cyano components have been completely consumed by the cyclotetramerization to form the core phthalocyanine structure^{1,16}. Moreover, the emergence of unique absorption bands in the lower frequency window 450 to 482 cm^{-1} due to

(M-N) vibrations further corroborates the successful coordination of the metal in the macrocyclic cavity¹⁷.

The structure of the compounds was further confirmed by ^1H and ^{13}C NMR analysis in DMSO- d_6 . In the ^{13}C NMR spectrum of the Schiff base intermediate (1), a characteristic low-field signal at $\delta=162\text{--}166$ ppm was observed, confirming the formation of the azomethine carbon (C=N). Aromatic carbon shifts were recorded in the region of $\delta=120\text{--}150$ ppm, while the cyano carbons (C≡N) produced signals between $\delta=100\text{--}110$ ppm²⁷.

In the profiles, the azomethine proton (-CH=N-) was observed as a distinct singlet at $\delta=8.0\text{--}9.0$ ppm. Following macrocycle formation, the aromatic proton signals in the region of $\delta=7.0\text{--}9.0$ ppm showed significant broadening, which is typical of extended conjugated phthalocyanine frameworks due to aggregation and strong macrocyclic ring currents¹⁶. Aliphatic olefinic groups produced a singlet within the $\delta=4.5\text{--}6.0$ ppm range, while the residual solvent peak of DMSO- d_6 was centered at $\delta=2.50$ ppm.

The electronic absorption data for the compounds dissolved in DMSO are presented in Table 3. While the Schiff base ligand (1) lacked macrocyclic absorption features, all phthalocyanine structures displayed intense Q-bands in the red visible window spanning 708.0-724.5 nm. These intense bands stem from characteristic $\pi\text{--}\pi^*$ transitions from the HOMO to the LUMO of the highly conjugated macrocyclic ring^{9,28}.

The optical band gap energies (E_g) were calculated from the absorption edge wavelengths (λ_{edge}) by using the standard equation: $E_g=1240/\lambda_{\text{edge}}$. The optical bandgap values were narrow and shifted slightly depending on the coordinated central metal as shown in Table 2: Zn (1.63 eV) < Sch < Fe (1.68 eV) < Co (1.69 eV) [26, 27]. This narrow band gap behavior indicates that these pigments can be readily excited by visible light frequencies, which makes them very suitable for photocatalytic applications²⁹⁻³⁰.

The prepared macrocycles were comparatively studied as photocatalysts in the degradation of anionic Congo Red (CR) and cationic Methylene Blue (MB) dyes under visible light irradiation. The degradation efficiency increased with the irradiation time up to 60 min³¹. The order of the photocatalytic activity was Fe > Zn > Co. The Fe complex Pc-Fe(4) exhibited the highest efficiency (70.6%) of Congo Red degradation, due to its enhanced charge transfer, Fe²⁺/Fe³⁺ redox property and reduced electron-hole recombination^{7,11,32}. Zn (47.9%) complexes^{33,34} were obtained moderate activity. Methylene Blue demonstrated significantly lower degradation (12.2%)

under similar circumstances. This difference is attributed to the stronger electrostatic attraction and π - π interactions between the anionic Congo Red and the catalyst surface^{7,35}. While the cationic Methylene Blue is subjected to electrostatic repulsion that limits the adsorption and reduces the photocatalytic efficiency^{36,37}.

The most active derivative, Fe (II) Phthalocyanine (4) was optimized for the effect of catalyst loading on the kinetics of photo-oxidation against a 25 ppm Congo Red solution. The removal efficiency increased significantly from 23.52% to 74.18% by increasing the amount of catalyst from 0.01 g to 0.20 g in 60 min as shown in Table 5. This substantial improvement is directly related to the expanded total surface area and the increased availability of photoactive sites^{8,38}. A higher catalyst concentration yields an increased generation of reactive oxygen species ($\cdot\text{OH}$ and $\cdot\text{O}_2^-$ radicals) per unit time, accelerating the oxidative cleavage of the dye molecules. The optimal catalyst configuration was established at 0.20 g. The initial concentration of the target dye also strongly influenced the photo-oxidation efficiency. Using a fixed dosage of 0.2 g of Fe(II) phthalocyanine, the initial Congo Red content was varied from 5 to 25 mg L⁻¹. The degradation profiles (Table 6) showed that the highest removal efficiency (68.23%) was achieved at a lower dye concentration (5 mg L⁻¹). The efficiency decreases with increasing dye concentration as a result of two phenomena:

At higher concentrations, more dye molecules compete for the limited active sites on the catalyst surface, leading to site saturation^{8,38}. Concentrated dye solutions absorb and scatter a large portion of incident visible light³⁹. This hinders effective penetration of photons into the solution, decreasing the absorption of light by the catalyst surface, and limiting the excitation of the photocatalyst, leading to a lower generation of reactive radicals per dye molecule, greatly affecting overall mass transfer³⁸⁻⁴⁰. ADMET analysis of Co(II)(2), Zn(II)(3) and Fe(II)(4) complexes exhibited similar physicochemical and pharmacokinetic properties. The complexes were characterized by high molecular weight, lipophilicity, hydrogen-bonding capacity and topological polar surface area resulting in low QED values, and violation of the Lipinski rule indicating limited oral drug-likeness. However, the strong P-glycoprotein inhibition, high plasma protein binding, low blood-brain barrier penetration, and long half-lives suggest systemic persistence with limited CNS exposure. Metabolism predictions indicated a moderate inhibition of CYP450 enzymes and low

substrate potential. Toxicity screening indicated a potential interaction with nuclear receptors and stress response pathways⁴¹. The ADMET-AI predictions compared to the approved Drug Bank compounds suggest that these compounds have promising pharmacokinetic and safety features and may be considered as candidates for further biological and pharmacological evaluation.

Conclusion

The present work was successful in the synthesis of a new Metallo phthalocyanine complexes and from a Schiff base intermediate. Spectroscopic characterization confirmed the formation of the macrocyclic framework and successful metal coordination in the core cavity. All complexes display sharp absorption features in the visible region with narrow band gap energies (1.63-1.69 eV). Photocatalytic tests showed that the degradation efficiency is strongly dependent on the central metal ion and the surface charge of the target dye. The macrocycle (Pc-Fe) with iron center showed higher photo-oxidation activity, due to the effective charge transfer. The catalysts exhibited high selectivity towards degradation of the anionic Congo Red in comparison to Methylene Blue due to favorable electrostatic attraction and π - π^* stacking. Moreover, the optimization of operational conditions revealed that increasing the catalyst dose enhance the degradation kinetics significantly, while high initial dye concentrations hinder the performance due to the light shielding effect. These results showcase the potential of modified phthalocyanine pigments as efficient and sustainable materials for solar-driven wastewater treatment. The ADMET evaluation demonstrated the drug-like potential of the synthesized compounds with good pharmacokinetic and safety profiles. These results indicate the possibility of synthesized compounds for future therapeutic development and biological applications.

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None

Conflict of interest:

The authors would like to state that there is no conflict of interest in this work.

Financial Disclosure

External funding was not obtained for this research.

Authors' contributions

The entire work was done by Mays Saeed Obied under the supervision of Mohanad Mousa Kareem and Ahmed F. Halbus; All authors approved the final manuscript.

Data Availability

Any questions regarding the availability of the study's supporting data should be addressed to the corresponding author, who can provide it upon justifiable request.

Ethics Approval and Consent to Participate

The study was conducted in accordance with the ethical standards of the institutional research committee. Ethical approval was obtained from the relevant institutional ethics committee (approval code: CSEC/1025/0148 October 27, 2025). Written informed consent was obtained from all participants prior to inclusion in the study.

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