

Characterization of Protoporphyrin IX as a Lead Compound of Photosensitizer for PDT

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Characterization of Protoporphyrin IX as a Lead Compound of Photosensitizer for PDT

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Abstract

The tetrapyrrolic compound protoporphyrin IX and related structures are receiving considerable interest as a potential drug for PDT [1-3]. Due to its chemical structure, protoporphyrin IX can be a lead compound for synthesis of new photosensitizer. The present research reports the characterization of protoporphyrin IX. The visible absorption spectrum showed an intensive absorption band at 406 nm (Soret band, $\epsilon = 155,953 \text{ cm}^{-1} \text{ M}^{-1}$) and four weak Q band at 505, 539, 576, and 630 nm with a value of ϵ , 14064, 11472, 6886, and $5275 \text{ cm}^{-1} \text{ M}^{-1}$, respectively. Protoporphyrin IX compounds showed emission wavelength fluorosensi at 635 nm. The absorption band of CO group appears at 1700.9 cm^{-1} and a broad band at 3313 cm^{-1} (OH group) of IR spectrum showed the presence of carboxylic group in the compound. The structure was also confirmed by ^1H NMR and MS.

Introduction

The tetrapyrrolic compound of protoporphyrin IX (PpIX) and related structures are receiving considerable interest as a potential drug for PDT [1-3]. PpIX has two peripheral carboxylic acids available and vinyl groups side chains. Due to its chemical structure, protoporphyrin IX can be a lead compound for synthesis of new photosensitizer. The aim of this work was undertaken to confirm the structure and optical properties of protoporphyrin-IX as a lead compound for PDT

Methods

PpIX (Sigma-Aldrich) was dissolved in dimethylformamide (DMF) in the case of absorption spectra and fluorescence emission measurements. UV/vis absorption spectra were taken with the use of the Beckman Coulter DU® 720. The fluorescence spectra were taken by a Shimadzu spectrofluorophotometer RF-540. The IR measurements were performed with a Jasco FT/IR-4200. NMR spectra were recorded in a spectrometer JEOL ECP500 (1H, 500 MHz, DMSO-d₆).

Results

The absorption spectral profiles of PpIX in DMF are shown in Fig. 1a. The UV-vis spectral characteristics showed an intensive absorption bands at 404 nm (Soret band, $\epsilon = 155,953 \text{ cm}^{-1} \text{ M}^{-1}$) and four weak Q band at 505, 539, 576, and 630 nm with a value of ϵ , 14064, 11472, 6886, and $5275 \text{ cm}^{-1} \text{ M}^{-1}$, respectively.

Fig 1a illustrates the fluorescence emission spectra of PpIX (excitation at 428 nm). Protoporphyrin IX compounds showed emission wavelength fluorosensi at 635 nm. Due to its optical properties, PpIX can be used for photodetection.

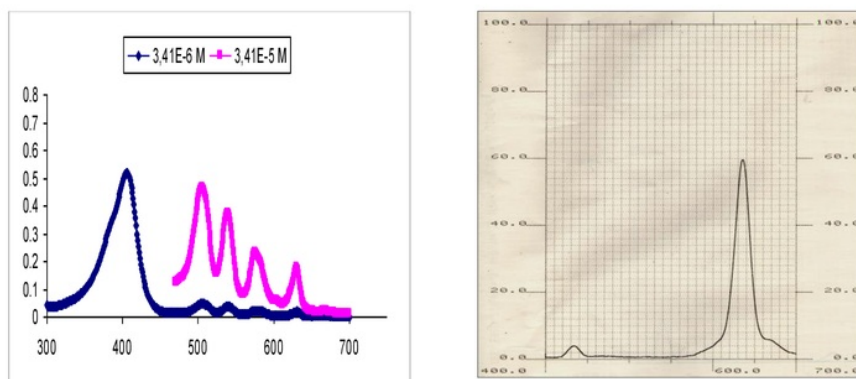


Fig 1. (a) Absorption spectra for Protoporphyrin IX.
(b) Fluorescence emission spectra for Protoporphyrin IX.

The IR spectra of PpIX are shown in Fig 2. The absorption band of CO group appears at 1700.9 cm^{-1} and a broad band at 3313 cm^{-1} (OH group) of IR spectrum showed the presence of carboxylic group in the compound.

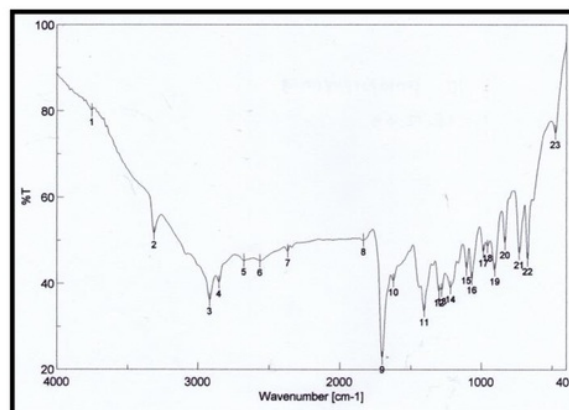


Fig 2. IR spectrum of protoporphyrin IX.

The ^1H NMR spectra of PpIX in DMSO- d_6 is shown in Fig 3. The signals (including the carboxylic acid protons) were evident in the spectrum. Due to the anisotropic effect from the porphyrin ring current, the shielded N-H protons appear at very high field (-4 ppm) in the ^1H -NMR spectrum, whereas the peripheral protons show up at low field (10.2 ppm) due to the presence of the deshielding environment resulting from the aromatic ring current. Furthermore, the mass spectra showed a molecular ion (m/z) 561 (Fig 4.).

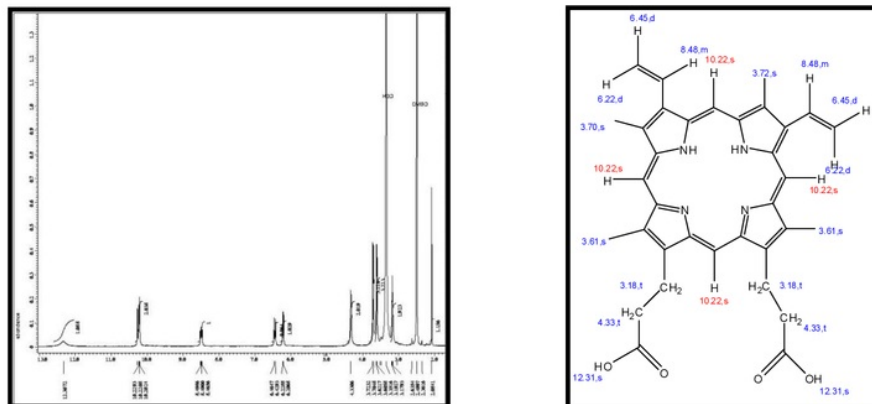


Fig 3. ¹H NMR spectra for PpIX.

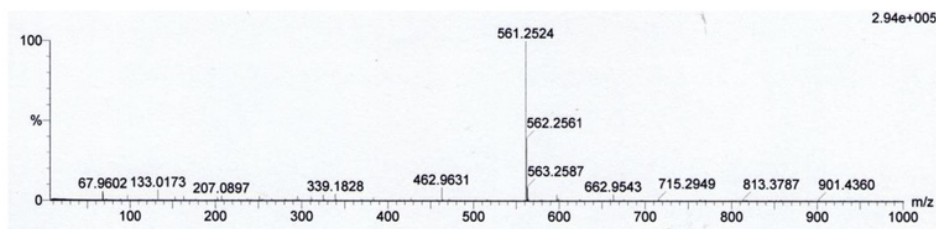


Fig 4. MS spectra for PpIX .

Conclusions

Due to its chemical structure and optical properties, protoporphyrin IX can be potential as a lead compound for synthesis of new photosensitizer.

References

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