Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Supplementary Information

Parietin: an efficient photo-screening pigment *in vivo* with good photosensitizing and photodynamic antibacterial effects *in vitro*

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Parietin (PTN) identification

General Experimental Procedures

UV spectra were recorded on a Cary Win UV-VIS spectrophotometer (Agilent Technologies, California, USA). NMR spectra were acquired in $CDCl_3$ on a Bruker Advance II 400 (400 MHz for ^1H and 100 MHz for ^{13}C) spectrometer (Bruker BioSpin GmbH, Silberstreifen 4-76287 Rheinstetten, Germany). Chemical shifts (δ) are reported in ppm relative to TMS as internal standard and coupling constants (J value) in Hz. EIMS were obtained on a Variant Mat CH-7A at 70 eV.

PTN was identified by comparison of their experimental spectroscopic data (UV-Vis, 1D and 2D NMR, and MS) with those previously reported in the literature. Their spectroscopic and spectrometric data are reported herein.

UV-Vis absorption maxima (nm) in MeOH

This work	251; 265; 285; 434
Fairbairn et al. 1972	255; 267; 288; 432

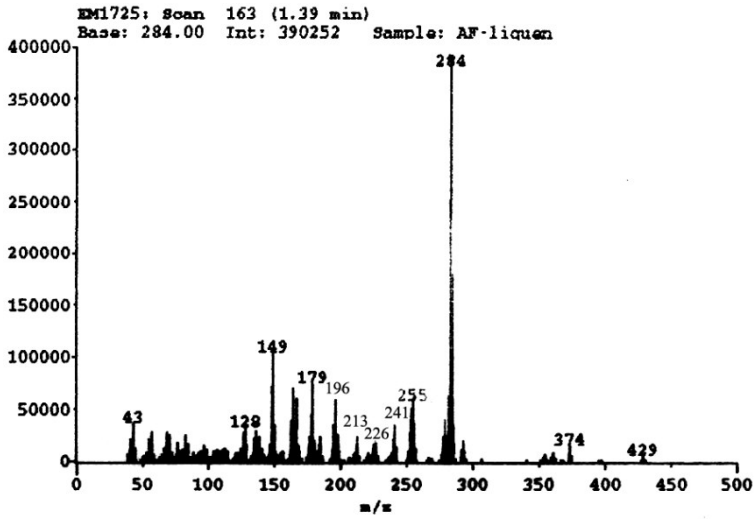

Figure 1: Mass spectra of PTN

Mass spectrometric data according Wu et al 1987.

EM-AR: m/z (relative intensity)	284 (M^+, 100%), 255, 241, 227, 226, 213, 198, 185

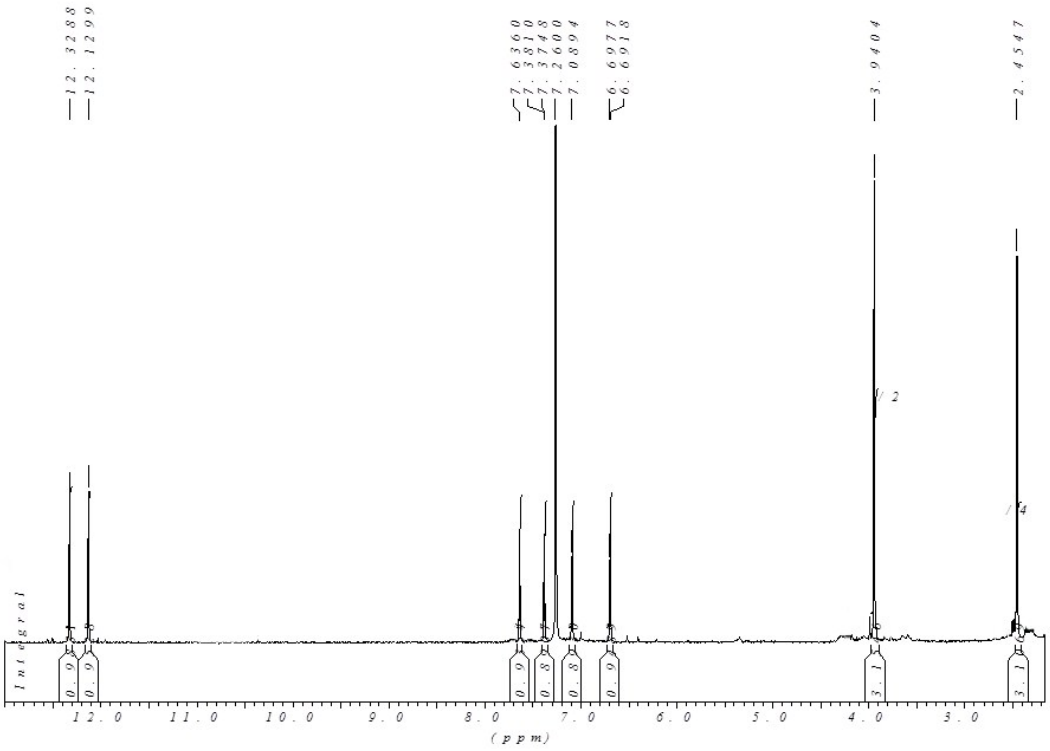

Figure 2: ^{1}H NMR spectra of PTN in $CDCl_3$

^{1}H NMR spectroscopic data according Wu et al 1987.

Position	^{1}H NMR δ (ppm) ($CDCl_3$)
2	6.69 (d, 1H, J= 2.5)
4	7.38 (d, 1H, J=2.5)
5	7.64 (s br, 1H)
7	7.09 (s br, 1H)
3-O-$\underline{CH_3}$	3.94 (s, 3H)
6-$\underline{CH_3}$	2.46 (s, 3H)
1-OH	12.32 (s, 1H)
8-OH	12.13 (s, 1H)

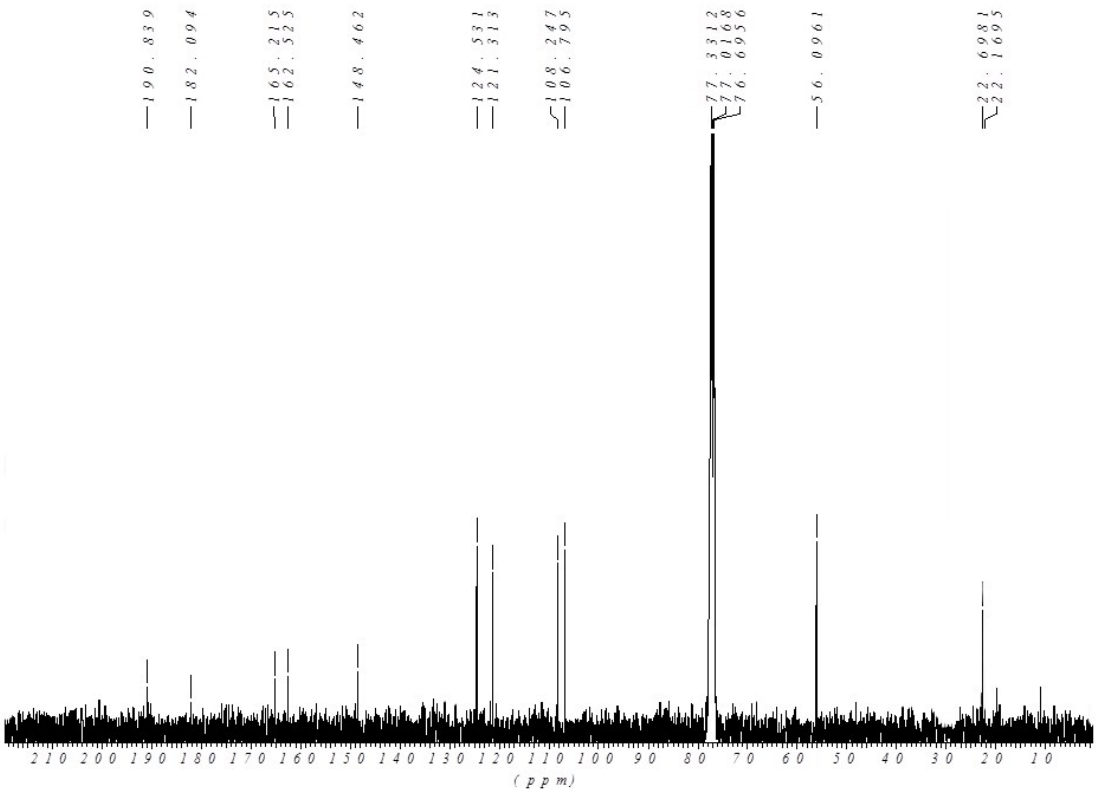

Figure 3: ^{13}C NMR spectra of PTN in $CDCl_3$

^{13}C NMR spectroscopic data according Canaviri at al 2006.

Position	^{13}C NMR δ (ppm) ($CDCl_3$)
1a	110.4
1	165.4
2	107.0
3	166.8
4	108.4
4a	135.3
5a	132.2
5	121.5
6	148.7
7	124.7
8	162.7
8a	113.9
9	191.3
10	182.2
3-O-$\underline{C}H_3$	55.4
6-$\underline{C}H_3$	21.7

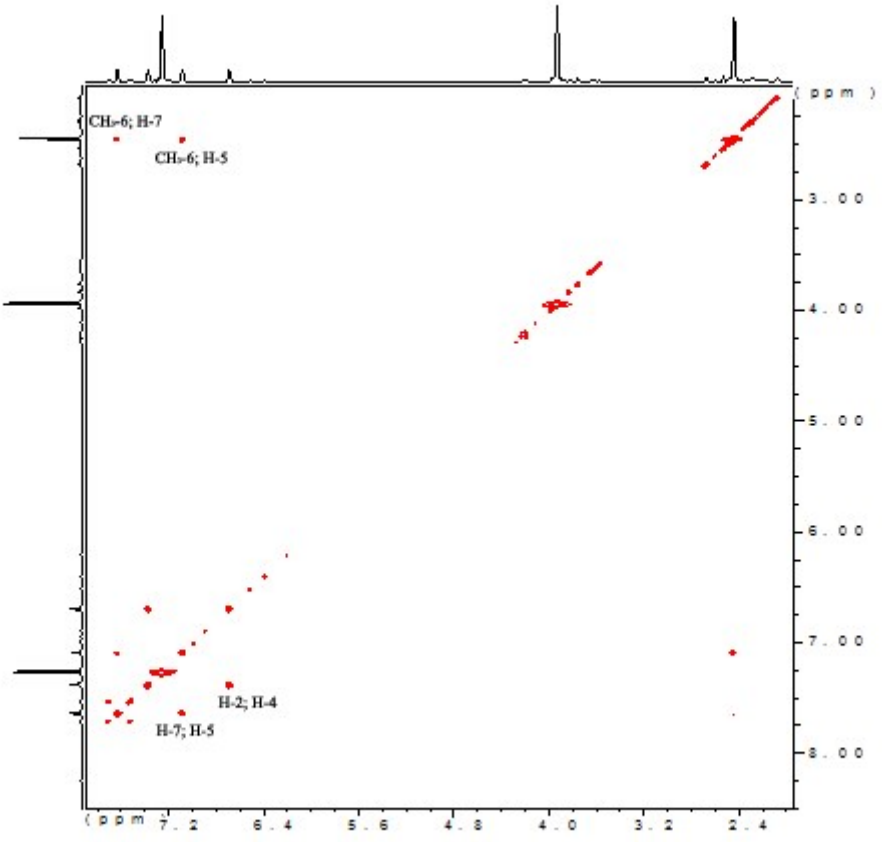

Figure 4: COSY spectra of PTN in $CDCl_3$

COSY spectroscopic data according Canaviri at al 2006.

Position	^{1}H NMR δ (ppm) ($CDCl_3$)	Cosy (^{1}H-^{1}H)
2	6.7 (d, 1H, J=2.0)	H4
4	7.4 (d, 1H, J=2.0)	H2
5	7.6 (d, 1H, J=2.0)	H7
7	7.1 (d, 1H, J=2.0)	H5

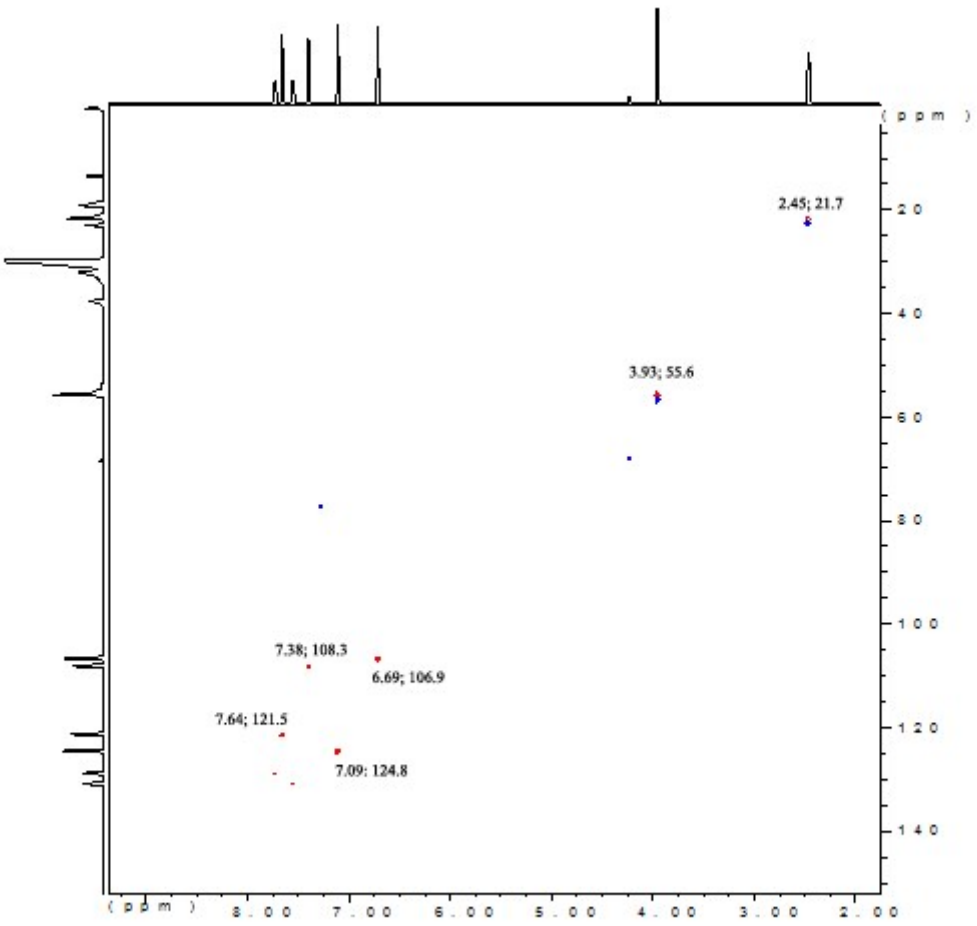

Figure 5: HSQC-DEPT spectra of PTN in $CDCl_3$

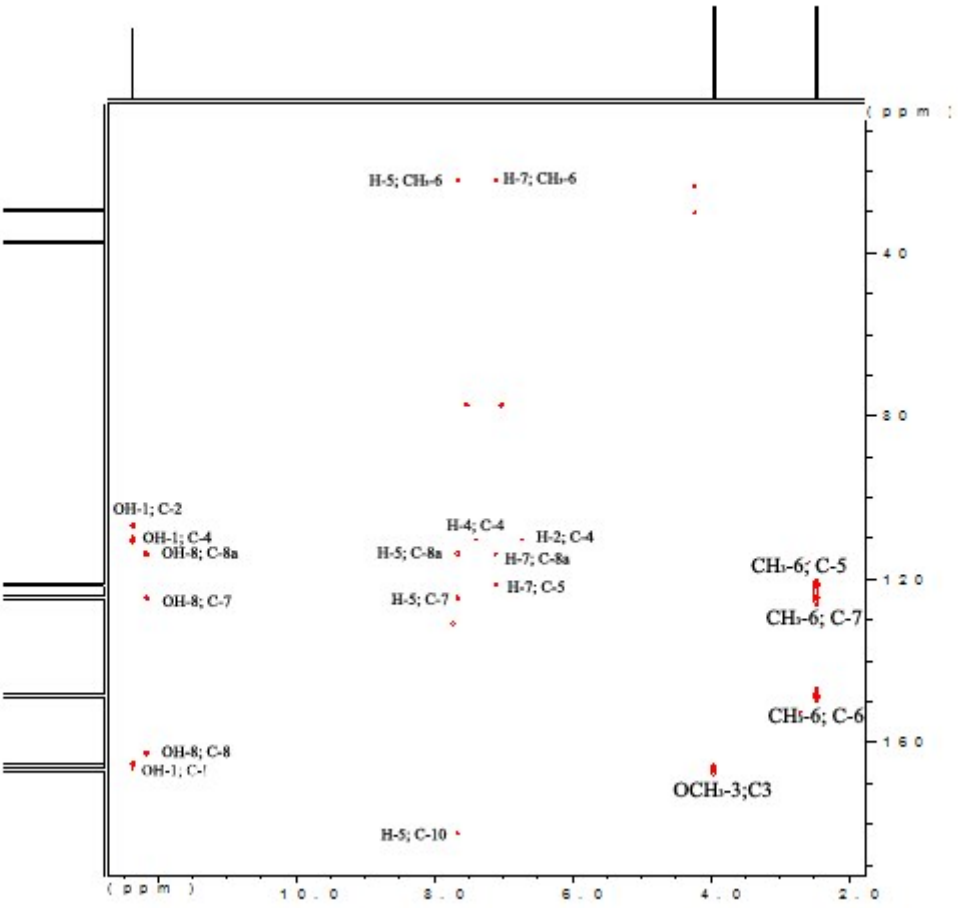

Figure 6: HMBC spectra of PTN in $CDCl_3$

HMBC spectroscopic data according Canaviri at al 2006.

Position	^{1}H NMR δ (ppm) ($CDCl_3$)	HMBC (^{1}H-^{13}C)
2	6.7 (d, 1H, J=2.0)	C-4, C-1a, C-1, C-3
4	7.4 (d, 1H, J=2.0)	C-3, C-1a, C-10
5	7.6 (d, 1H, J=2.0)	CH_3-6, C-8a, C-7, C-10
7	7.1 (d, 1H, J=2.0)	CH_3-6, C-8a, C-5, C-8
3-O-$\underline{CH_3}$	3.0	C3
6-$\underline{CH_3}$	1.8	C-5, C-6, C-7

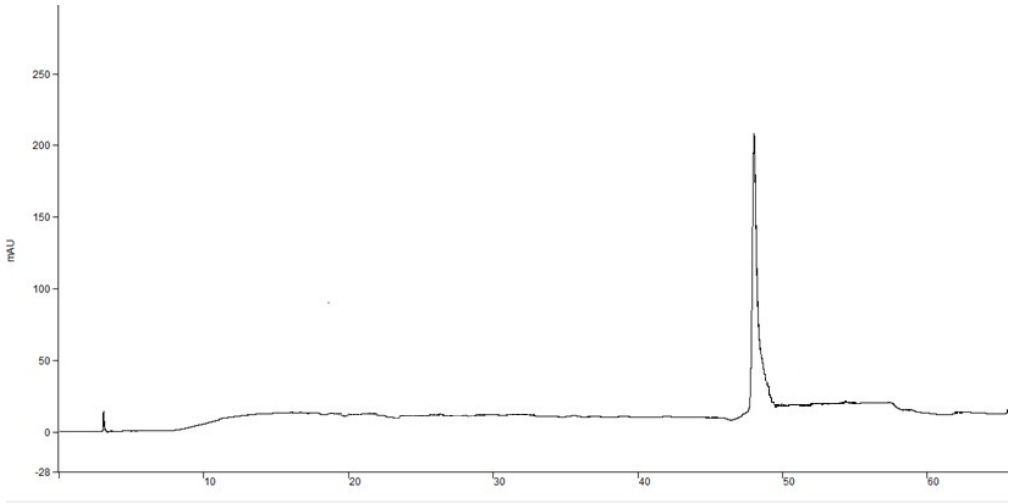

Figure 7: HPLC chromatogram of purified PTN

A Varian Pro Star chromatography apparatus (model 210, series 04171, California, USA), equipped with an UV-Vis detector and a Microsorb-MV column 100-5 C-18 (250 x 4.6 mm i.d., Agilent) was used at 25 °C. The mobile phase was a gradient elution of solvent A formic acid 0.16 M (ultra-pure water) and solvent B: MeOH 0.6% formic acid; the composition varied from 65 to 0 % of A in 66 min, at a variable flow from 1 at 0.7 mL/min. Detection was performed at 265 nm. Sample dissolved in MeOH (HPLC, Sintorgan, Buenos Aires, Argentina) and filtered through cellulose (Merck Millipore, Sao Paulo, Brasil) was manual injected (20 µL). Data analysis was performed using Varian software (Star Chromatography Workstation 6.41, California, USA).

References

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