Supporting Information

Isomeric effect on the properties of tetraplatinated porphyrins showing optimized phototoxicity for photodynamic therapy

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Figures:

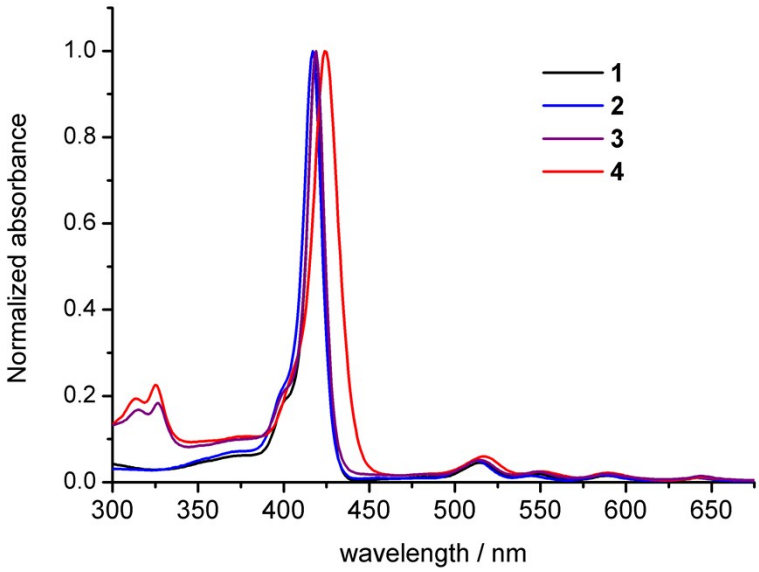

Figure S1: Absorption spectra of porphyrins **1-4** in DMSO solution. The Soret band of porphyrin **4** is broader and red-shifted compared to the other porphyrins.

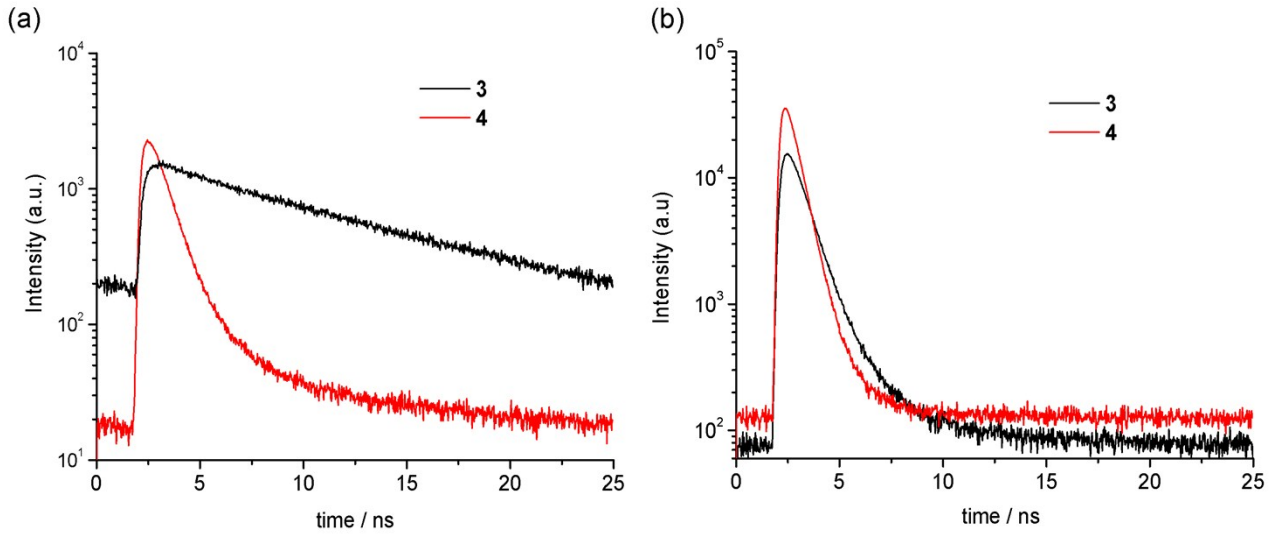

Figure S2: Fluorescence decay curves for **3** (black) and **4** (red) in (a) DMSO and (b) aqueous solution.

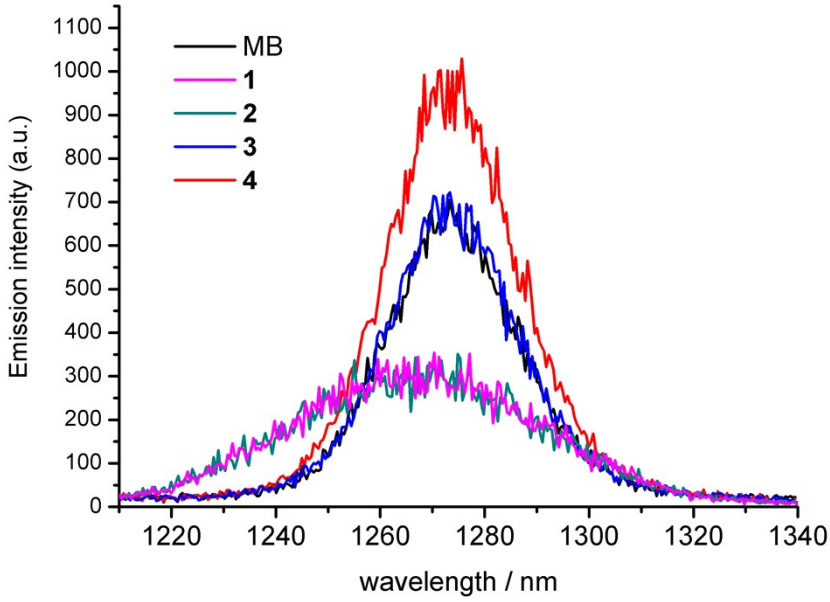

Figure S3: Singlet oxygen phosphorescence emission spectra for porphyrins **1-4** and methylene blue (MB) in acetonitrile.

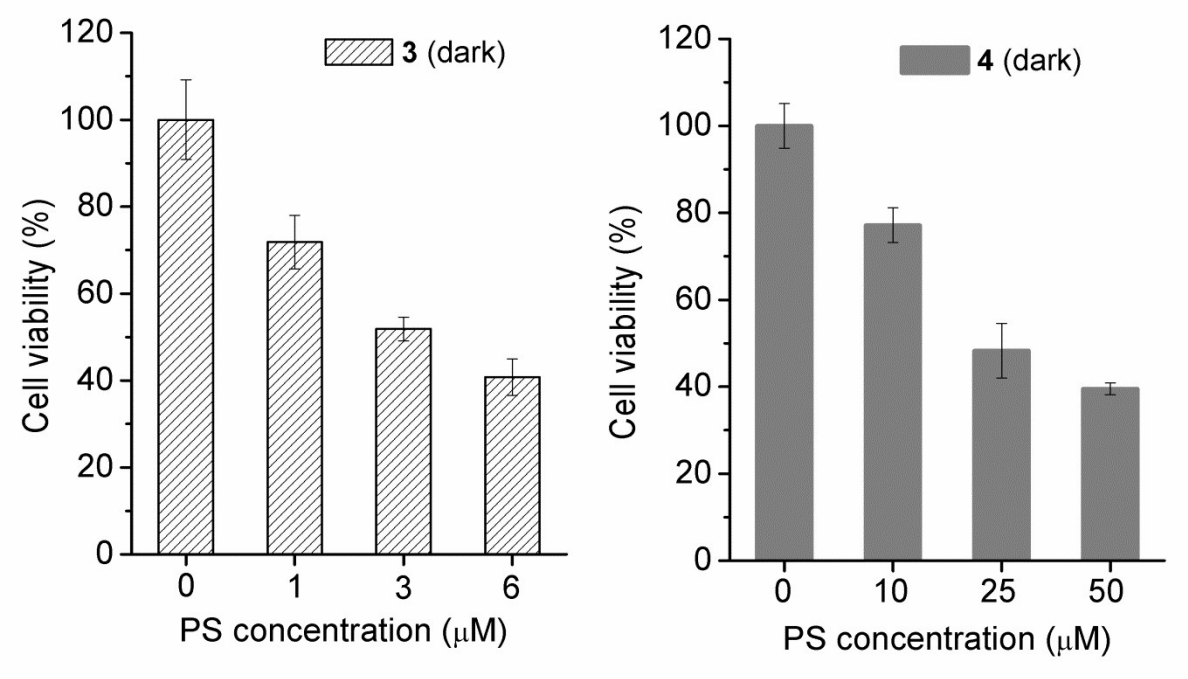

Figure S4: Cell viability (%) of HeLa incubated with **3** (hashed) and **4** (gray) for 24 h in the dark.

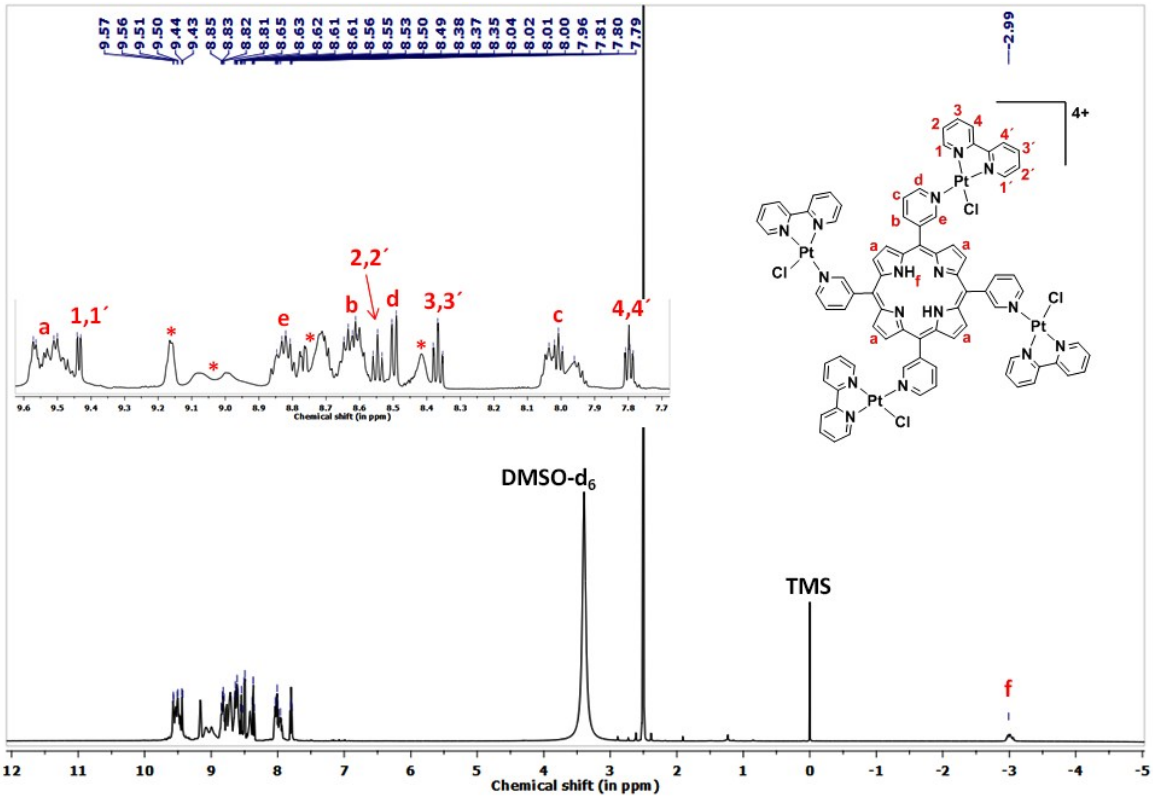

Figure S5: ^{1}H NMR spectrum of compound **3**, in (600 MHz, DMSO-d_6).*residual peaks.

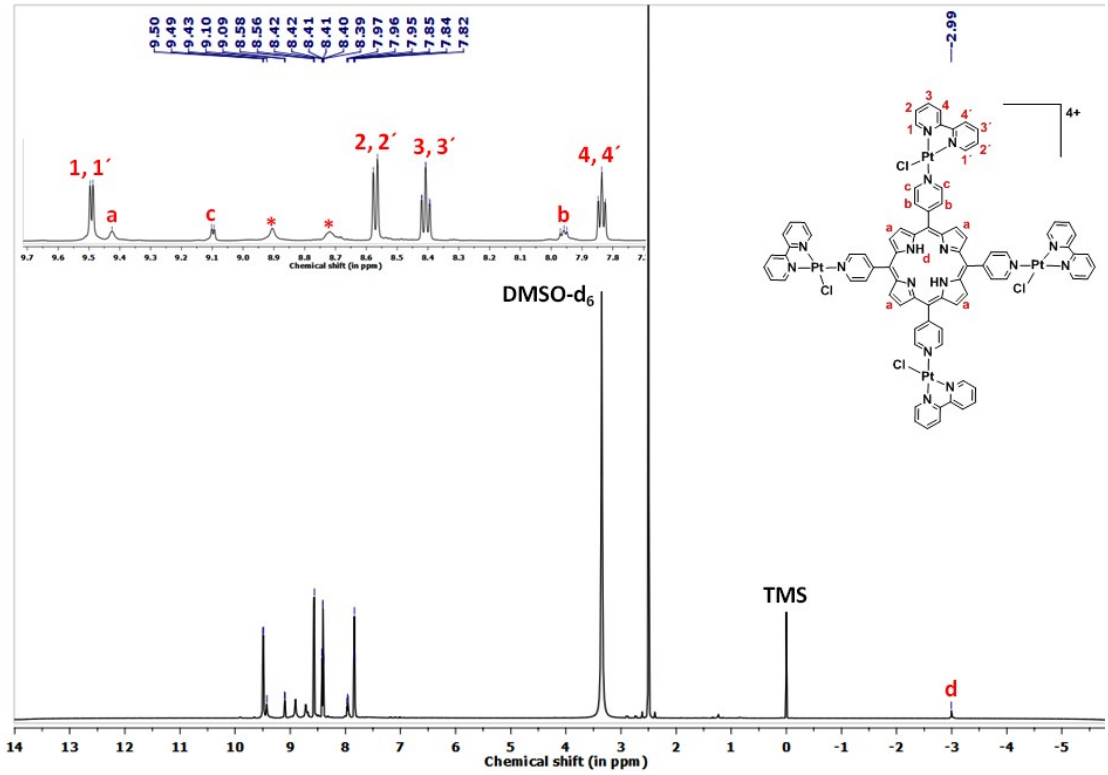

Figure S6: ^{1}H NMR spectrum of compound **4**, in (600 MHz, DMSO-d_6).*residual peaks.

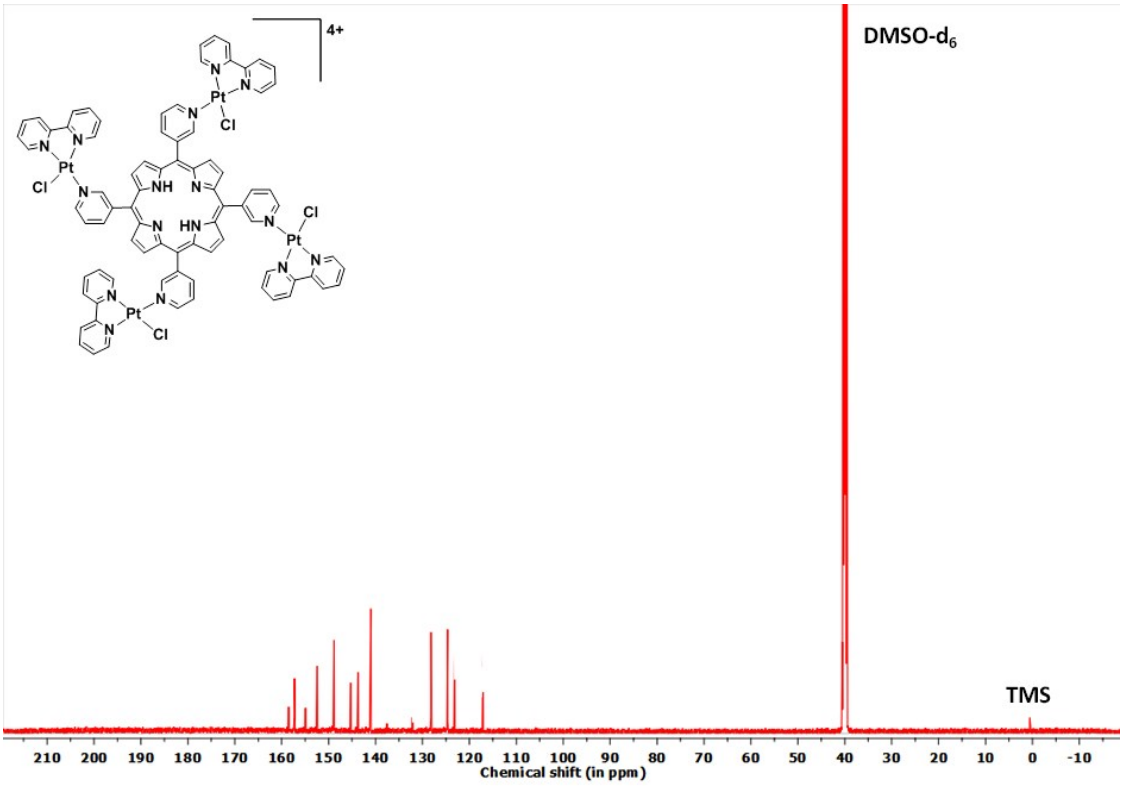

Figure S7: ^{13}C NMR spectrum of compound **3**, in (100 MHz, DMSO-d_6).

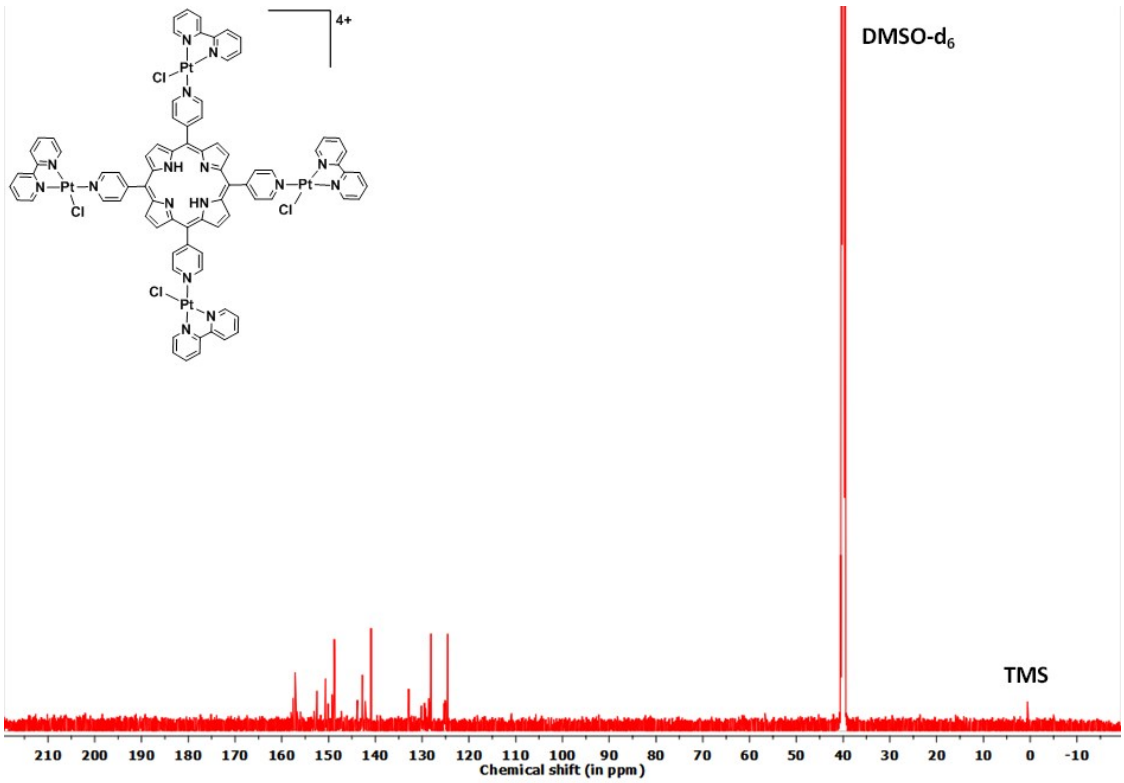

Figure S8: ^{13}C NMR spectrum of compound **4**, in (100 MHz, DMSO-d_6).

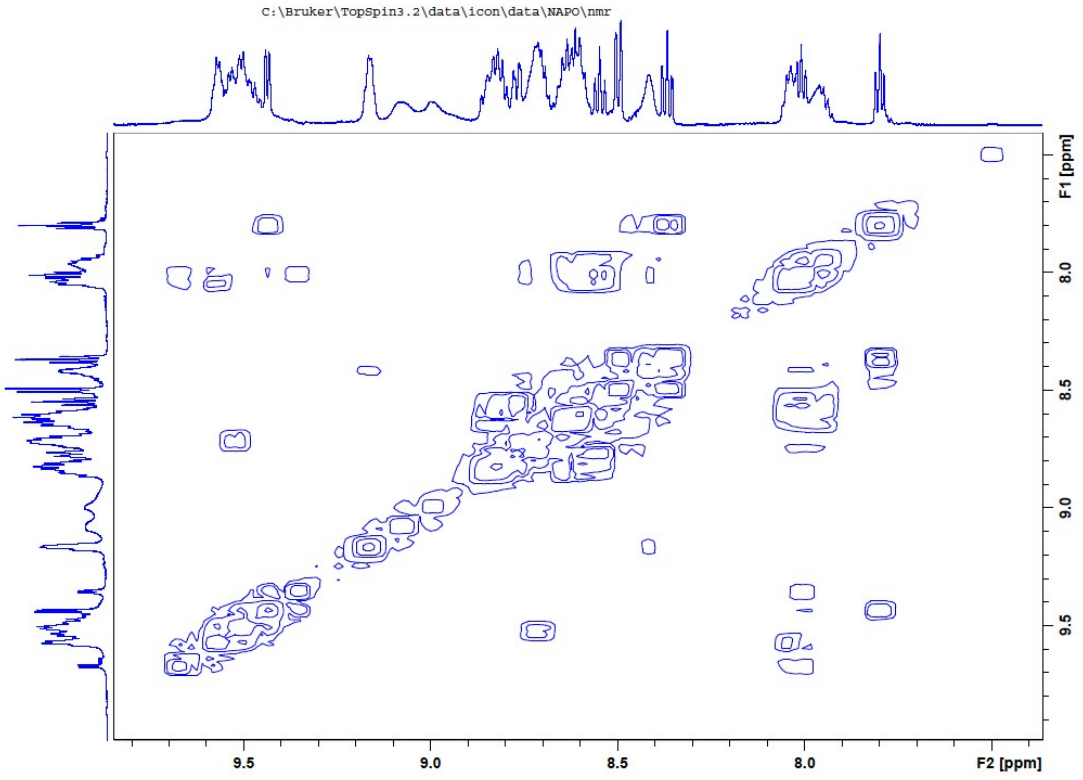

Figure S9: COSY 2D NMR spectrum of compound **3**, in DMSO-d_6.

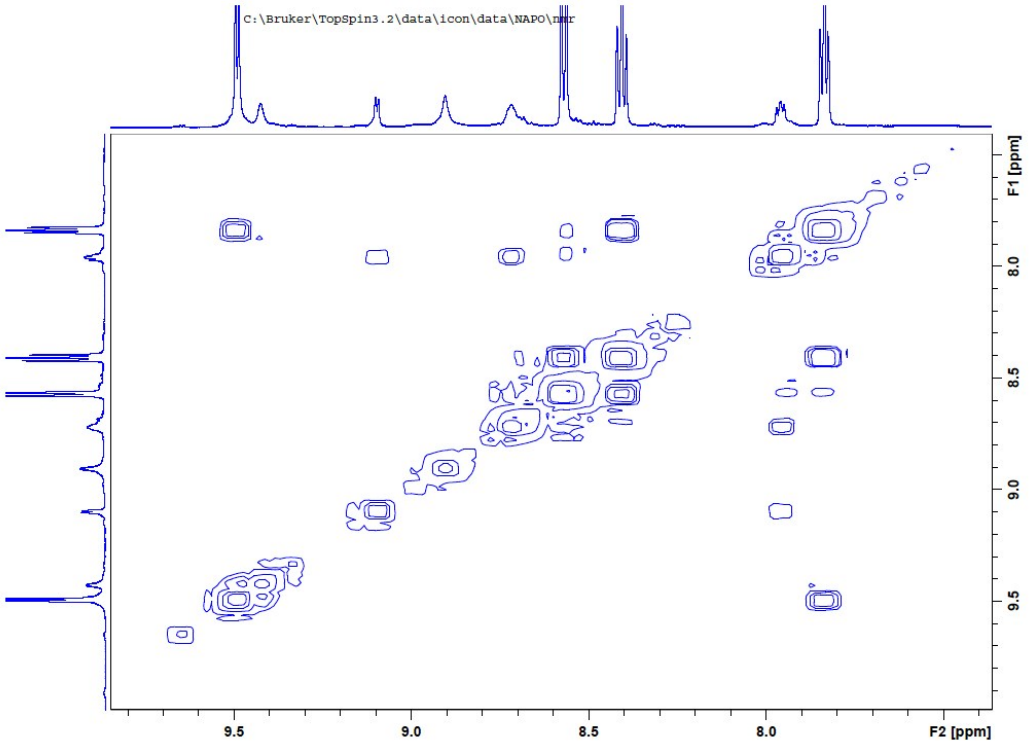

Figure S10: COSY 2D NMR spectrum of compound **4**, in DMSO-d_6.

Table S1: Elemental analysis and NMR data of porphyrins **3** and **4**.

	Elemental analysis, exp. (calc.)[1] - $[C_{80}H_{58}Cl_4N_{16}Pt_4](PF_6)_4 \cdot 8H_2O$
Porphyrin 3	%C: (33.25) 33.27; %H: (2.58) 2.61; %N: (7.76) 7.81
Porphyrin 4	%C: (33.25) 33.26; %H: (2.58) 2.60; %N: (7,76) 7.80

Compound	**^{1}H NMR, DMSO-d_6**
Porphyrin 3	-2.99 (2H, bs, NH); 7.81 (8H, dd, *J* = 6.0 Hz, 4,4´); 8.04 (8H, m, Hc); 8.38 (8H, dd, *J* = 6.0 Hz, 3,3´); 8.50 (4H, d, *J* = 12.0 Hz, Hd); 8.56 (8H, dd, *J* = 6.0 Hz, 2,2´); 8.65 (4H, m, Hb); 8.85 (4H, m, He); 9.44 (8H, d, *J* = 6.0 Hz, 1,1´) and 9.57-9.50 (8H, d, *J* = 6.0 Hz, Ha)
Porphyrin 4	-2.99 (2H, bs, NH); 7.85 (8H, dd, *J* = 6.0 Hz, 4,4´); 7.97 (8H, d, *J* = 5.8 Hz, Hb); 8.42 (8H, dd, *J* = 6.0 Hz, 3,3´); 8.58 (8H, d, *J* = 5.6 Hz, 2,2´); 9.10 (8H, d, *J* = 5.7 Hz, Hc); 9.43 (8H, s, β-H) and 9.50 (8H, d, *J* = 6.0 Hz, 1,1´)
Compound	**^{13}C NMR, DMSO-d_6**
Porphyrin 3	158.7, 157.3, 155.3, 153.06, 148.9, 145.07, 144.7, 141.0, 137.5, 133.9, 128.2, 124.6, 123.2, 117.05
Porphyrin 4	157.5, 157.1, 152.4, 150.6, 150.1, 149.2, 148.8, 143.8, 142.7, 142.2, 140.9, 132.8, 128.1, 124.5

[1]J. A. Naue, S. H. Toma, J. A. Bonacin, K. Araki and H. E. Toma, *J. Inorg. Biochem.*, **2009**, 103, 182–189.