

## Electronic Supplementary Information

**Manuscript Title:** Synthesis, Photophysical Properties and *in vitro* Photodynamic Activity of Axially Substituted Subphthalocyanines

**Authors:** Hu Xu, Xiong-Jie Jiang, Elaine Y. M. Chan, Wing-Ping Fong and Dennis K. P. Ng\*

### Contents:

**Fig. S1** UV-Vis and fluorescence spectra of **2-5** in the DMEM and RPMI media.

**Fig. S2** Changes in the Q-band absorbance of **2-5** in the RPMI medium with time, both in the absence and presence of light.

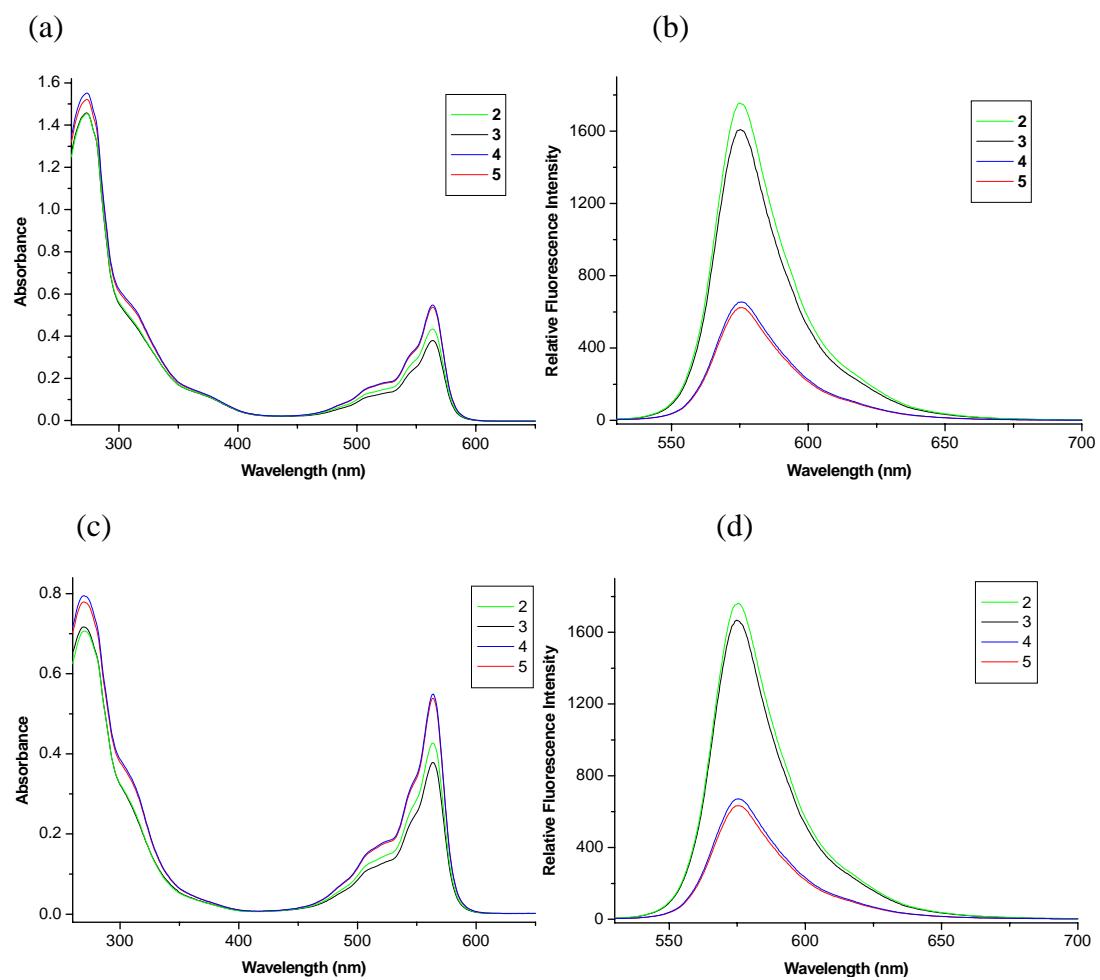
**Fig. S3** Changes in absorption spectra of **2-5** in the presence of RNO and imidazole in the RPMI medium upon irradiation with time.

**Fig. S4** (a)  $^1\text{H}$  and (b)  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **2** in  $\text{CDCl}_3$ .

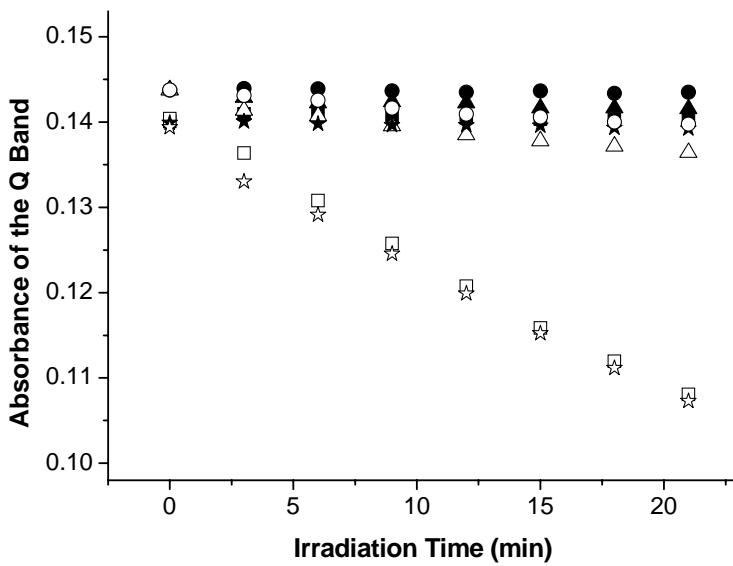
**Fig. S5** (a)  $^1\text{H}$  and (b)  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **3** in  $\text{CDCl}_3$ .

**Fig. S6** (a)  $^1\text{H}$  and (b)  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **4** in  $\text{CDCl}_3$ .

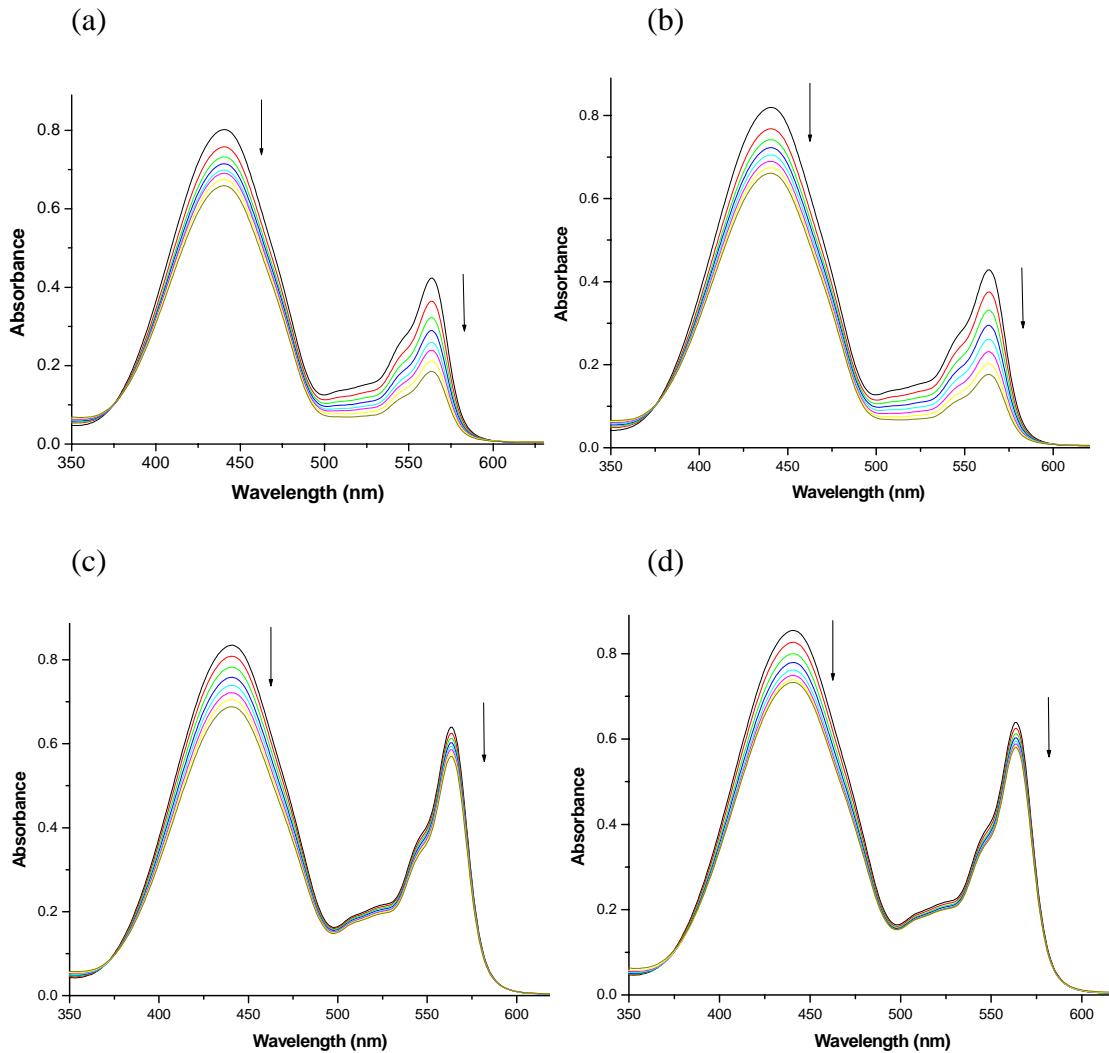
**Fig. S7** (a)  $^1\text{H}$  and (b)  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **5** in  $\text{CDCl}_3$ .



**Fig. S1** (a) UV-Vis and (b) fluorescence spectra of **2-5** in the DMEM medium (8.0  $\mu\text{M}$ ). The corresponding spectra in the RPMI medium are shown in (c) and (d).

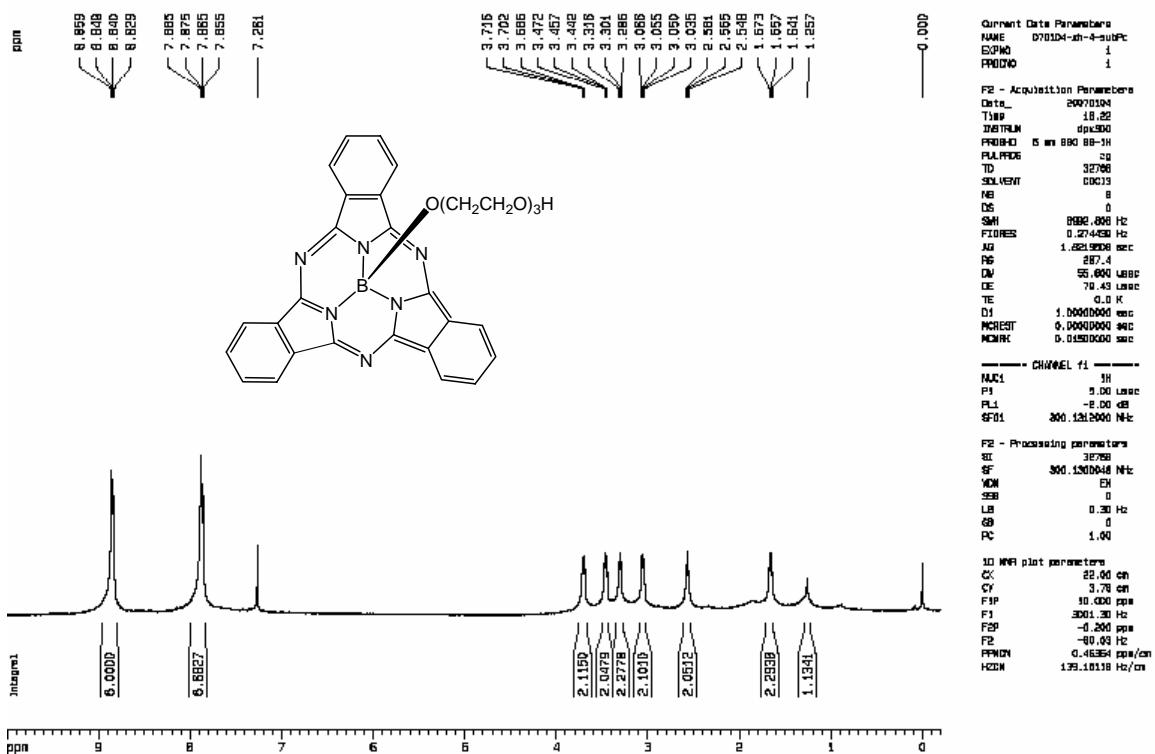


**Fig. S2** Changes in the Q-band absorbance of **2** (stars), **3** (squares), **4** (circles) and **5** (triangles) in the RPMI medium (all at 2.0  $\mu\text{M}$ ) with time, both in the absence (closed symbols) and presence (open symbols) of light ( $\lambda > 515$  nm, 9 mW  $\text{cm}^{-2}$ ). The data were taken at 3-min intervals.

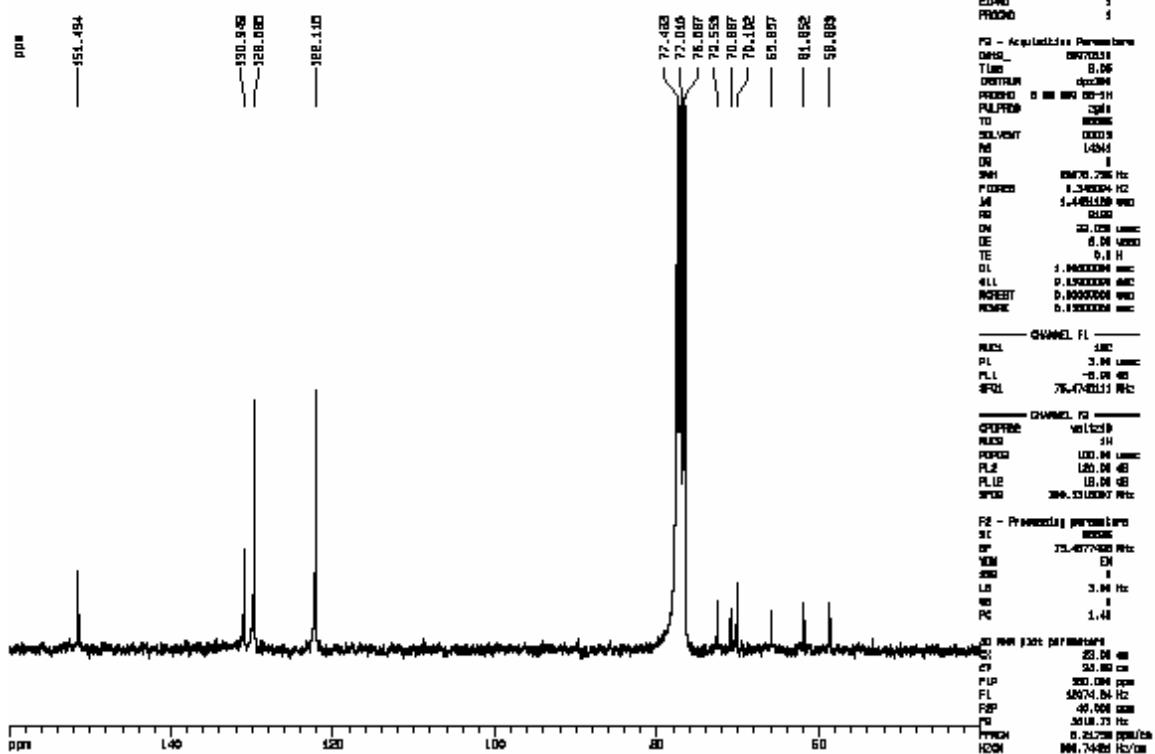


**Fig. S3** Changes in absorption spectra of (a) **2**, (b) **3**, (c) **4** and (d) **5** (all at 8.0  $\mu$ M) in the presence of RNO (0.02 mM) and imidazole (5.0 mM) in the RPMI medium upon irradiation ( $\lambda > 515$  nm) with time. The spectra were taken at 3-min intervals. The relative rates of decay of RNO and the photosensitiser can be compared by monitoring the decrease in absorbance at 440 and 563-564 nm, respectively.

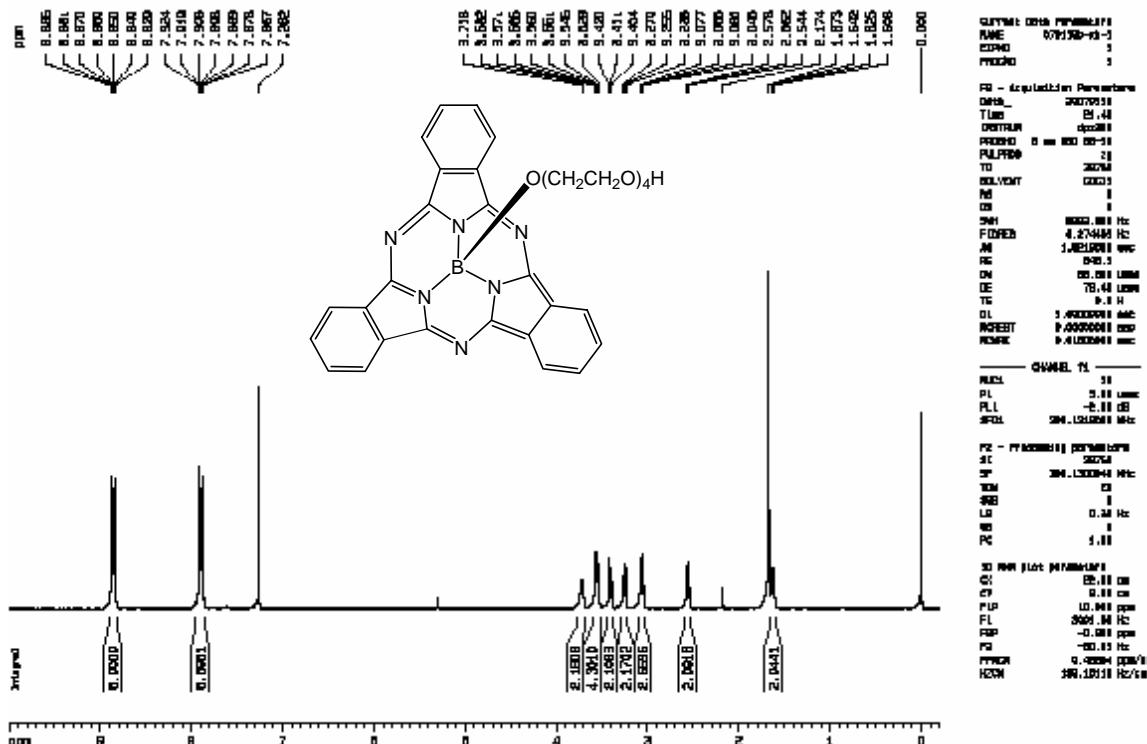
(a)

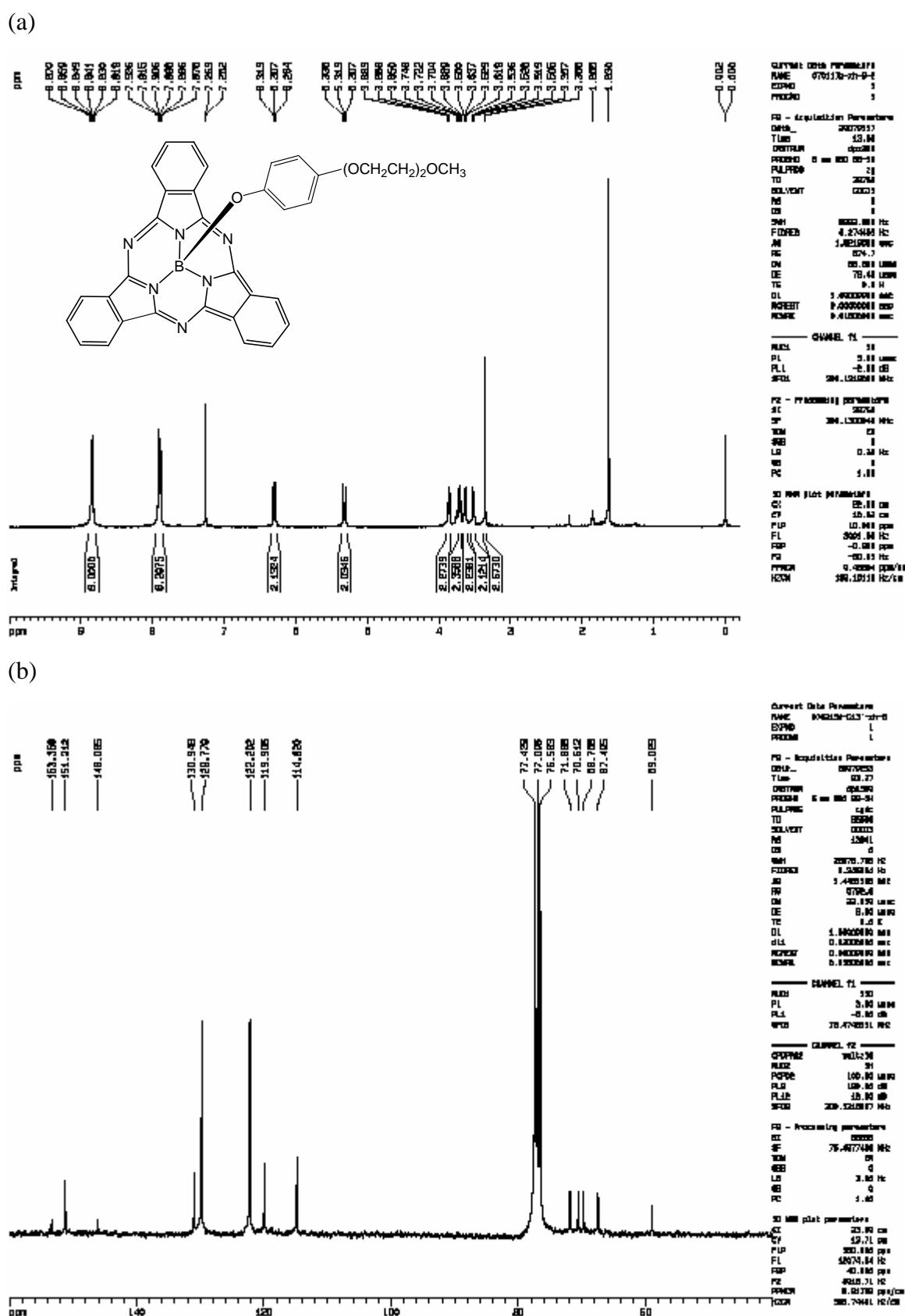


(b)

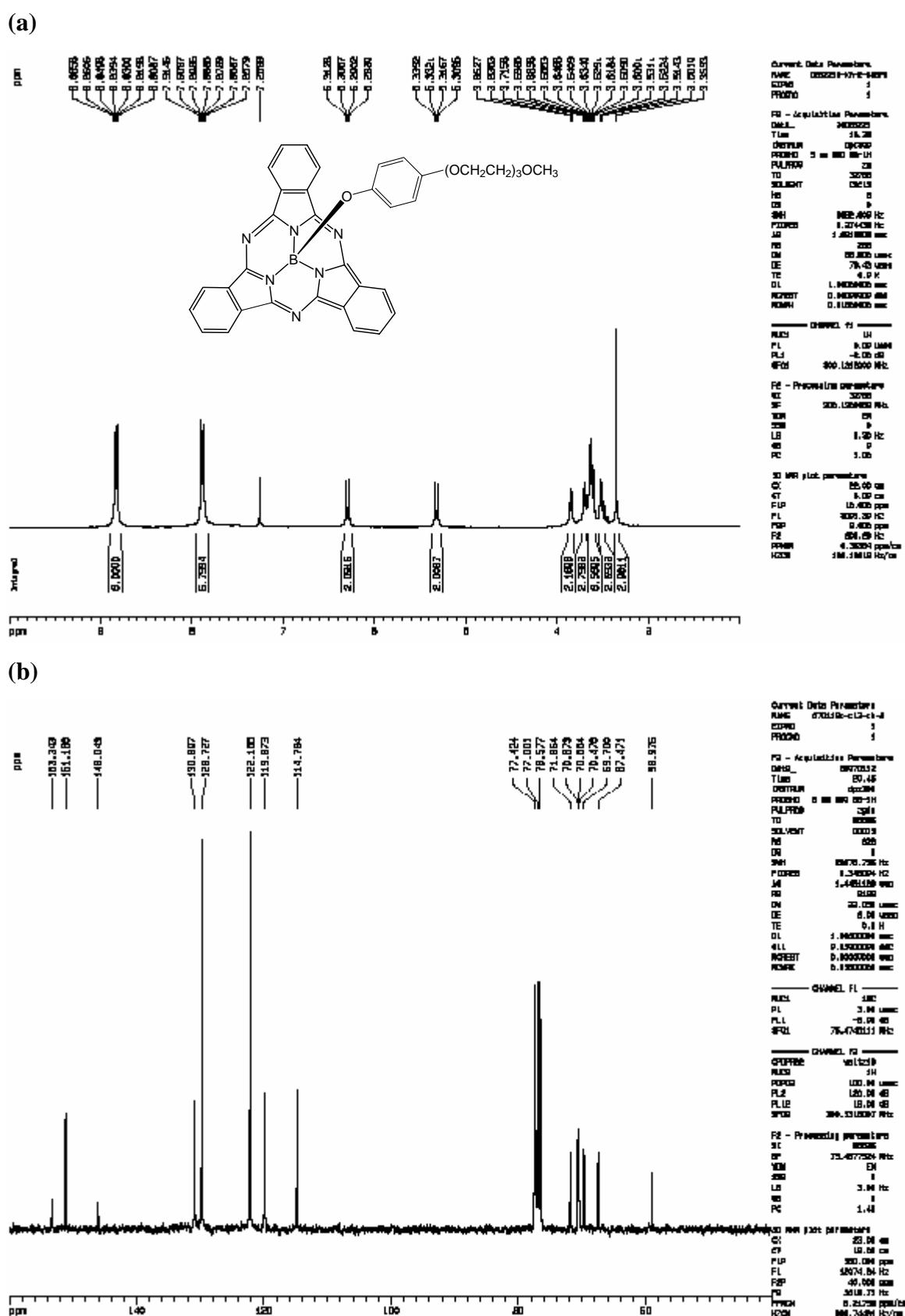
Fig. S4 (a)  $^1\text{H}$  and (b)  $^{13}\text{C}\{\text{H}\}$  NMR spectra of **2** in  $\text{CDCl}_3$ .

(a)





**Fig. S6** (a)  $^1\text{H}$  and (b)  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **4** in  $\text{CDCl}_3$ .



**Fig. S7** (a)  $^1\text{H}$  and (b)  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **5** in  $\text{CDCl}_3$ .