

Electronic Supplementary Information:

**Self-Assembly with Fluorescence Readout in a Free Base Dipyrrin–Polymer
Triggered by Metal Ion Binding in Aqueous Solution**

Rui Liu, Pothiappan Vairaprakash and Jonathan S. Lindsey*

Department of Chemistry
North Carolina State University
Raleigh, North Carolina 27695-8204

Email: jlindsey@ncsu.edu

Table of Contents

Topic	Page
1. Complexation with ZnX_2 species	S2–S3
2. NMR spectra of new compounds	S4–S13

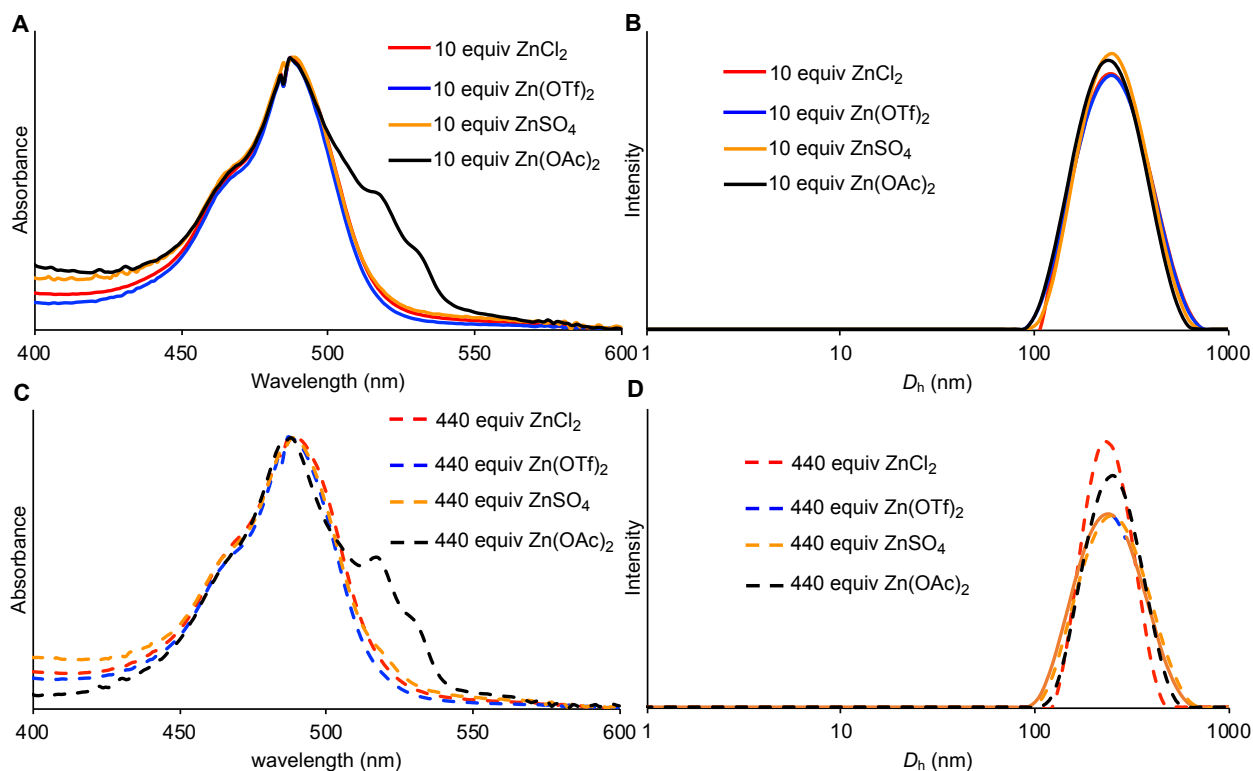


Figure S1. Data of **Pod-Dipyrrin** treated with Zn(II) in water (1.0 mg/mL) at room temperature.

(A) Absorption spectra of **Pod-Dipyrrin** treated with 10 equiv of ZnCl₂ (red line), Zn(OTf)₂ (blue line), ZnSO₄ (orange line), and Zn(OAc)₂ (black line);

(B) DLS data of **Pod-Dipyrrin** treated with 10 equiv of ZnCl₂ ($D_h = 273$ nm, red line), Zn(OTf)₂ ($D_h = 270$ nm, blue line), ZnSO₄ ($D_h = 284$ nm, orange line), and Zn(OAc)₂ ($D_h = 269$ nm, black line);

(C) absorption spectra of **Pod-Dipyrrin** treated with 440 equiv of ZnCl₂ (red dashed line), Zn(OTf)₂ (blue dashed line), ZnSO₄ (orange dashed line), and Zn(OAc)₂ (black dashed line); and

(D) DLS data of **Pod-Dipyrrin** treated with 440 equiv of ZnCl₂ ($D_h = 243$ nm, red dashed line), Zn(OTf)₂ ($D_h = 256$ nm, blue dashed line), ZnSO₄ ($D_h = 268$ nm, orange dashed line), and Zn(OAc)₂ ($D_h = 260$ nm, black dashed line). The change in particle size in going from 10 to 440 equiv is -30 nm (ZnCl₂), -14 nm (Zn(OTf)₂), -16 nm (ZnSO₄), and -9 nm (Zn(OAc)₂).

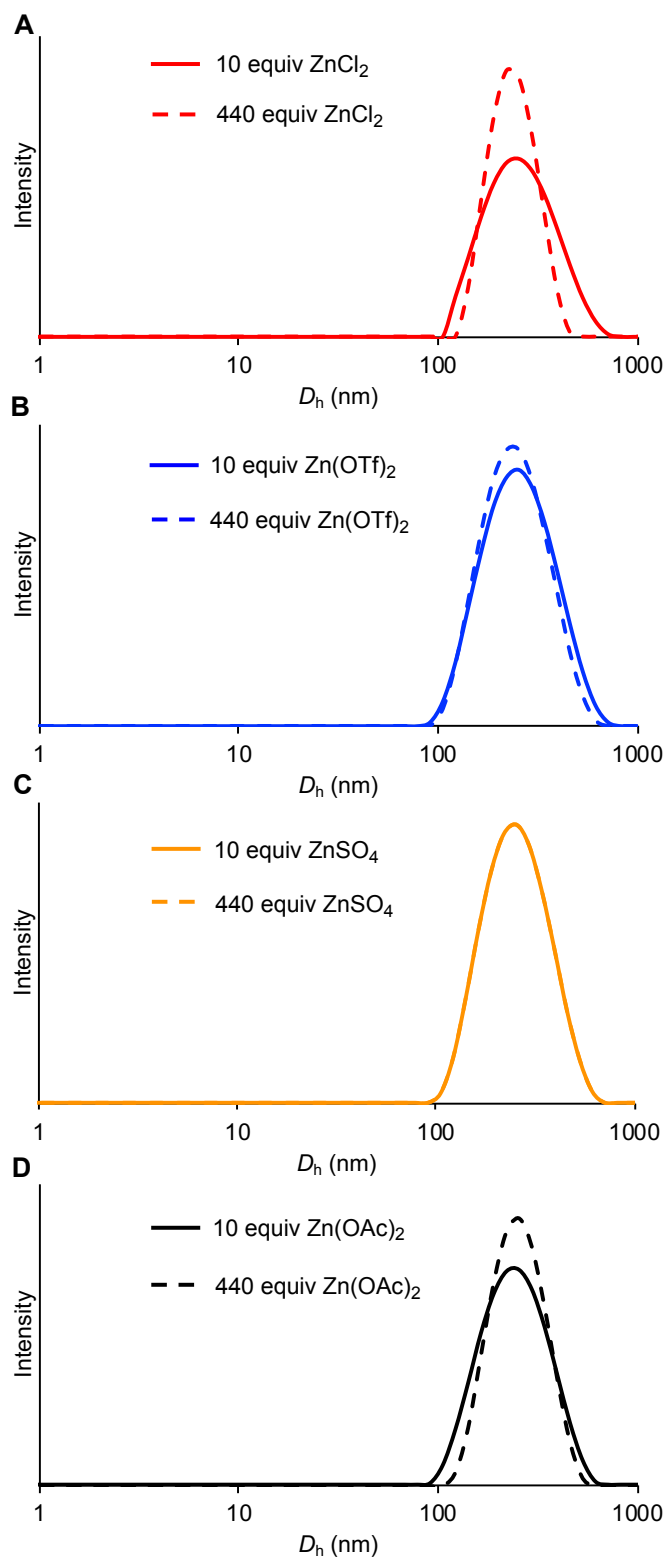


Figure S2. DLS data of **Pod-Dipyrrin** in water (1.0 mg/mL) treated with 10 equiv Zn(II) (solid line) and 440 equiv Zn(II) (dashed line) at room temperature. (A) ZnCl₂; (B) Zn(OTf)₂; (C) ZnSO₄ (the data are essentially identical); and (D) Zn(OAc)₂.

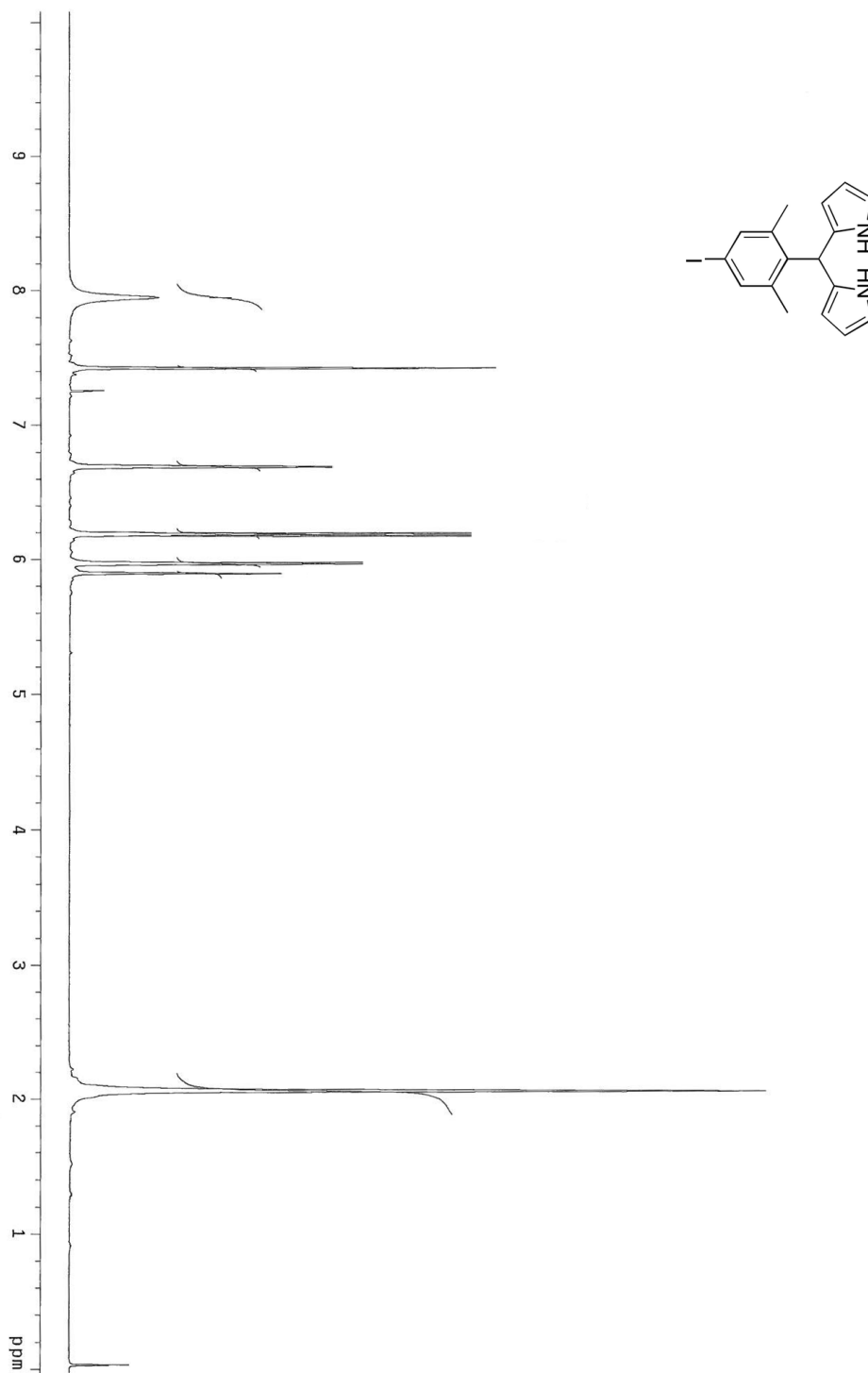


Figure S3. ^1H NMR spectrum of **2**.

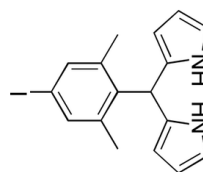
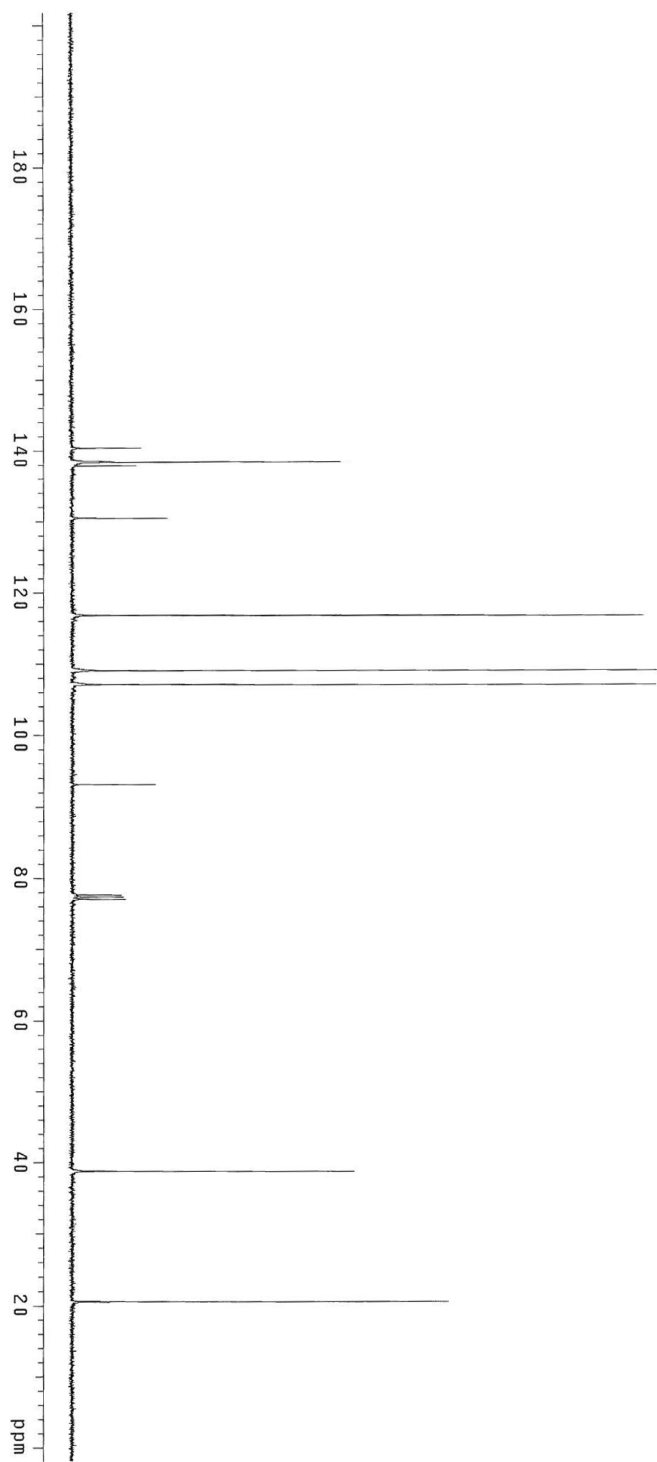


Figure S4. ^{13}C NMR spectrum of **2**.

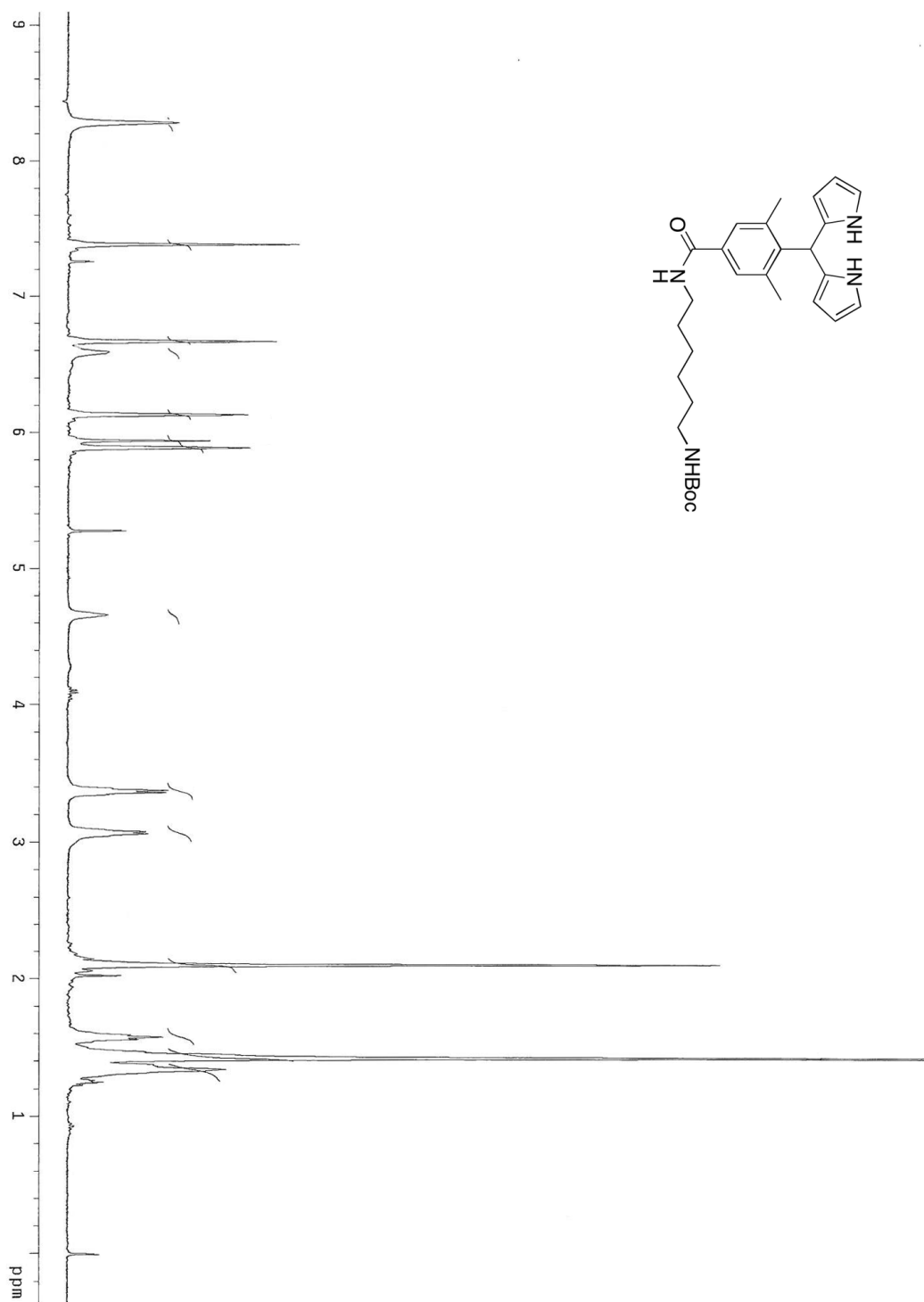


Figure S5. ^1H NMR spectrum of **3**.

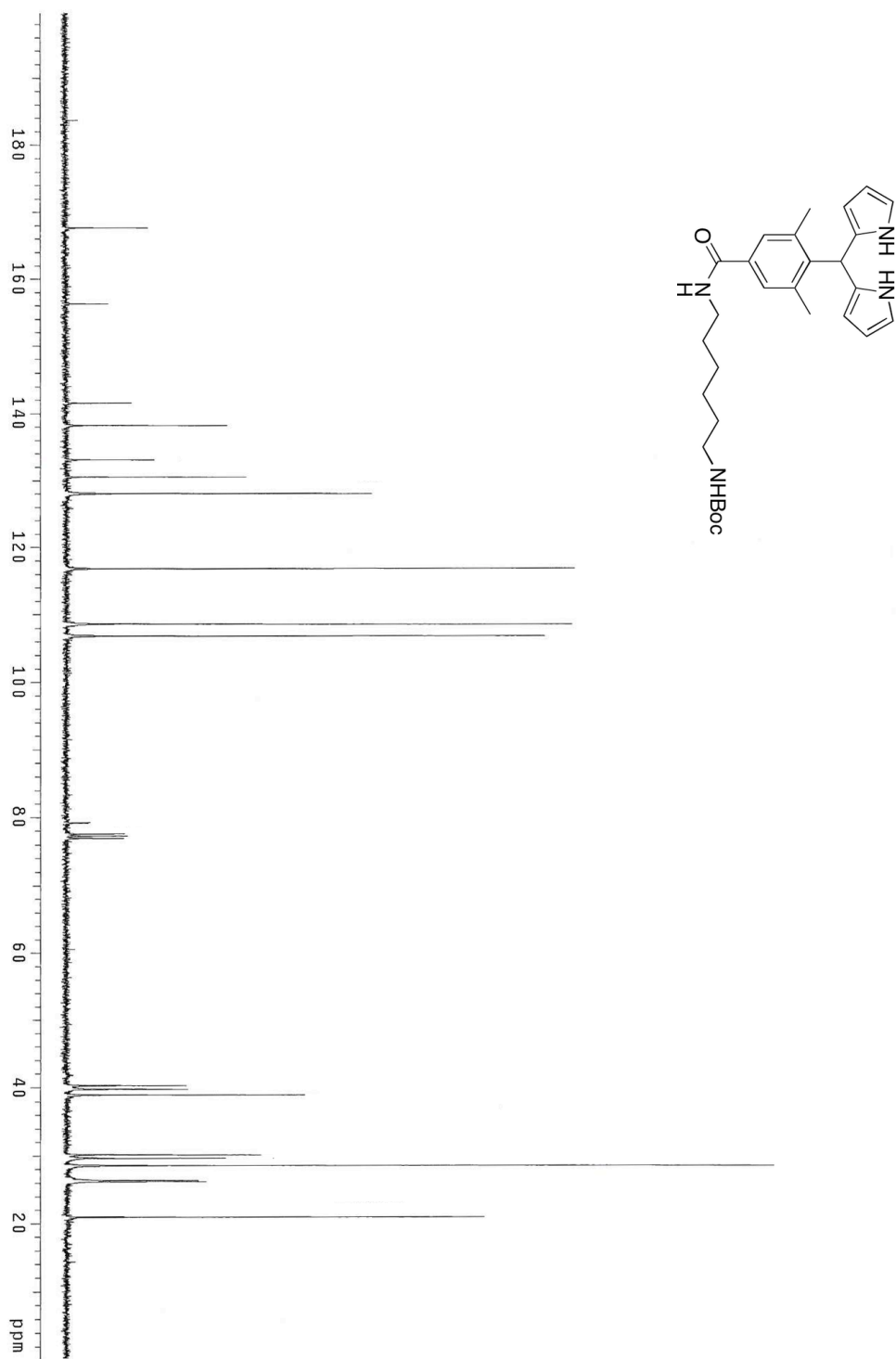


Figure S6. ^{13}C NMR spectrum of **3**.

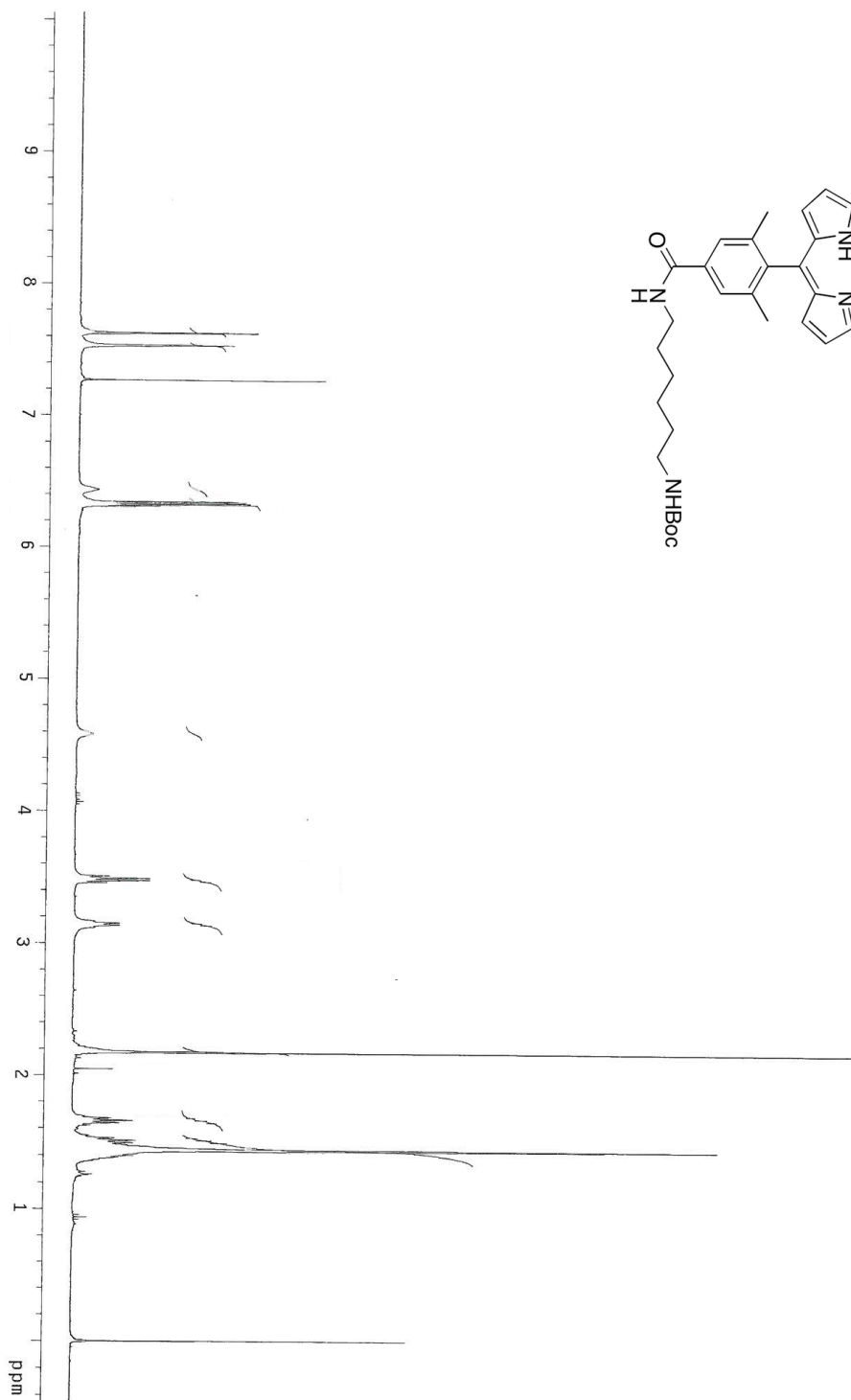


Figure S7. ¹H NMR spectrum of 4.

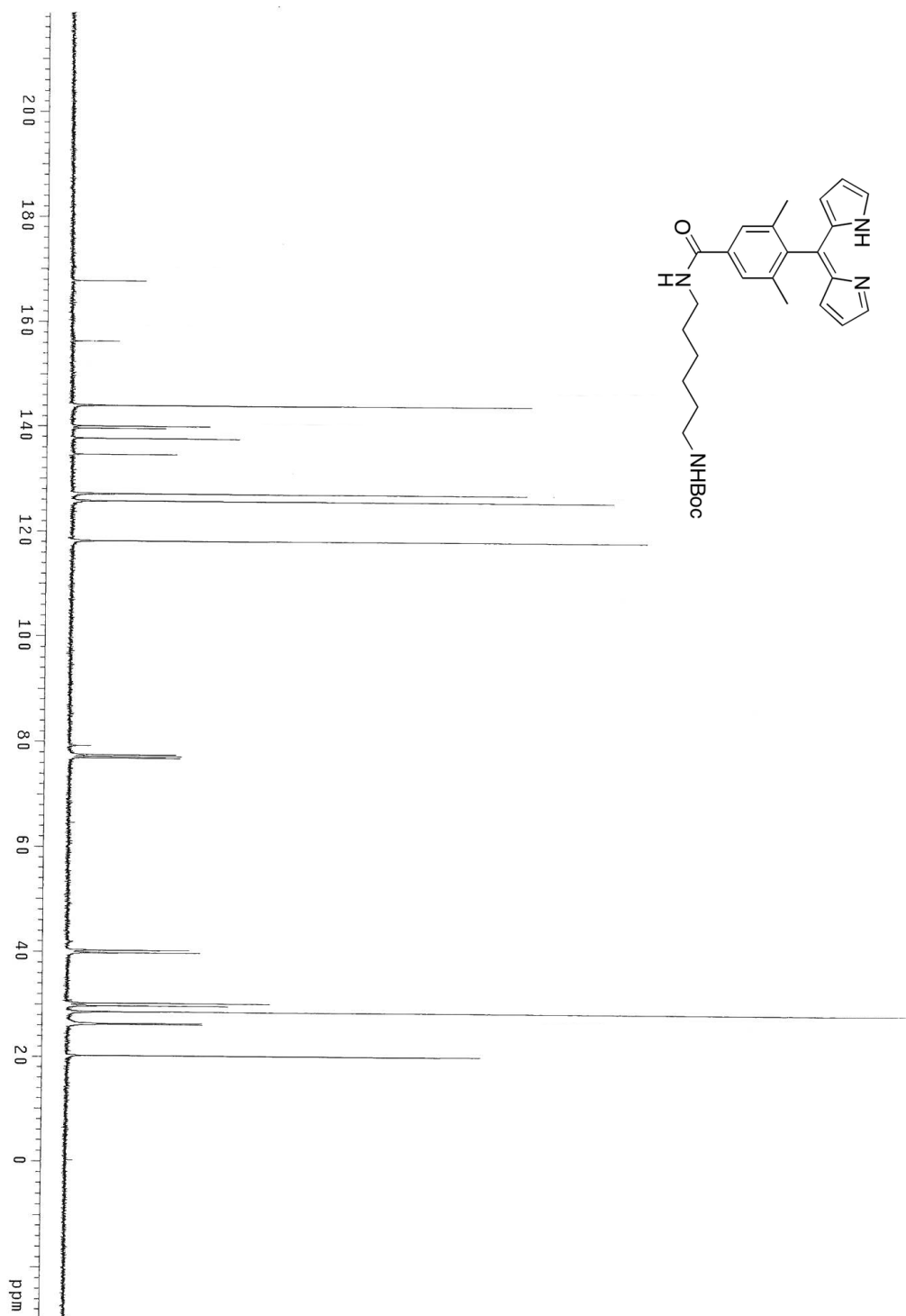


Figure S8. ^{13}C NMR spectrum of 4.

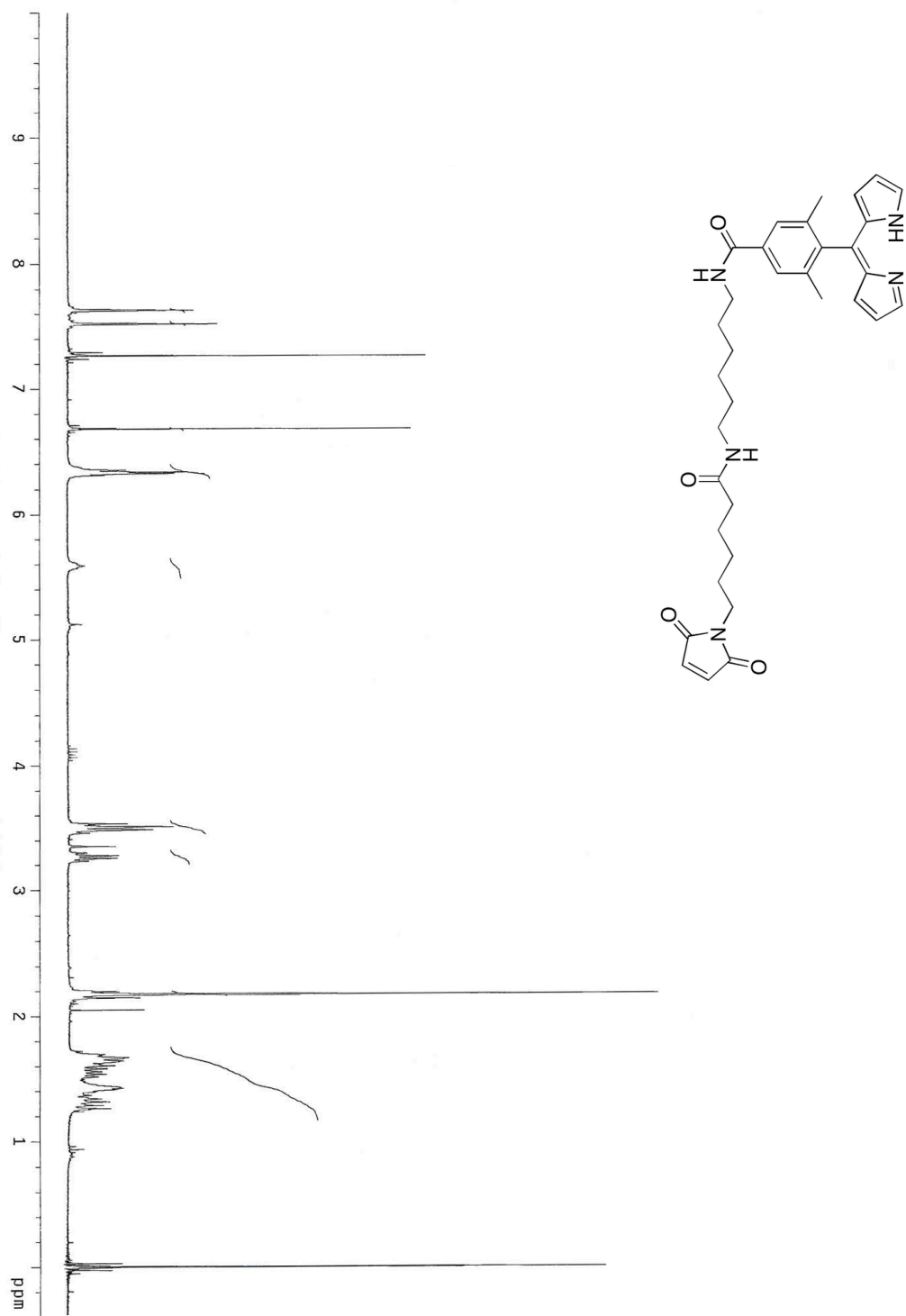


Figure S9. ^1H NMR spectrum of **5**.

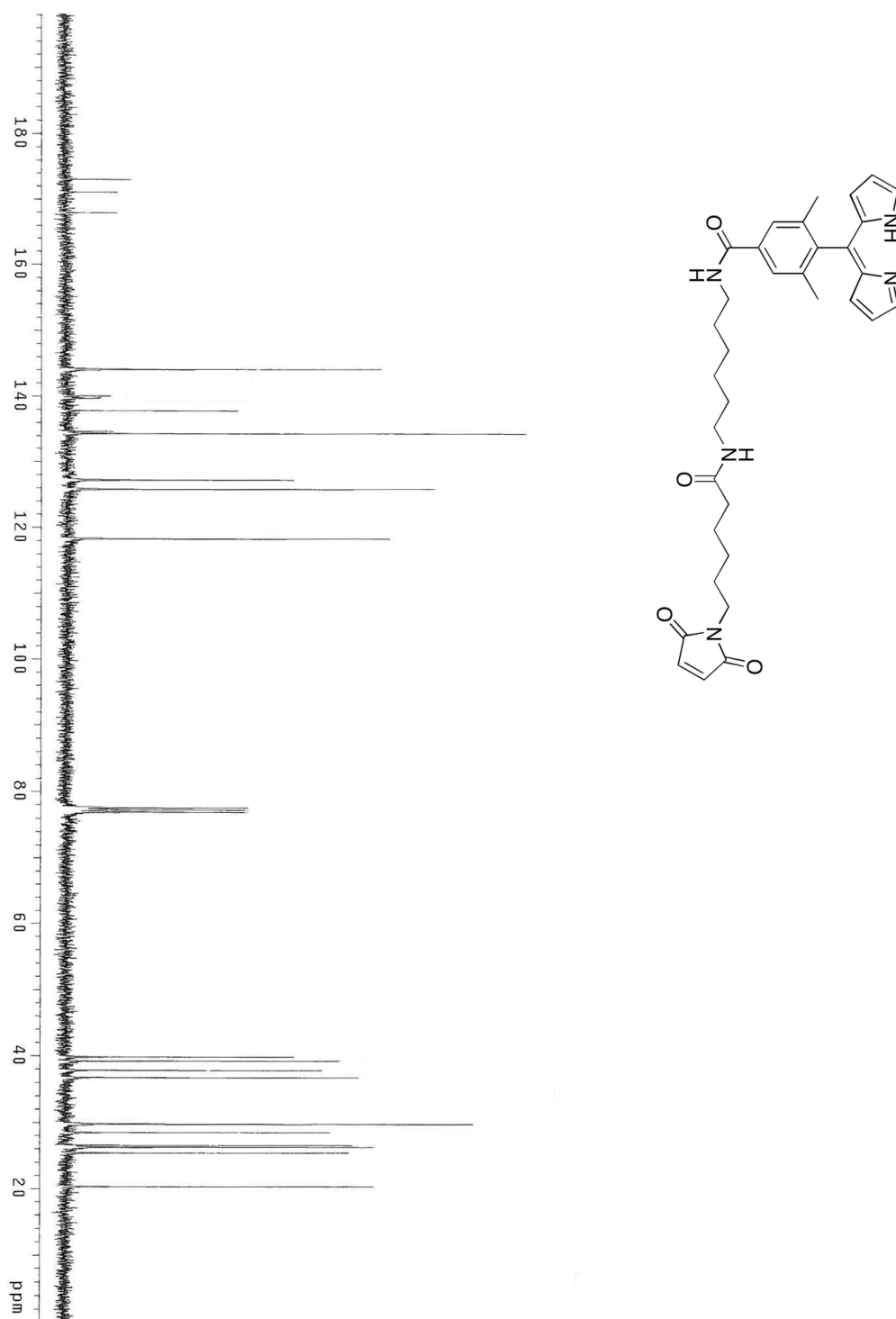


Figure S10. ^{13}C NMR spectrum of **5**.

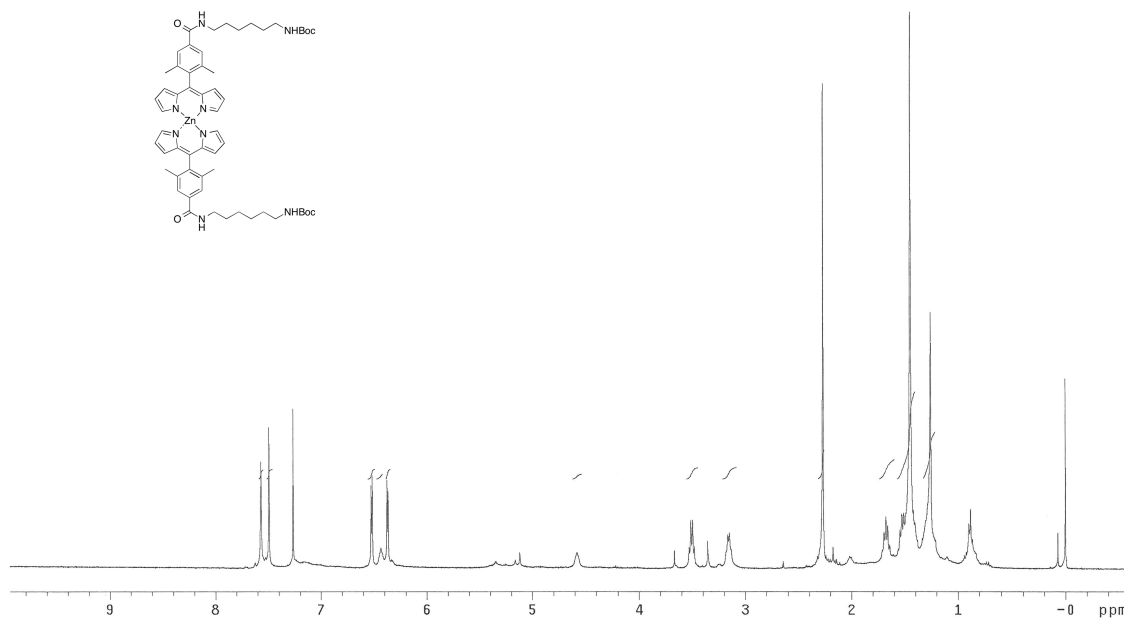


Figure S11. ¹H NMR spectrum of **6**.

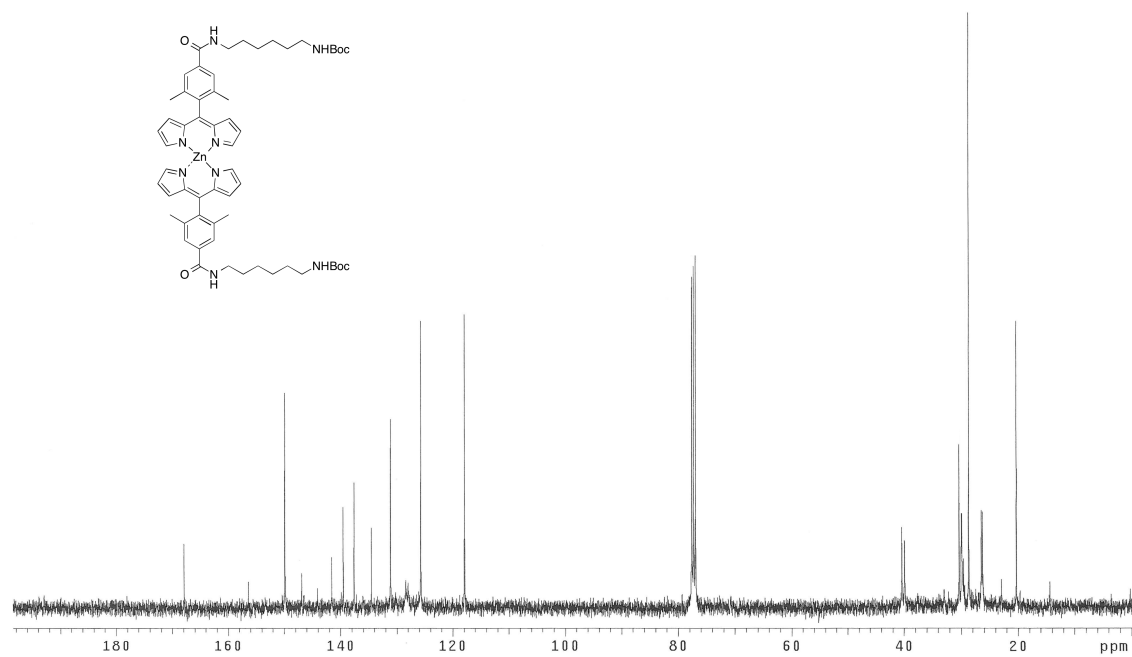


Figure S12. ^{13}C NMR spectrum of 6.