

Electronic Supplementary Information (ESI) to:

**Oxazolochlorins 13. PEGylated *meso*-arylporpholactone metal complexes as
optical cyanide sensors in water**

Jill L. Worlinsky, Steven Halepas, and Christian Brückner*

*Department of Chemistry
University of Connecticut, Unit 3060
Storrs, CT 06269-3060.
U.S.A.
Fax: (+01) 860-486-2981; E-mail: c.bruckner@uconn.edu*

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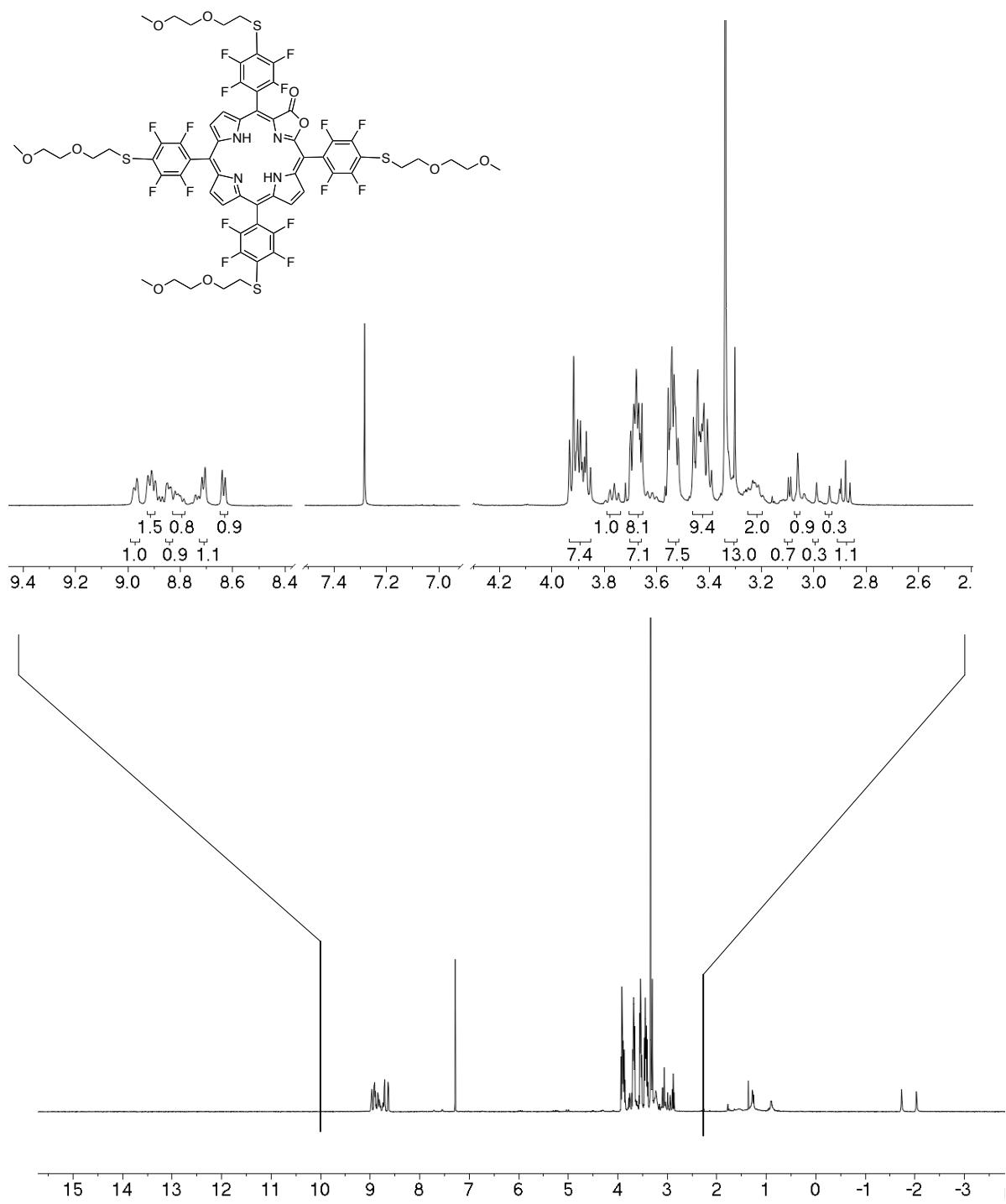


Figure 1. ¹H NMR spectrum (400 MHz, CDCl₃) of **6-MET**.

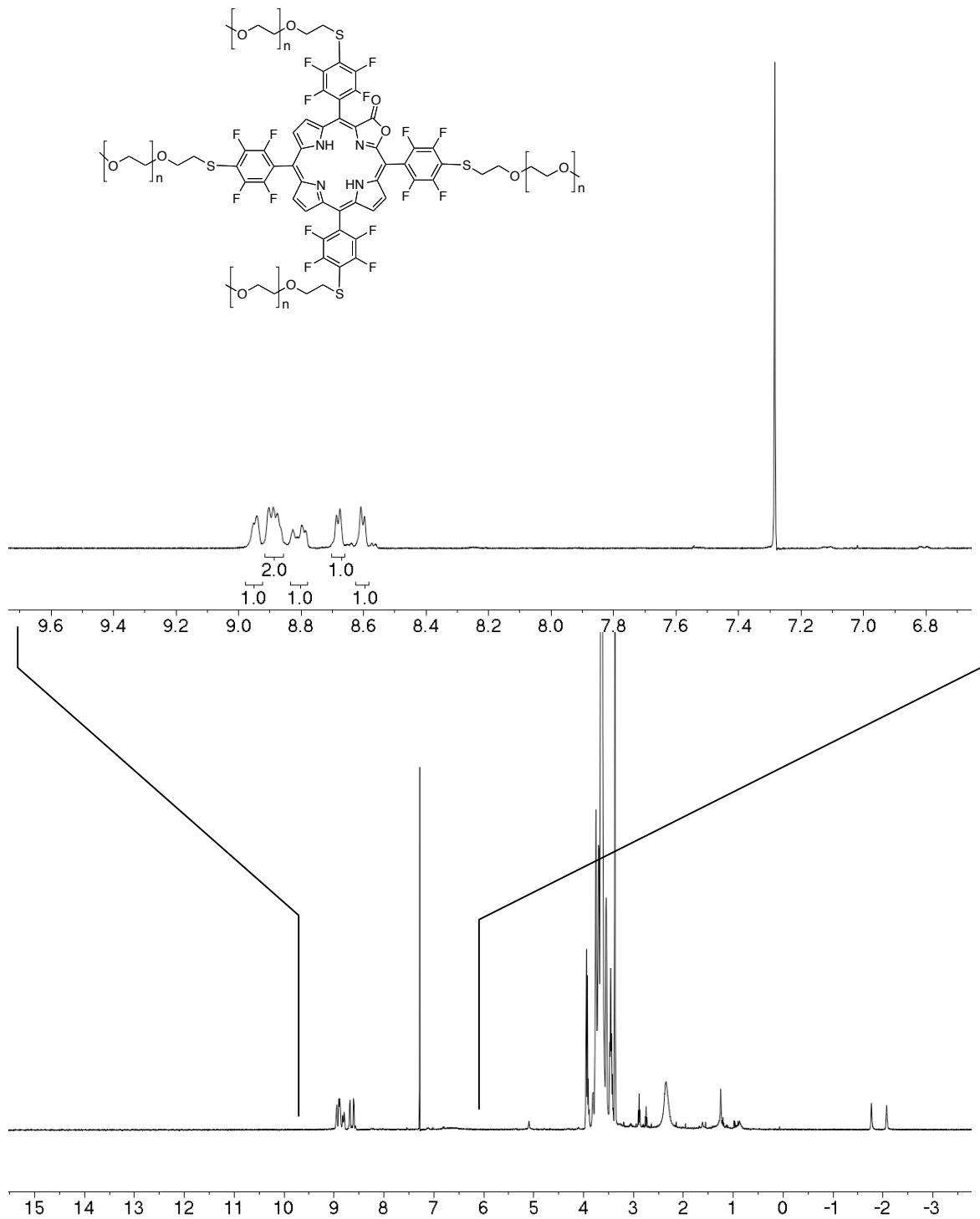


Figure 2. ^1H NMR spectrum (400 MHz, CDCl_3) of **6-PEG₁₀₀₀** ($n \sim 20$).

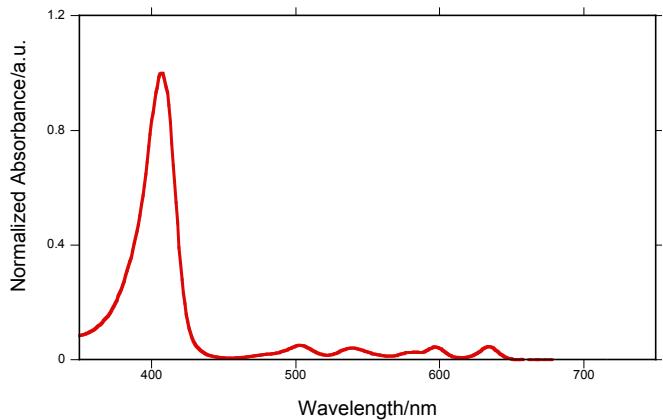


Figure 3. UV-vis spectrum (CH_2Cl_2) of **6-MET**.

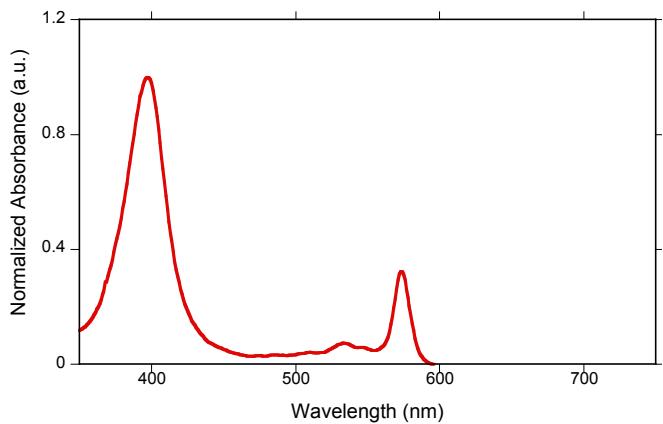


Figure 4. UV-vis spectrum (CH_2Cl_2) of **6Pt-PEG₁₀₀₀**.

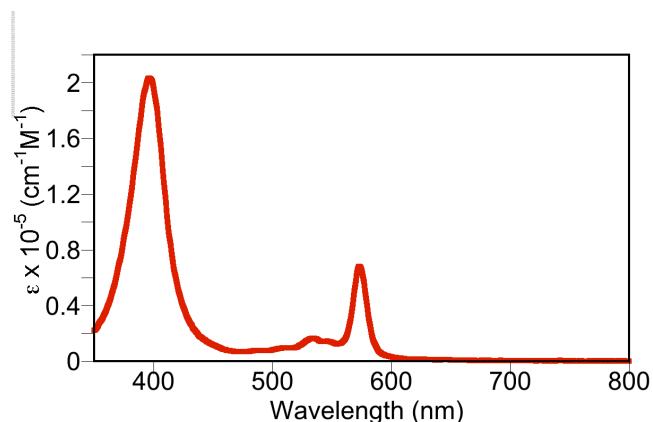


Figure 5. UV-vis spectrum (pH 7 phosphate buffer) of **6Pt-PEG₁₀₀₀**.

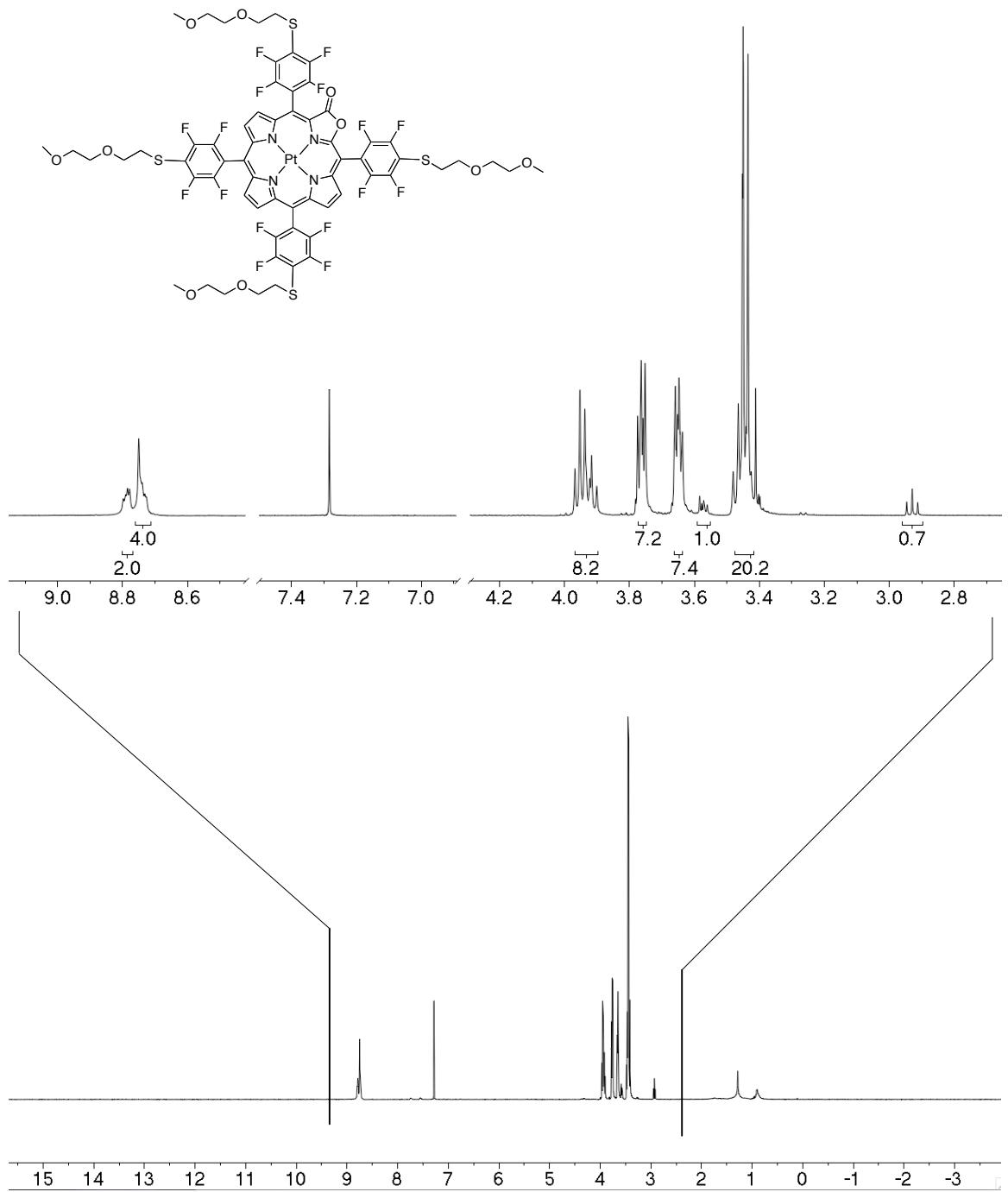


Figure 6. ^1H NMR spectrum (400 MHz, CDCl₃) of **6Pt-MET**.

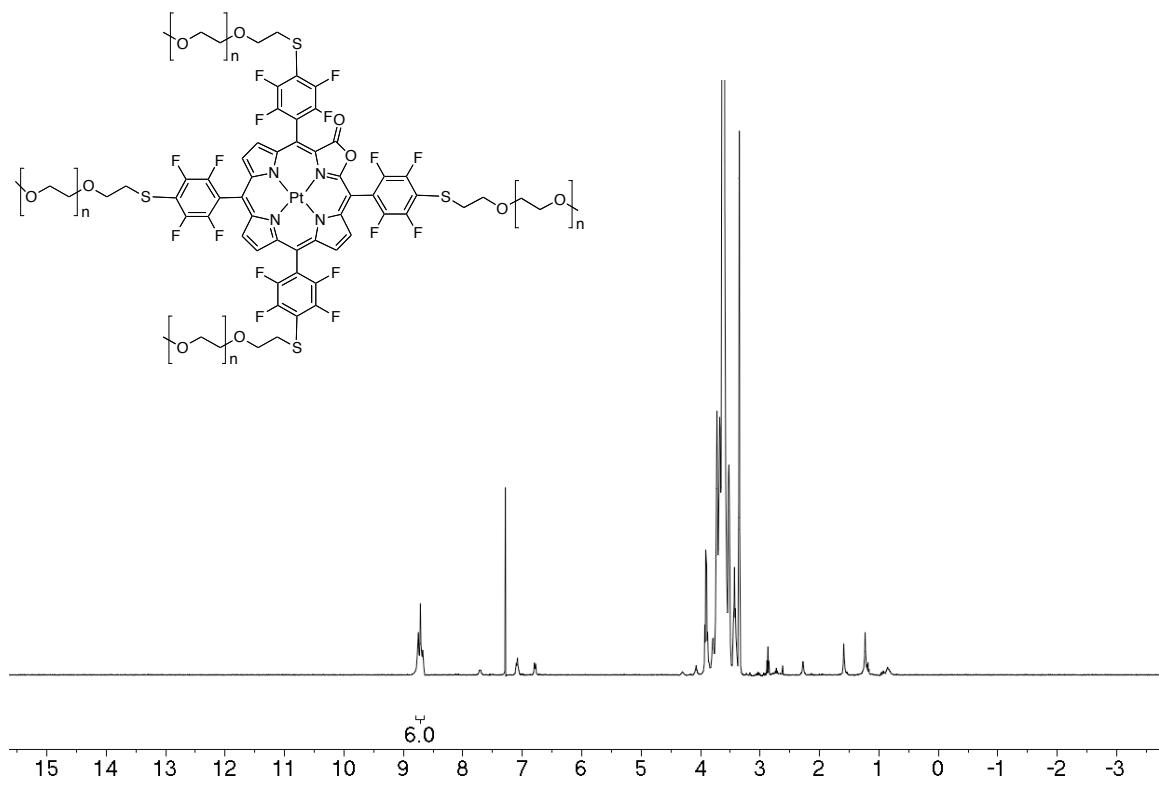


Figure 7. ^1H NMR spectrum (400 MHz, CDCl_3) of **6Pt-PEG₁₀₀₀** ($M_n \sim 1000$).

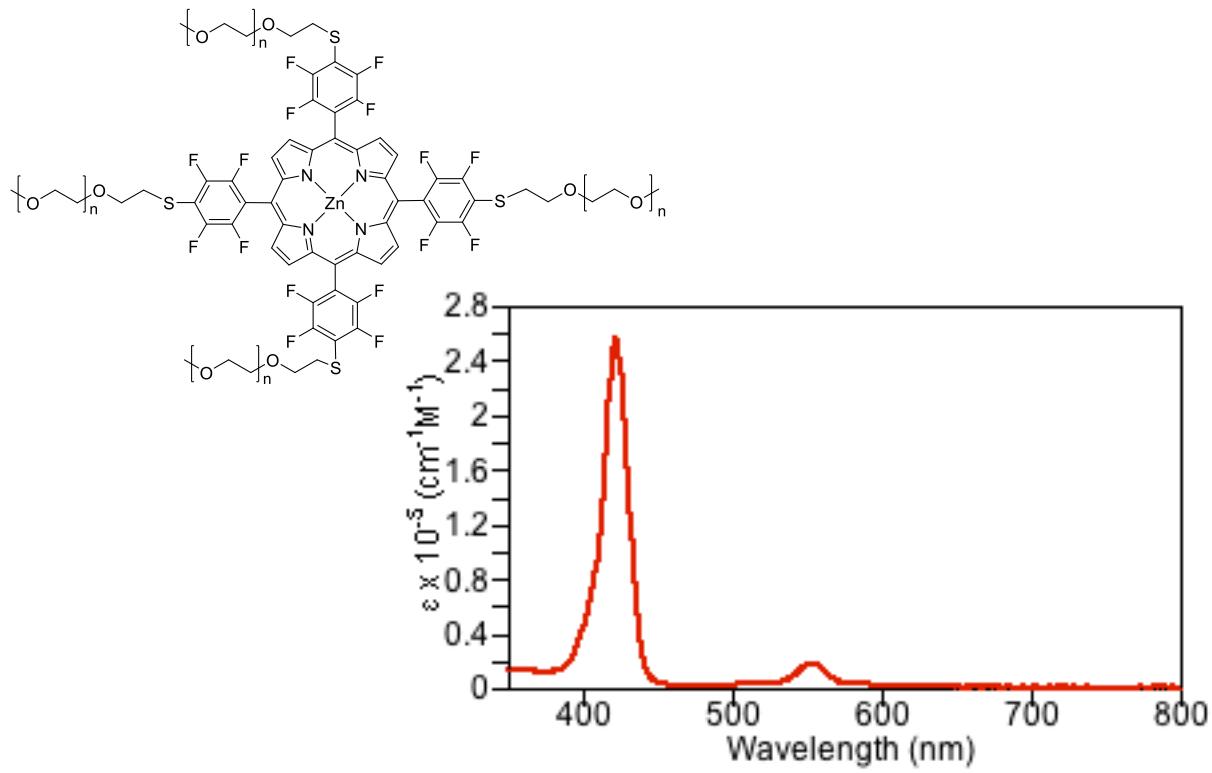


Figure 8. UV-vis spectrum (pH 7 phosphate buffer) of **1Zn-PEG₁₀₀₀**.

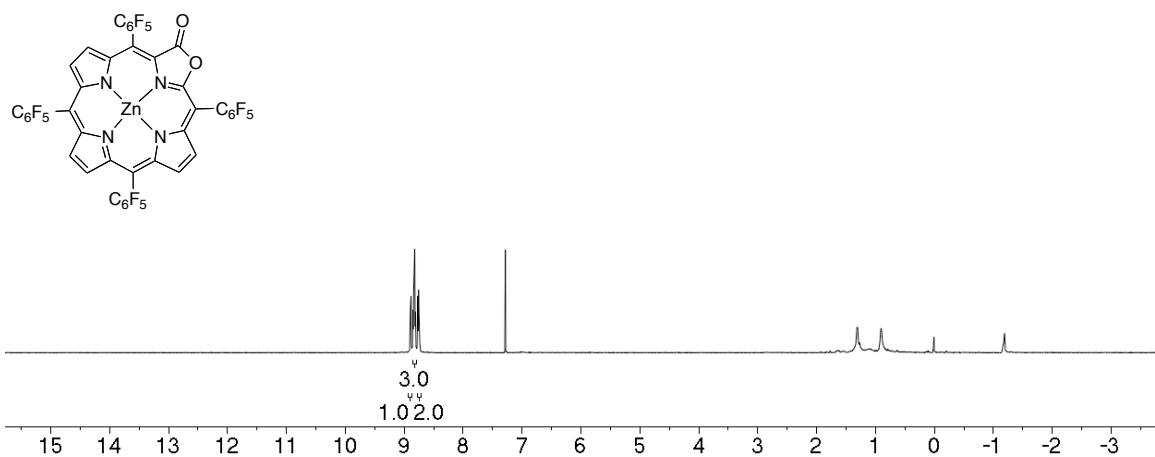


Figure 9. ¹H NMR spectrum (400 MHz, CDCl₃) of **6Zn**.

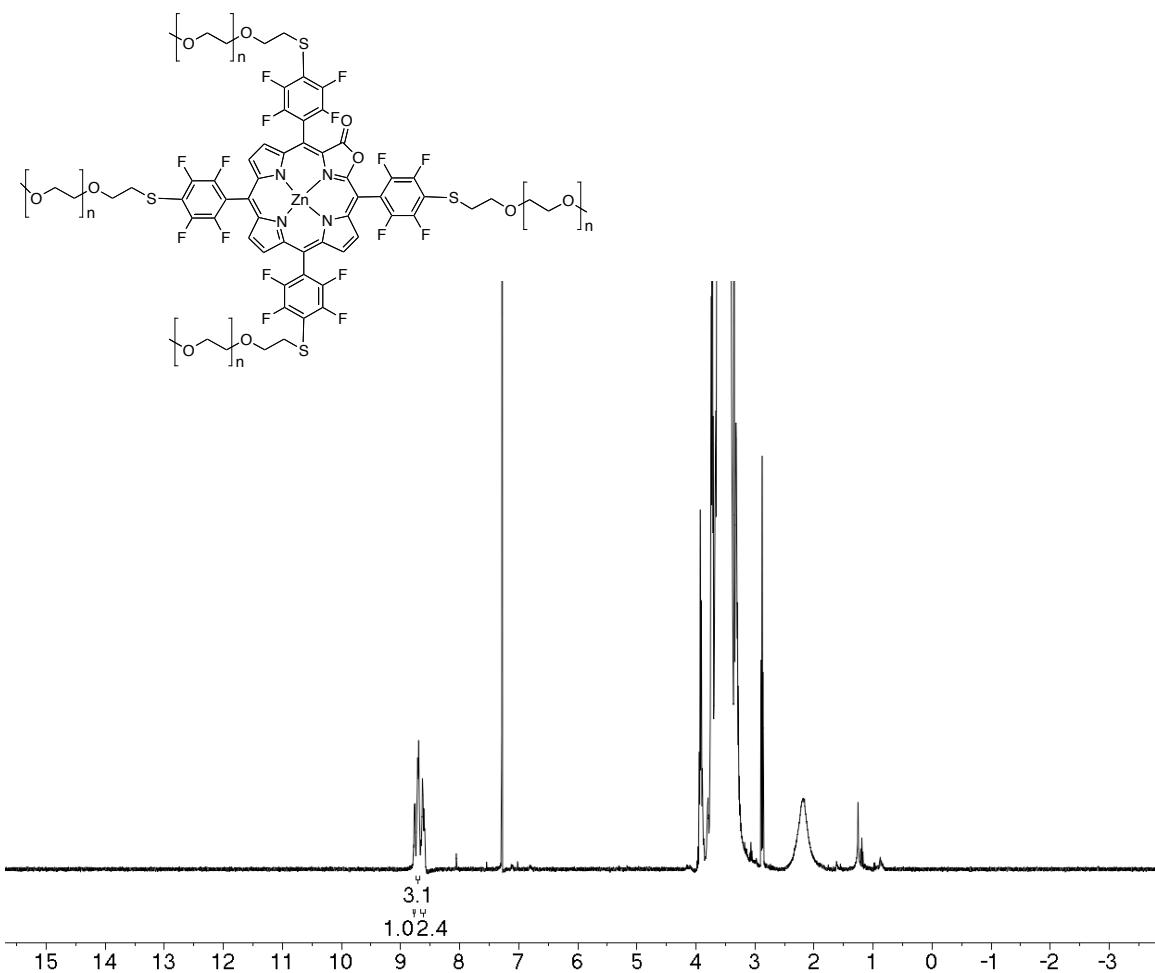


Figure 10. ¹H NMR spectrum (400 MHz, CDCl₃) of **6Zn-PEG₁₀₀₀**.

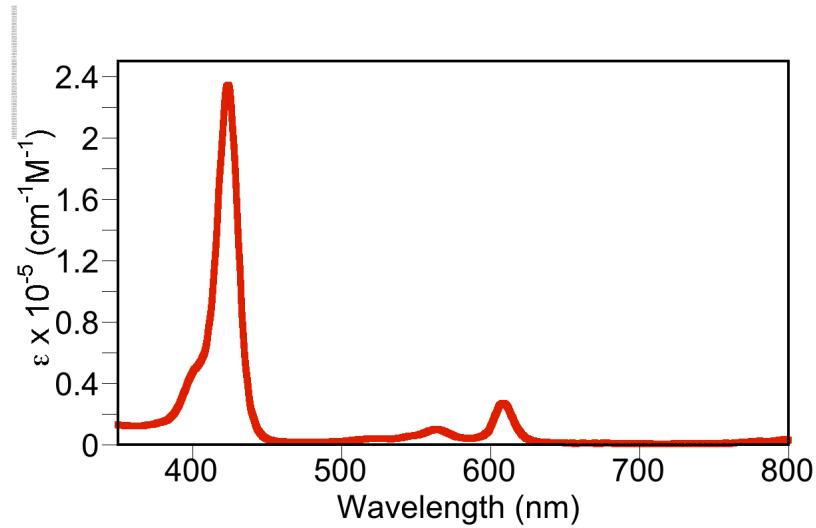


Figure 11. UV-vis spectrum (pH 7 phosphate buffer) of **6Zn-PEG₁₀₀₀**.

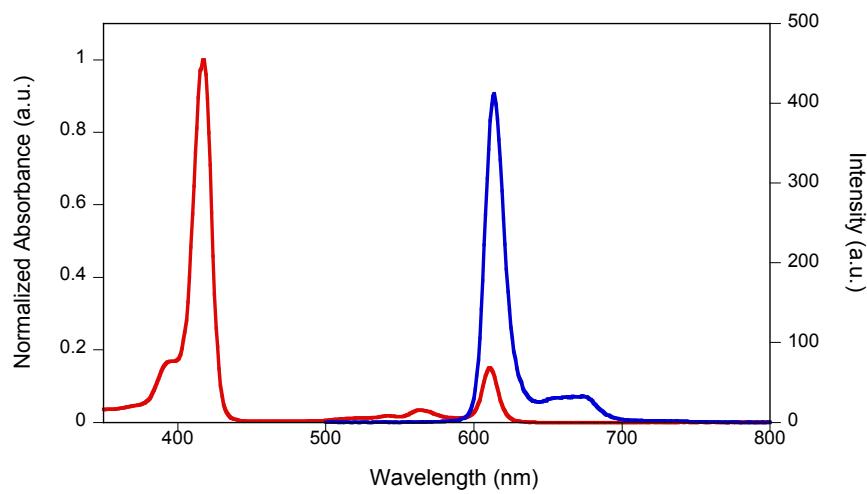


Figure 12. UV-vis and fluorescence spectrum (CH_2Cl_2) of **6Ga**.

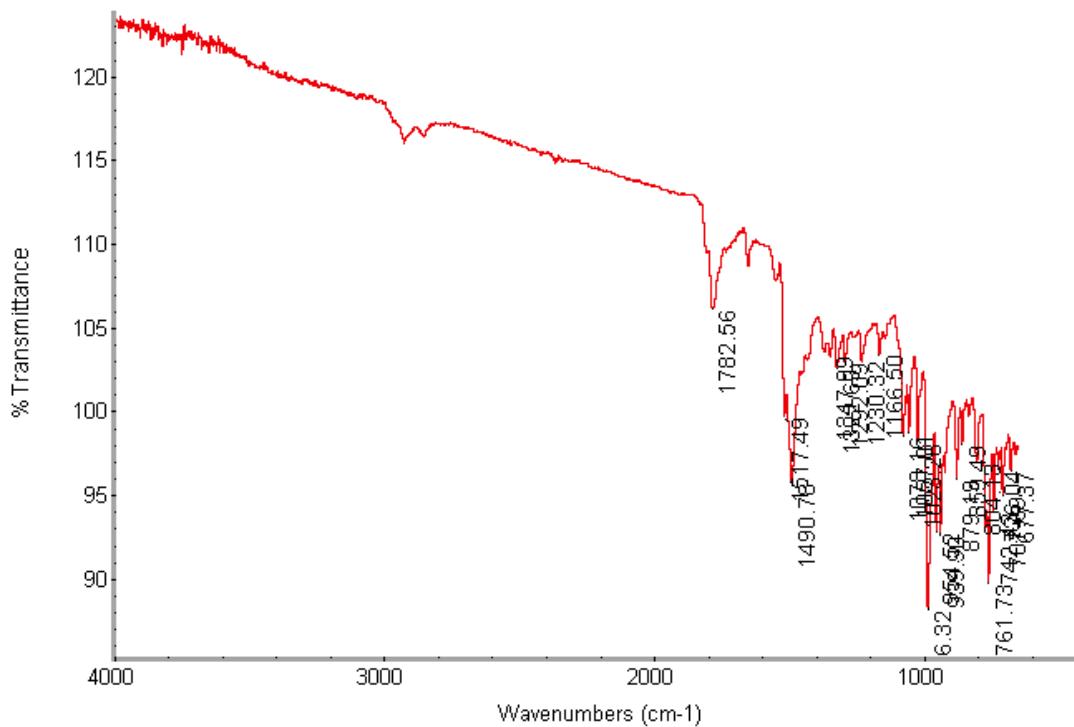


Figure 13. FT-IR spectrum (neat, diffuse reflectance) of **6Ga**.

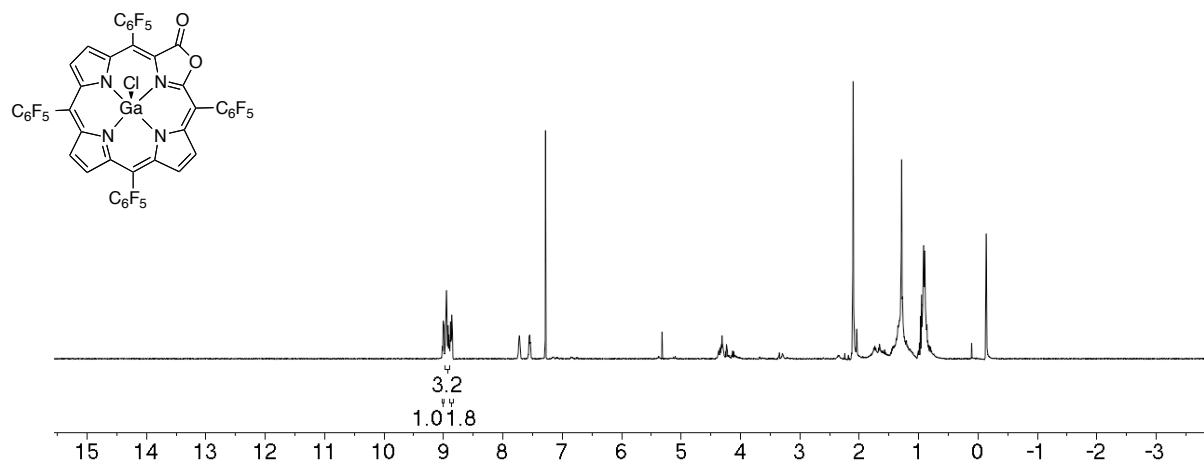


Figure 14. ^1H NMR spectrum (400 MHz, CDCl_3) of **6Ga**.

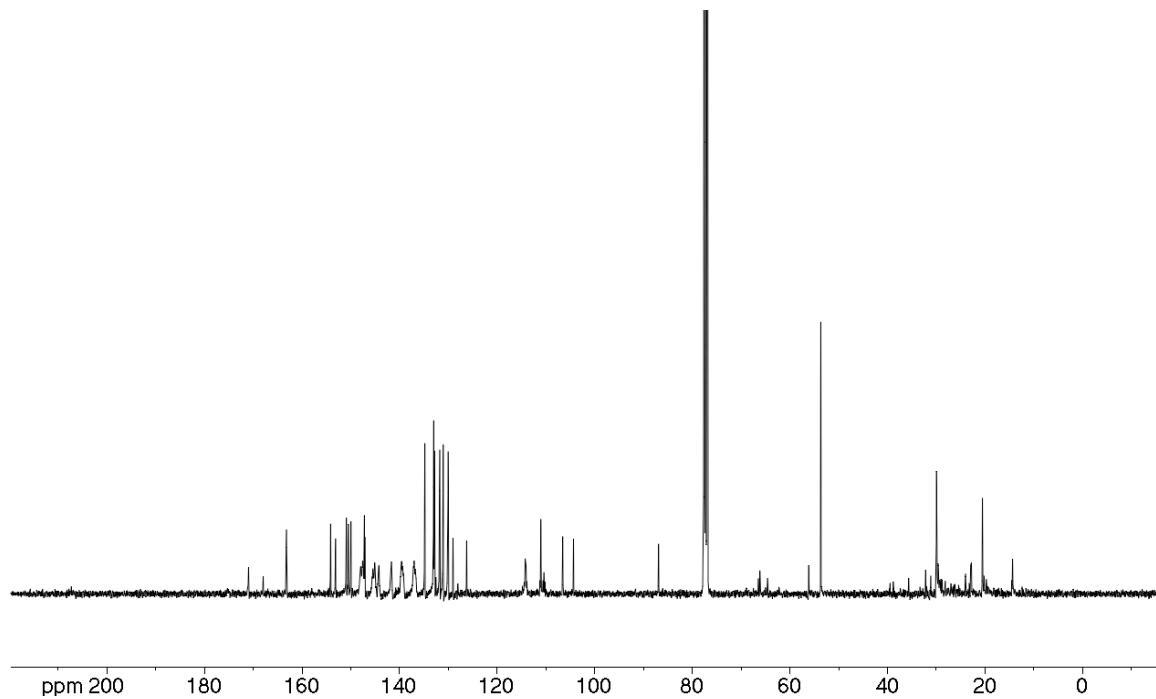


Figure 15. ¹³C NMR spectrum (100 MHz, CDCl₃) of **6Ga**.



Figure 16. UV-vis spectrum (CH₂Cl₂) of **6Ga-MET**.

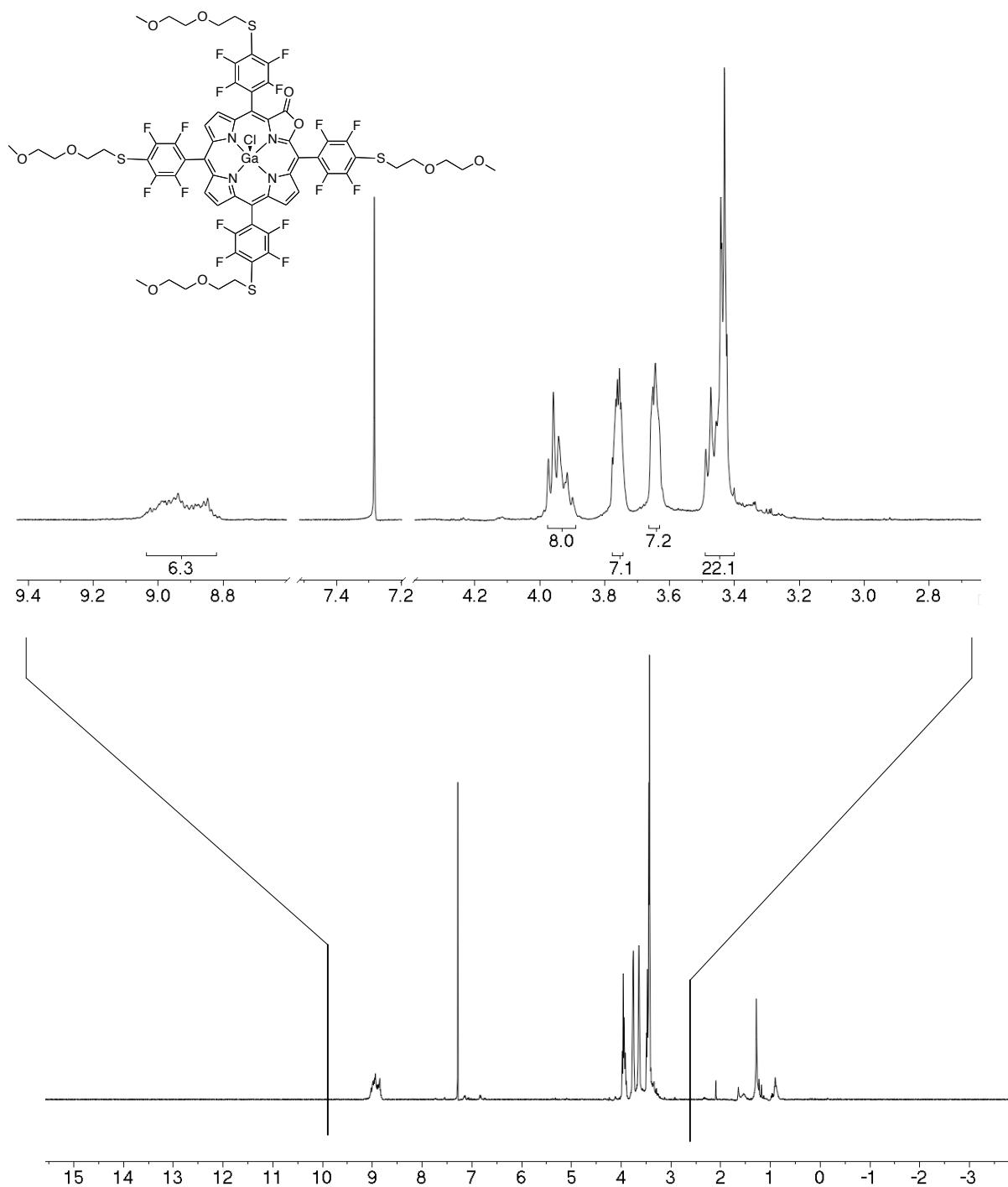


Figure 17. ^1H NMR spectrum (400 MHz, CDCl_3) of **6Ga-MET**.

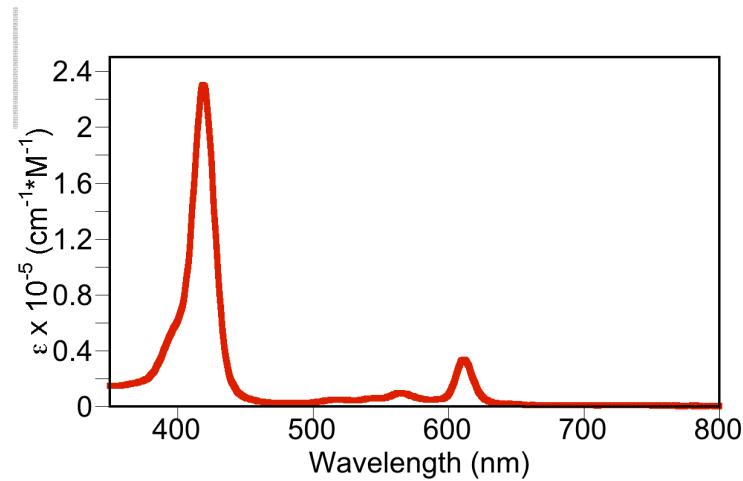


Figure 18. UV-vis spectrum (pH 7 phosphate buffer) of **6Ga-PEG₁₀₀₀**.

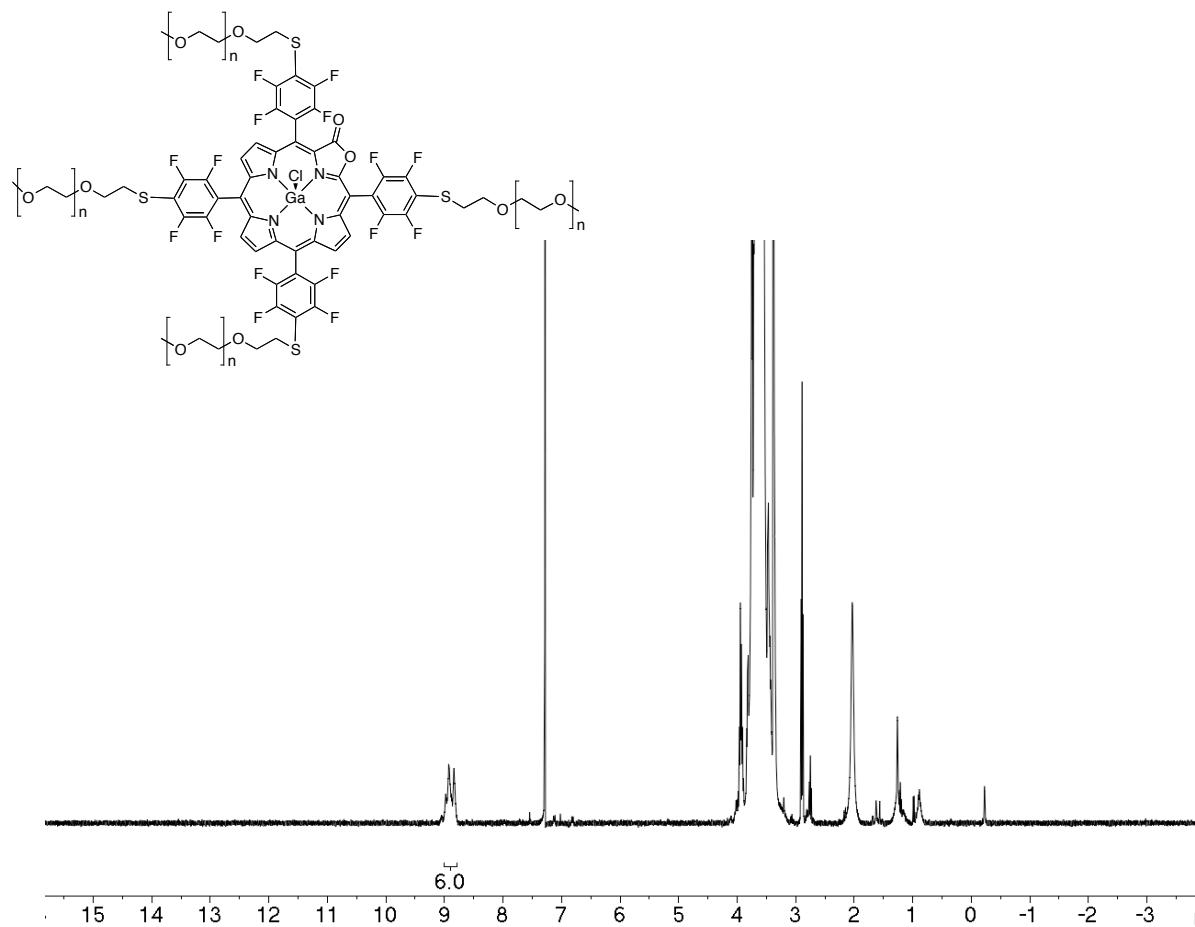


Figure 19. ¹H NMR spectrum (400 MHz, CDCl₃) of **6Ga-PEG₁₀₀₀**.

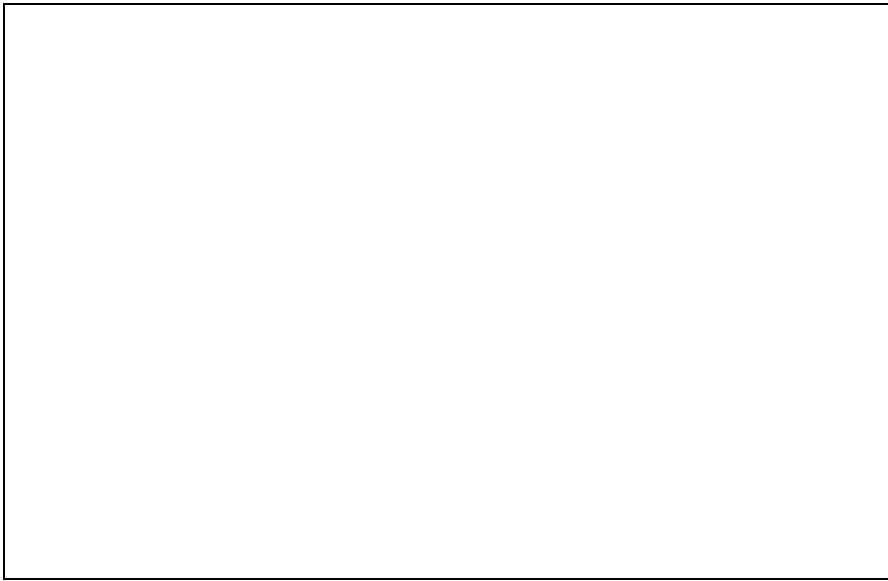


Figure 20. Spectrophotometric CN^- titration of **6Zn-PEG₁₀₀₀** (H_2O) and CN^- in the form of NaCN.

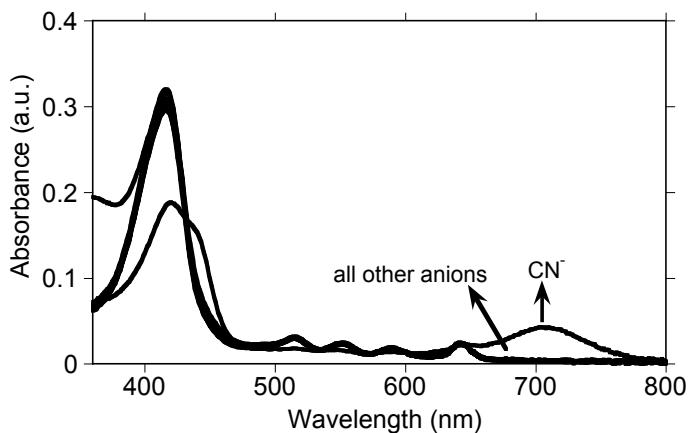


Figure 21. UV-vis spectrum of **6-PEG₁₀₀₀** upon the addition of various anions (50 equiv) in water: CN⁻, F⁻, Cl⁻, Br⁻, I⁻, AcO⁻, ClO₄⁻, NO₃⁻, NO₂⁻, H₂PO₄⁻, N₃⁻.

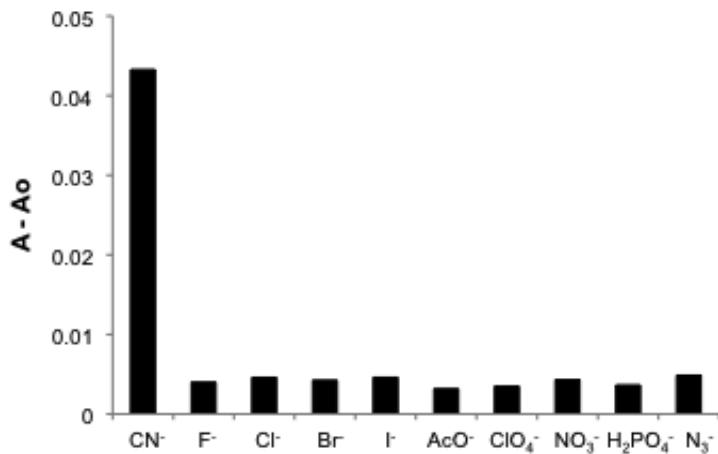


Figure 22. Absorbance intensity (A-A₀) response of a solution of **6-PEG₁₀₀₀** upon the addition of various anions (50 equiv) in water: CN⁻, F⁻, Cl⁻, Br⁻, I⁻, AcO⁻, ClO₄⁻, NO₃⁻, NO₂⁻, H₂PO₄⁻, N₃⁻.

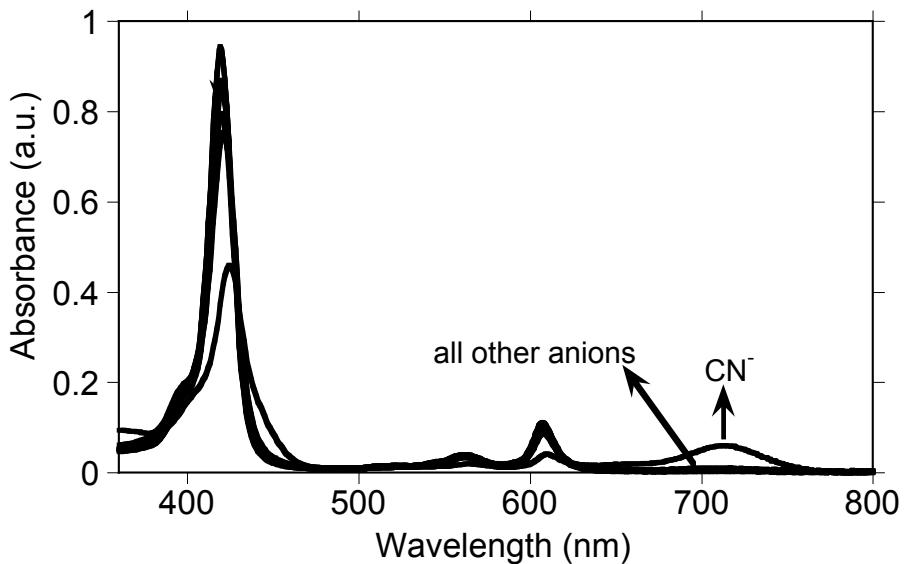


Figure 23. UV-vis spectrum of **6Ga-PEG₁₀₀₀** upon the addition of various anions (50 equiv) in water: CN⁻, F⁻, Cl⁻, Br⁻, I⁻, AcO⁻, ClO₄⁻, NO₃⁻, NO₂⁻, H₂PO₄⁻, N₃⁻.

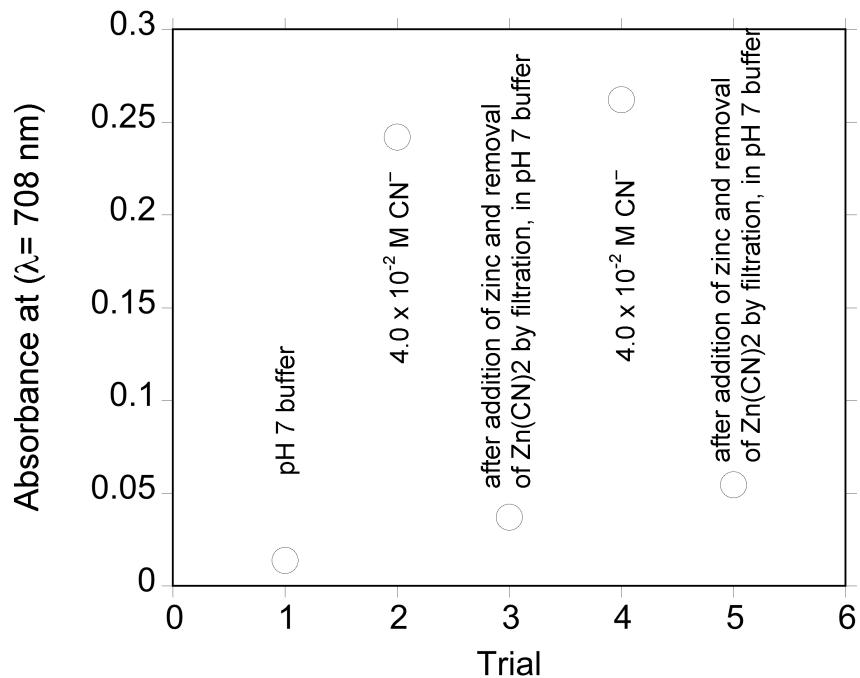


Figure 24. Absorbance intensity at $\lambda_{\max} = 708 \text{ nm}$ of **6Ga-PEG₁₀₀₀** ($7.9 \times 10^{-6} \text{ M}$, 3 mL initial volume) in pH 7 phosphate buffer after repeated exposures to NaCN ($4.0 \times 10^{-2} \text{ M}$), followed by precipitation of the cyanide with ZnCl₂ (200 μL of 100 mM ZnCl₂), followed by filtration through a plug of Celite®.

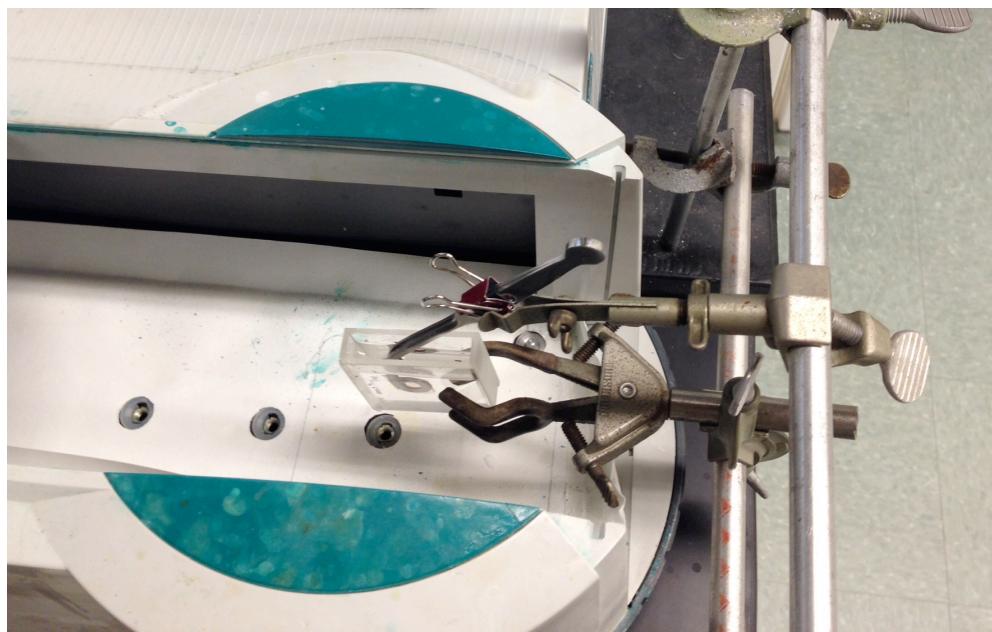


Figure 25. Experimental setup for the Nafion® membrane measurements: Membrane held by stainless steel washers in a cuvette held into the beam of the Cary 50 UV-vis spectrophotometer.

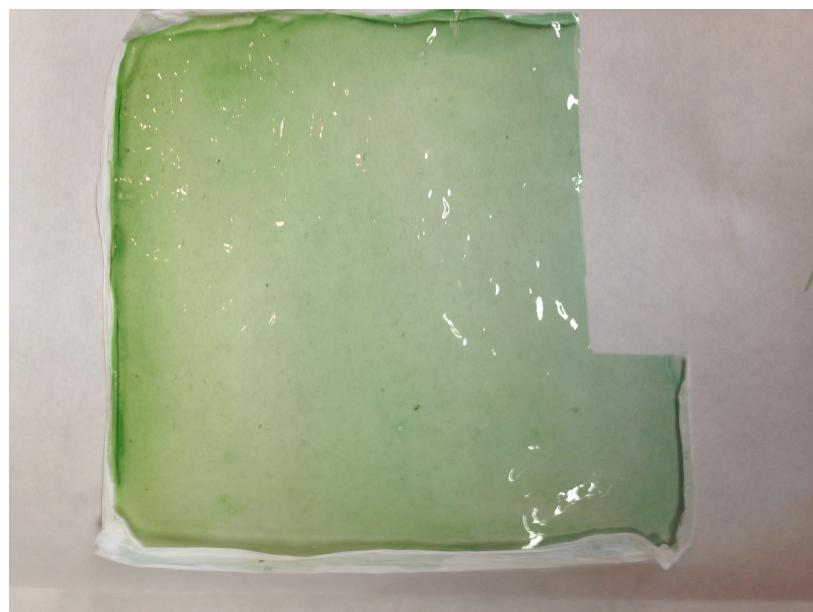


Figure 26. Photograph of the finished 5 x 5 in Nafion® membrane with embedded **6Ga-PEG₁₀₀₀** (some small membrane samples taken).