Supporting Information for:

A Highly Fluorescent PN-Heterocycle-fused Pyrene Derivative with Strong Self-dimerization through Hydrogen Bonding

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Additional Crystallographic Figures

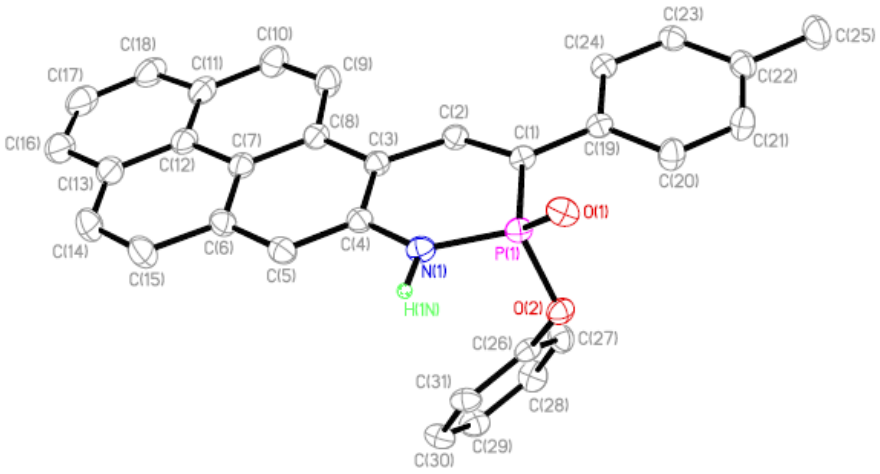

Figure S1. ORTEP drawing of PN-fused pyrene **2**; thermal ellipsoids drawn at 30% probability. Crystals grown from slow layering of pentane into a concentrated solution of **2** in chloroform.

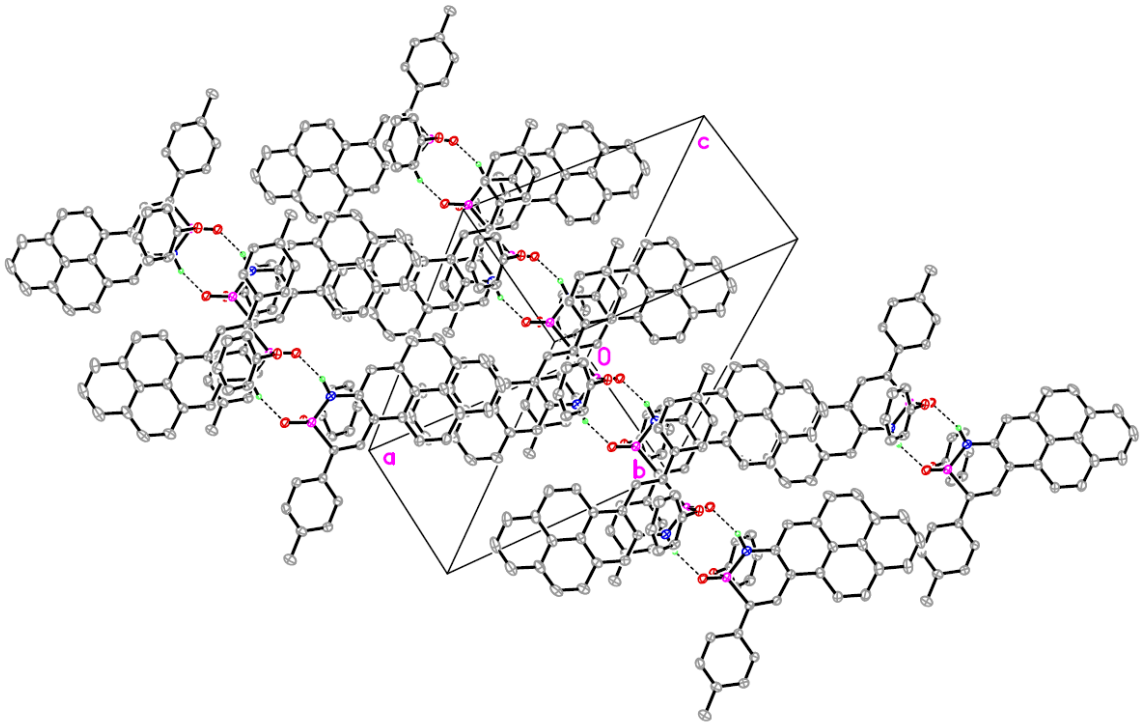

Figure S2. ORTEP drawing of the crystal packing of **2**. Crystals grown from slow layering of pentane into a concentrated solution of **2** in chloroform.

Photophysical Studies in Different Solvents and the Solid-state

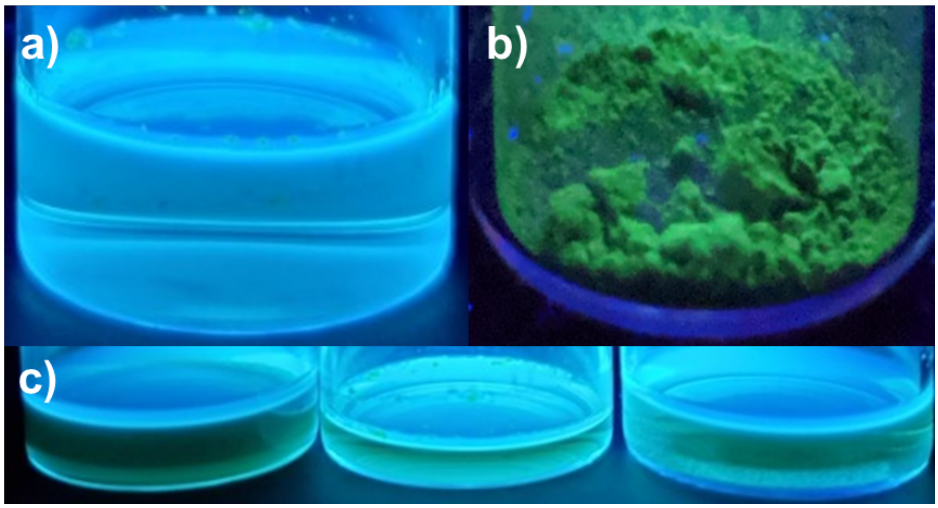

Figure S3. Fluorescence images of **2** in a) chloroform (*ca.* 1 μM), b) the solid state, and c) (left to right) toluene, chloroform, and methanol at *ca.* 4 mM in concentration. All samples were excited at 365 nm.

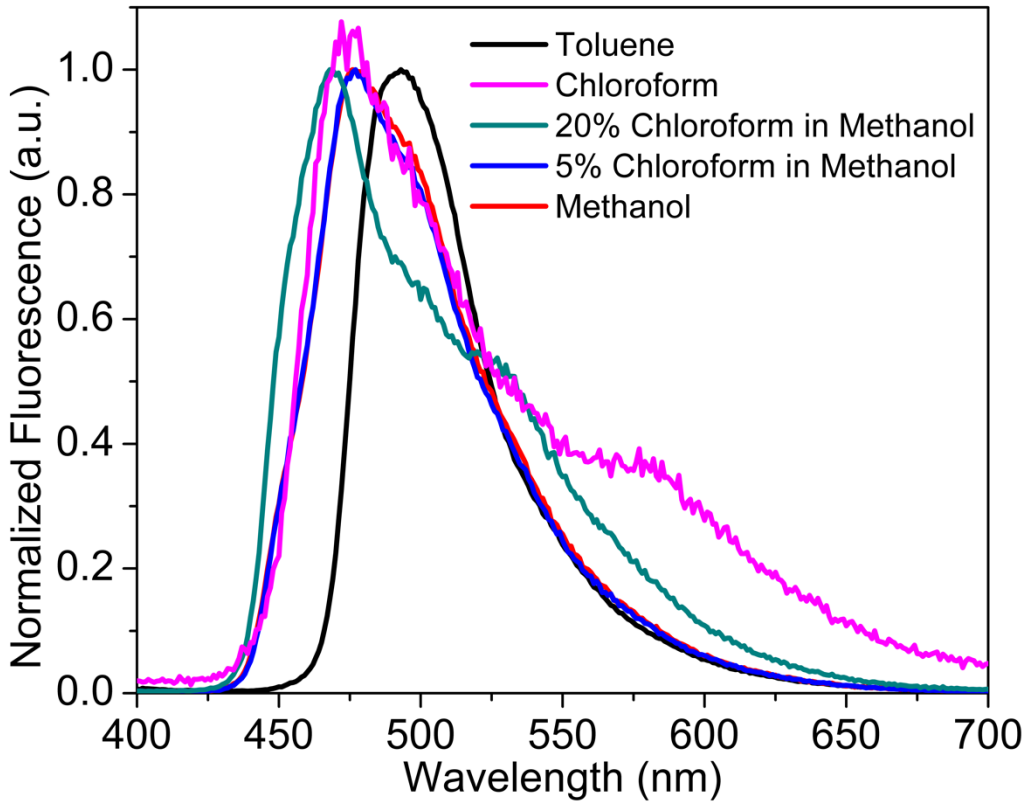

Figure S4. Fluorescence spectra of 4 mM solutions of **2** in a variety of solvents. Samples excited at 365 nm.

Copies of NMR Spectra for New Compounds

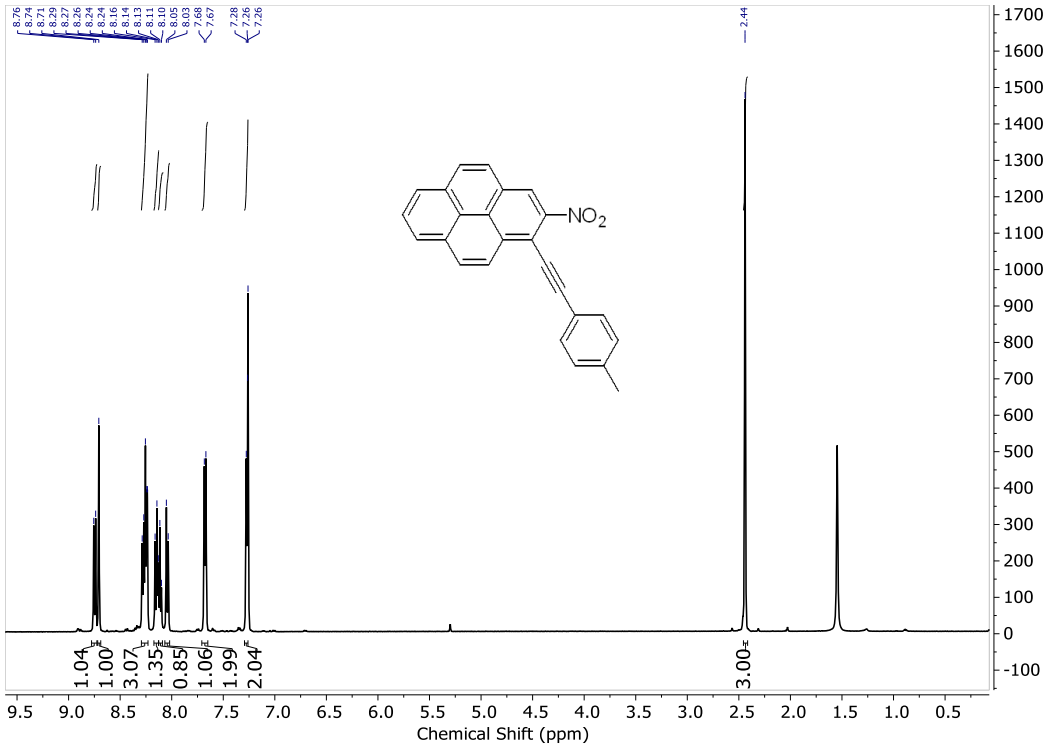

Figure S5. ^{1}H NMR spectrum of **4** in $CDCl_3$.

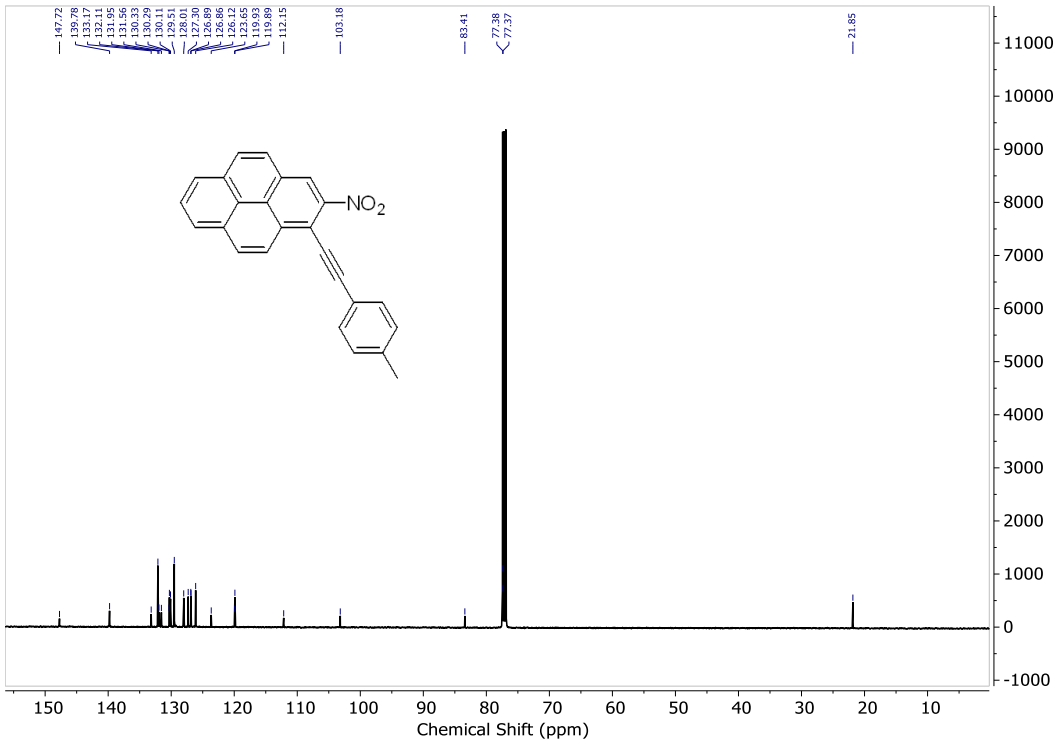

Figure S6. ^{13}C NMR spectrum of **4** in $CDCl_3$.

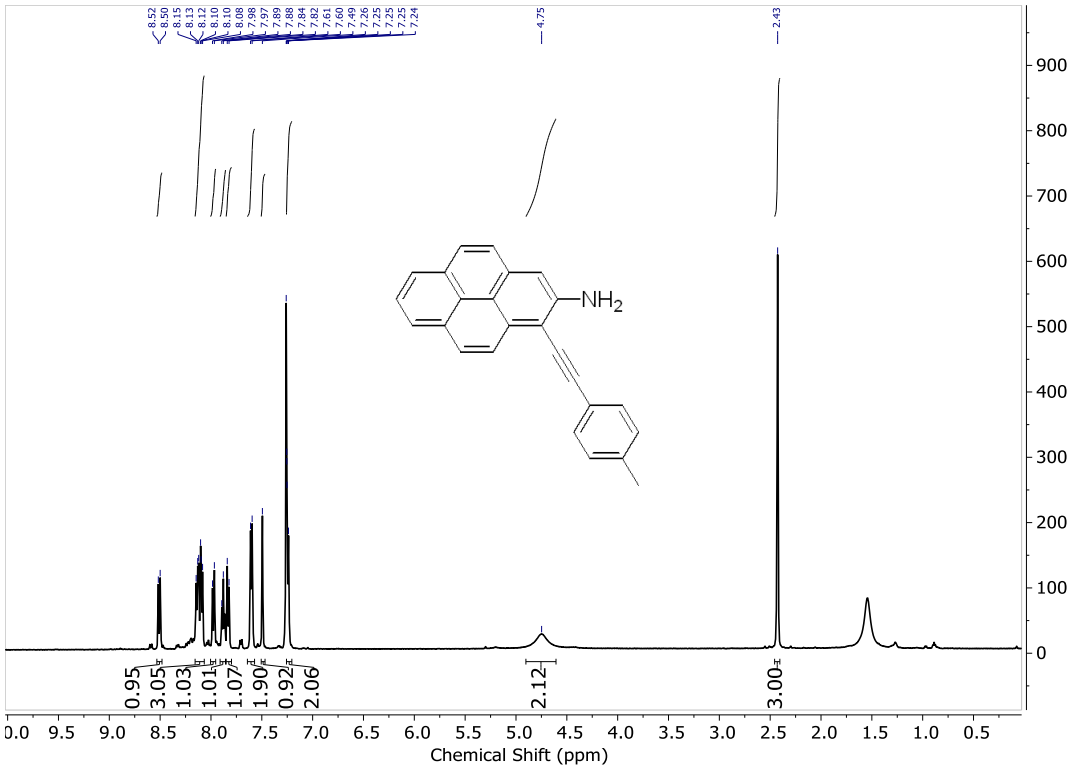

Figure S7. ^{1}H NMR spectrum of **5** in $CDCl_3$.

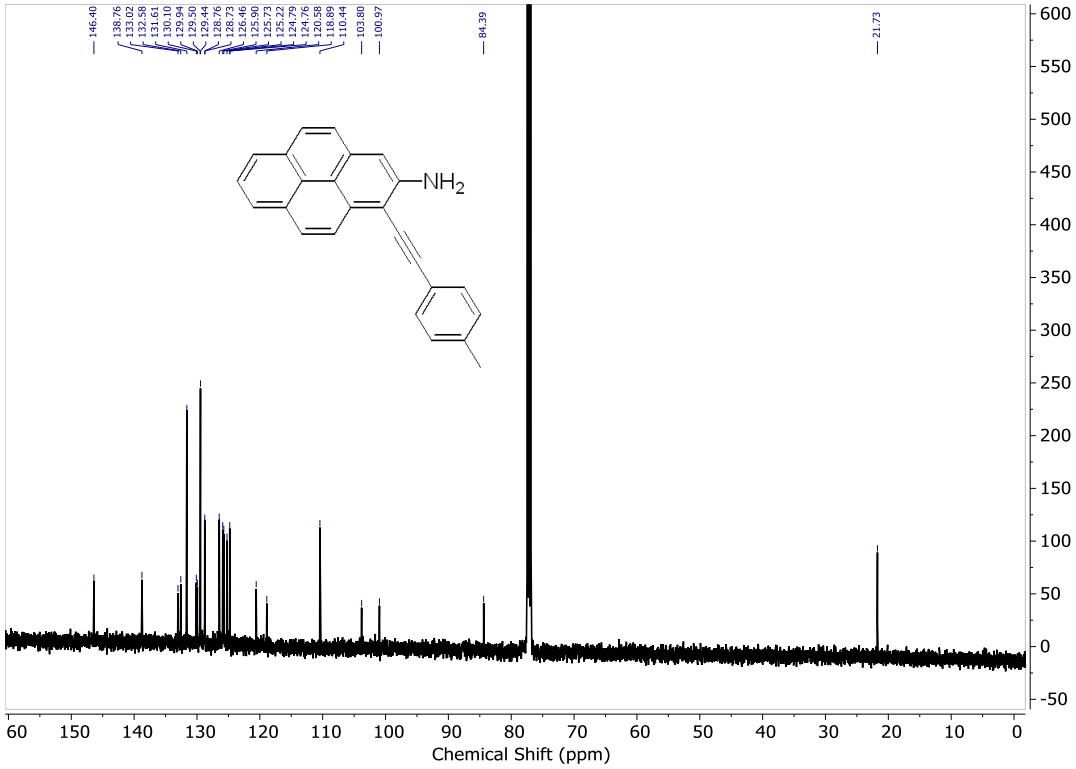

Figure S8. ^{13}C NMR spectrum of **5** in $CDCl_3$.

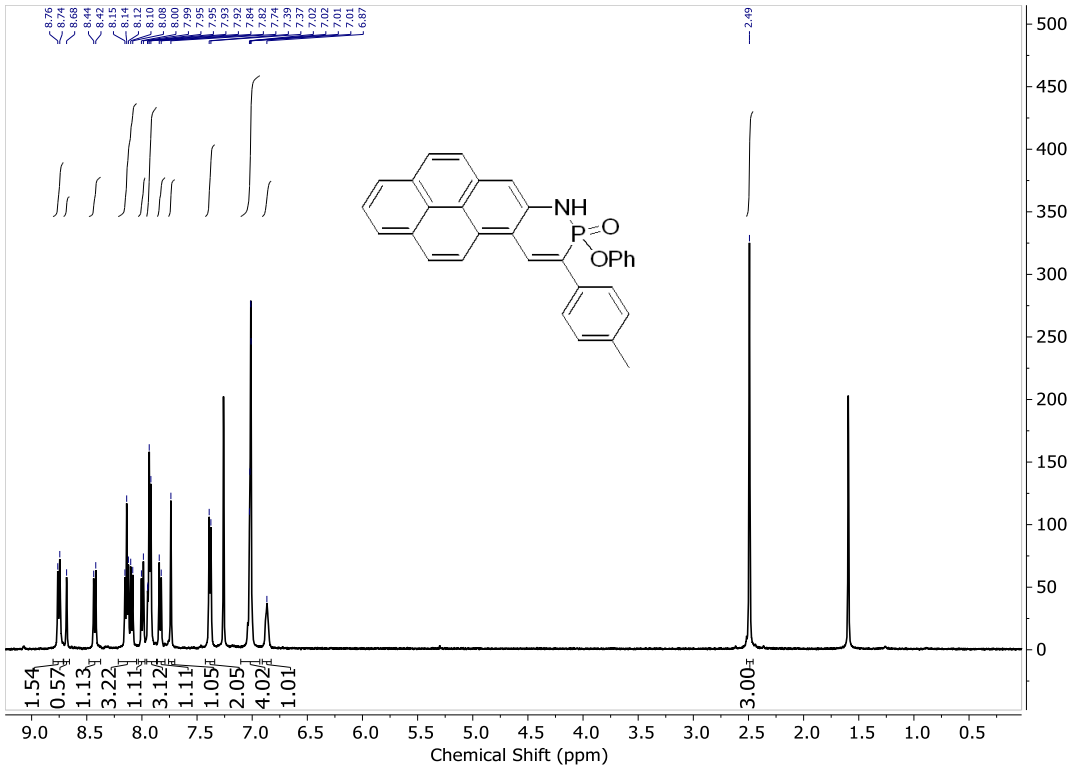

Figure S9. ^{1}H NMR spectrum of **2** in $CDCl_3$.

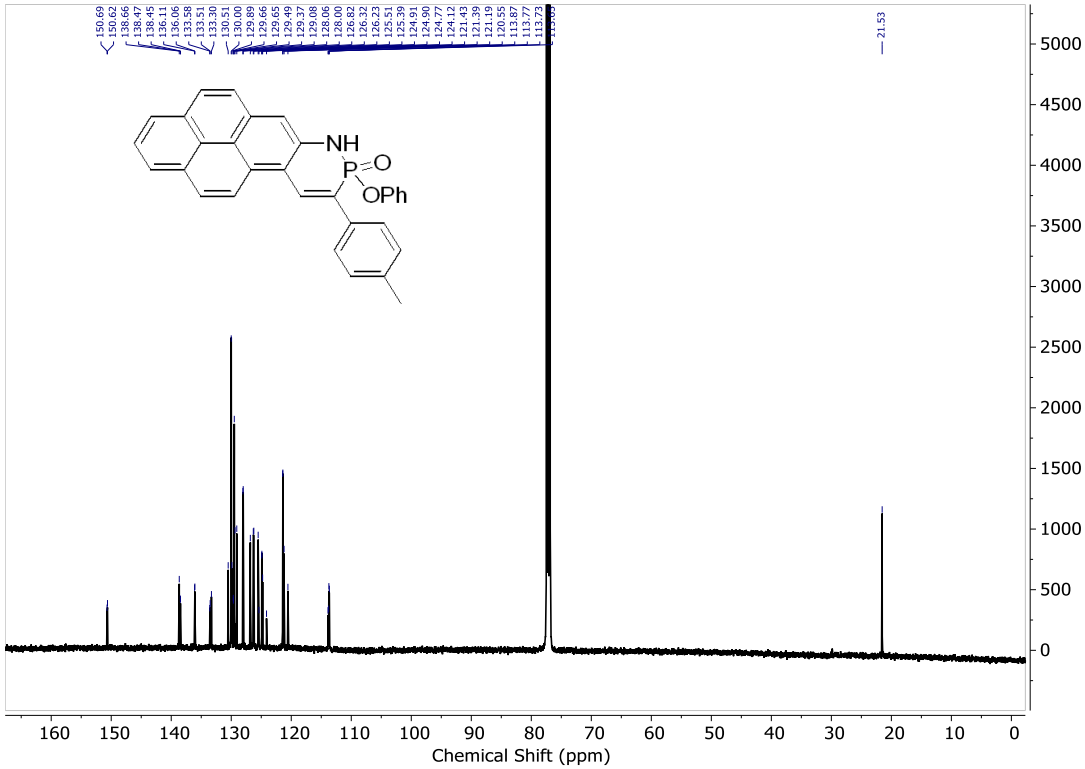

Figure S10. ^{13}C NMR spectrum of **2** in $CDCl_3$.

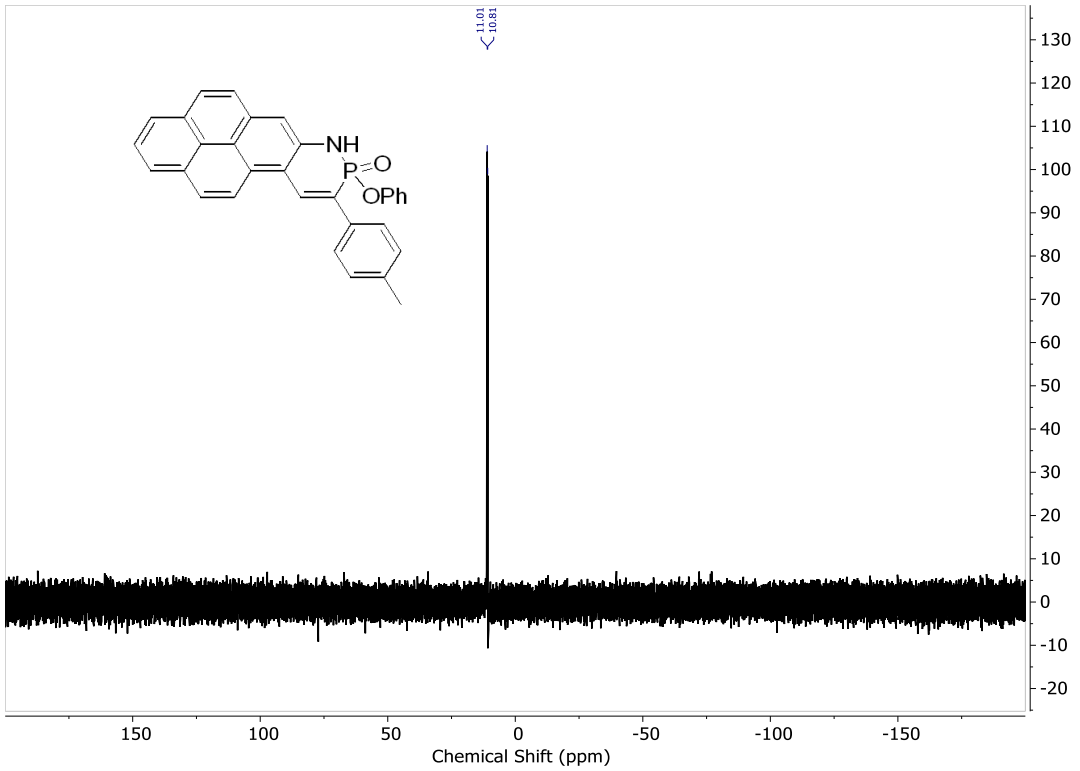

Figure S11. ^{31}P NMR spectrum of **2** in $CDCl_3$.