

SUPPORTING INFORMATION

Iodine-Catalyzed Functionalization of Primary Aliphatic Amines to Oxazoles, 1,4-Oxazines, and Oxazinones

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Section I: ^1H and ^{13}C NMR spectra

Figure S1. ^1H and ^{13}C NMR of 4a

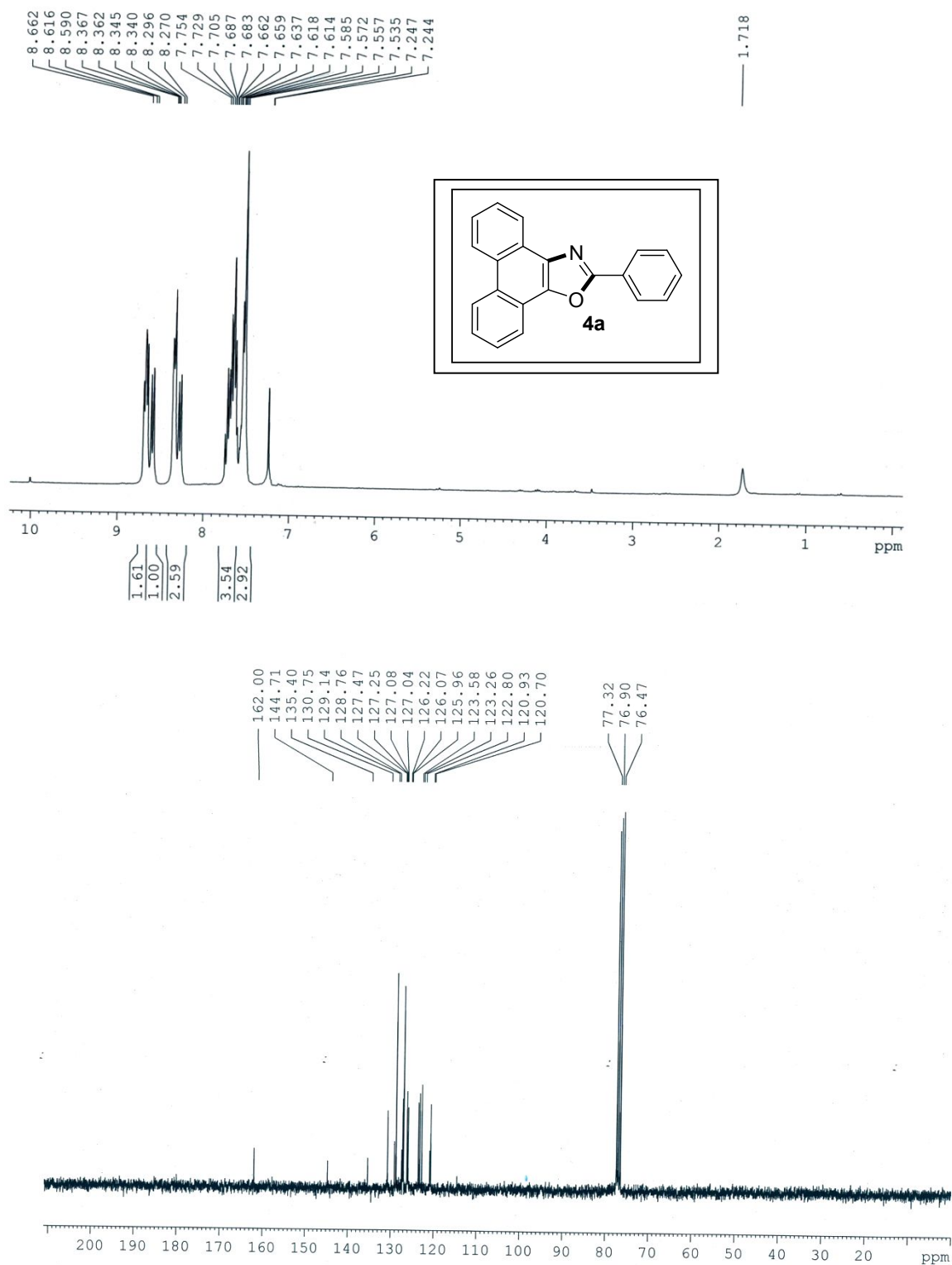


Figure S2. ¹H and ¹³C NMR of 4b

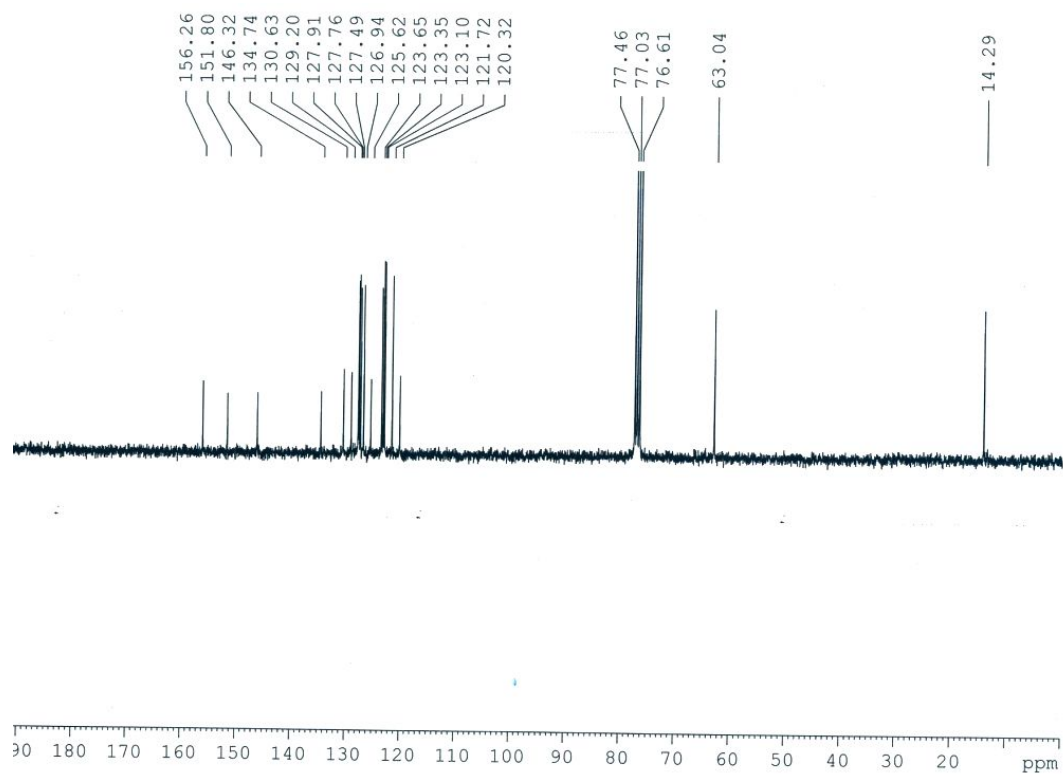
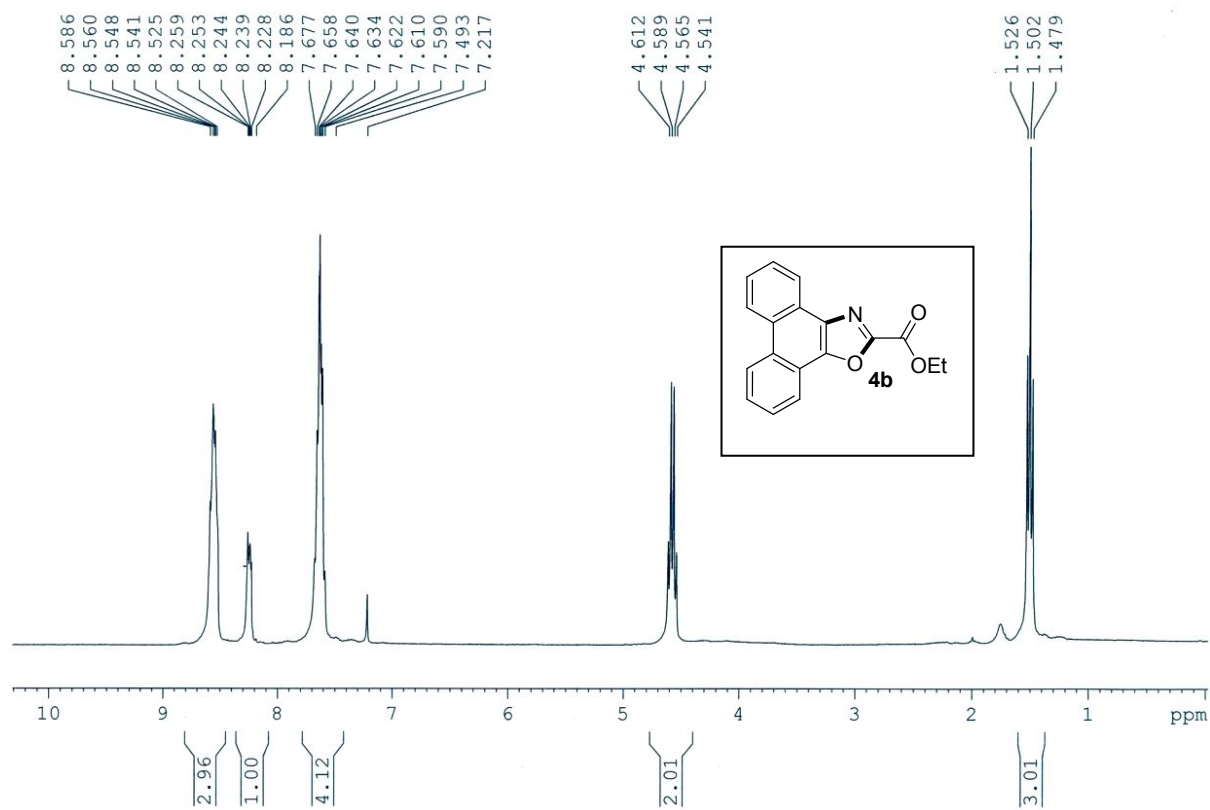


Figure S3. ^1H and ^{13}C NMR of **4c**

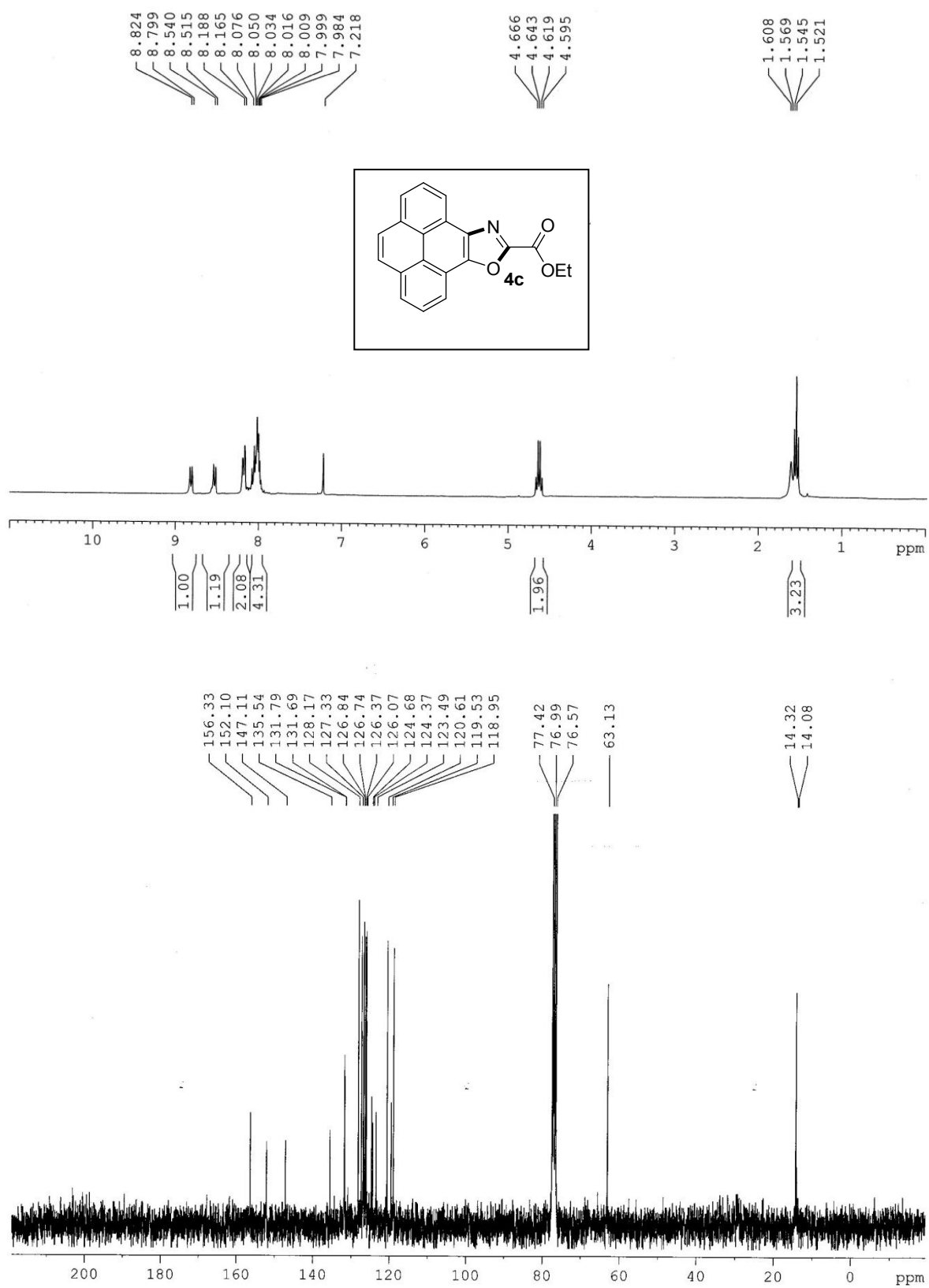


Figure S4. ^1H and ^{13}C NMR of 4d

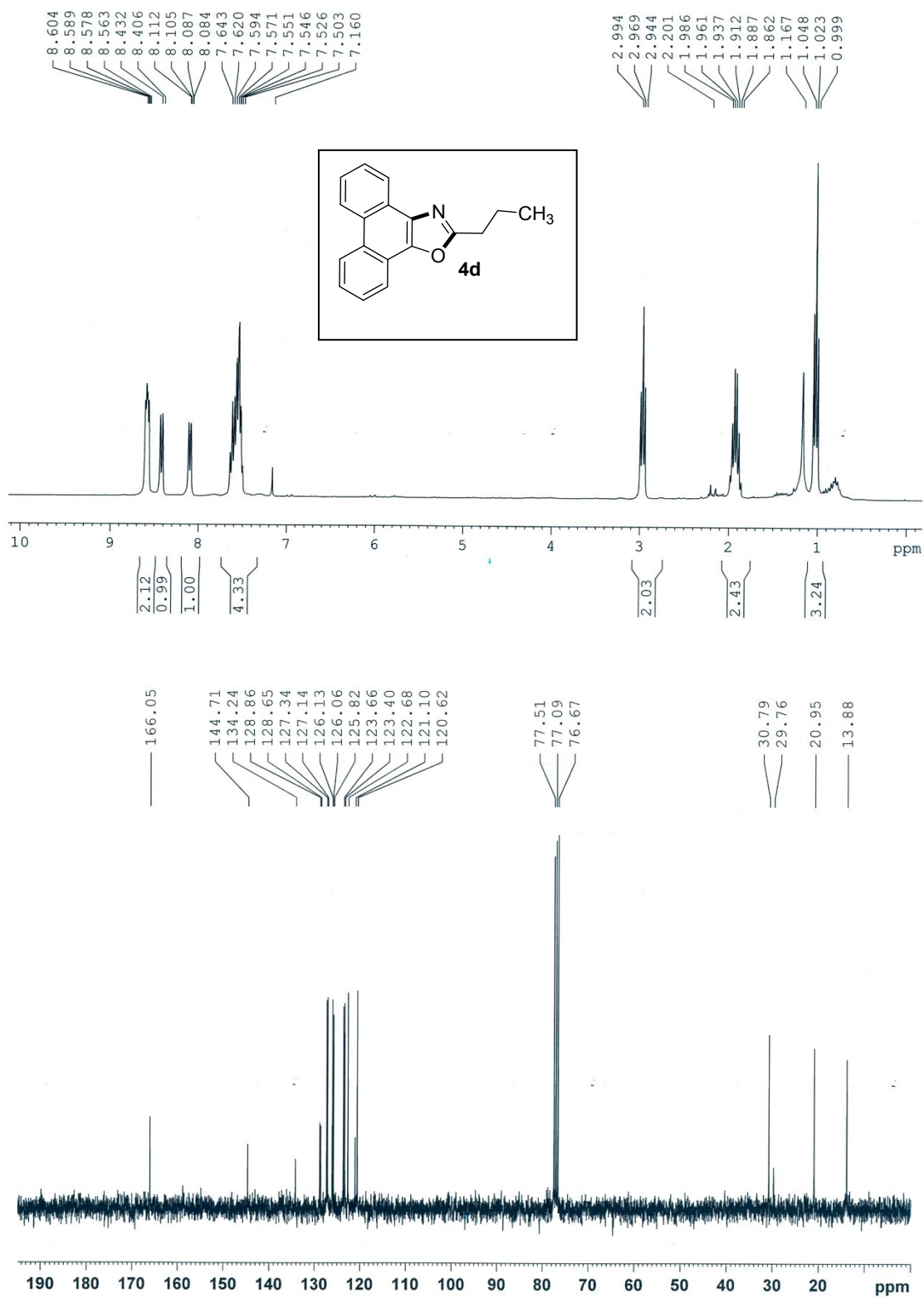


Figure S5. ^1H and ^{13}C NMR of 4e

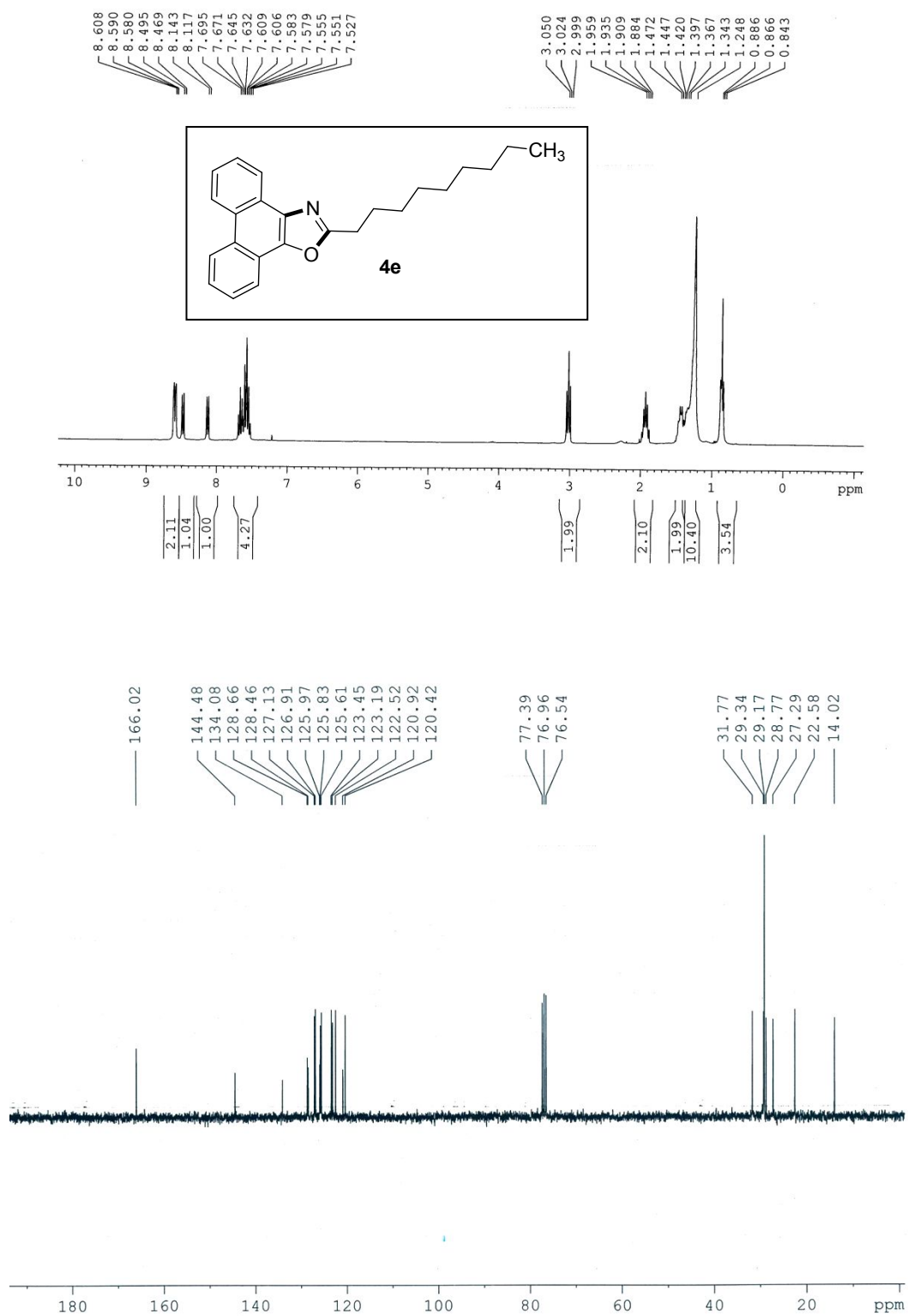


Figure S6. ^1H and ^{13}C NMR of 4f

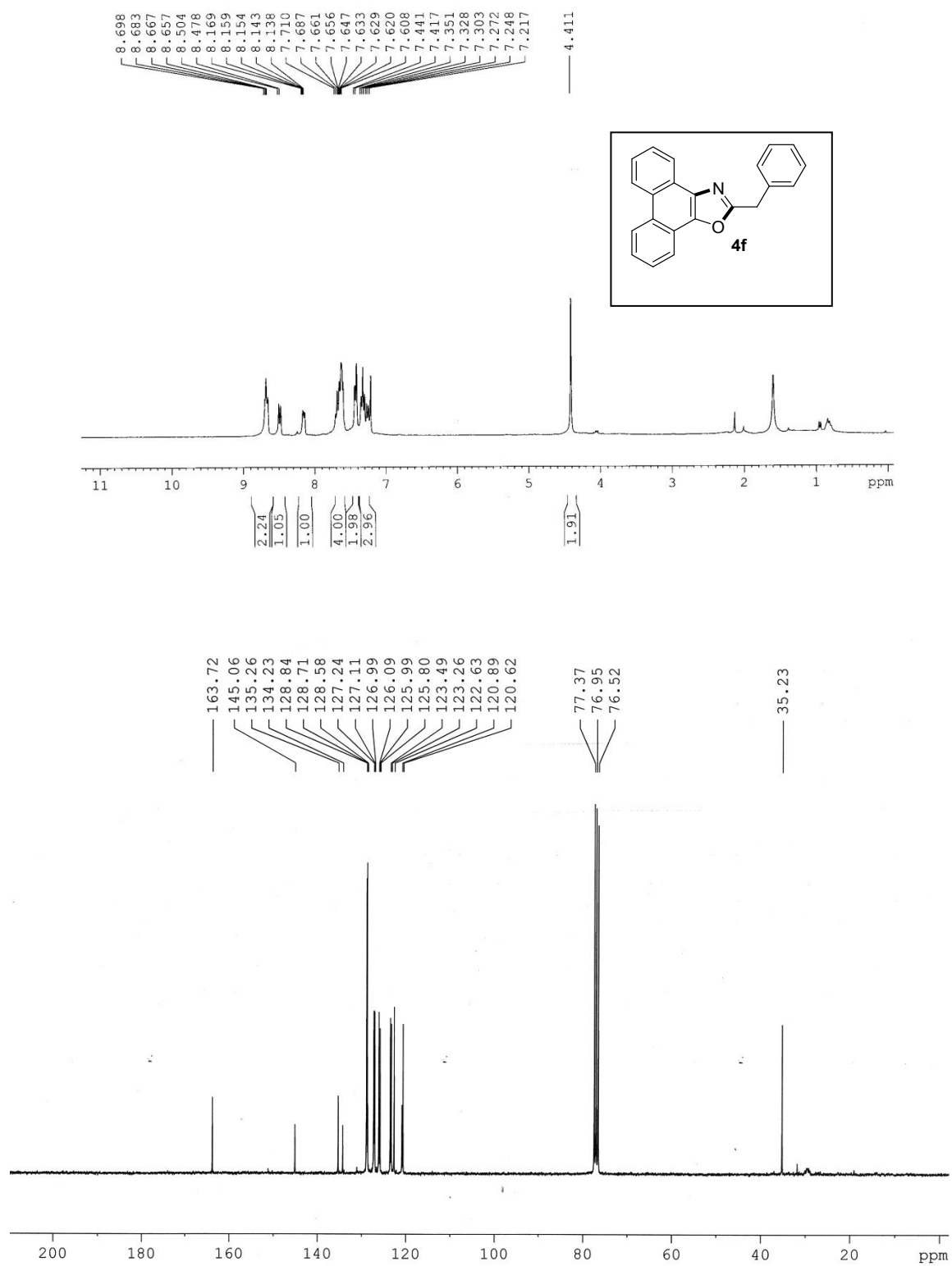


Figure S7. ^1H and ^{13}C NMR of 4g

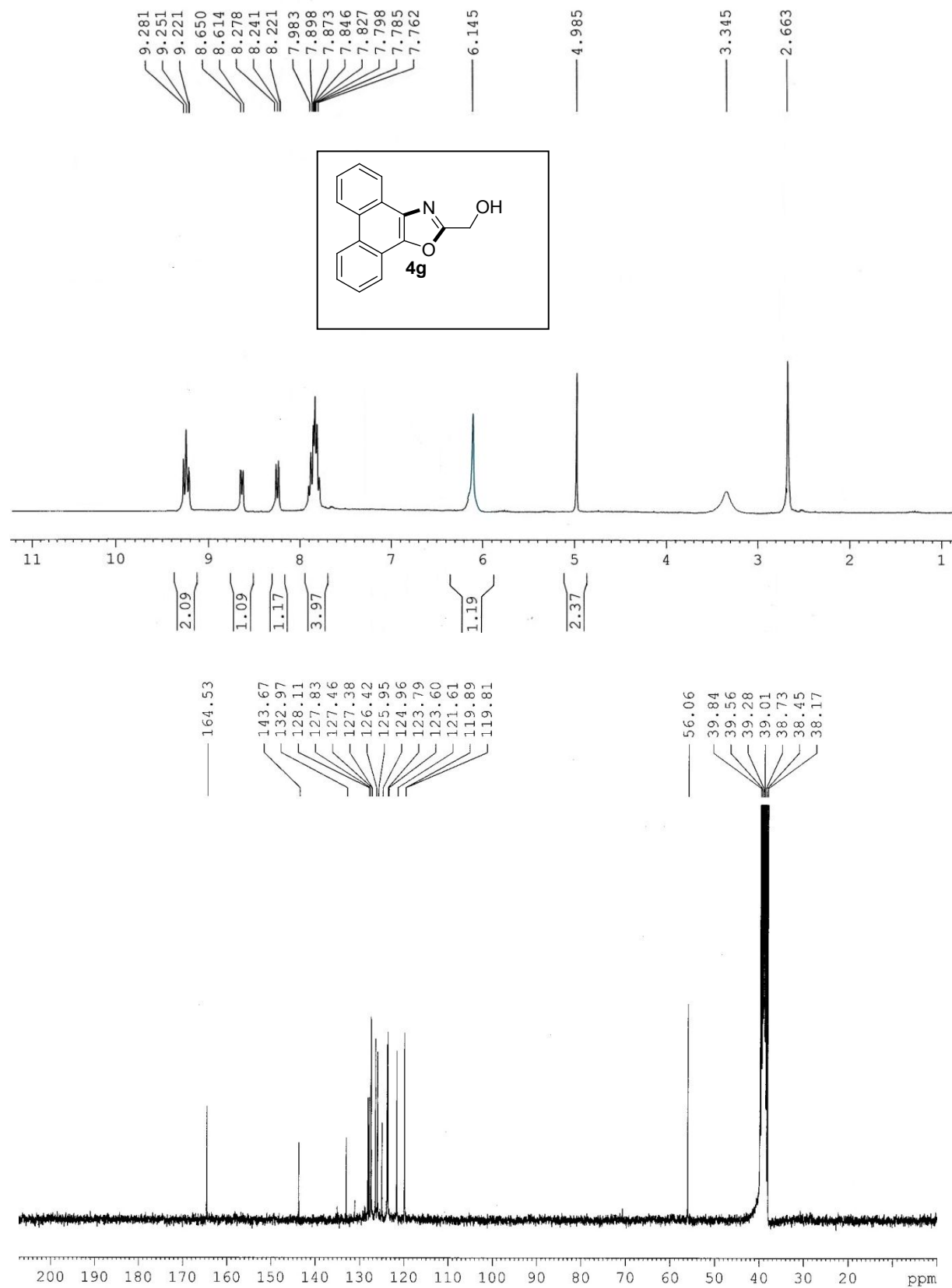


Figure S8. ^1H and ^{13}C NMR of 4h

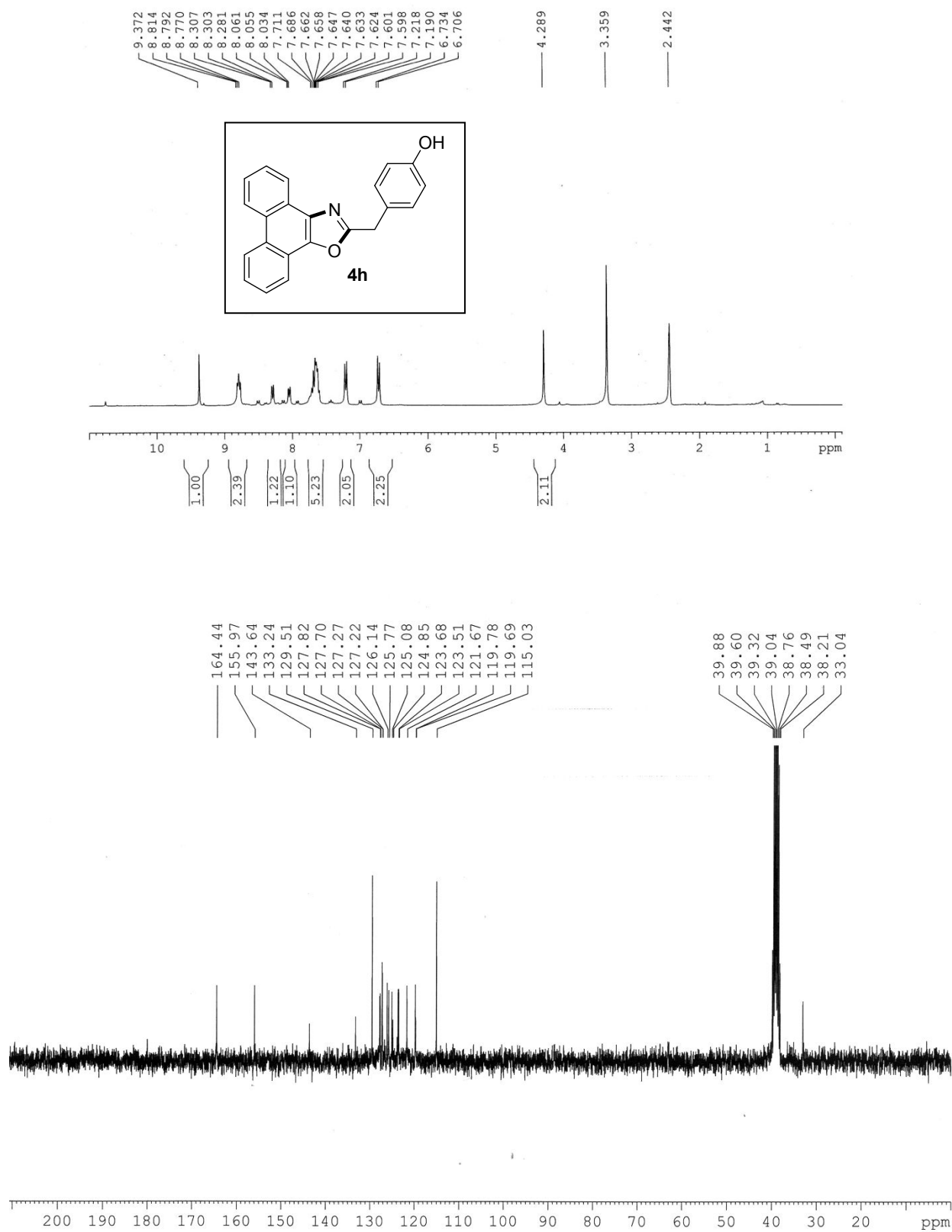


Figure S9. ¹H and ¹³C NMR of 4i

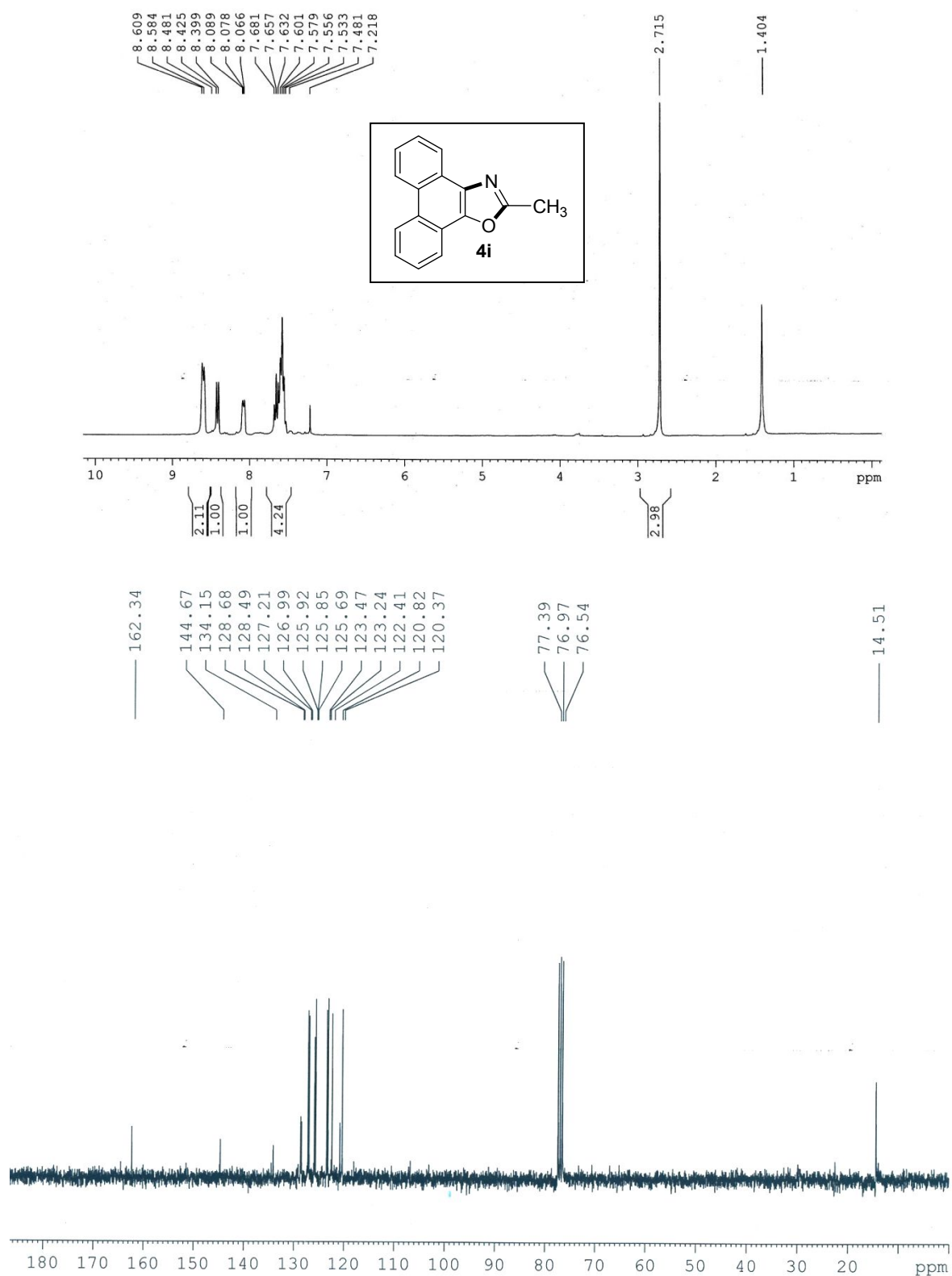


Figure S10. ¹H and ¹³C NMR of 4j

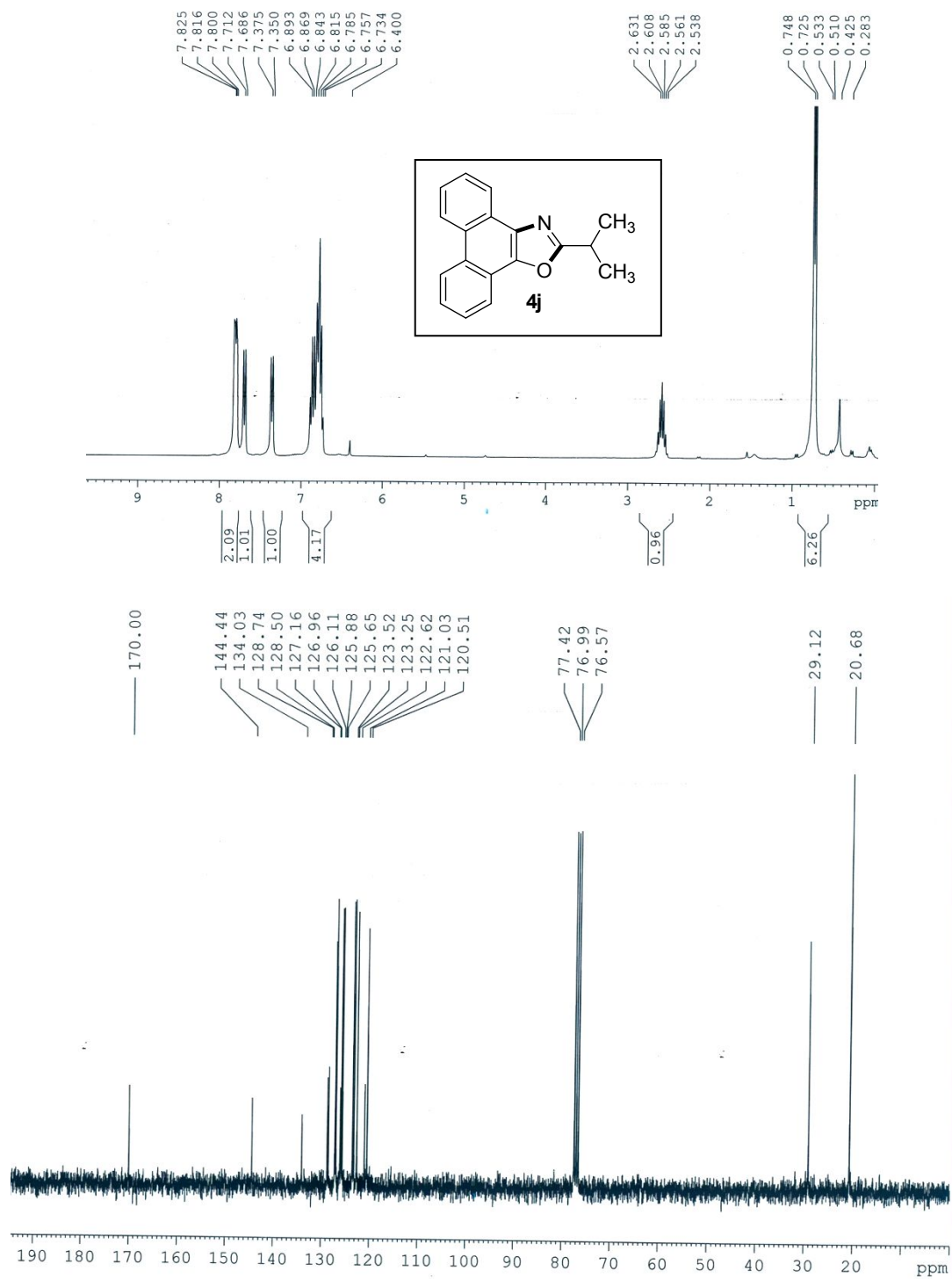


Figure S11. ¹H and ¹³C NMR of 4k

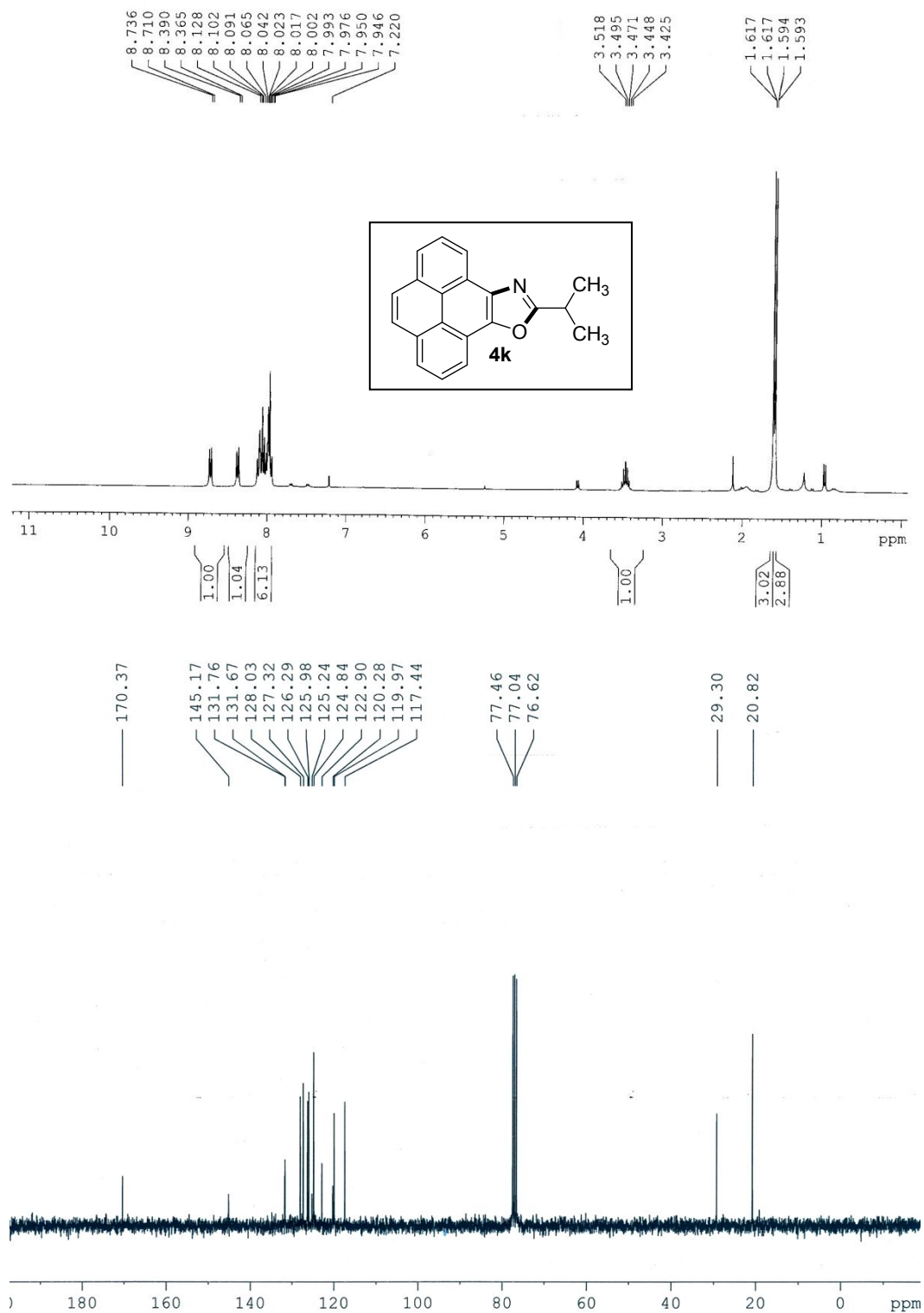


Figure S12. ^1H and ^{13}C NMR of 4I

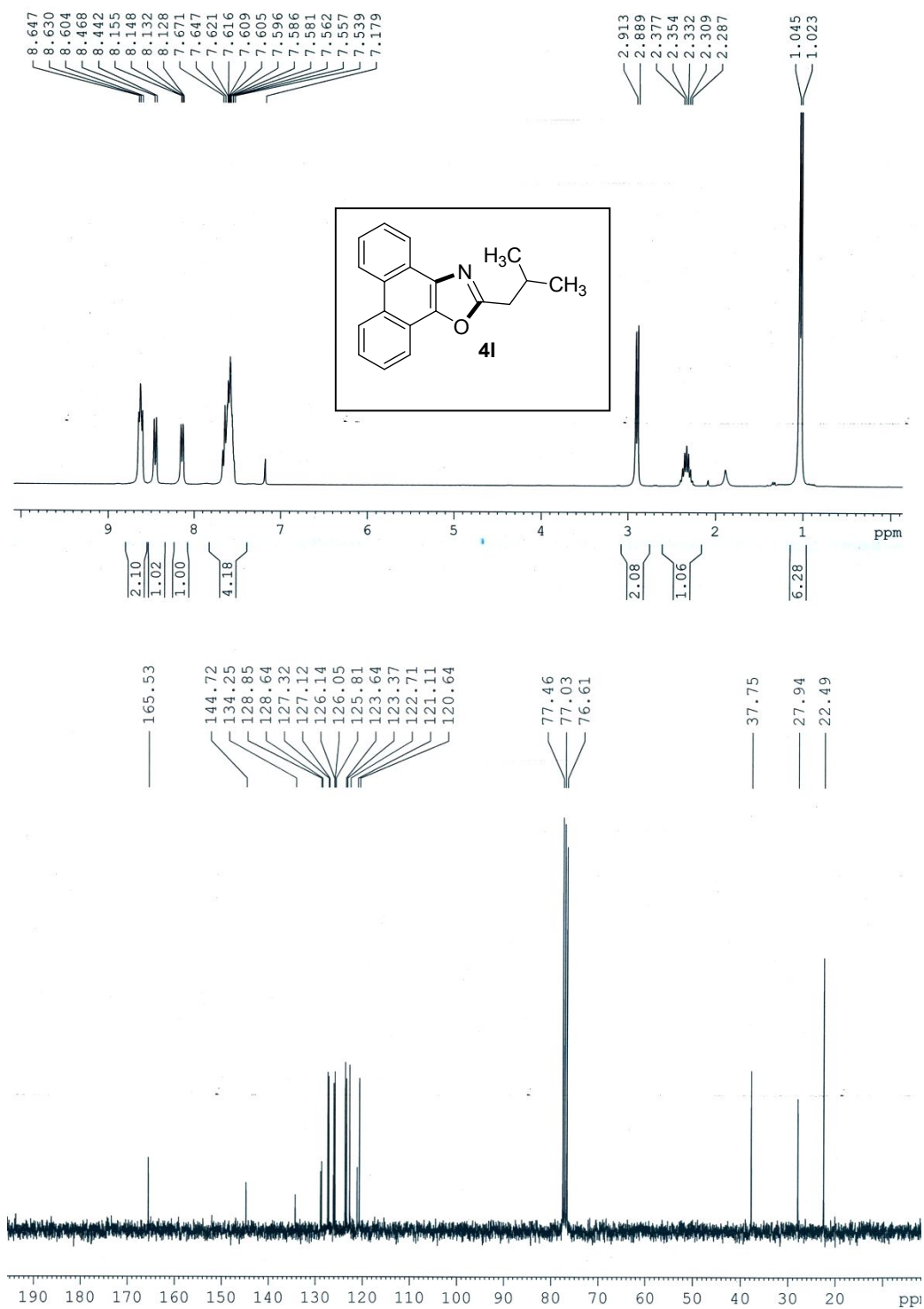


Figure S13. ¹H and ¹³C NMR of 4m

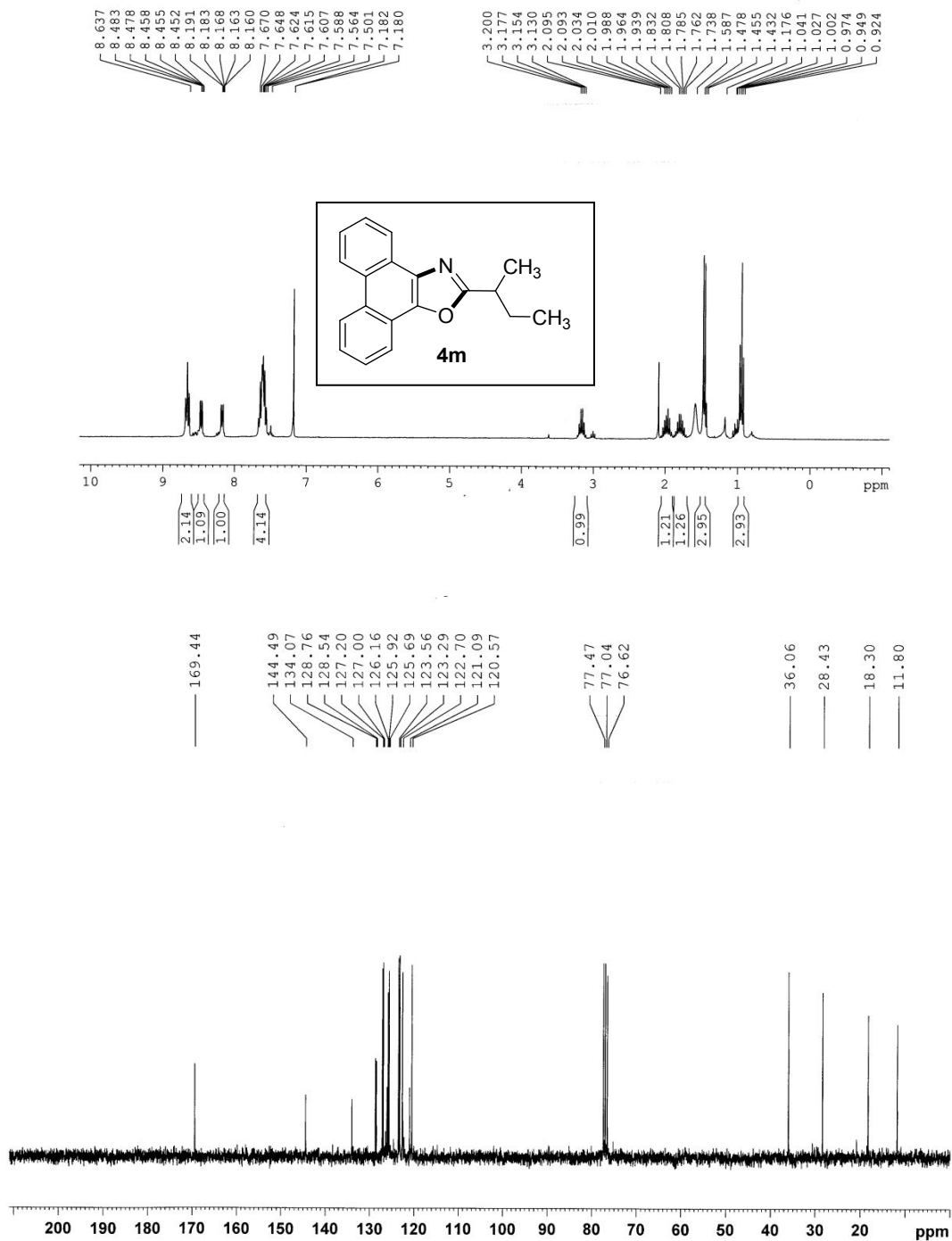


Figure S14. ^1H and ^{13}C NMR of **4n**

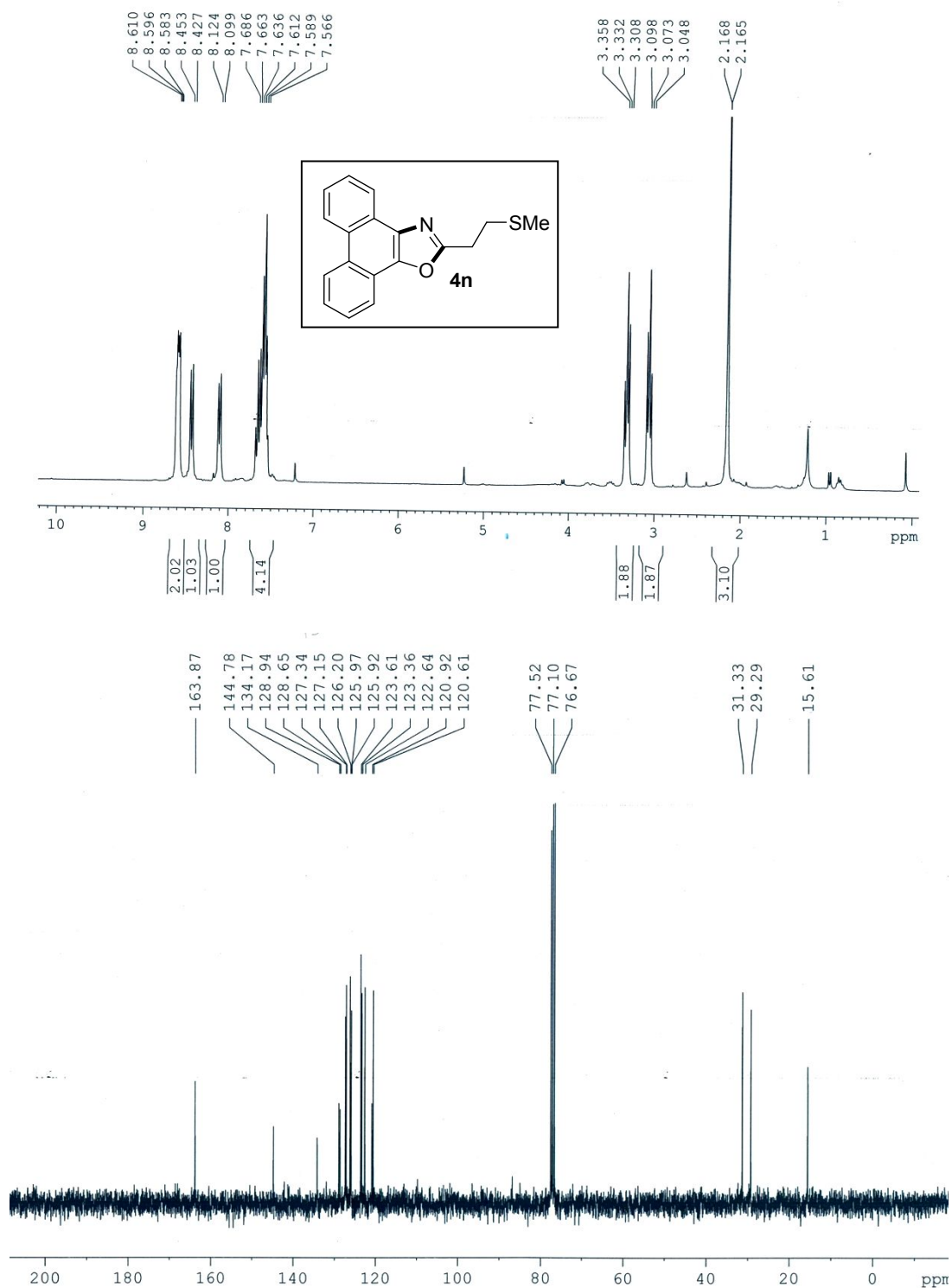


Figure S15. ¹H and ¹³C NMR of 4o

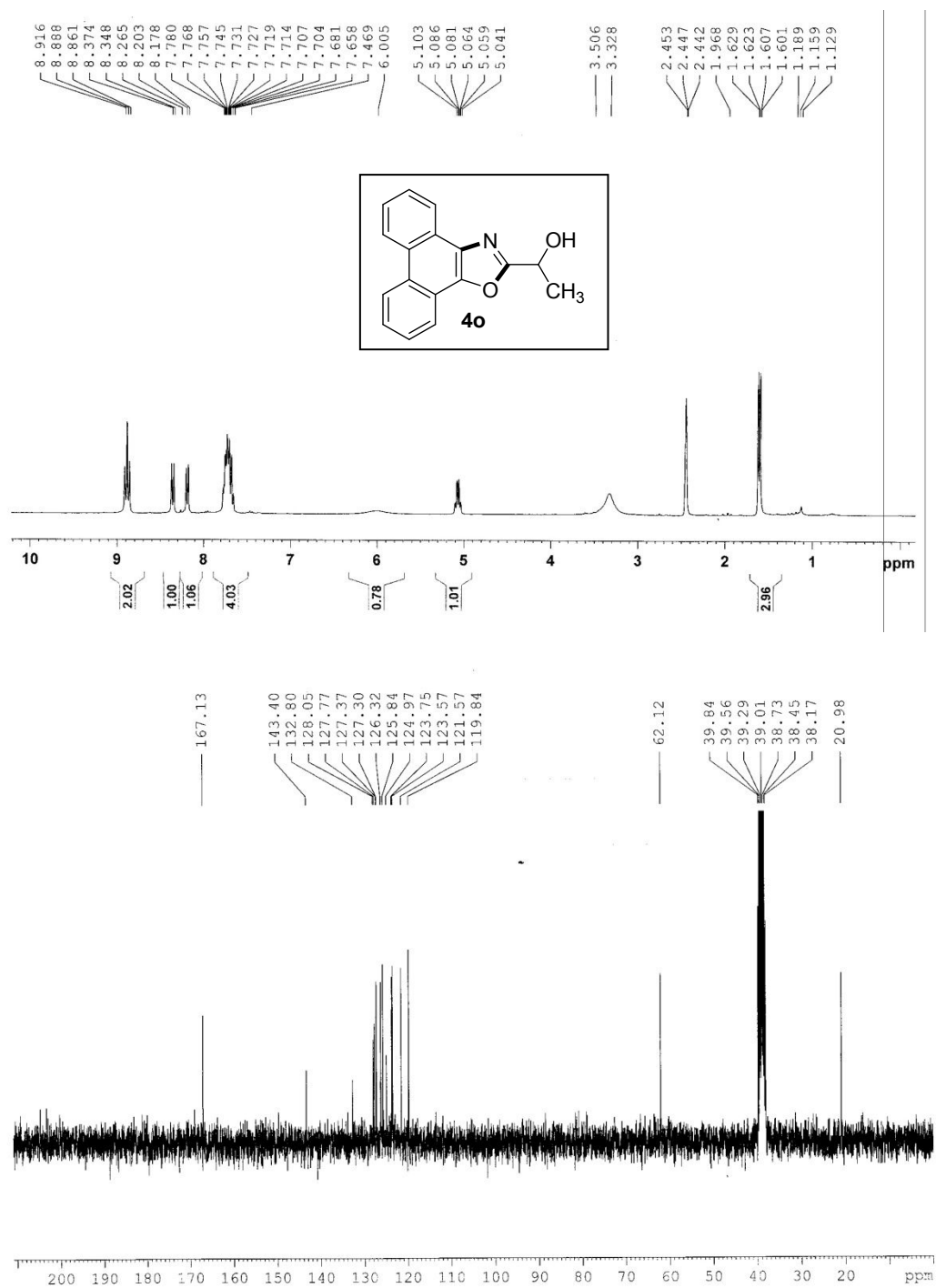


Figure S16. ^1H and ^{13}C NMR of 4p

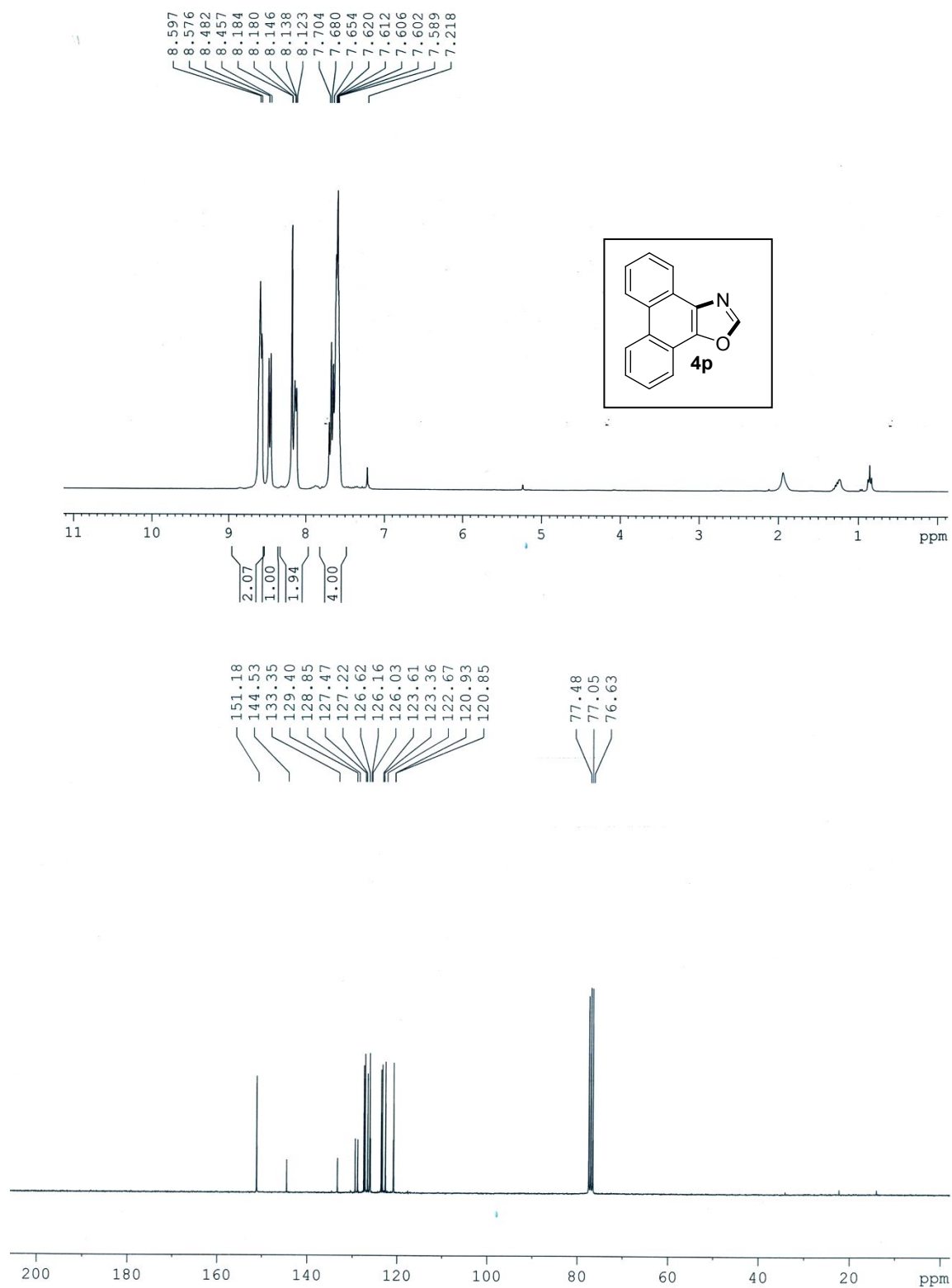


Figure S17. ^1H and ^{13}C NMR of 4r

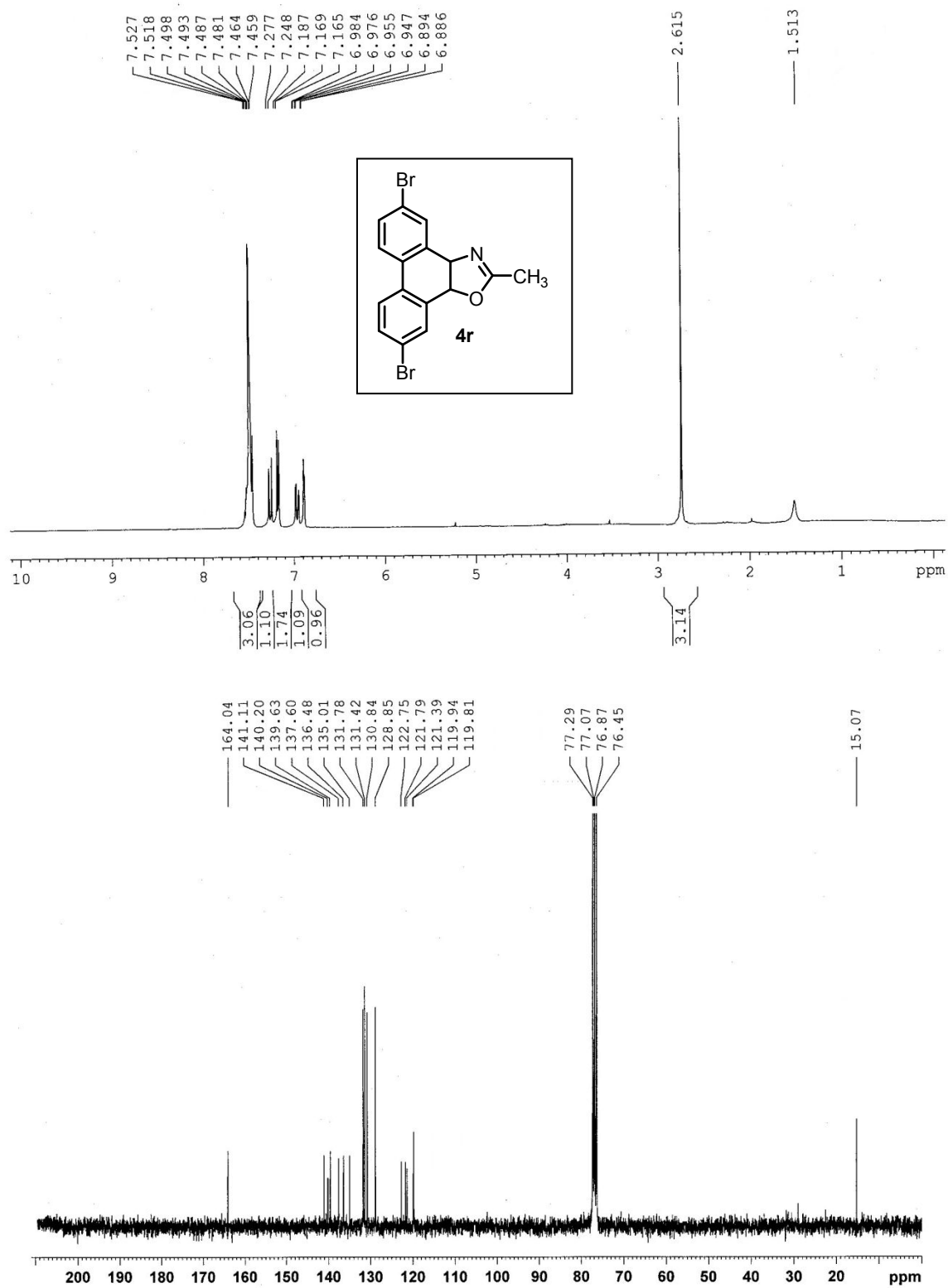


Figure S18. ^1H and ^{13}C NMR of 4s

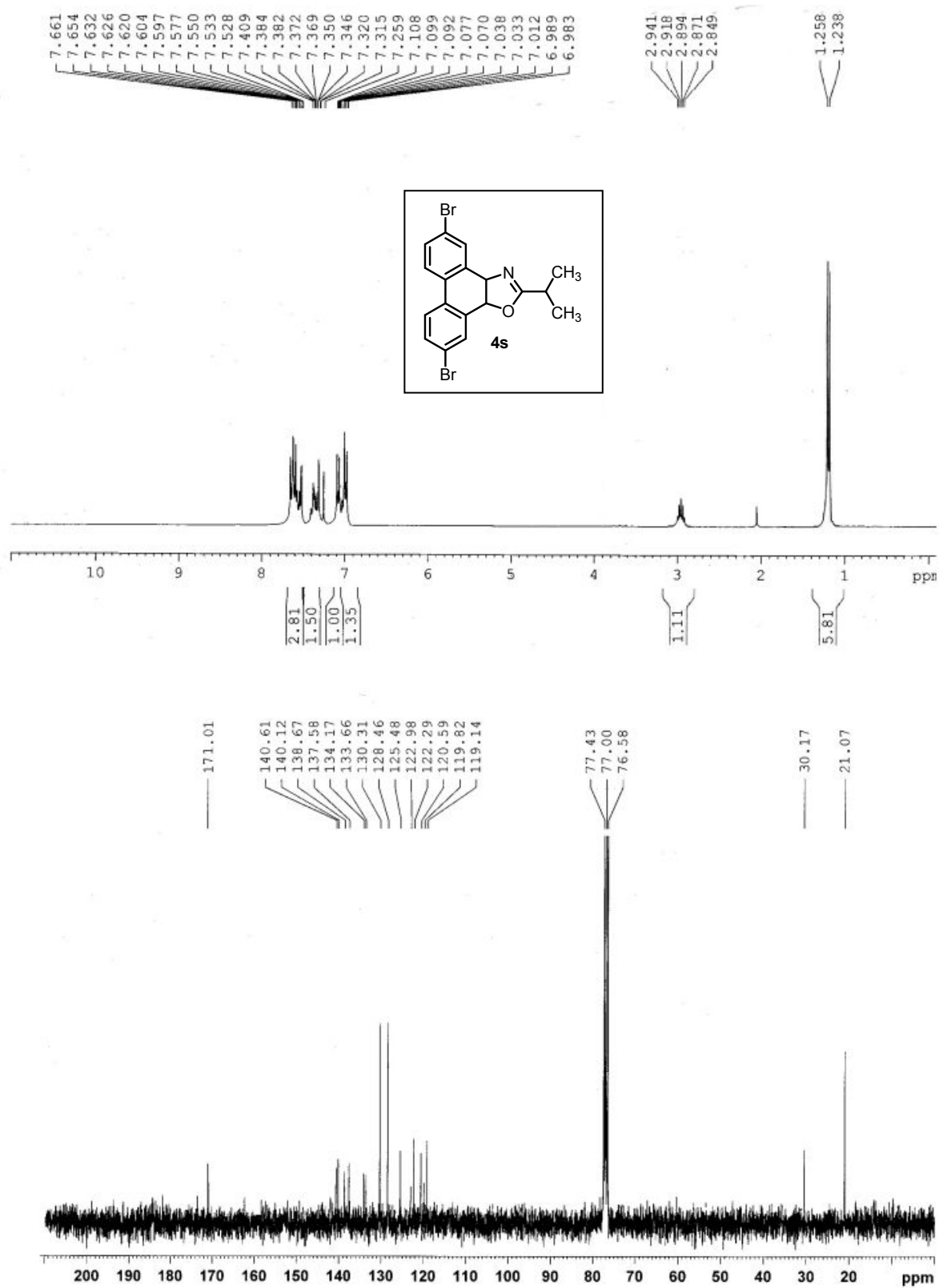


Figure S19. ^1H and ^{13}C NMR of **6a**

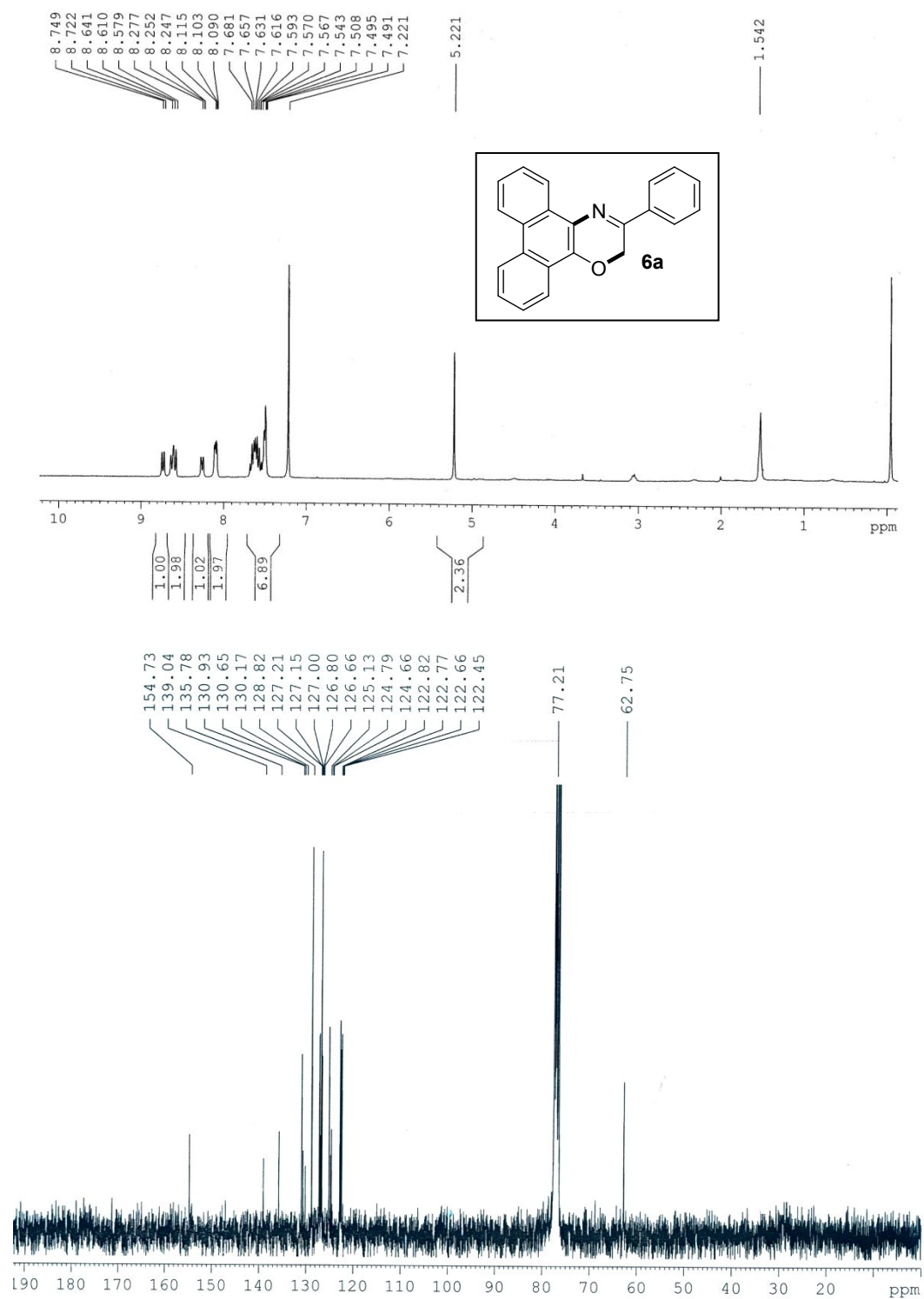


Figure S20. ^1H and ^{13}C NMR of **6b**

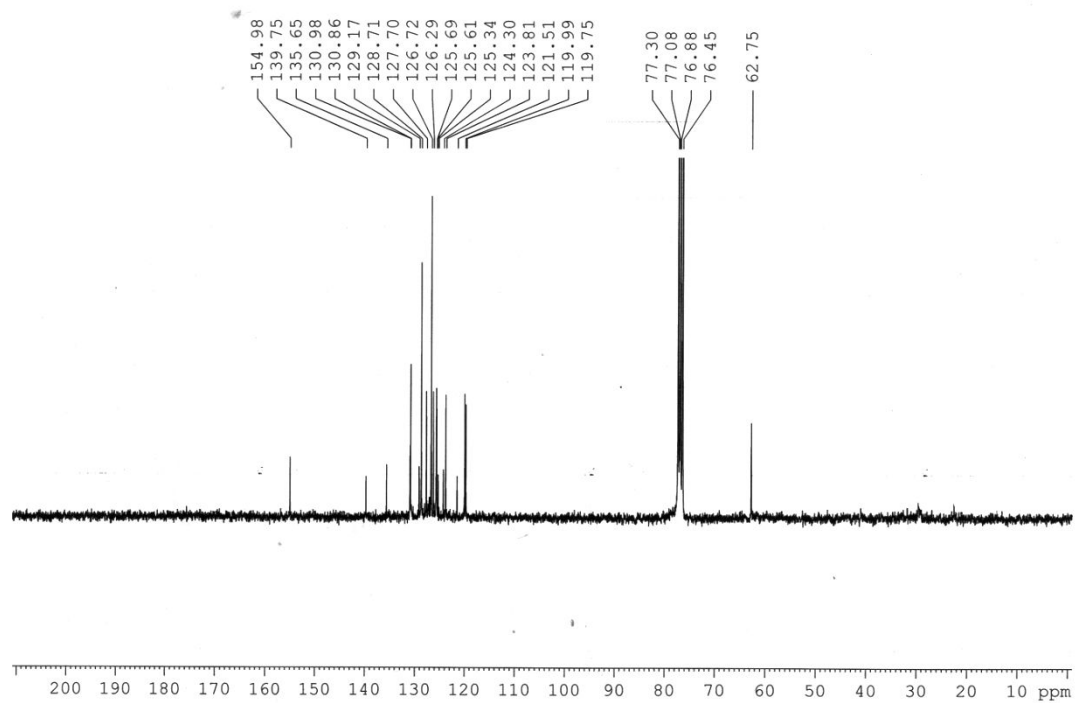
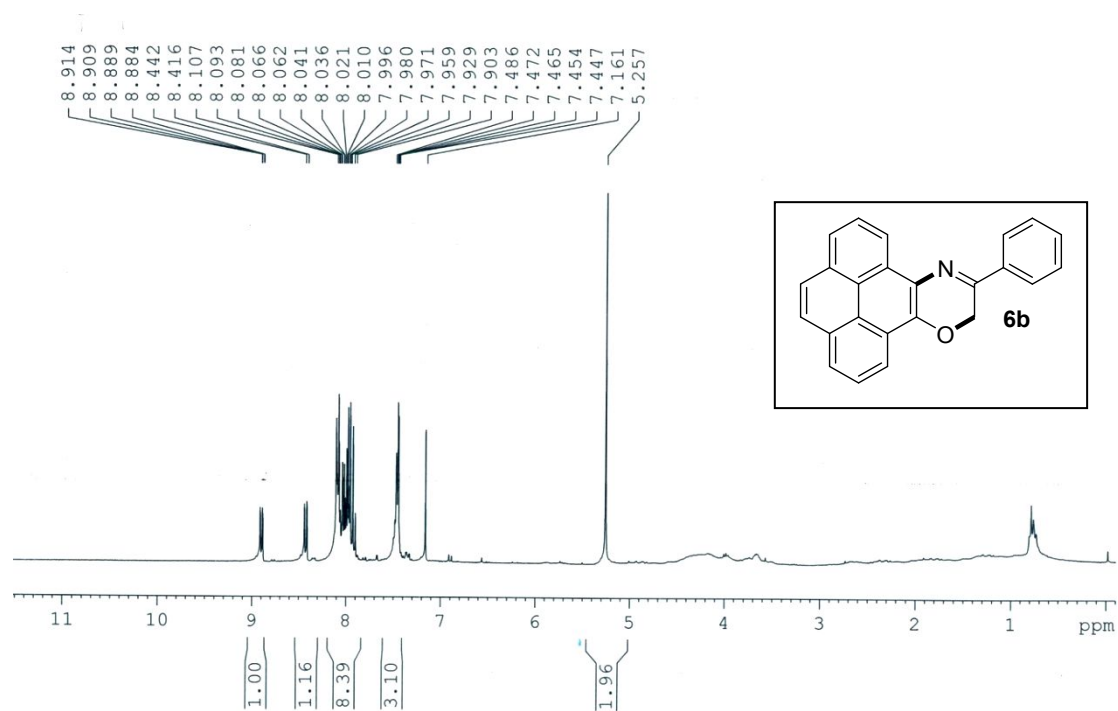


Figure S21. ¹H and ¹³C NMR of 6c

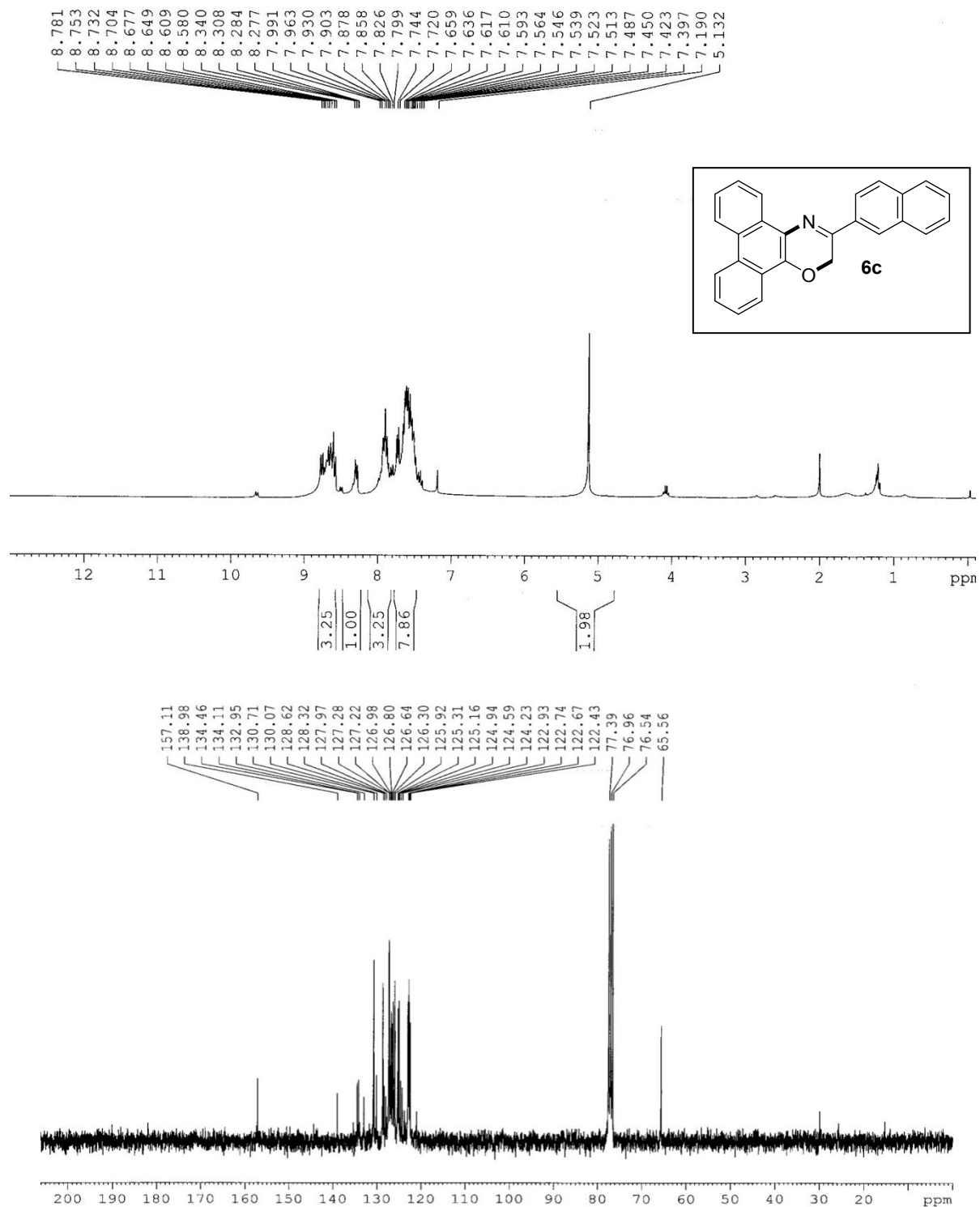


Figure S22. ^1H and ^{13}C NMR of 6d

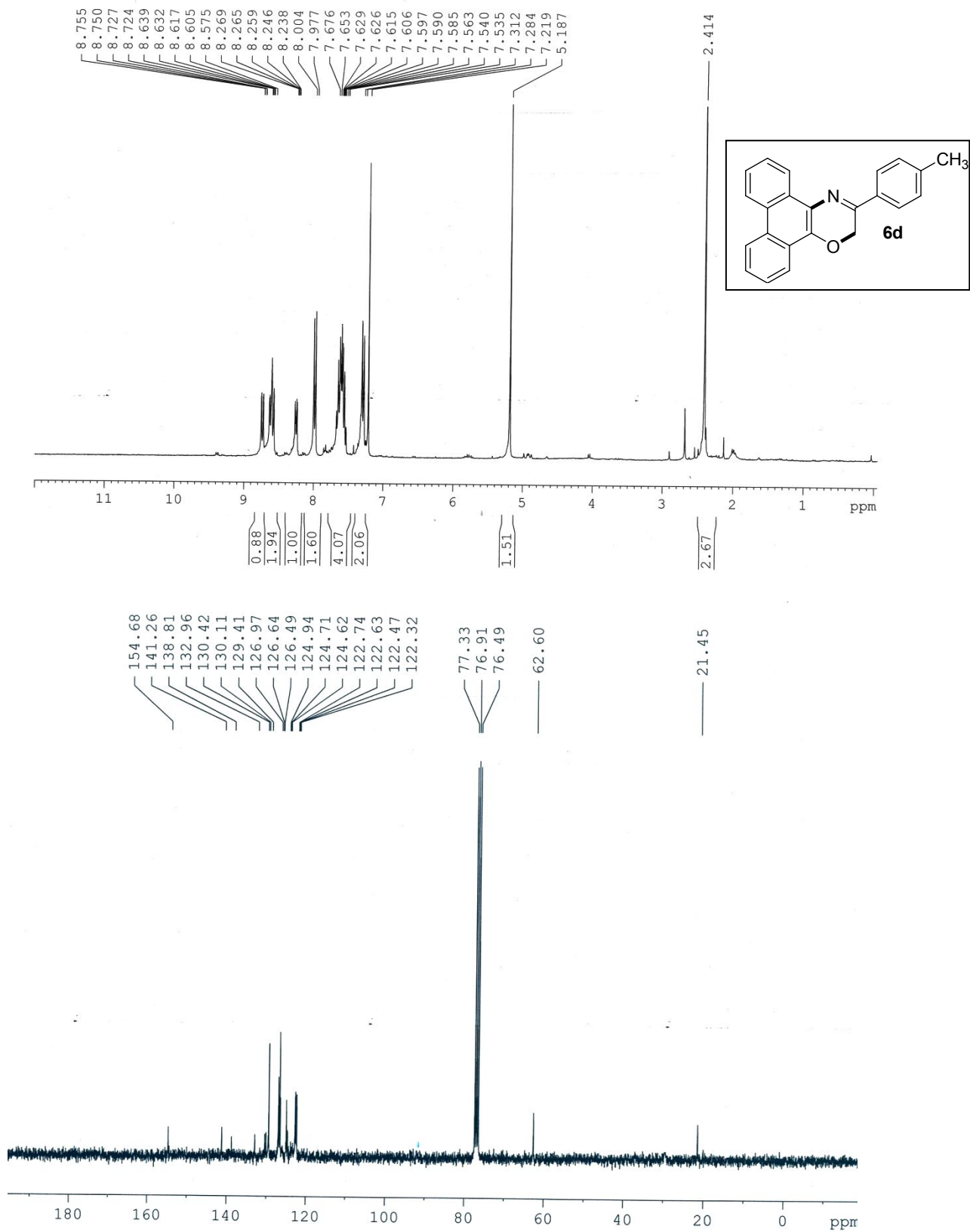


Figure S23. ^1H and ^{13}C NMR of **6e**

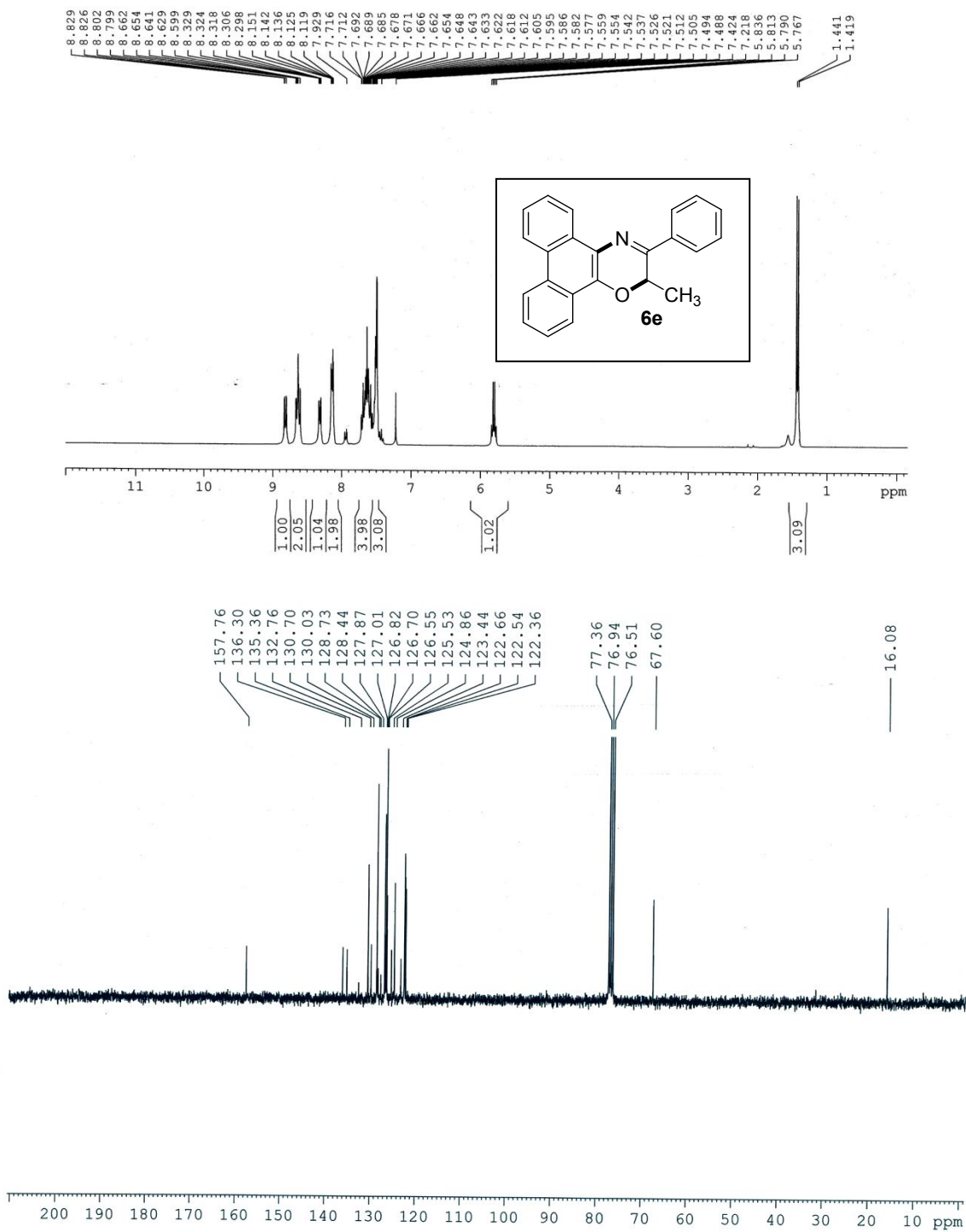


Figure S24. ^1H and ^{13}C NMR of **6f**

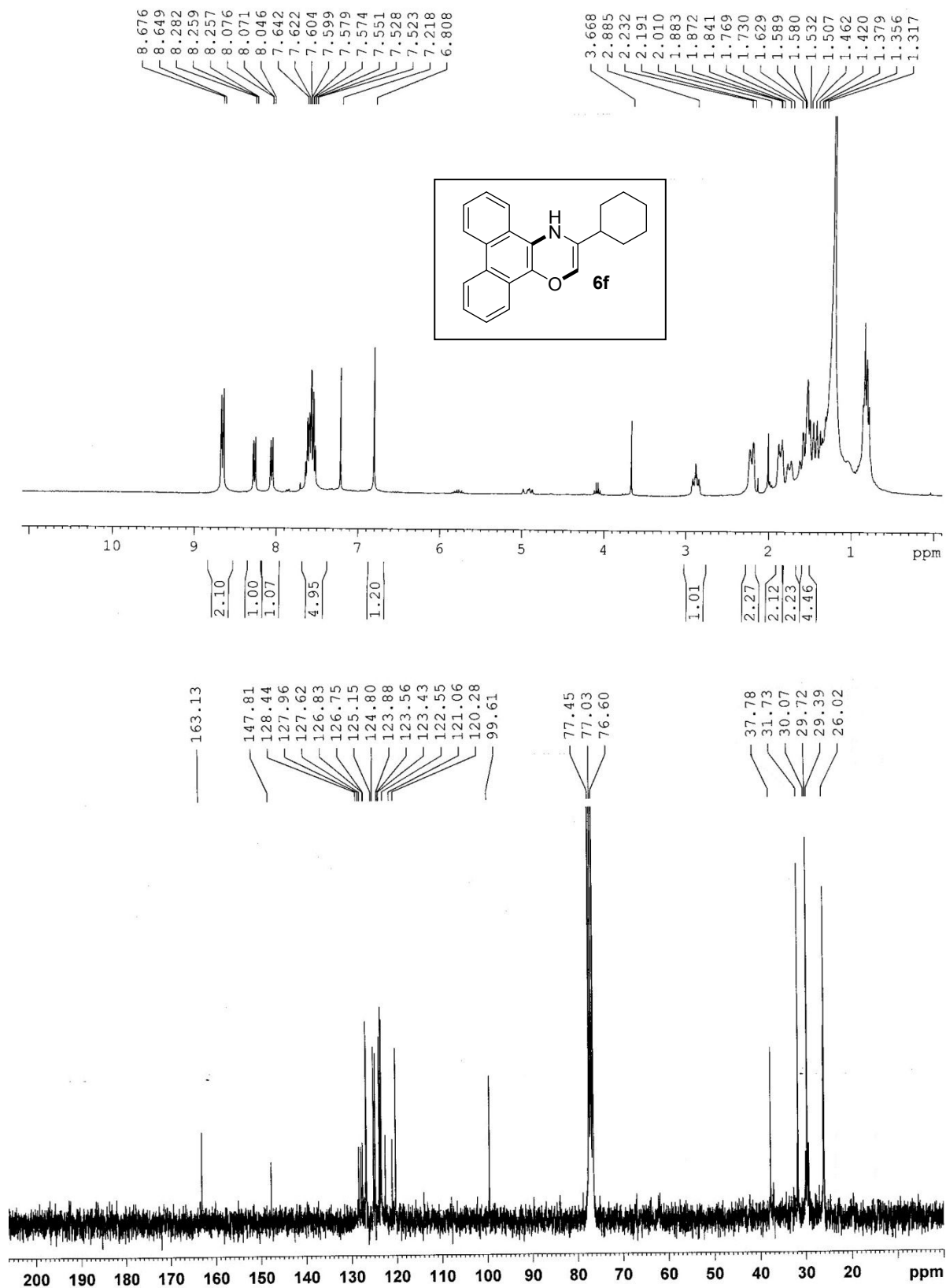


Figure S25. ^1H and ^{13}C NMR of **6g**

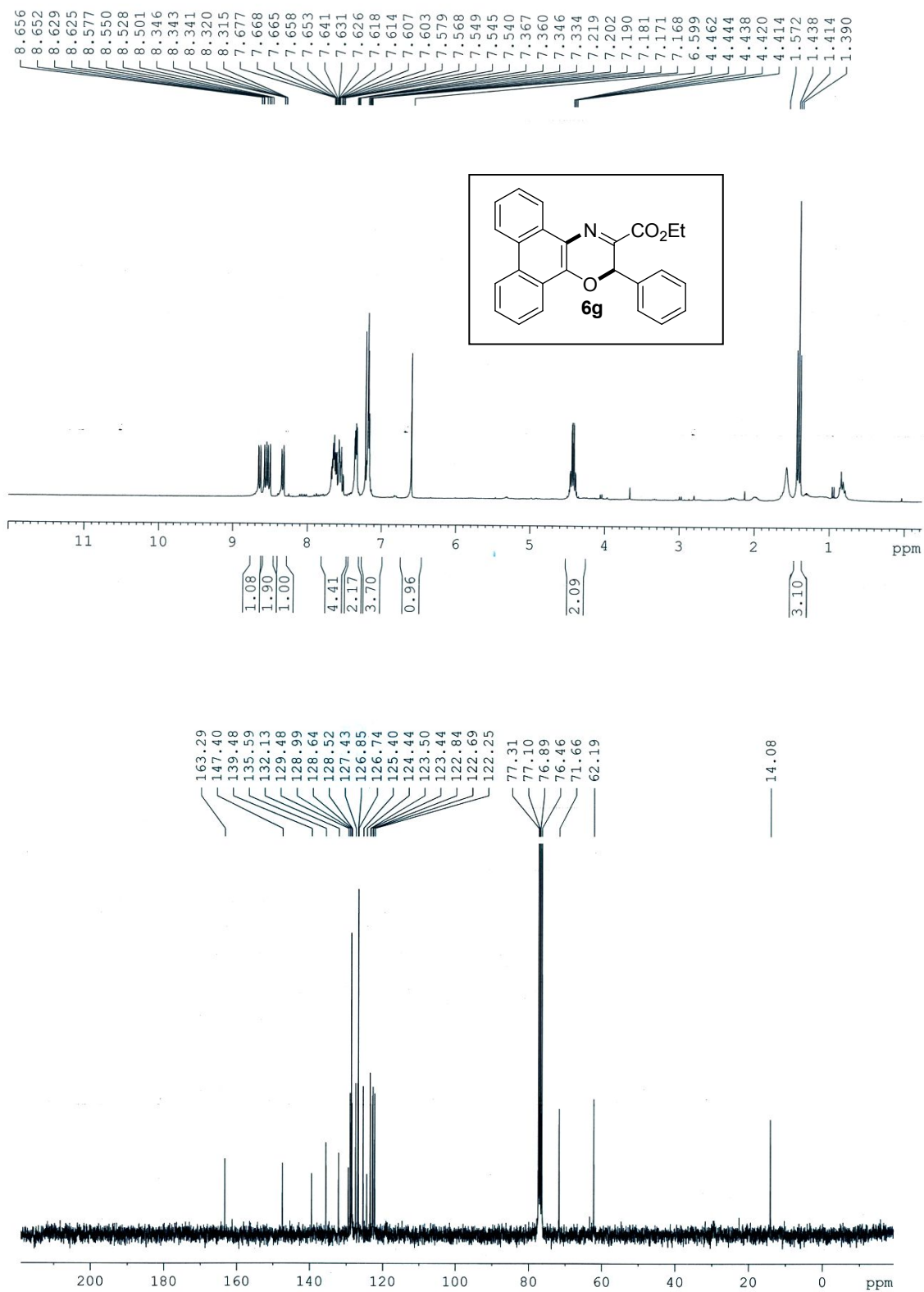


Figure S26. ¹H and ¹³C NMR of 6h

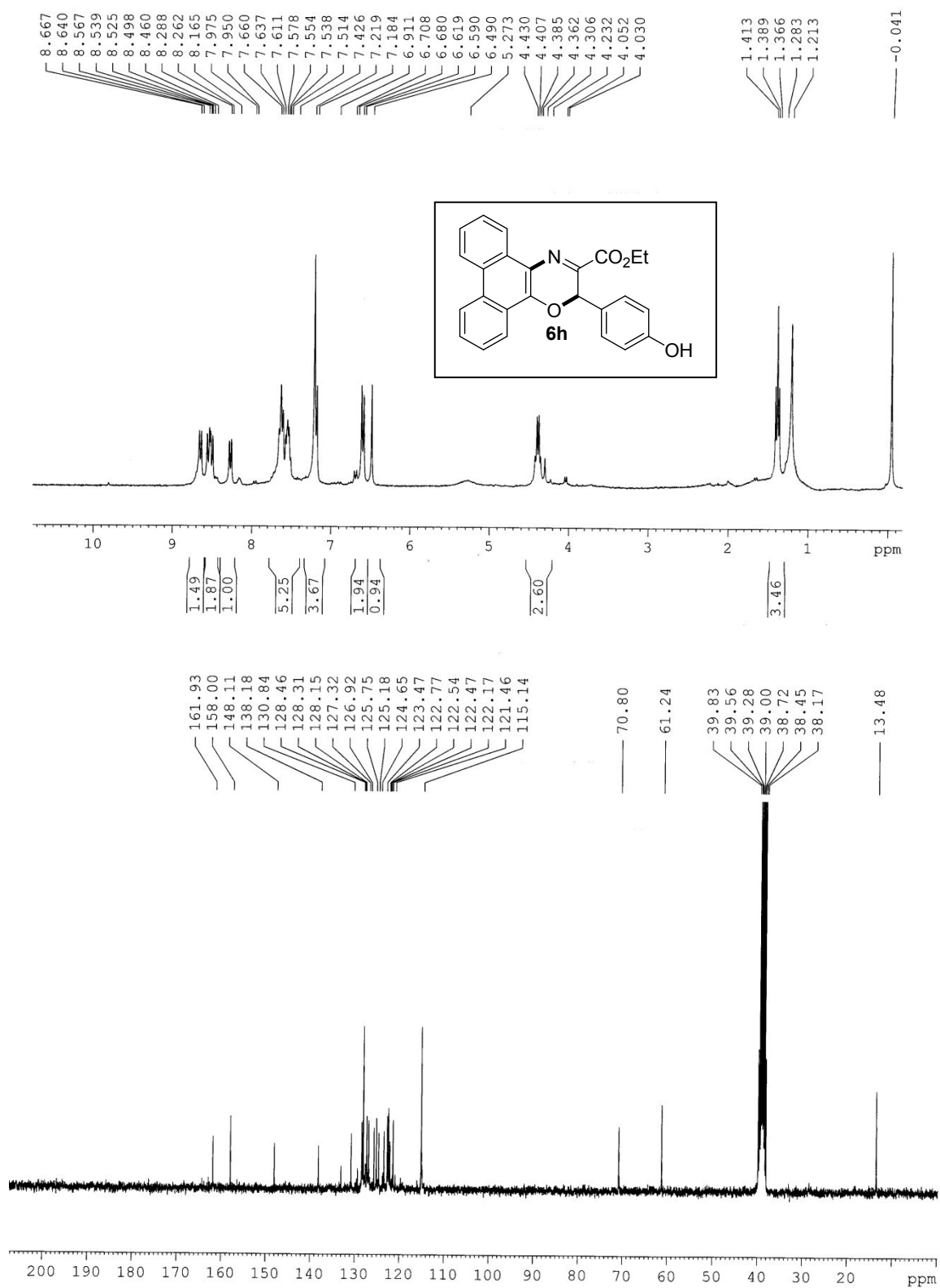


Figure S27. ^1H and ^{13}C NMR of **6i**

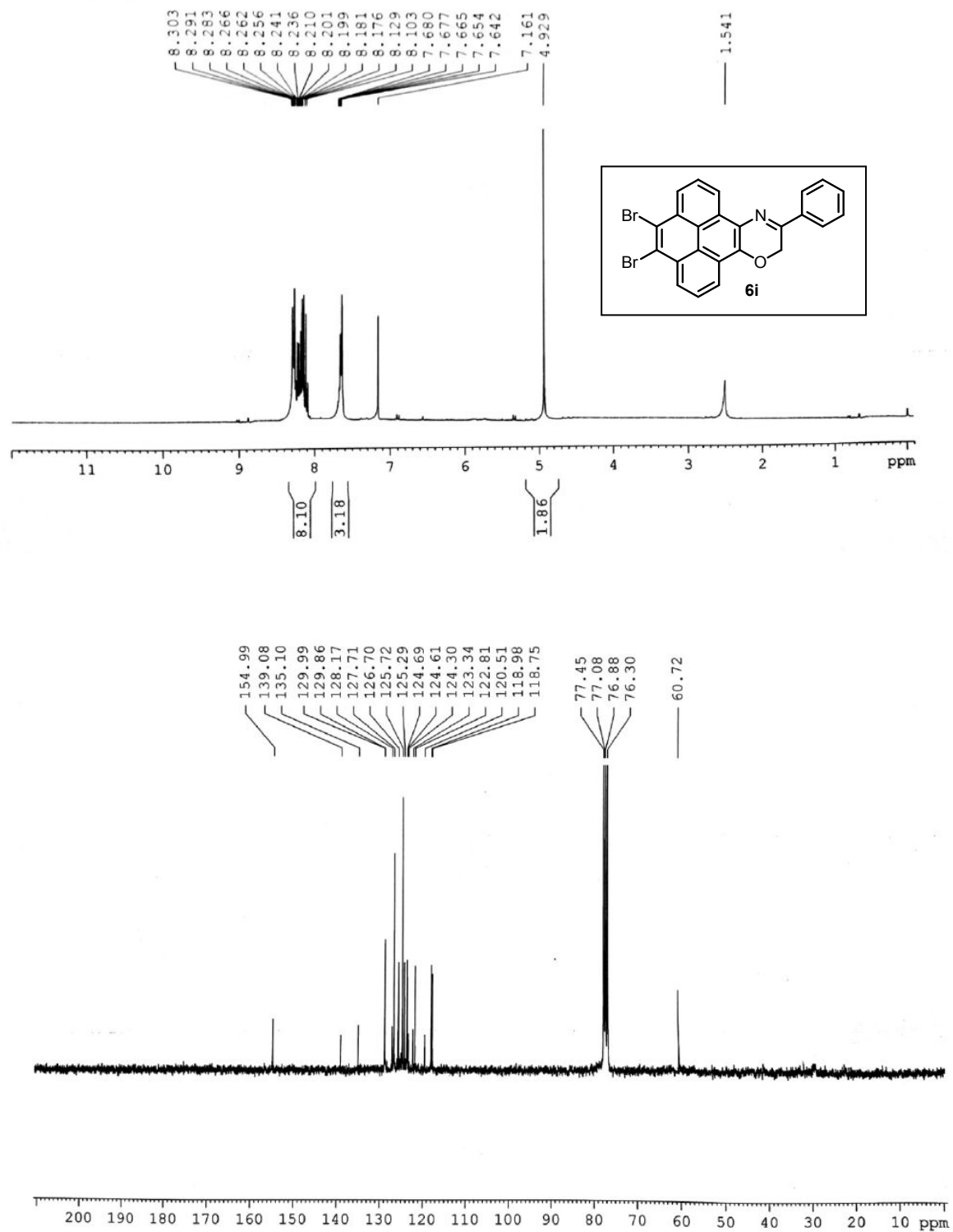


Figure S28. ^1H and ^{13}C NMR of 8a

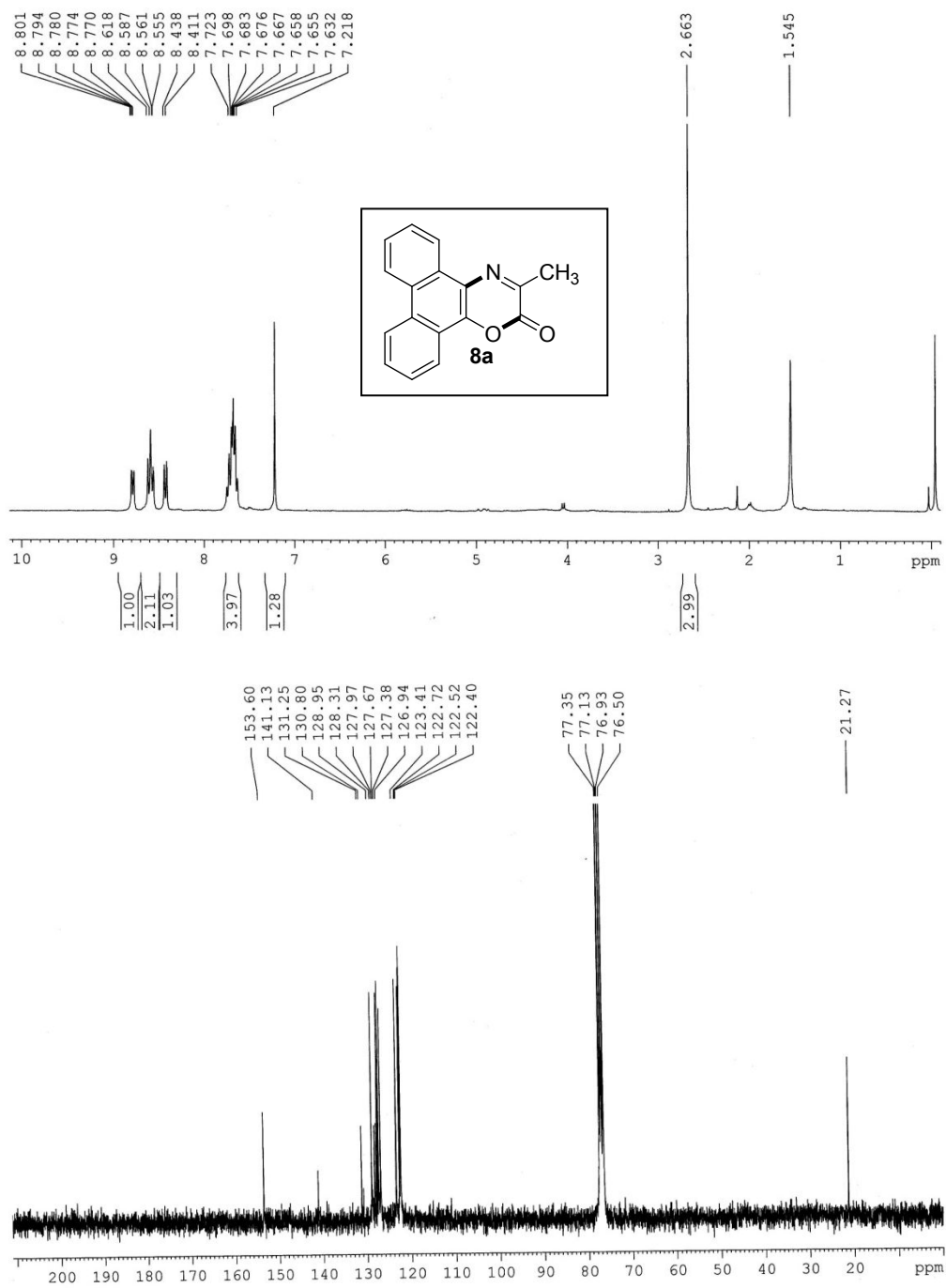


Figure S29. ^1H and ^{13}C NMR of **8b**

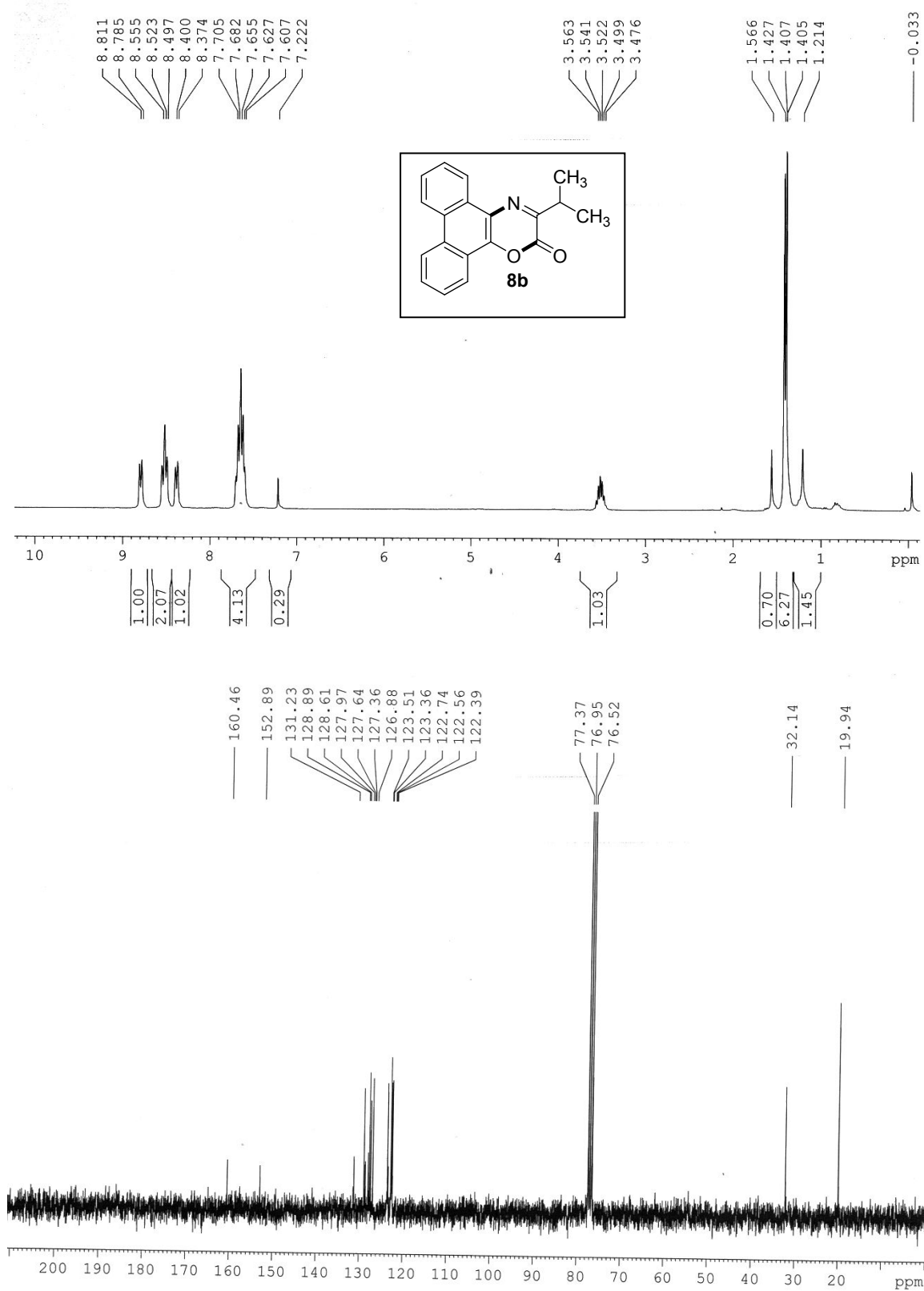
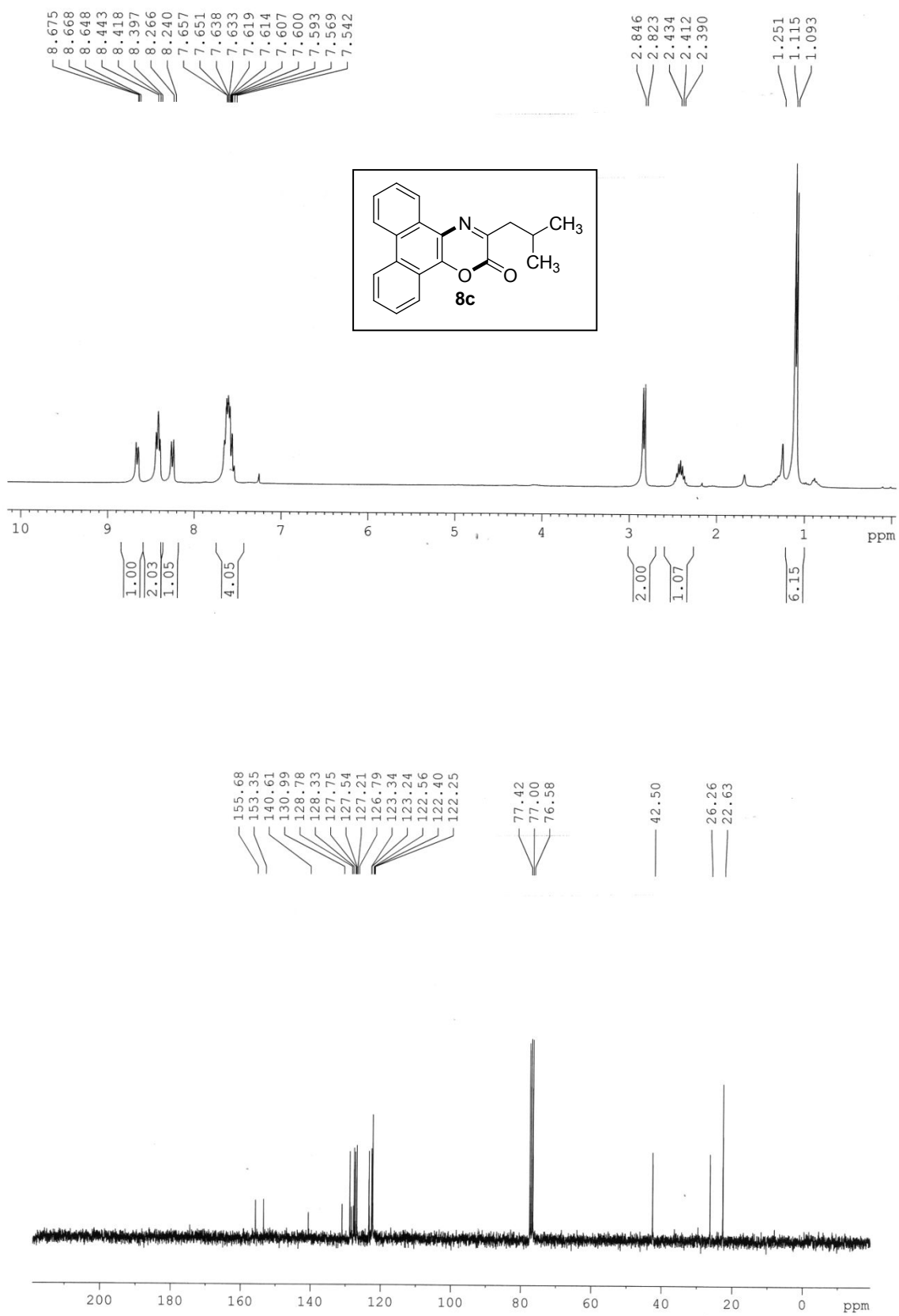


Figure S30. ^1H and ^{13}C NMR of **8c**



Section II: X-ray diffraction data of compounds 4j and 6a

X-ray diffraction data of 4j(CCDC 1551936)

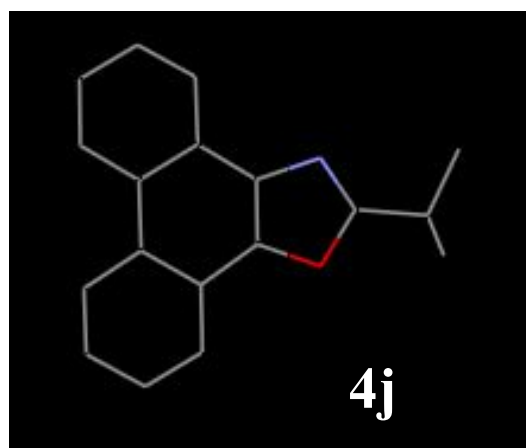
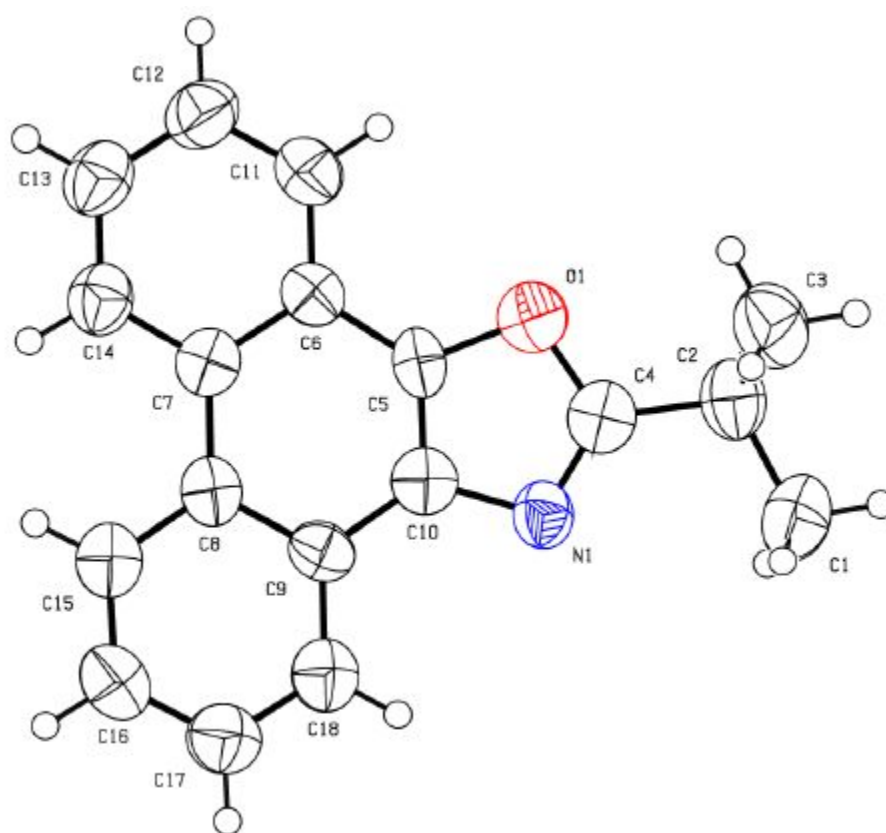


Figure S31. Thermal ellipsoid plot of 4j with ellipsoids at 50% of probability.

X-ray diffraction data of 6a (CCDC 1551938)

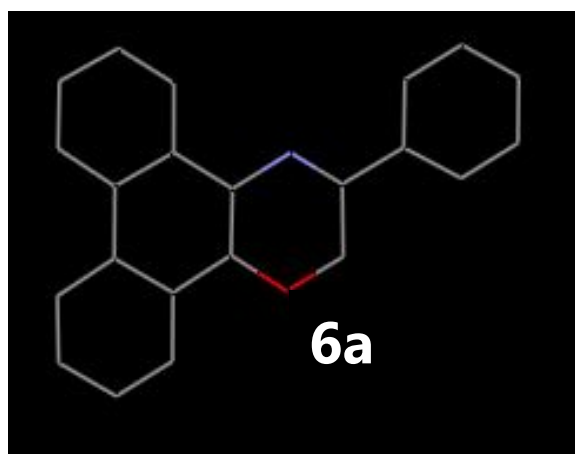
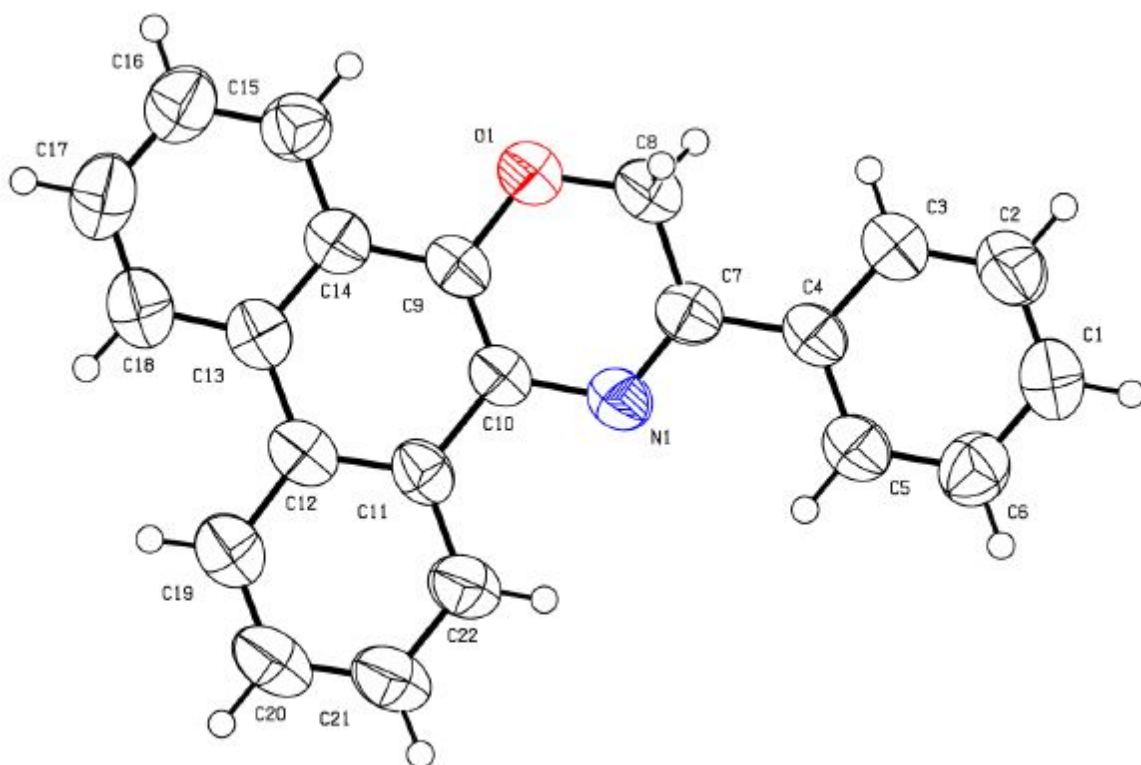


Figure S32. Thermal ellipsoid plot of 6a with ellipsoids at 50% of probability.

Crystal structure experimental protocol:

Single crystal of compound **4j** and **6a** were mounted on a Bruker-AXS SMART APEX II diffractometer equipped with a graphite monochromator and Mo K α ($\lambda = 0.71073 \text{ \AA}$) radiation. The crystal was placed 60 mm from the CCD, and frames (360) were measured with a counting time of 5s. The structures were solved using the Patterson method using the SHELXS 97 program. Non-hydrogen atoms were refined with independent anisotropic displacement parameters, while difference Fourier synthesis and least-squares refinement showed the positions of any remaining non-hydrogen atoms. The non-hydrogen atoms were refined with anisotropic thermal parameters. Successful convergence was indicated by the maximum shift/error of 0.001 for the last cycle of the least-squares refinement. All other crystallographic details such as h, k, l ranges, 2θ ranges, and R-factors can be found above (Table S1 and S2).

Section III: Mass spectra data

Mass spectra were taken in infusion method.

Parameters

Source - capillary (kv): 3.06, Sampling cone: 85, source offset: 80

Temp($^{\circ}$ C) - Source: 120, Desolvation: 300

Gas flows– Cone gas (L/h) 50, Desolvation gas (L/h) 600, Lock spray capillary (kv) 2.50

ESI-MS Study of the ongoing reaction

Herein, we have also carried out the HRMS study of the two reaction mixtures separately. In all cases a certain amount of aliquot was withdrawn from the reaction mixture which was subjected to mass analysis. The following spectra are the spectra of intermediates (**IA-B** and **IIIA-B**) and each of the spectrum is followed by their simulated pattern.

Figure S33. ESI-MS spectra of IA

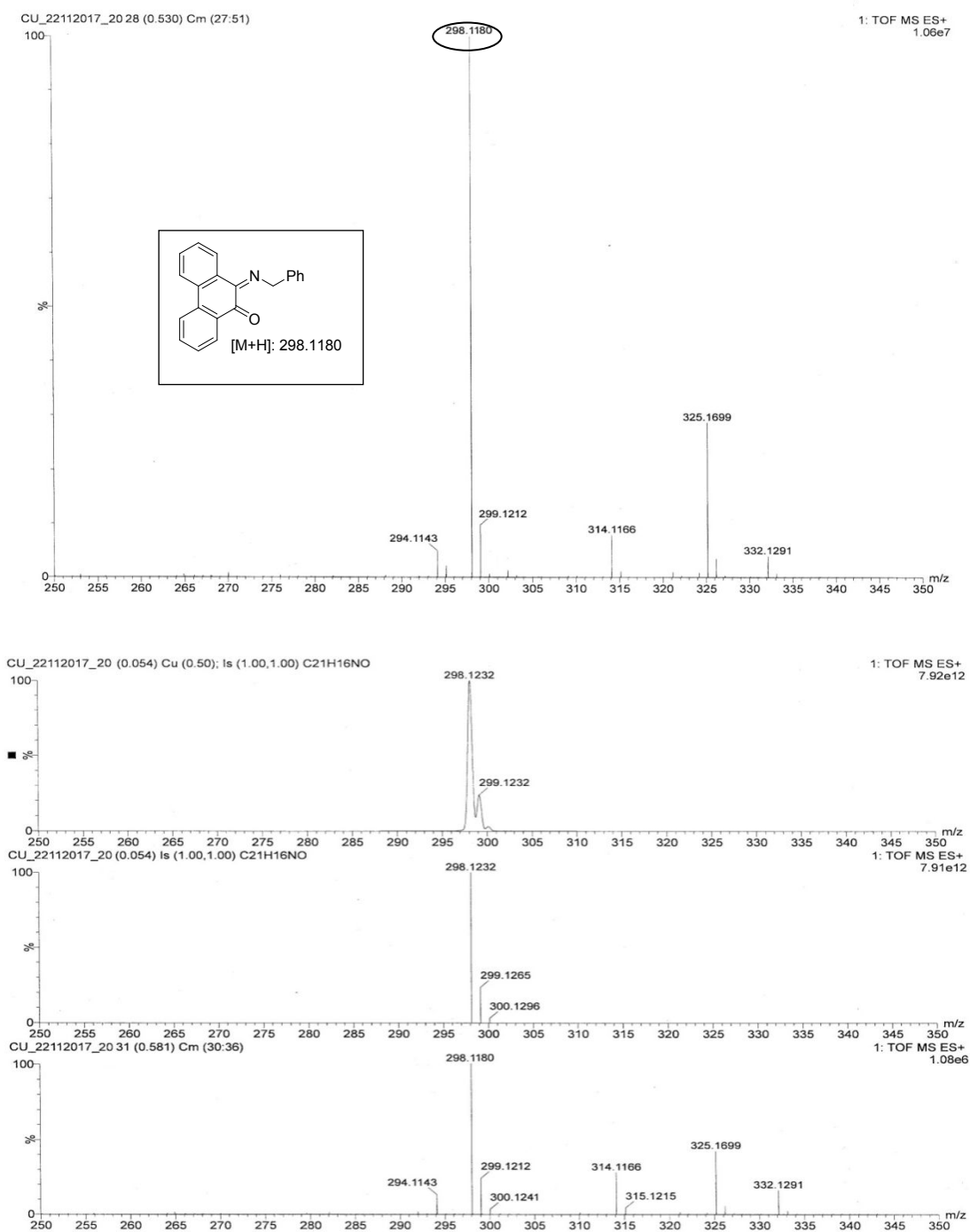


Figure S34. ESI-MS spectra of IB

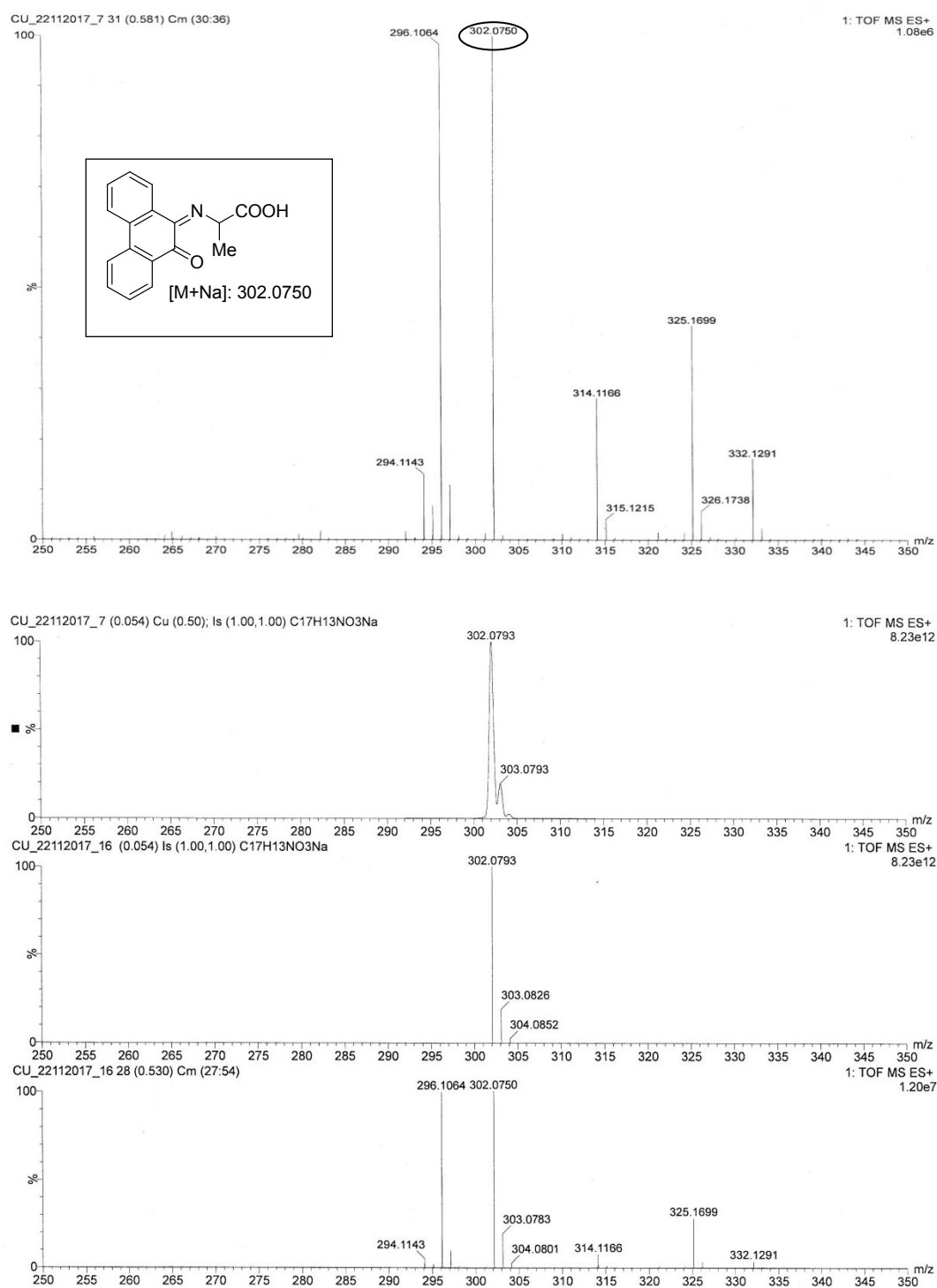


Figure S35. ESI-MS spectra of IIIA

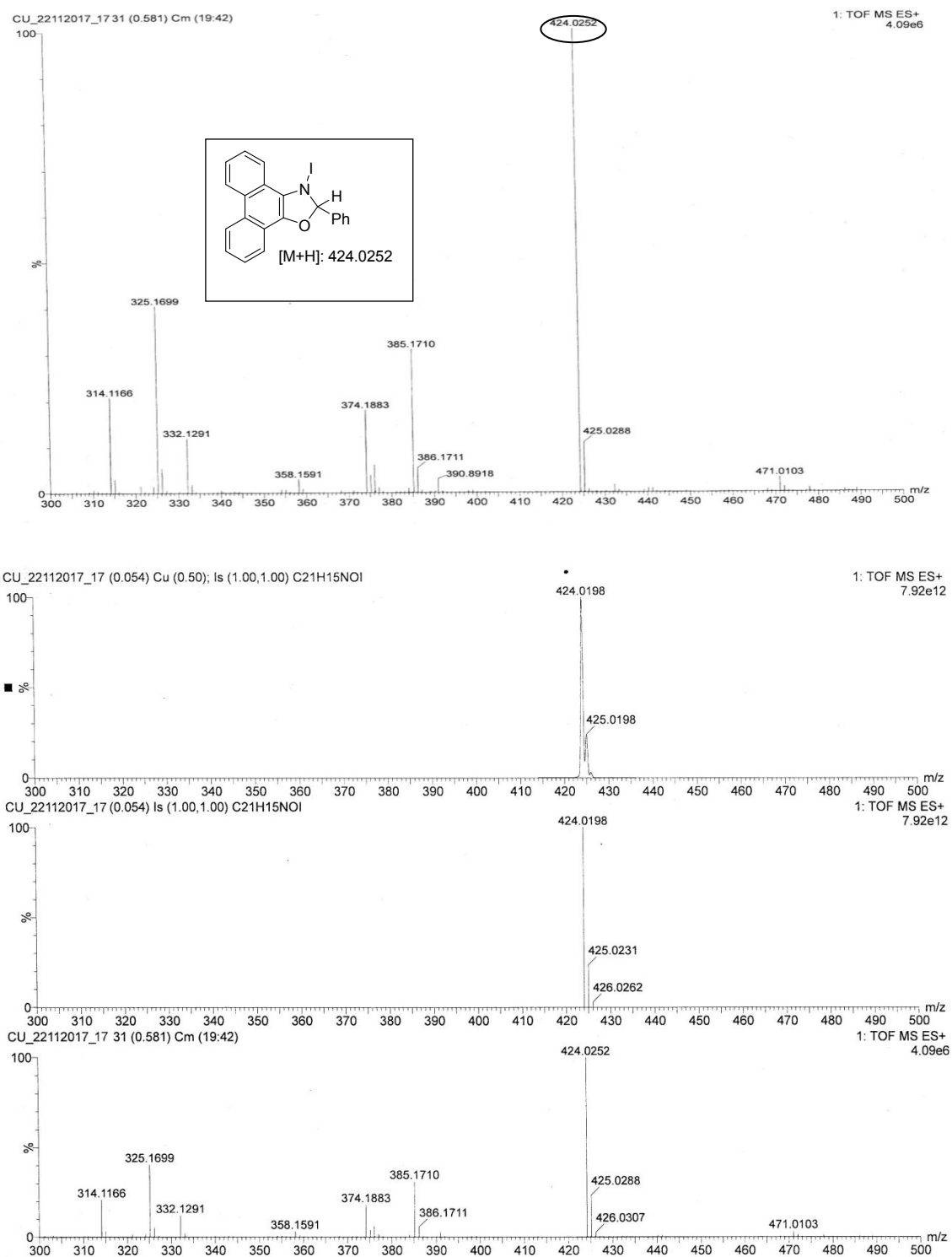


Figure S36. ESI-MS spectra of IIIB

