

Supporting Information

Pyridine-Based Small-Molecule Fluorescent Probes as Optical Sensors for Benzene and Gasoline Adulteration

Thiago J. Peglow, Marcelo M. Vieira, Nathalia B. Padilha, Bianca T. Dalberto,
Henrique C. S. Junior, Fabiano S. Rodembusch* and Paulo H. Schneider*

Instituto de Química, Laboratory of Molecular Catalysis (LAMOCA),
Universidade Federal do Rio Grande do Sul (UFRGS), P.O. Box
15003, 91501-970, Porto Alegre-RS, Brazil.

* Correspondence: paulos@iq.ufrgs.br (P.H.S.),
fabiano.rodembusch@ufrgs.br (F.S.R)

Table of Contents

	Page
1. Spectroscopic characterization	S2
2. Additional photophysical data	S24
3. Additional theoretical data	S30

Spectroscopic characterization

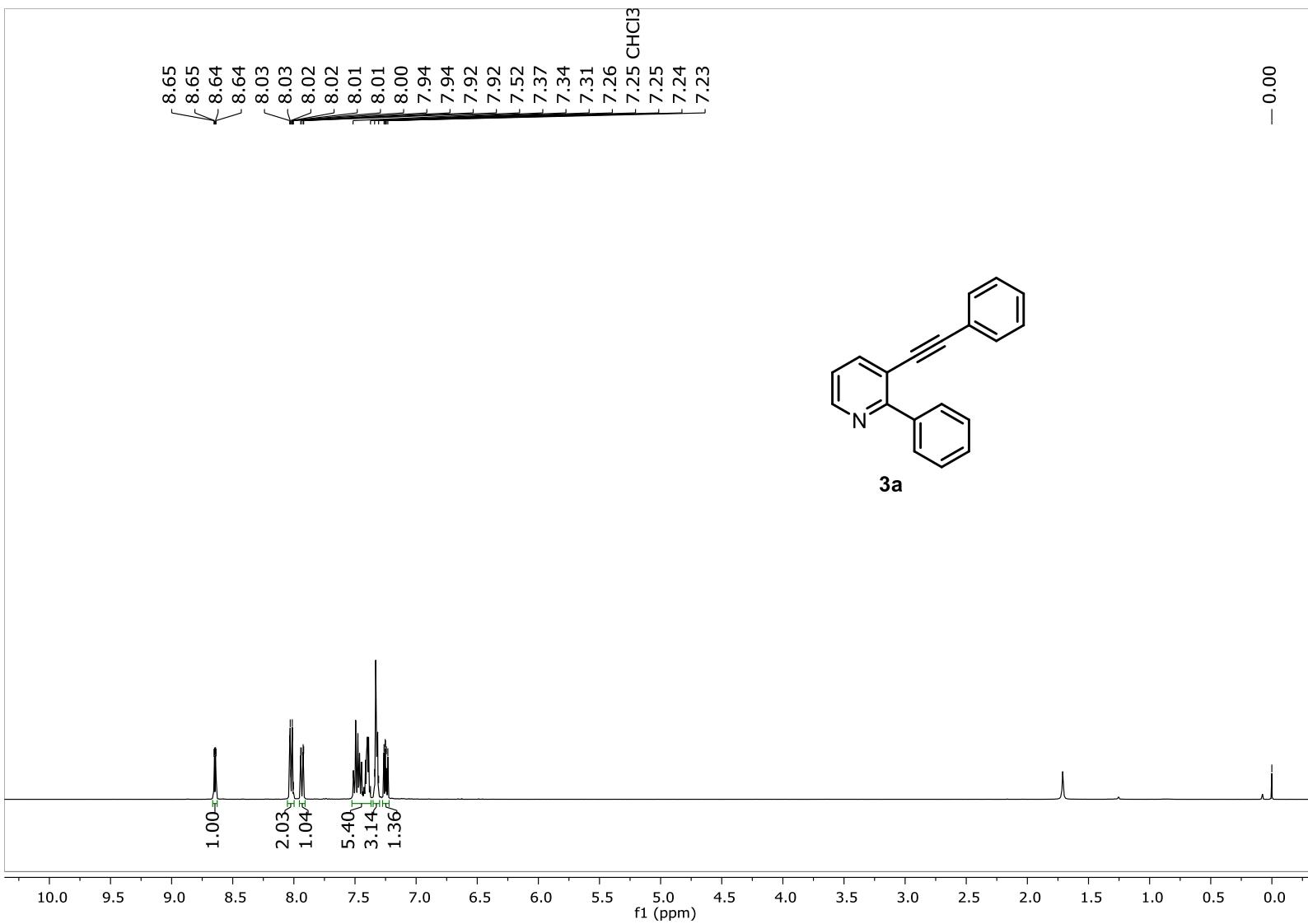


Figure S1: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3a**.

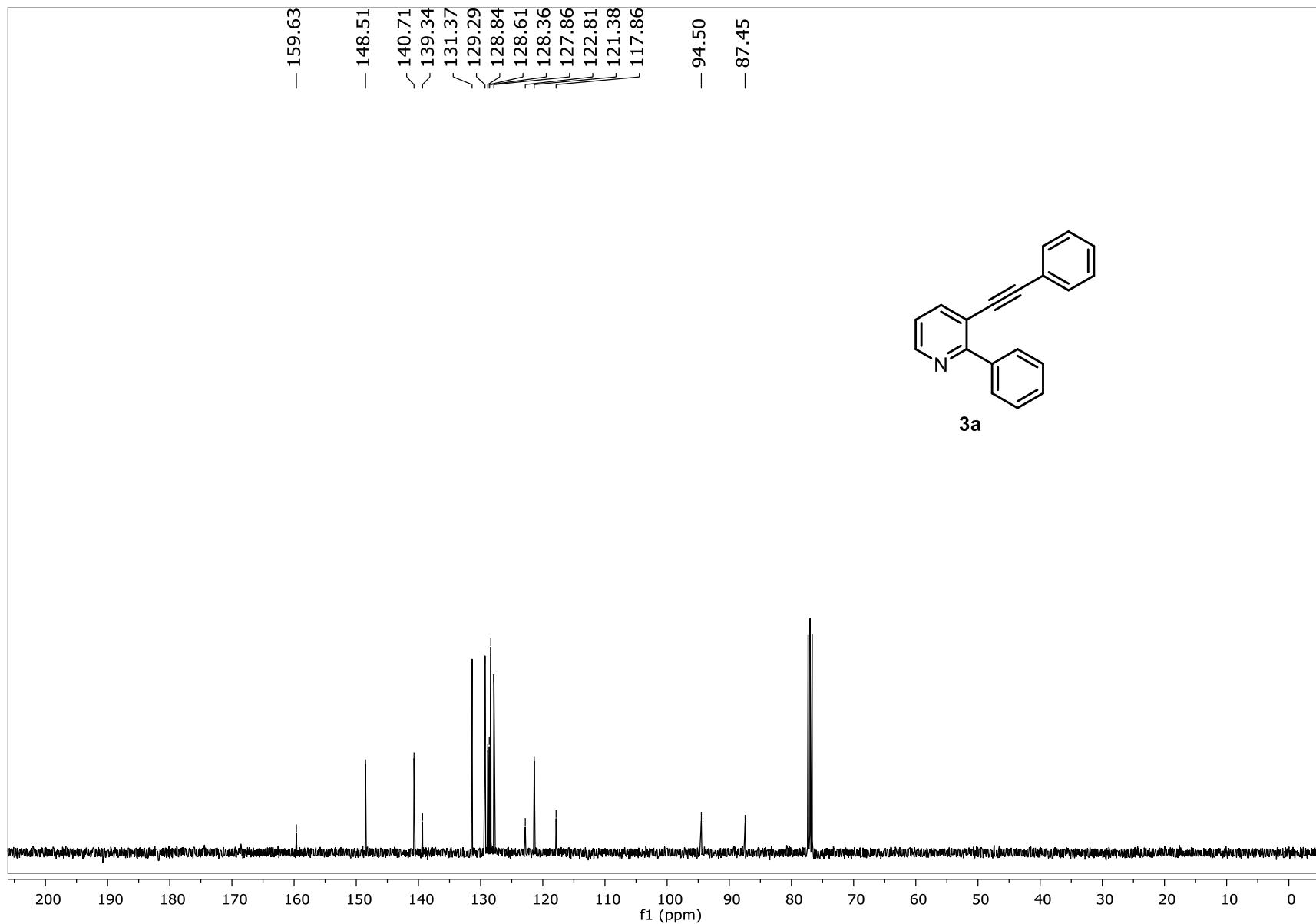


Figure S2: $^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3a**.

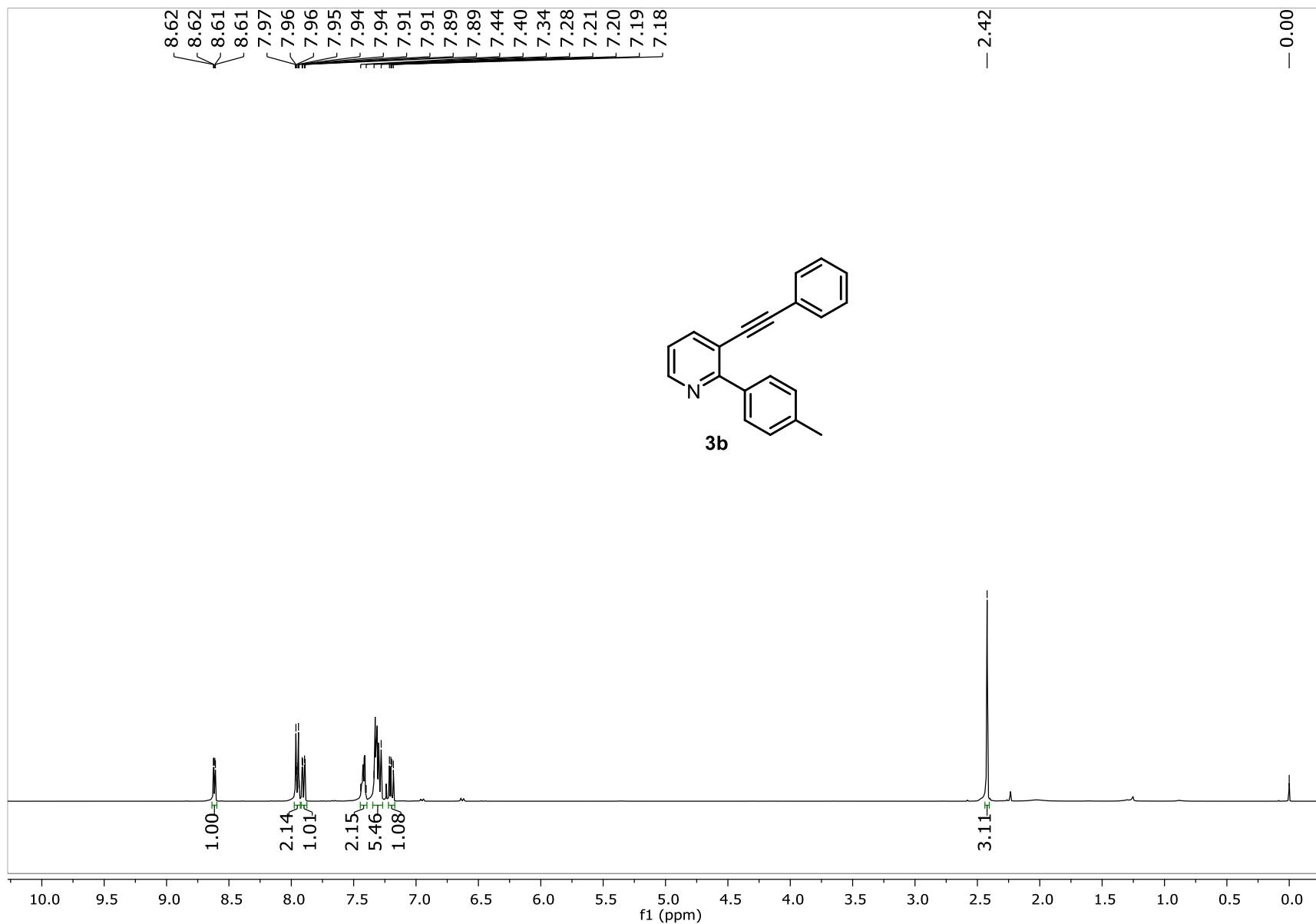


Figure S3: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3b**.

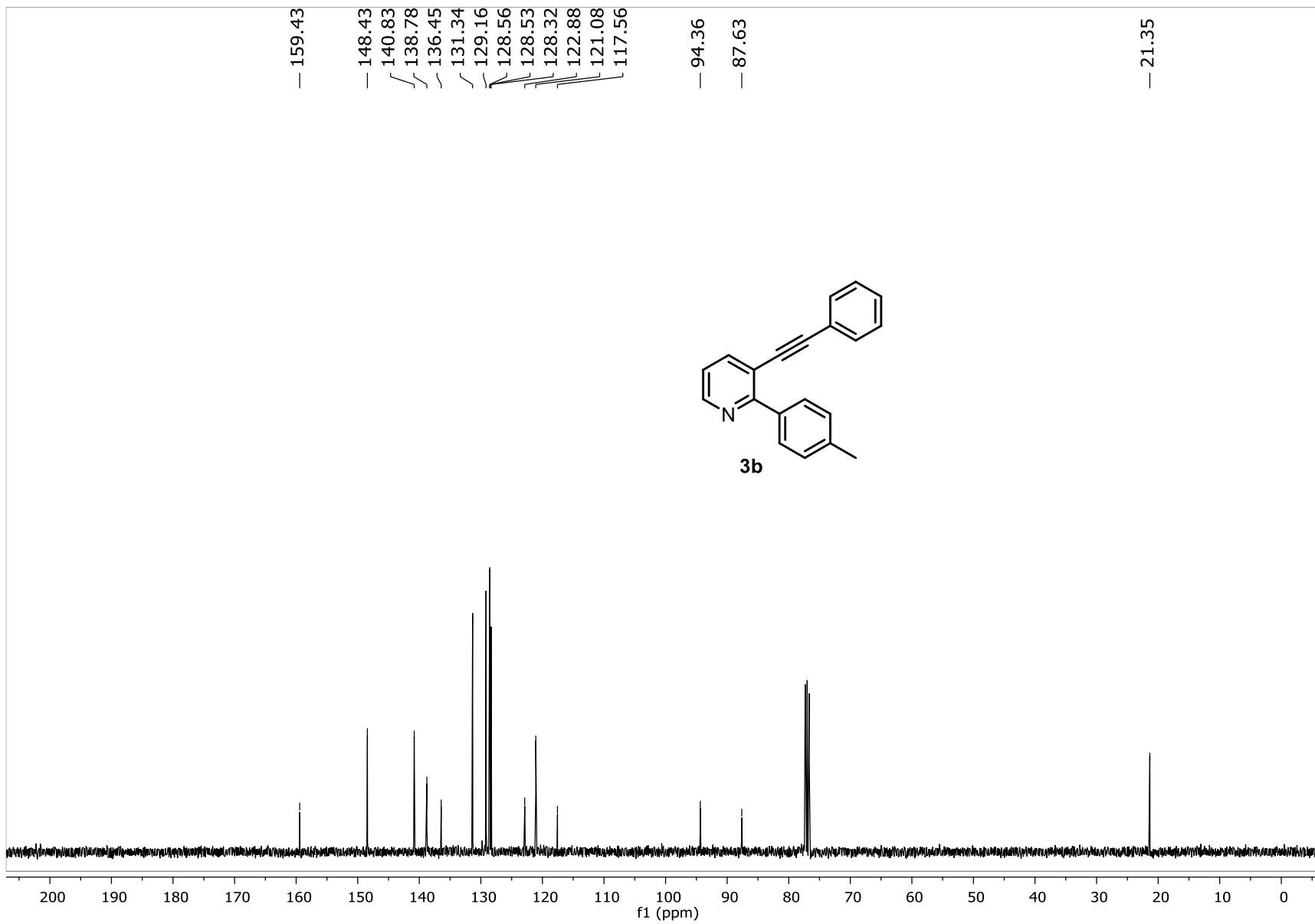


Figure S4: $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3b**.

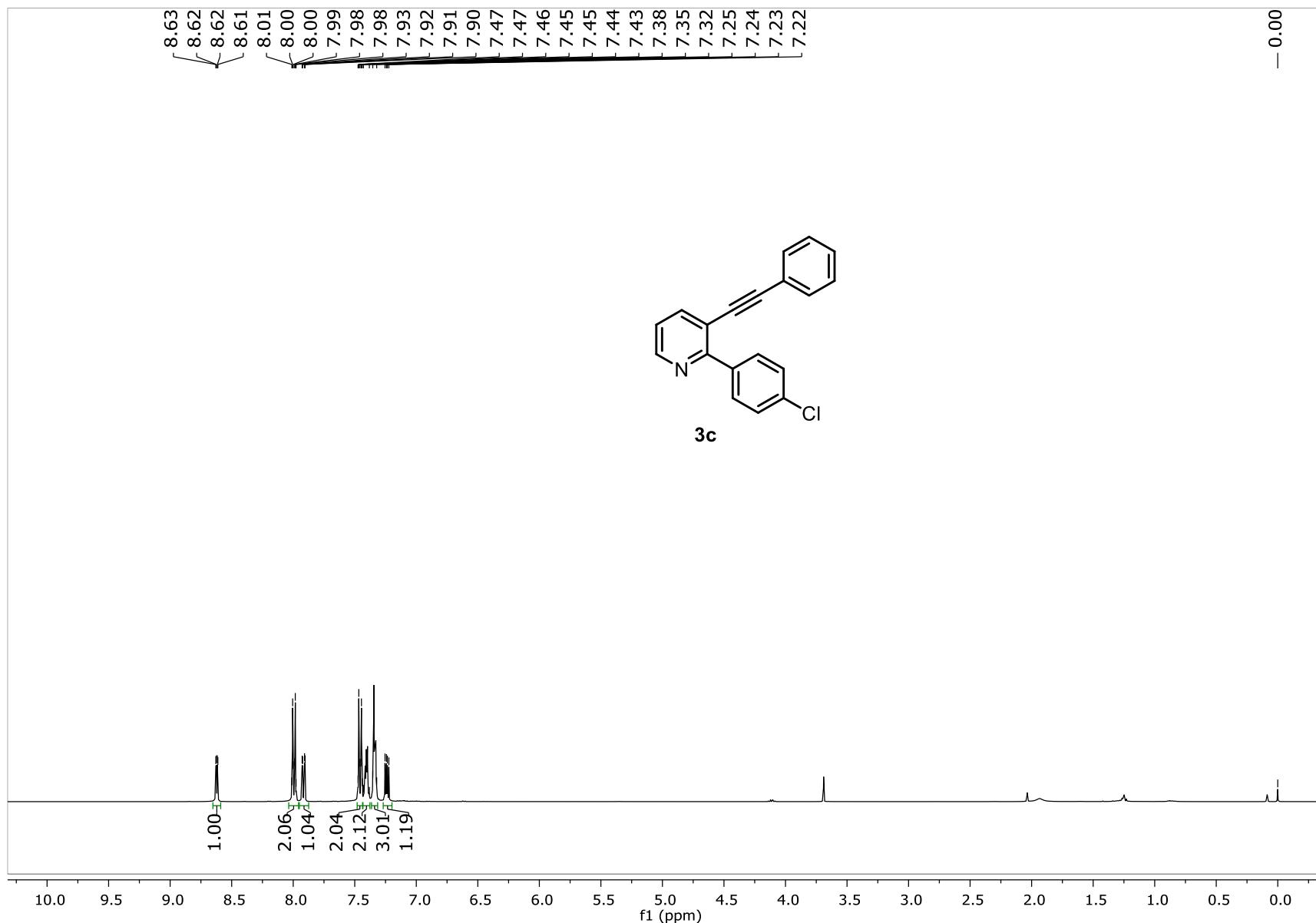


Figure S5: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3c**.

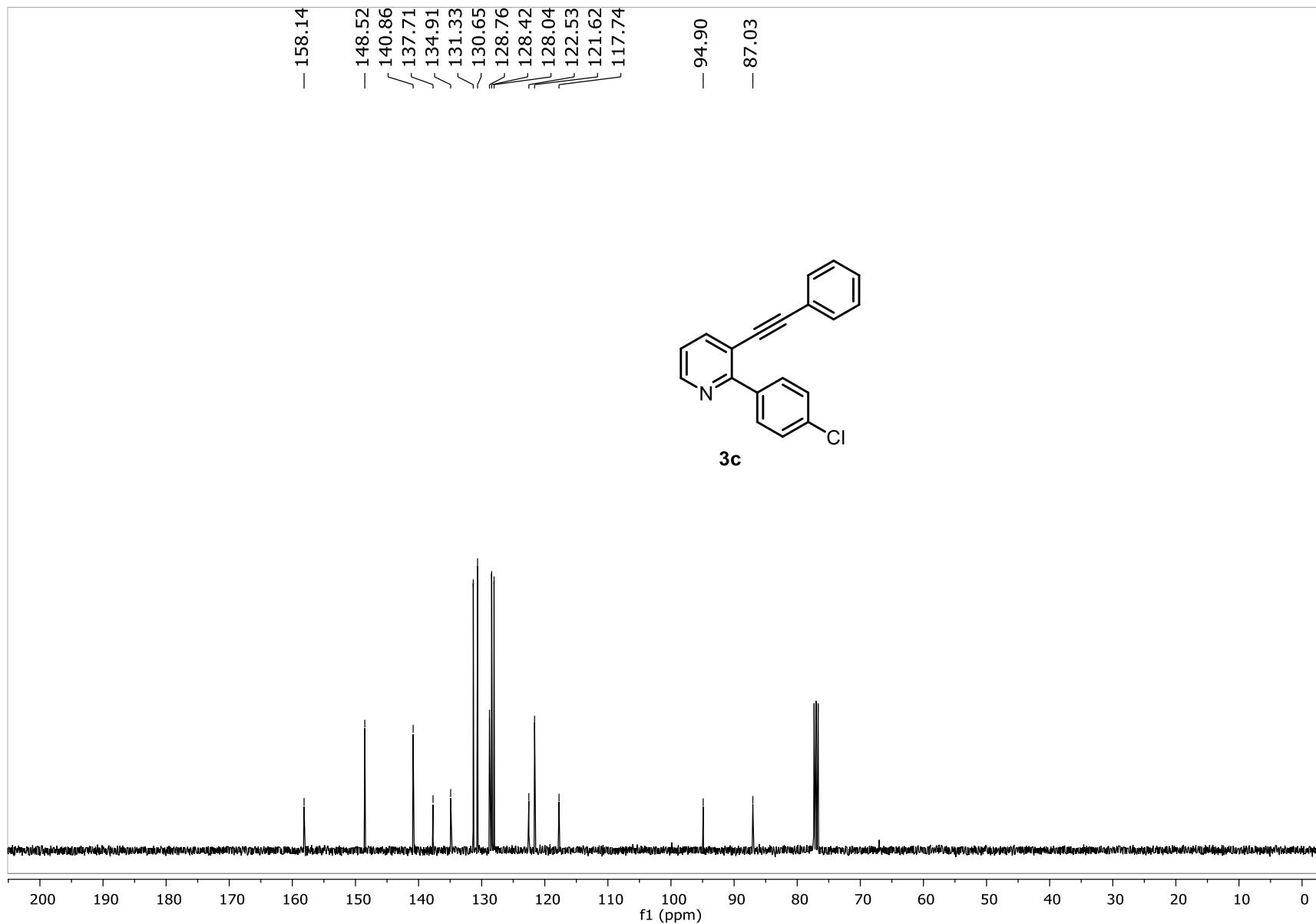


Figure S6: $^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3c**.

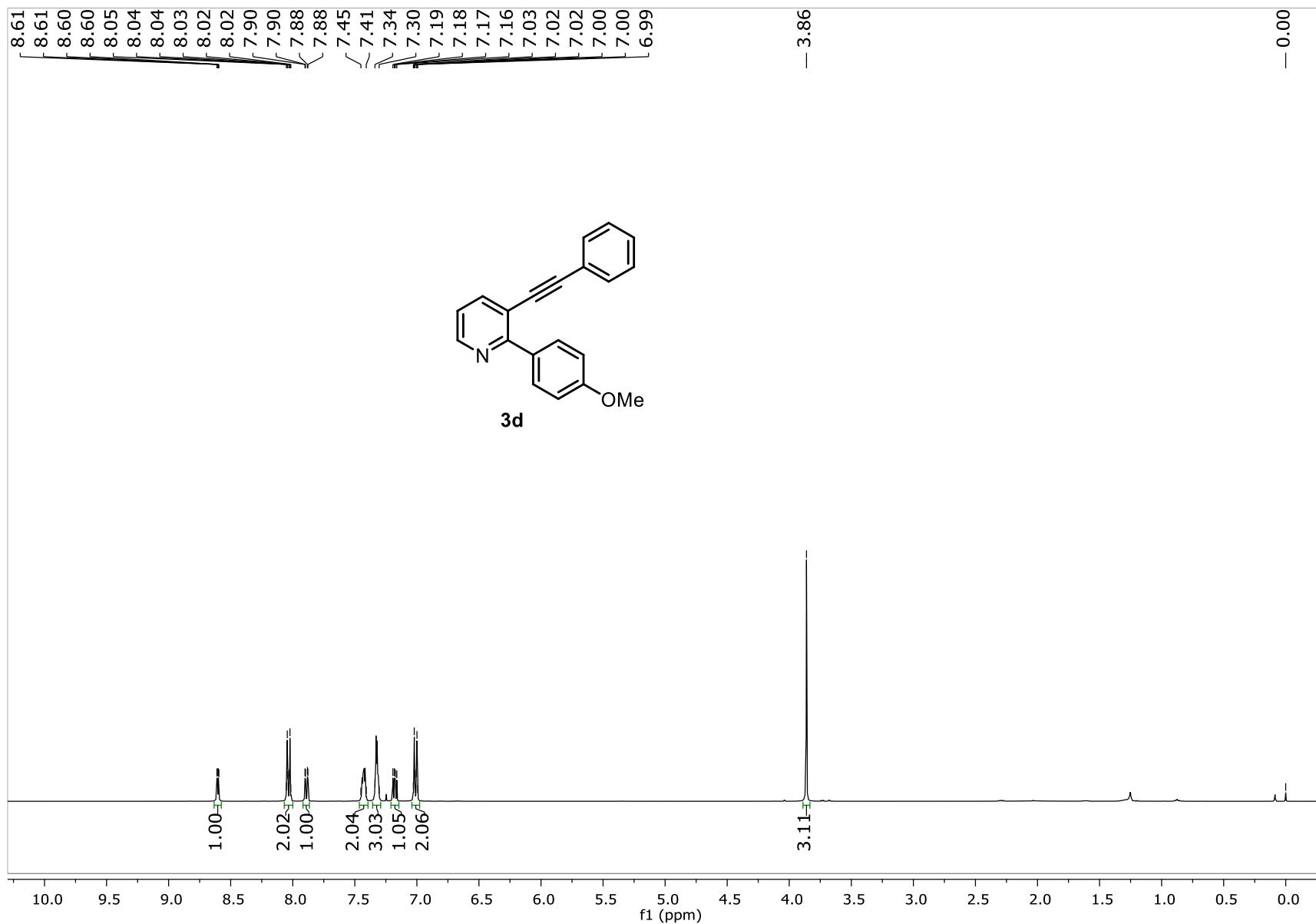


Figure S7: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3d**.

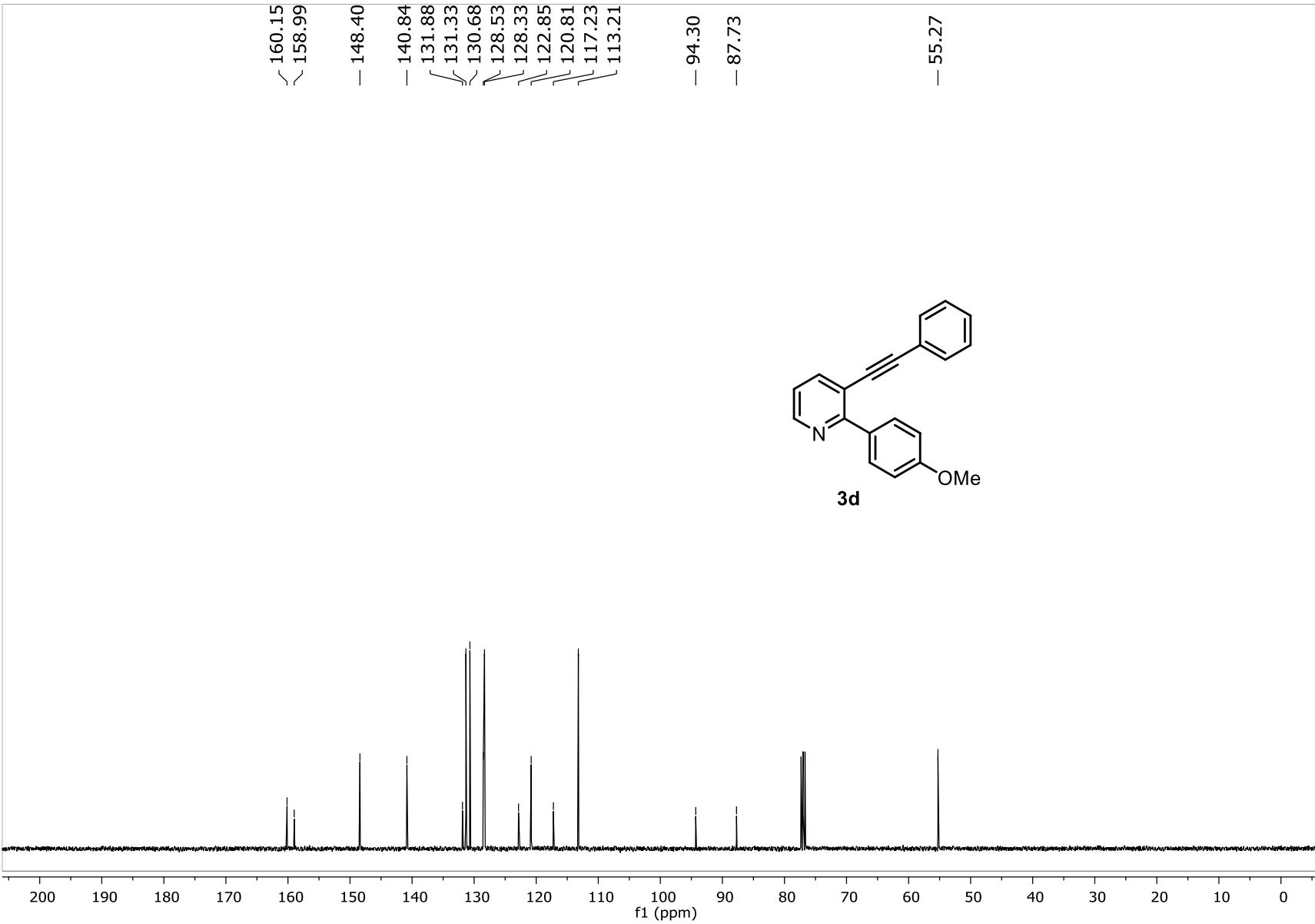


Figure S8: $^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3d**.

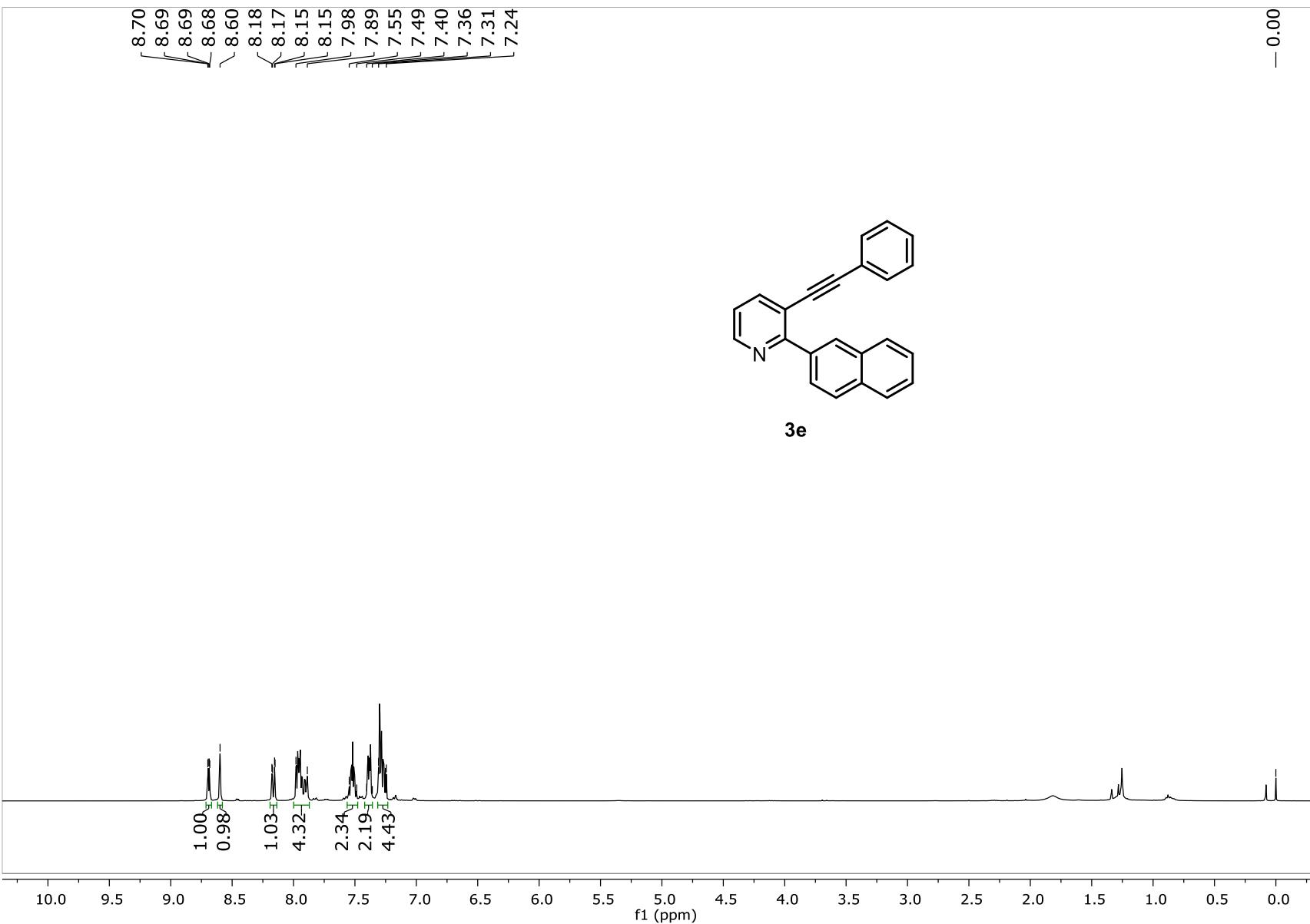


Figure S9: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3e**.

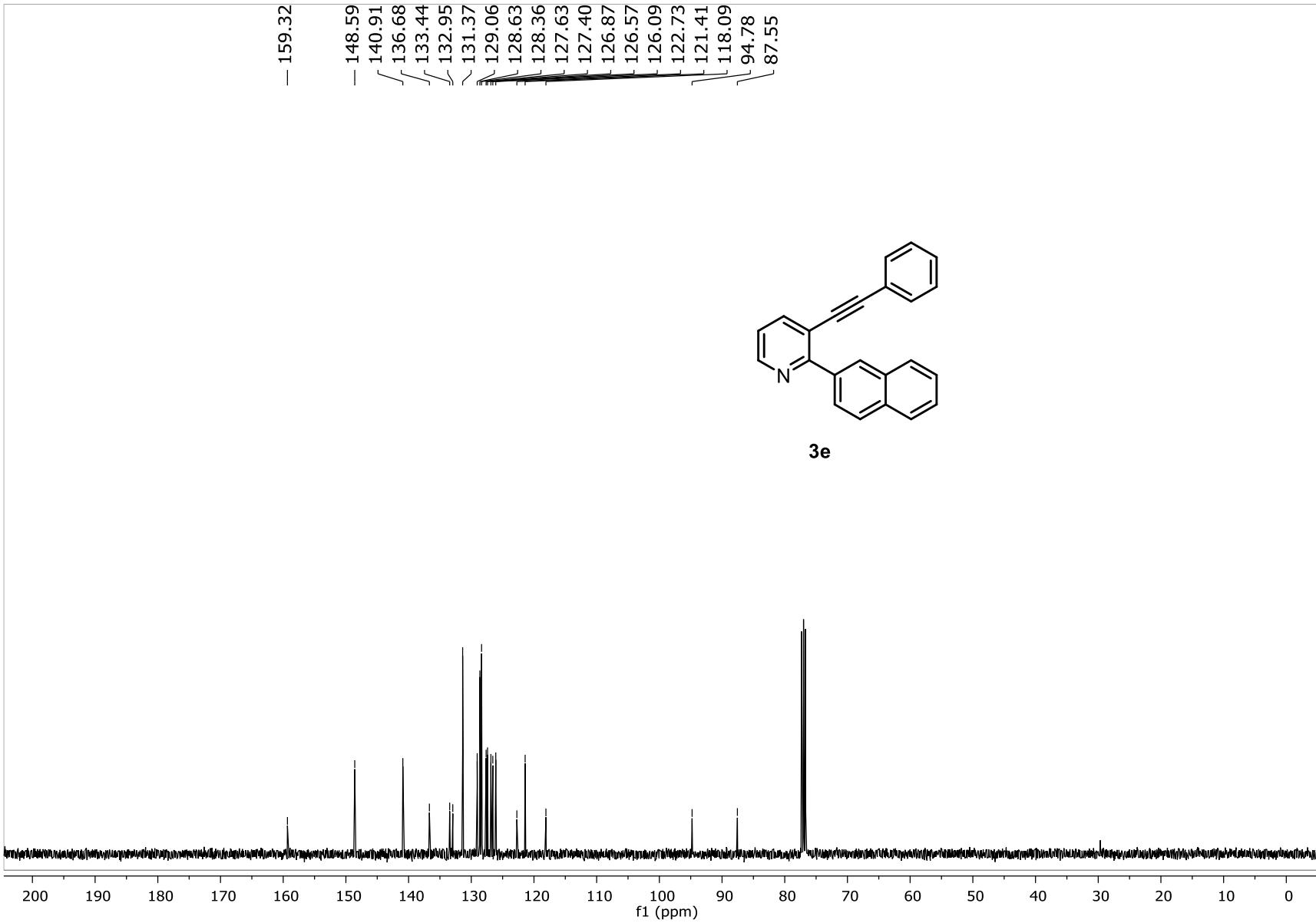


Figure S10: $^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3e**.

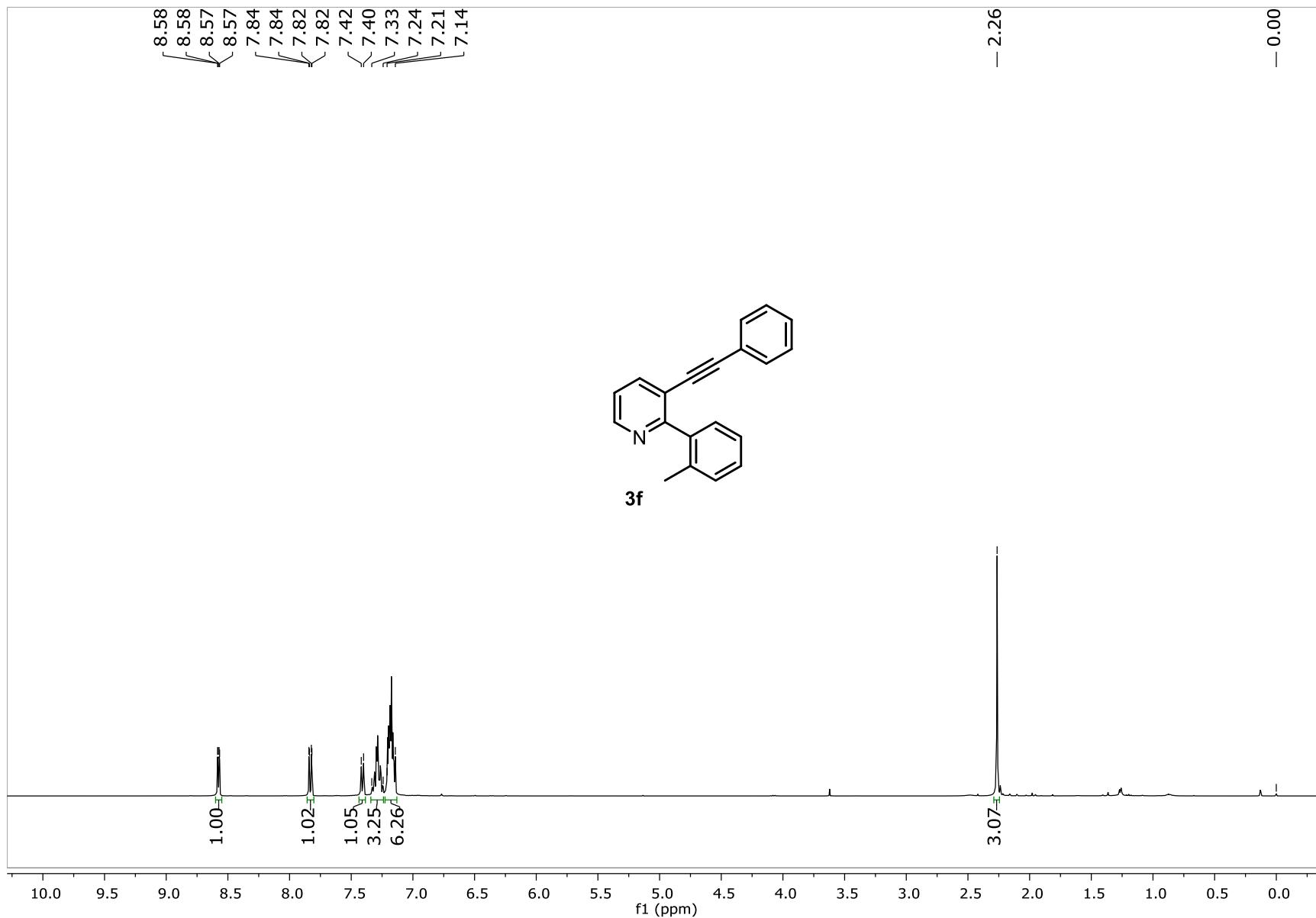


Figure S11: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3f**.

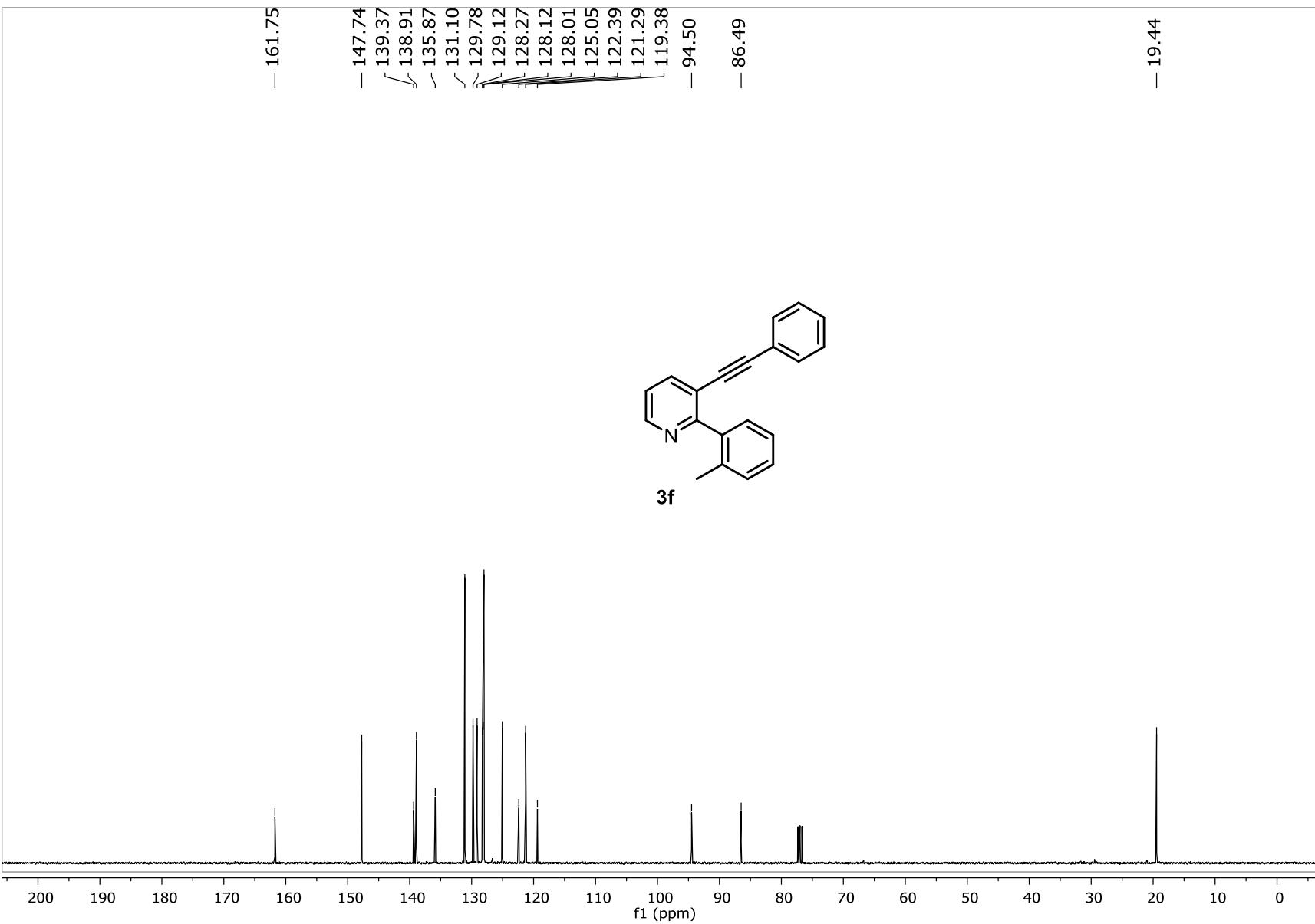


Figure S12: $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3f**.

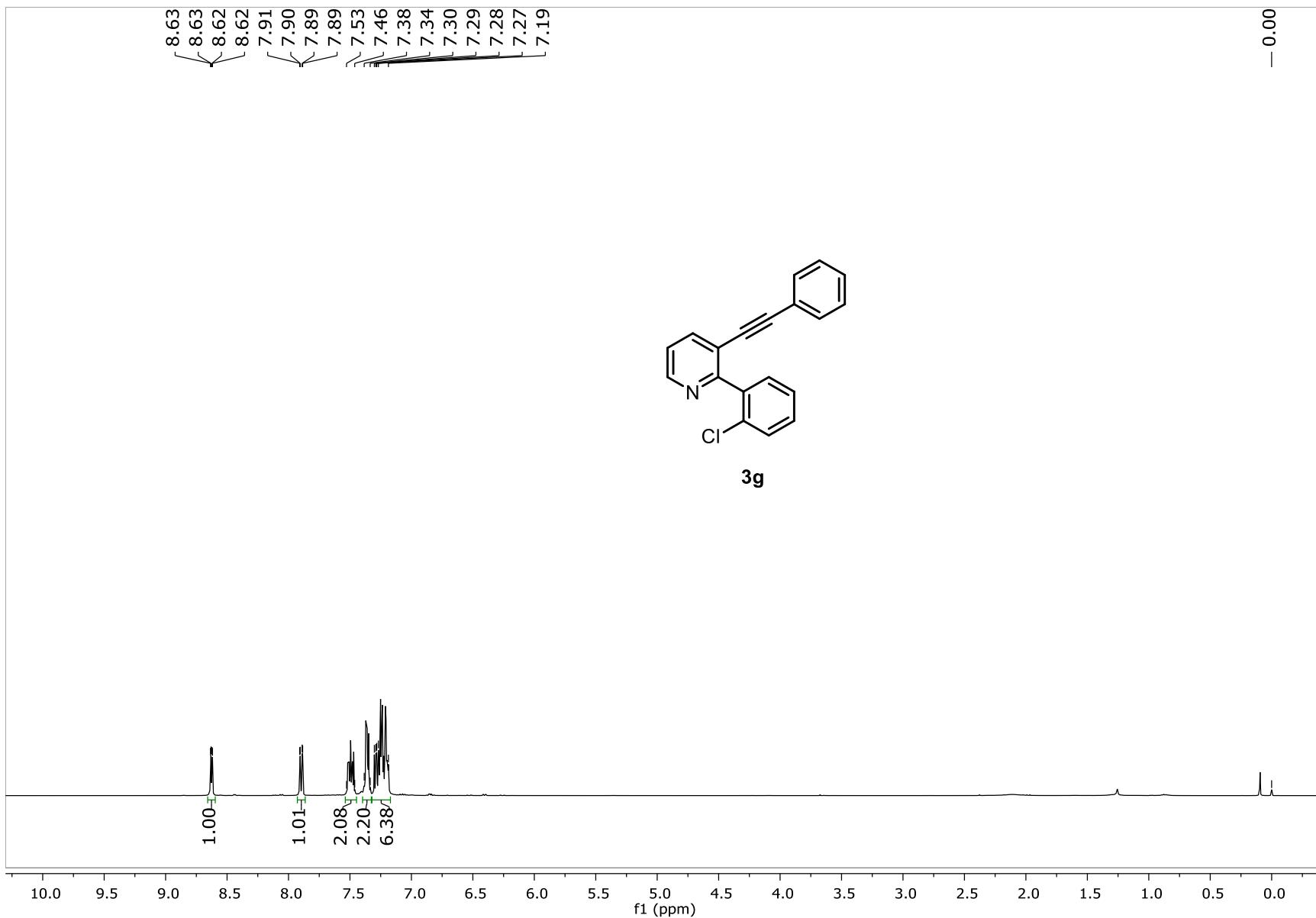


Figure S13: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3g**.

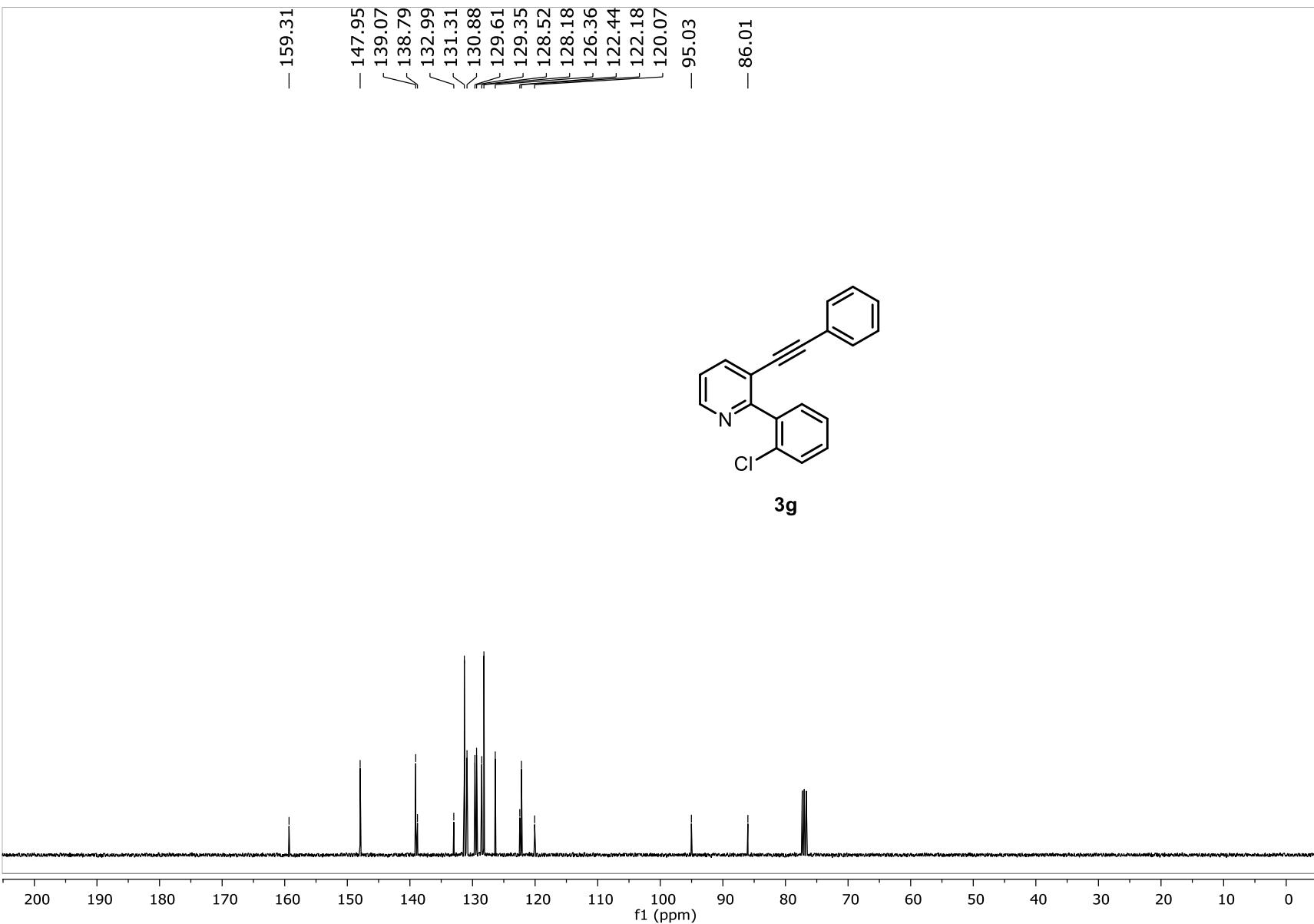


Figure S14: $^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3g**.

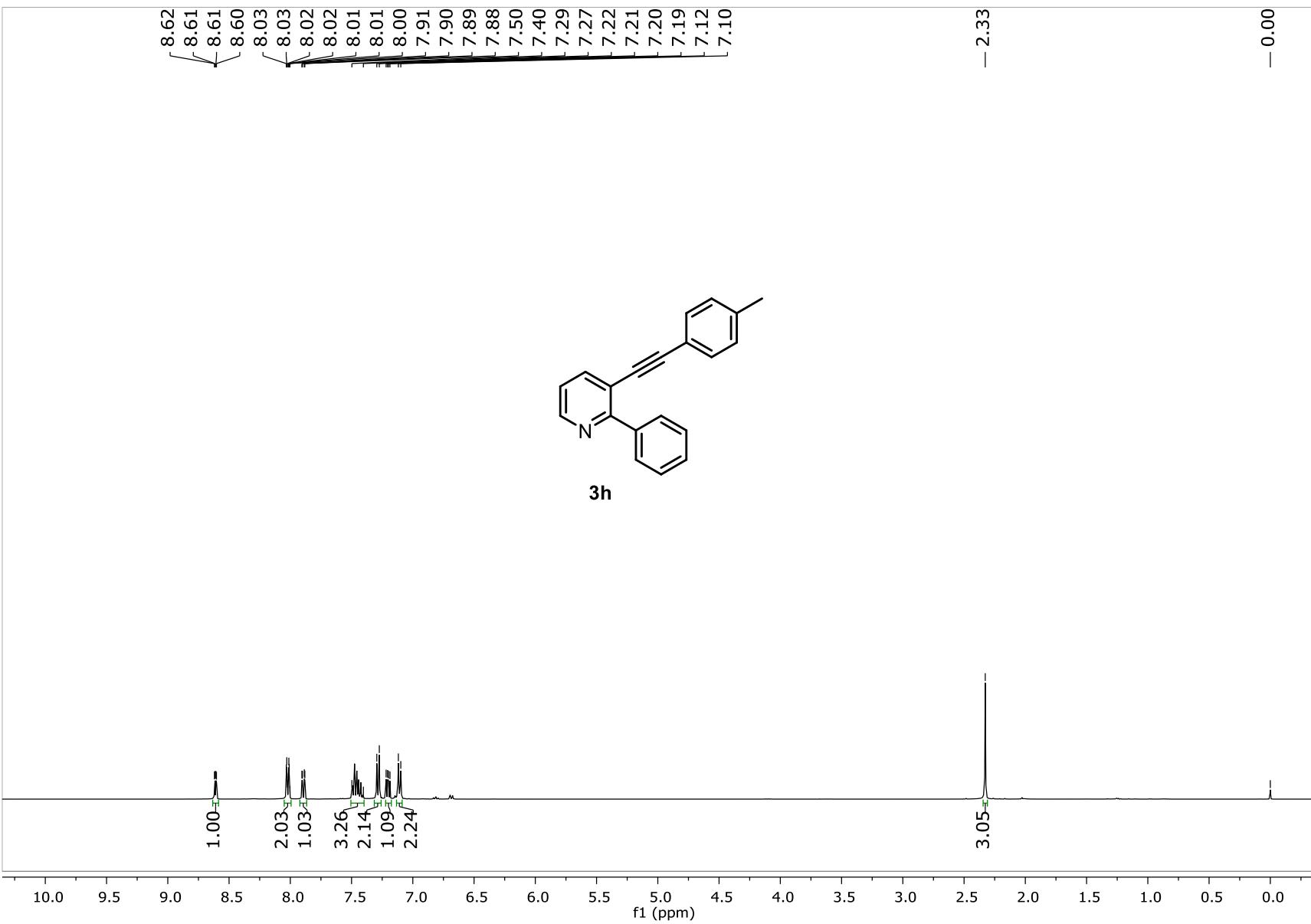


Figure S15: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3h**.

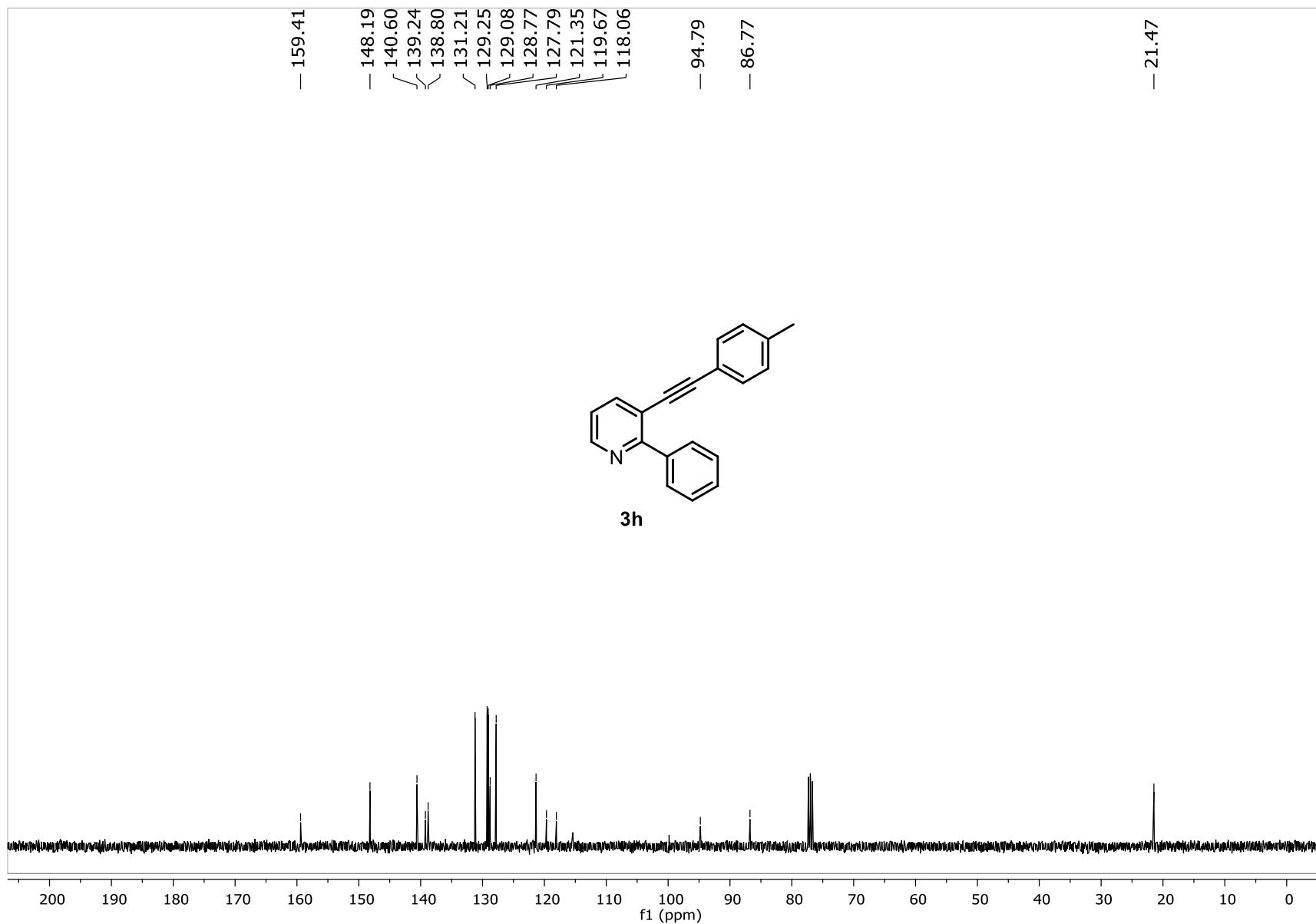


Figure S16: $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3h**.

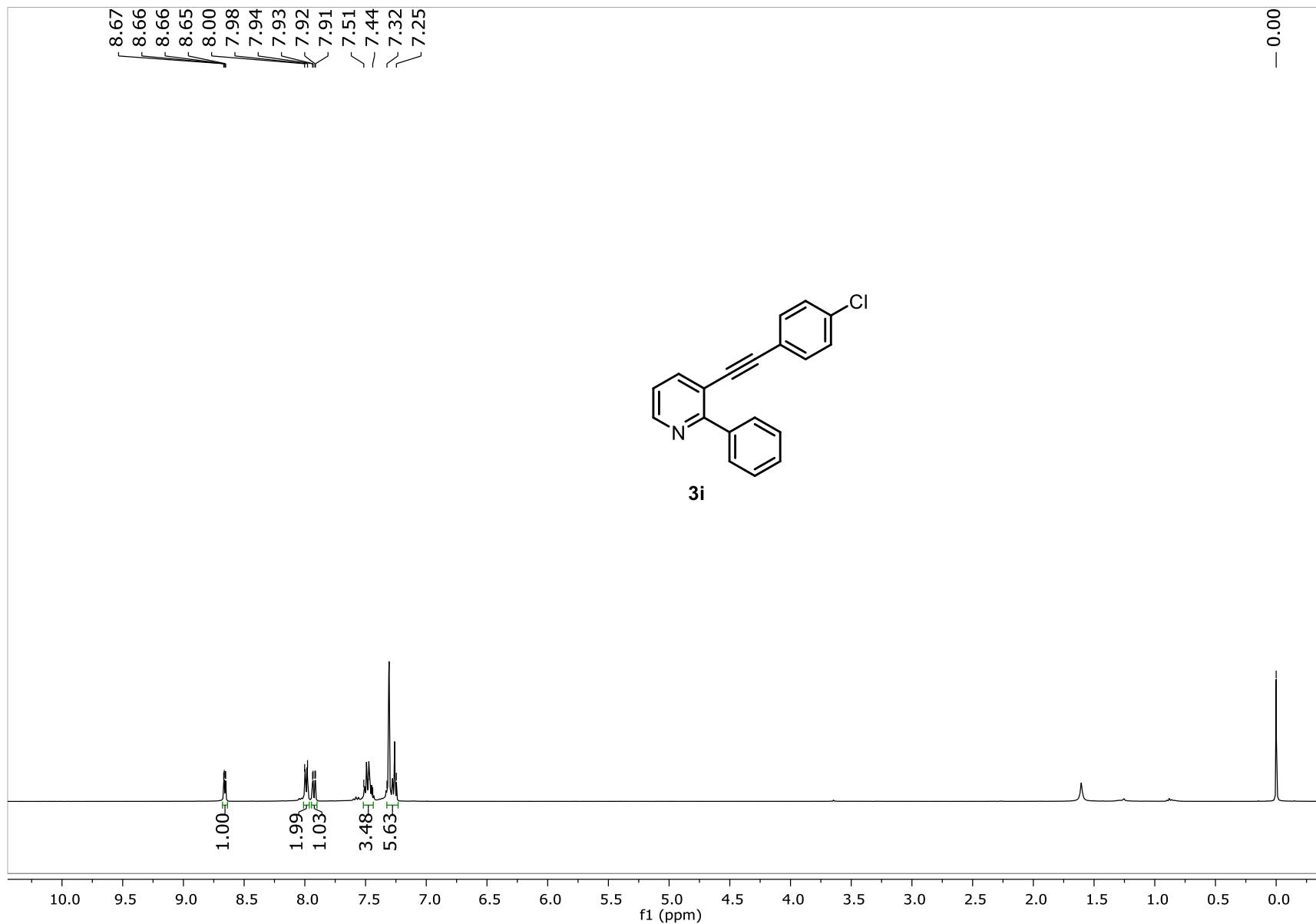


Figure S17: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3i**.

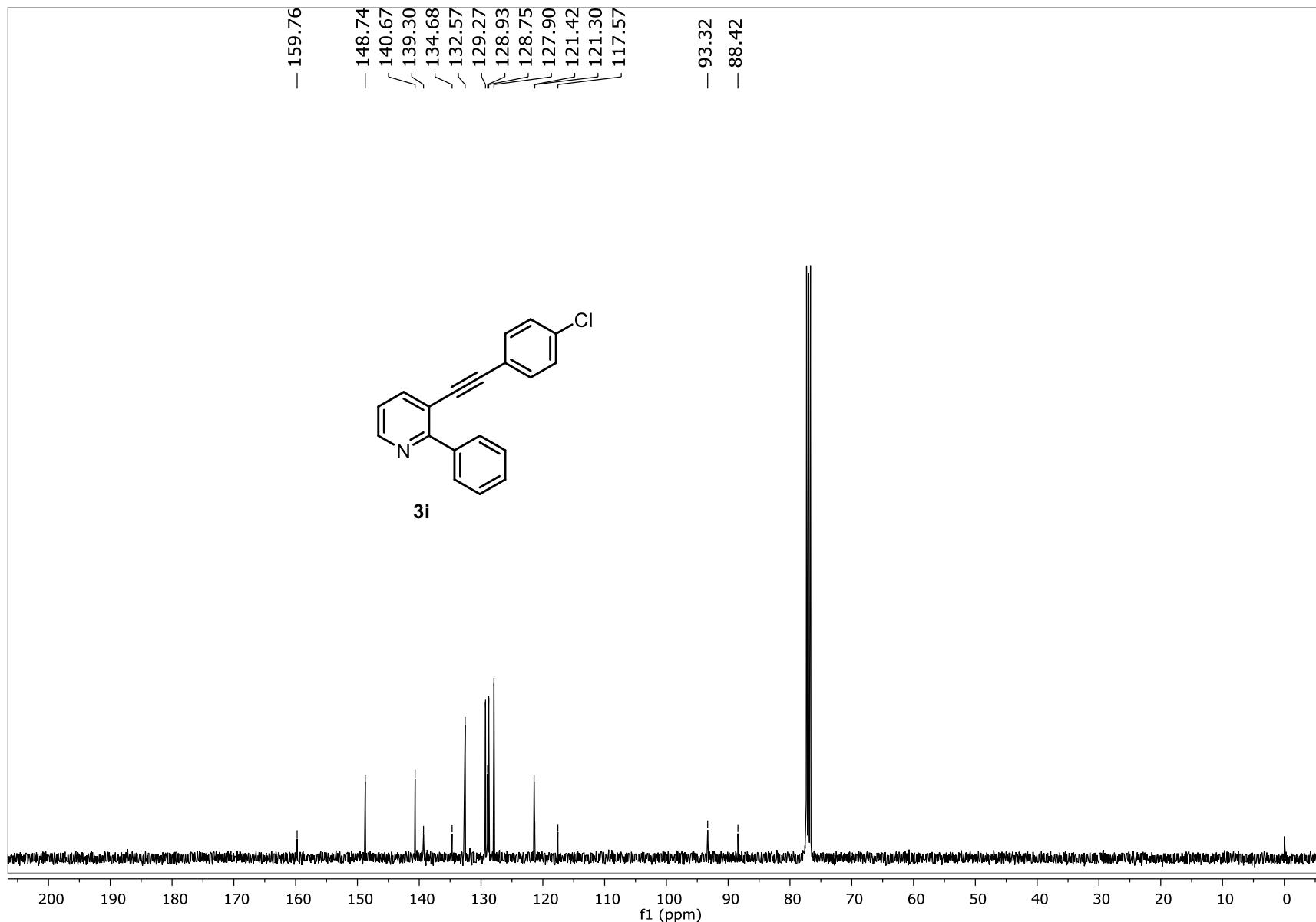


Figure S18: $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3i**.

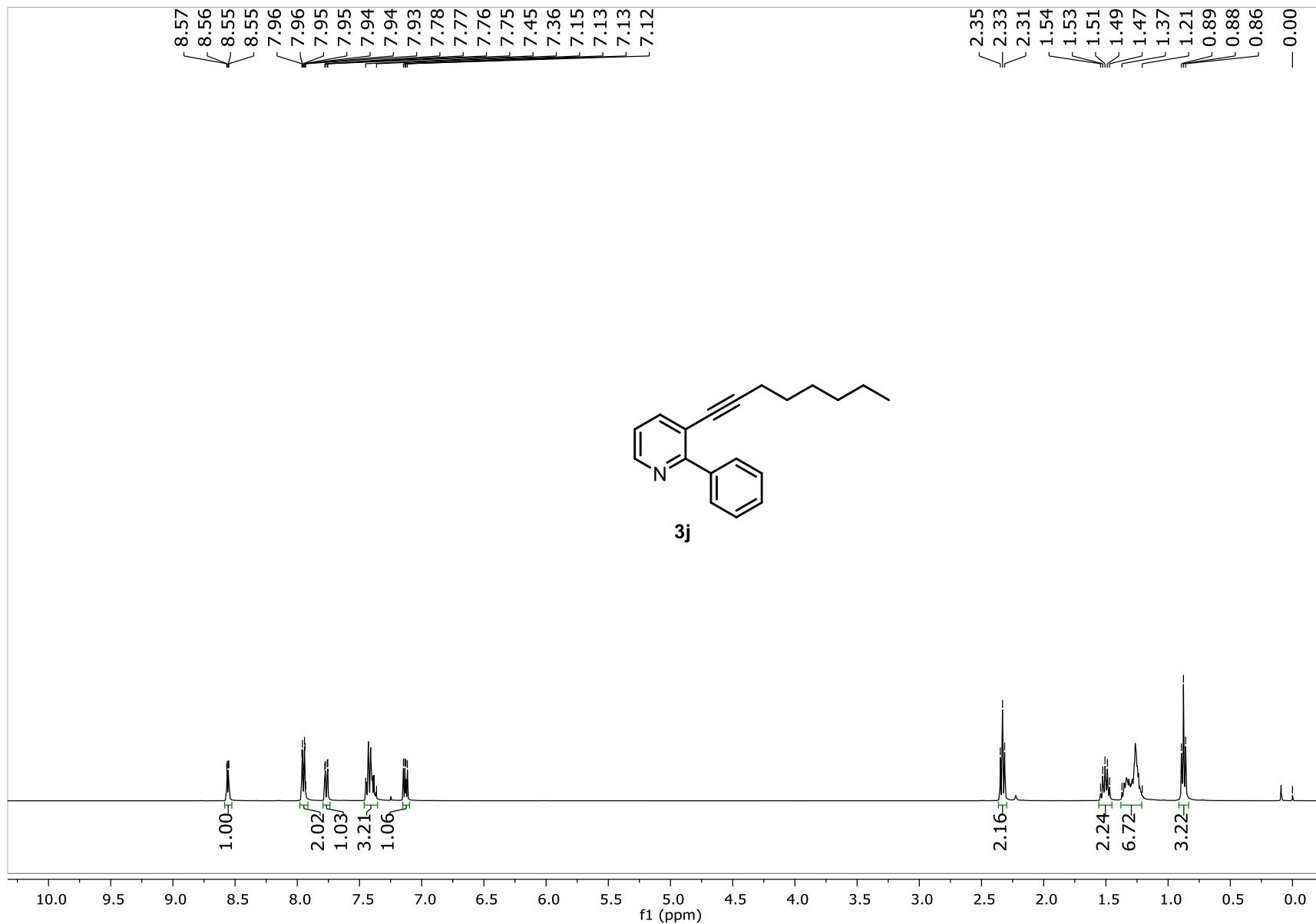


Figure S19: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3j**.

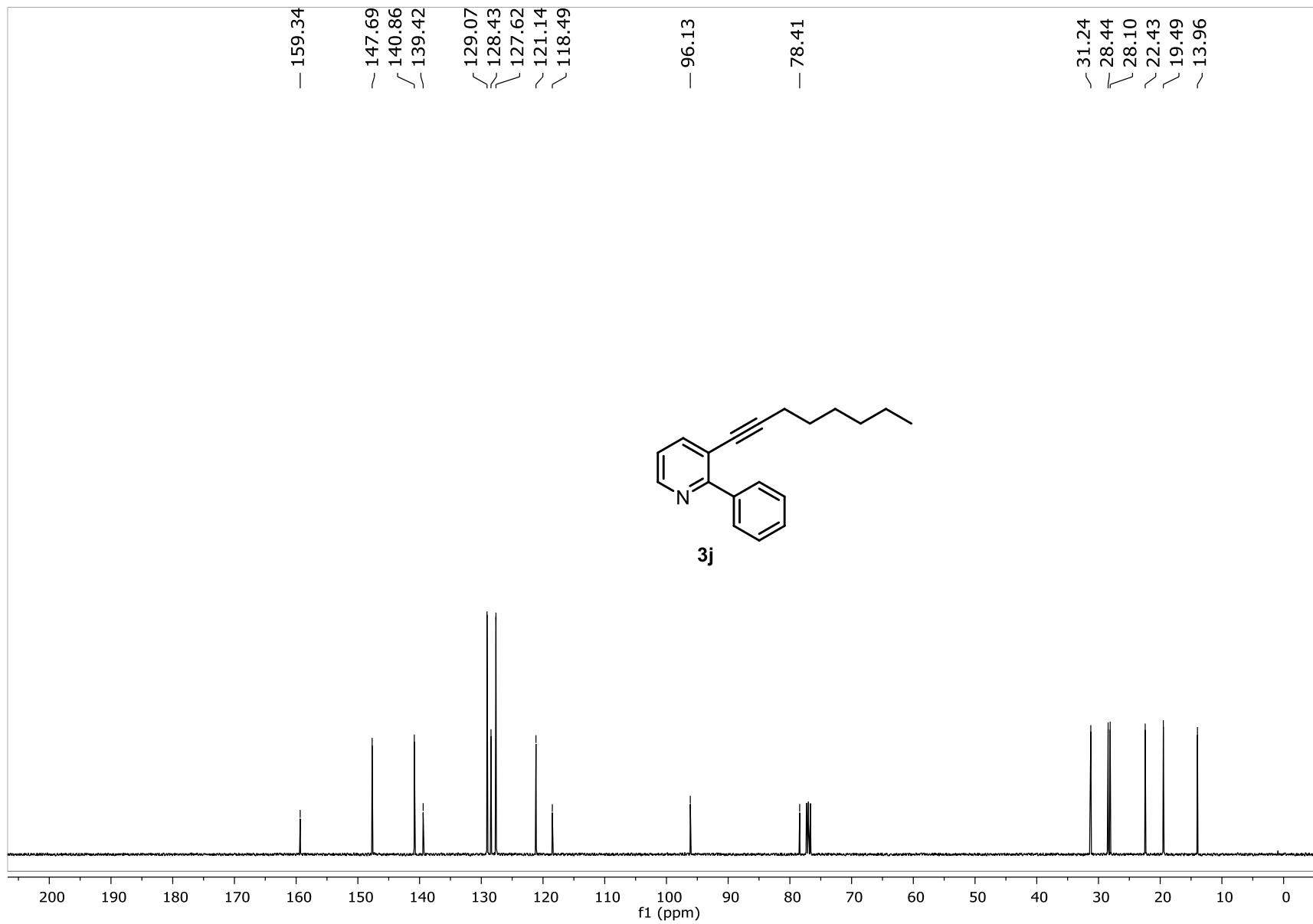


Figure S20: $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3j**.

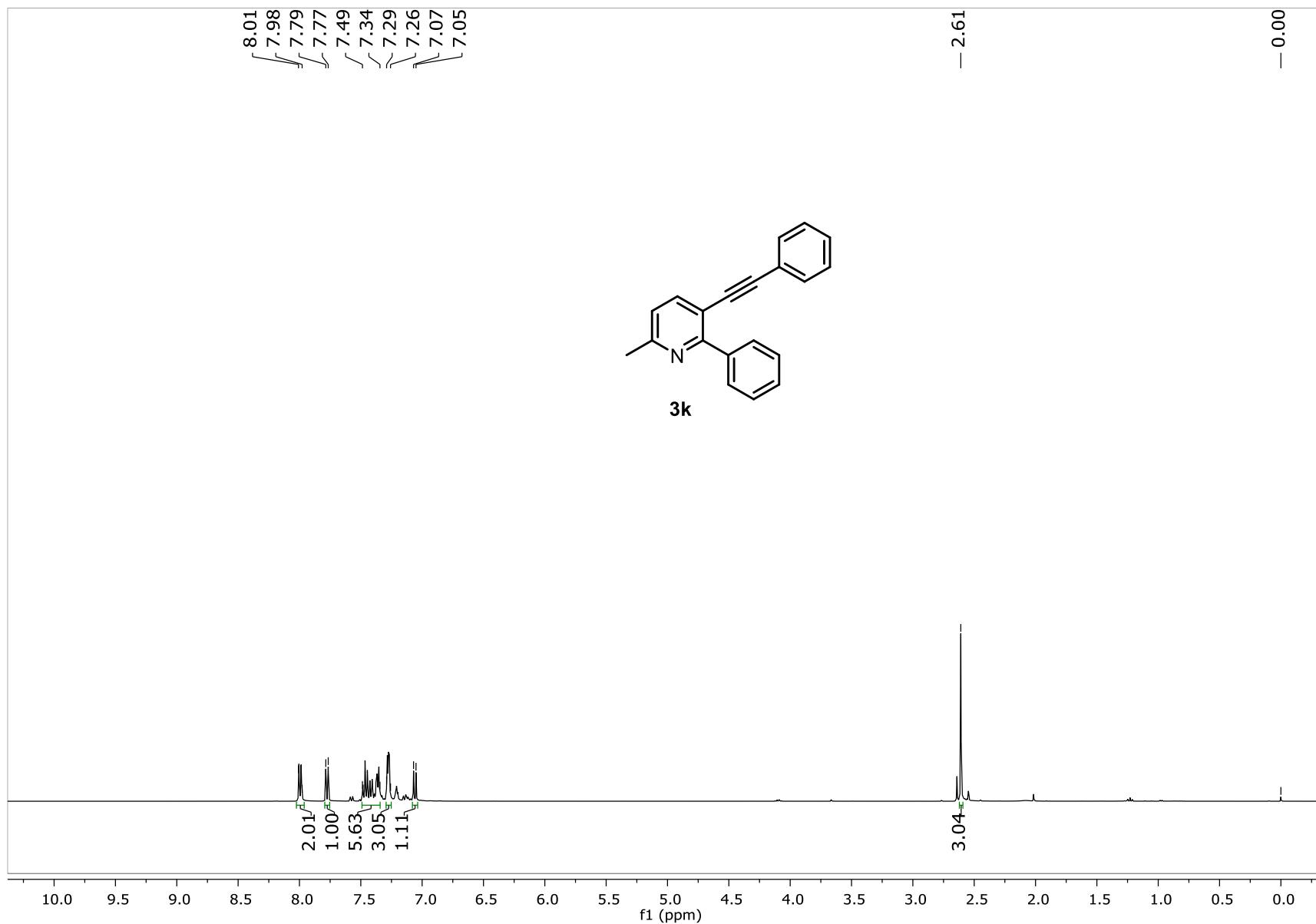


Figure S21: ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3k**.

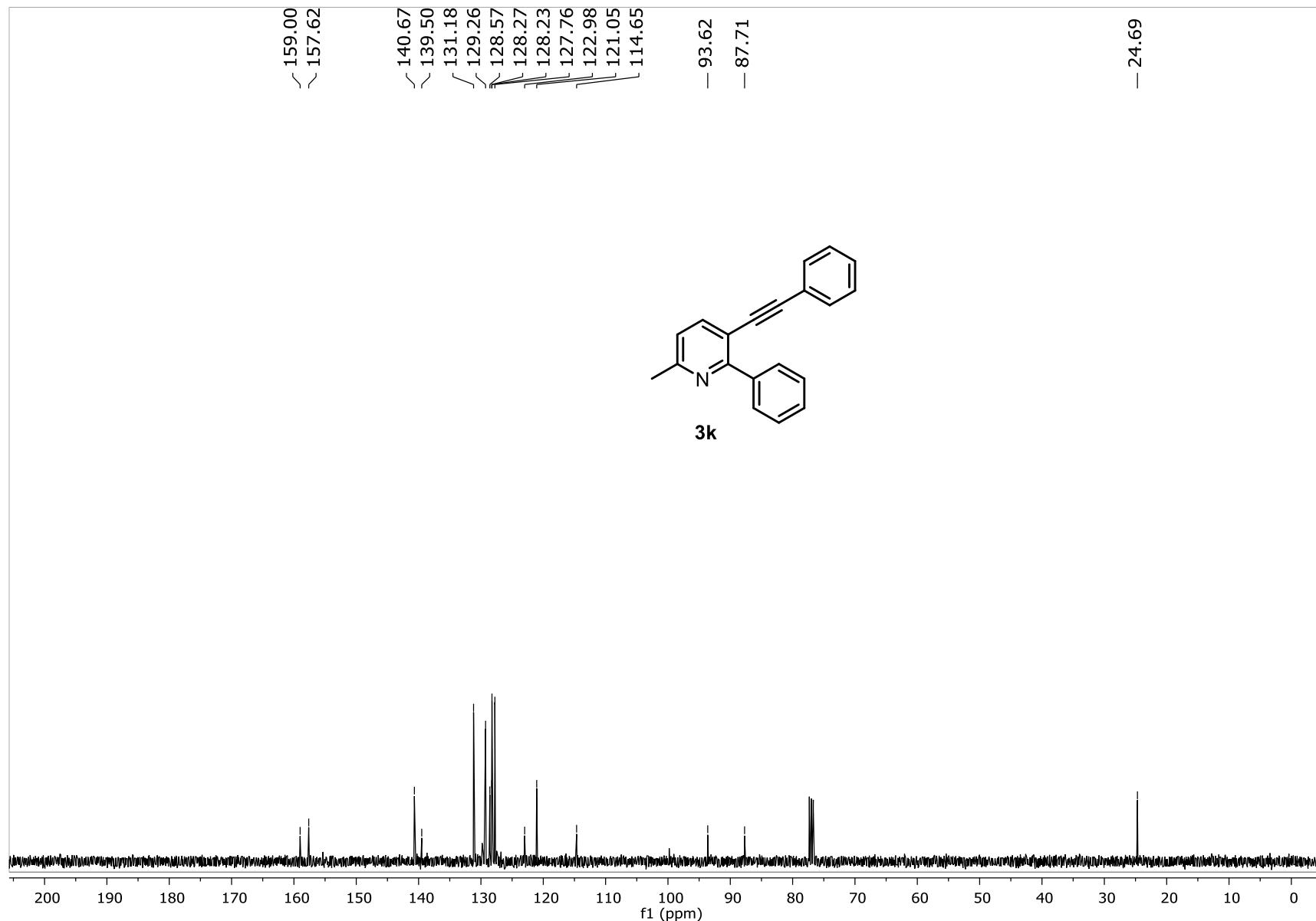


Figure S22: $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of compound **3k**.

Additional photophysical data

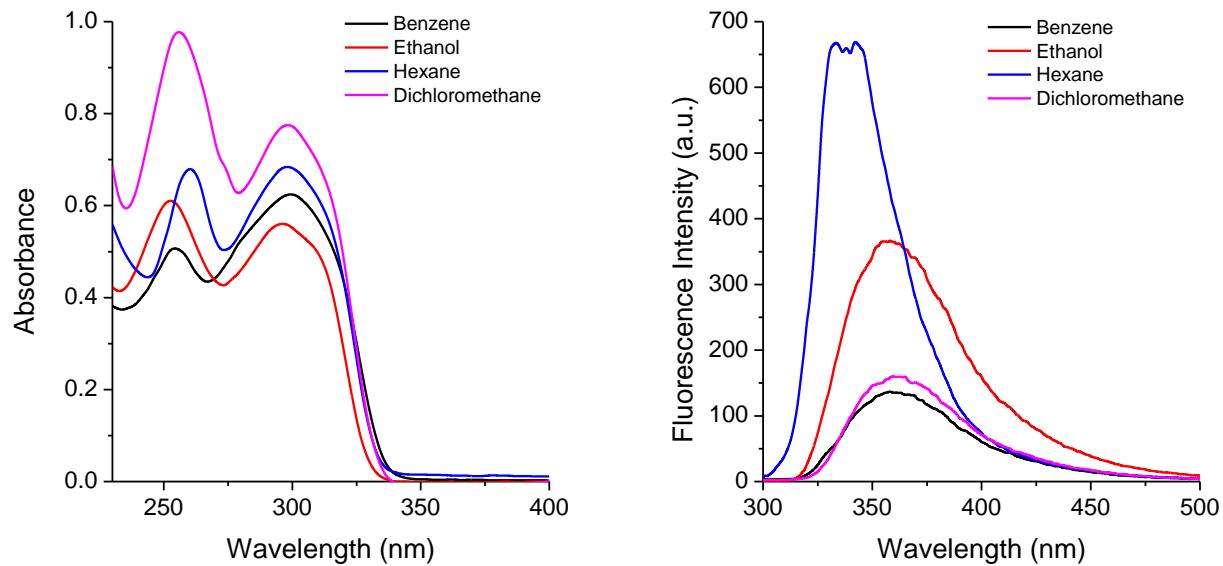


Figure S23. (left) UV-Vis absorption and (right) steady-state fluorescence emission spectra in solution [$\sim 10^{-5}$ M] of the pyridine-based fluorophore **3b**.

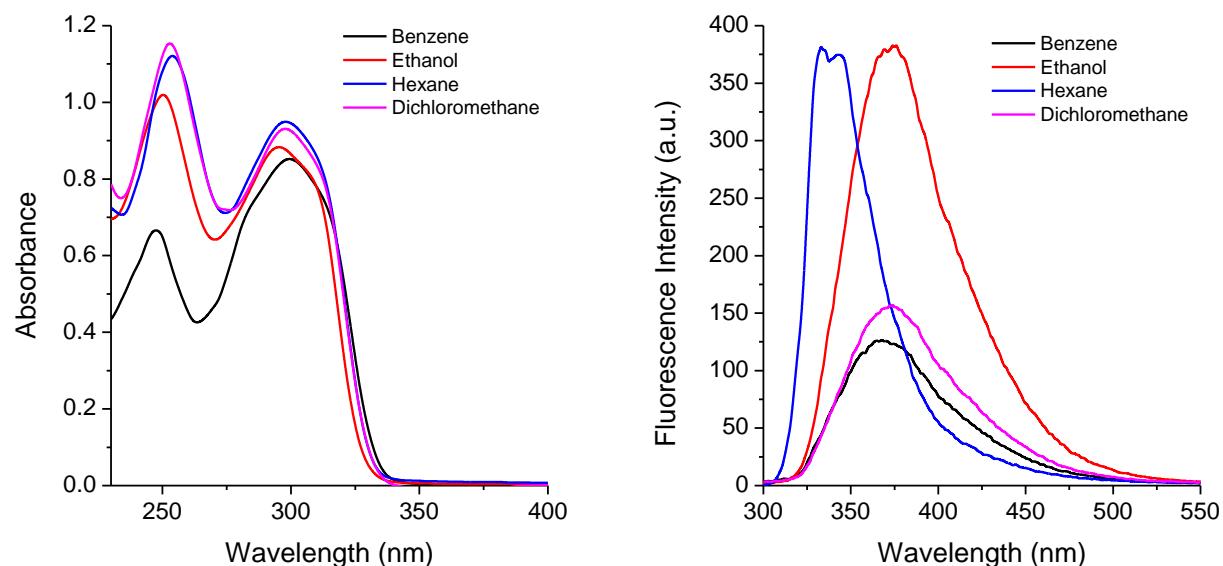


Figure S24. (left) UV-Vis absorption and (right) steady-state fluorescence emission spectra in solution [$\sim 10^{-5}$ M] of the pyridine-based fluorophore **3c**.

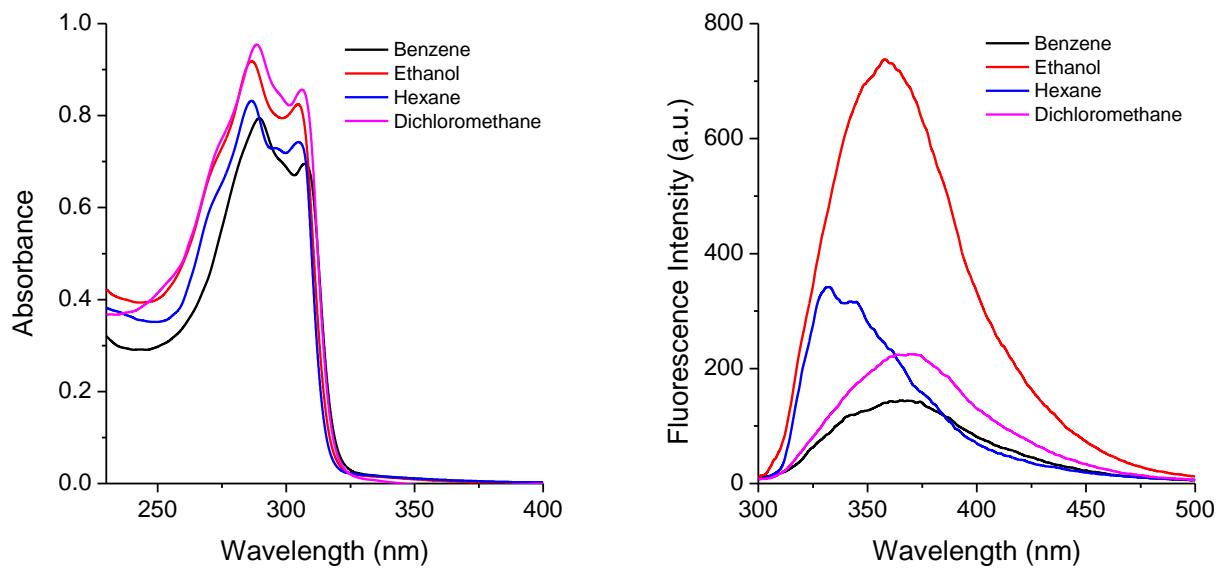


Figure S25. (left) UV-Vis absorption and (right) steady-state fluorescence emission spectra in solution [$\sim 10^{-5}$ M] of the pyridine-based fluorophore **3g**.

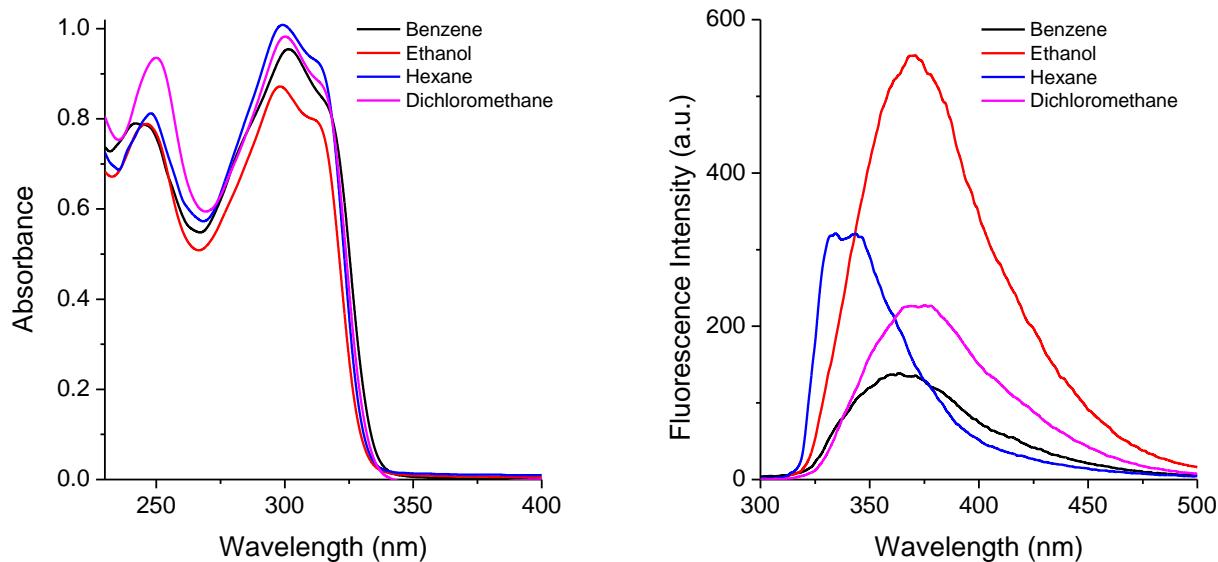


Figure S26. (left) UV-Vis absorption and (right) steady-state fluorescence emission spectra in solution [$\sim 10^{-5}$ M] of the pyridine-based fluorophore **3h**.

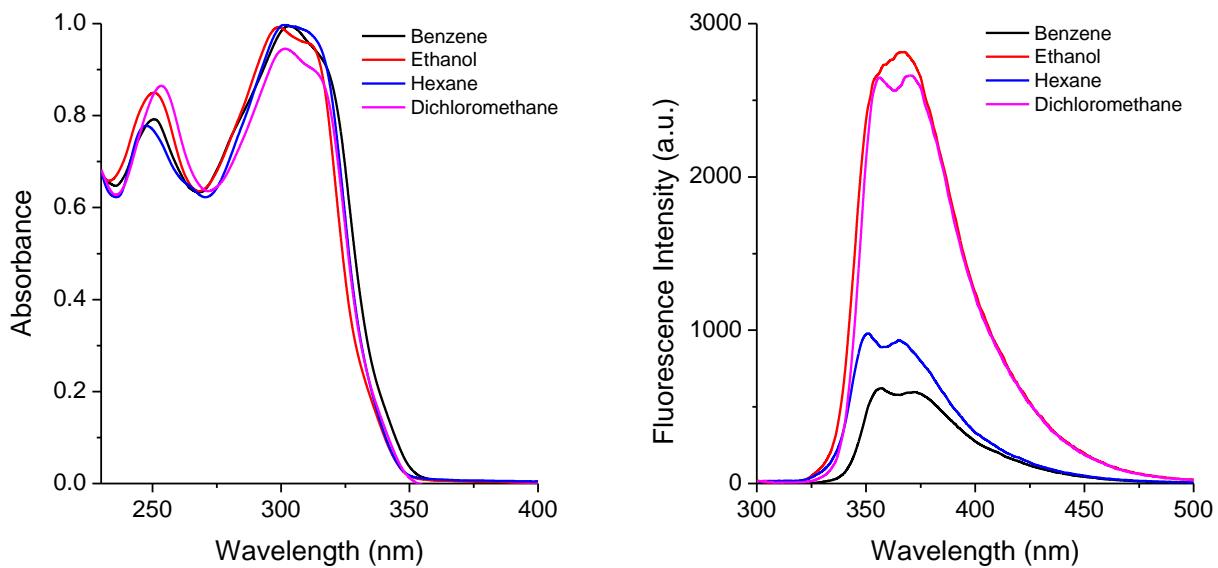


Figure S27. (left) UV-Vis absorption and (right) steady-state fluorescence emission spectra in solution [$\sim 10^{-5}$ M] of the pyridine-based fluorophore **3i**.

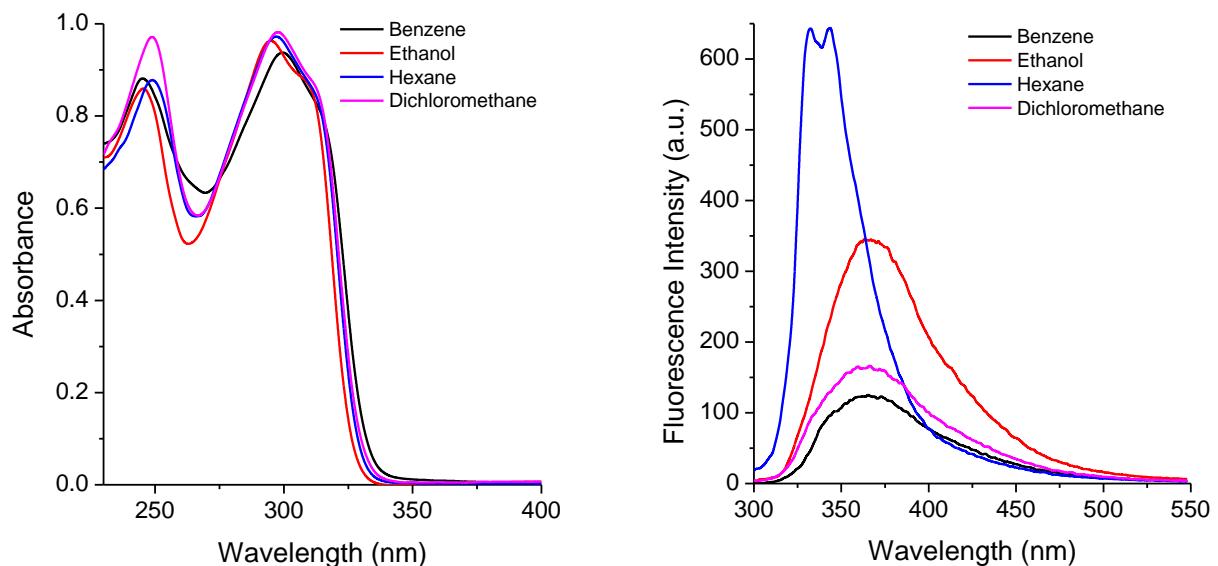


Figure S28. (left) UV-Vis absorption and (right) steady-state fluorescence emission spectra in solution [$\sim 10^{-5}$ M] of the pyridine-based fluorophore **3k**.

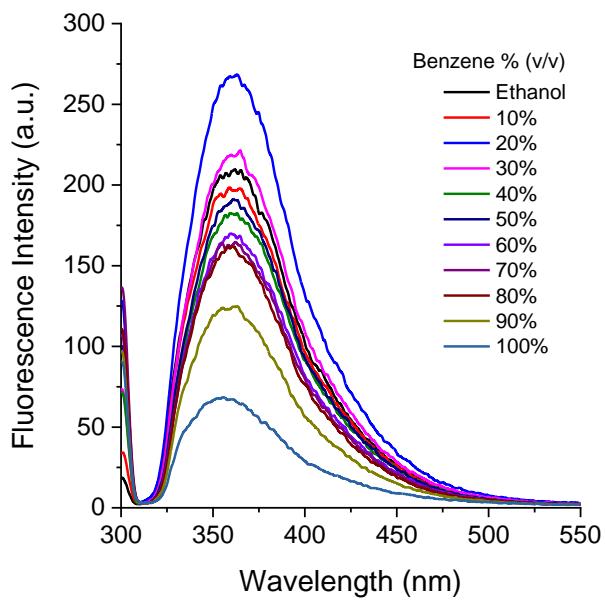


Figure S29. Fluorescence titration of fluorophore **3a** in ethanol upon different amounts of benzene (v/v).

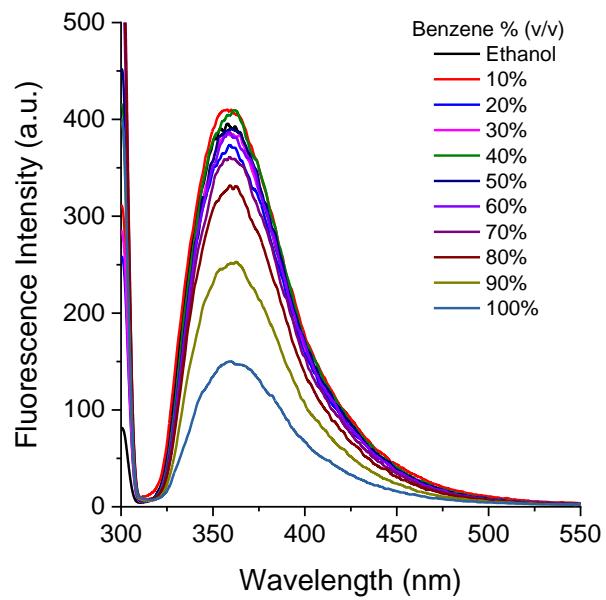


Figure S30. Fluorescence titration of fluorophore **3b** in ethanol upon different amounts of benzene (v/v).

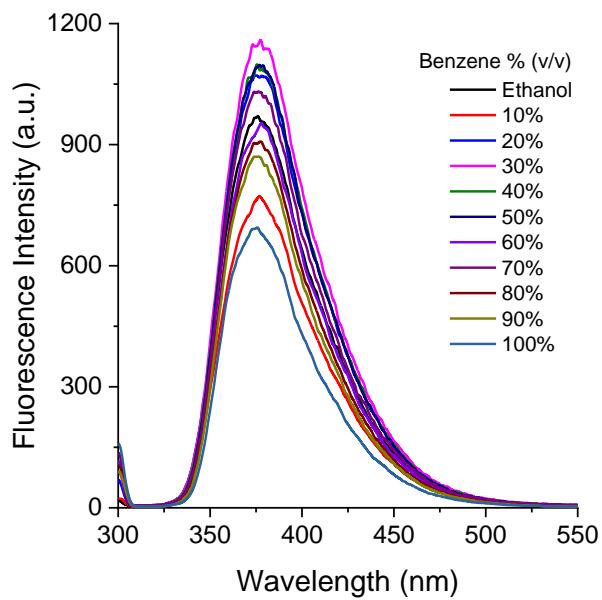


Figure S31. Fluorescence titration of fluorophore **3d** in ethanol upon different amounts of benzene (v/v).

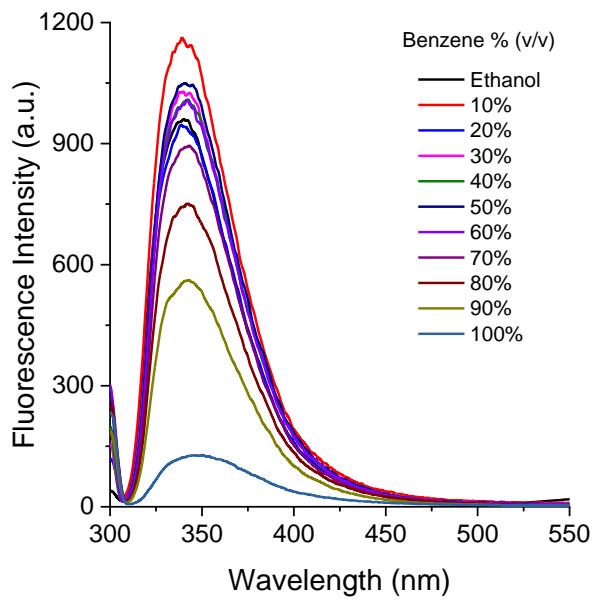


Figure S32. Fluorescence titration of fluorophore **3f** in ethanol upon different amounts of benzene (v/v).

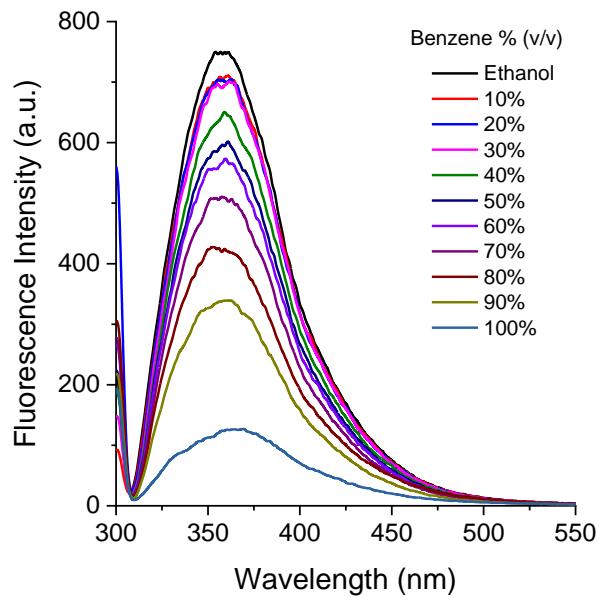


Figure S33. Fluorescence titration of fluorophore **3g** in ethanol upon different amounts of benzene (v/v).

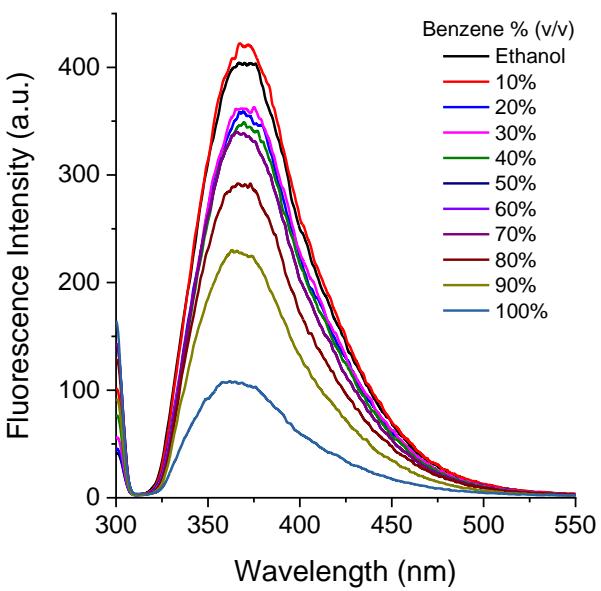


Figure S34. Fluorescence titration of fluorophore **3h** in ethanol upon different amounts of benzene (v/v).

Additional theoretical data

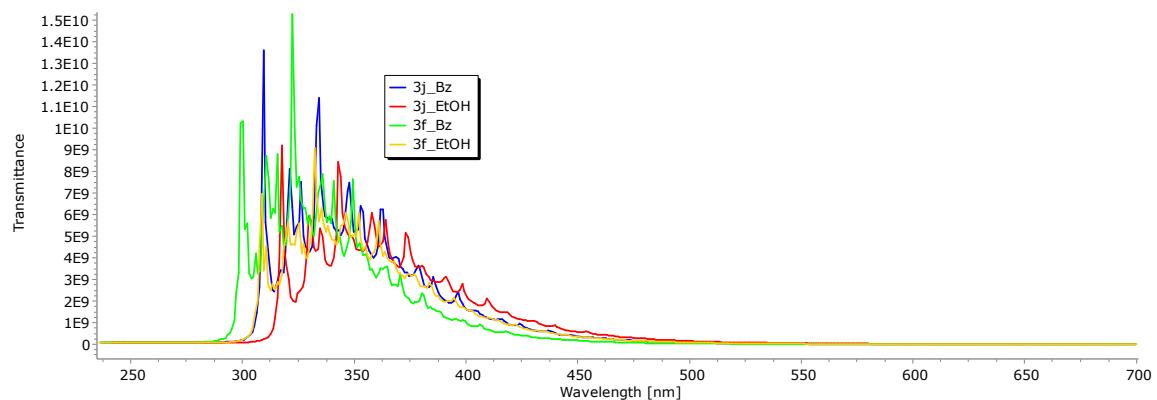


Figure S35. Emission spectra using the vertical gradient approach for **3f** and **3j** under implicit CPCM benzene and ethanol solvation.