

Electronic Supplementary Information

A Chemoselective Ugi-type reaction in Water Using TMSCN as Functional Isonitrile Equivalent:

Generation of Heteroaromatic Molecular Diversity

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General Information

^1H NMR spectra were recorded on a Bruker Avance III-400 (400 MHz) spectrometer using tetramethylsilane as an internal standard and NMR solvent CD_3OD or $\text{DMSO}-d_6$. Chemical shifts are in ppm. The ^1H NMR data includes the integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, td = triplet of doublet, dt = doublet of triplet, br = broad), and coupling constants (Hz). ^{13}C NMR spectra were recorded on a Bruker Avance III-400 (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are in ppm with NMR solvent as an internal standard. The acquisition of High-resolution mass spectra (HRMS) was performed on Bruker maxis Q-TOF. Infrared (IR) spectra were recorded on a Perkin Elmer FTIR with ATR and IR Microscope spectrometer. For thin layer chromatography (TLC) analysis, Merck precoated TLC plates (silica gel 60 GF 254, 0.25 mm) were used. Melting points determined are uncorrected. The starting materials and solvents were used as received from commercial sources without further purification.

Spectra of compounds (4a-r)

Table 1, entry 6; 4a: ^1H NMR

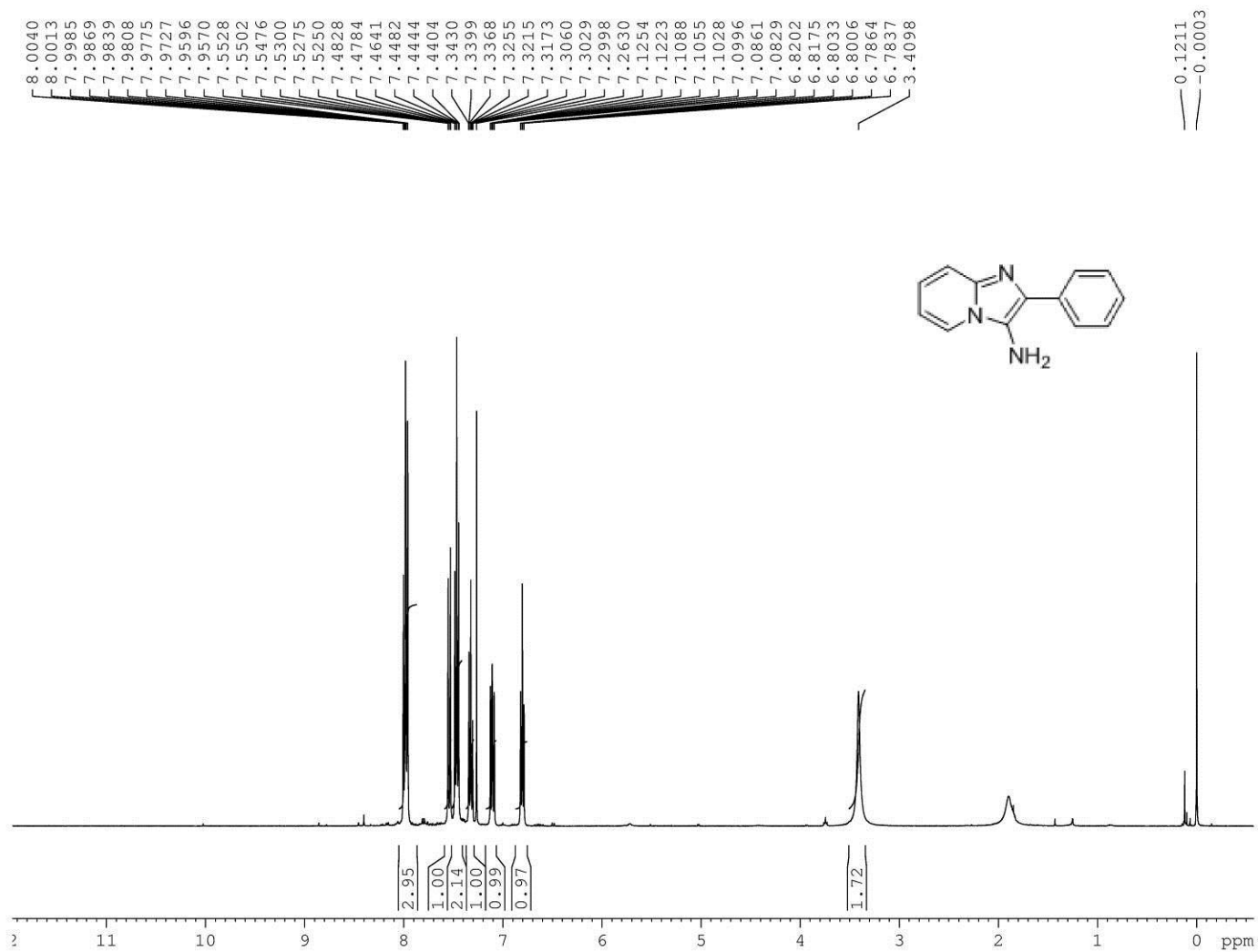


Table 1, entry 6; 4a: ^{13}C NMR

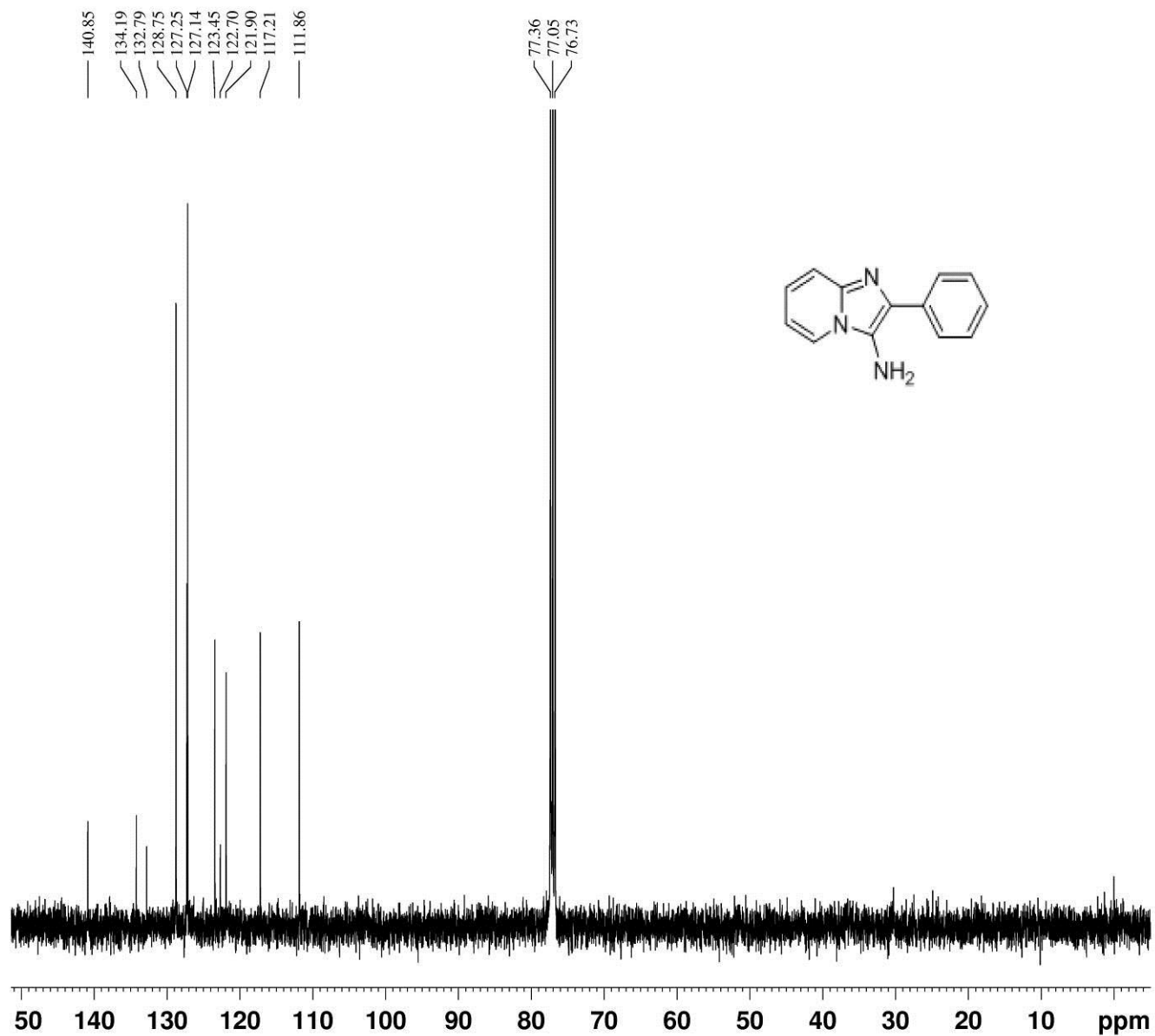


Table 2, entry 1; 4b: ^1H NMR

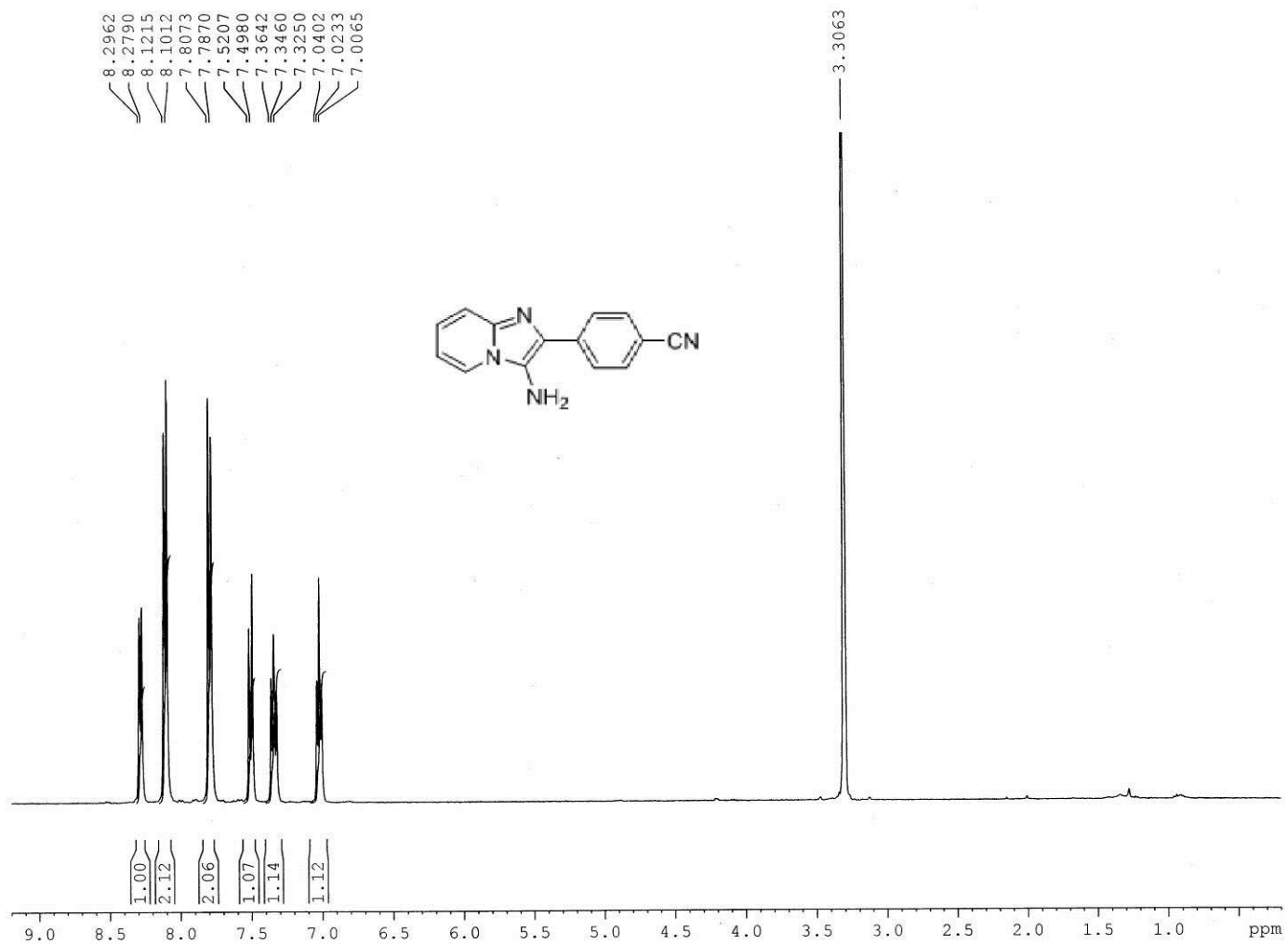


Table 2, entry 1; 4b: ^{13}C NMR

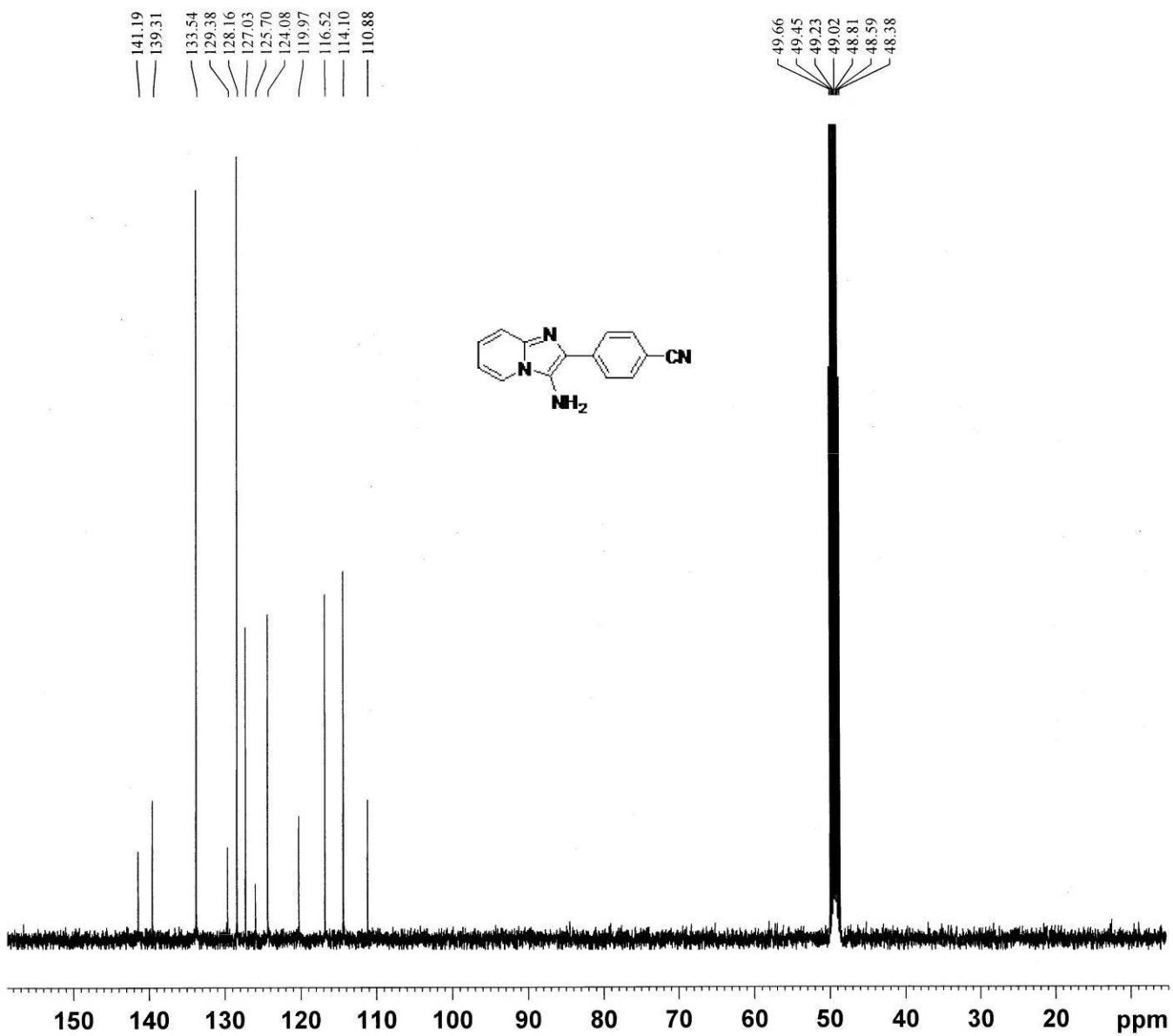


Table 2, entry 2; 4c: ^1H NMR

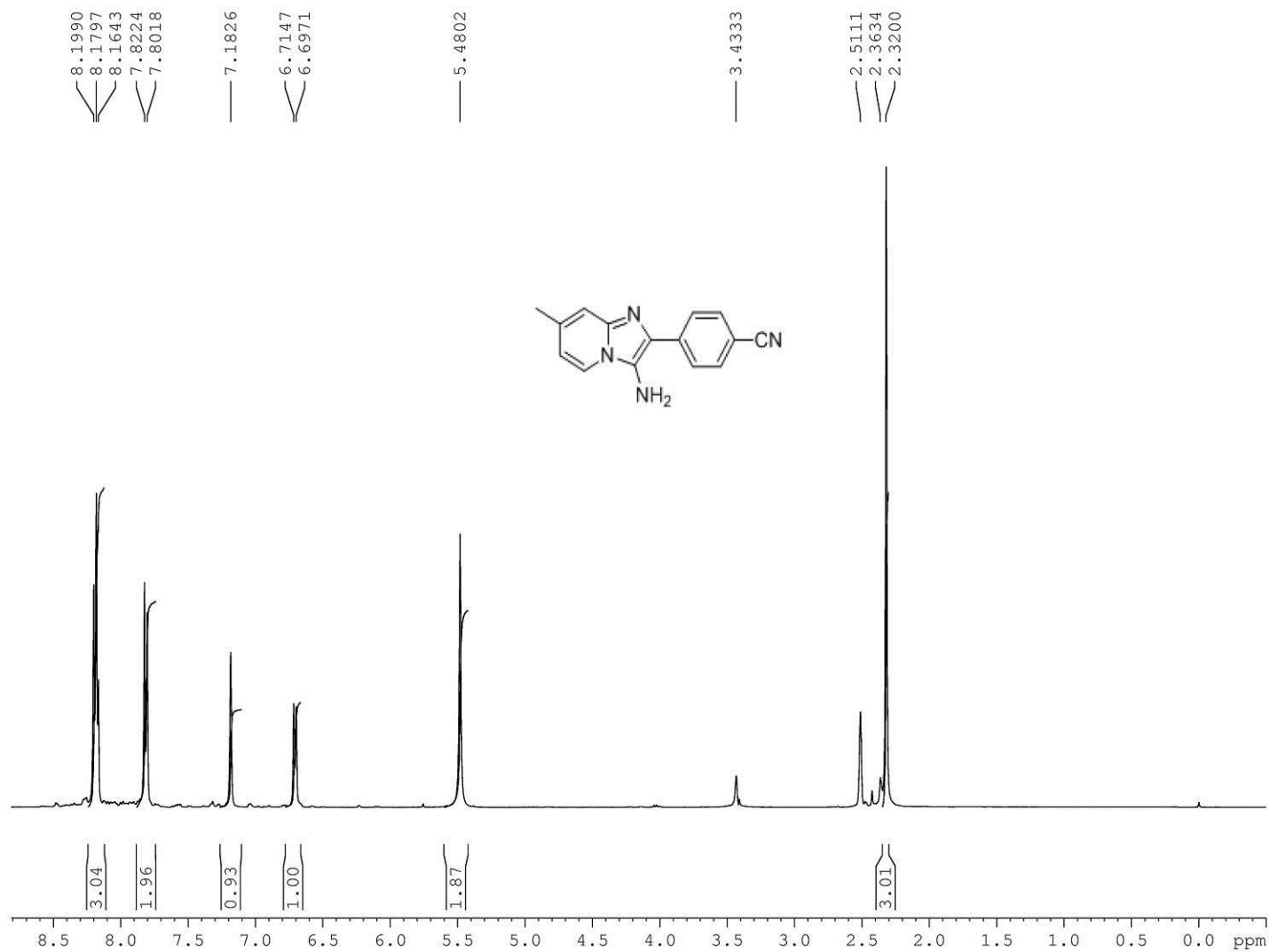


Table 2, entry 2; 4c: ^{13}C NMR

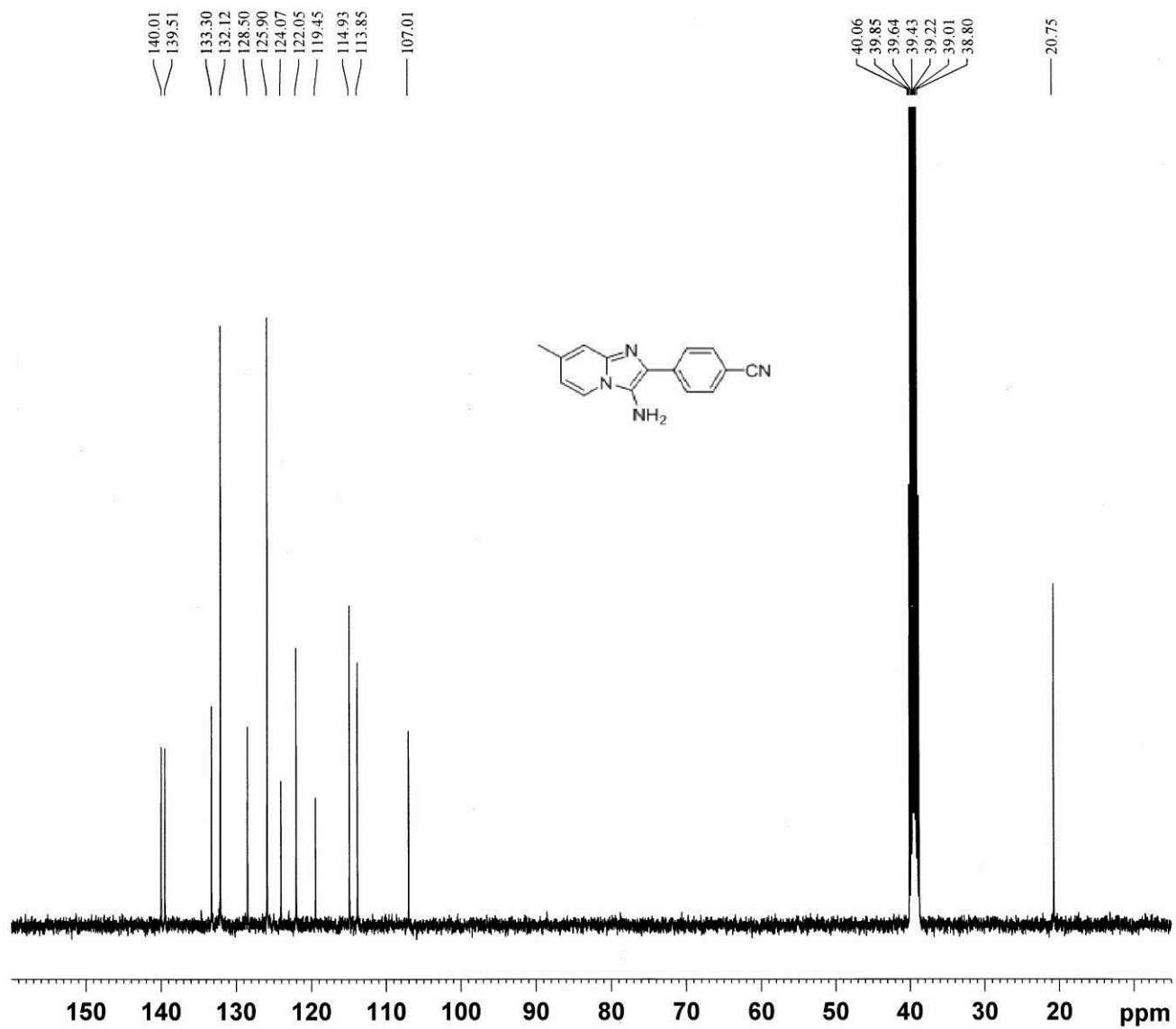


Table 2, entry 3; 4d: ^1H NMR

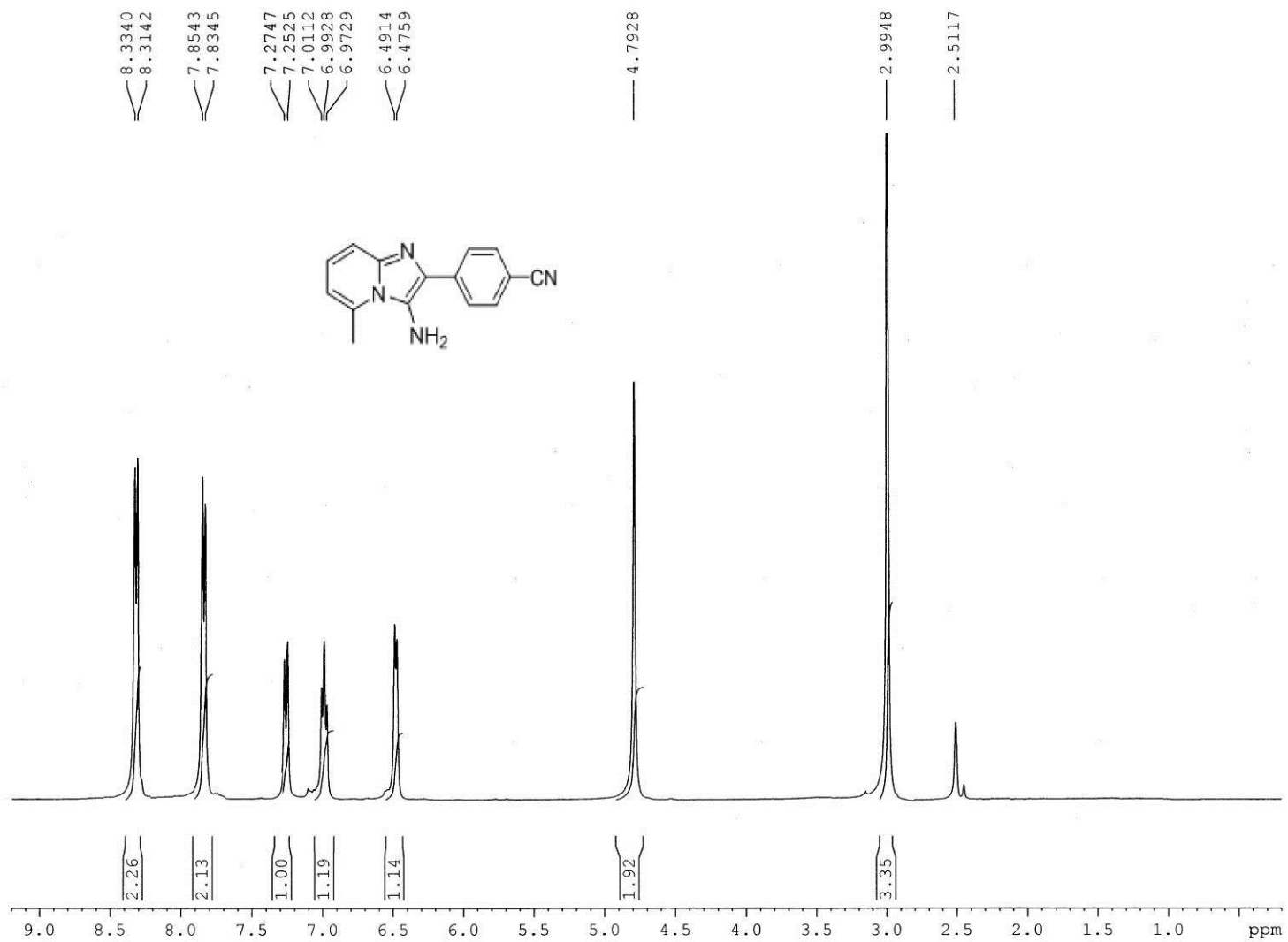


Table 2, entry 3; 4d: ^{13}C NMR

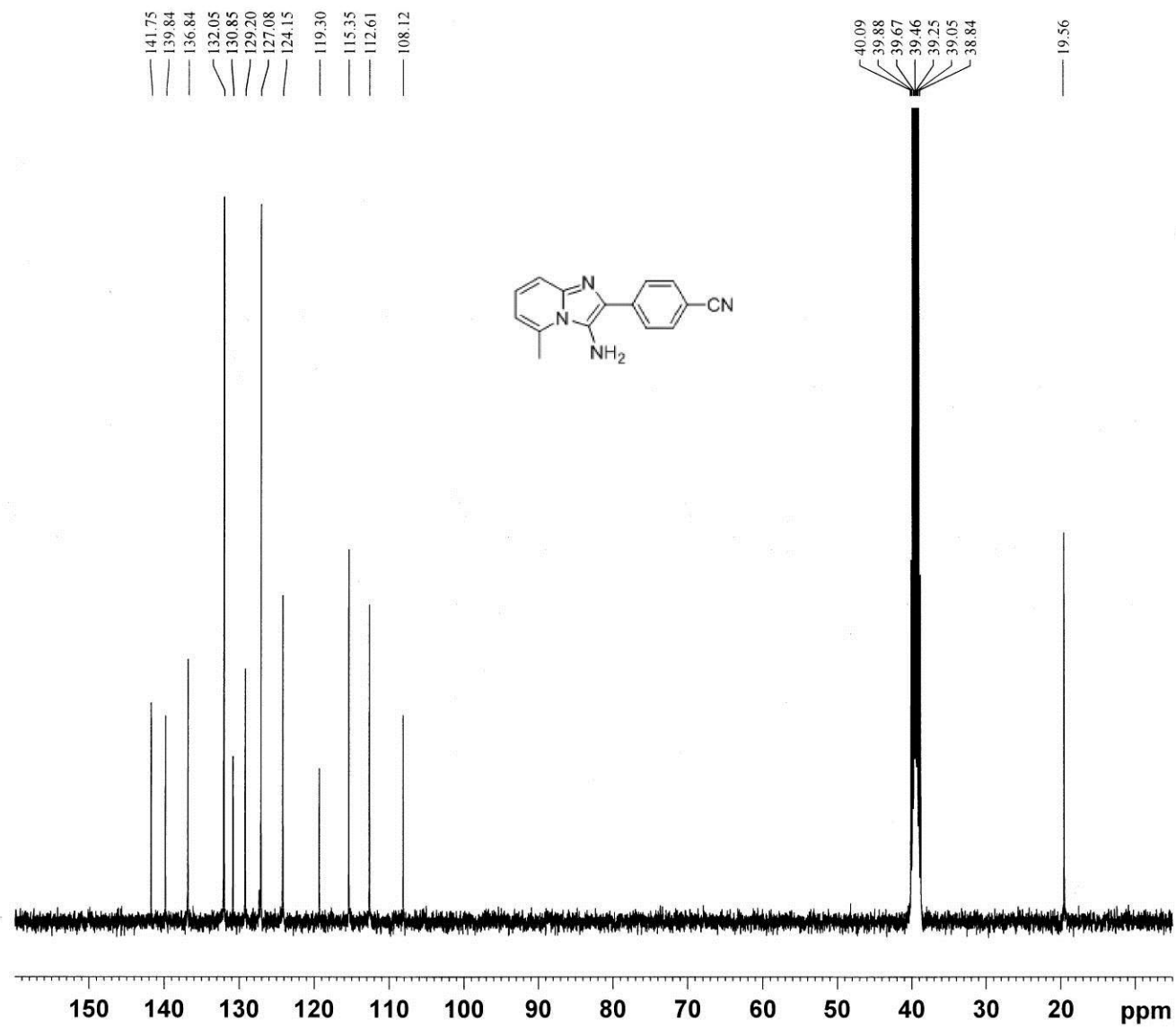


Table 2, entry 4; 4e: ^1H NMR

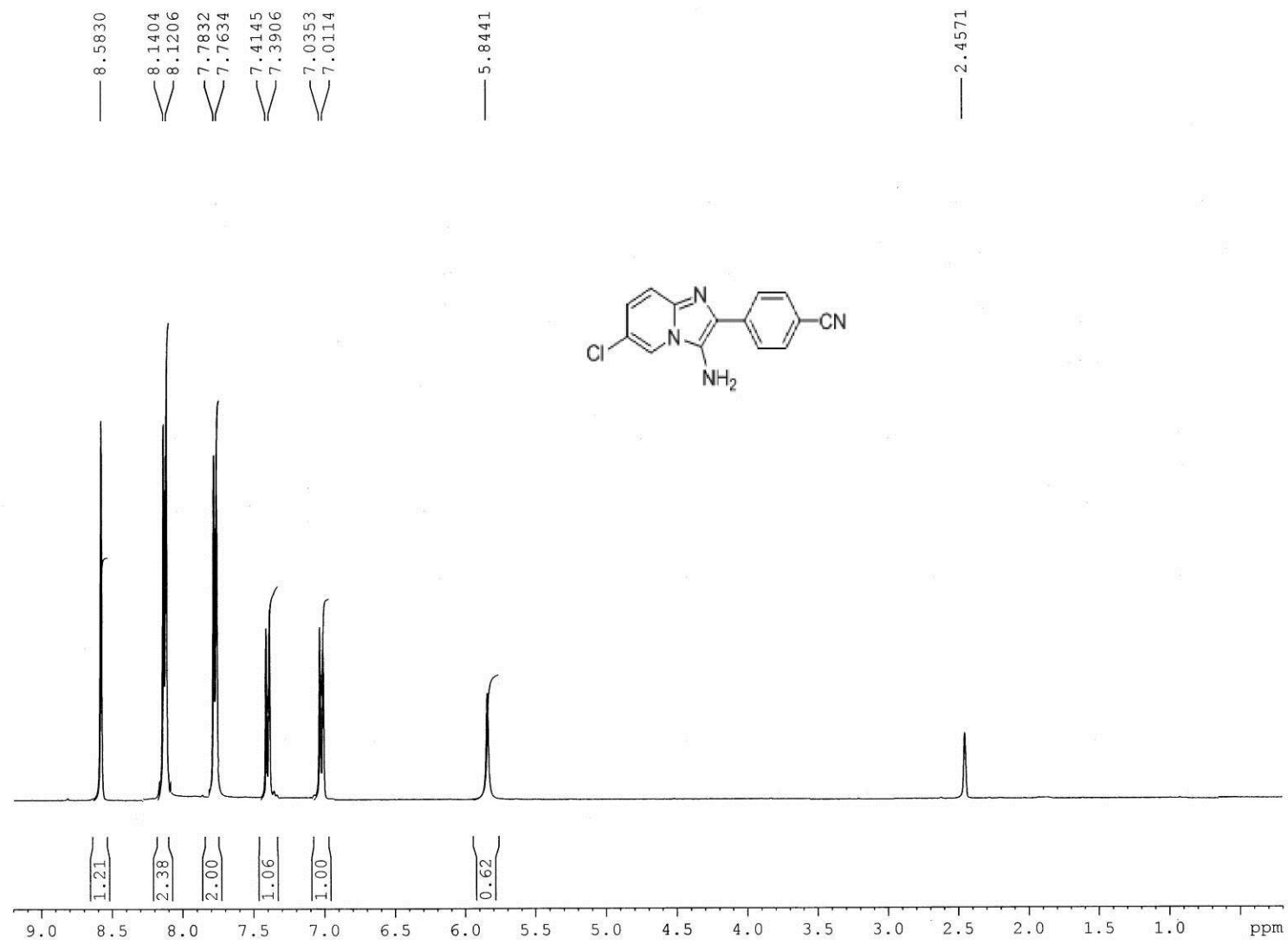


Table 2, entry 4; 4e: ^{13}C NMR

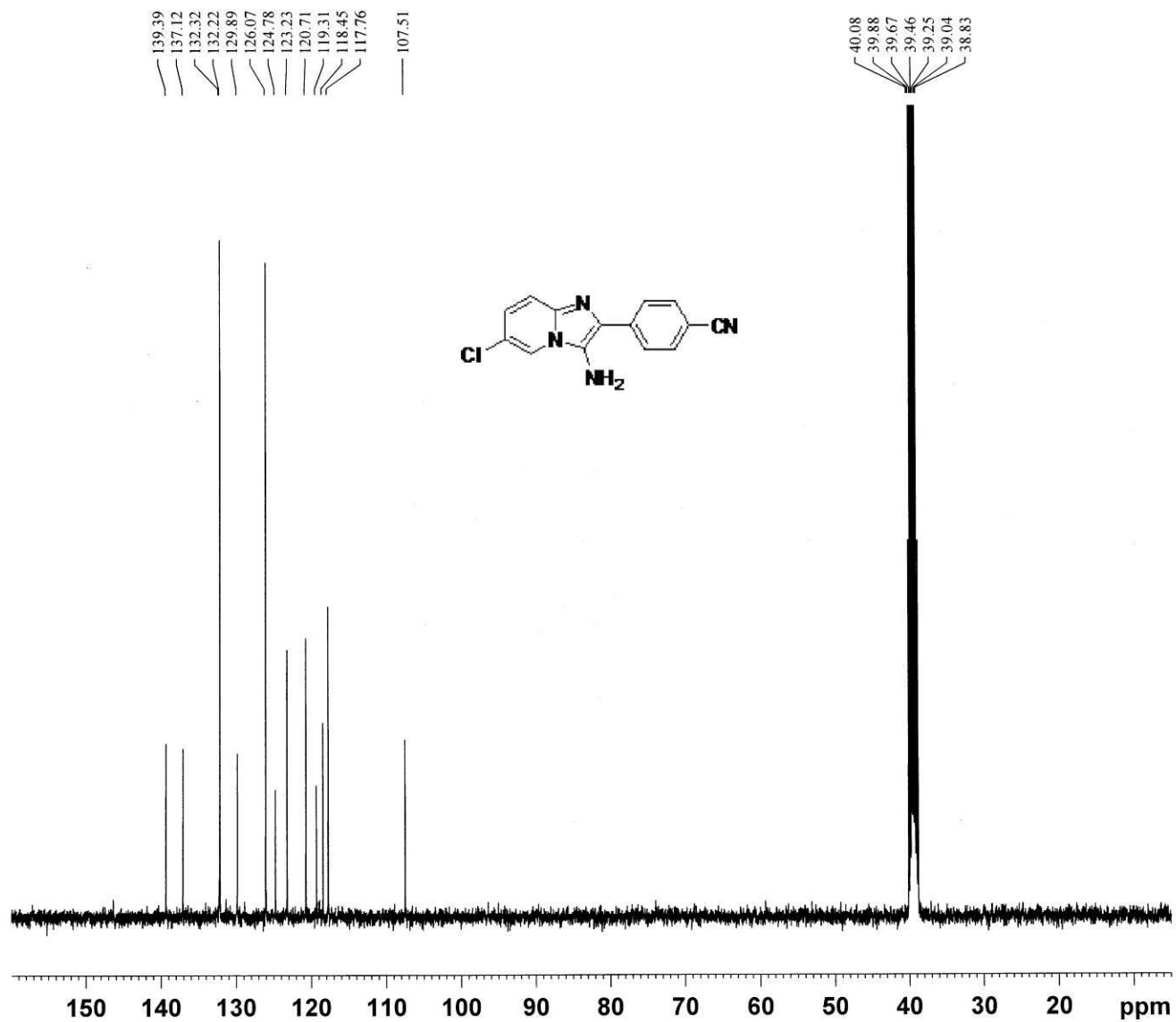


Table 2, entry 5; 4f: ^1H NMR

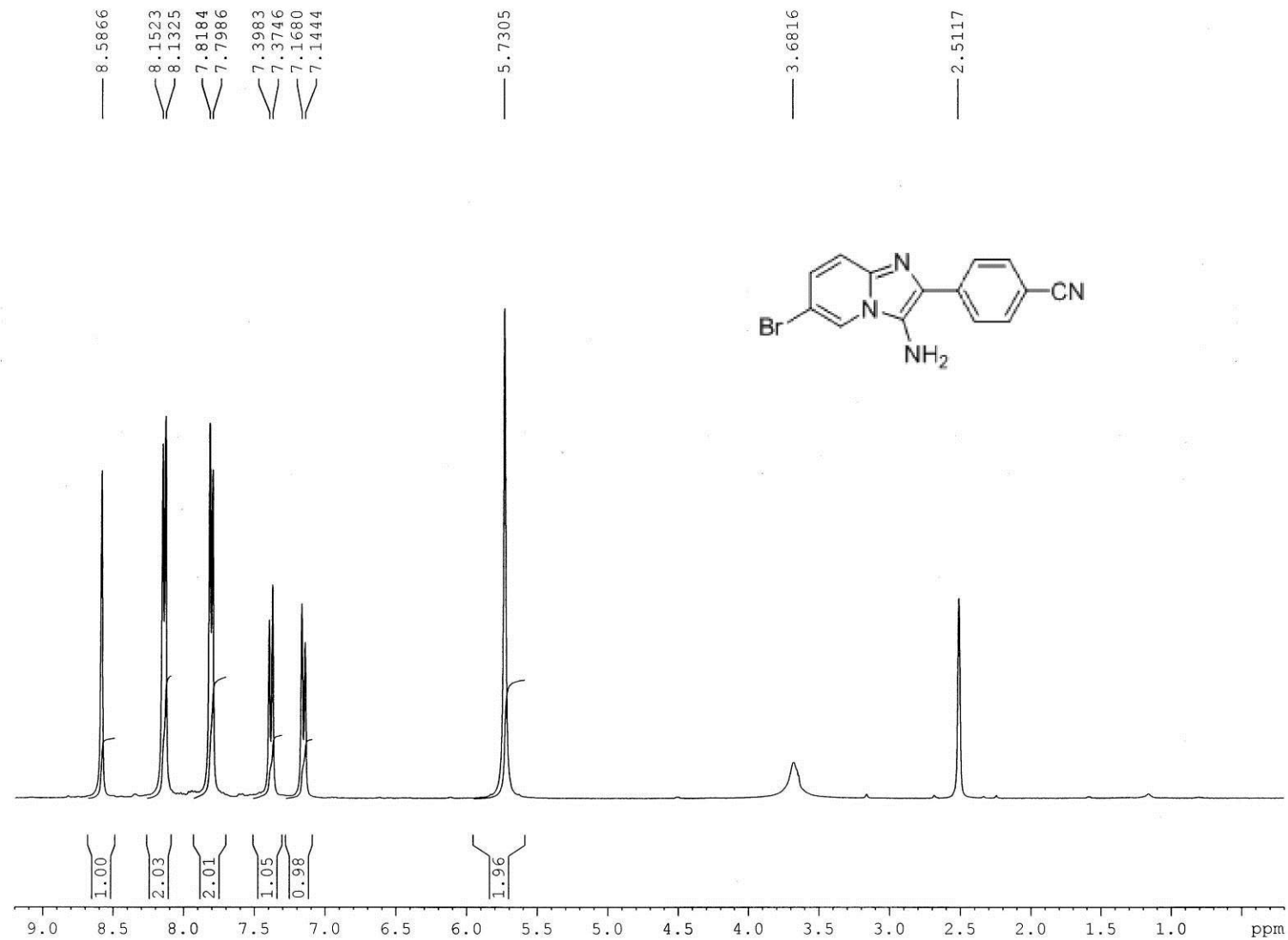


Table 2, entry 5; 4f: ^{13}C NMR

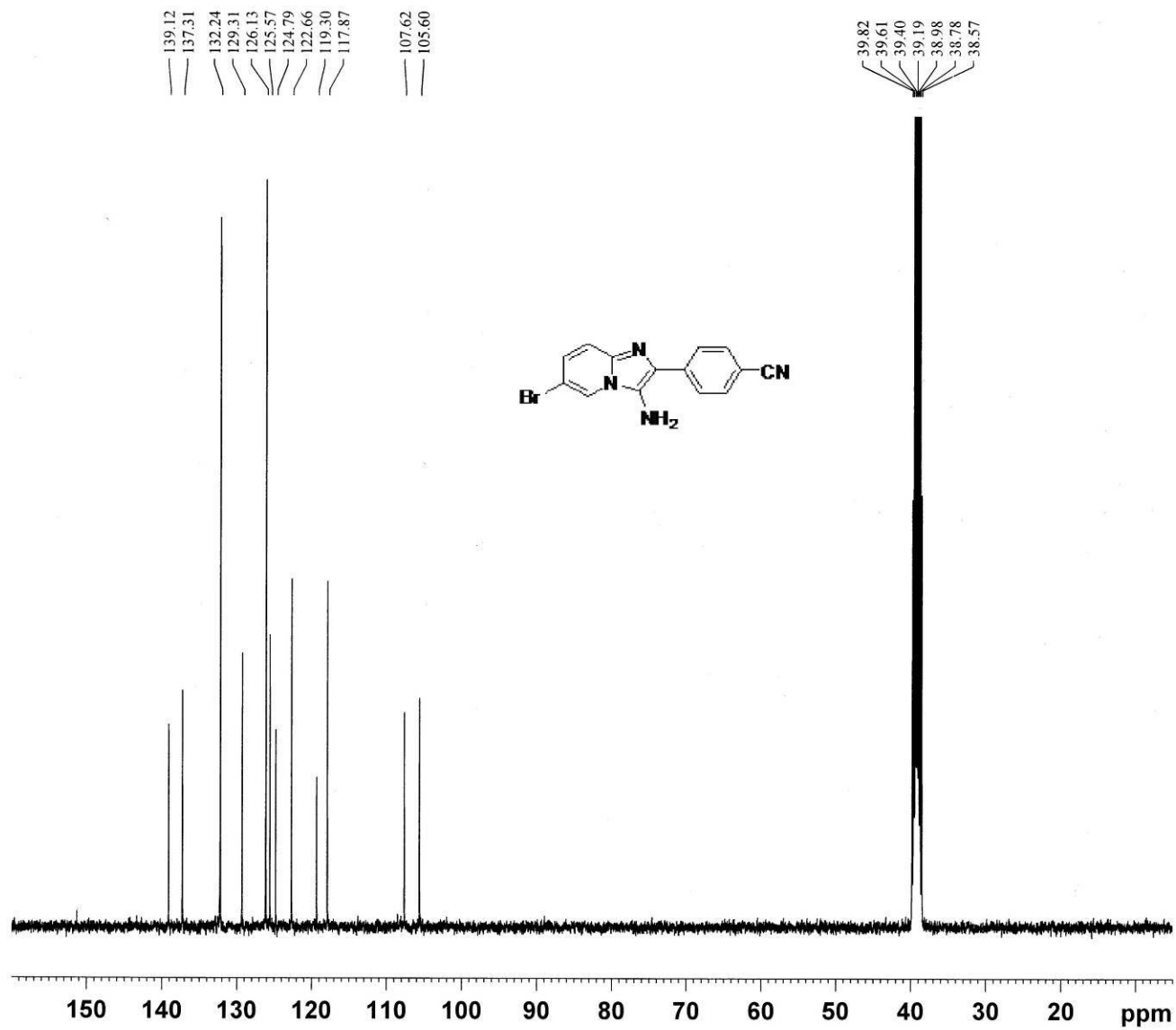


Table 2, entry 6; 4g: ^1H NMR

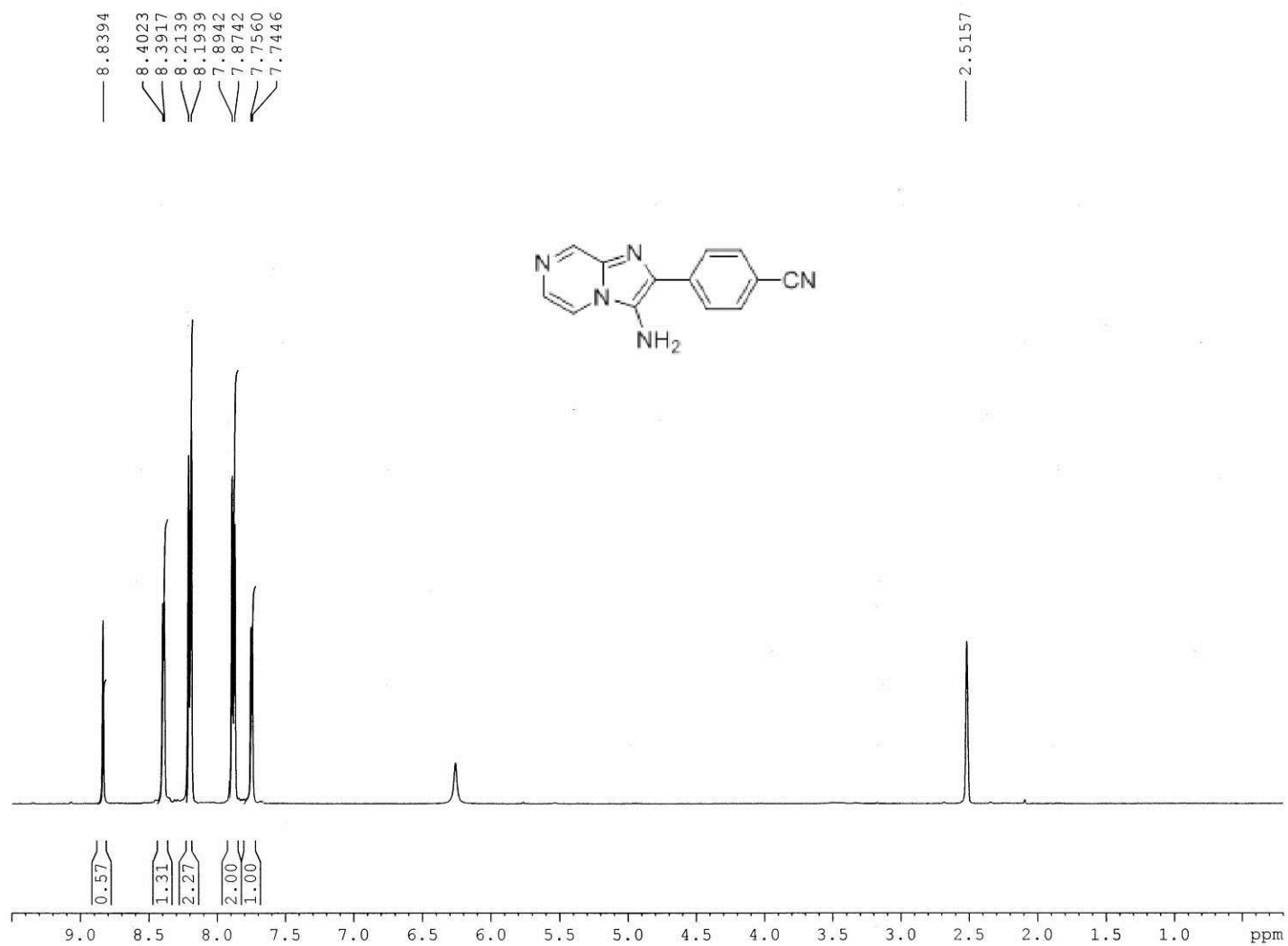


Table 2, entry 6; 4g: ^{13}C NMR

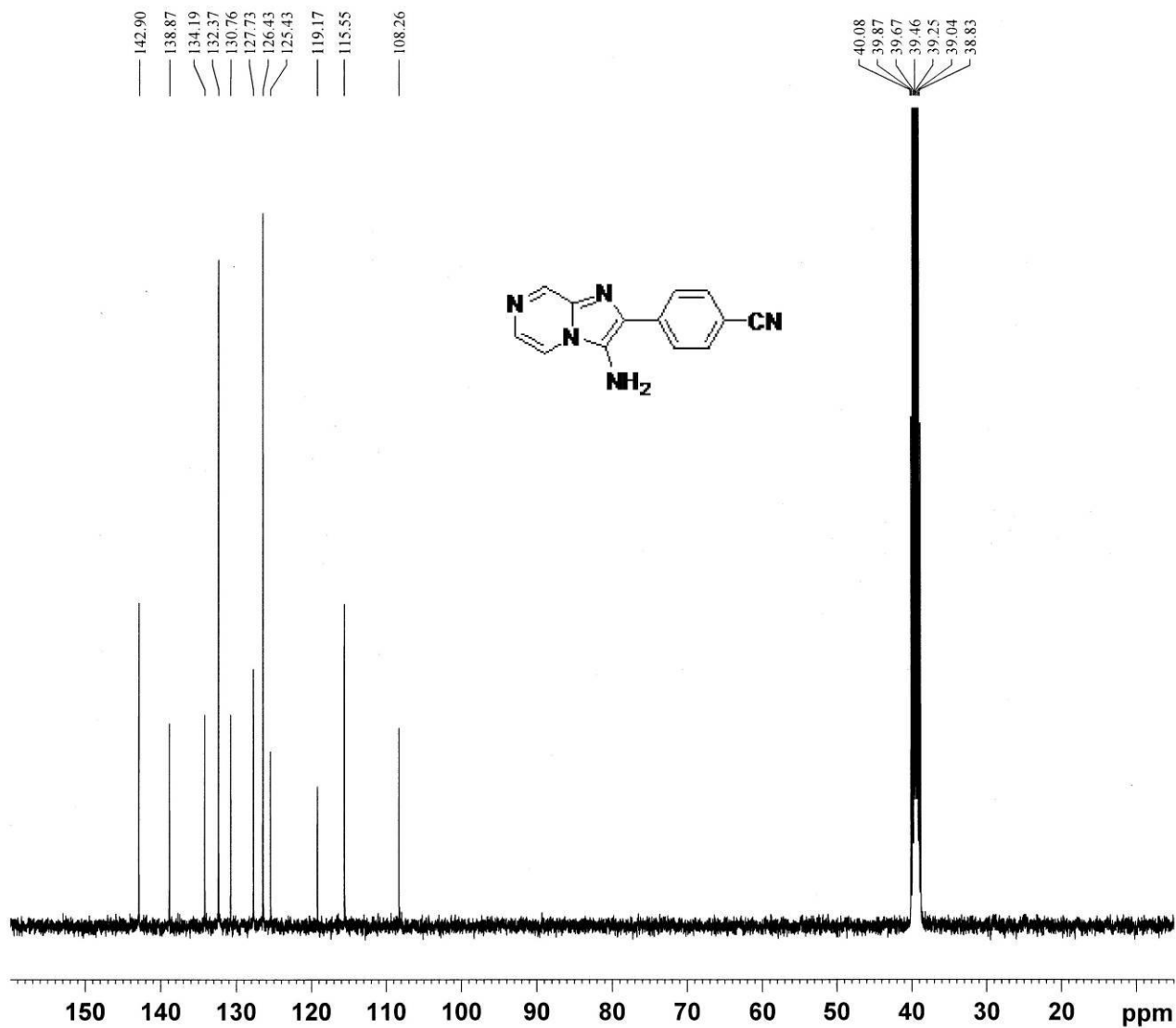


Table 2, entry 7; 4h: ^1H NMR

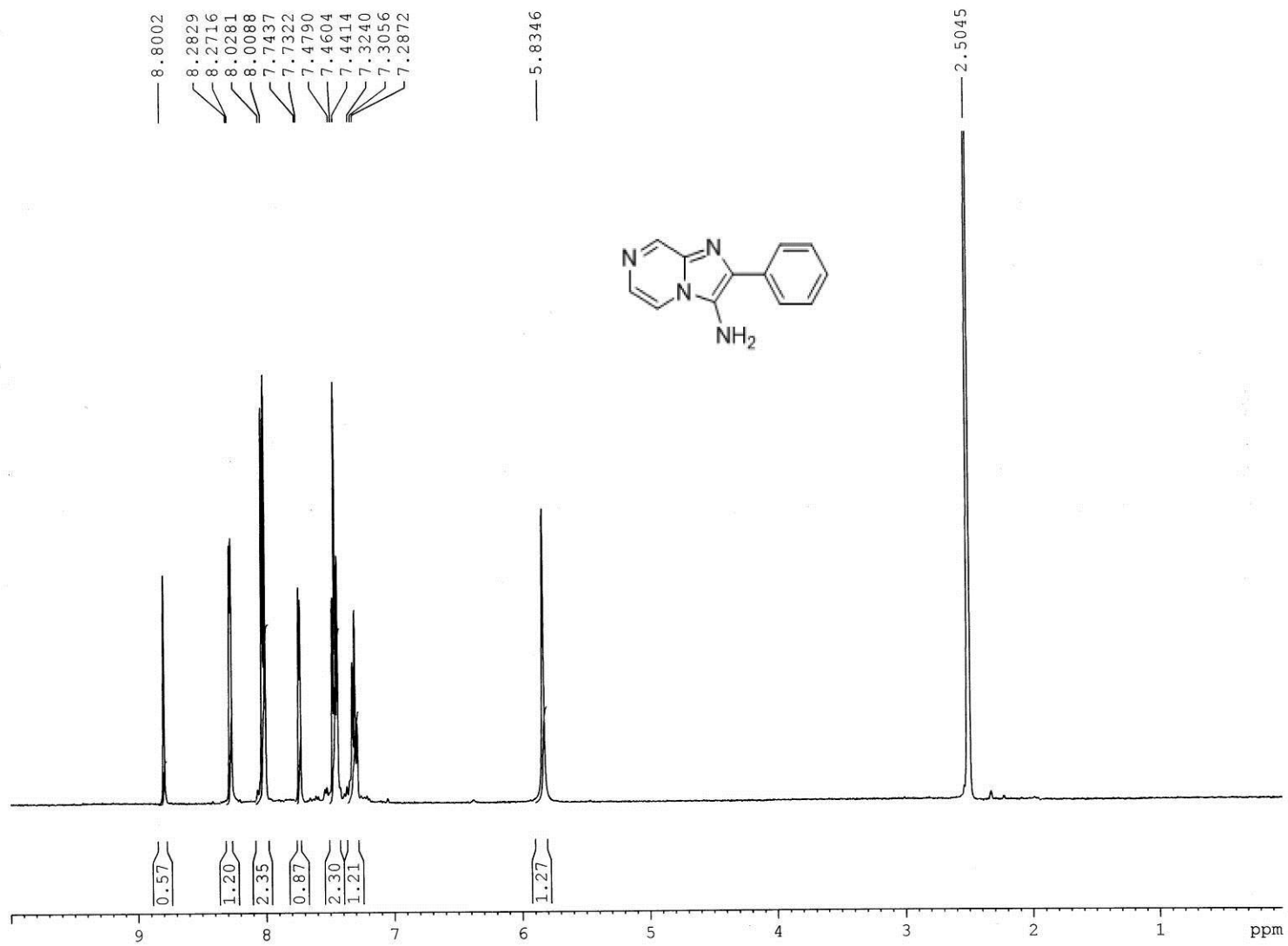


Table 2, entry 7; 4h: ^{13}C NMR

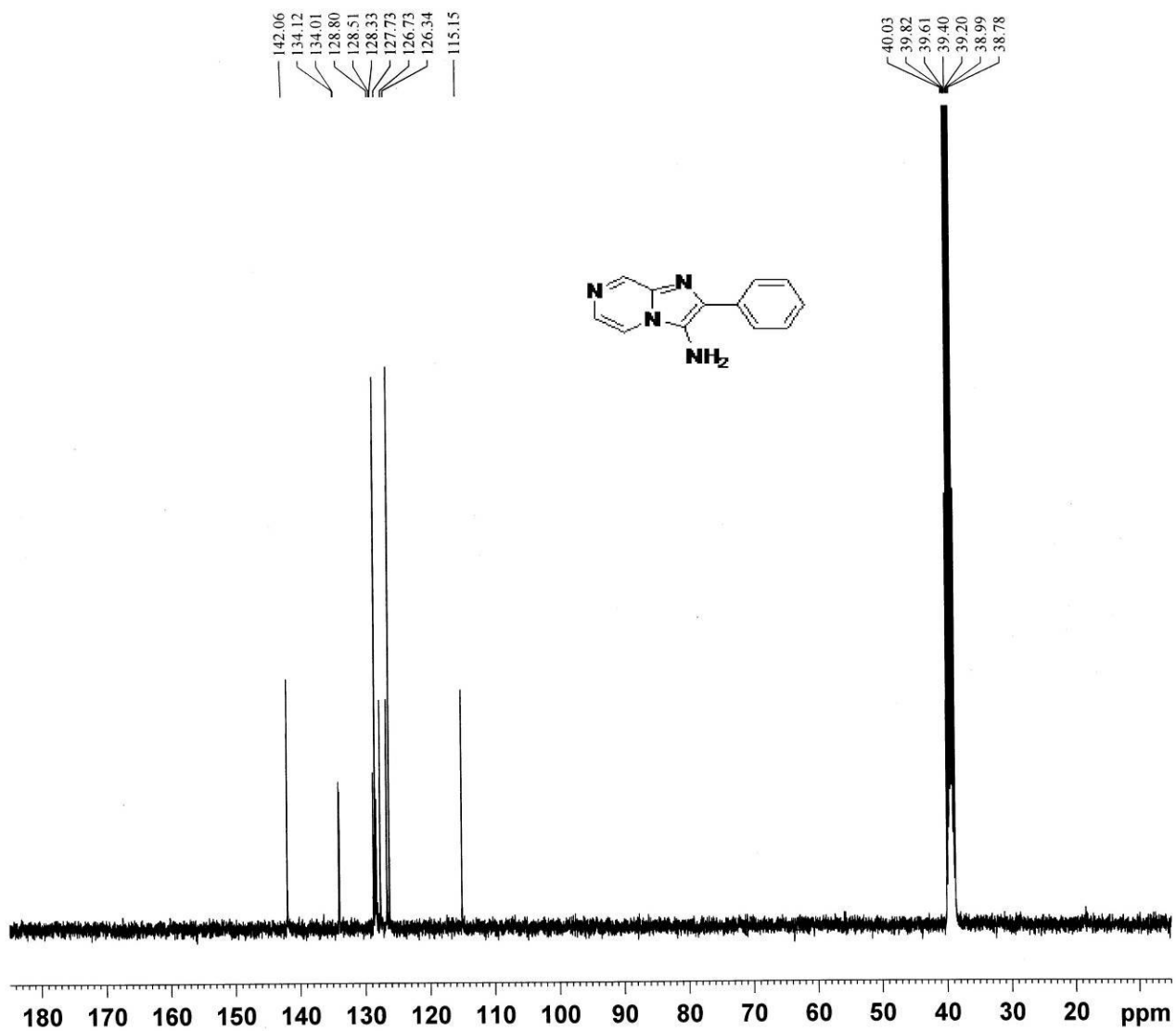


Table 2, entry 8; 4i: ^1H NMR

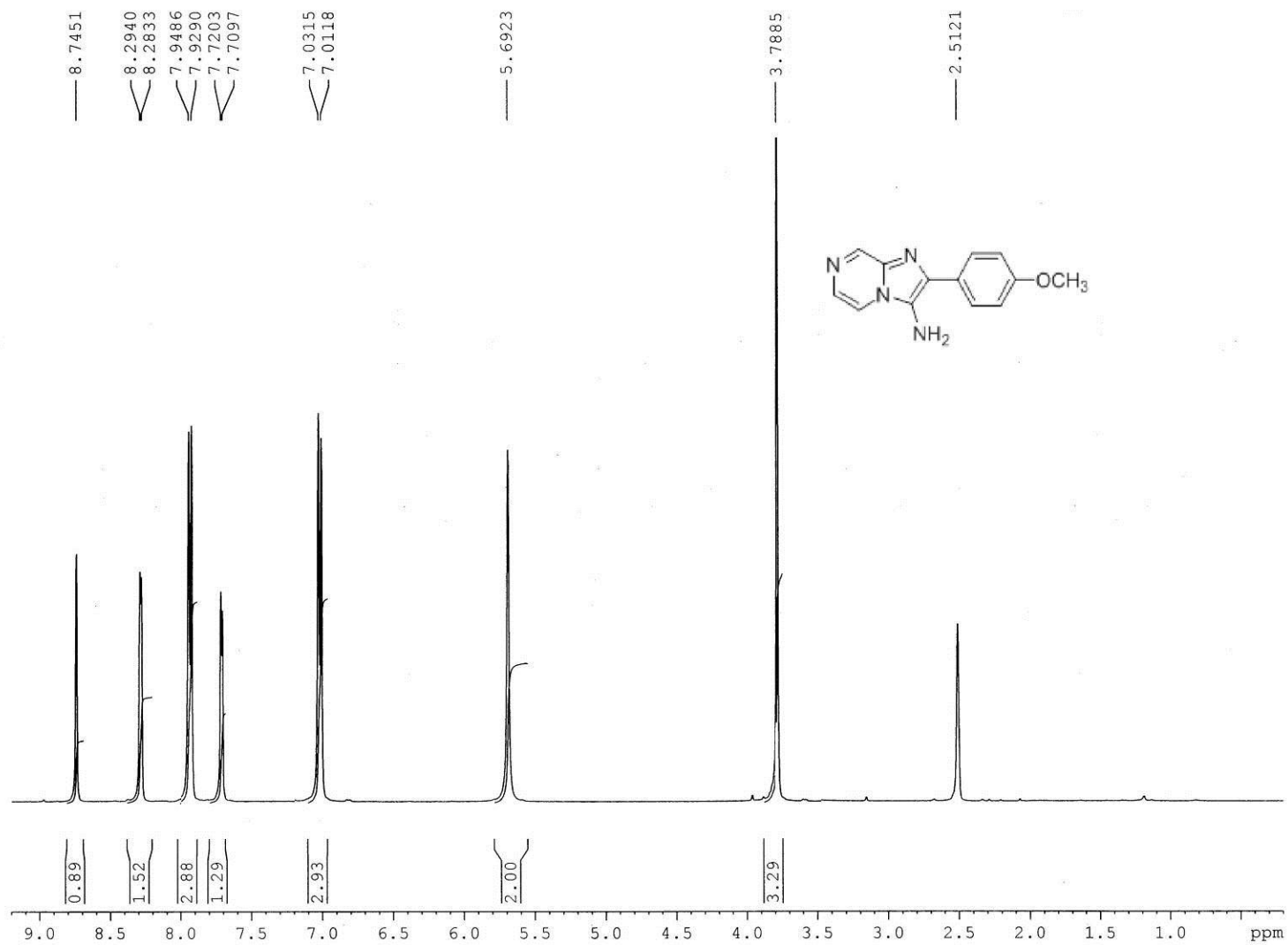


Table 2, entry 8; 4i: ^{13}C NMR

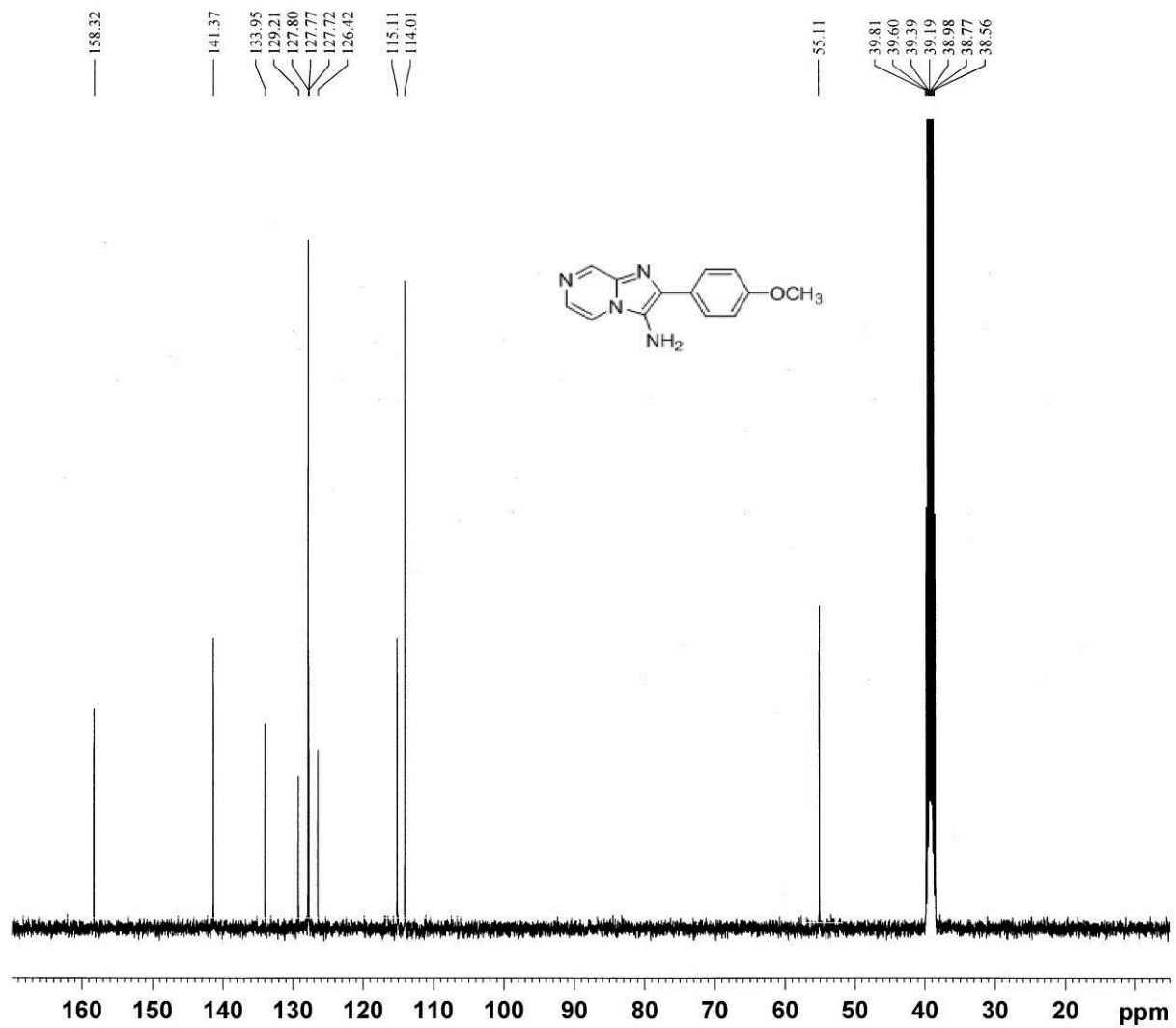


Table 2, entry 9; 4j: ^1H NMR

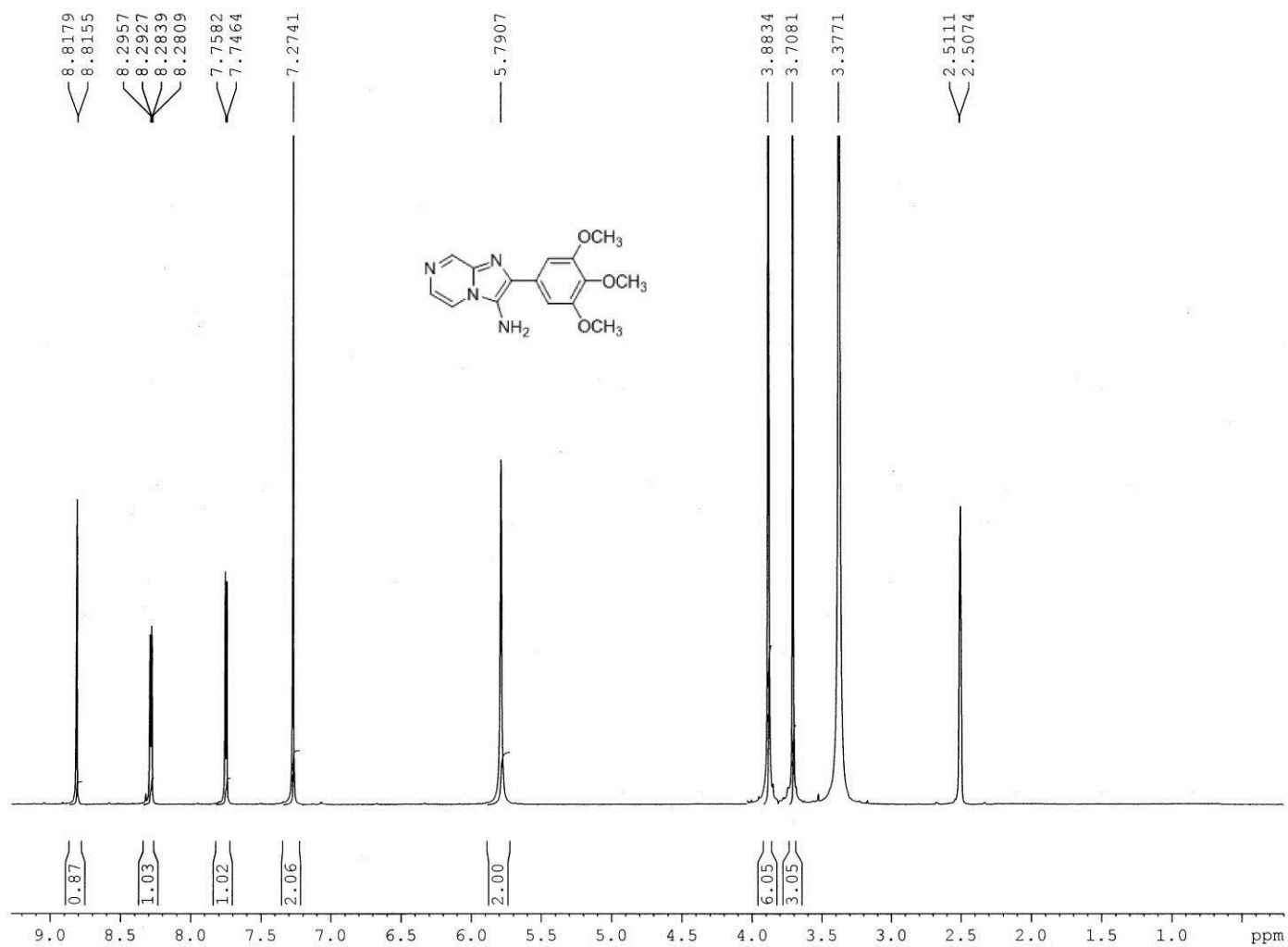


Table 2, entry 9; 4j: ^{13}C NMR

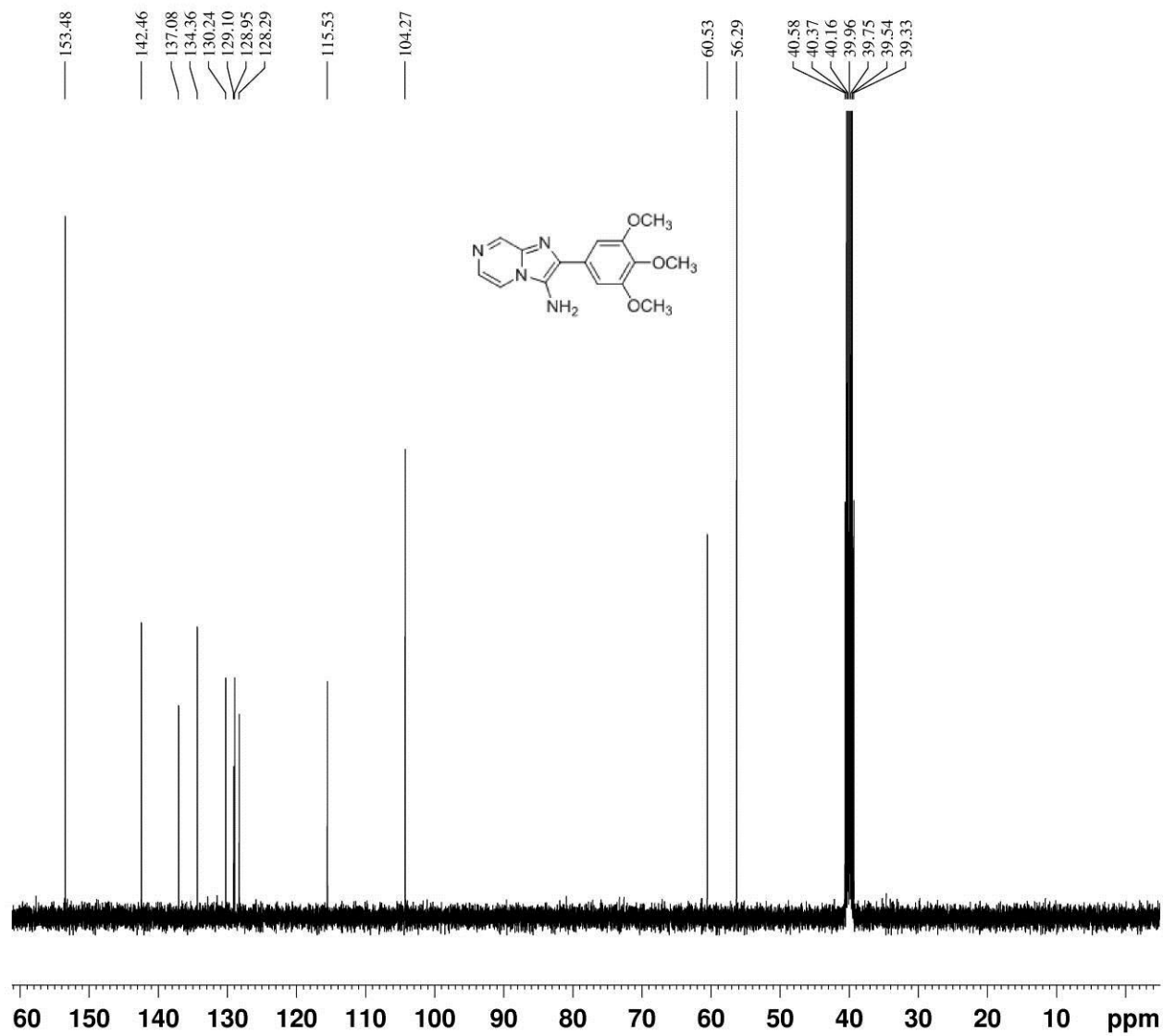


Table 2, entry 10; 4k: ^1H NMR

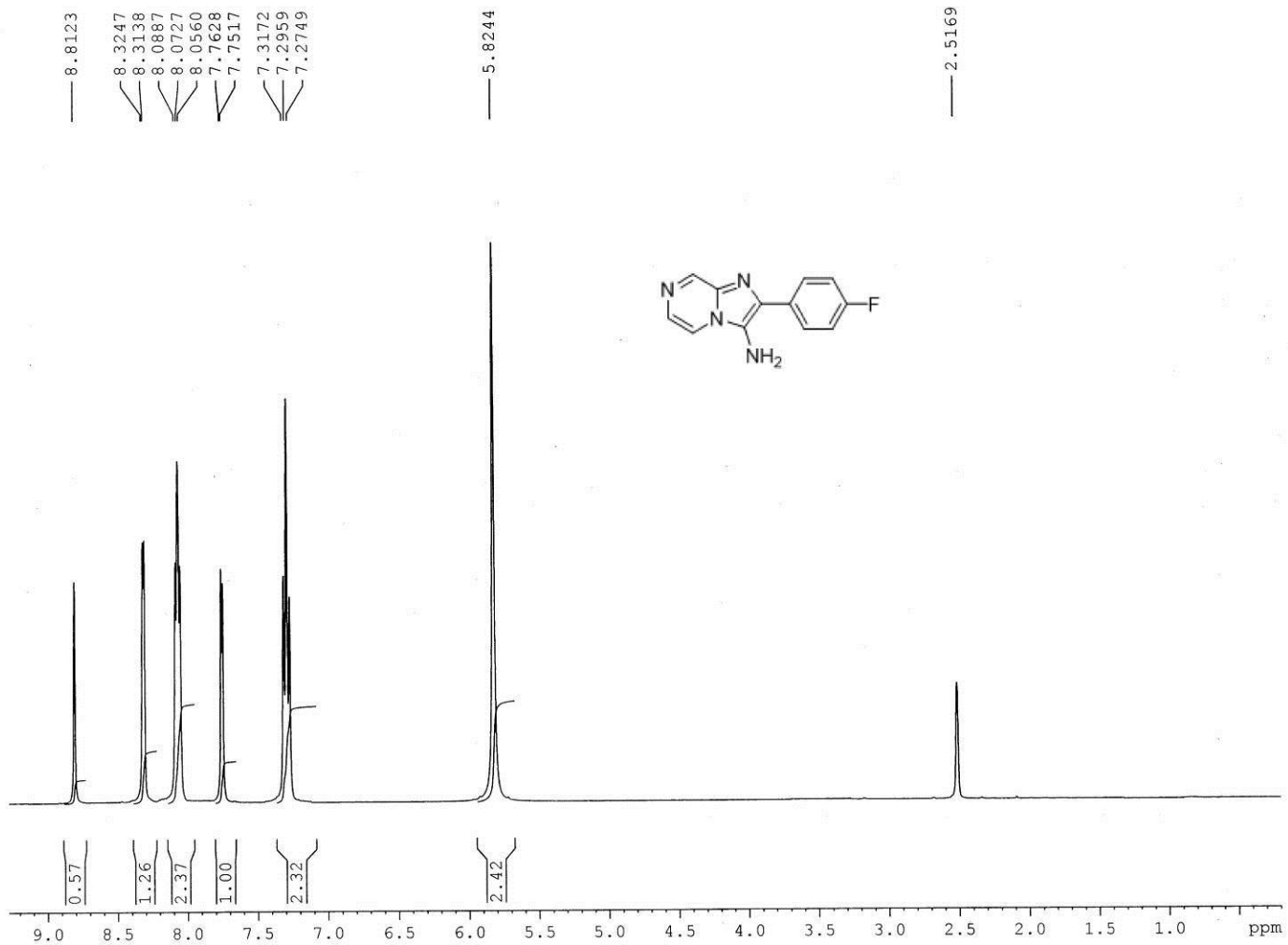


Table 2, entry 10; 4k: ^{13}C NMR

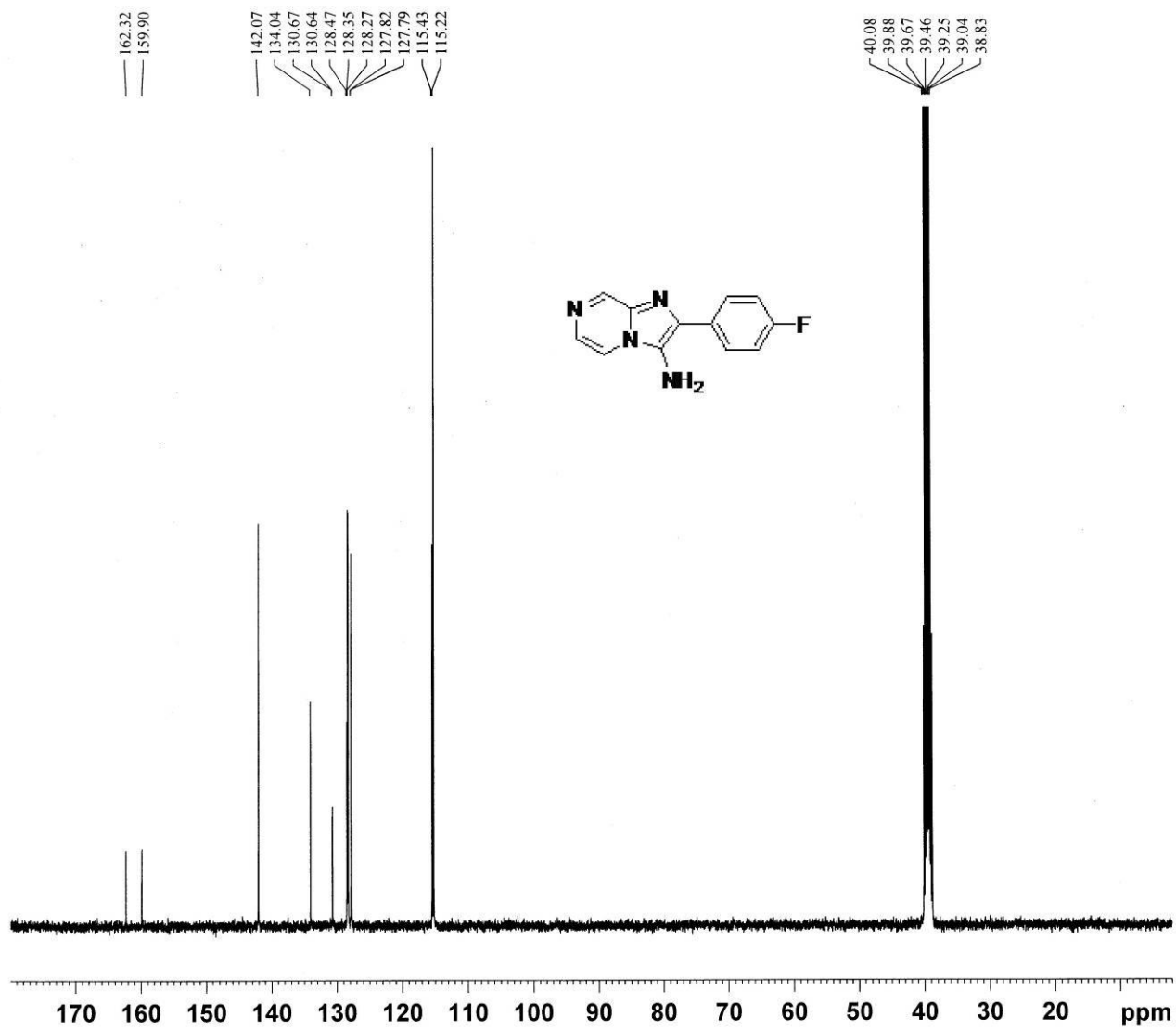


Table 2, entry 11; 4l: ^1H NMR

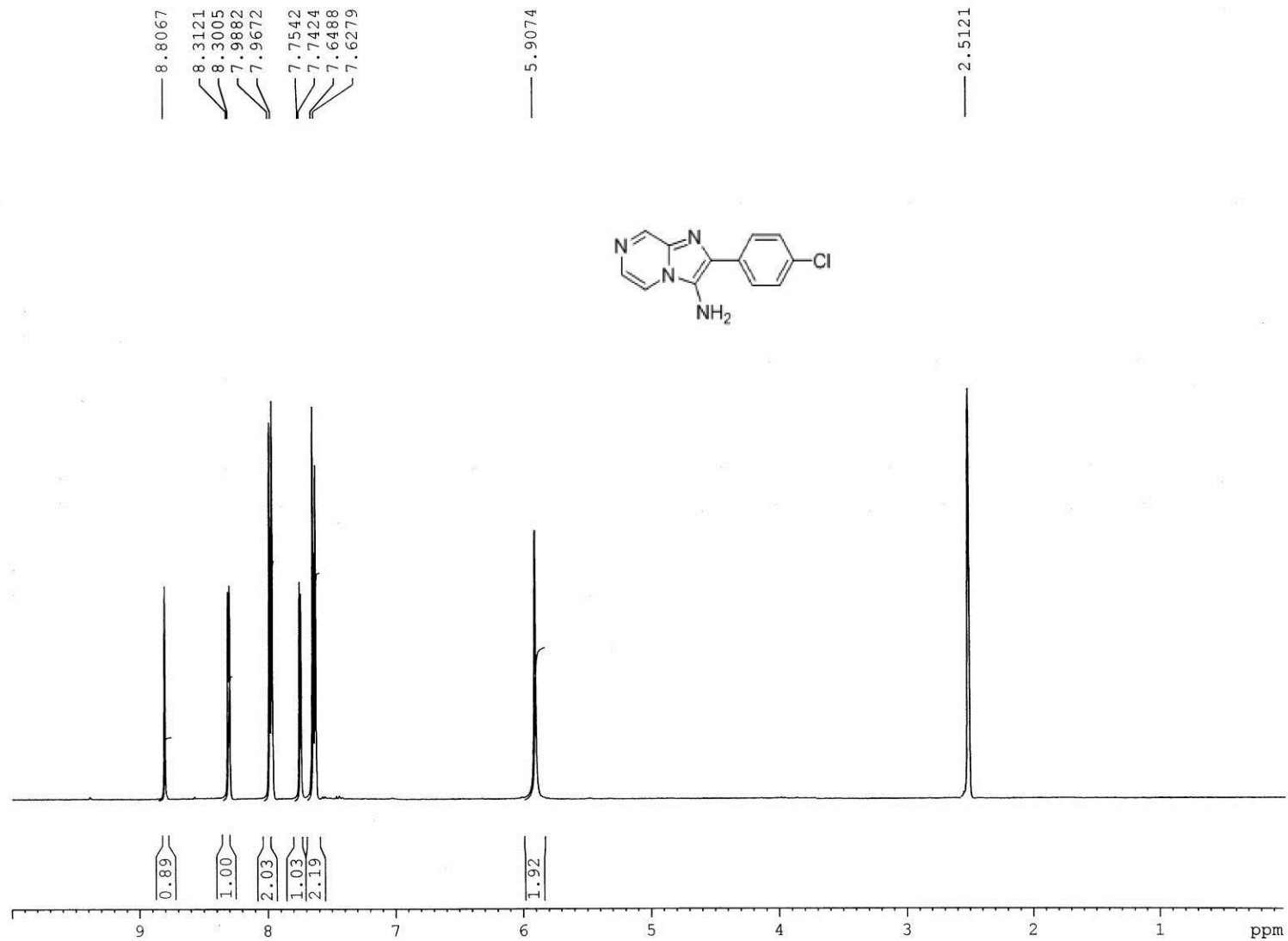


Table 2, entry 11; 4l: ^{13}C NMR

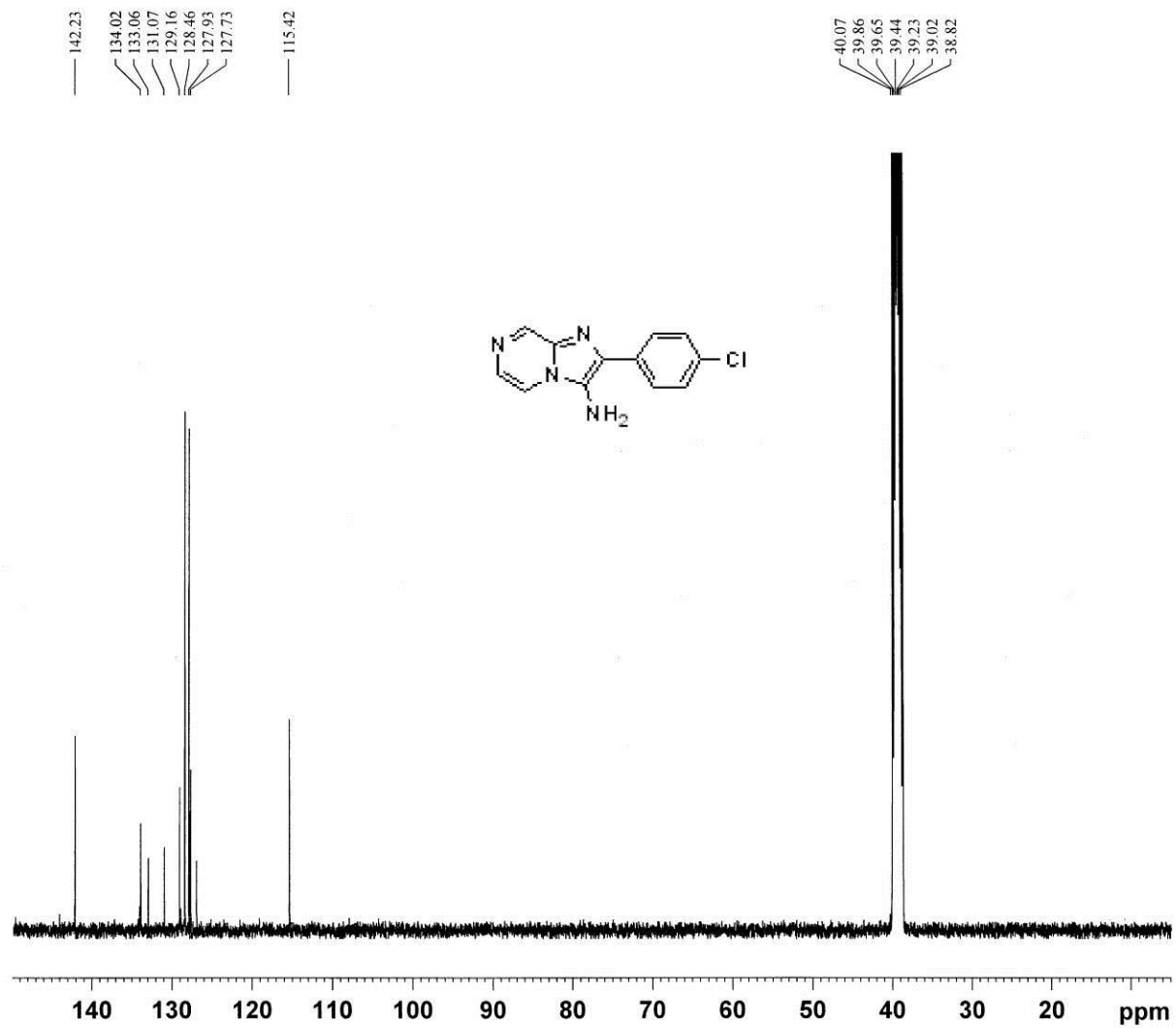


Table 2, entry 12; 4m: ^1H NMR

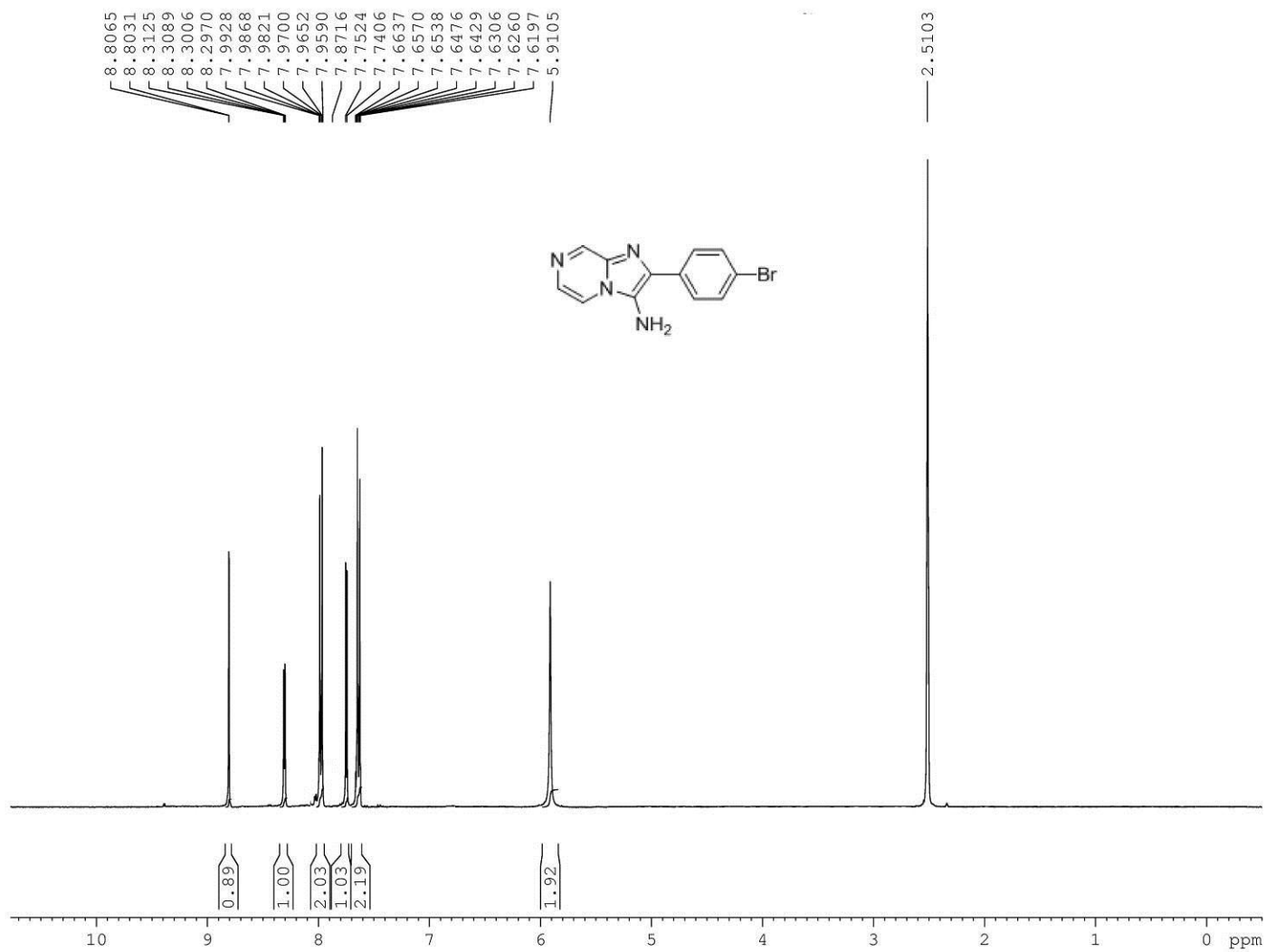


Table 2, entry 12; 4m: ^{13}C NMR

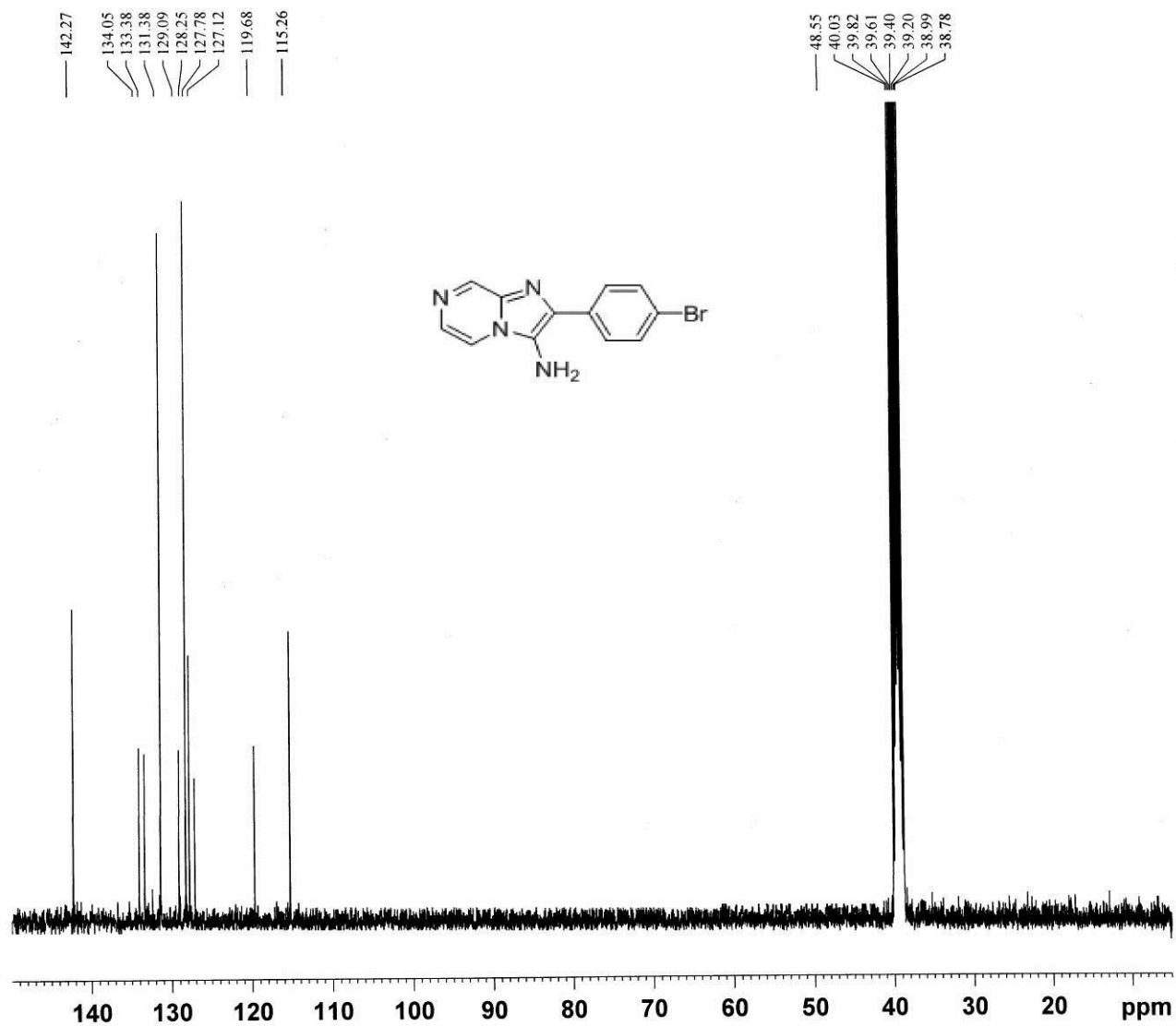


Table 2, entry 13; 4n: ^1H NMR

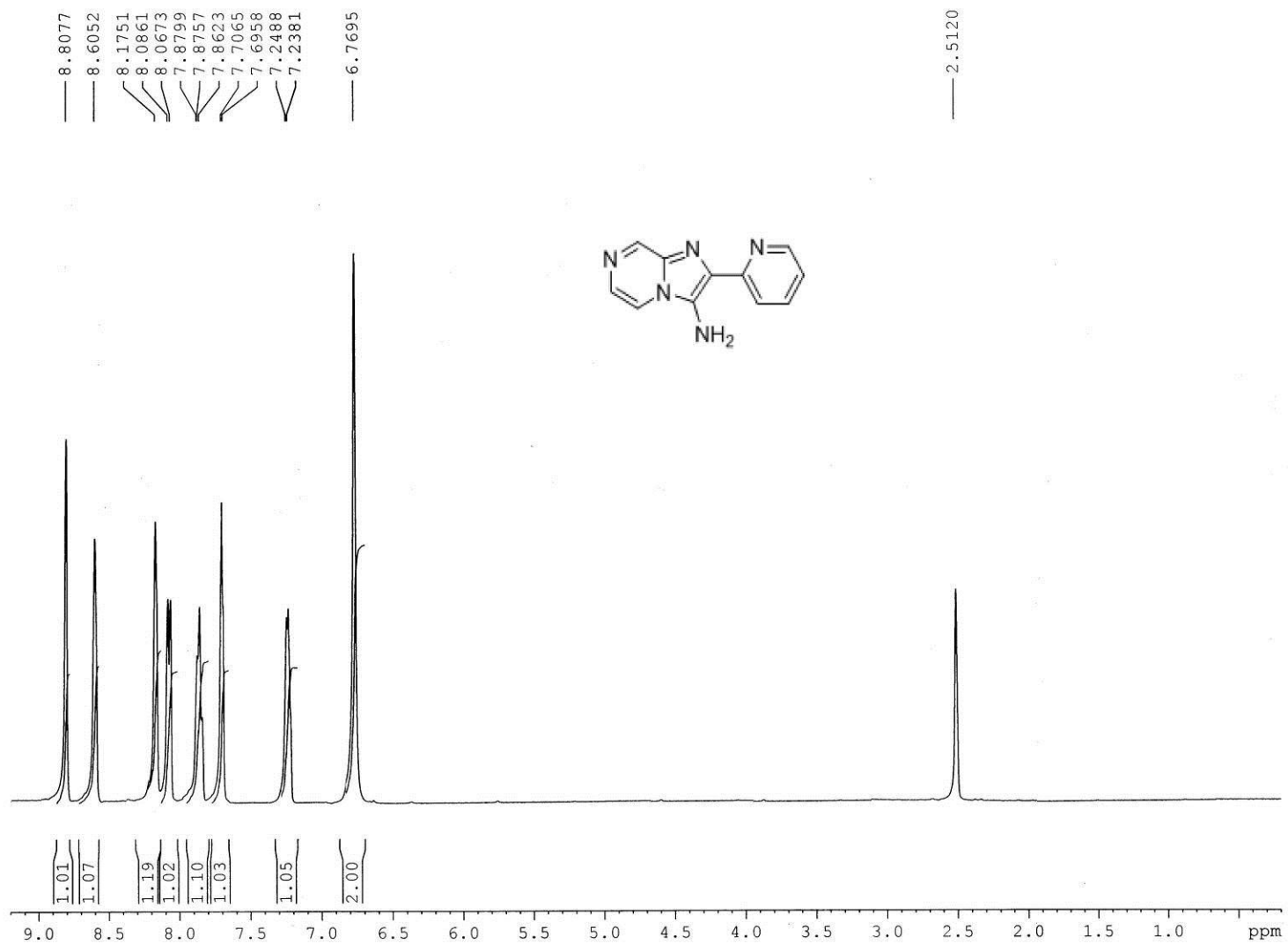


Table 2, entry 13; 4n: ^{13}C NMR

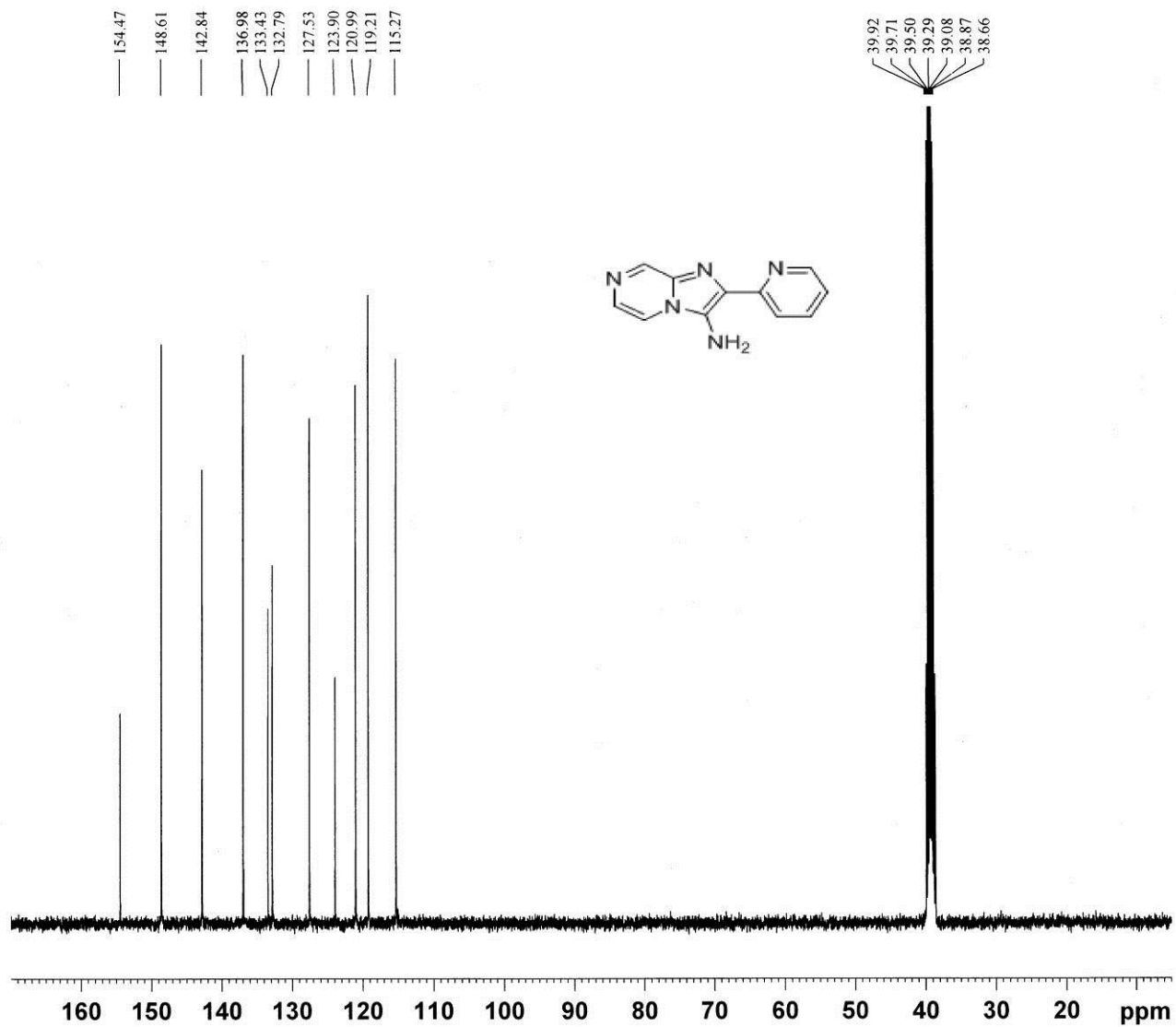


Table 2, entry 14; 4o: ^1H NMR

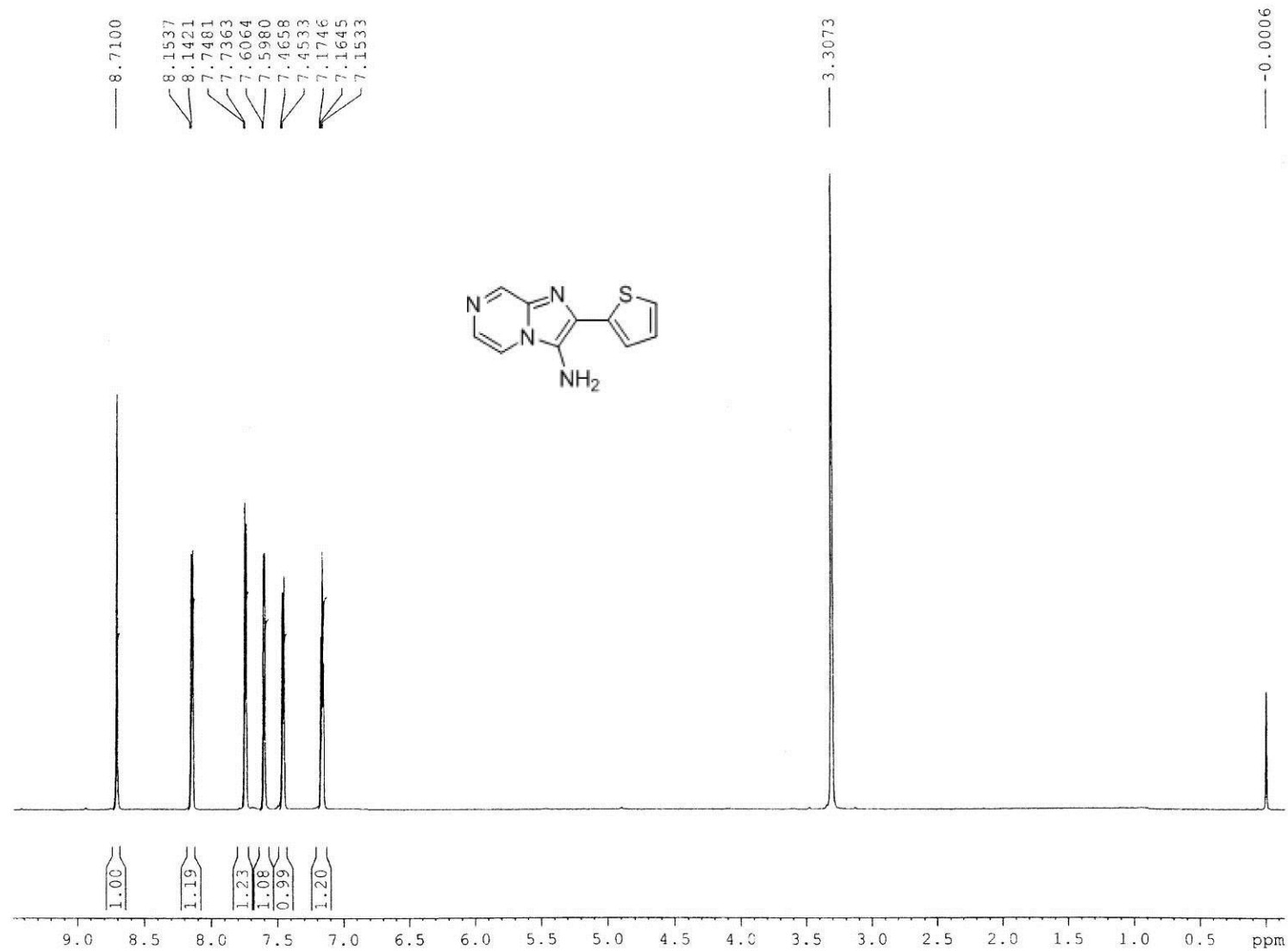


Table 2, entry 14; 4o: ^{13}C NMR

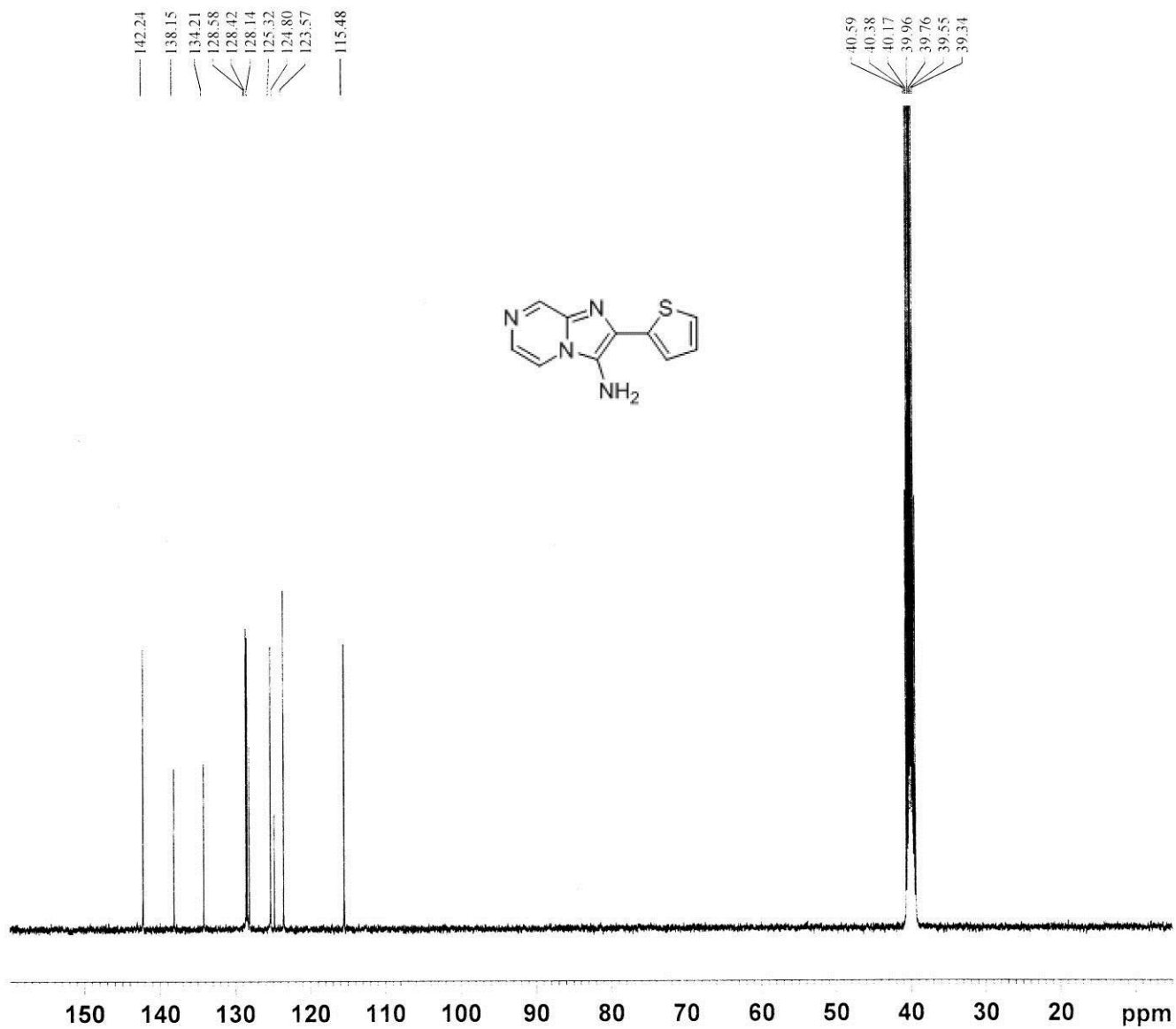


Table 2, entry 15; 4p: ^1H NMR

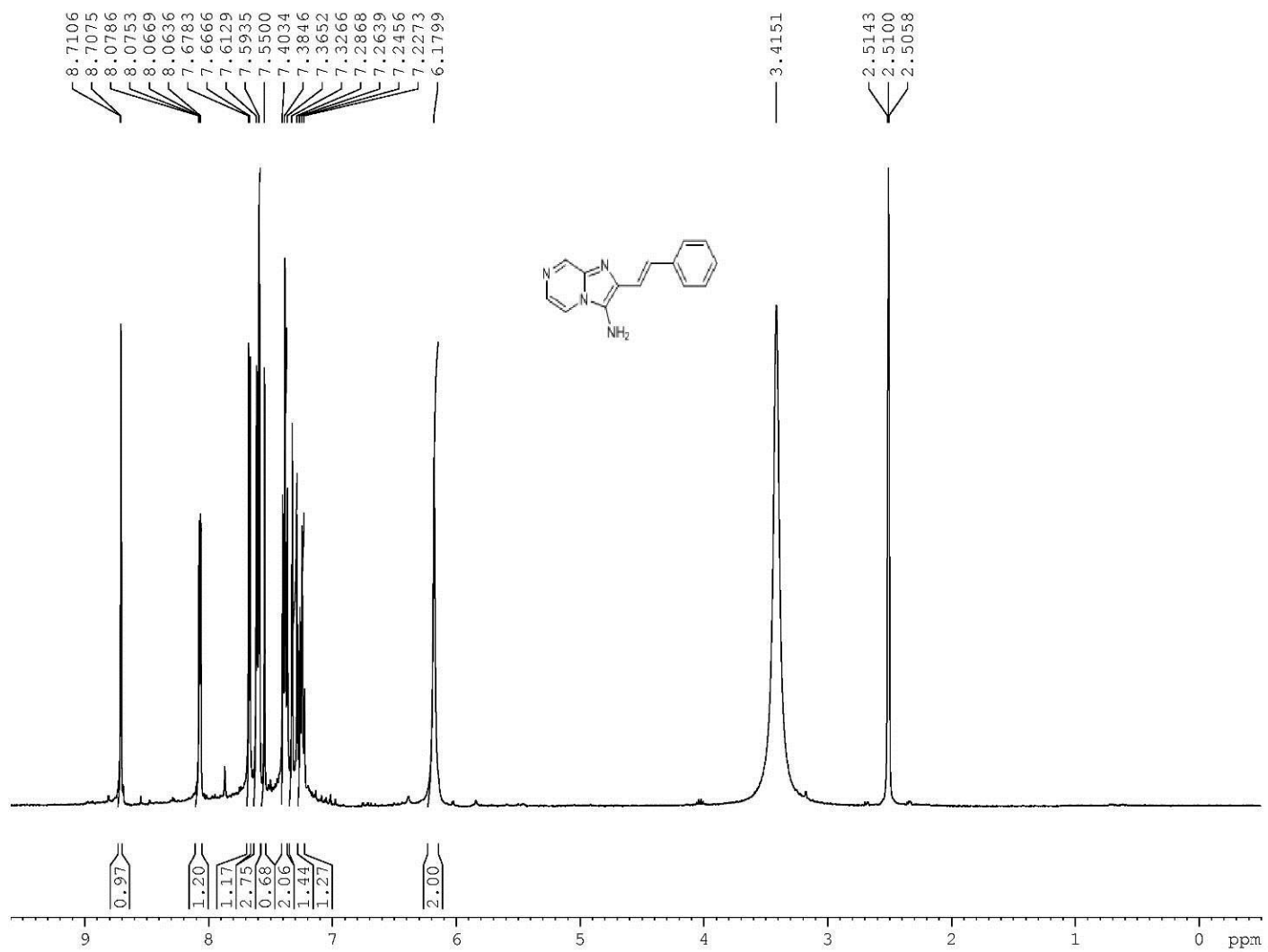


Table 2, entry 15; 4p: ^{13}C NMR

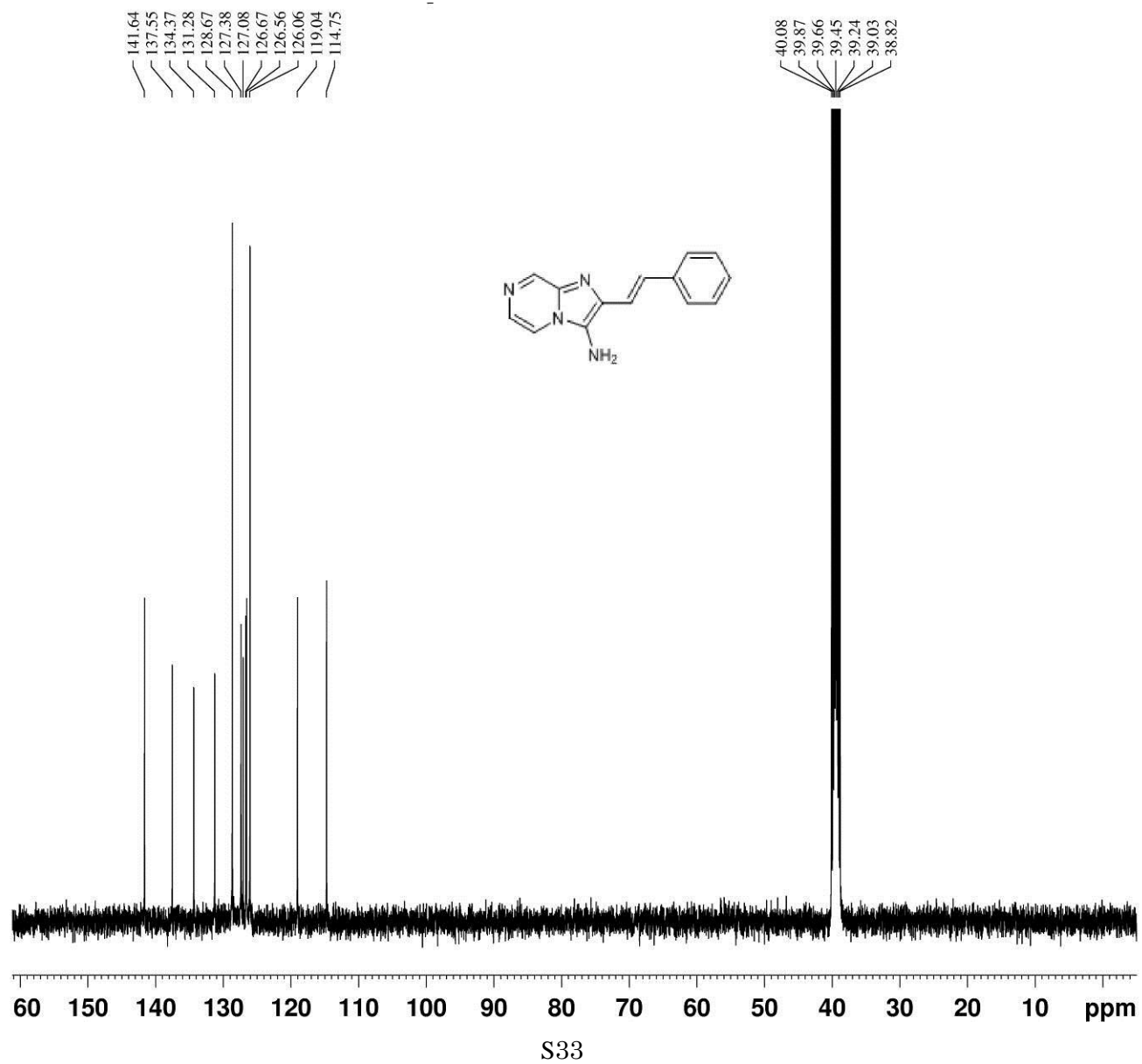


Table 2, entry 16; 4q: ^1H NMR

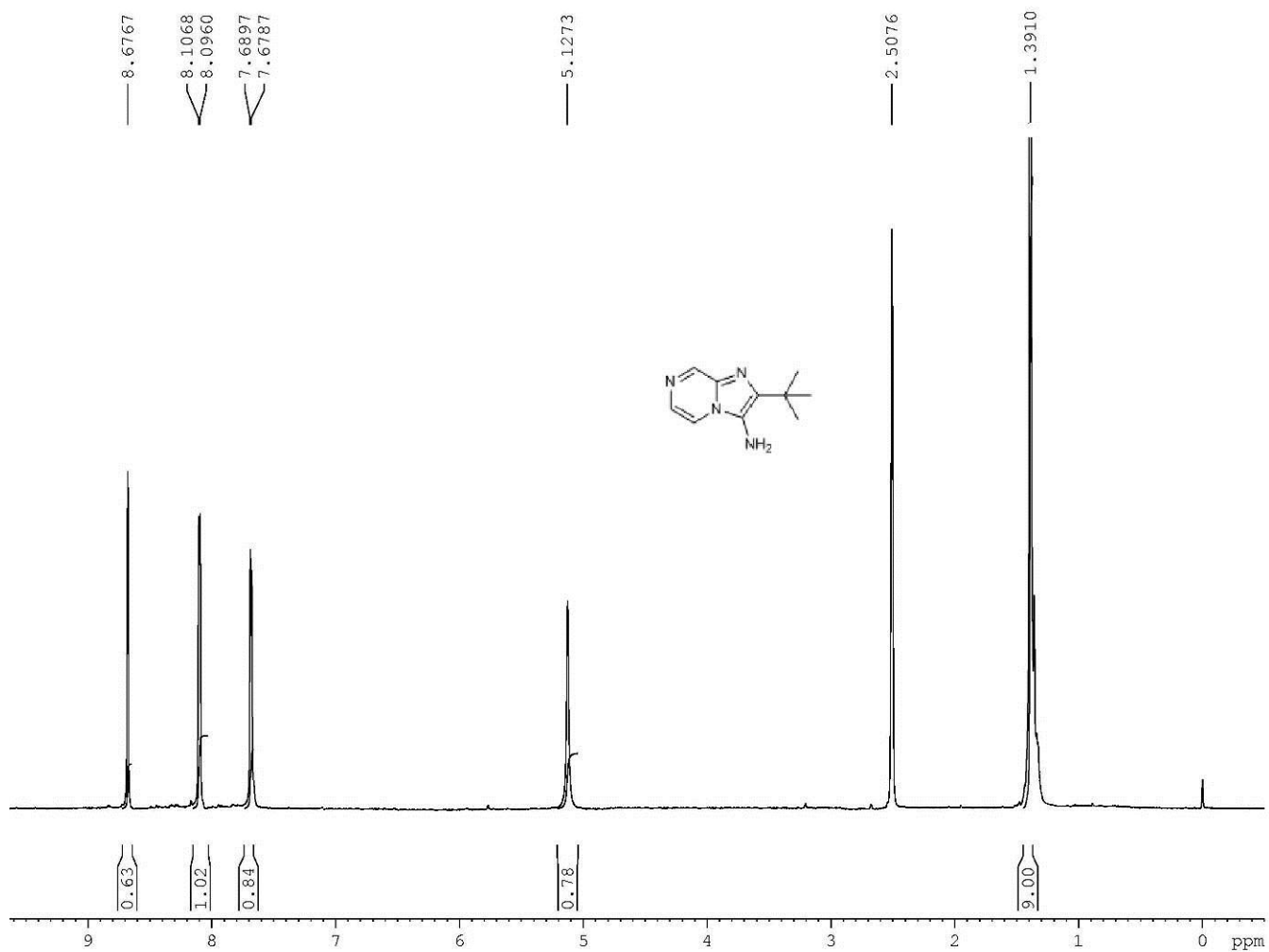


Table 2, entry 16; 4q: ^{13}C NMR

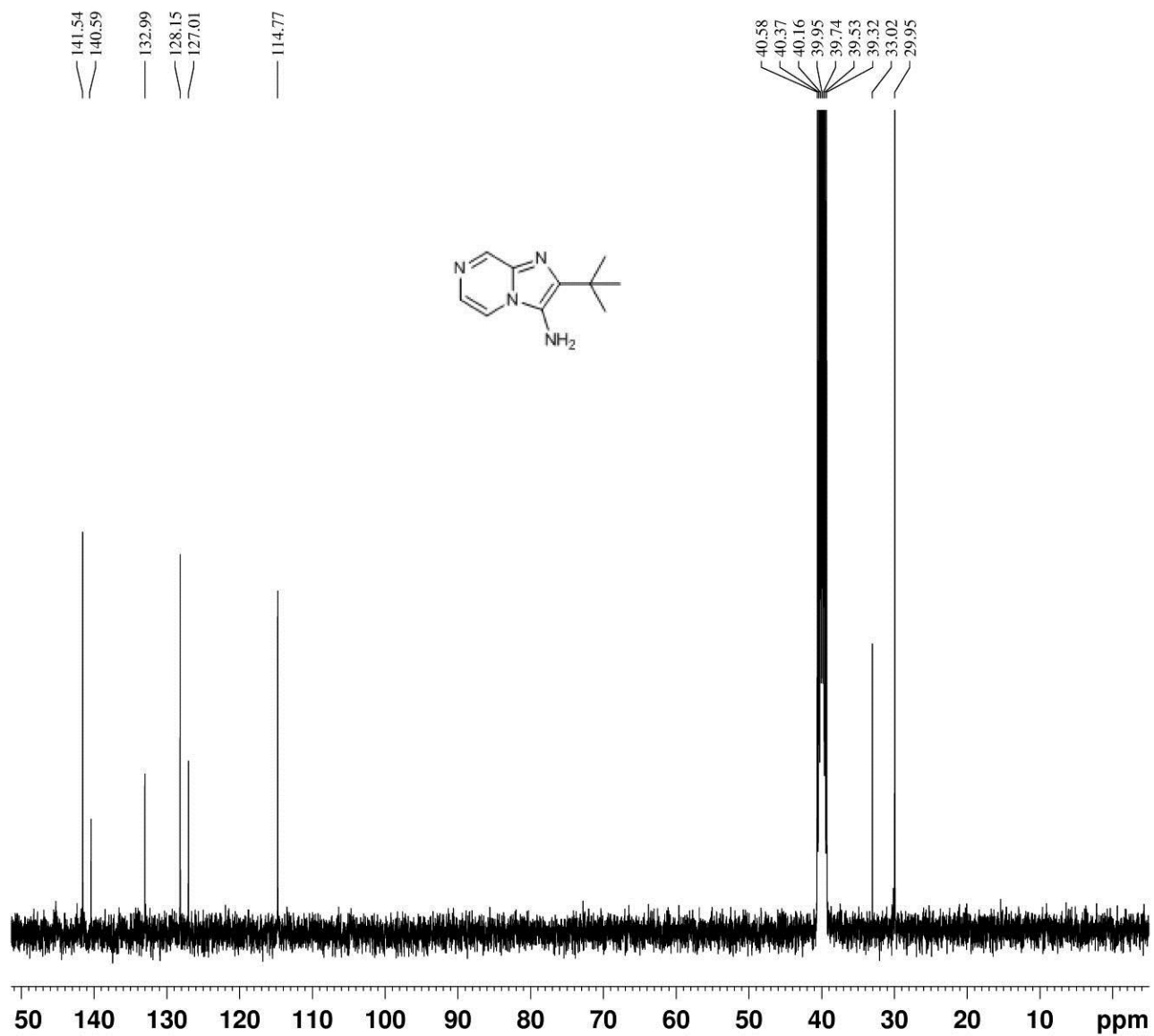


Table 2, entry 17; 4r: ^1H NMR

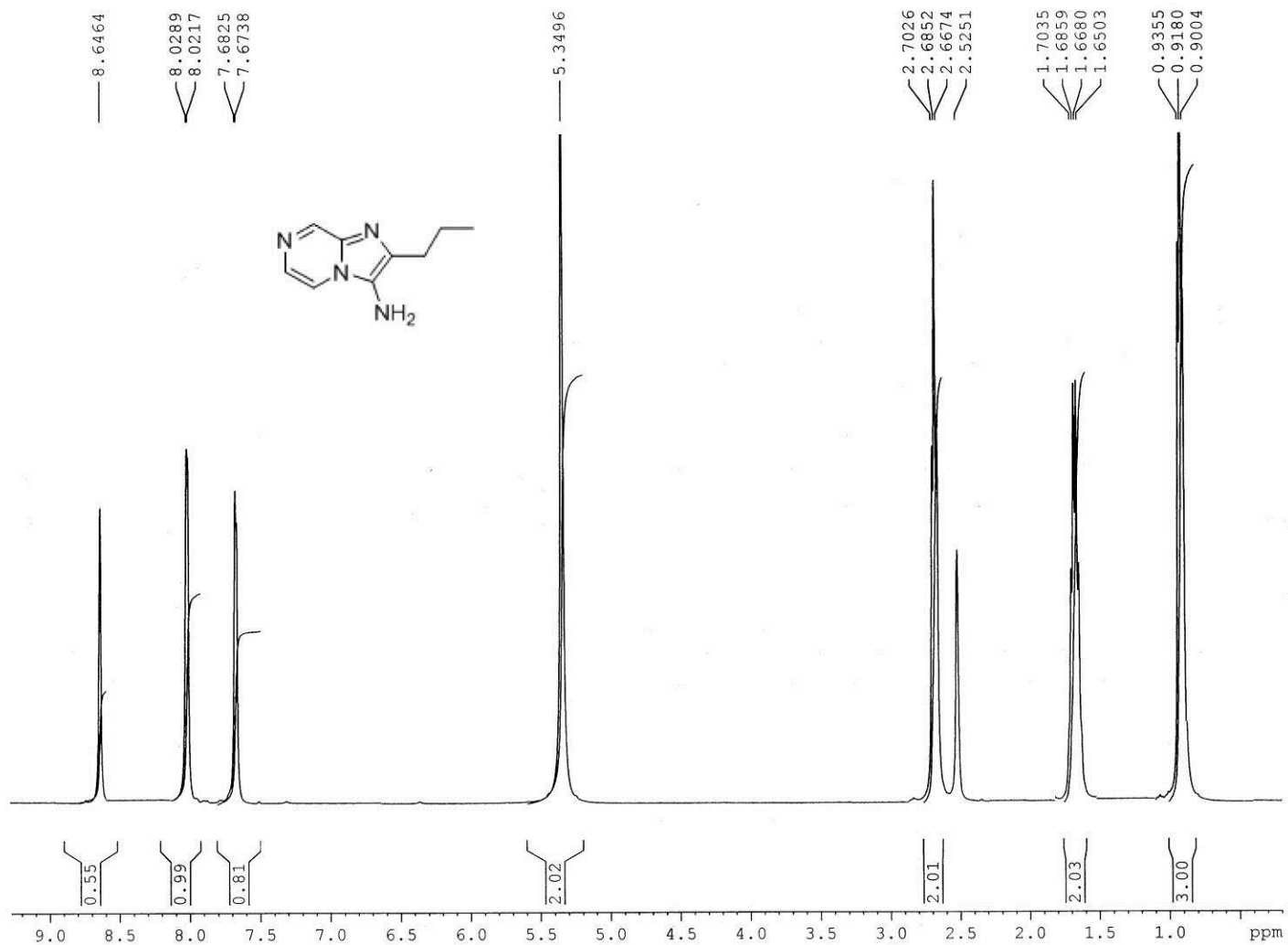
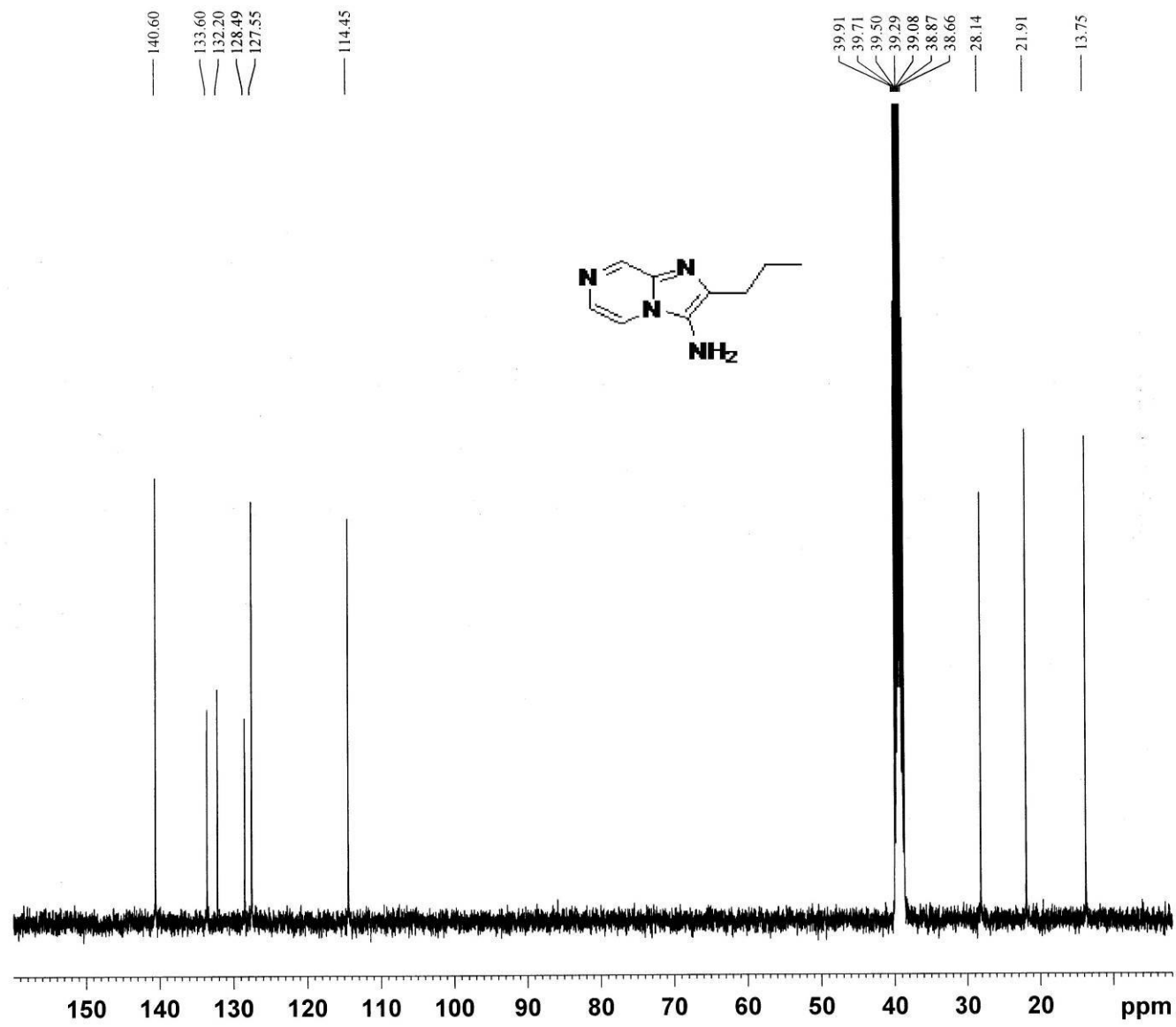


Table 2, entry 17; 4r: ^{13}C NMR



Spectra of compounds (7a-f)

Table 3, entry 1; 7a: ^1H NMR

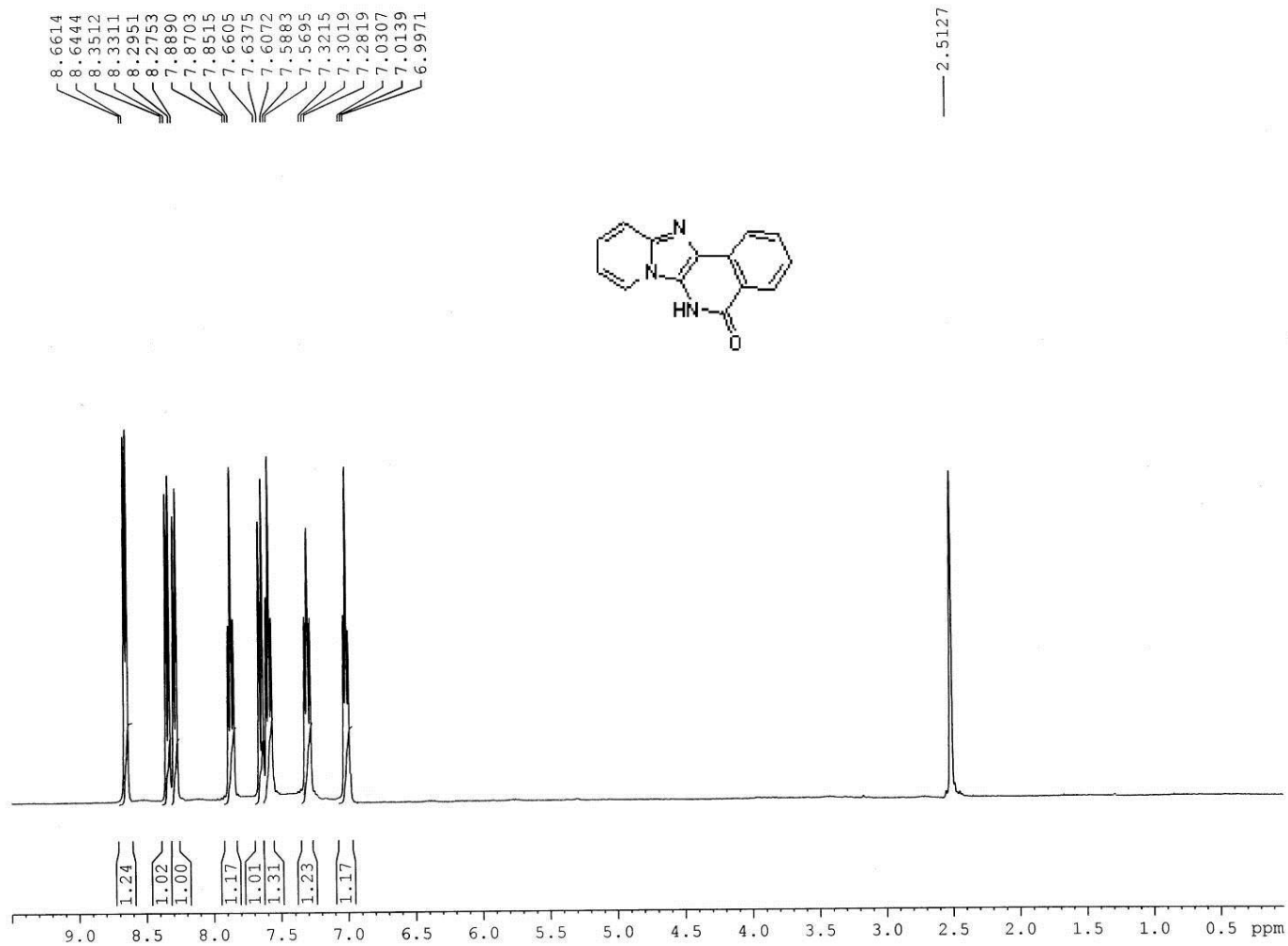


Table 3, entry 1; 7a: ^{13}C NMR

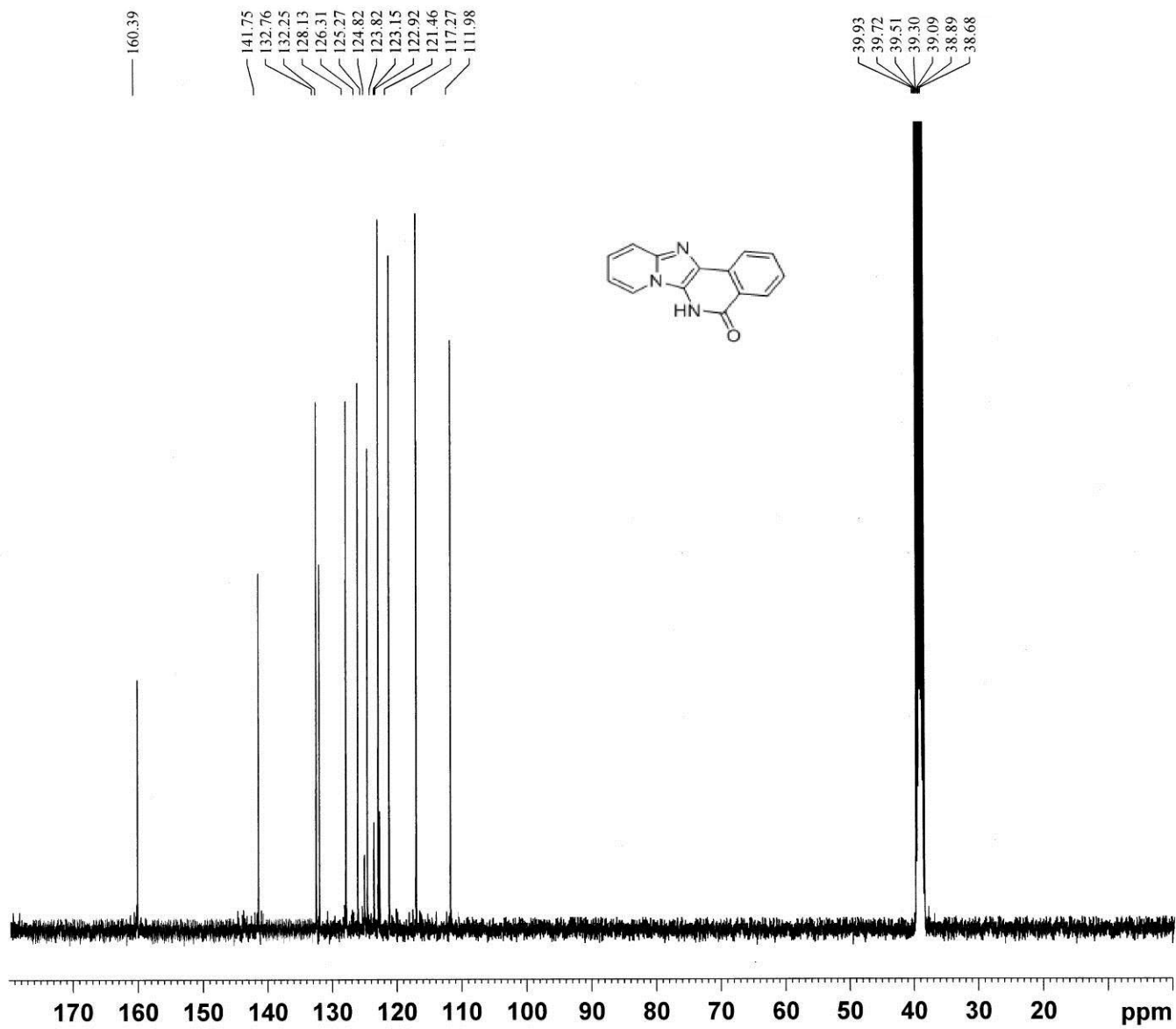


Table 3, entry 2; 7b: ^1H NMR

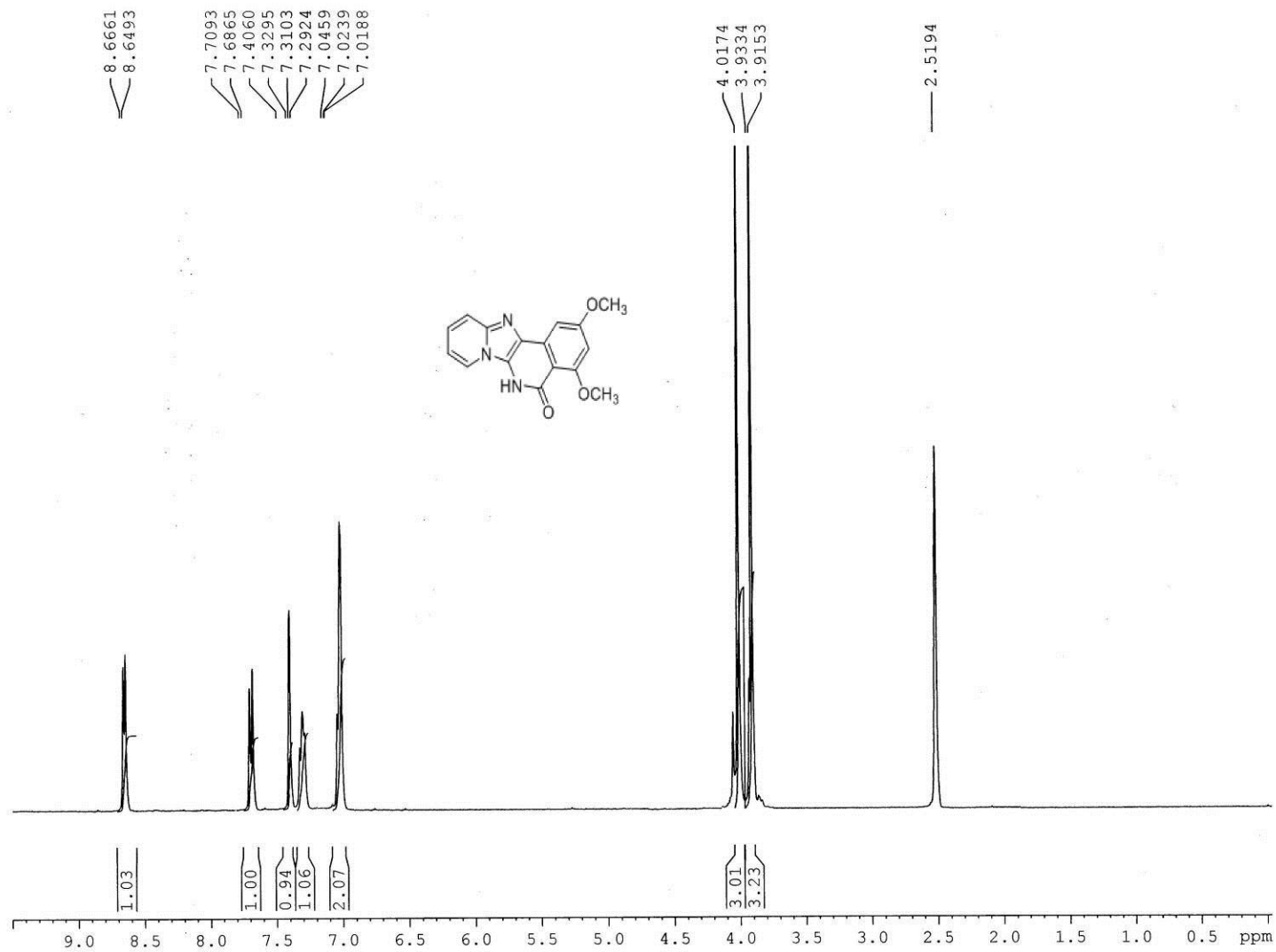


Table 3, entry 2; 7b: ^{13}C NMR

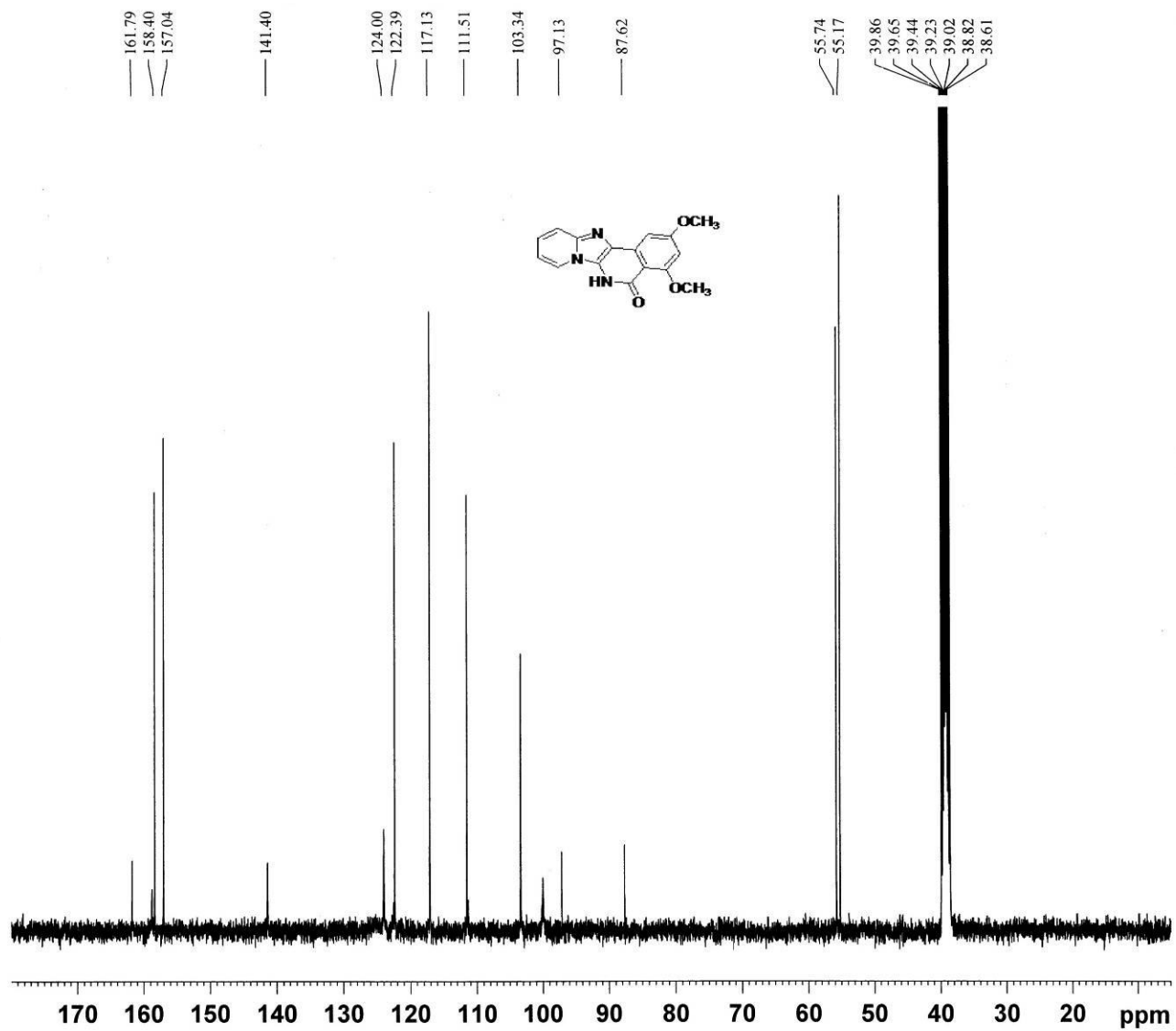


Table 3, entry 3; 7c: ^1H NMR

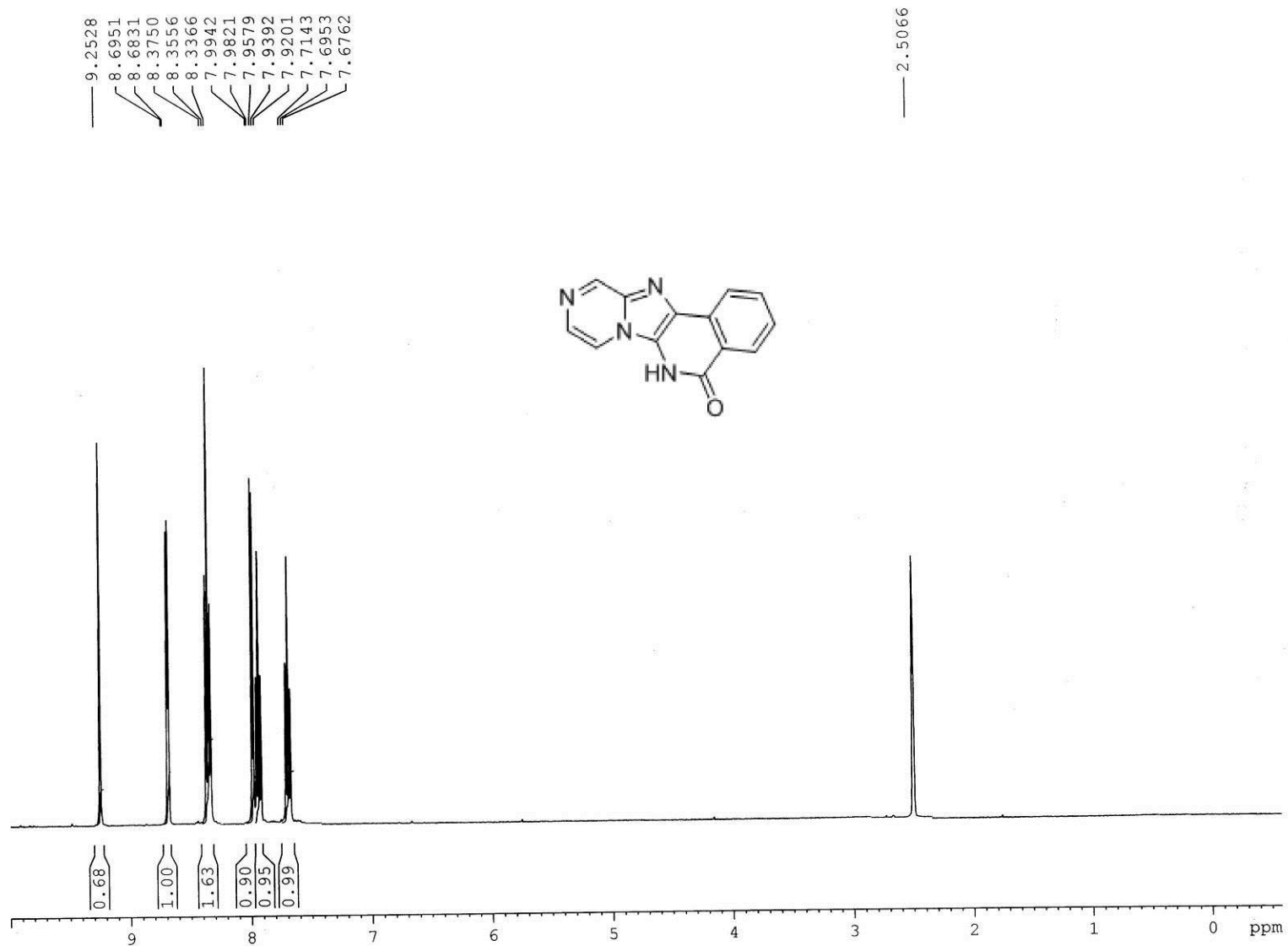


Table 3, entry 3; 7c: ^{13}C NMR

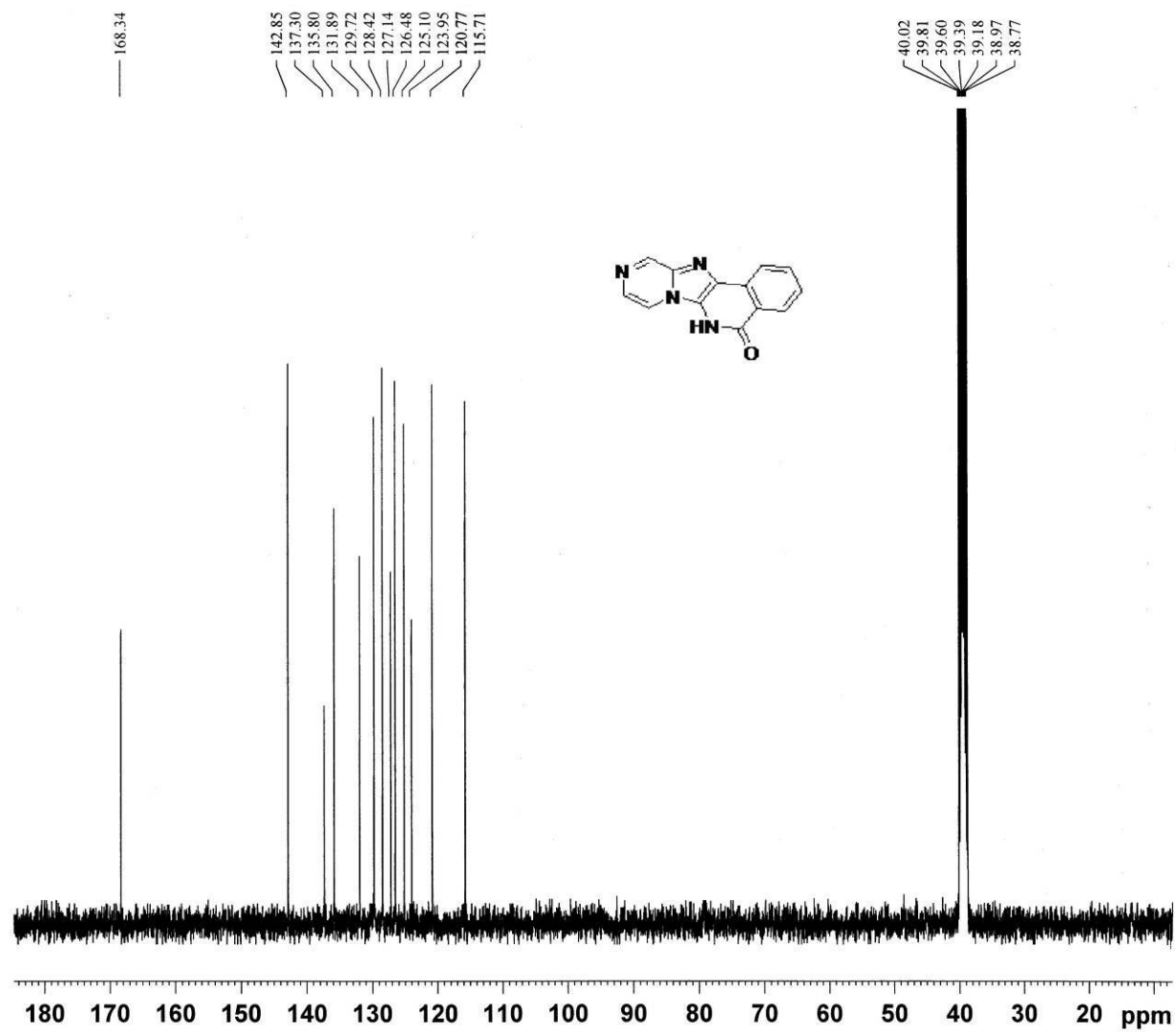


Table 3, entry 4; 7d: ^1H NMR

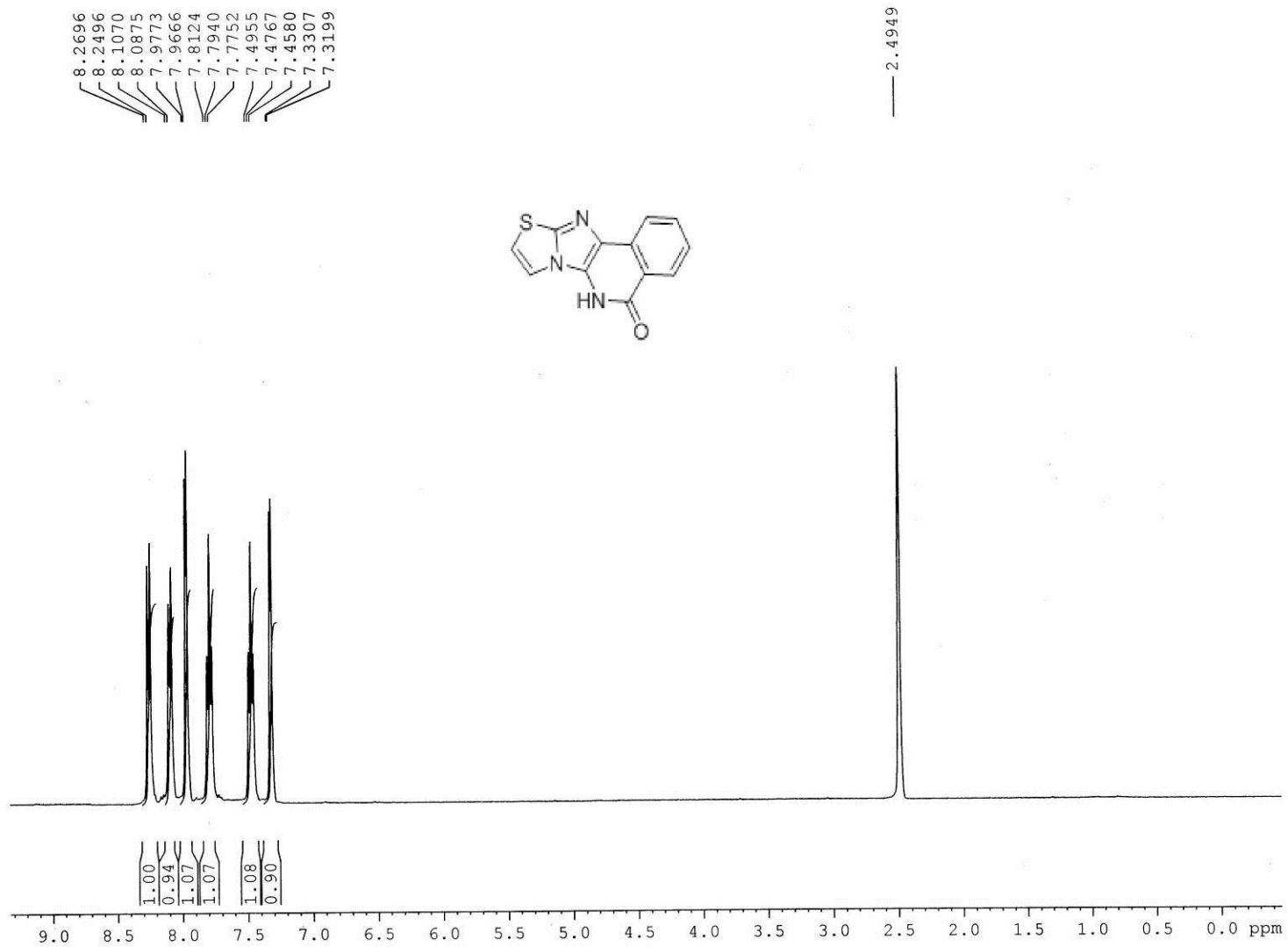


Table 3, entry 4; 7d: ^{13}C NMR

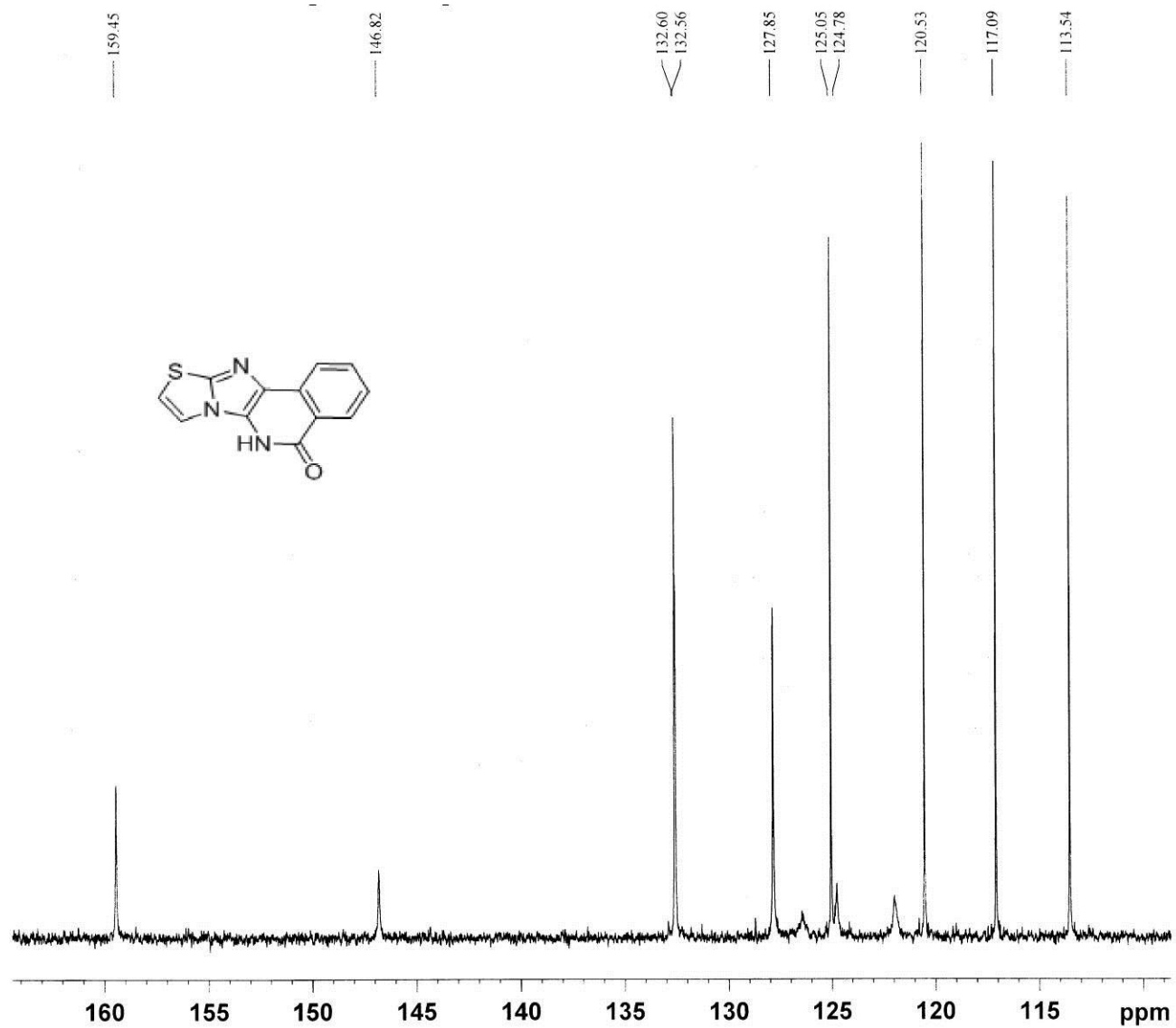


Table 3, entry 5; 7e: ^1H NMR

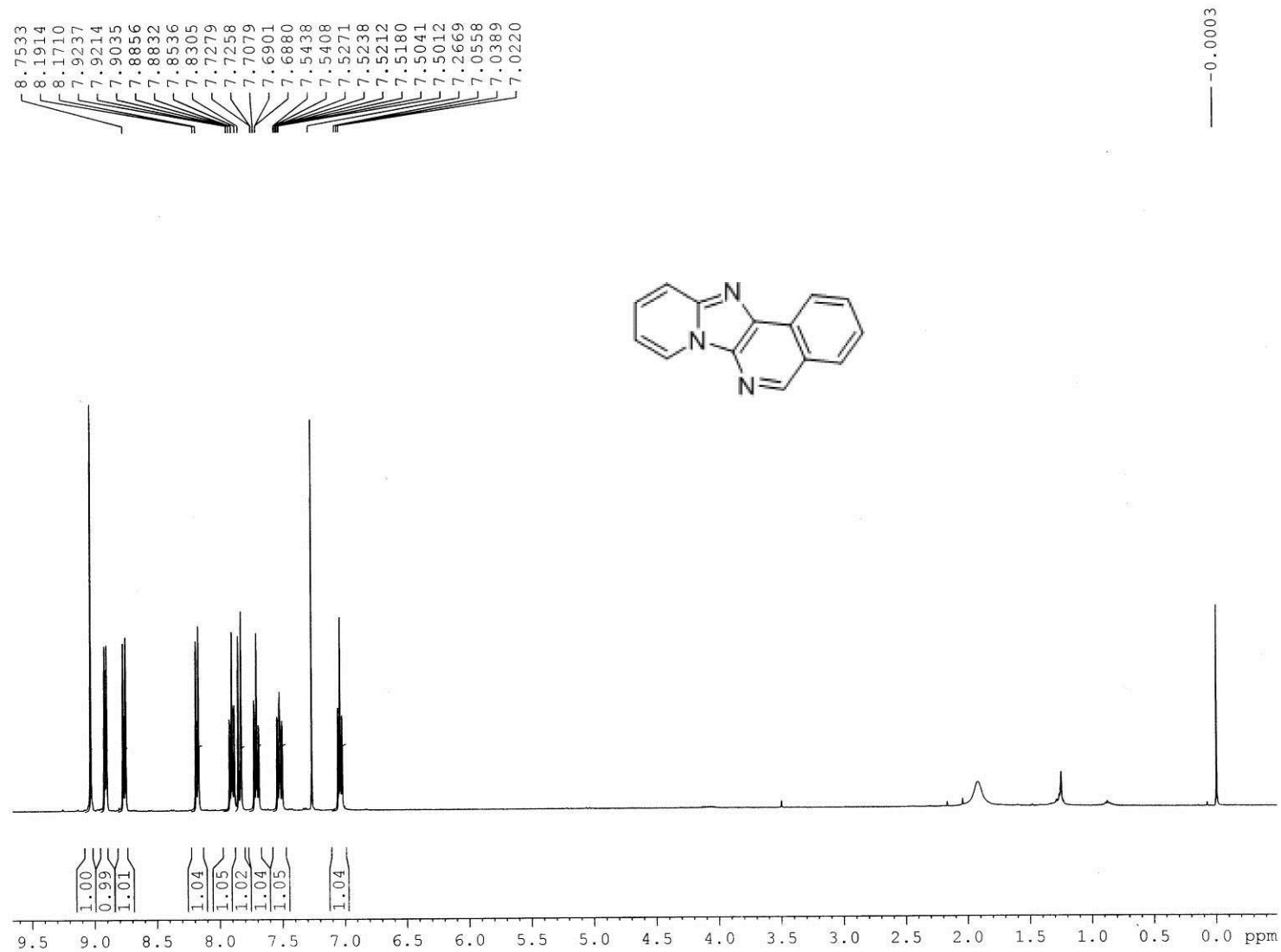


Table 3, entry 6; 7e: ^{13}C NMR

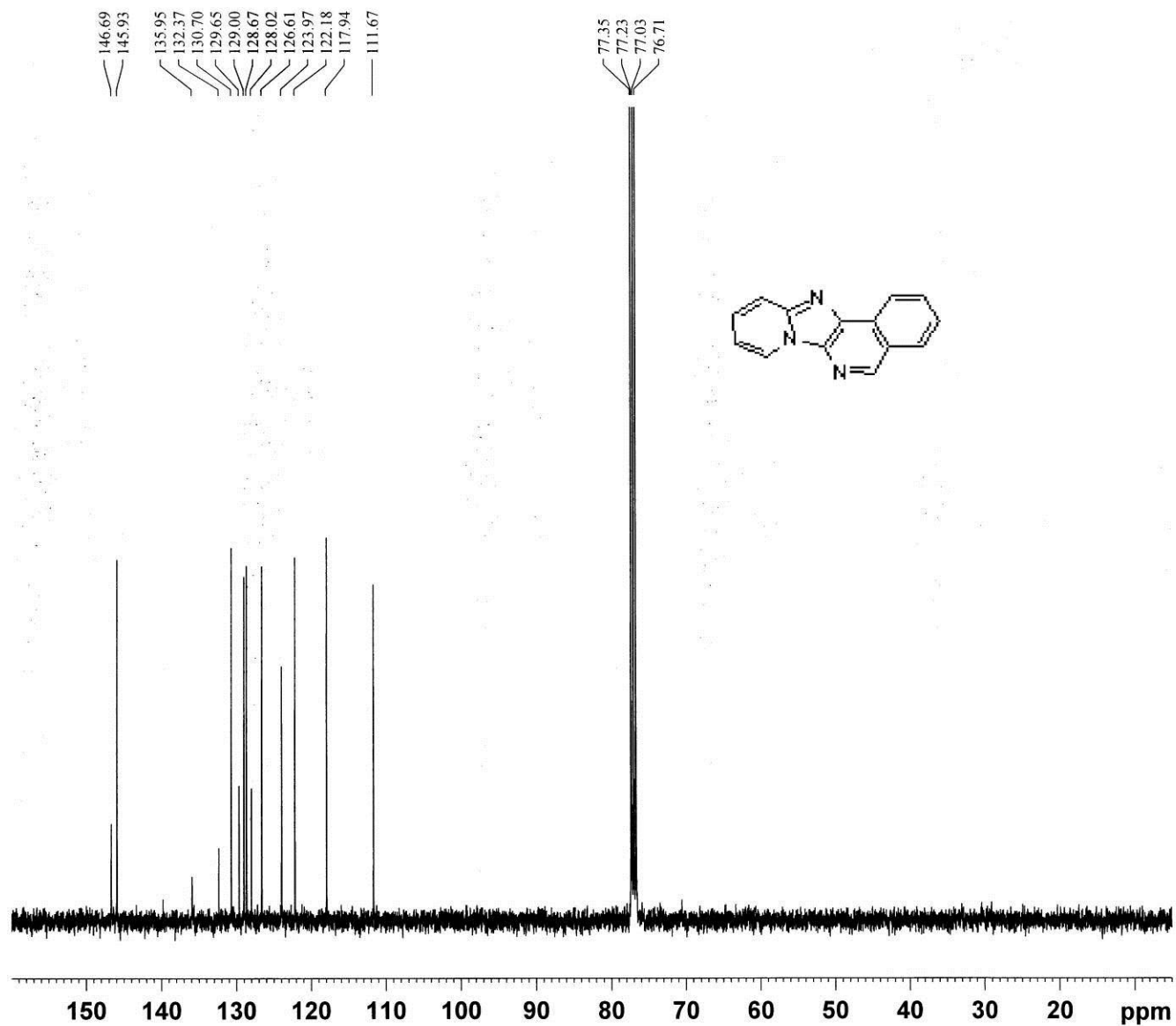


Table 3, entry 6; 7f: ^1H NMR

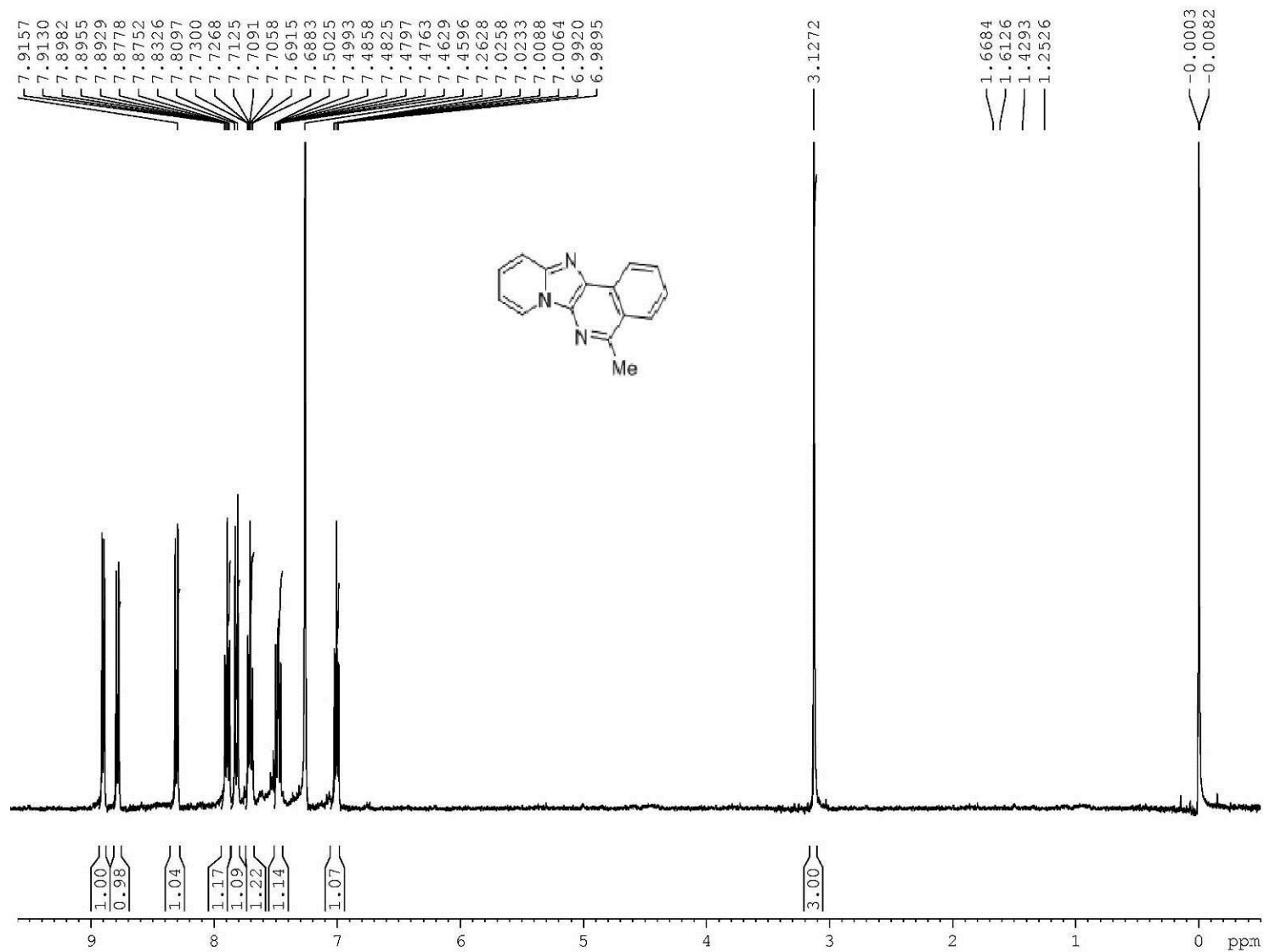


Table 3, entry 6; 7f: ^{13}C NMR

