Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

An eco-friendly Pictet-Spengler approach to pyrrolo- and indolo[1,2-a]quinoxalines using *p*-dodecylbenzenesulfonic acid as an efficient Brønsted acid catalyst

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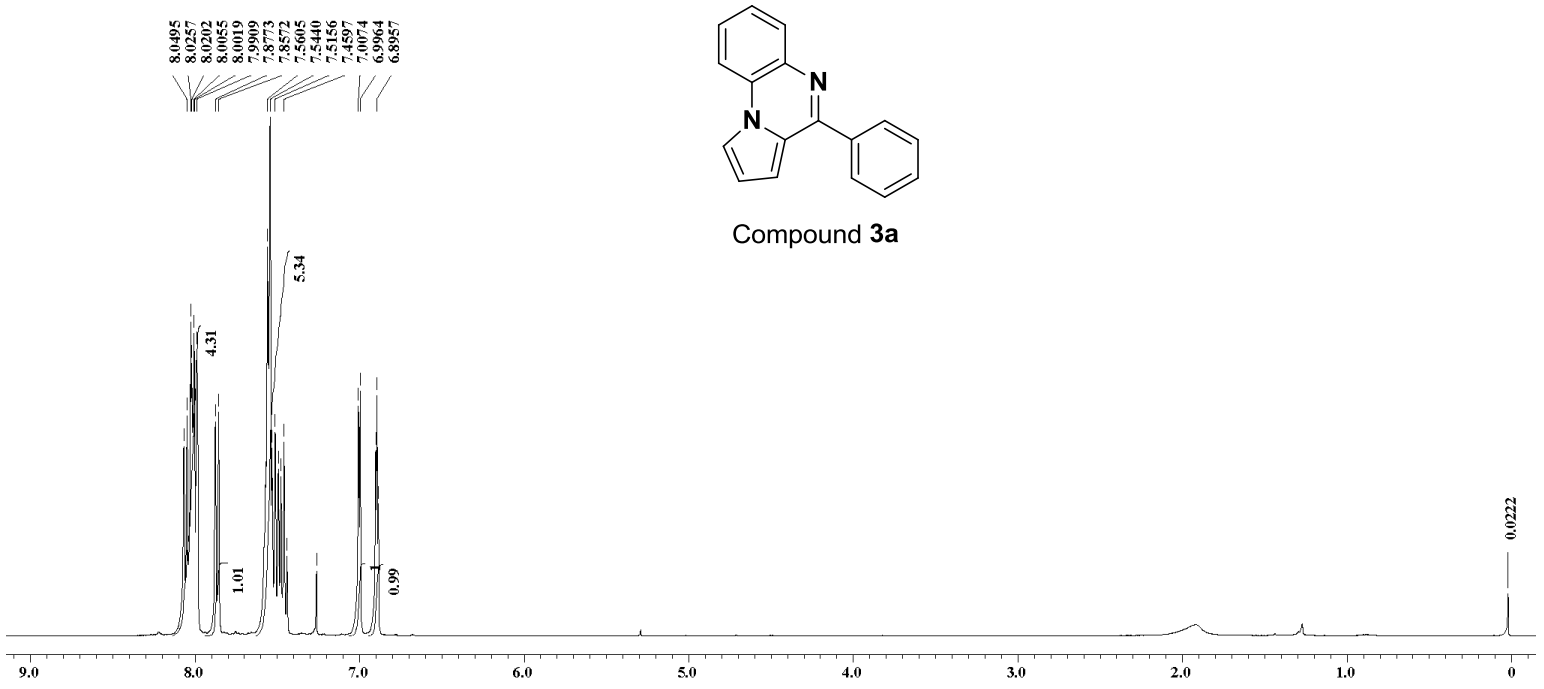


Compound **3a**

Figure 1: ^{1}H NMR spectrum of 3a

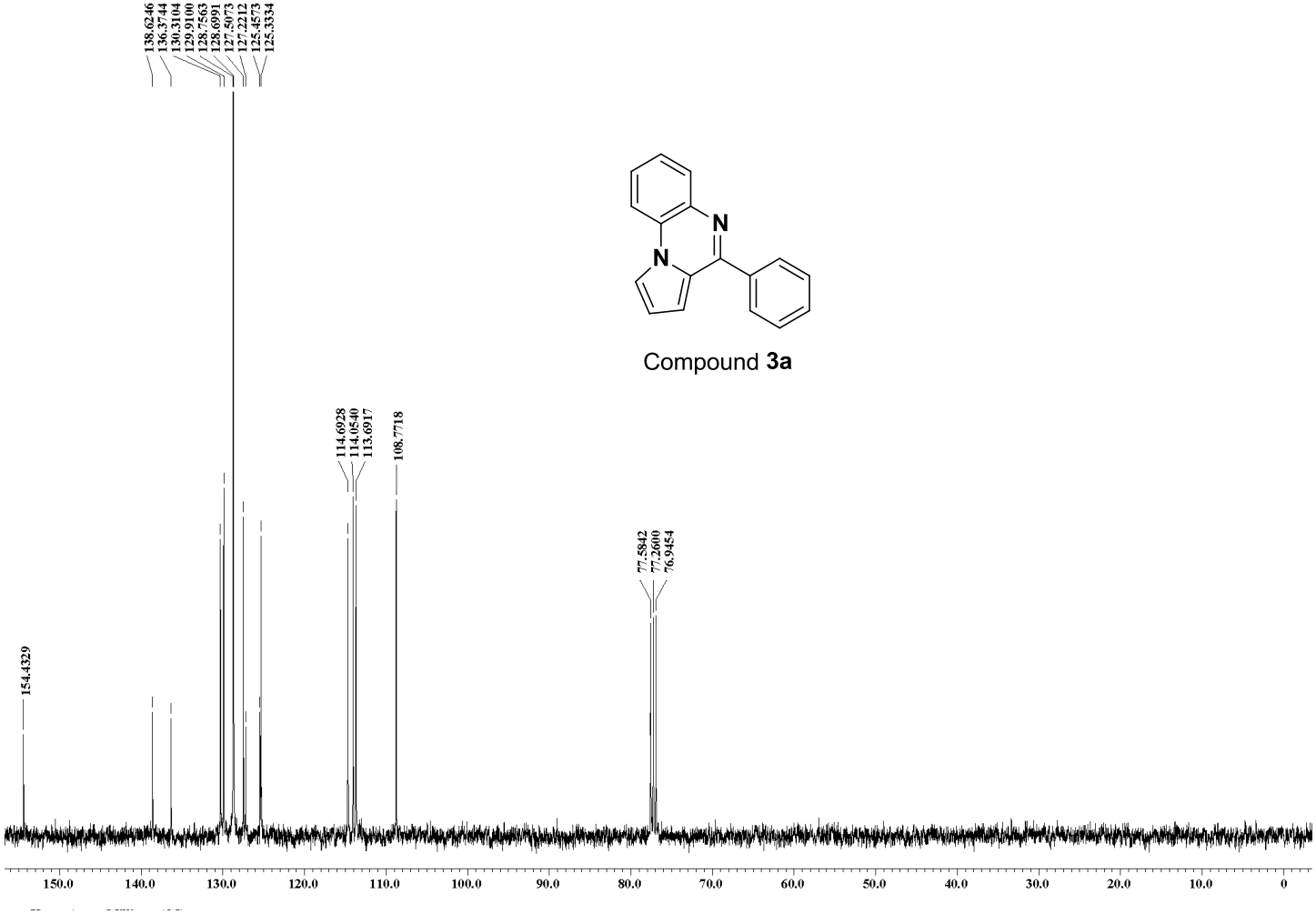


Figure 2: ^{13}C NMR spectrum of 3a

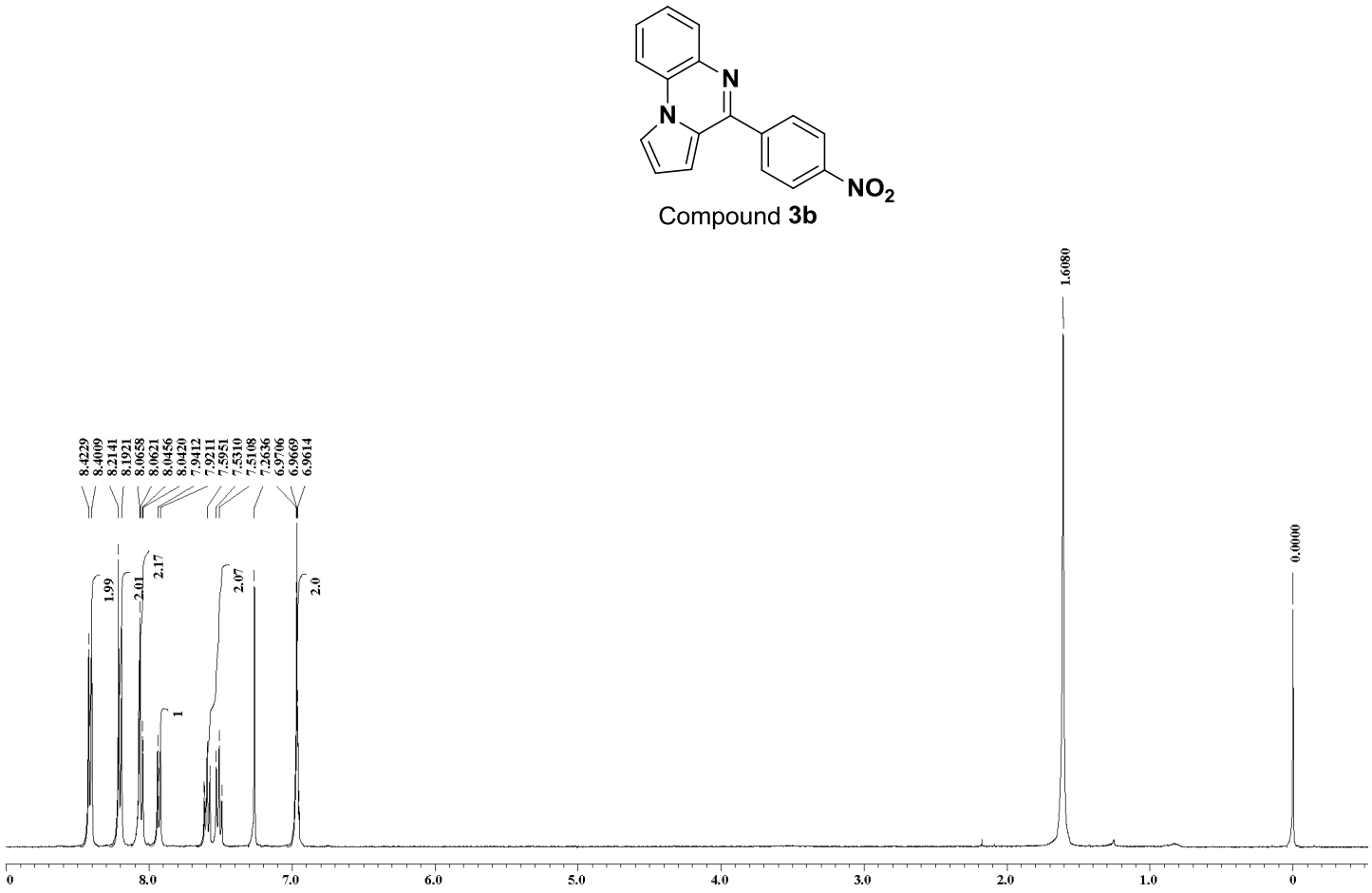


Figure 3: ^{1}H NMR spectrum of 3b

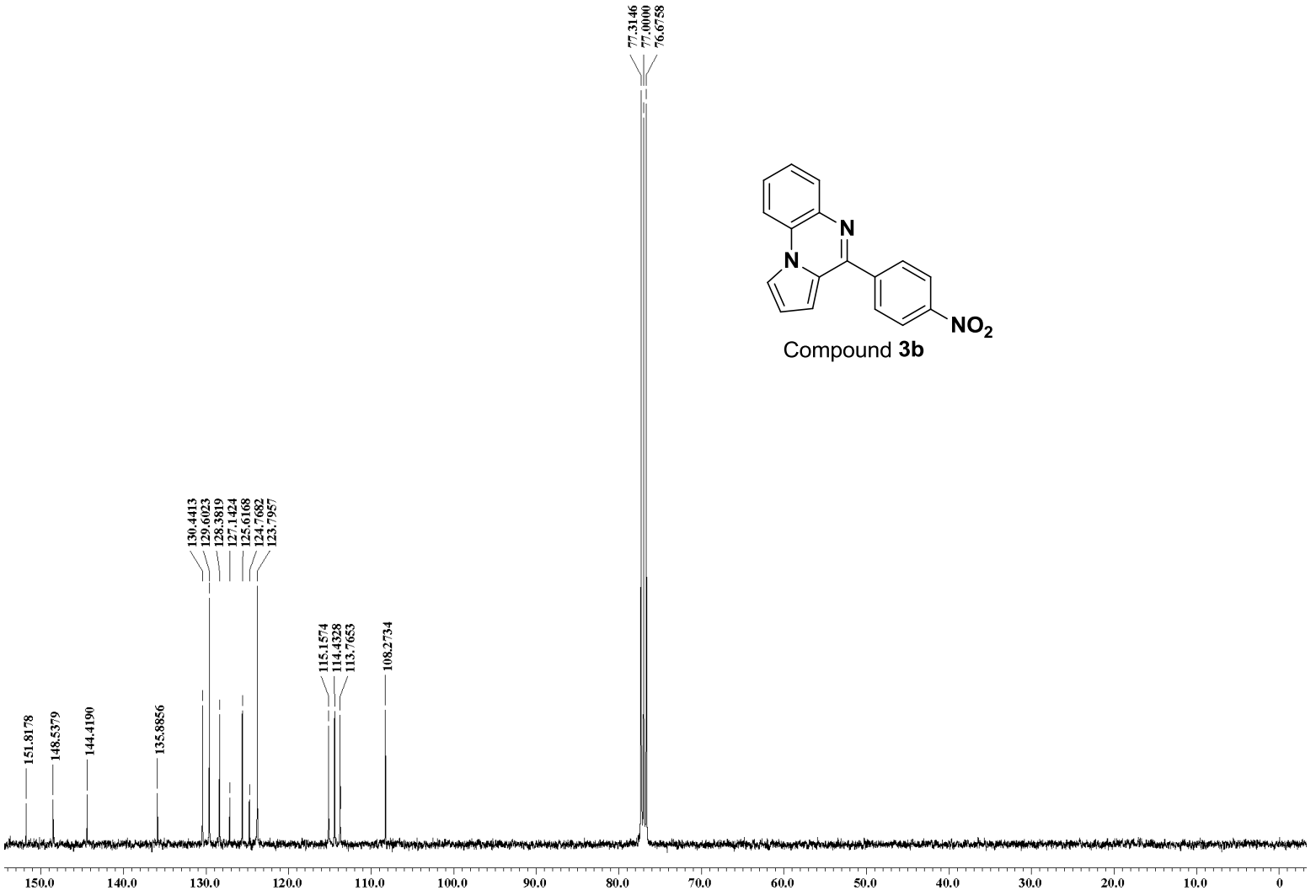
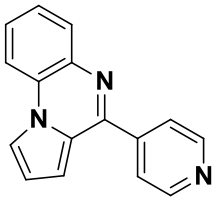


Figure 4: ^{13}C NMR spectrum of 3b



Compound **3c**

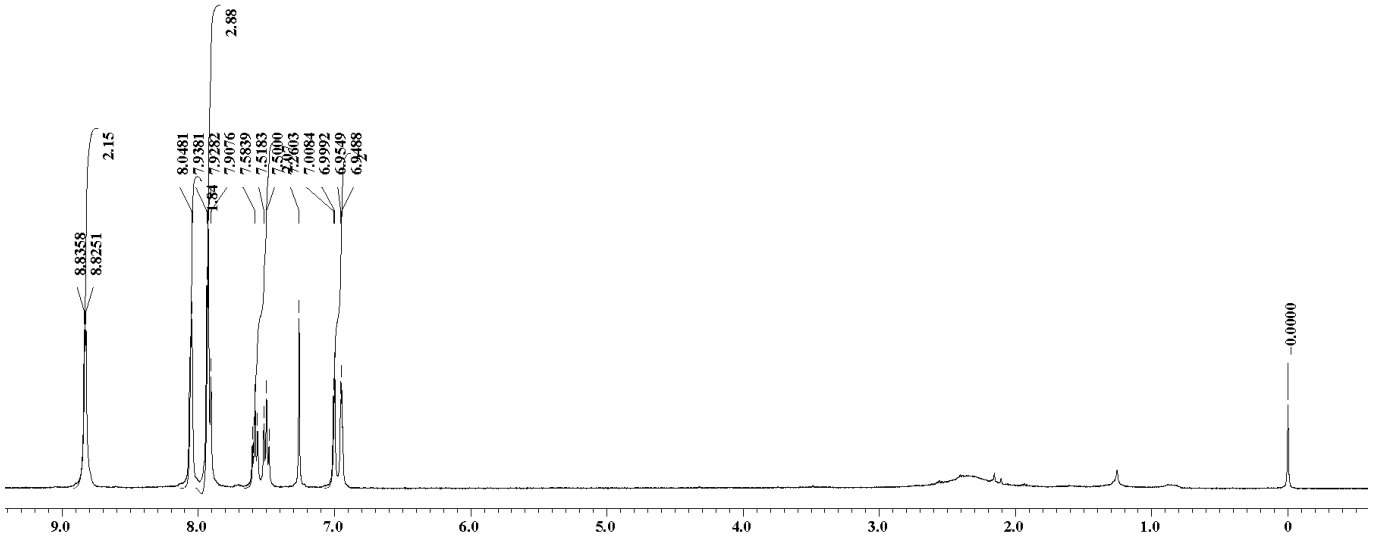


Figure 5: ^{1}H NMR spectrum of 3c

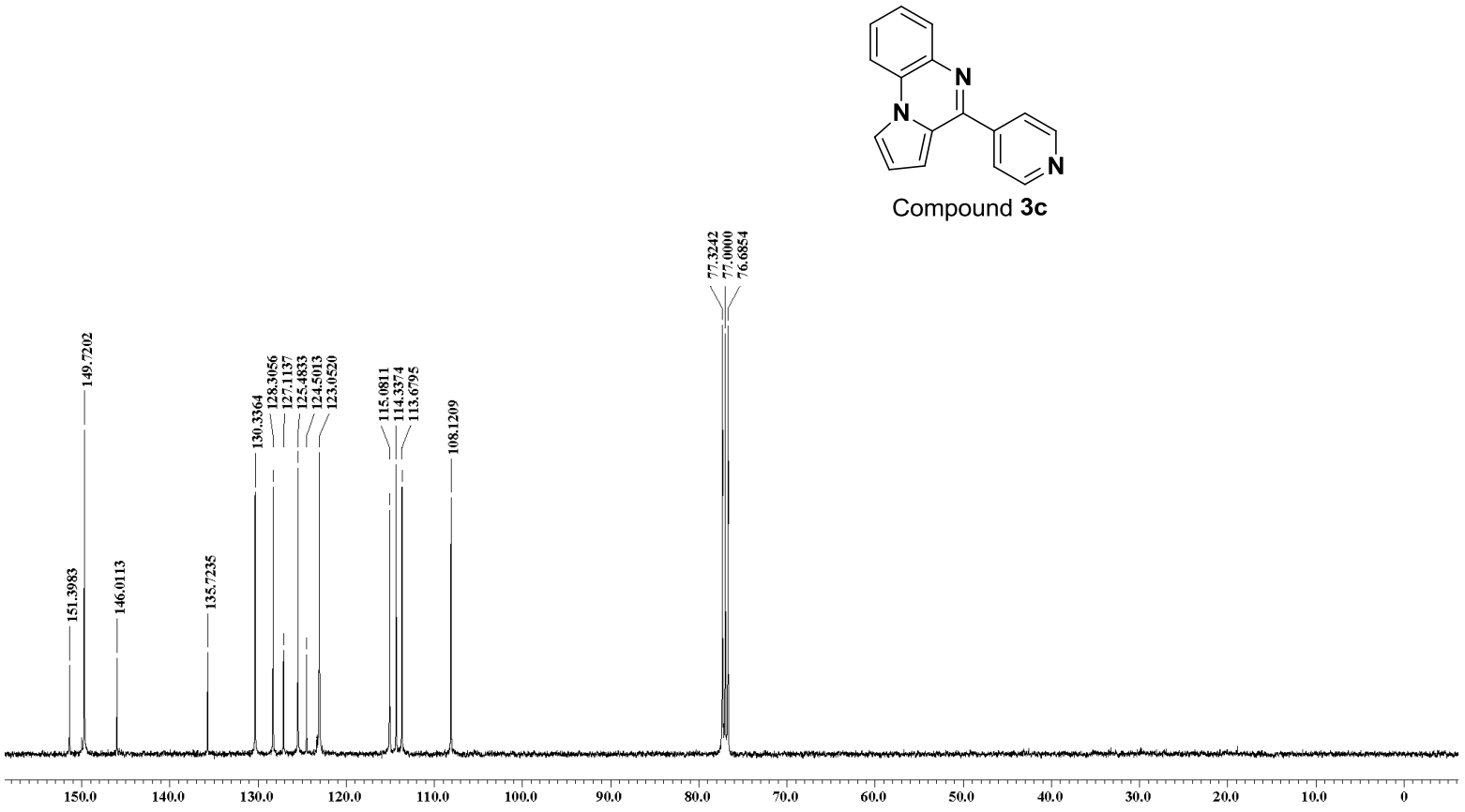
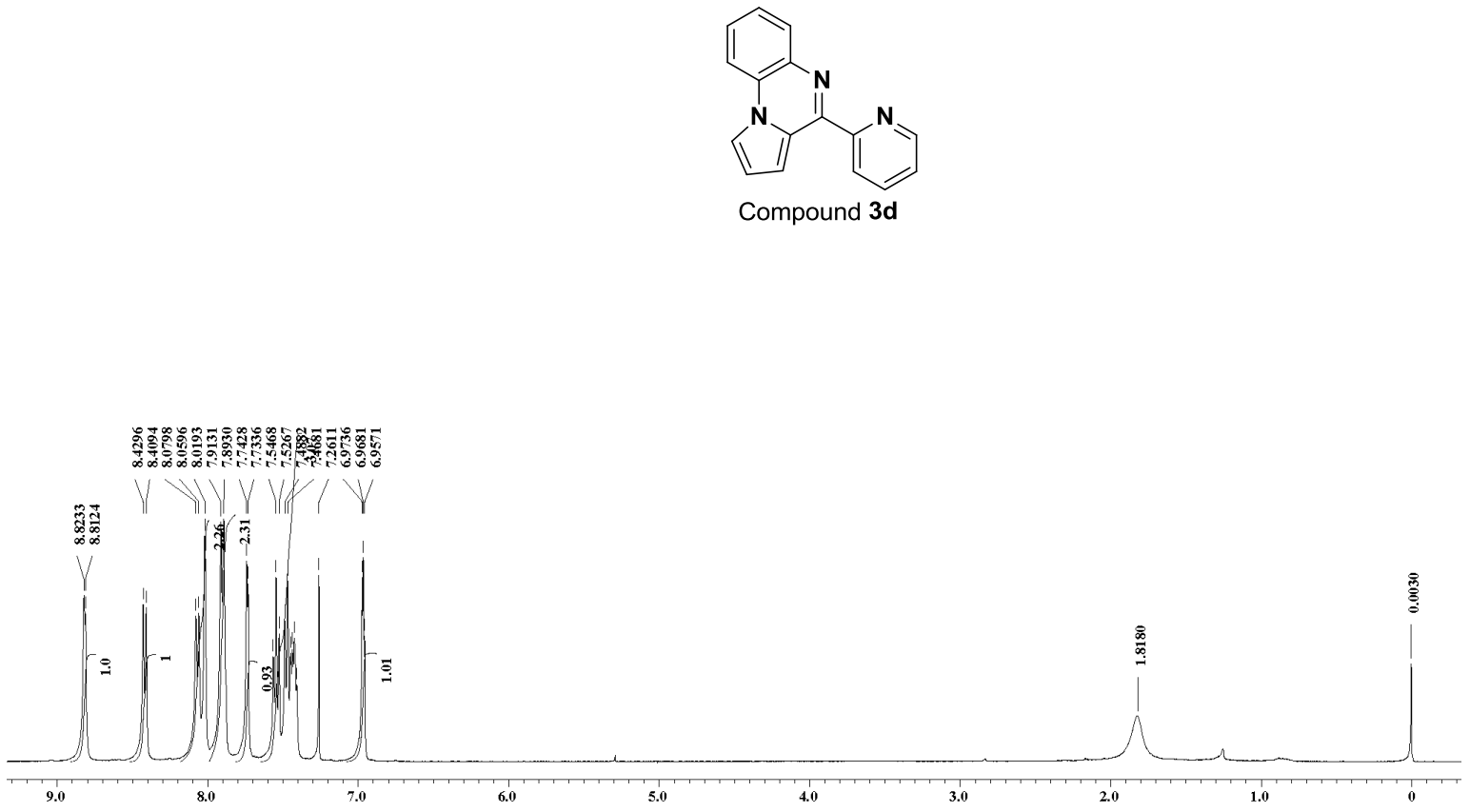


Figure 6: ^{13}C NMR spectrum of 3c



Compound **3d**

Figure 7: ^{1}H NMR spectrum of 3d

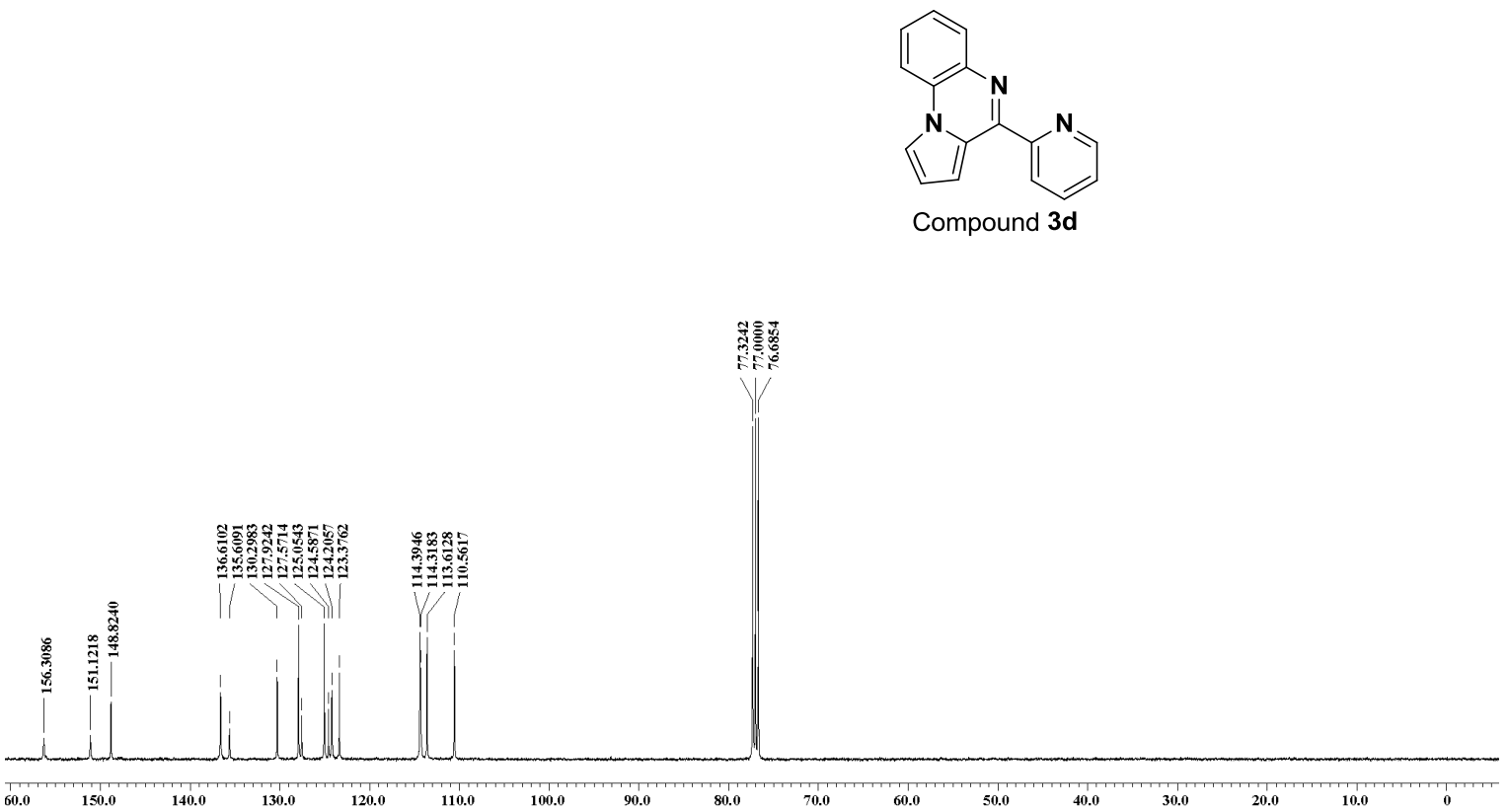


Figure 8: ^{13}C NMR spectrum of 3d

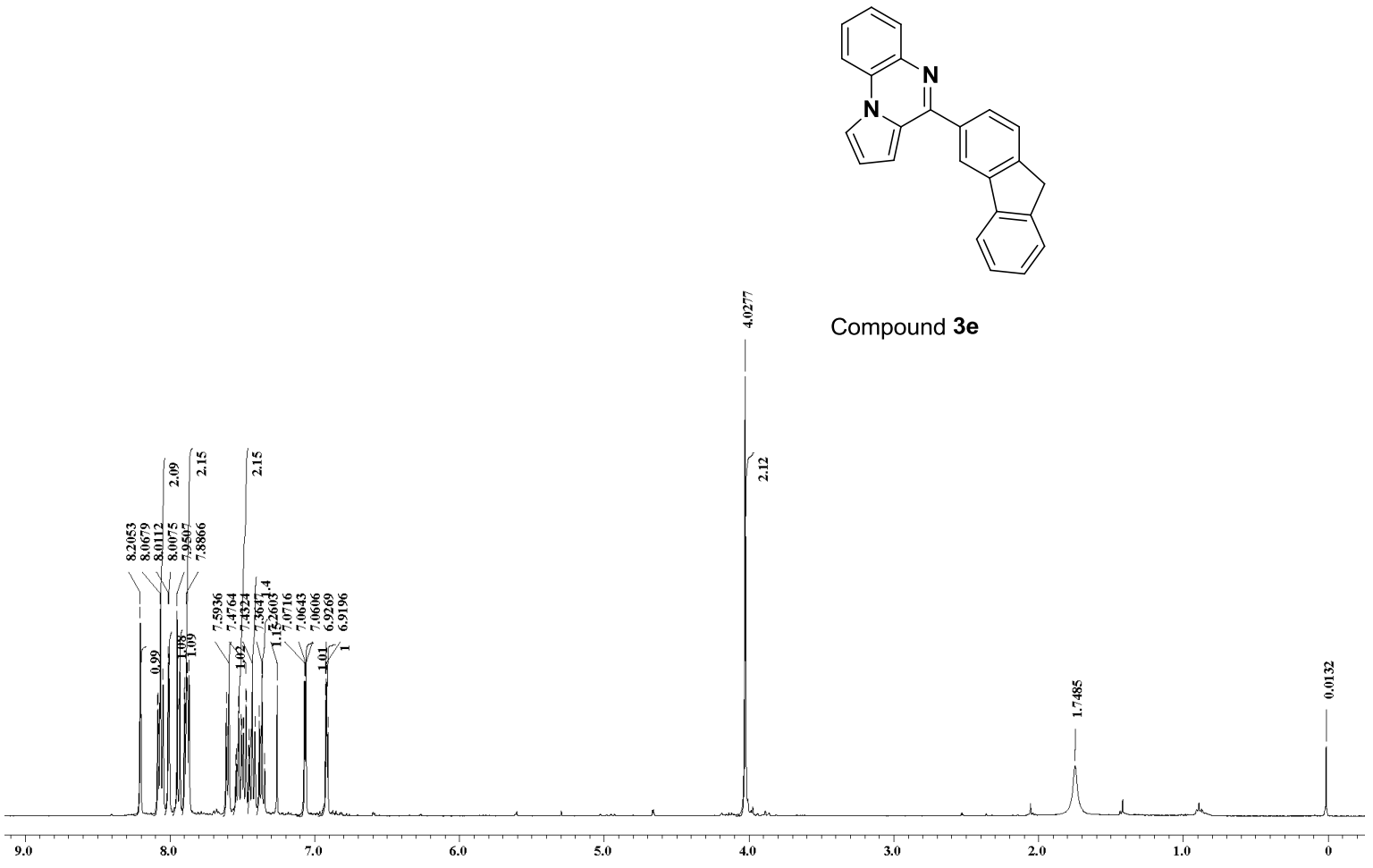


Figure 9: ^{1}H NMR spectrum of 3e

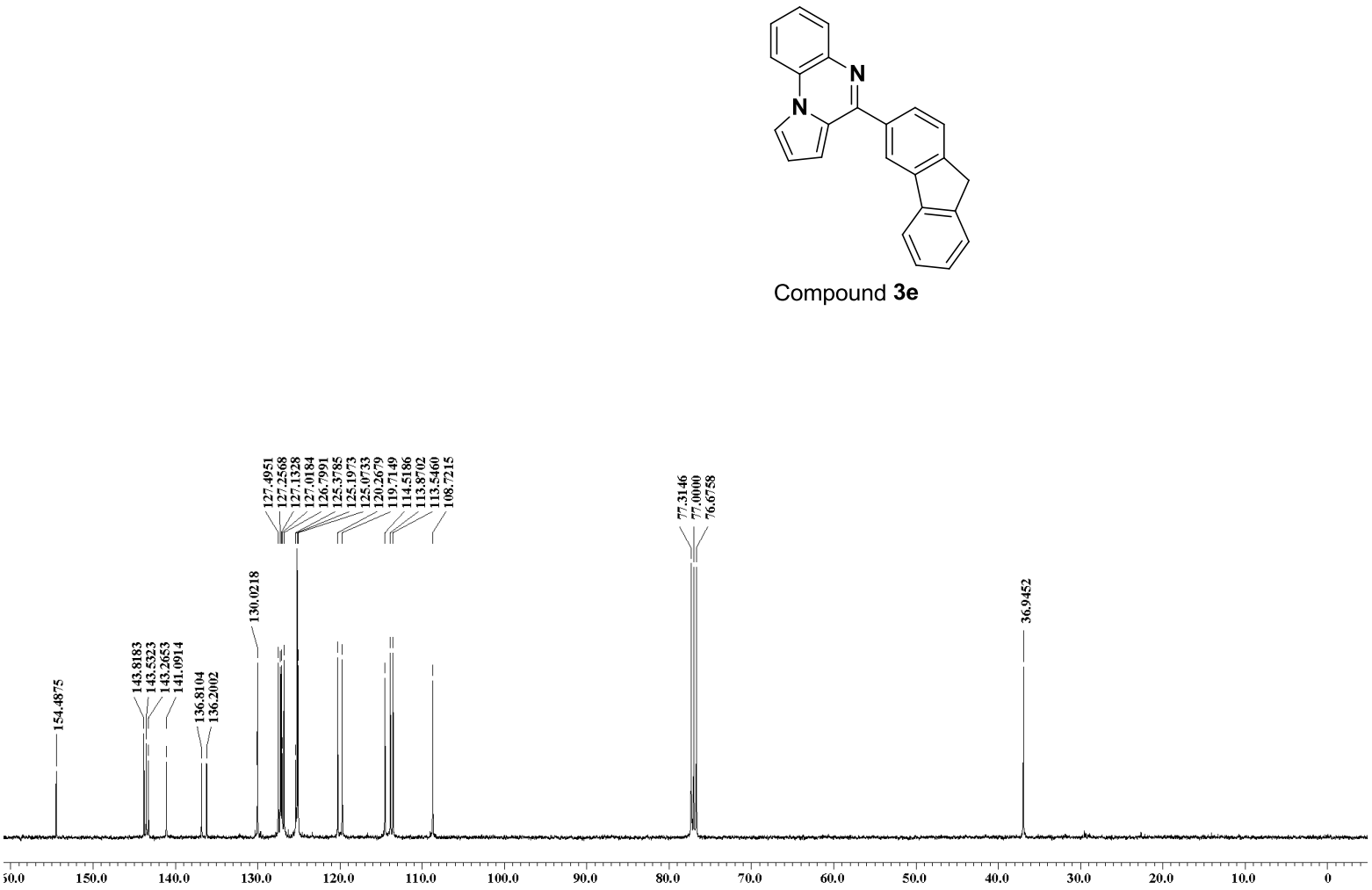
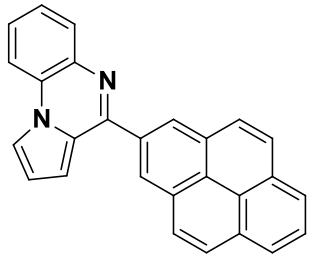


Figure 10: ^{13}C NMR spectrum of 3e



Compound **3f**

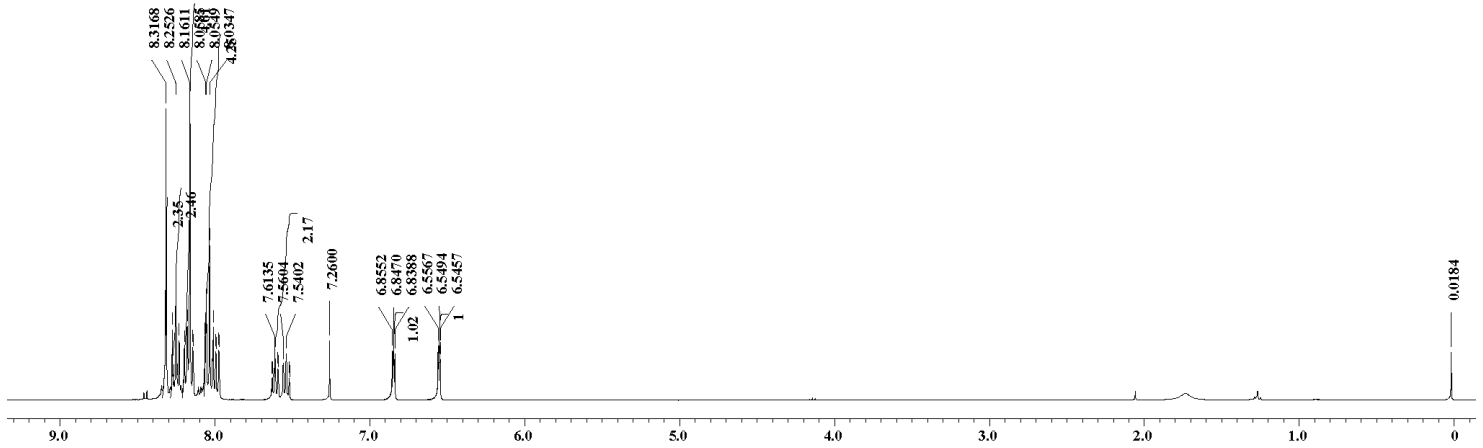


Figure 11: ^{1}H NMR spectrum of 3f

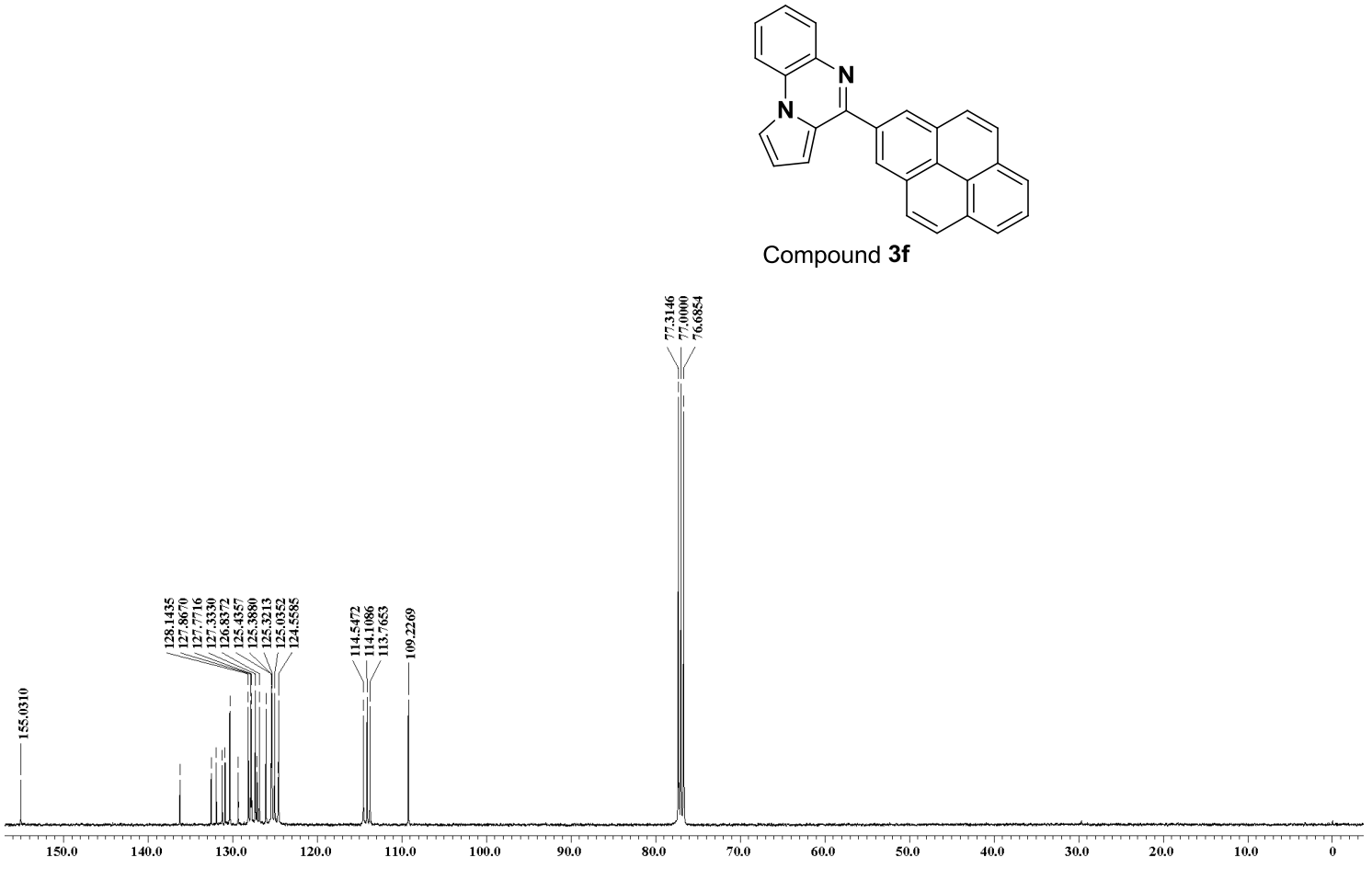
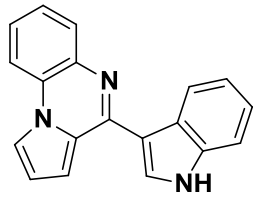


Figure 12: ^{13}C NMR spectrum of 3f



Compound **3g**

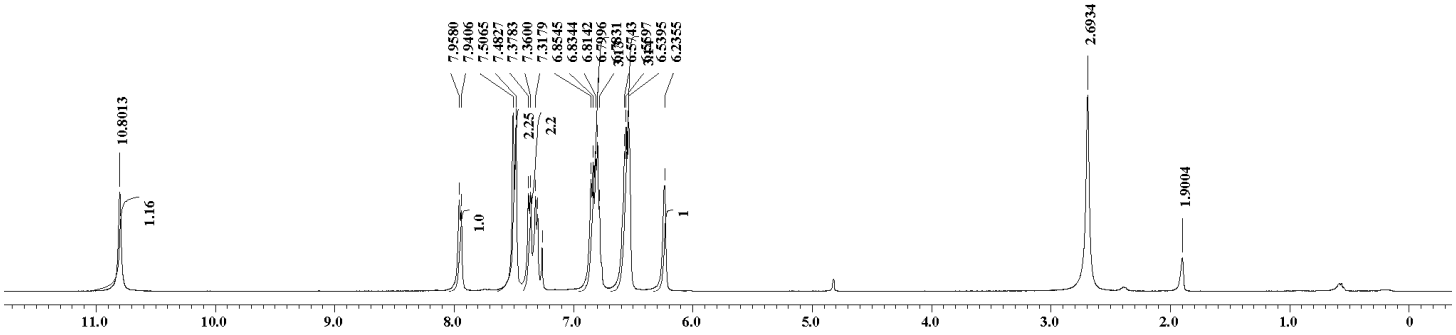


Figure 13: ^{1}H NMR spectrum of 3g

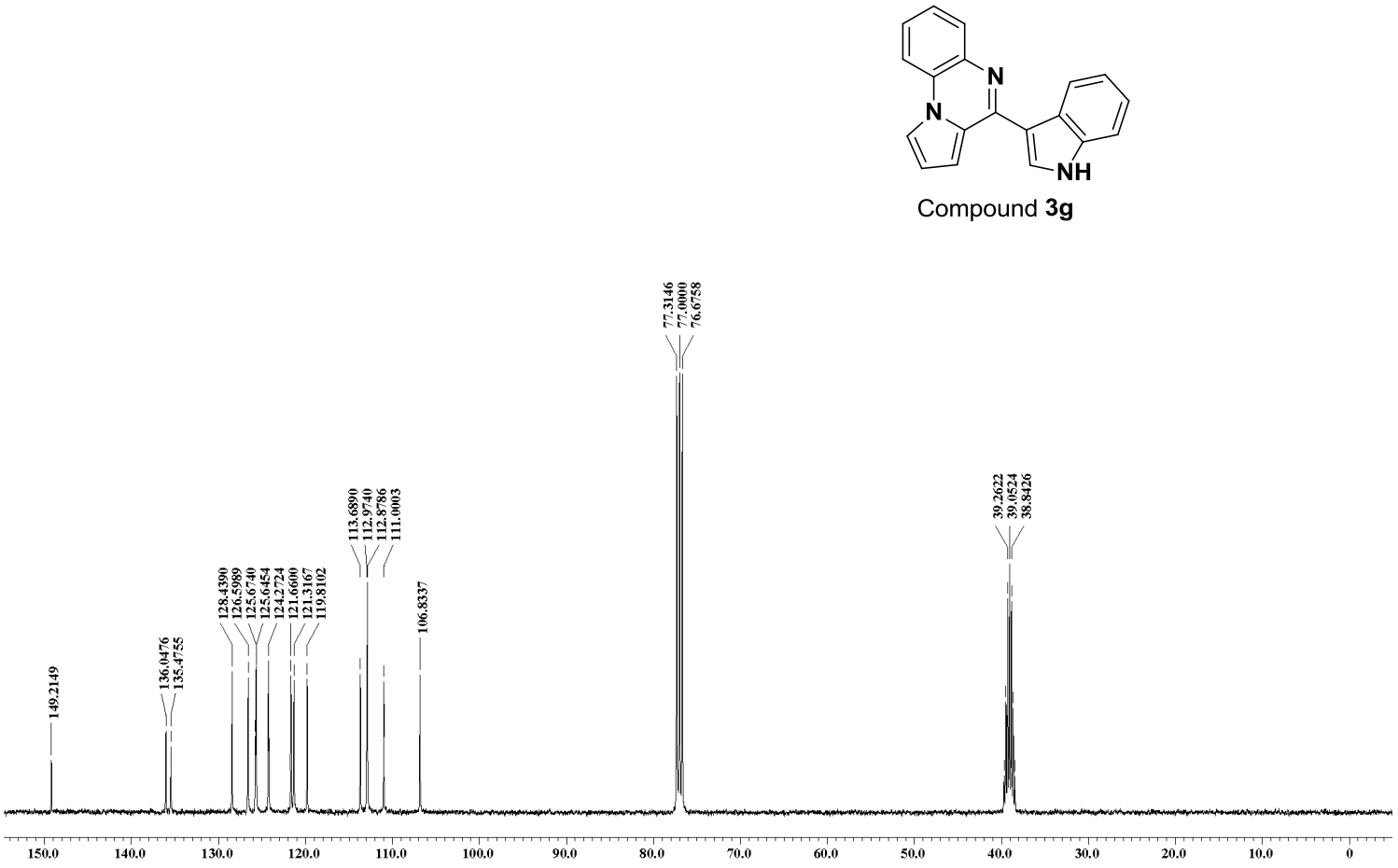


Figure 14: ^{13}C NMR spectrum of 3g

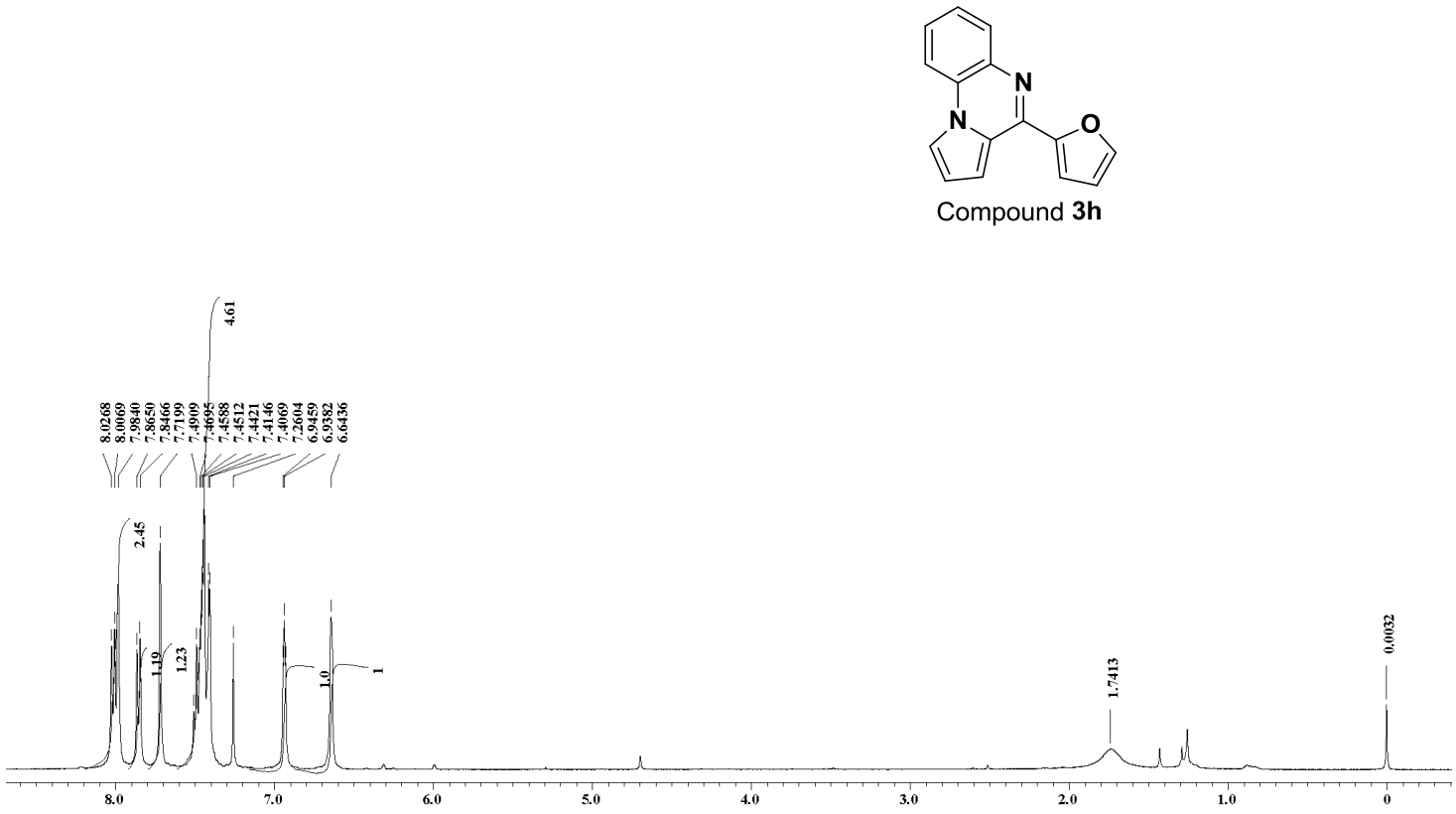
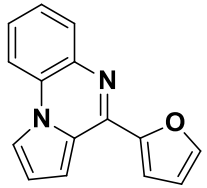


Figure 15: ^{1}H NMR spectrum of 3h



Compound **3h**

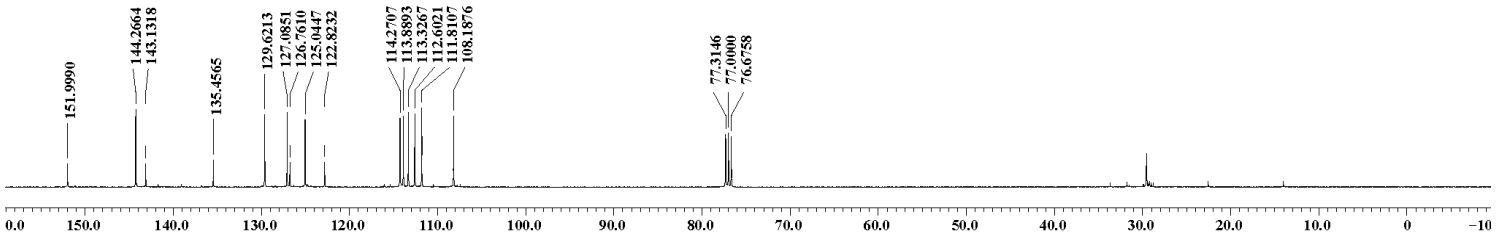
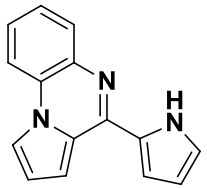


Figure 16: ^{13}C NMR spectrum of 3h



Compound **3i**

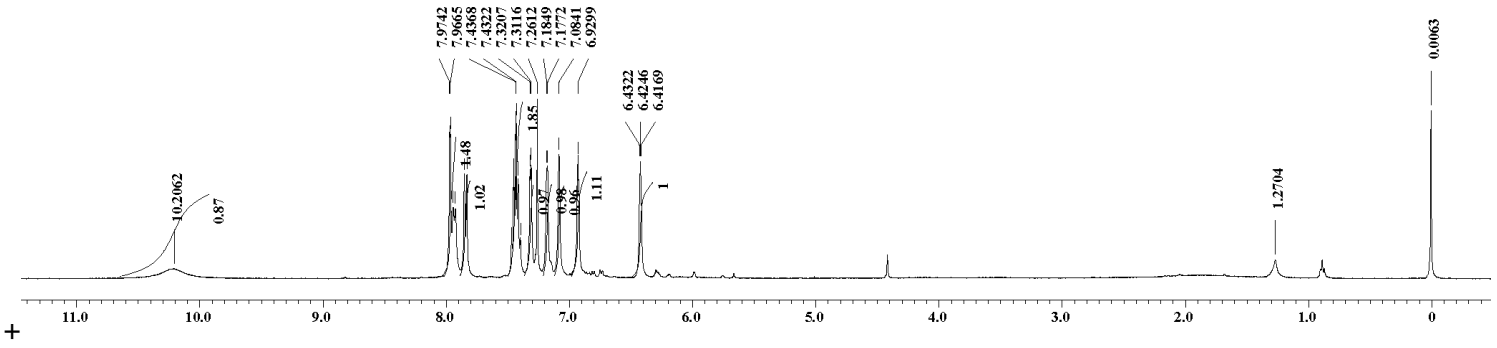


Figure 17: ^{1}H NMR spectrum of 3i

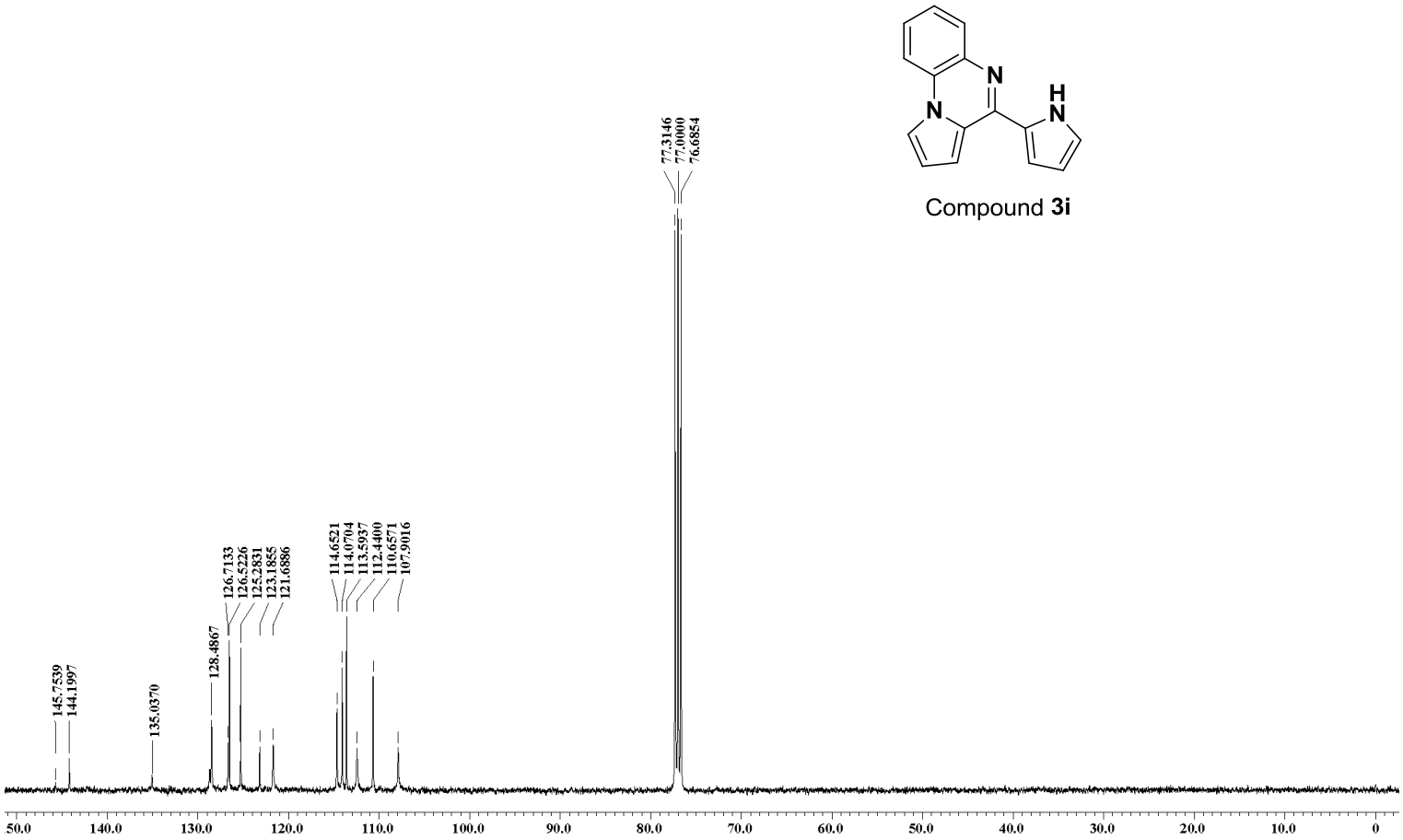


Figure 18: ^{13}C NMR spectrum of 3i

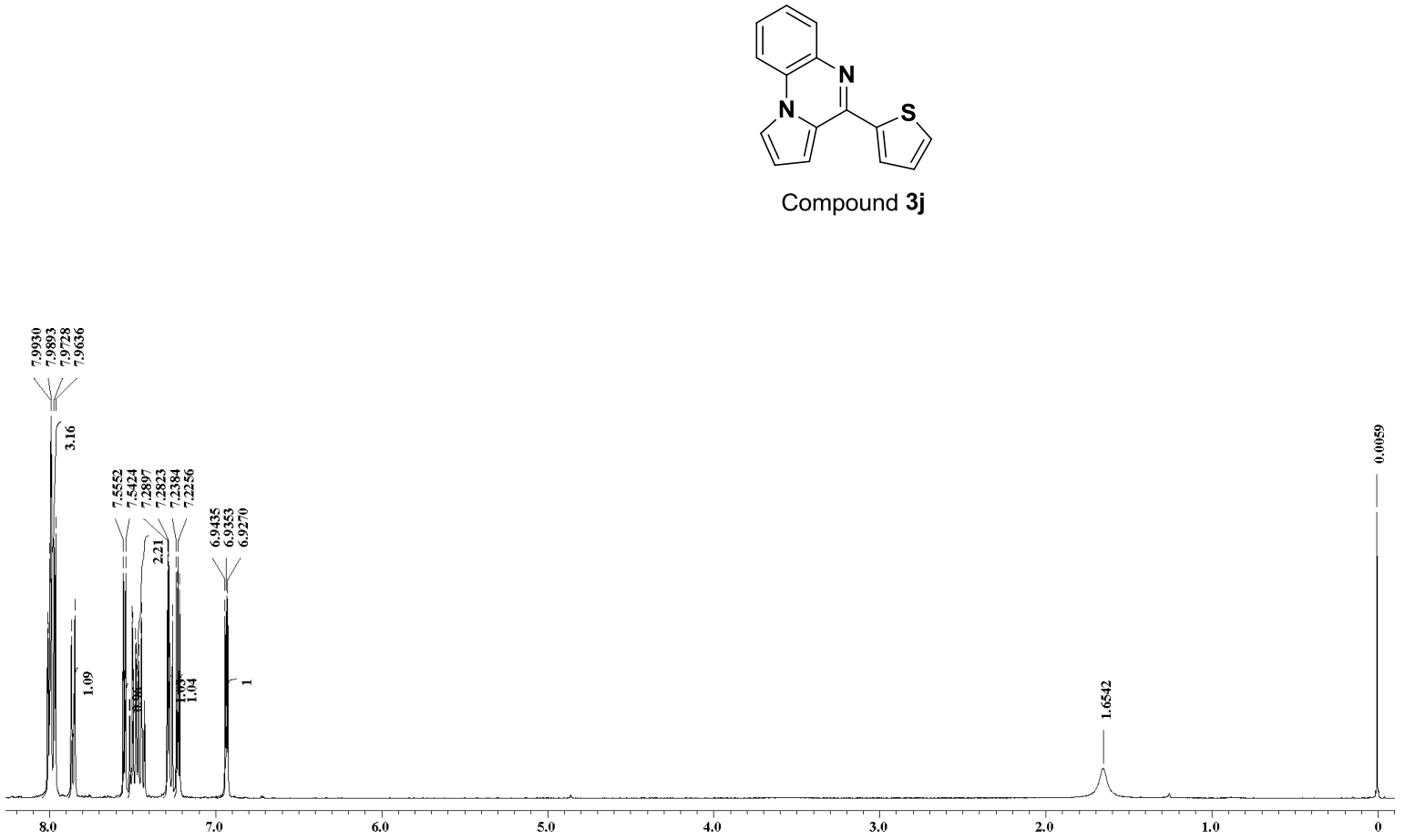


Figure 19: ^{1}H NMR spectrum of 3j

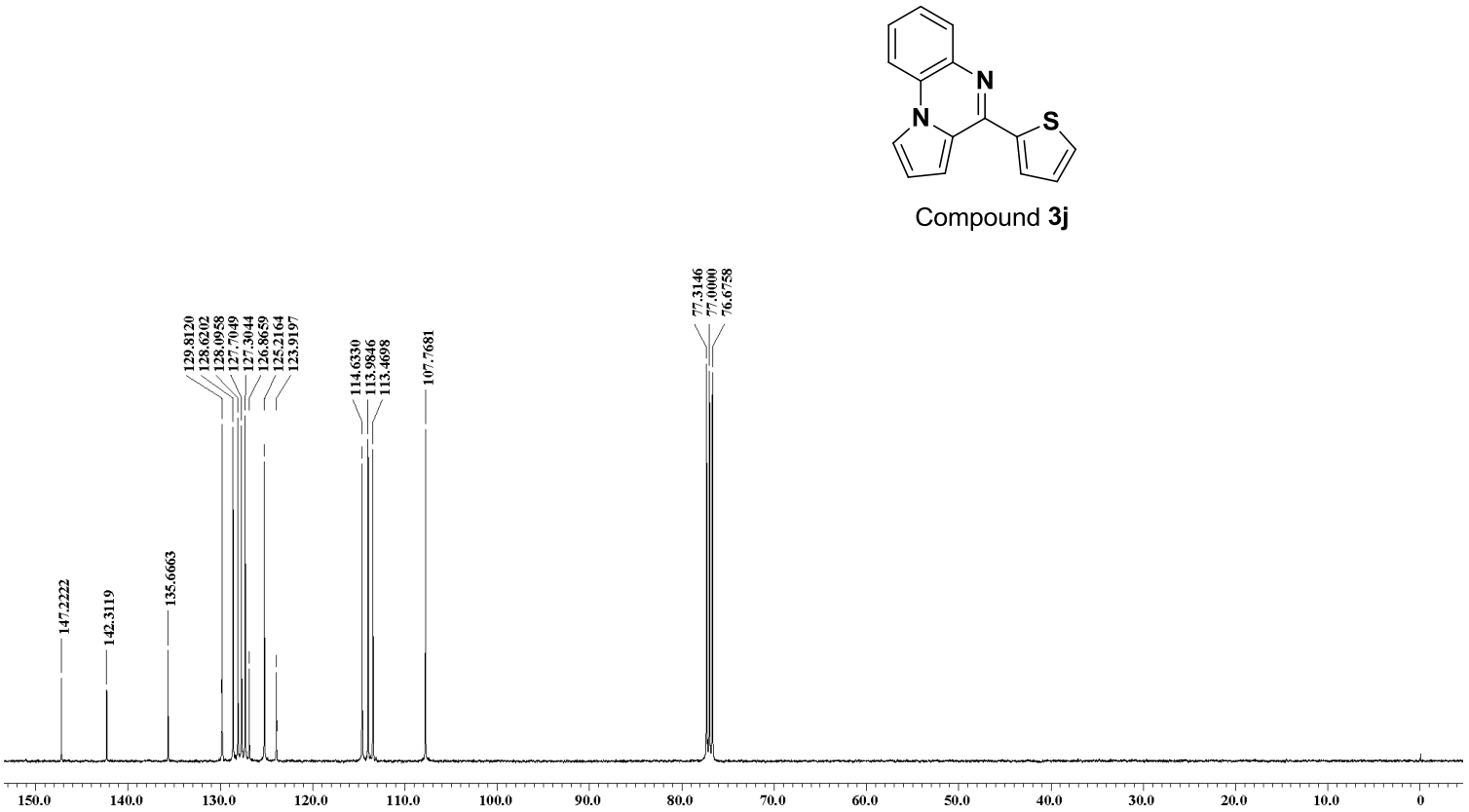


Figure 20: ^{13}C NMR spectrum of 3j

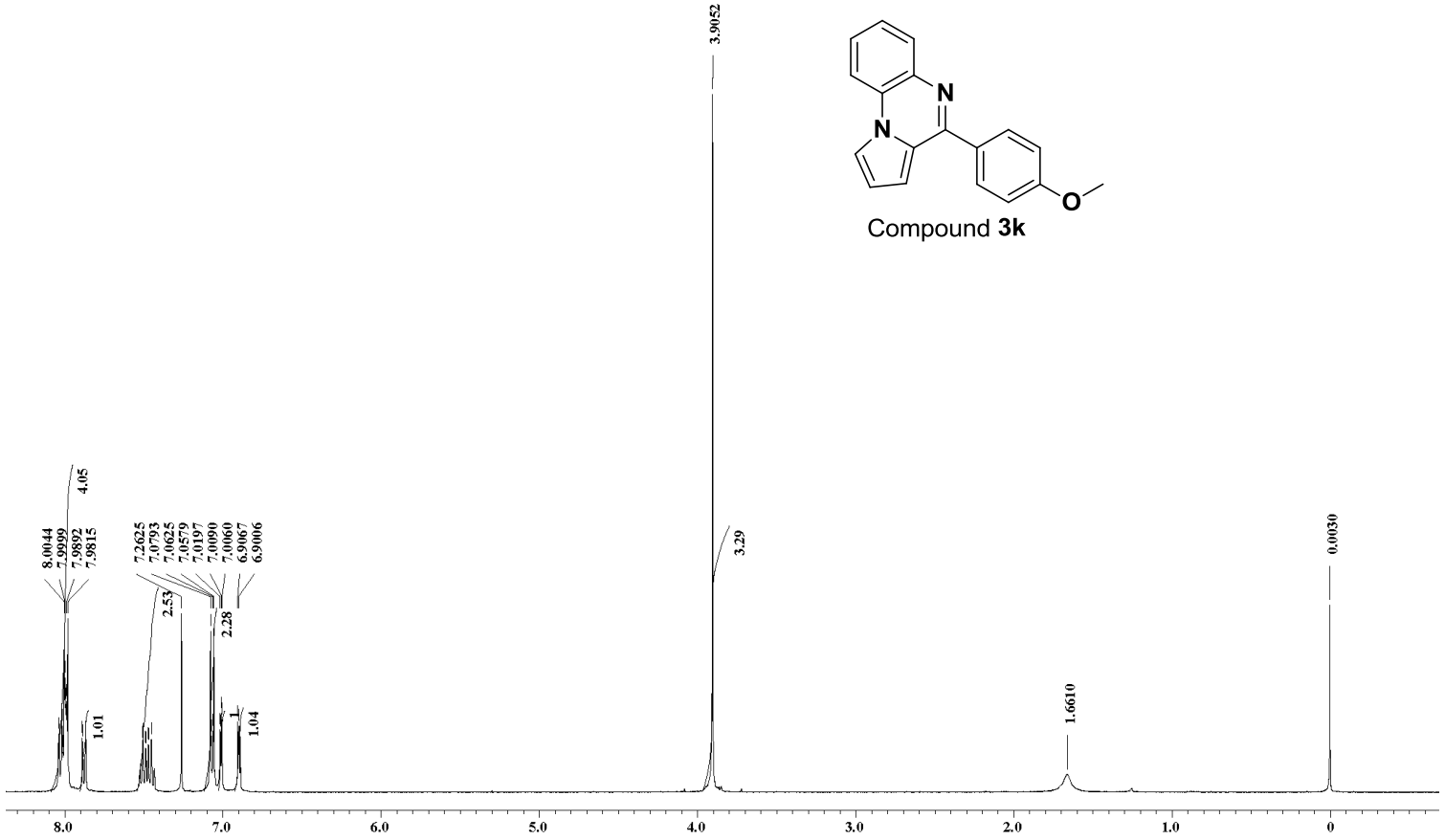


Figure 21: ^{1}H NMR spectrum of 3k

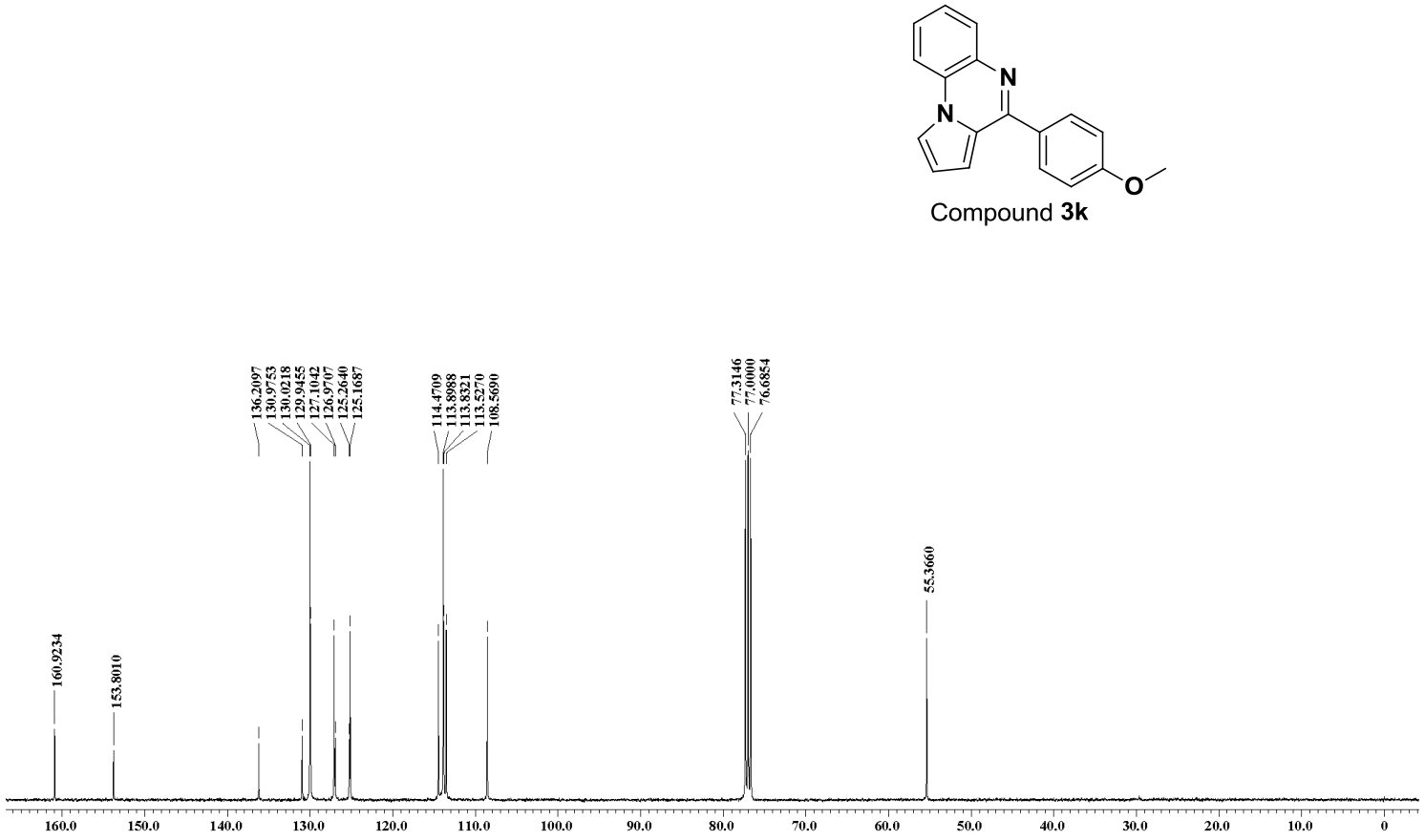


Figure 22: ^{13}C NMR spectrum of 3k

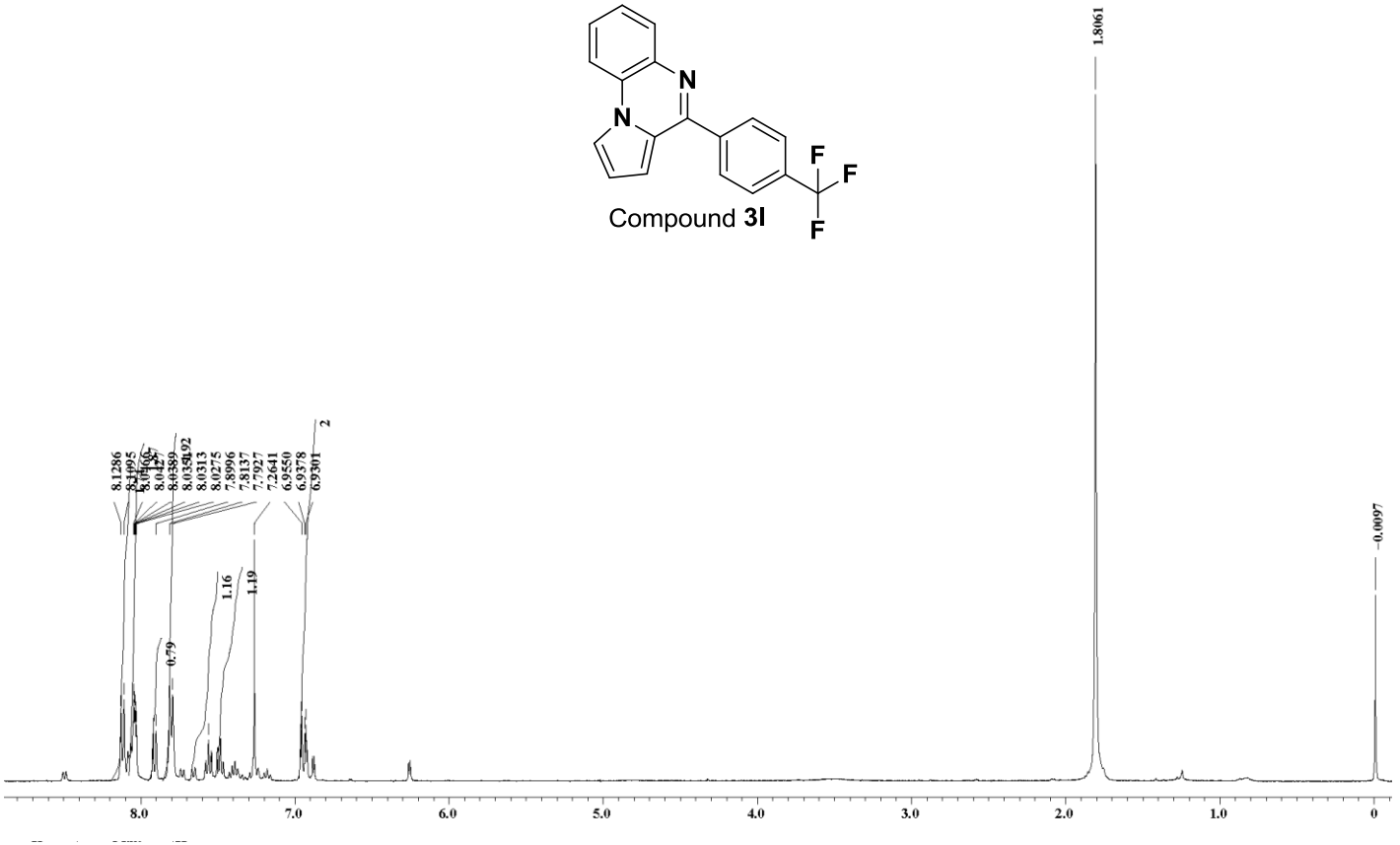


Figure 23: ^{1}H NMR spectrum of 3l

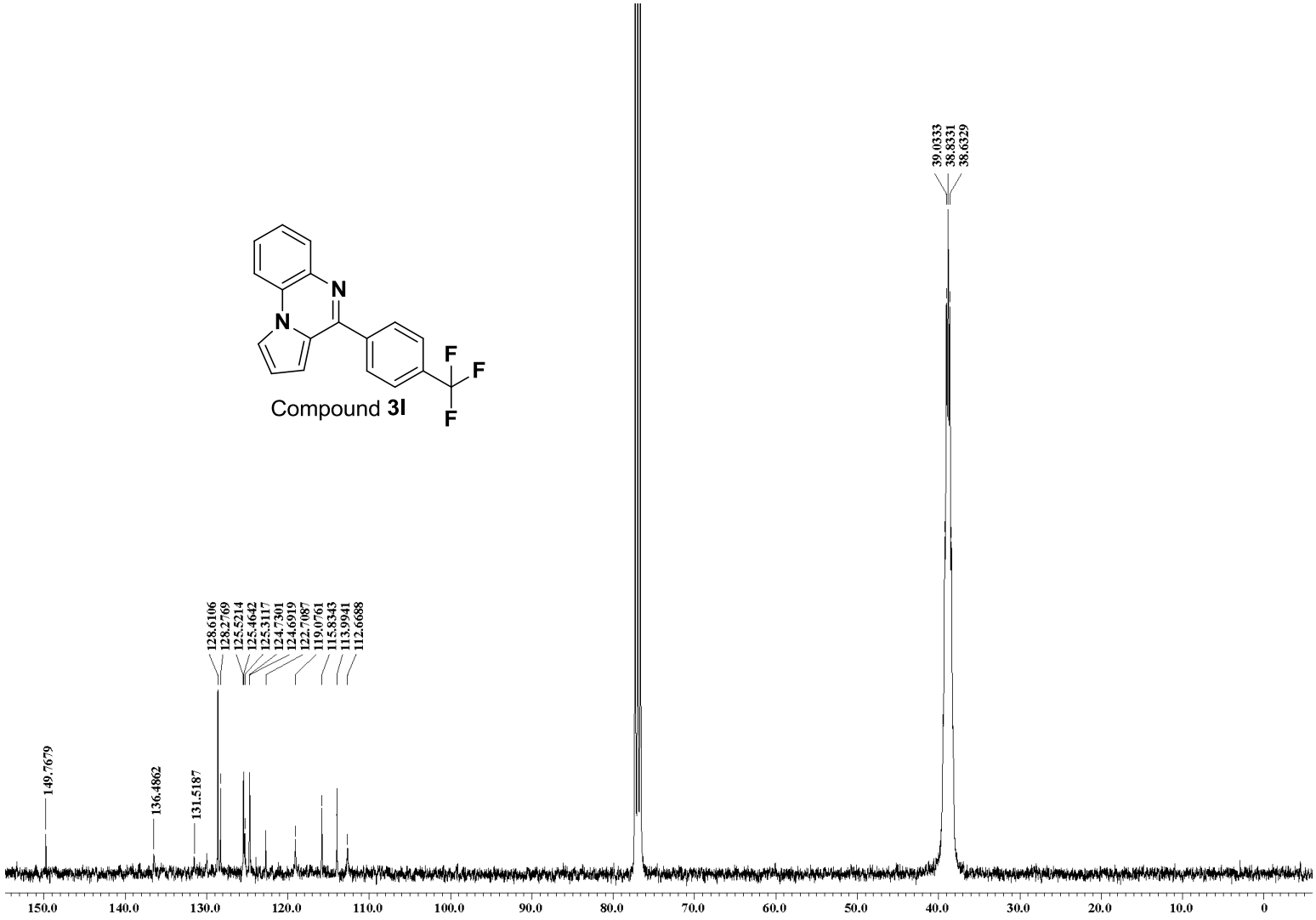
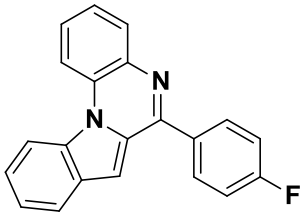


Figure 24: ^{13}C NMR spectrum of 3l



Compound **3m**

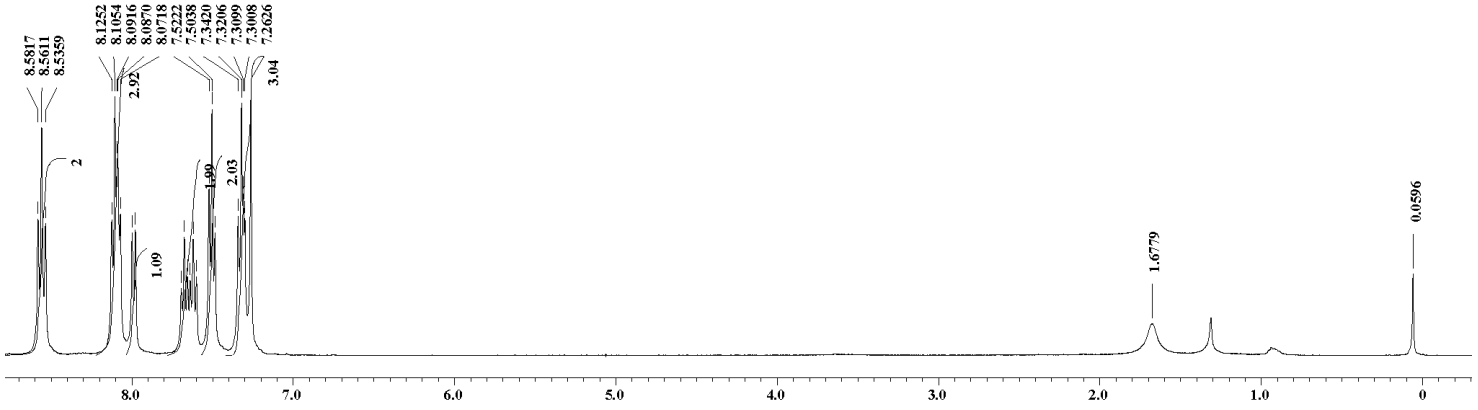


Figure 25: ^{1}H NMR spectrum of 3m

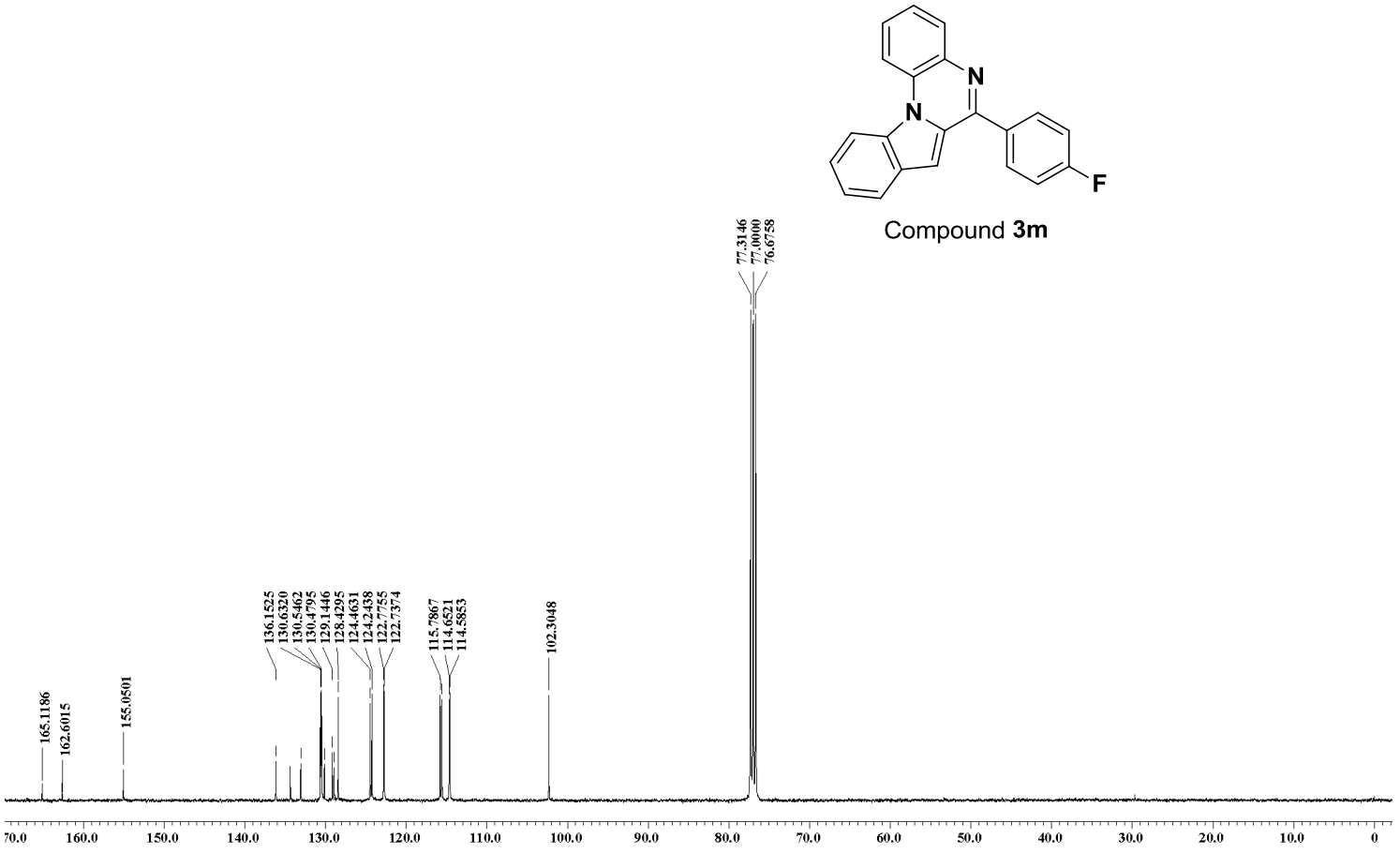


Figure 26: ^{13}C NMR spectrum of 3m

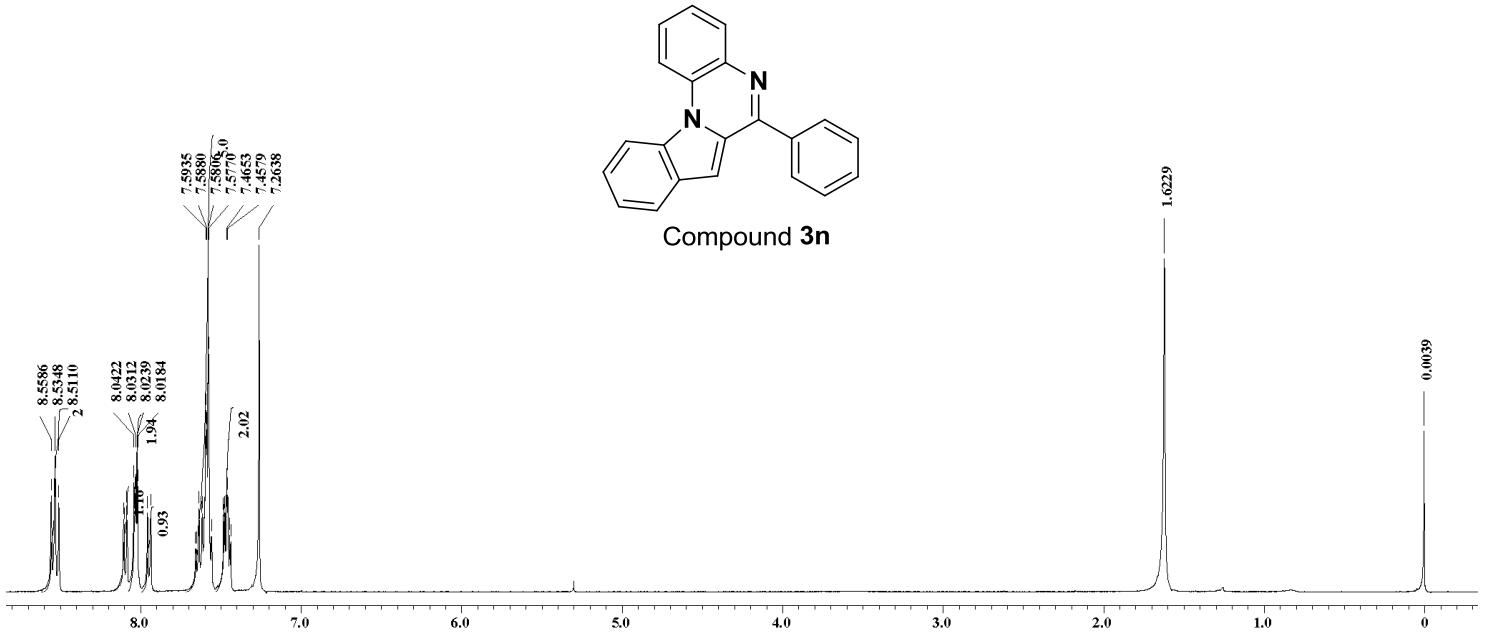


Figure 27: ^{1}H NMR spectrum of 3n

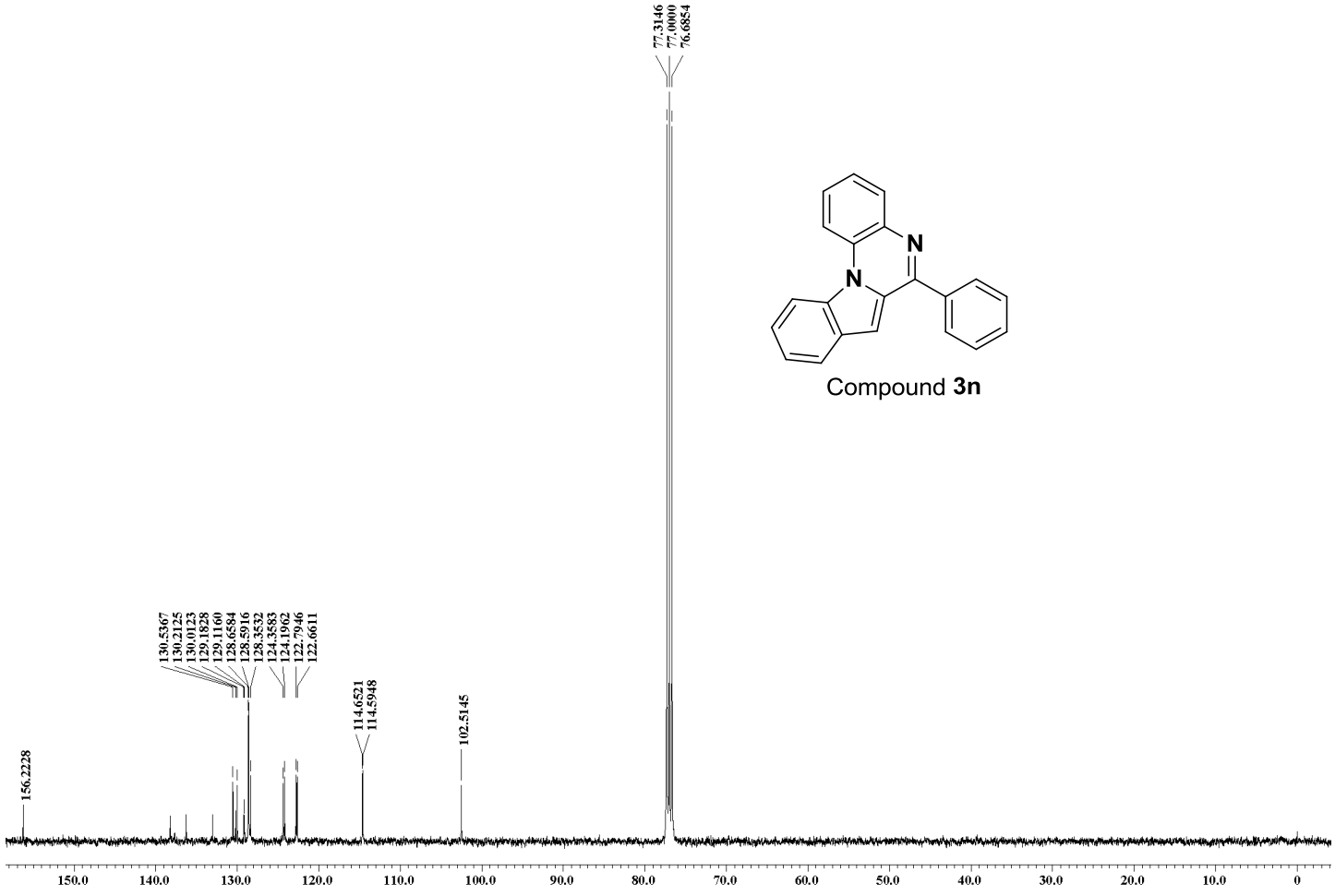


Figure 28: ^{13}C NMR spectrum of 3n

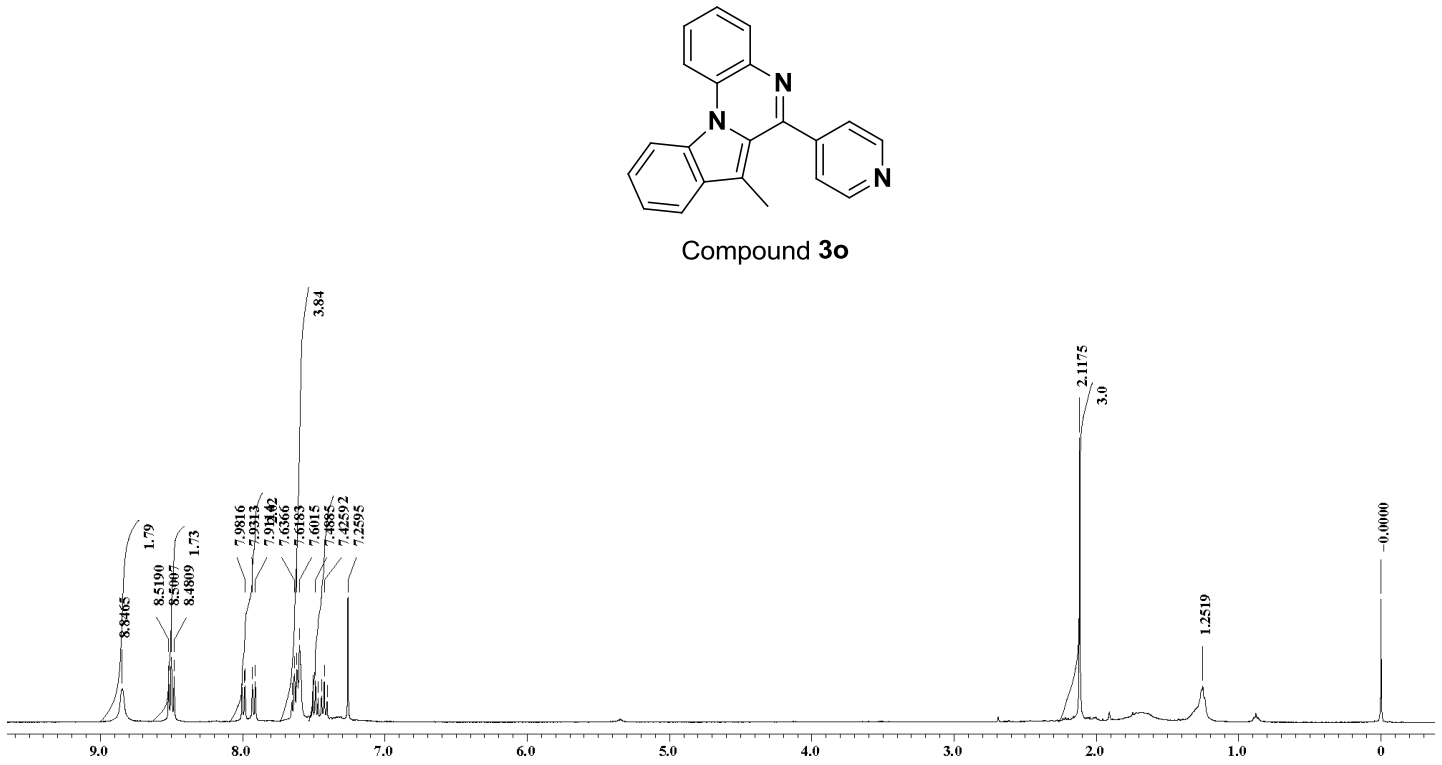


Figure 29: ^{1}H NMR spectrum of 3o

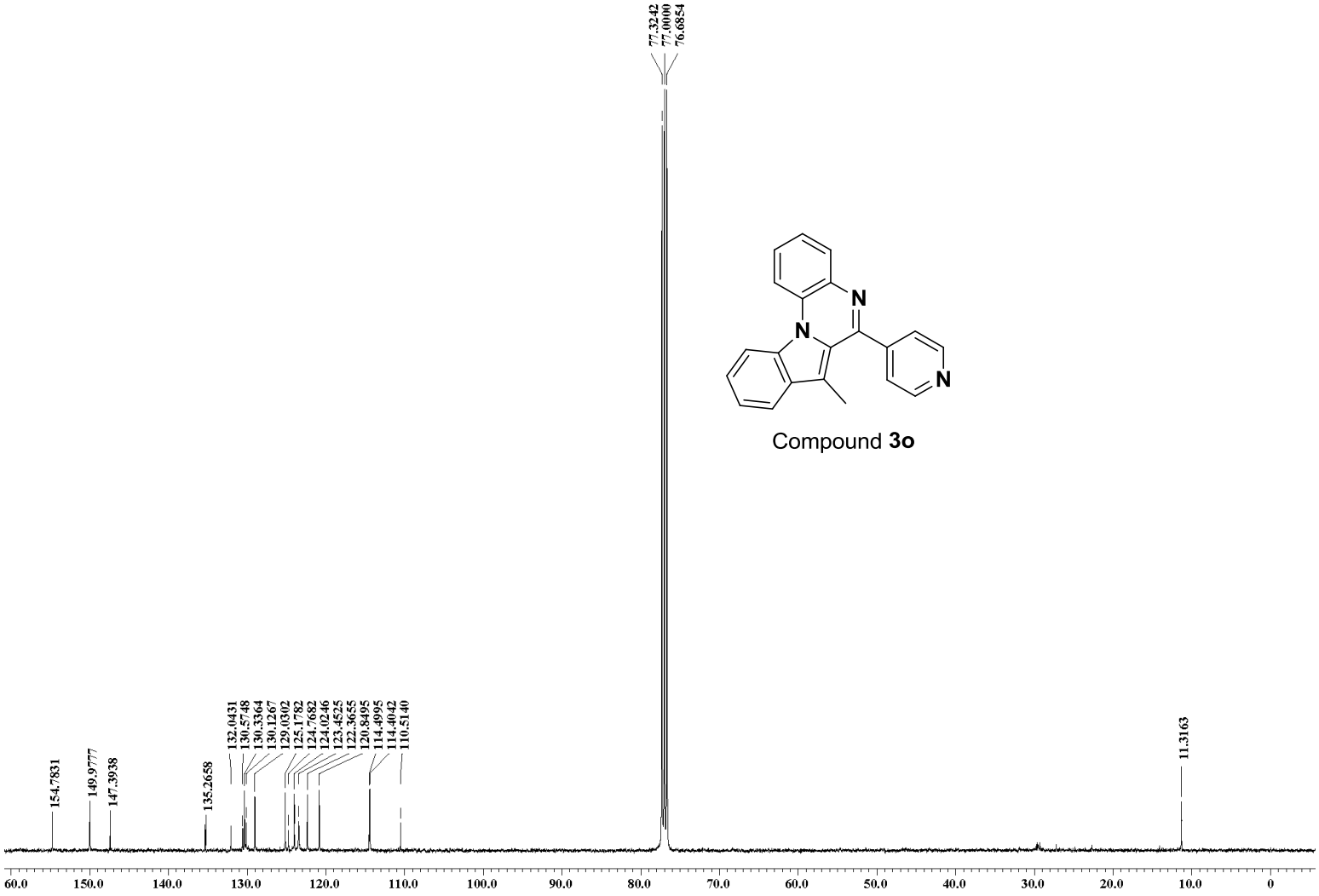


Figure 30 ^{13}C NMR spectrum of 3o

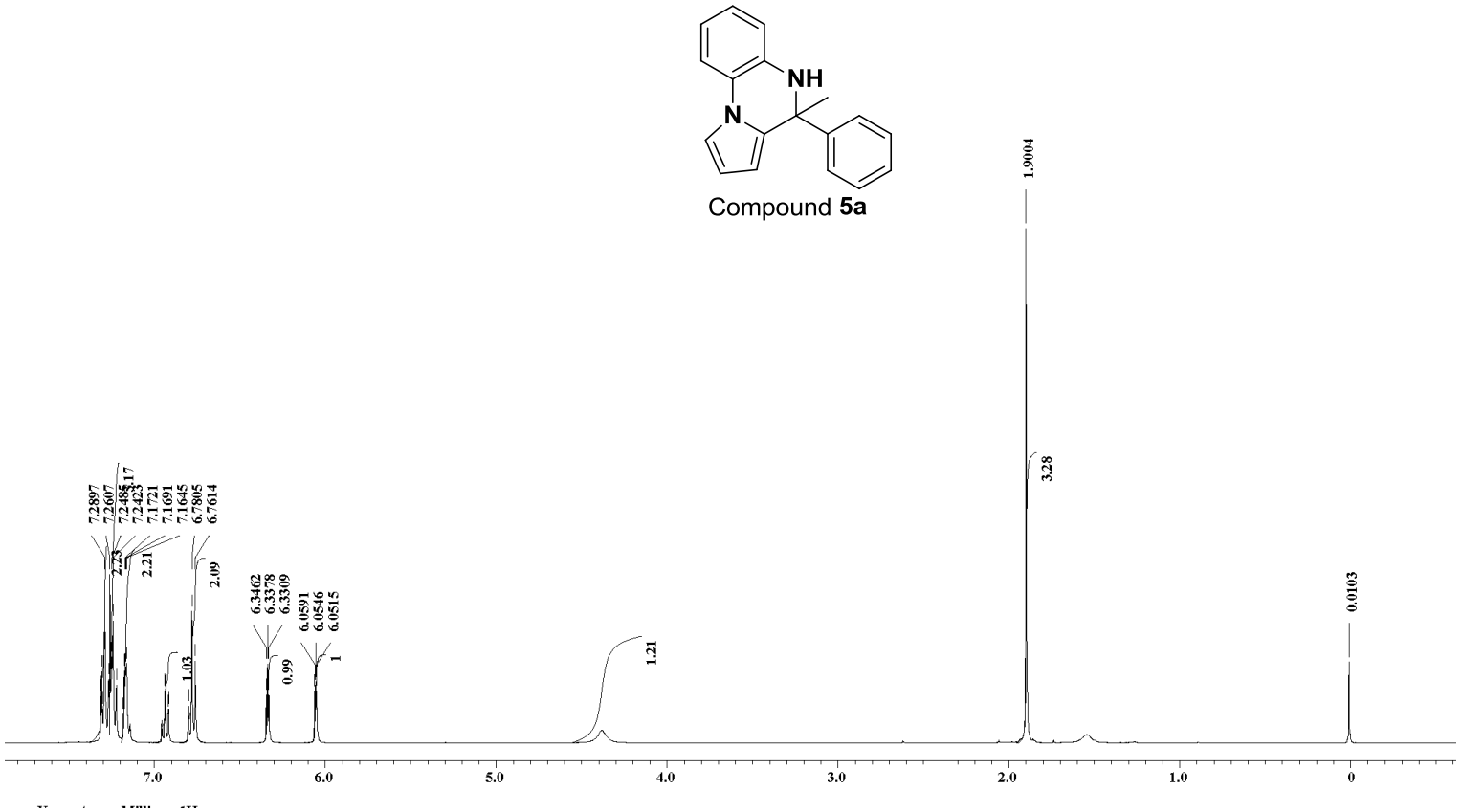


Figure 31: ^{1}H NMR spectrum of 5a

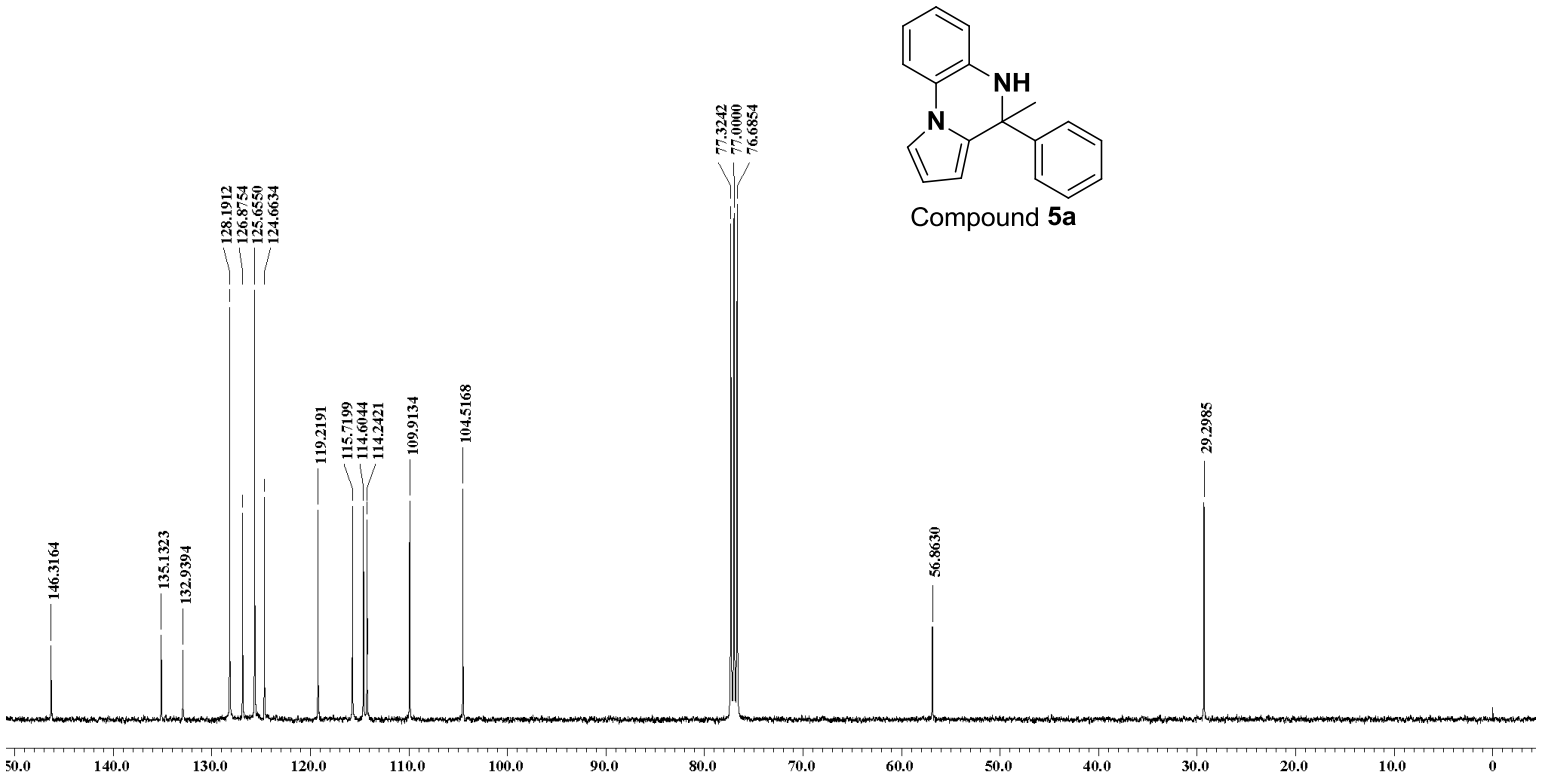


Figure 32: ^{13}C NMR spectrum of 5a

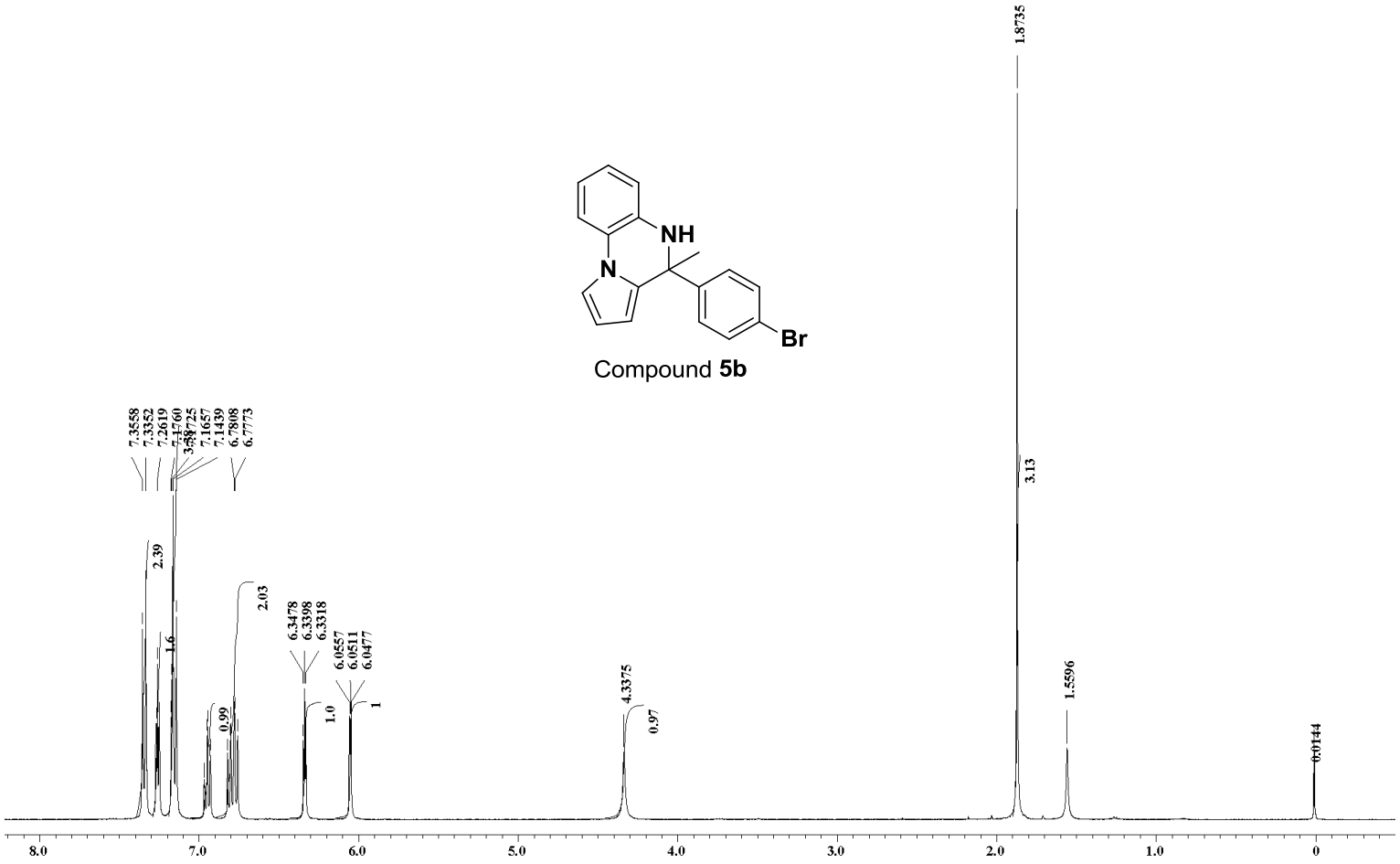


Figure 33: ^{1}H NMR spectrum of 5b

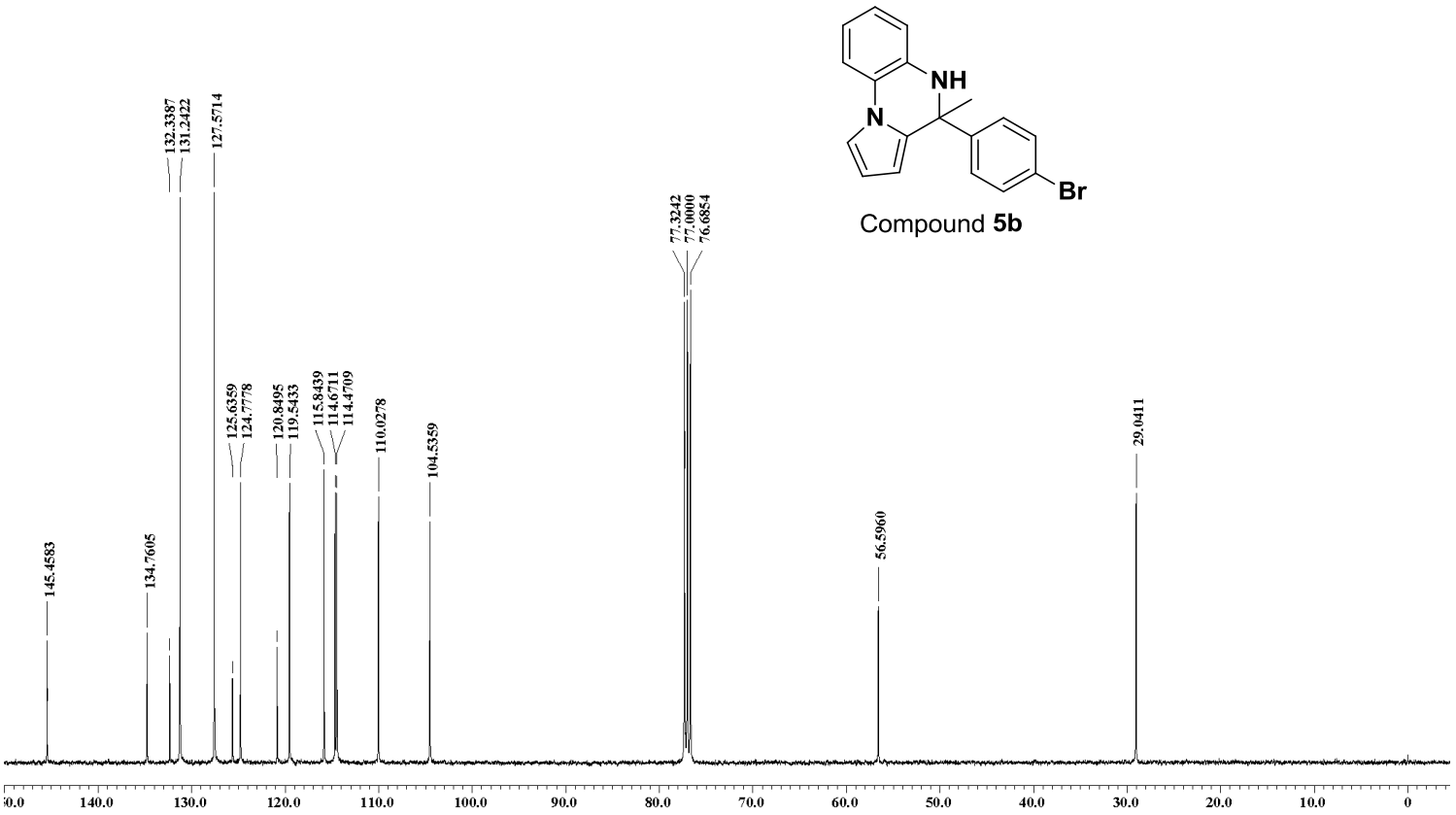


Figure 34: ^{13}C NMR spectrum of 5b

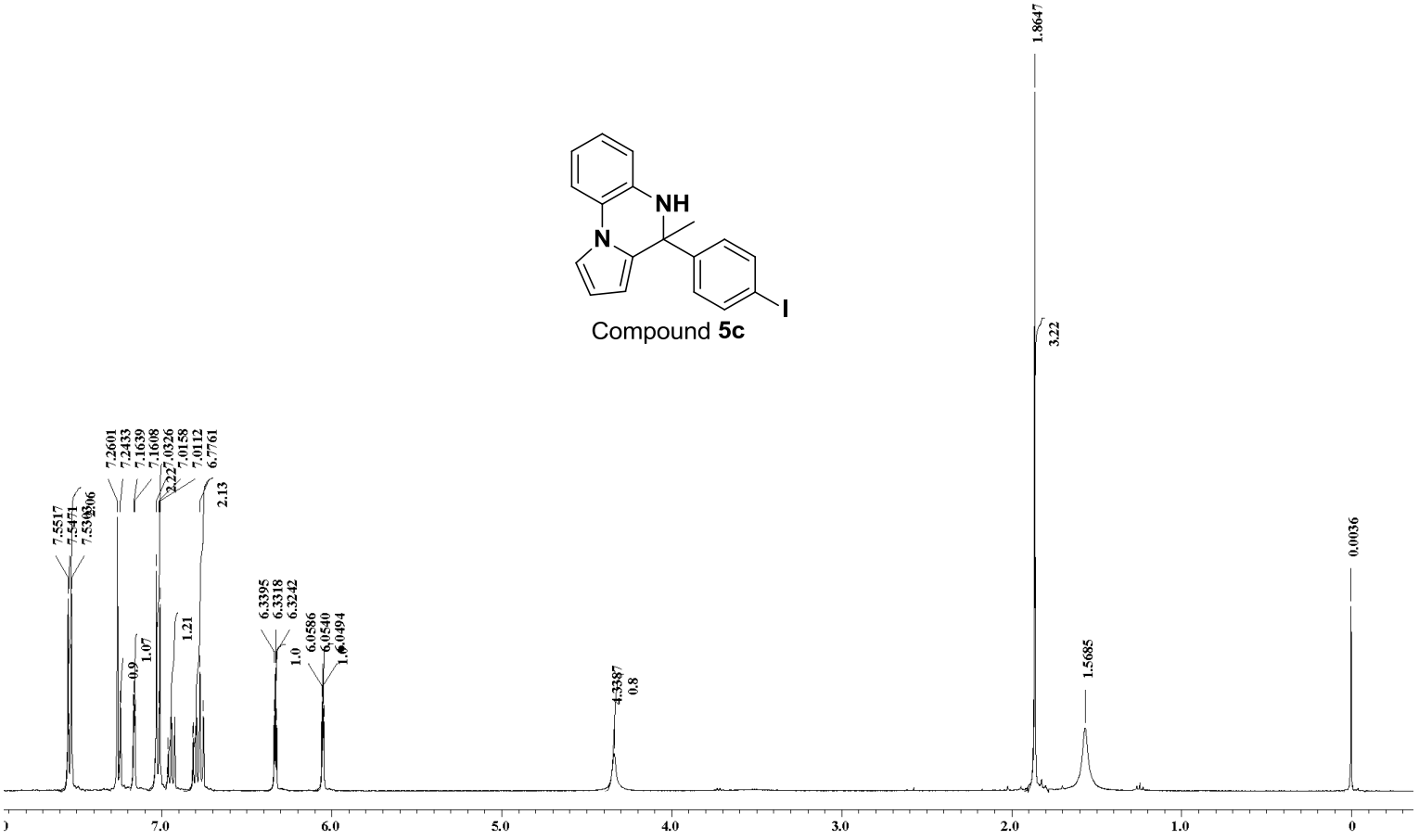


Figure 35: ^{1}H NMR spectrum of 5c

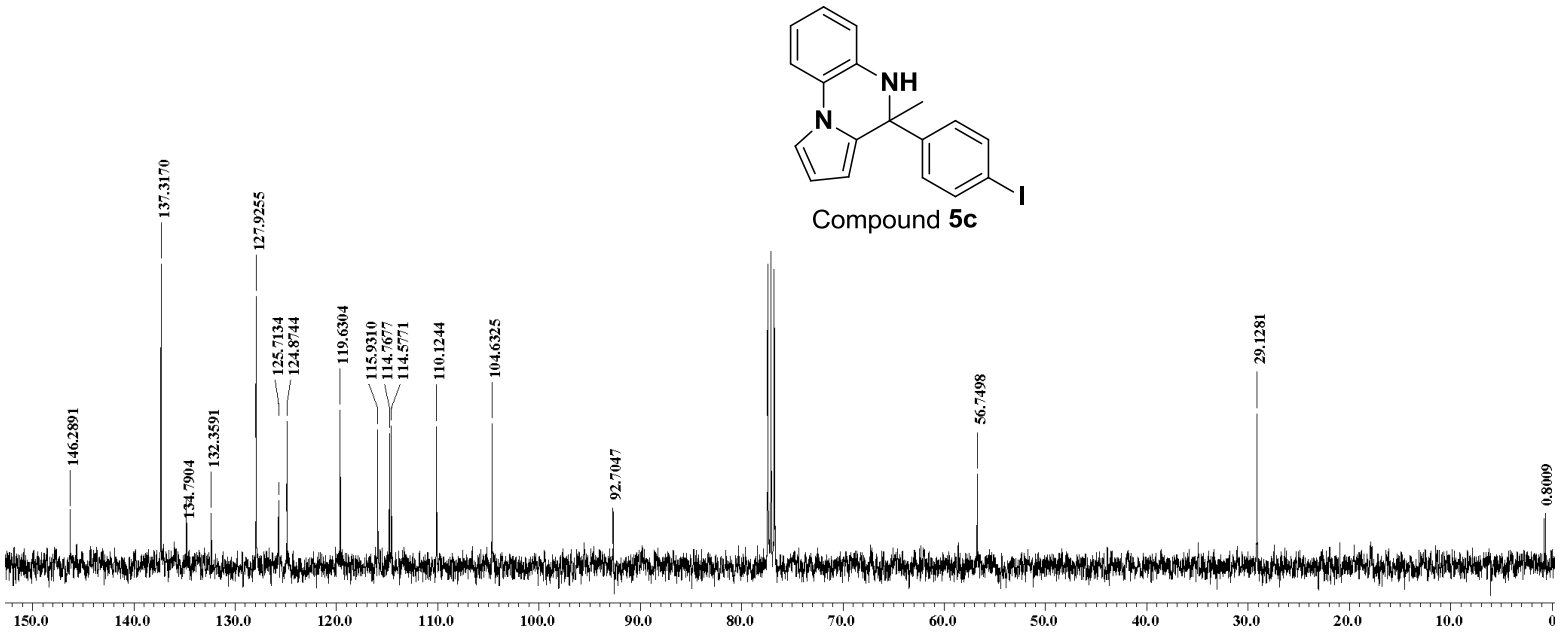


Figure 36: ^{13}C NMR spectrum of 5c

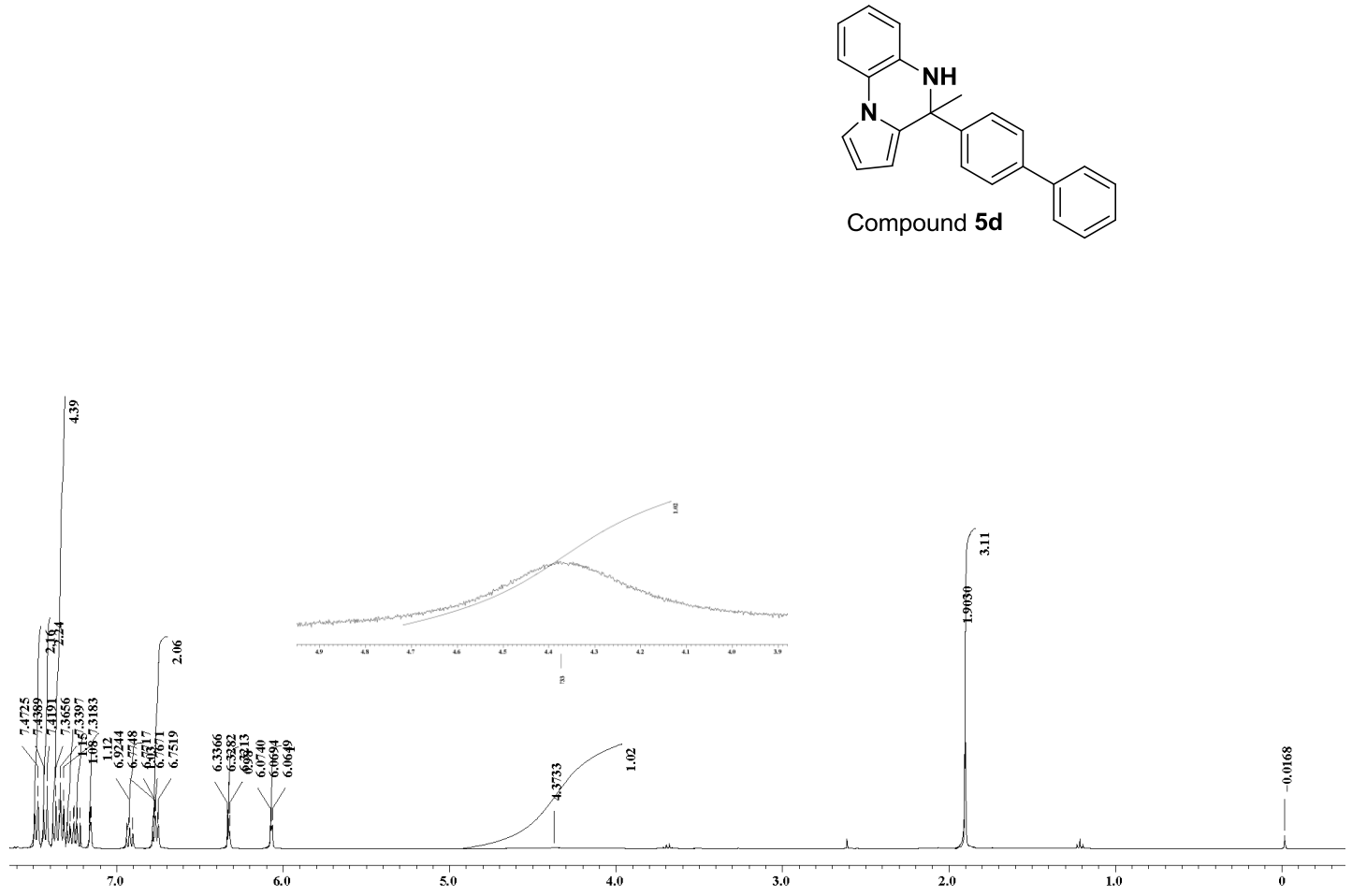


Figure 37: ^{1}H NMR spectrum of 5d

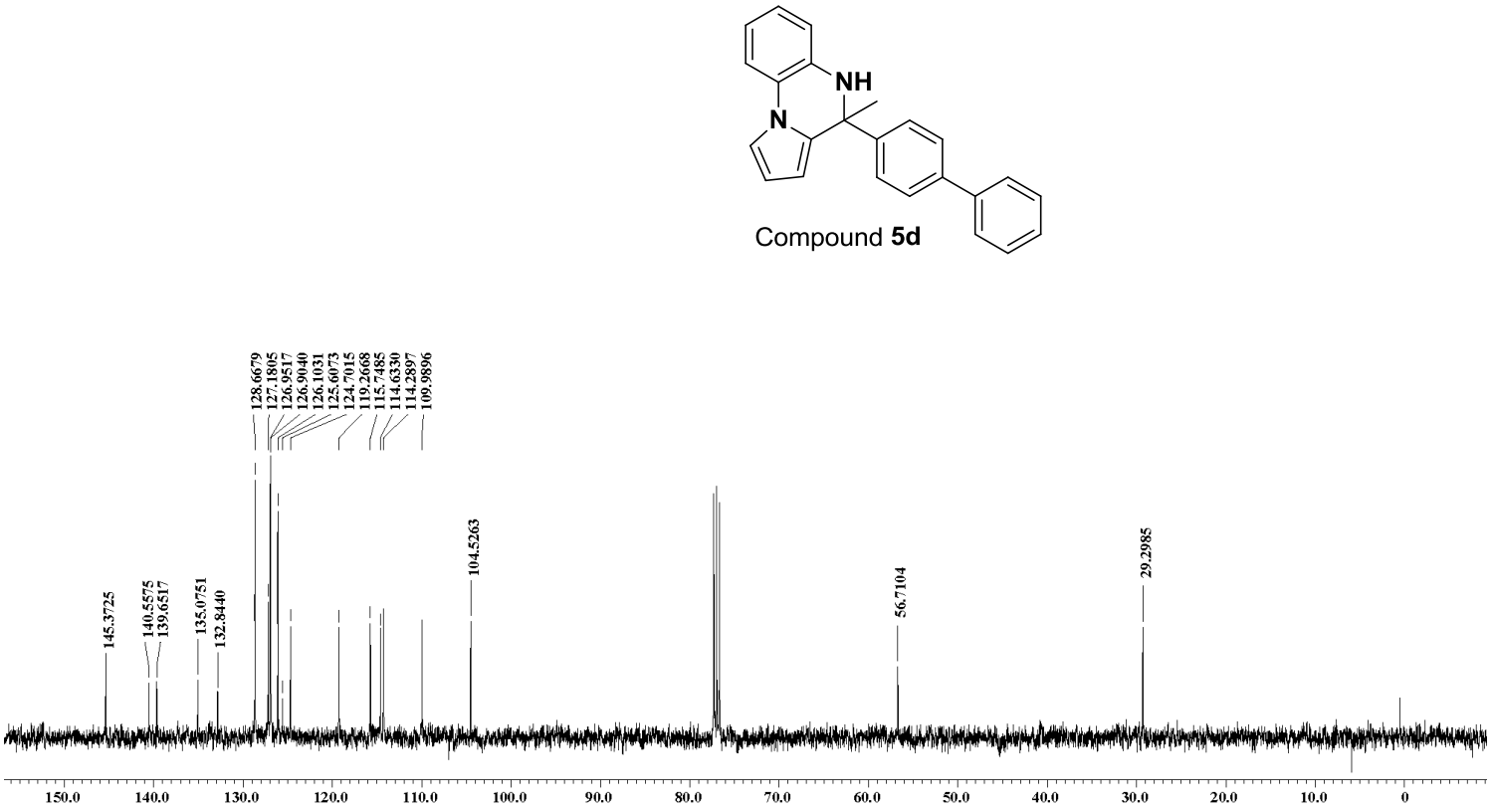


Figure 38: ^{13}C NMR spectrum of 5d

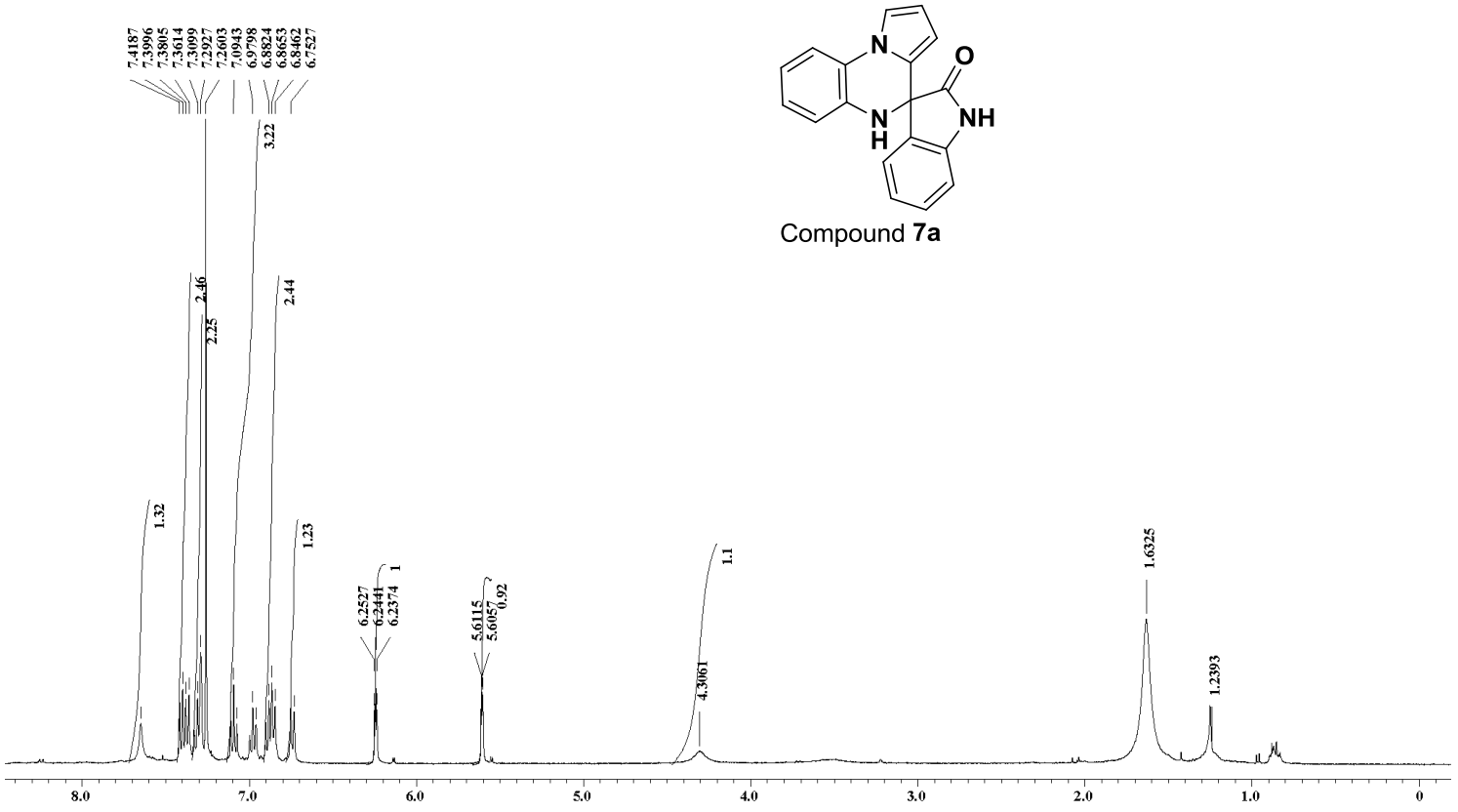


Figure 39: ^{1}H NMR spectrum of 7a

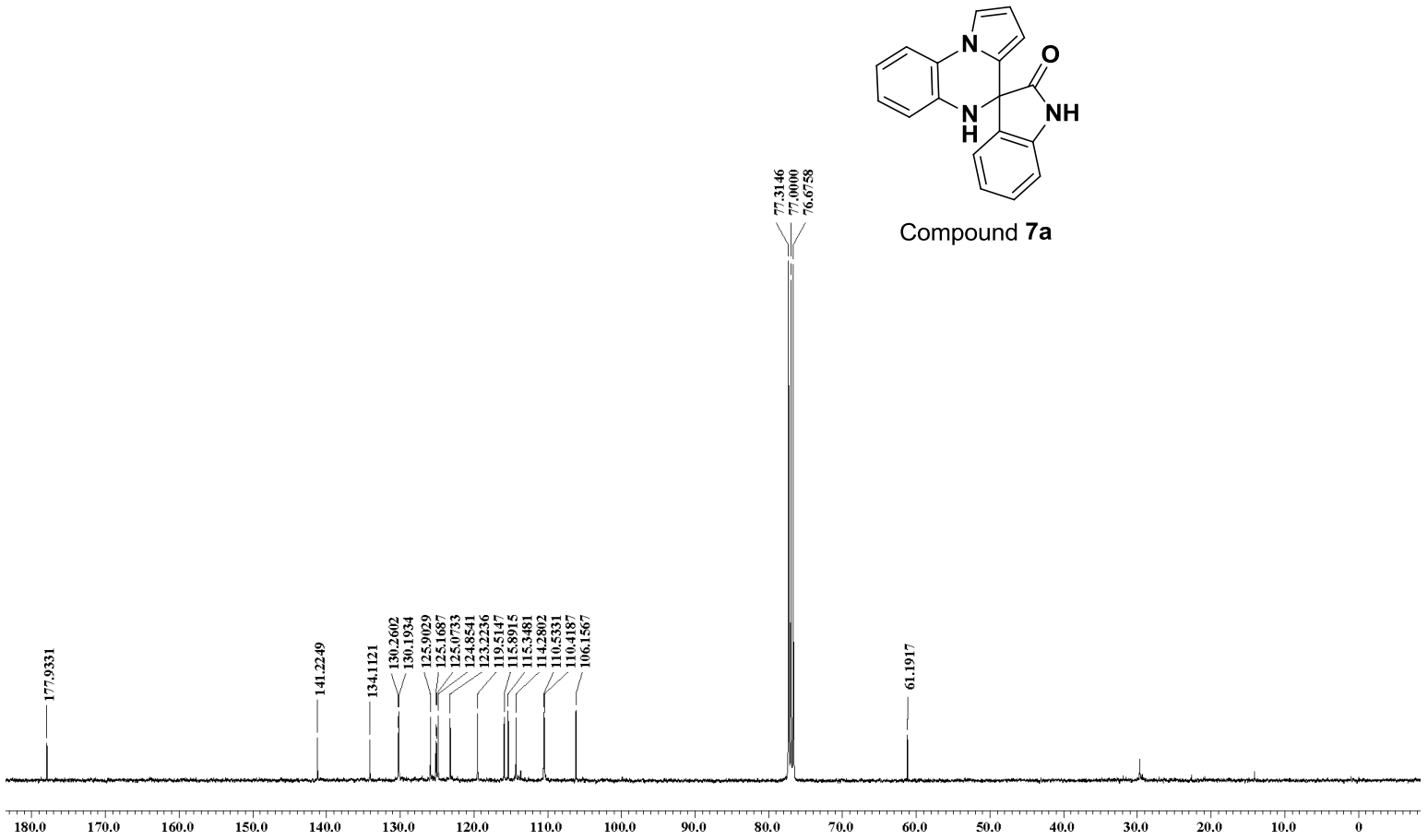


Figure 40: ^{13}C NMR spectrum of 7a

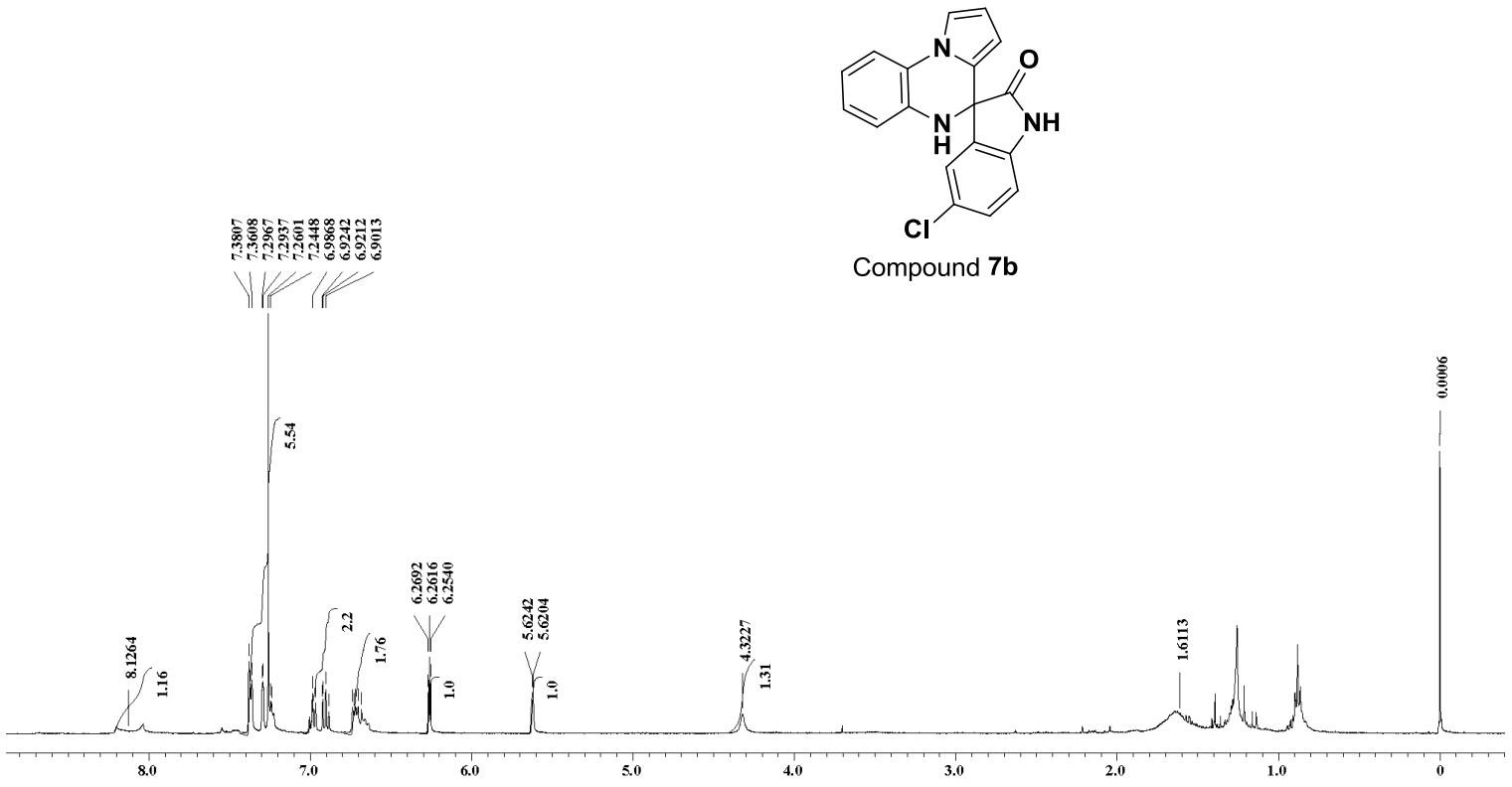
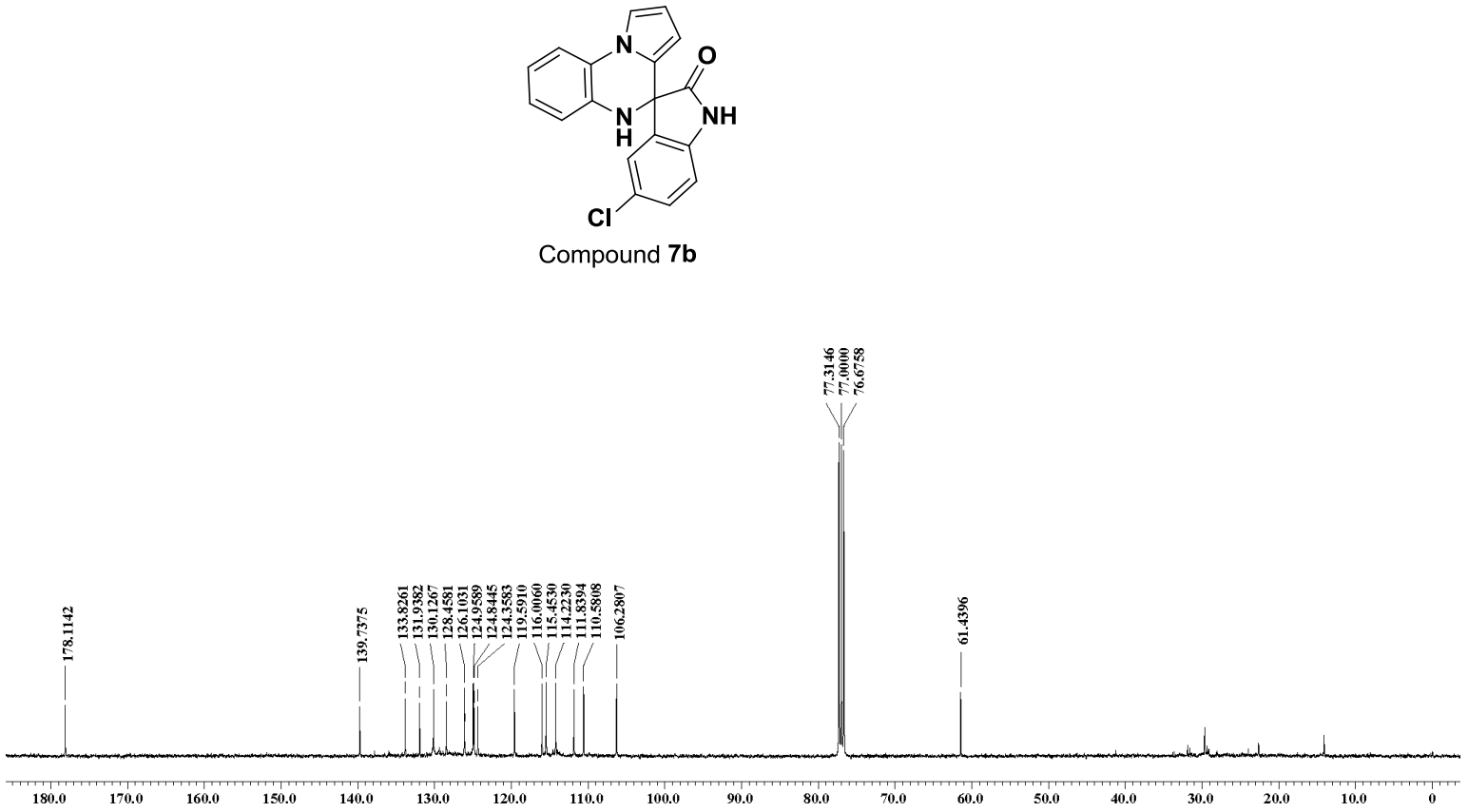
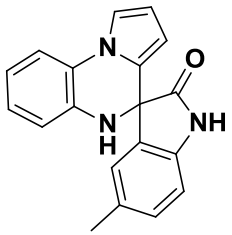


Figure 41: ^{1}H NMR spectrum of 7b



Compound **7b**

Figure 42: ^{13}C NMR spectrum of 7b



Compound **7c**

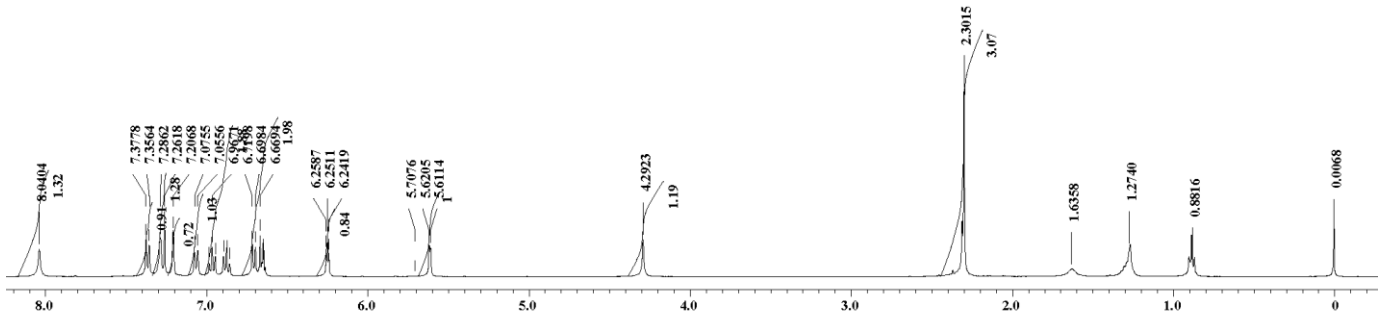


Figure 43: ^{1}H NMR spectrum of 7c

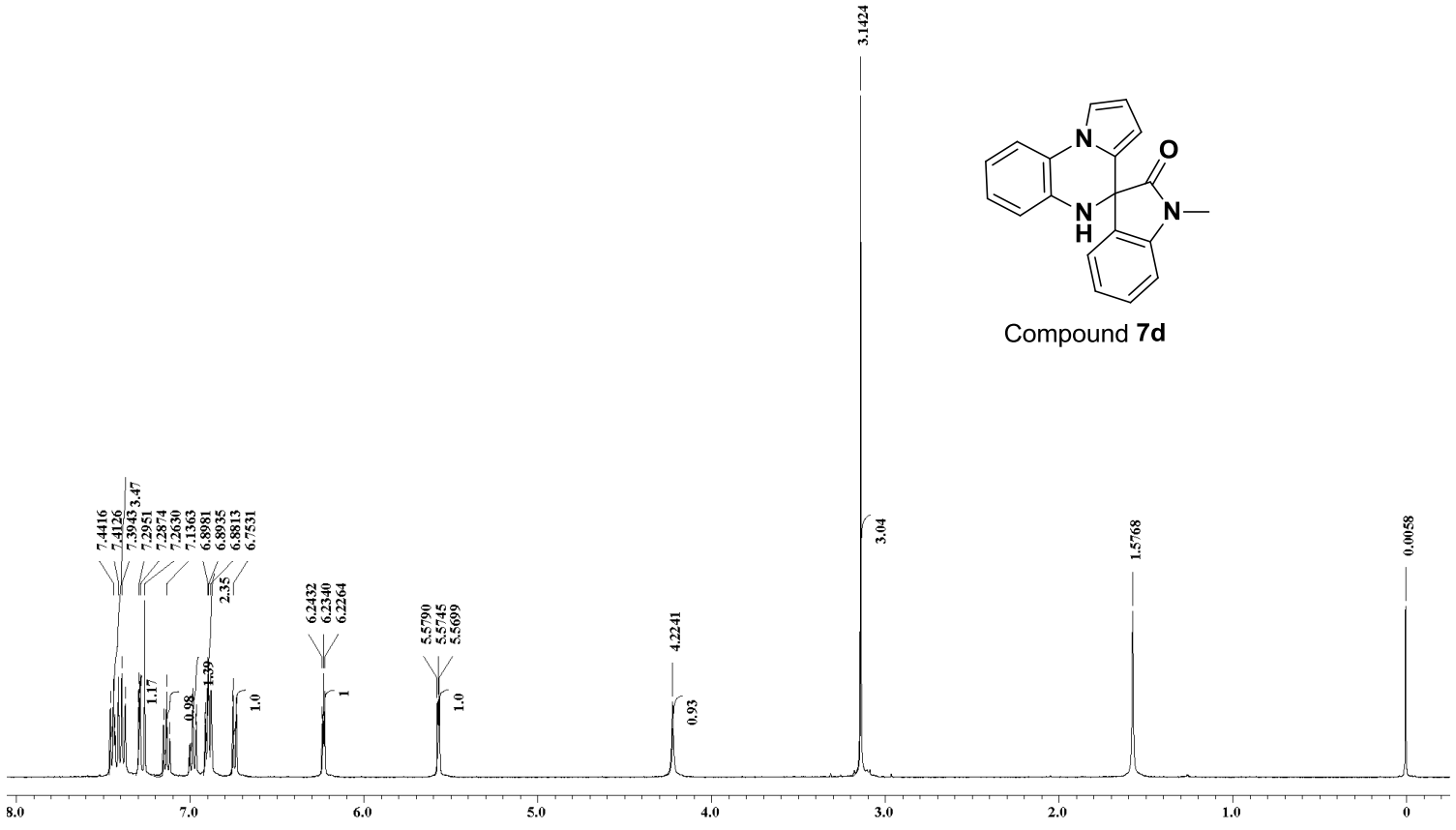


Figure 44: ^{1}H NMR spectrum of 7d

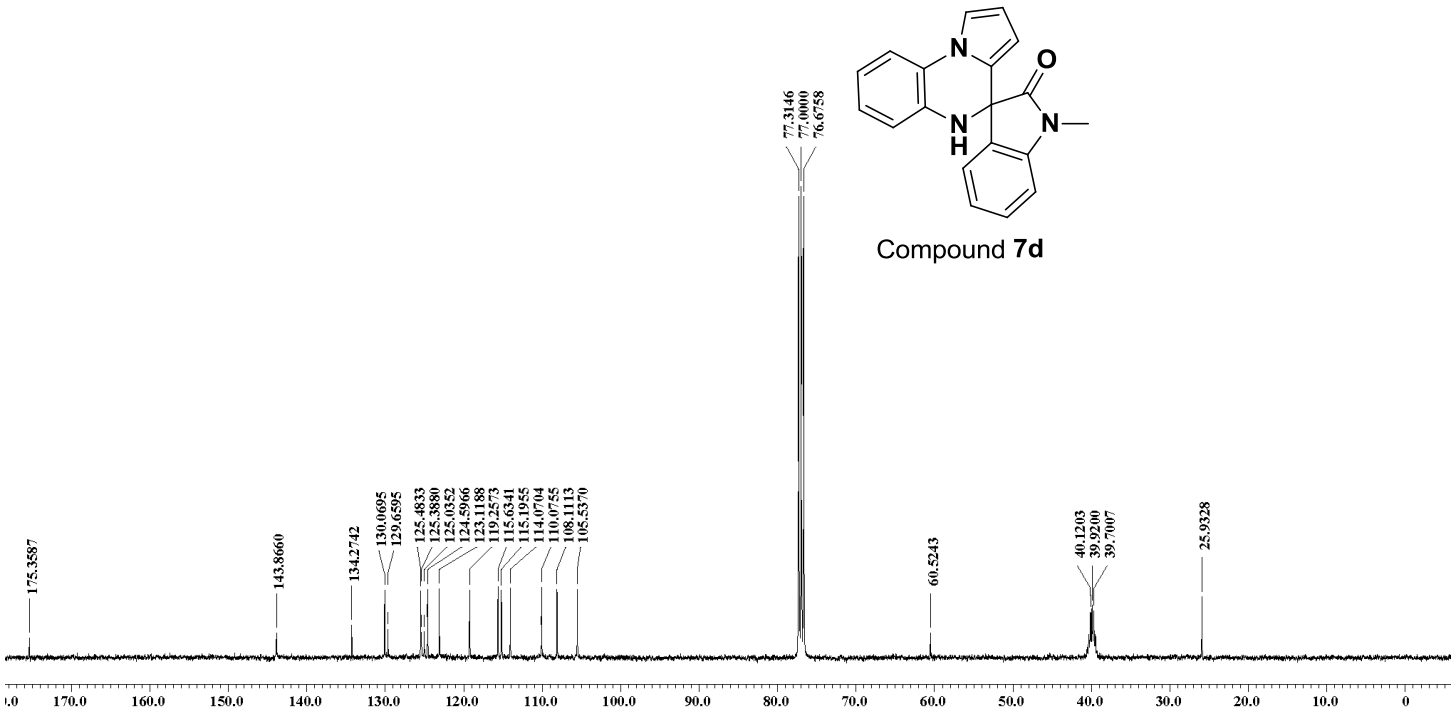


Figure 45: ^{13}C NMR spectrum of 7d

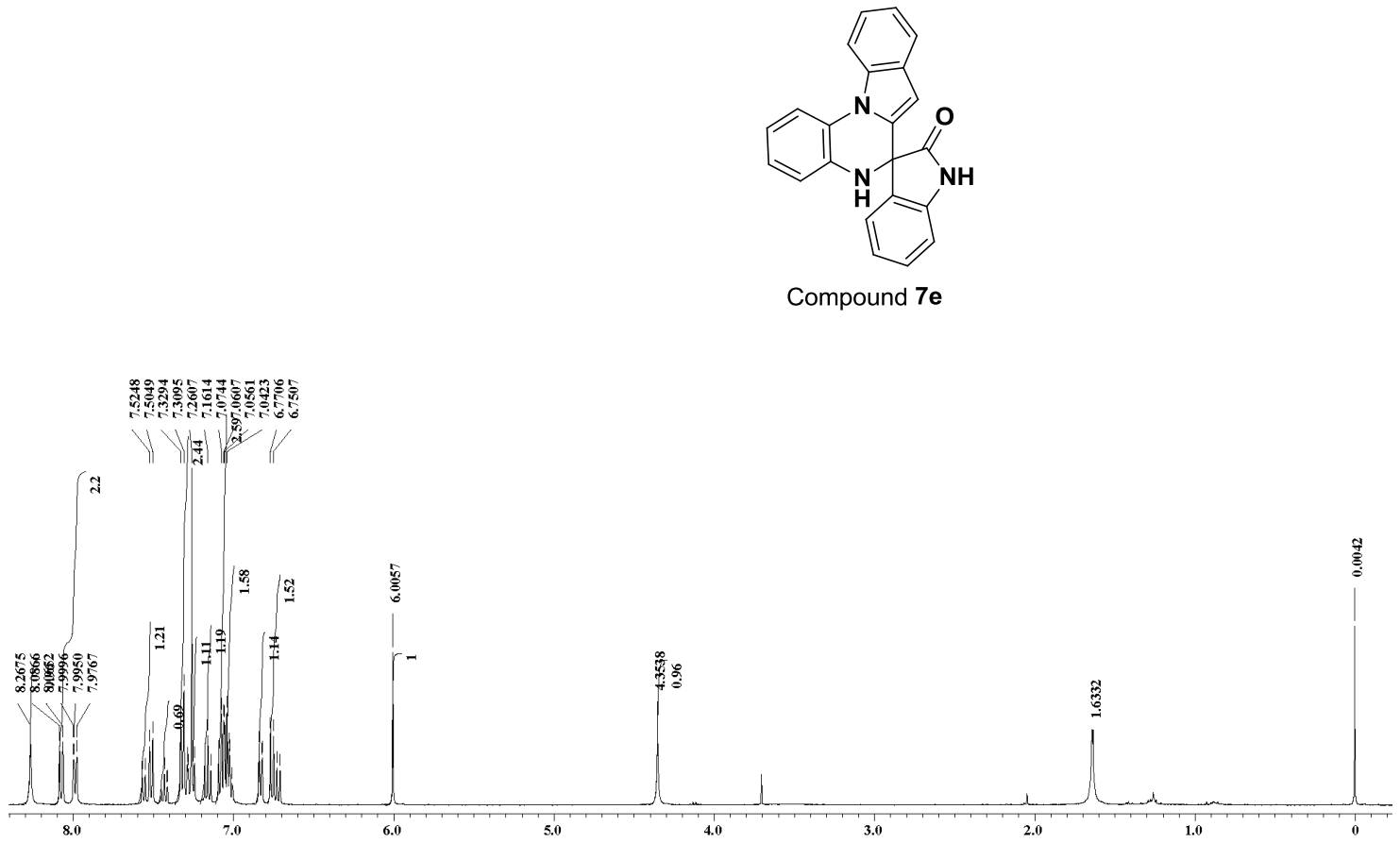
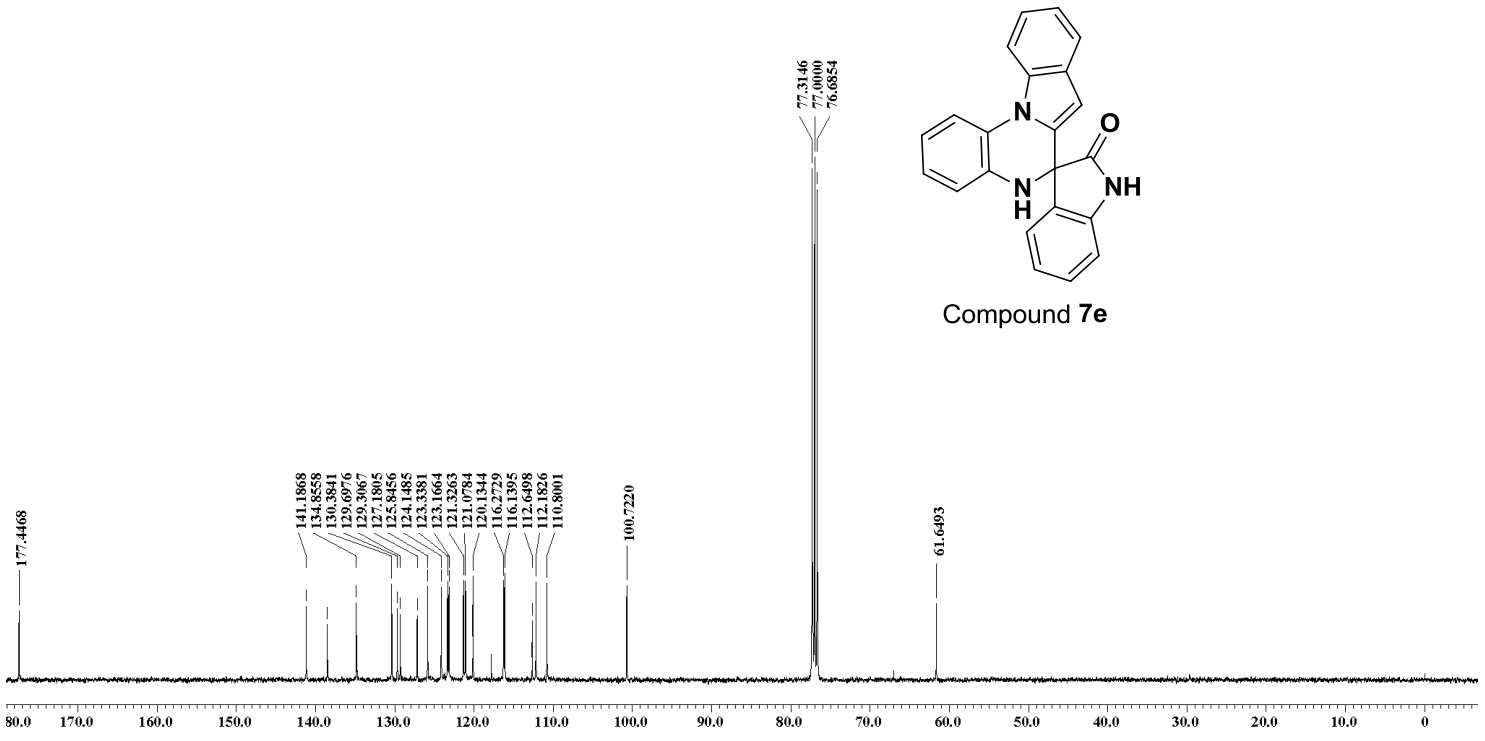


Figure 46: ^{1}H NMR spectrum of 7e



Compound **7e**

Figure 47: ^{13}C NMR spectrum of 7e

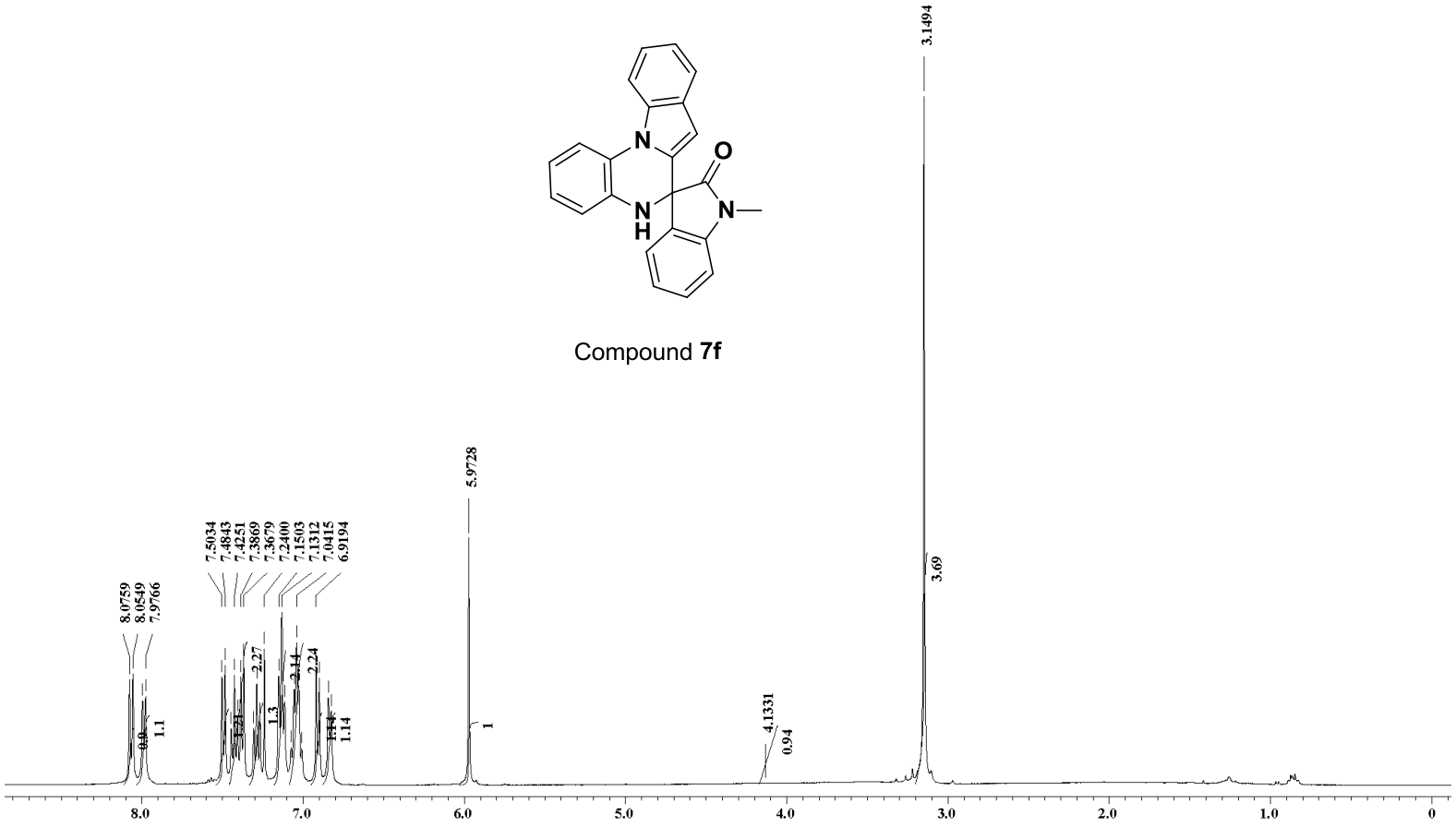


Figure 48: ^{1}H NMR spectrum of 7f

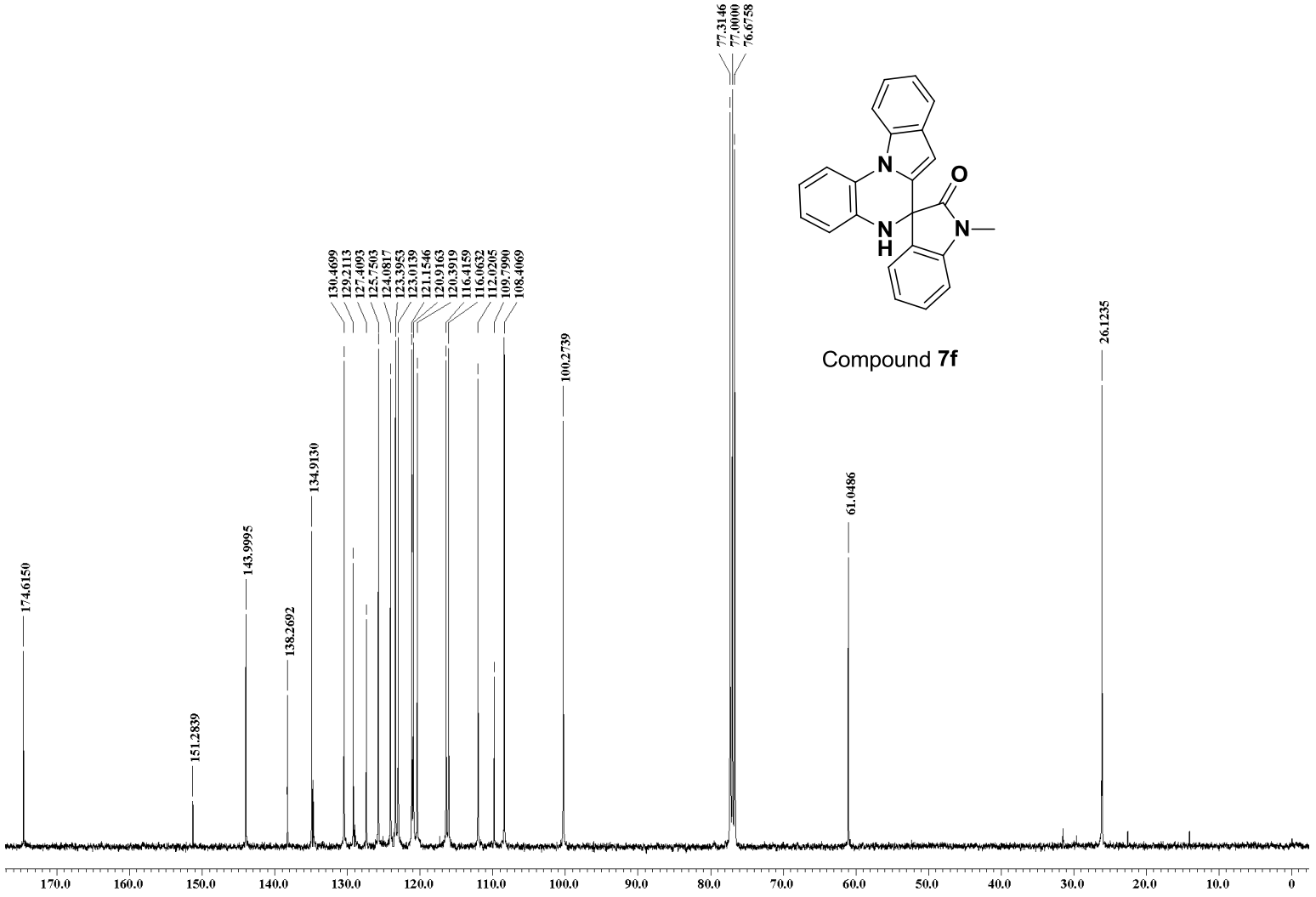


Figure 49: ^{13}C NMR spectrum of 7f

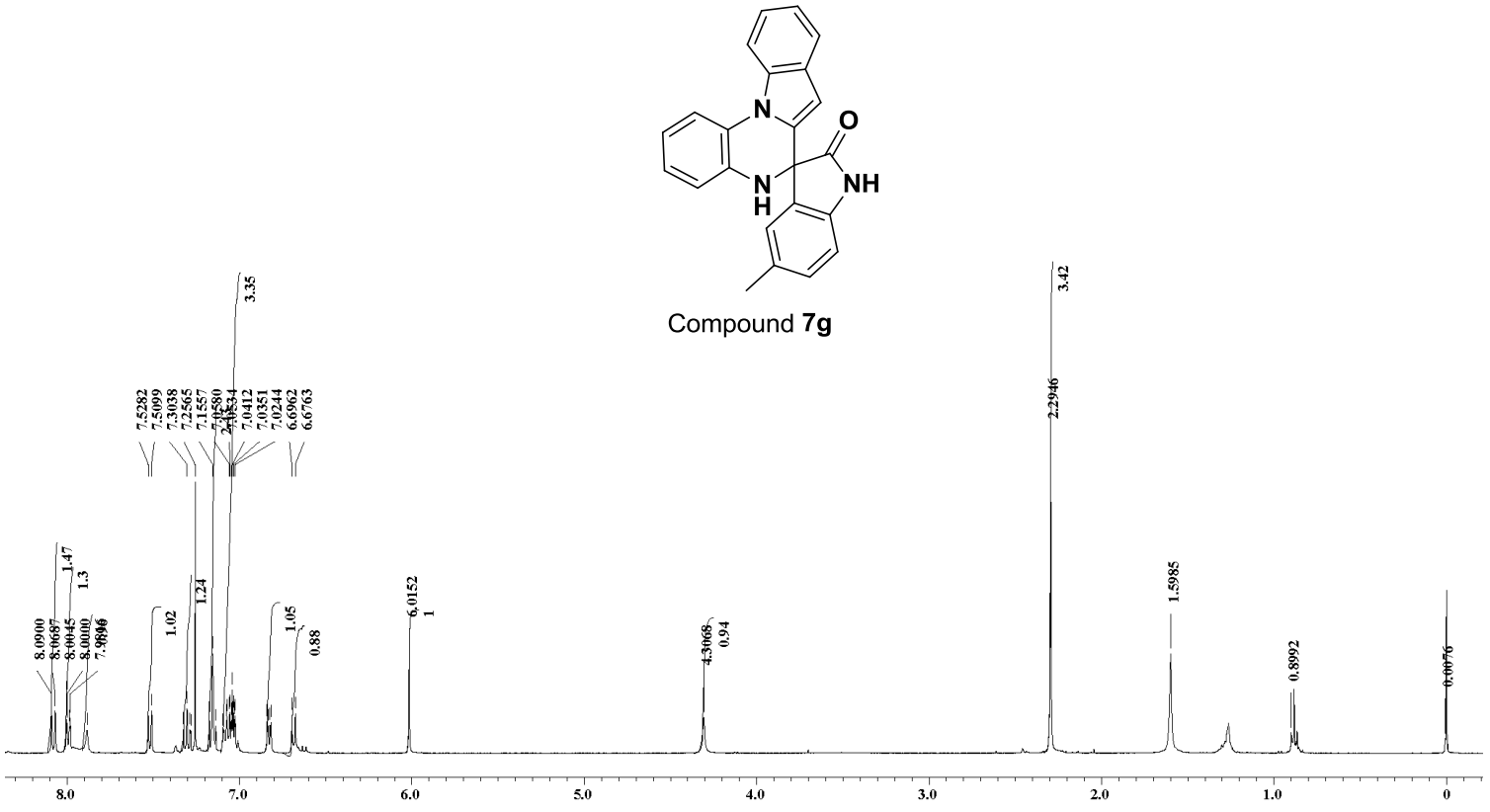
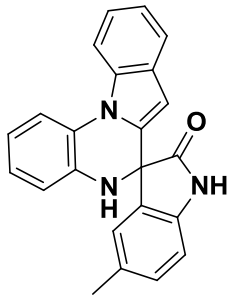


Figure 50: ^{1}H NMR spectrum of 7g



Compound **7g**

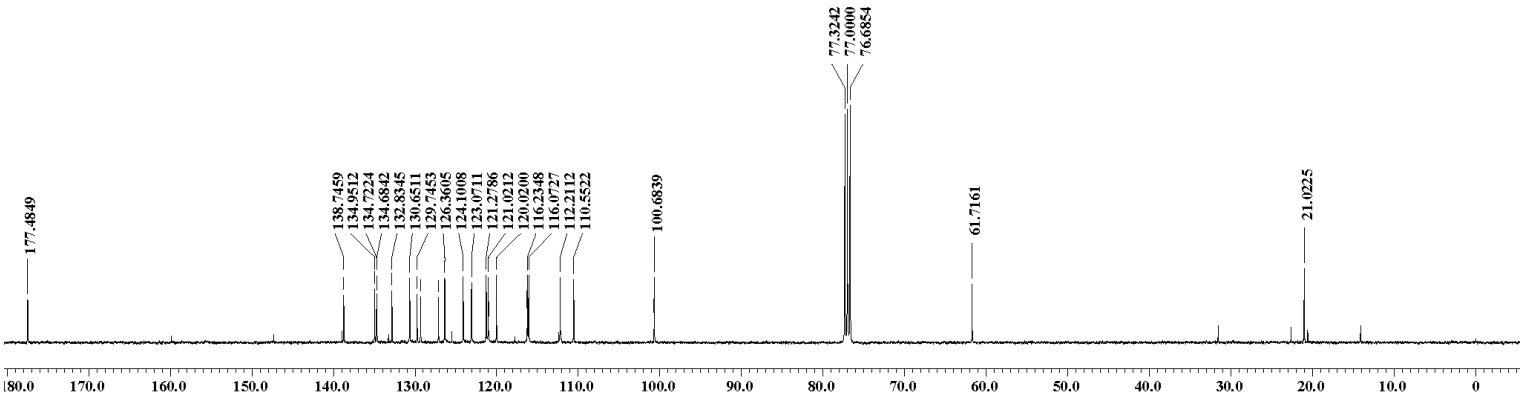


Figure 51: ^{13}C NMR spectrum of 7g

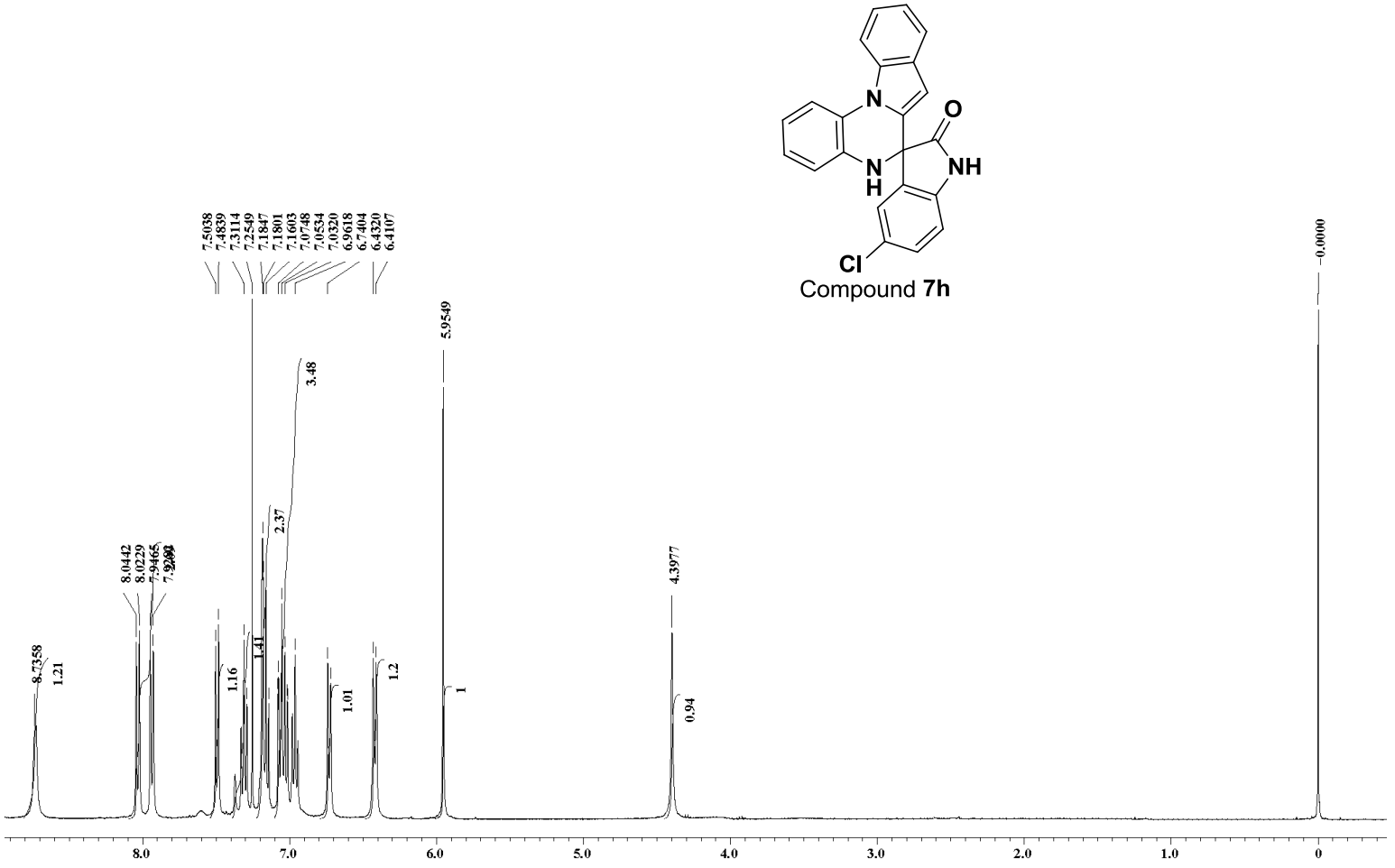


Figure 52: ^{1}H NMR spectrum of 7h

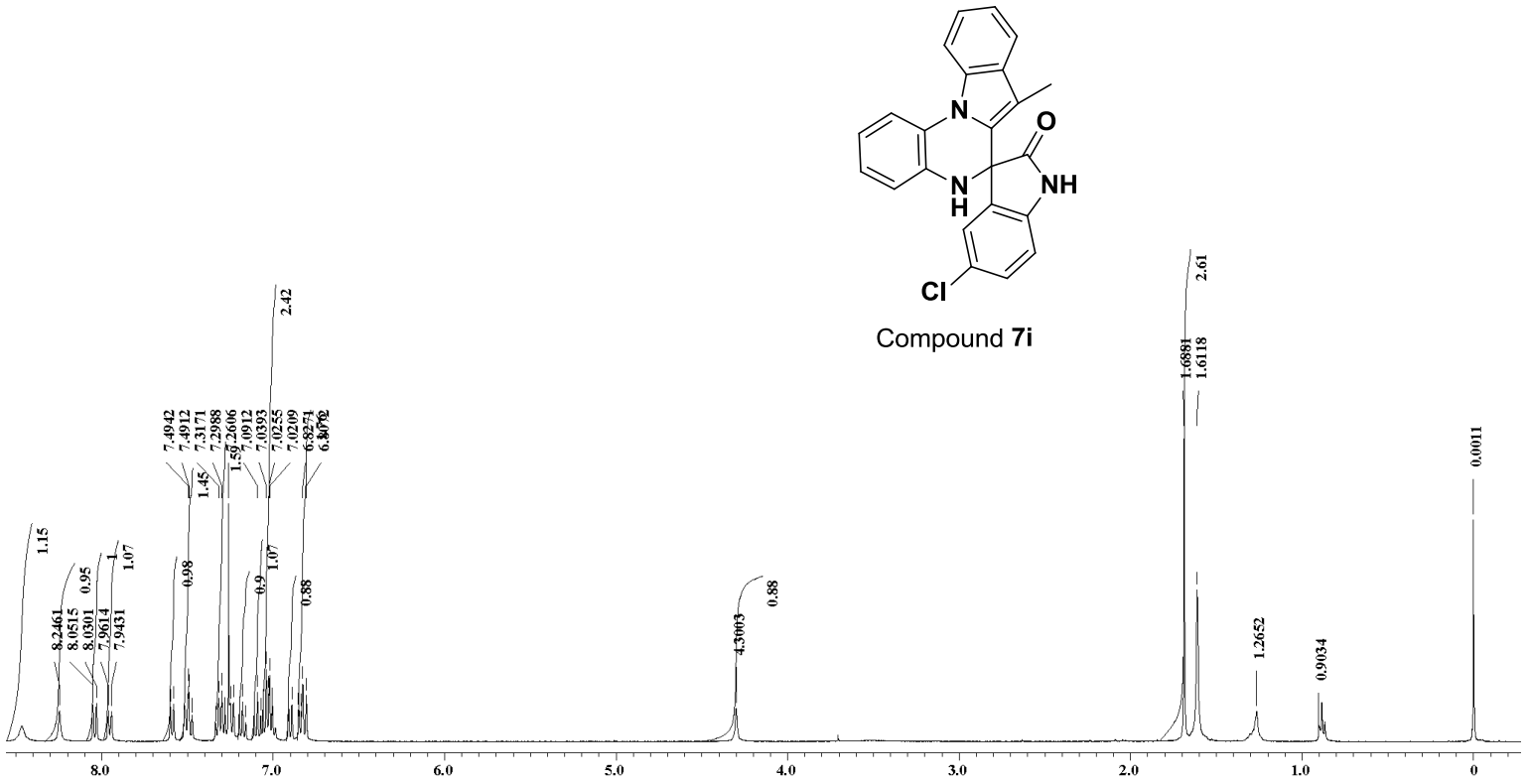


Figure 53: ^{1}H NMR spectrum of 7i

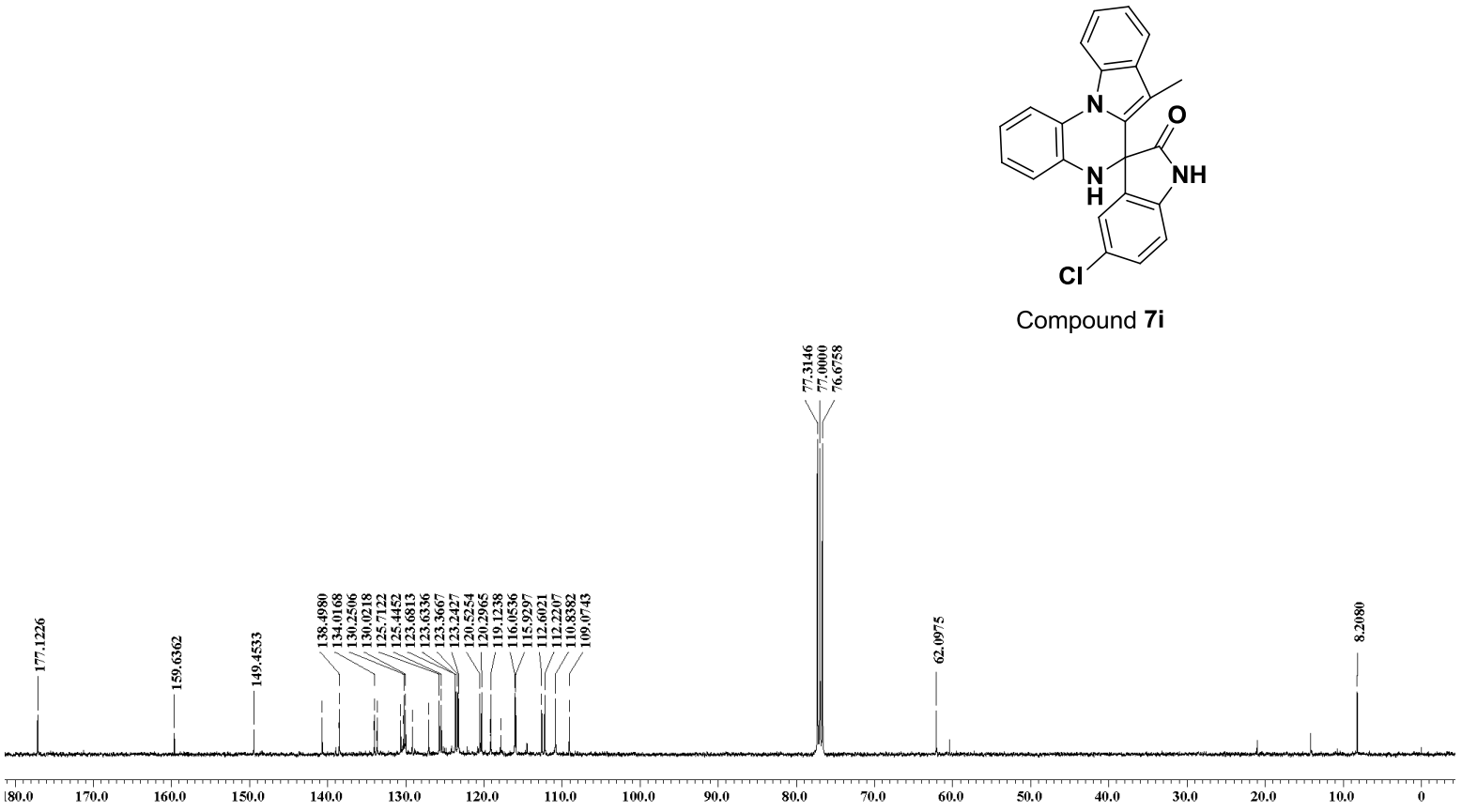


Figure 54: ^{13}C NMR spectrum of 7i

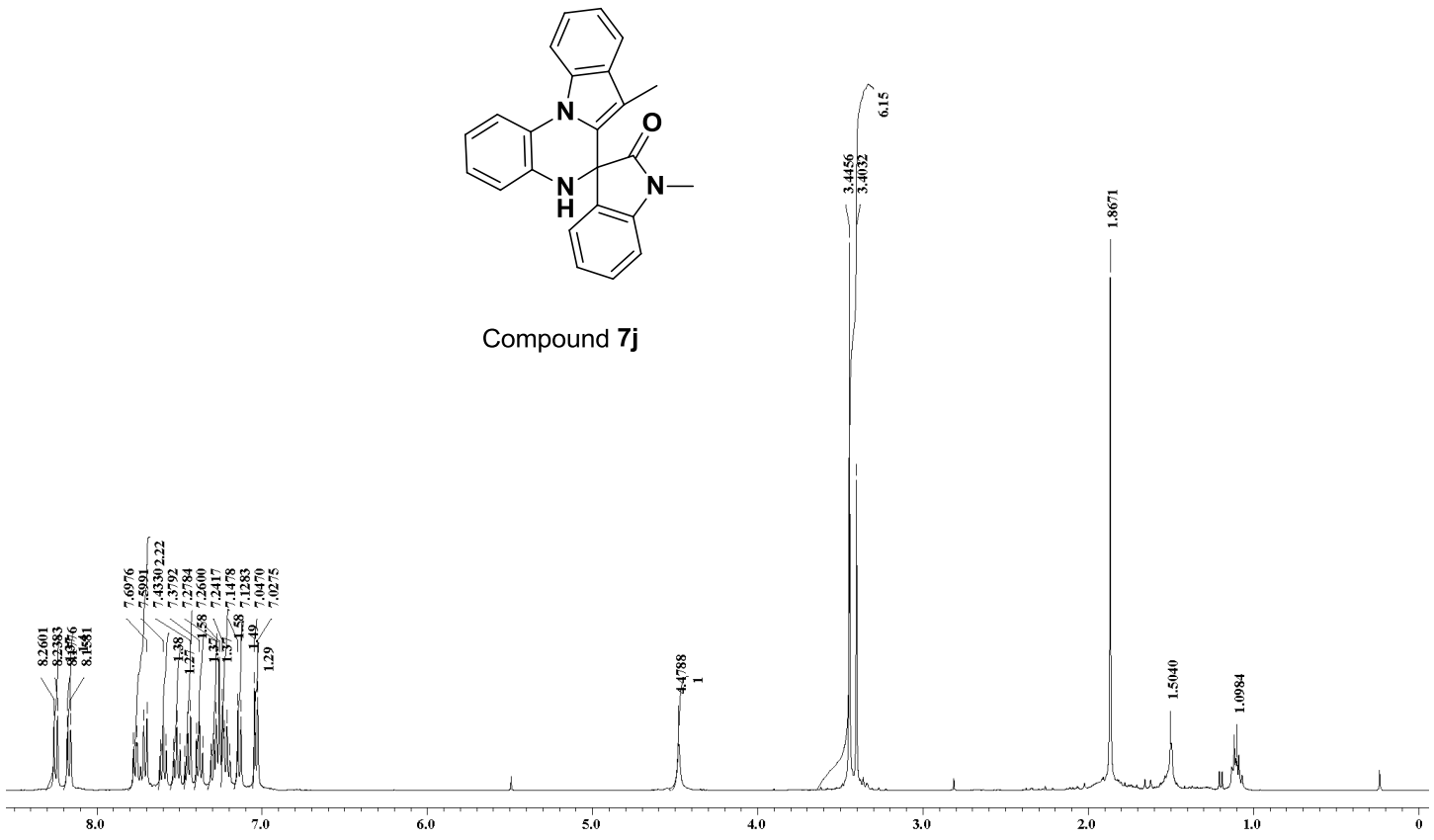
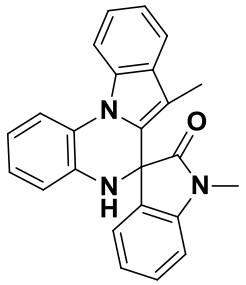


Figure 55: ^{1}H NMR spectrum of 7j



Compound **7j**

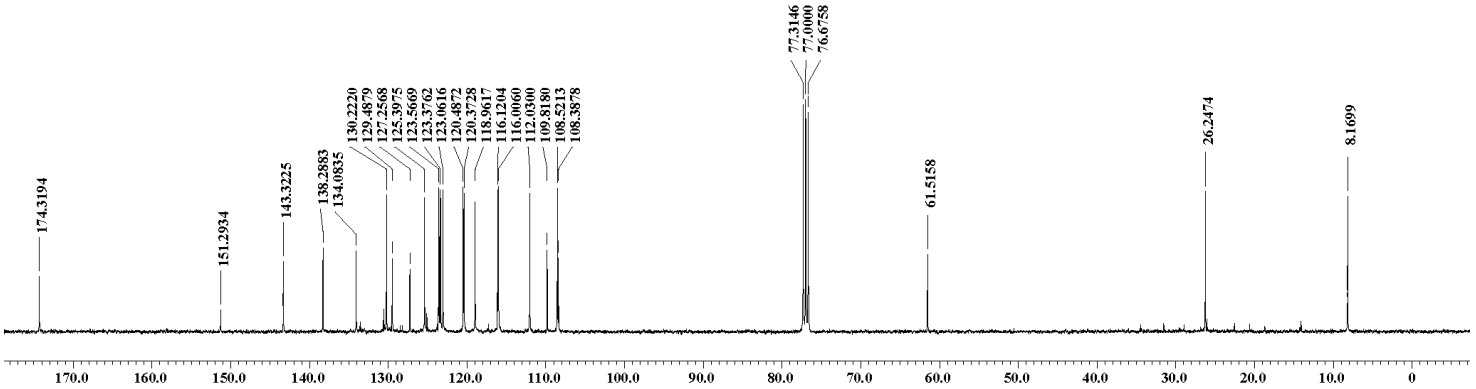


Figure 56: ^{13}C NMR spectrum of 7j

Single Crystal X-ray analysis of compound 7d:

The intensity data for compound **7d** was collected on an Oxford Xcalibur CCD diffractometer equipped with graphite monochromatic Mo-Ka radiation (λ = 0.71073 Å) at 293(2) K[1].A multi-scan correction was applied. The structure was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on F^2 using SHELXL97[2]. The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package[3].

References:

1. CrysAlisPro, Agilent Technologies, Version 1.171.34.49 (**2011**).

2. Sheldrick, G. M. Acta Cryst., 2008, A64, 112-122.

3. L. J. Farrugia, WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data;* Department of Chemistry, University of Glasgow (1997-2009).

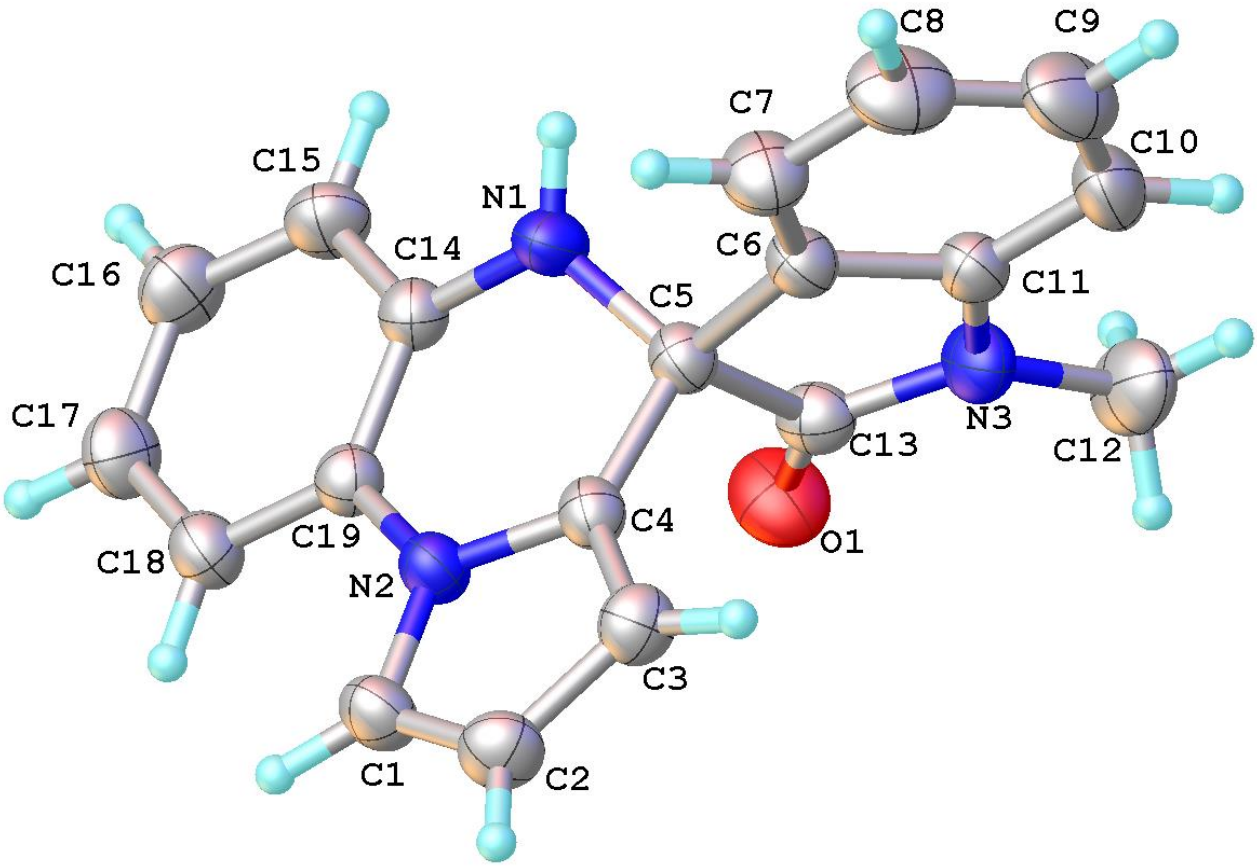


Figure **57**: Molecular structure for compound **7d** (thermal ellipsoids are drawn at 30% probability level).

Table: Crystallographic data and structure refinements for compound **7d**.

Empirical formula	$C_{19}H_{15}N_3O$
Formula weight	301.35
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P n m a
A	8.1561(4) Å
B	10.4240(4) Å
C	17.6525(10) Å
α	90°
β	97.994(5)°
γ	90°
Volume	1486.22(13) $Å^3$
Z	4
Density (calculated)	1.347 Mg/m^3
Absorption coefficient	0.086 mm^{-1}
F(000)	632
Crystal size	0.28 x 0.18 x 0.10 mm^3
Theta range for data collection	3.04 to 26.37°.
Index ranges	$-10 \leq h \leq 10$, $-12 \leq k \leq 13$, $-22 \leq l \leq 22$
Reflections collected	20207
Independent reflections	3031 [R(int) = 0.0236]
Completeness to theta = 26.37°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9915 and 0.9764
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3031/ 0 / 208
Goodness-of-fit on F^2	1.082
Final R indices [I>2sigma(I)][a, b]	R1 = 0.0515, wR2 = 0.1354
R indices (all data)	R1 = 0.0575, wR2 = 0.1394
Extinction coefficient	0.035(8)
Largest diff. peak and hole	0.453 and -0.412 $e.Å^{-3}$