

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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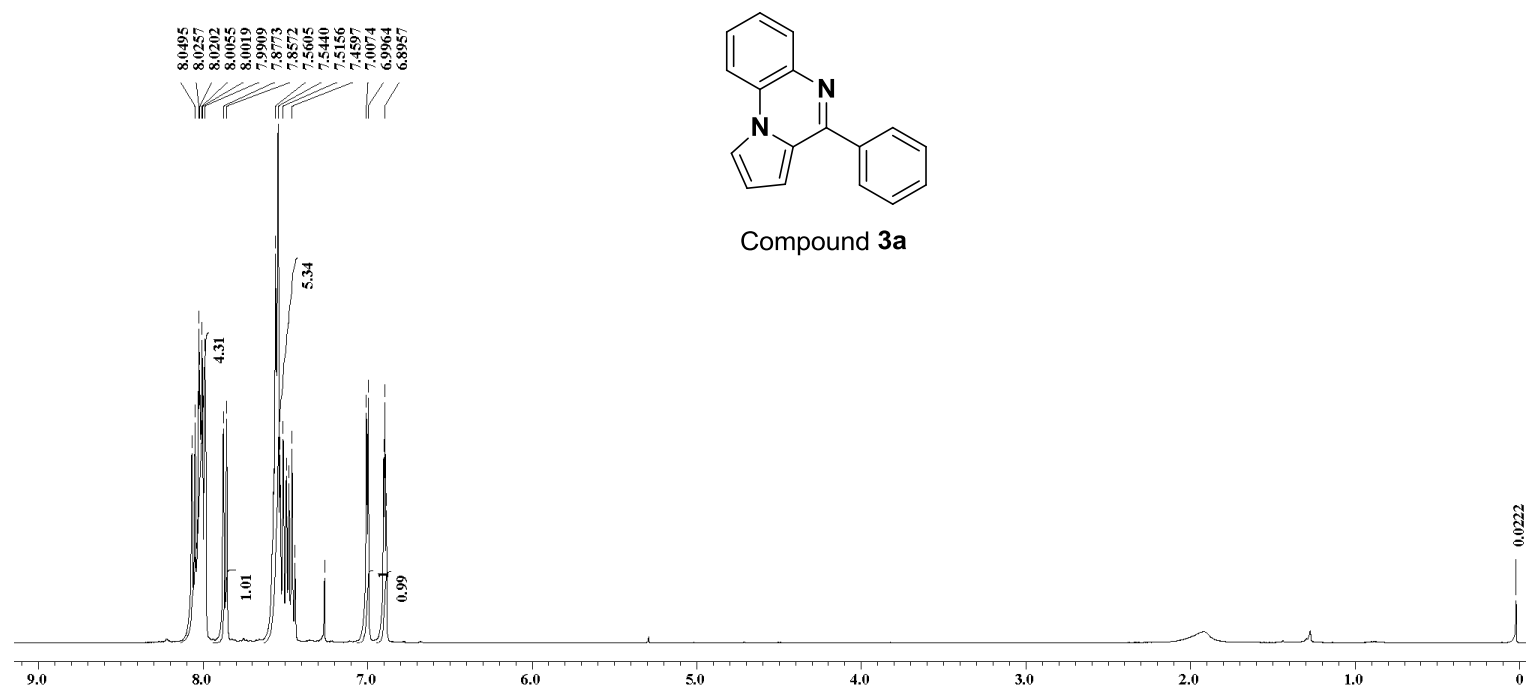


Figure 1: ^1H NMR spectrum of 3a

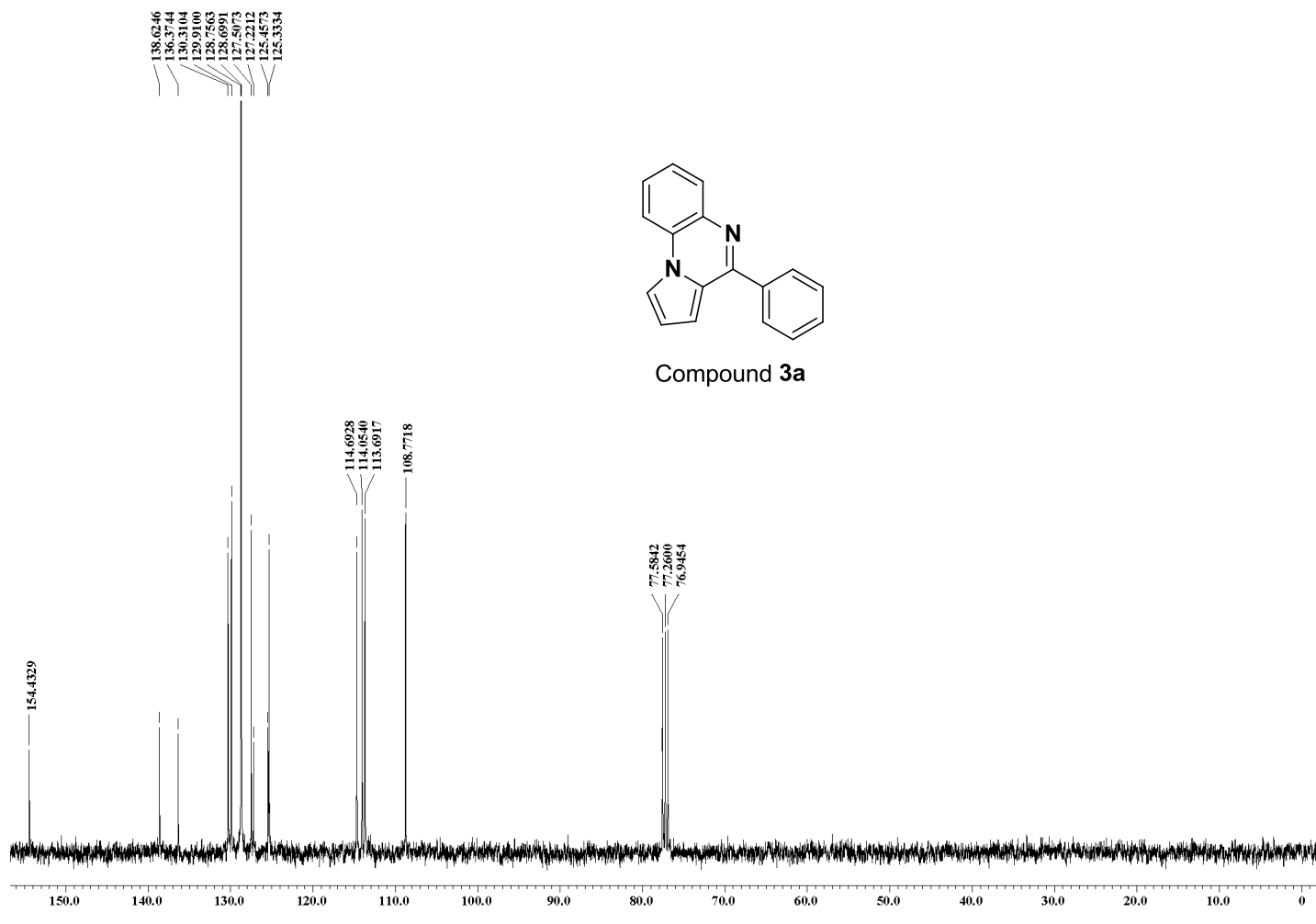


Figure 2: ^{13}C NMR spectrum of 3a

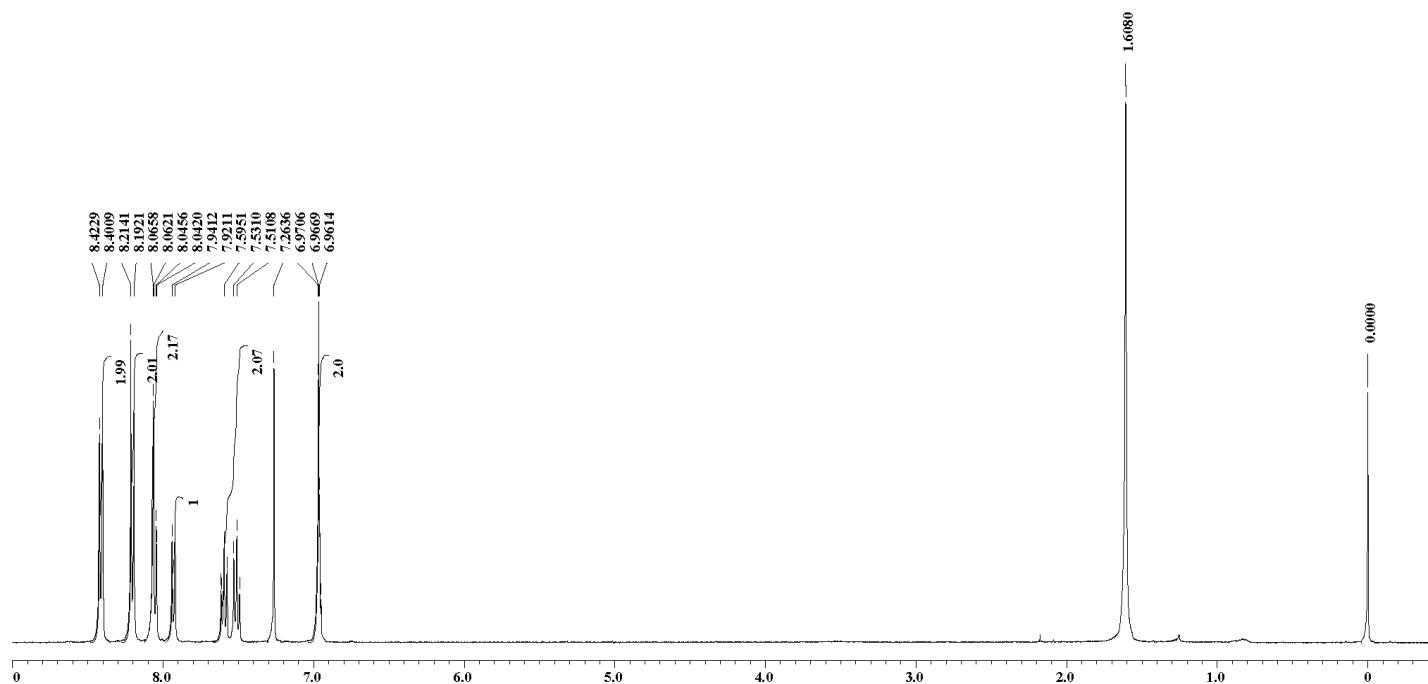
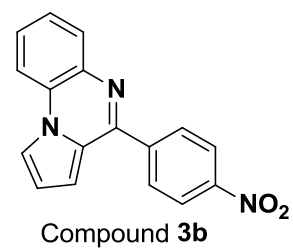


Figure 3: ¹H NMR spectrum of **3b**

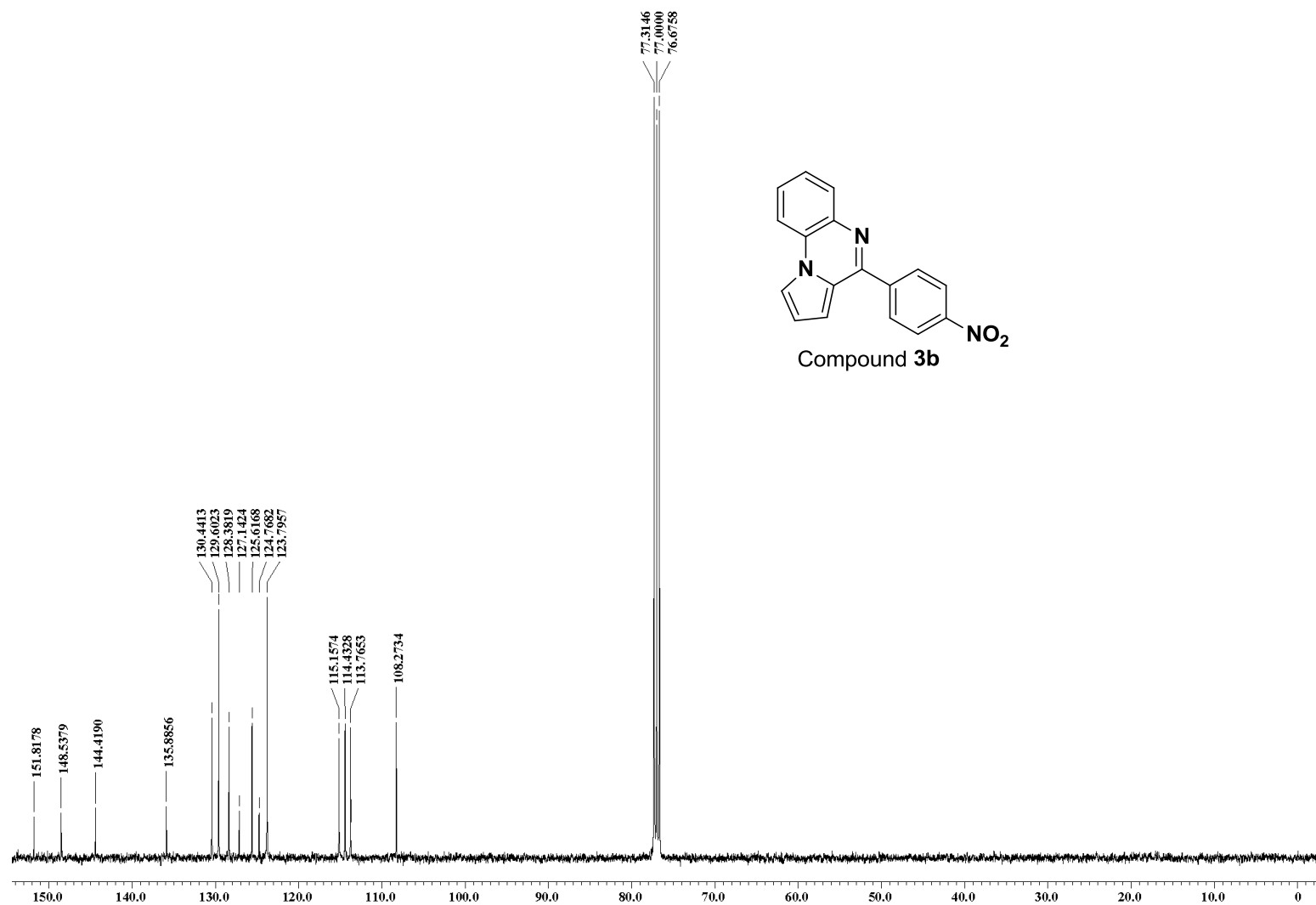


Figure 4: ¹³C NMR spectrum of 3b

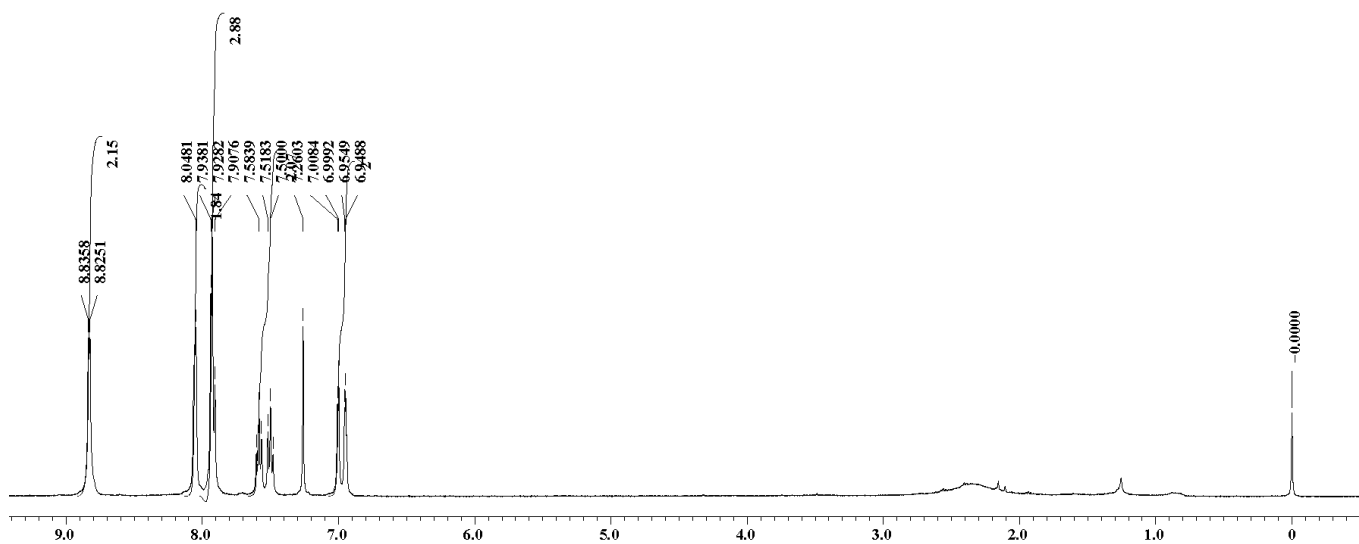
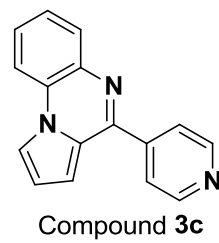
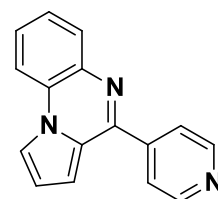


Figure 5: ¹H NMR spectrum of **3c**



Compound **3c**

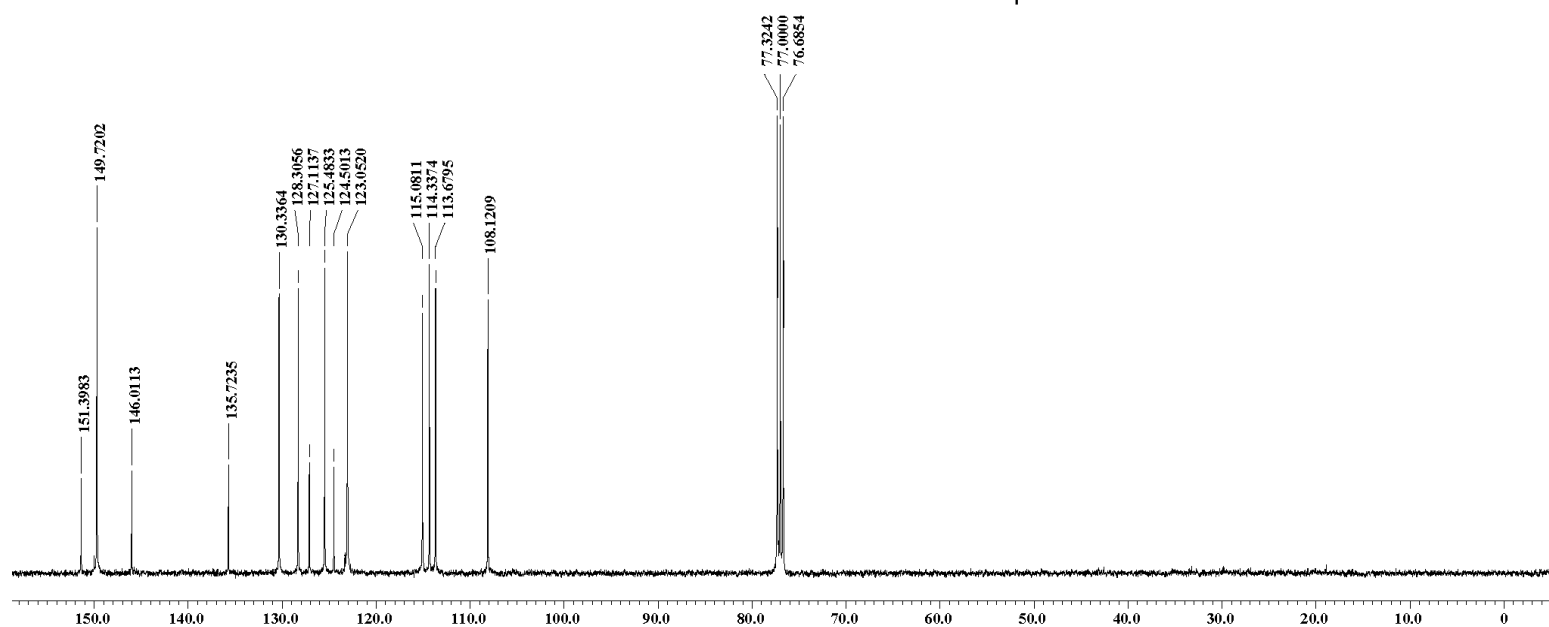
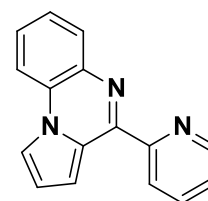


Figure 6: ^{13}C NMR spectrum of **3c**



Compound **3d**

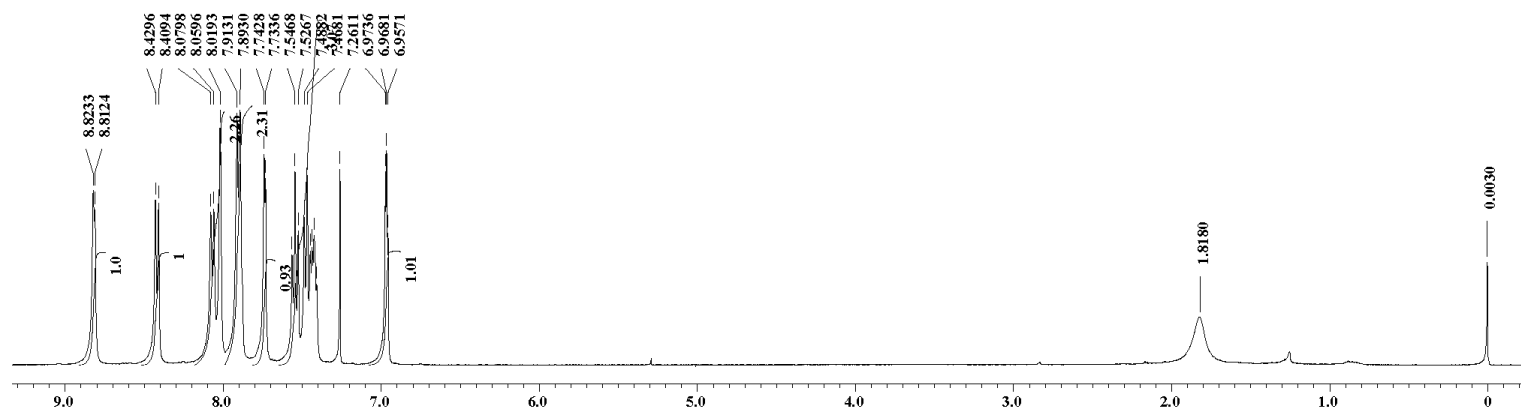


Figure 7: ^1H NMR spectrum of 3d

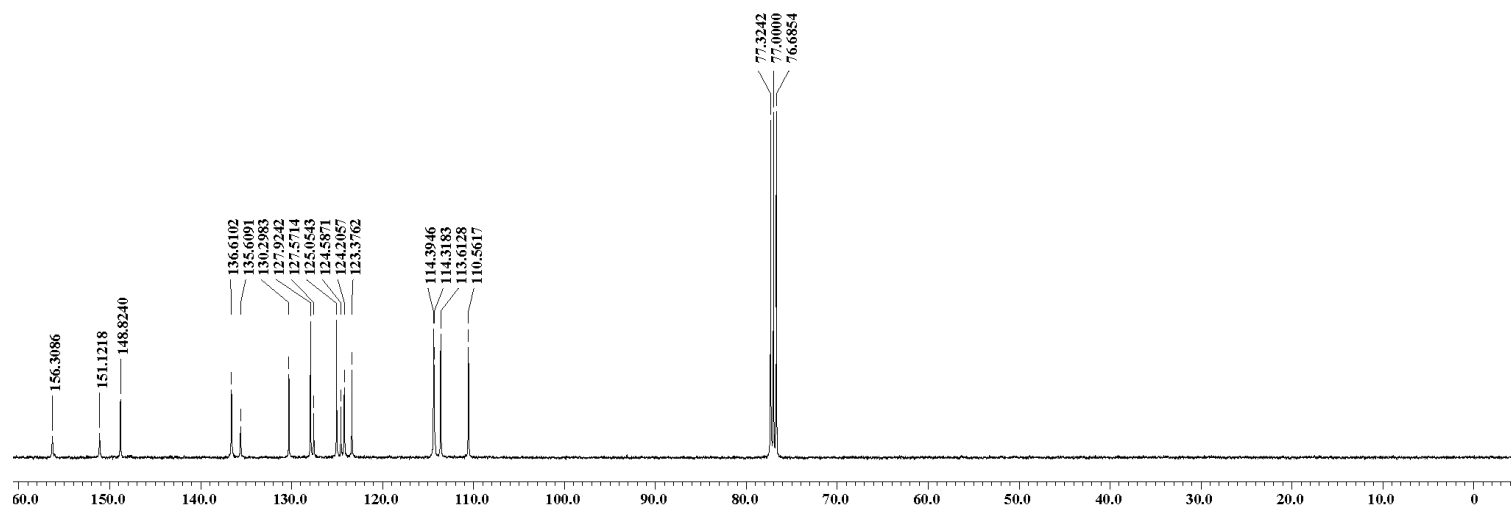
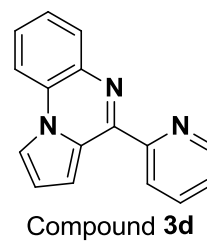
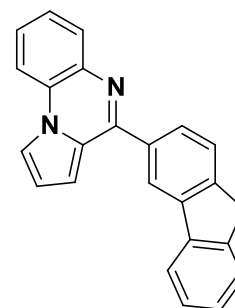


Figure 8: ¹³C NMR spectrum of **3d**



Compound **3e**

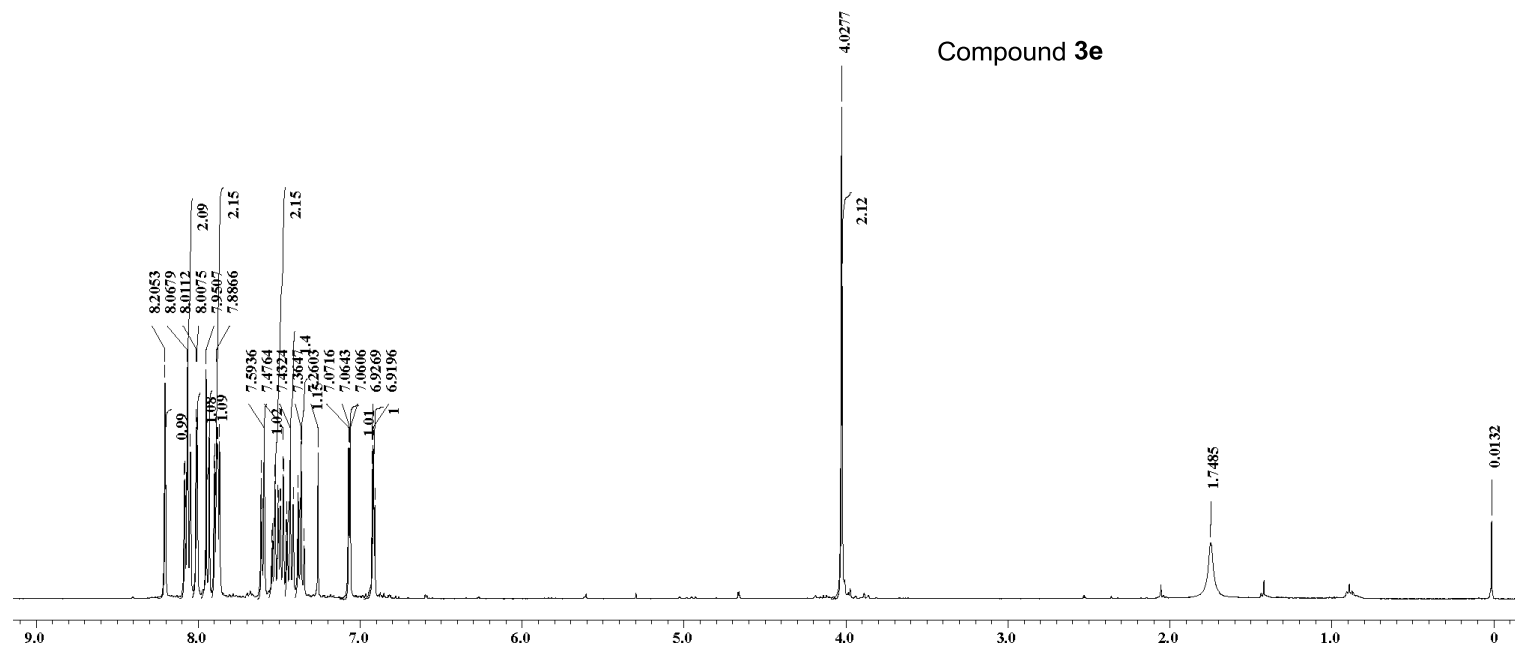
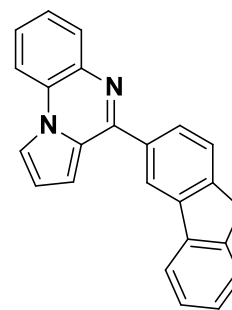


Figure 9: ¹H NMR spectrum of **3e**



Compound **3e**

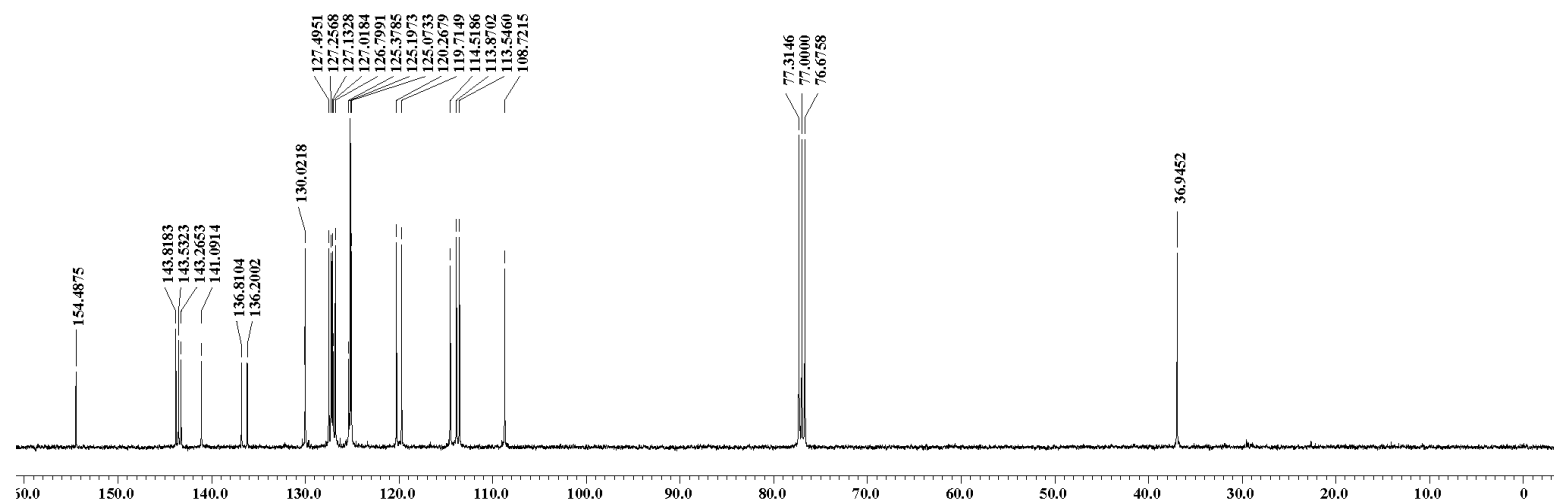
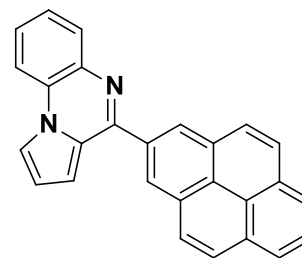


Figure 10: ^{13}C NMR spectrum of **3e**



Compound 3f

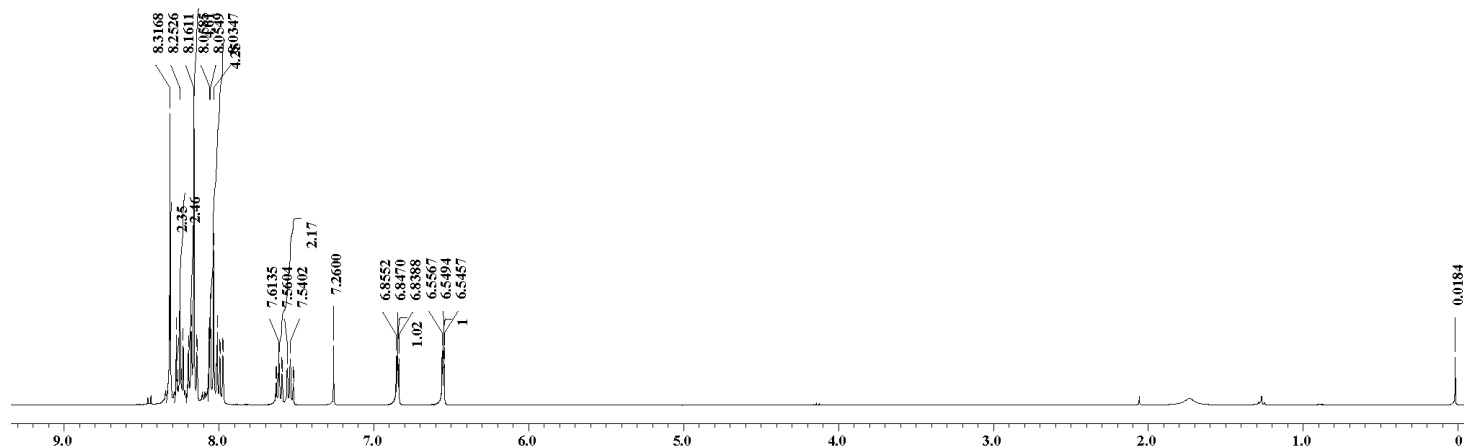
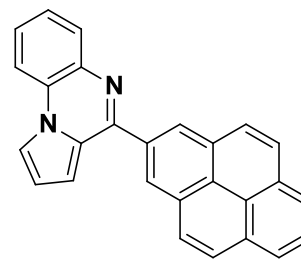


Figure 11: ¹H NMR spectrum of 3f



Compound **3f**

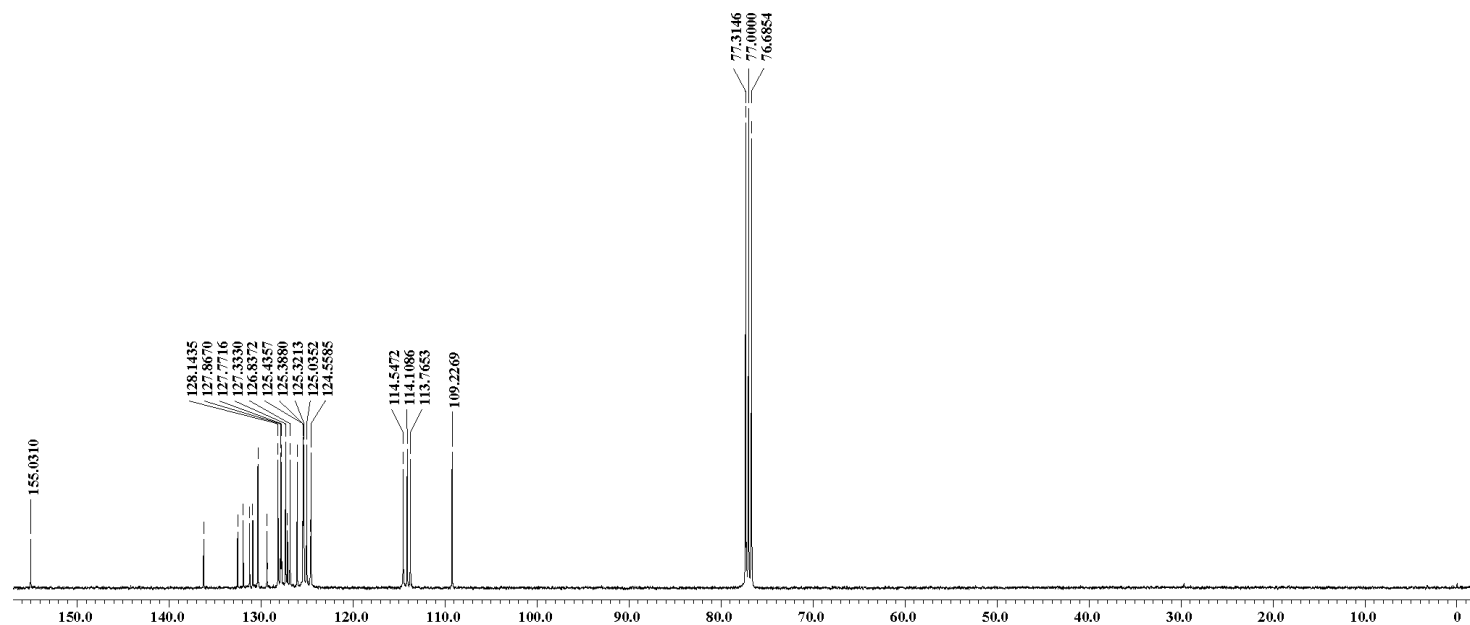
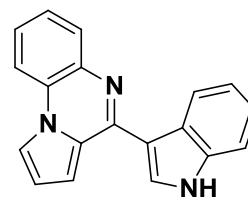


Figure 12: ^{13}C NMR spectrum of **3f**



Compound **3g**

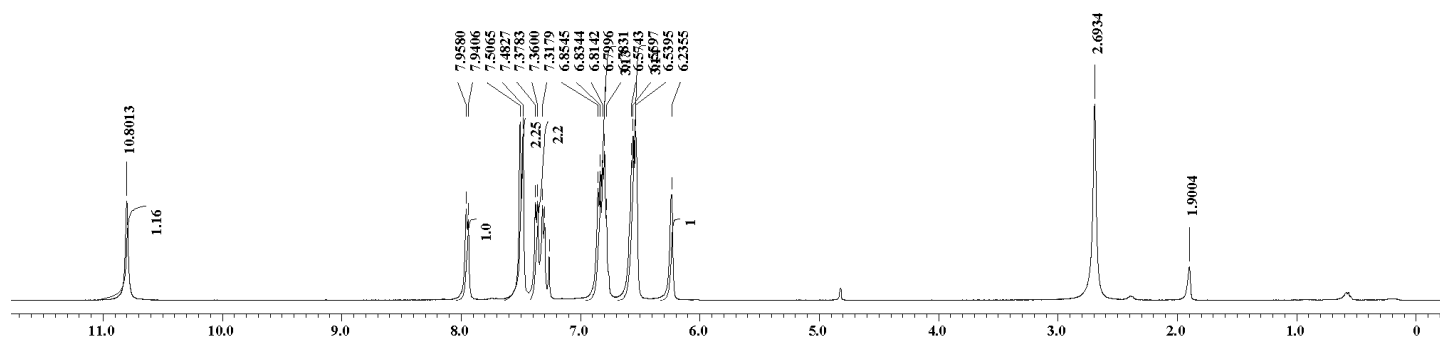
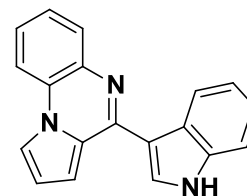


Figure 13: ^1H NMR spectrum of **3g**



Compound **3g**

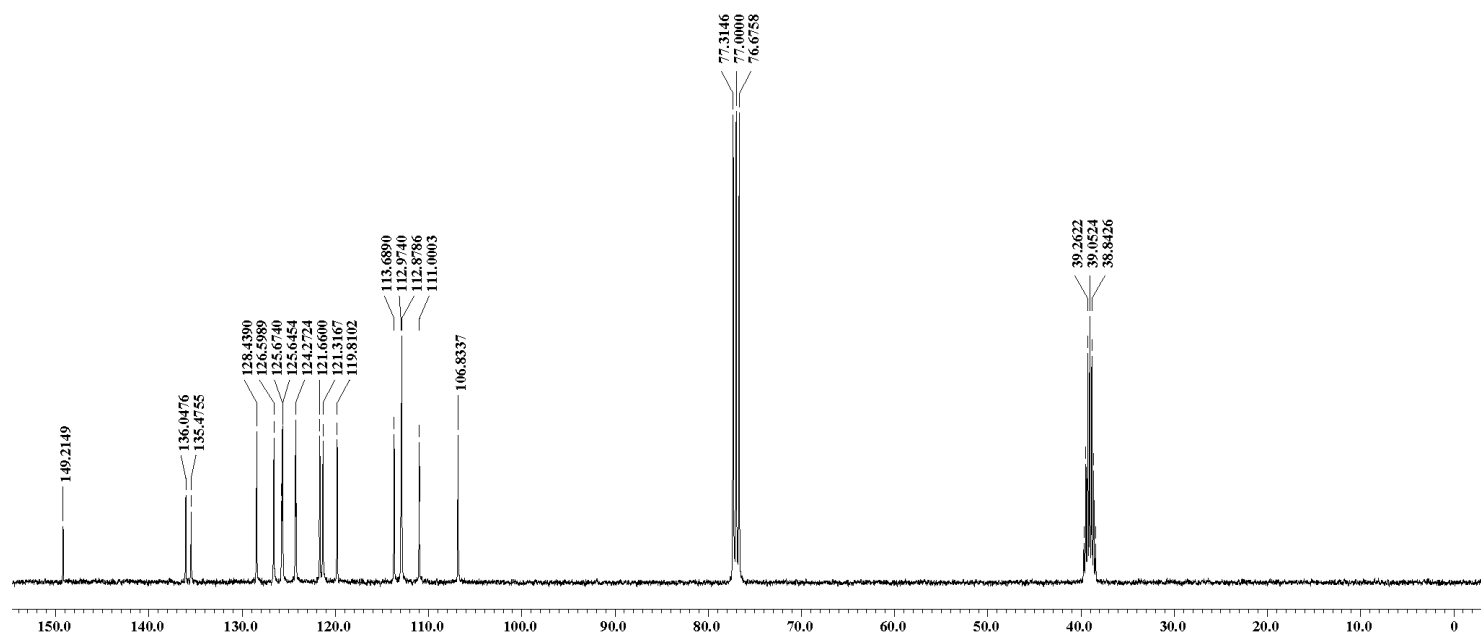


Figure 14: ^{13}C NMR spectrum of **3g**

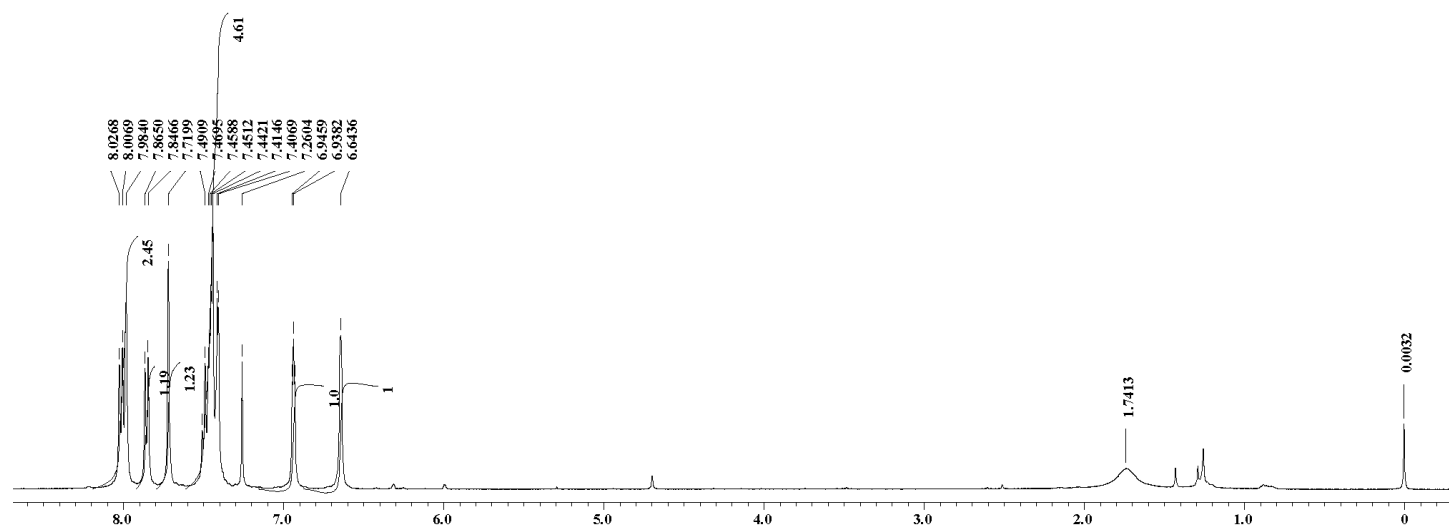
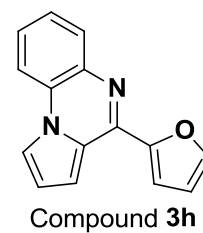
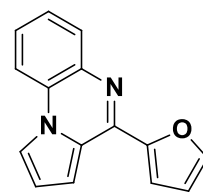


Figure 15: ¹H NMR spectrum of 3h



Compound **3h**

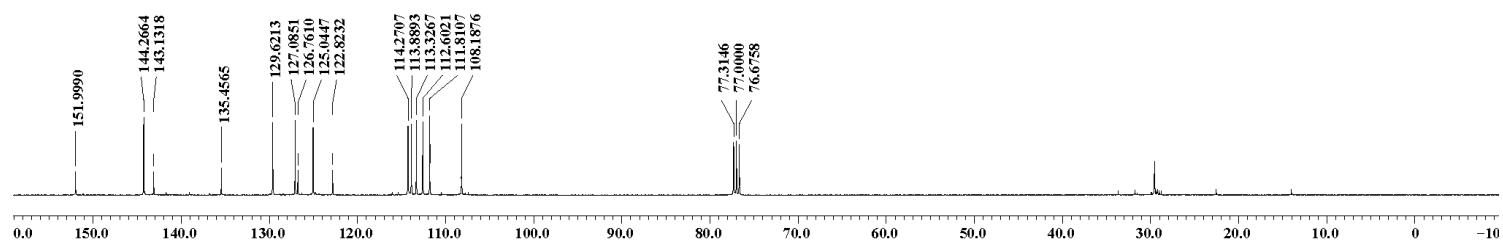
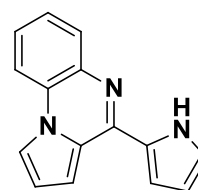


Figure 16: ^{13}C NMR spectrum of 3h



Compound **3i**

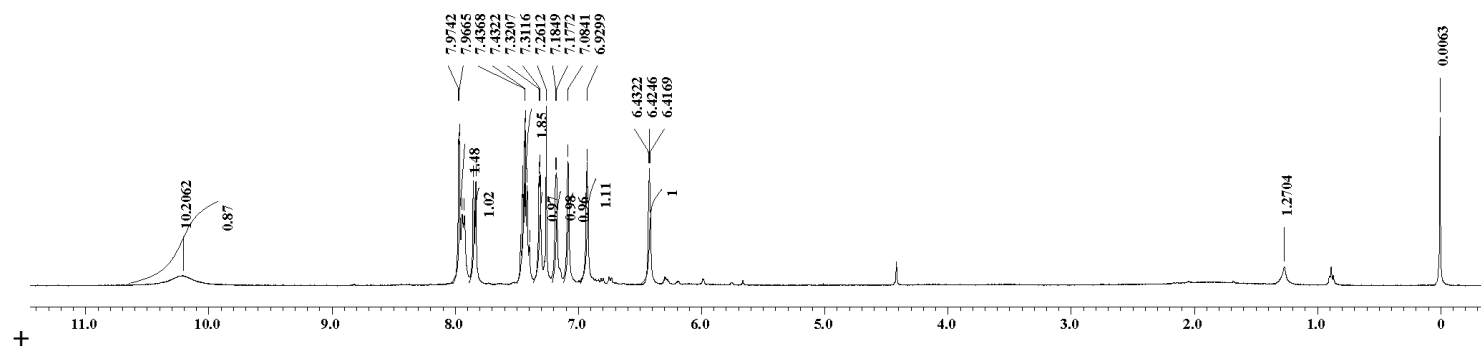


Figure 17: ^1H NMR spectrum of **3i**

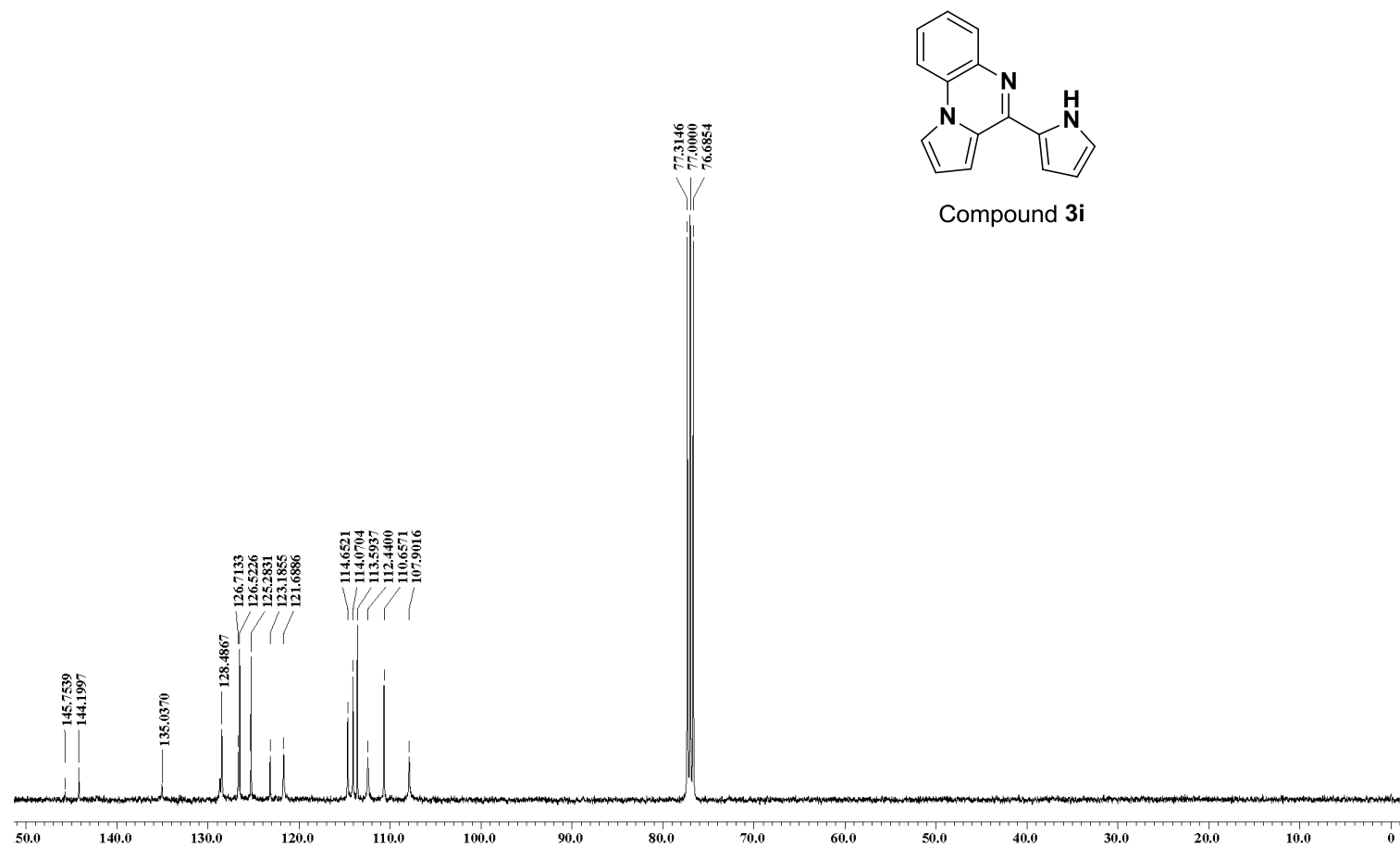
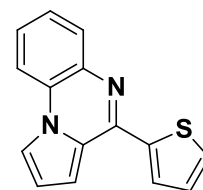


Figure 18: ^{13}C NMR spectrum of 3i



Compound **3j**

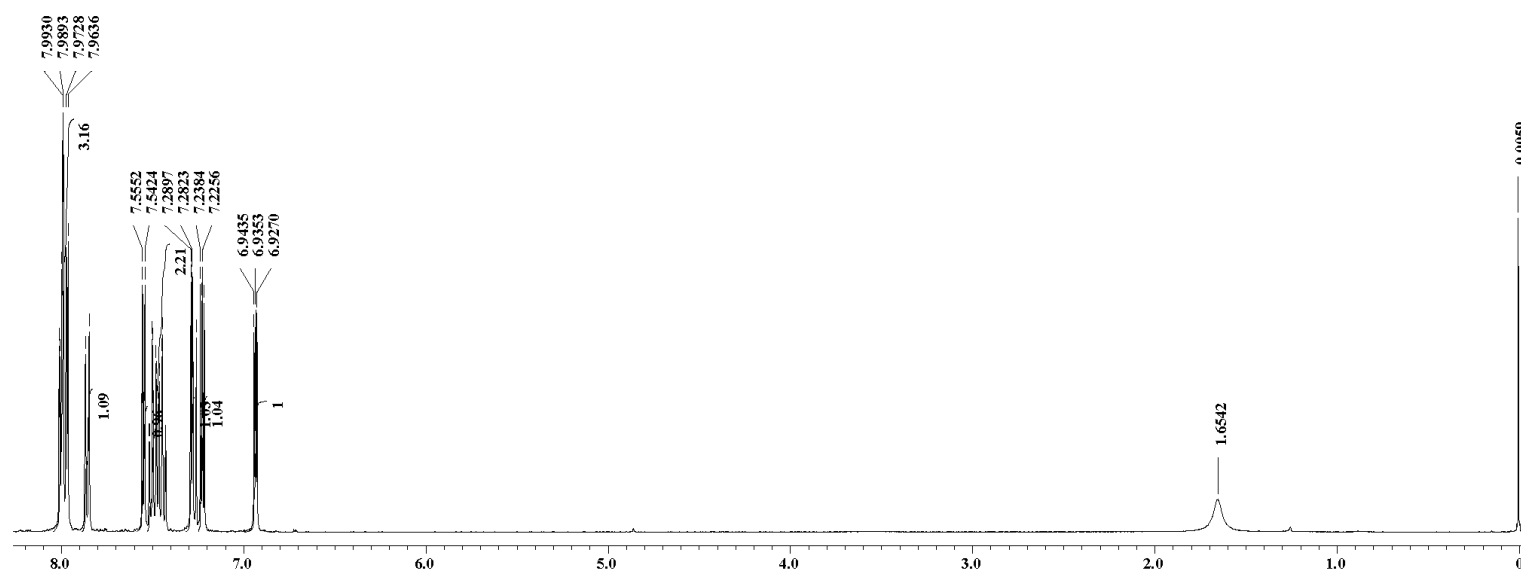
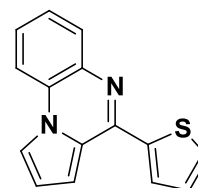


Figure 19: ^1H NMR spectrum of **3j**



Compound **3j**

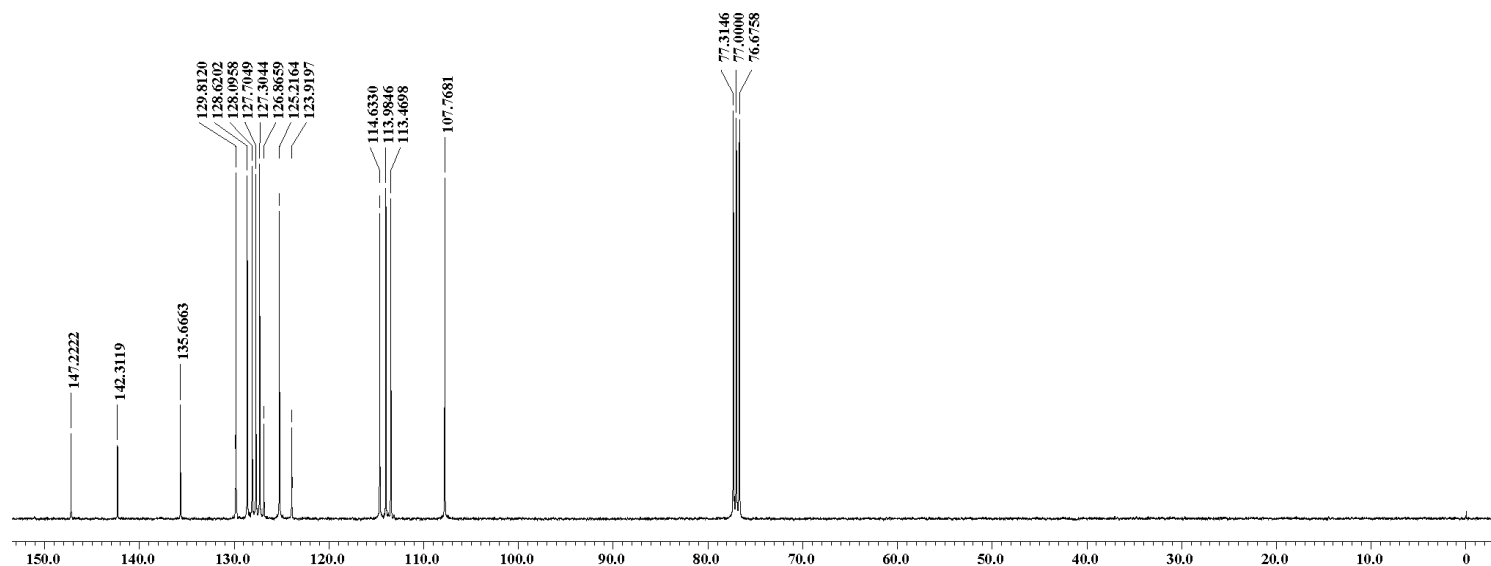


Figure 20: ^{13}C NMR spectrum of **3j**

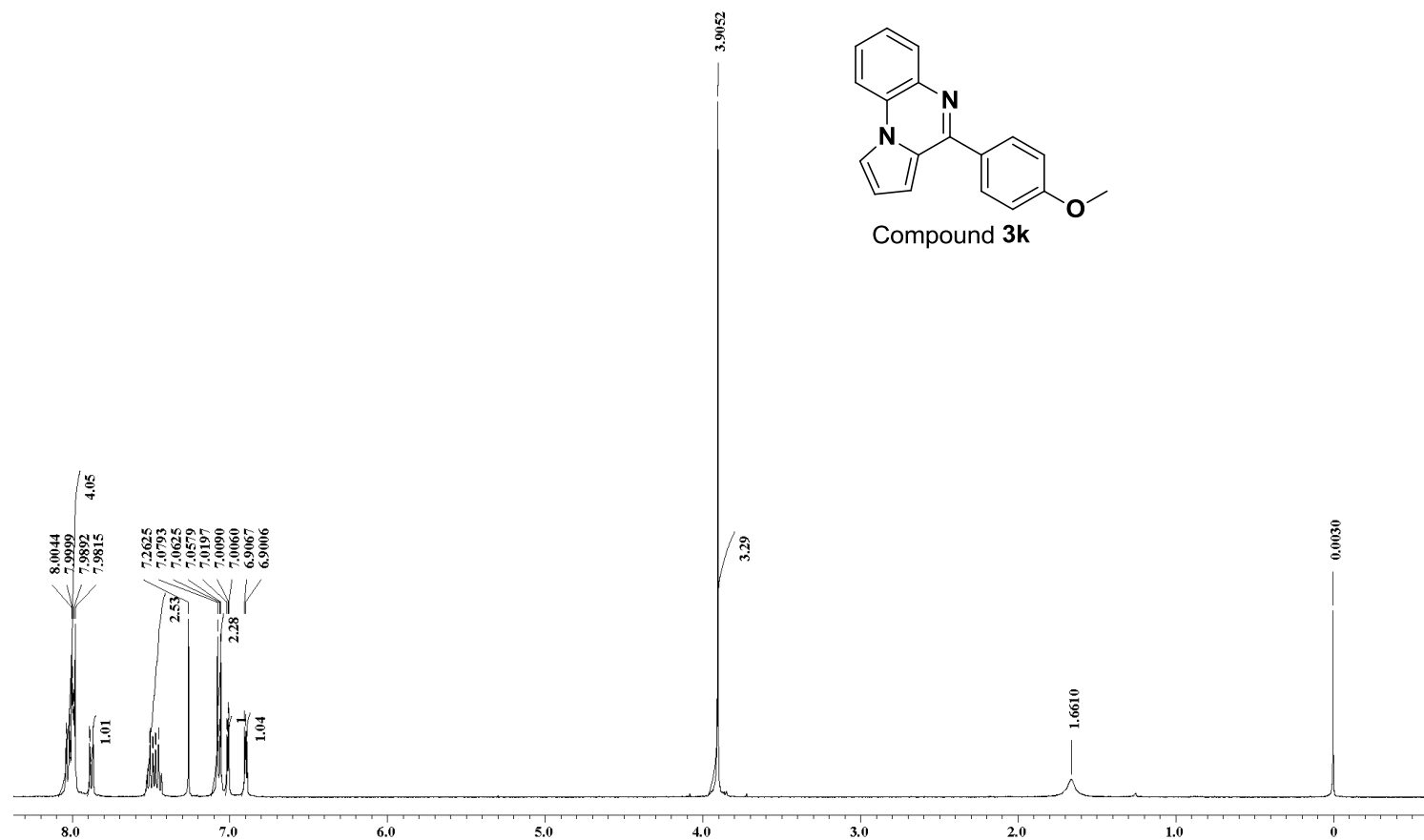


Figure 21: ¹H NMR spectrum of 3k

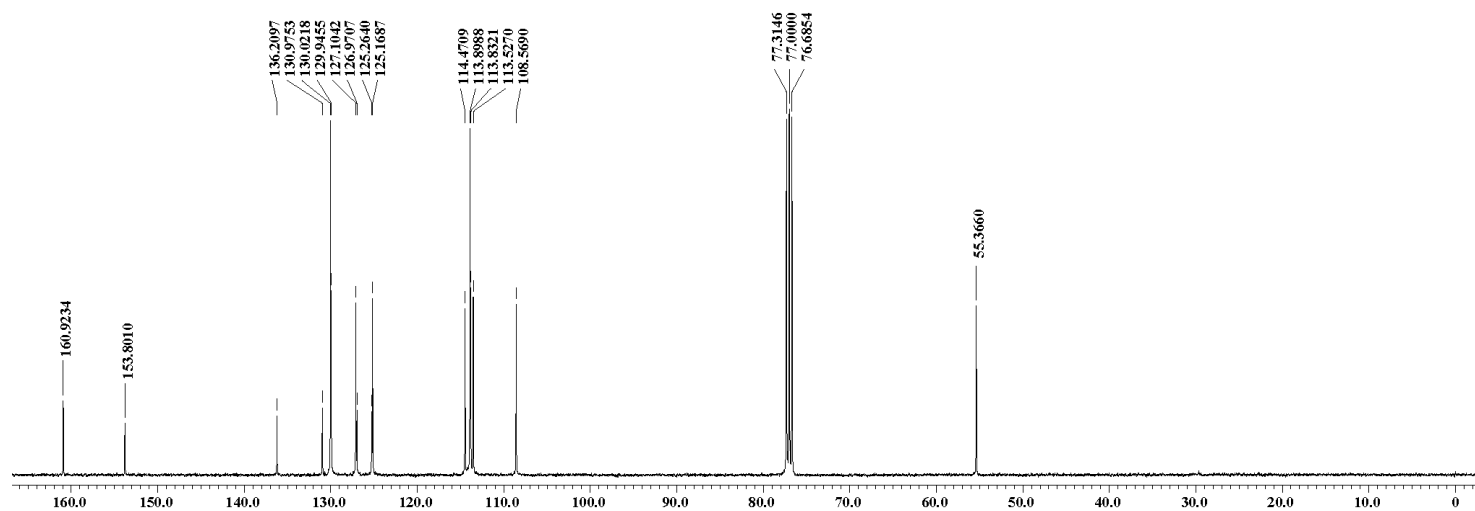
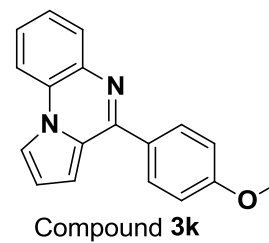


Figure 22: ^{13}C NMR spectrum of **3k**

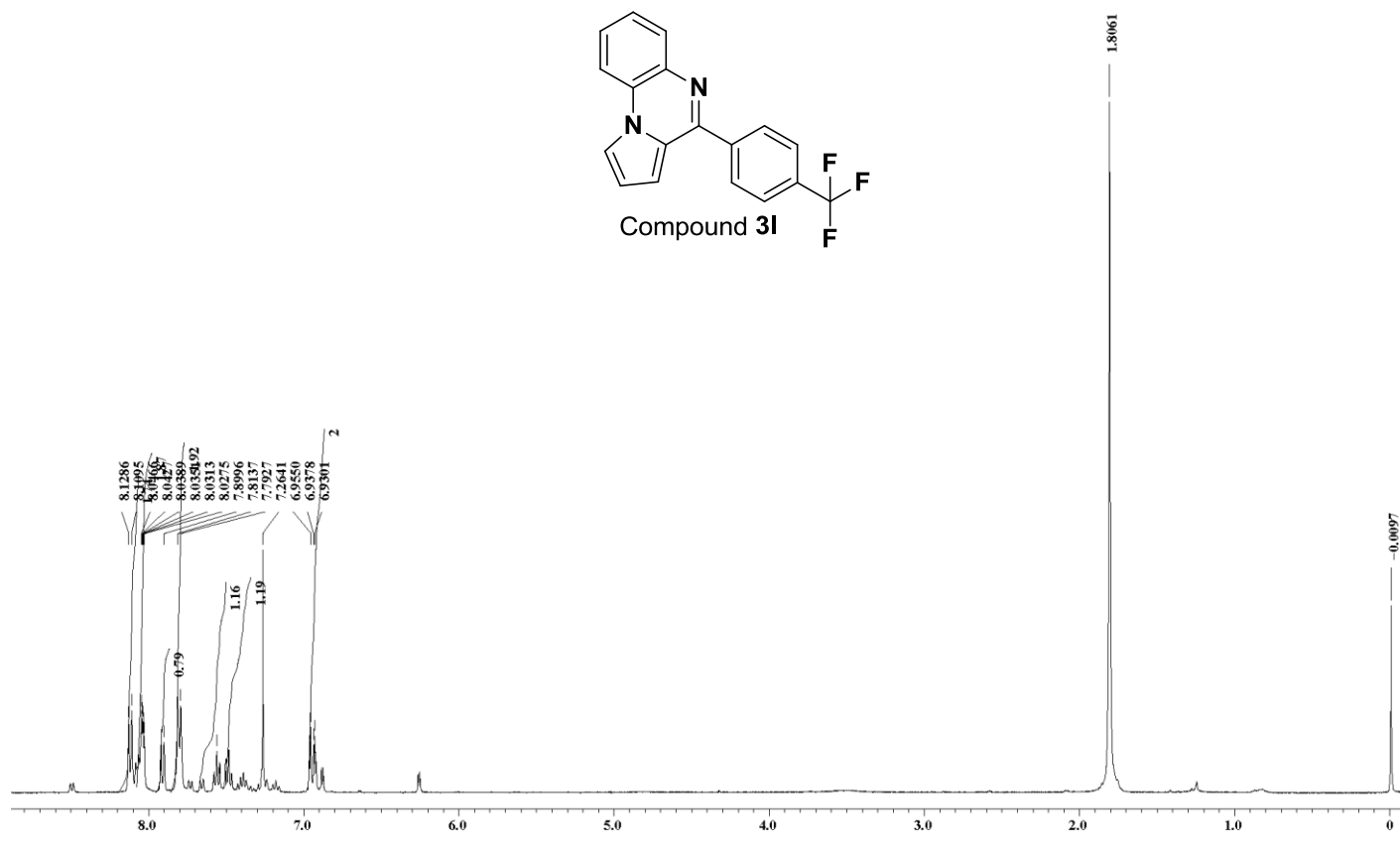


Figure 23: ^1H NMR spectrum of 3I

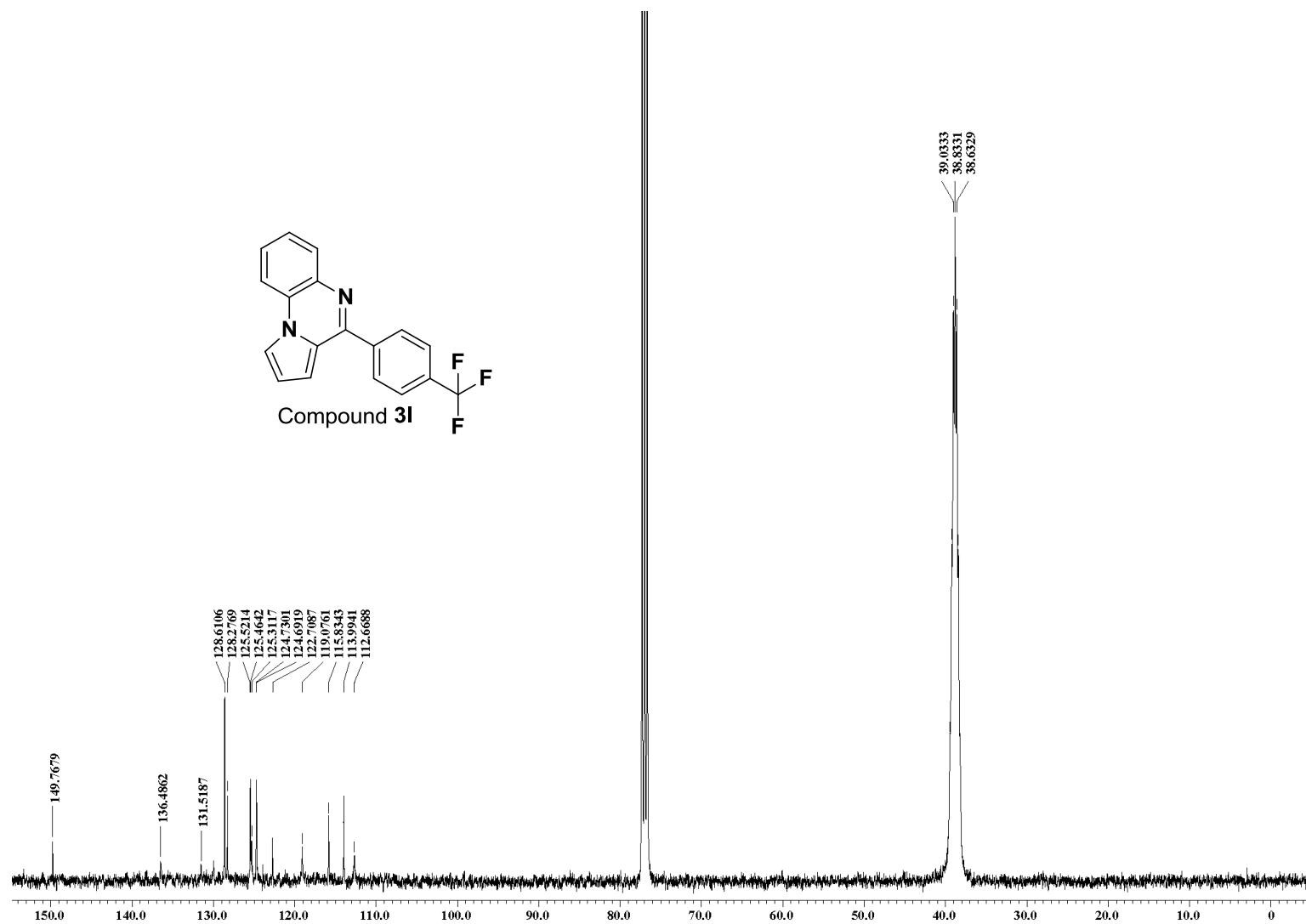
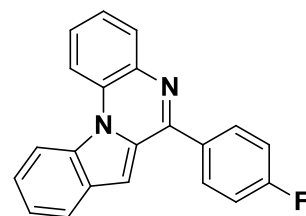


Figure 24: ^{13}C NMR spectrum of 3I



Compound **3m**

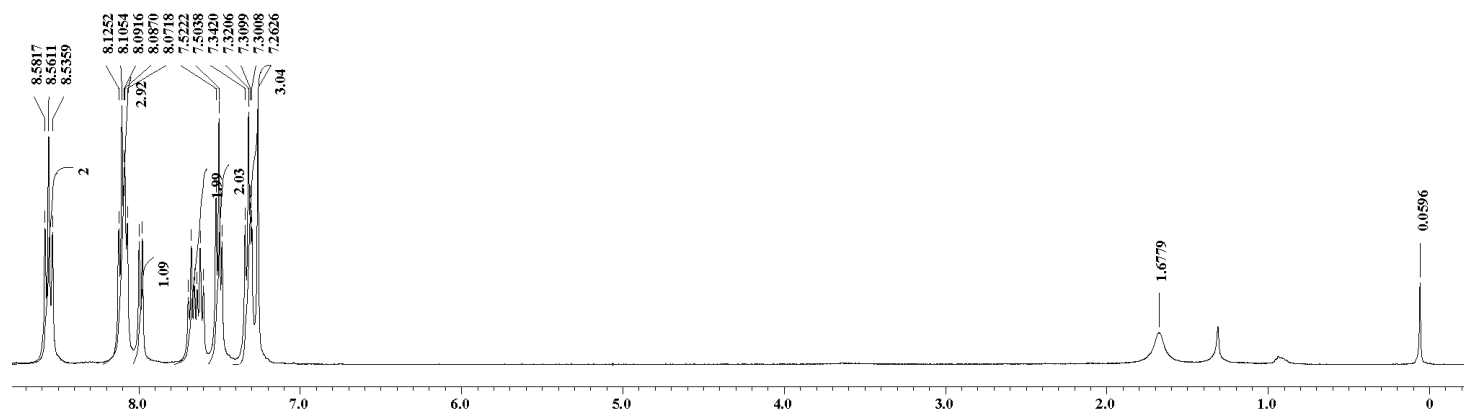


Figure 25: ^1H NMR spectrum of **3m**

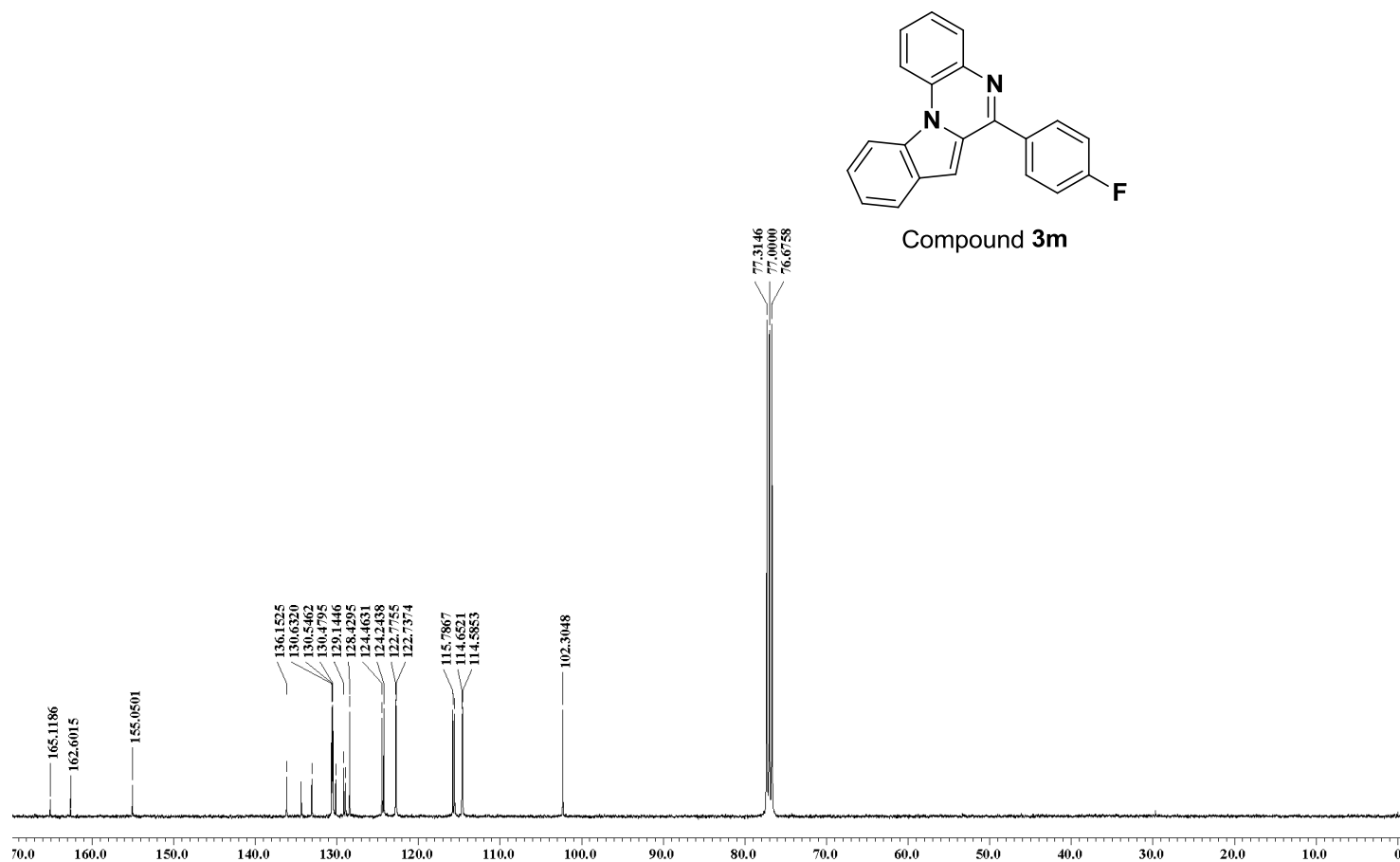


Figure 26: ¹³C NMR spectrum of 3m

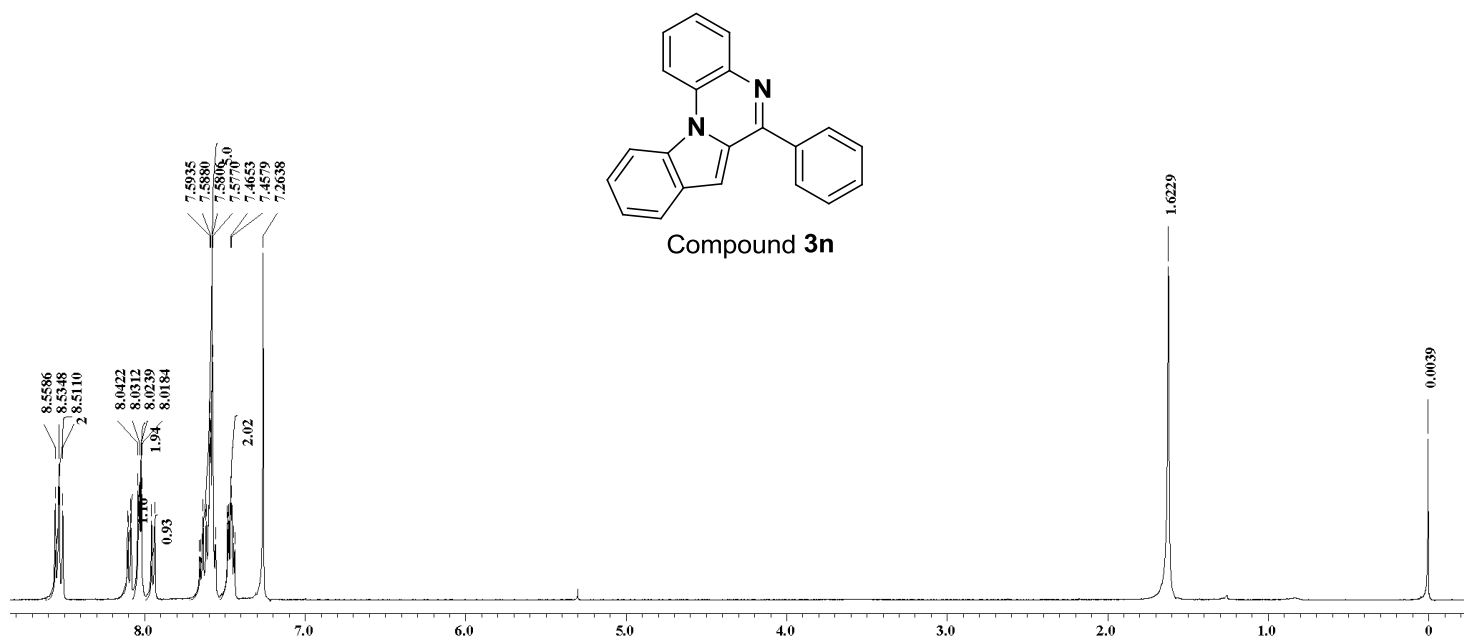


Figure 27: ¹H NMR spectrum of **3n**

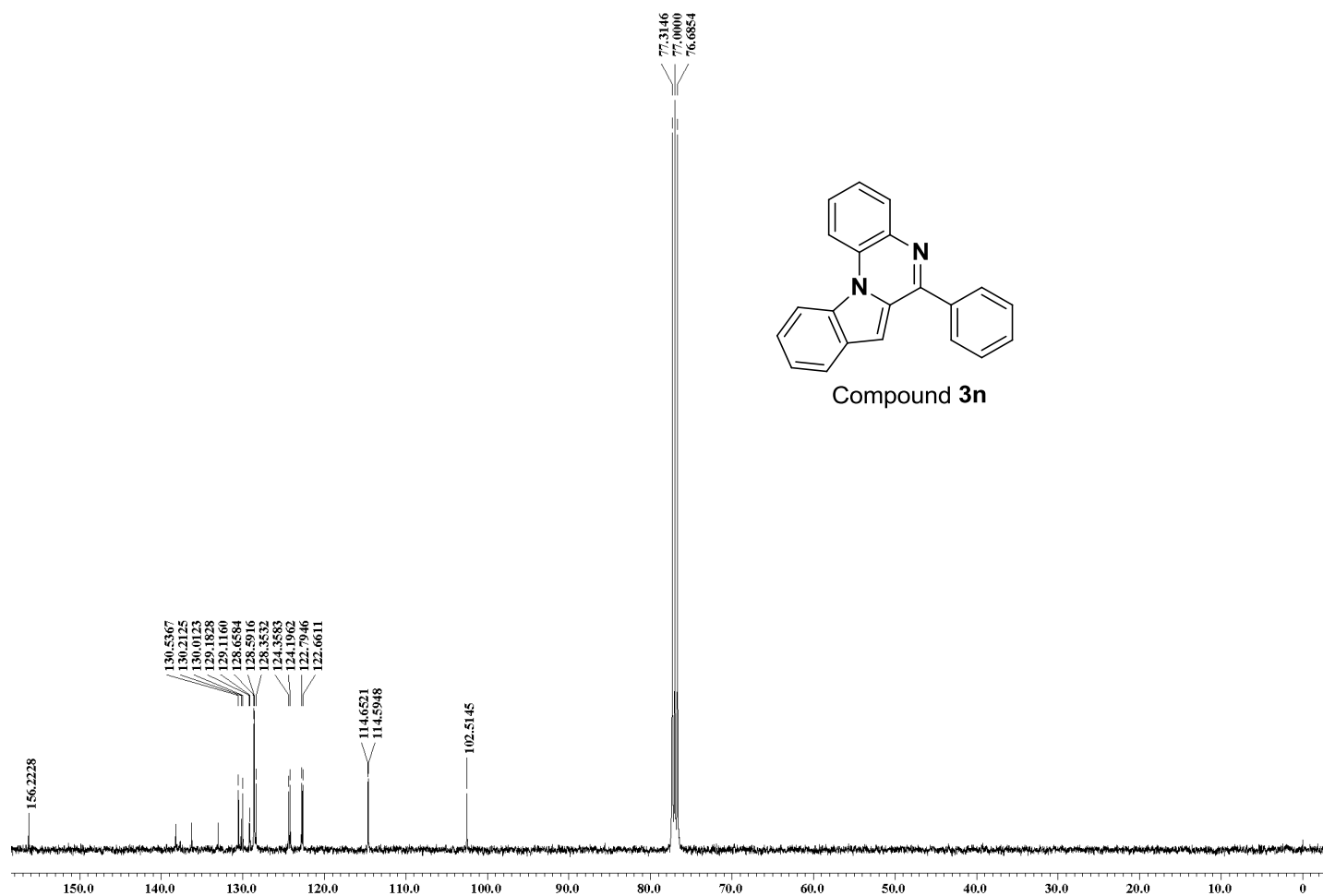
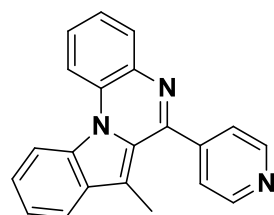


Figure 28: ^{13}C NMR spectrum of 3n



Compound **3o**

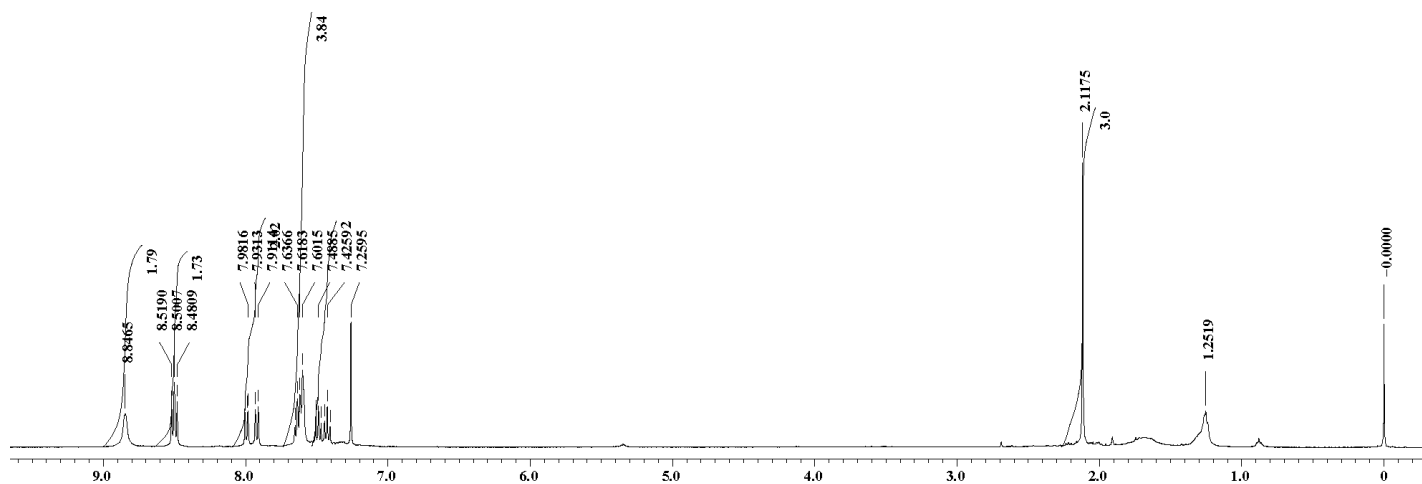


Figure 29: ^1H NMR spectrum of **3o**

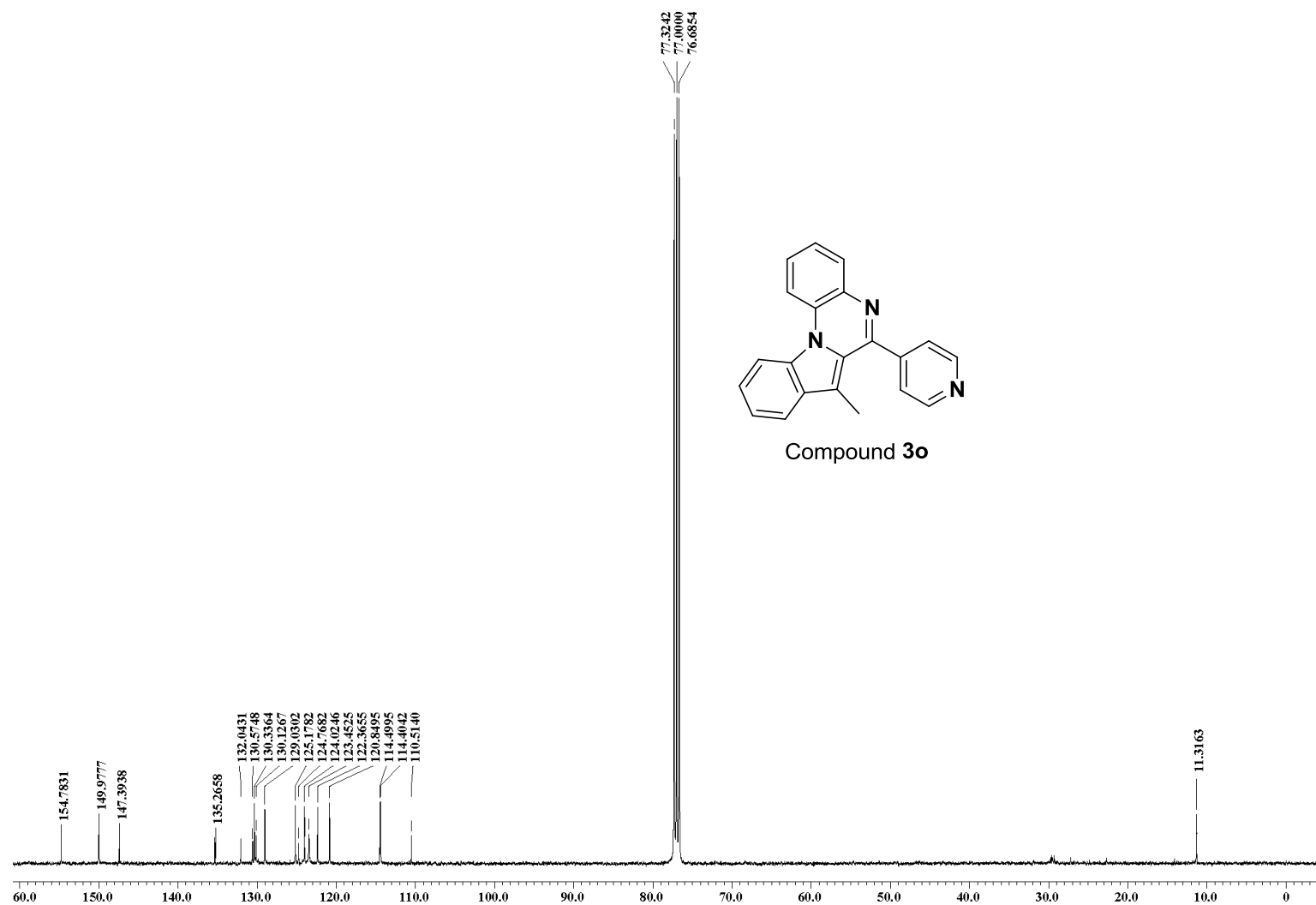


Figure 30 ¹³C NMR spectrum of 3o

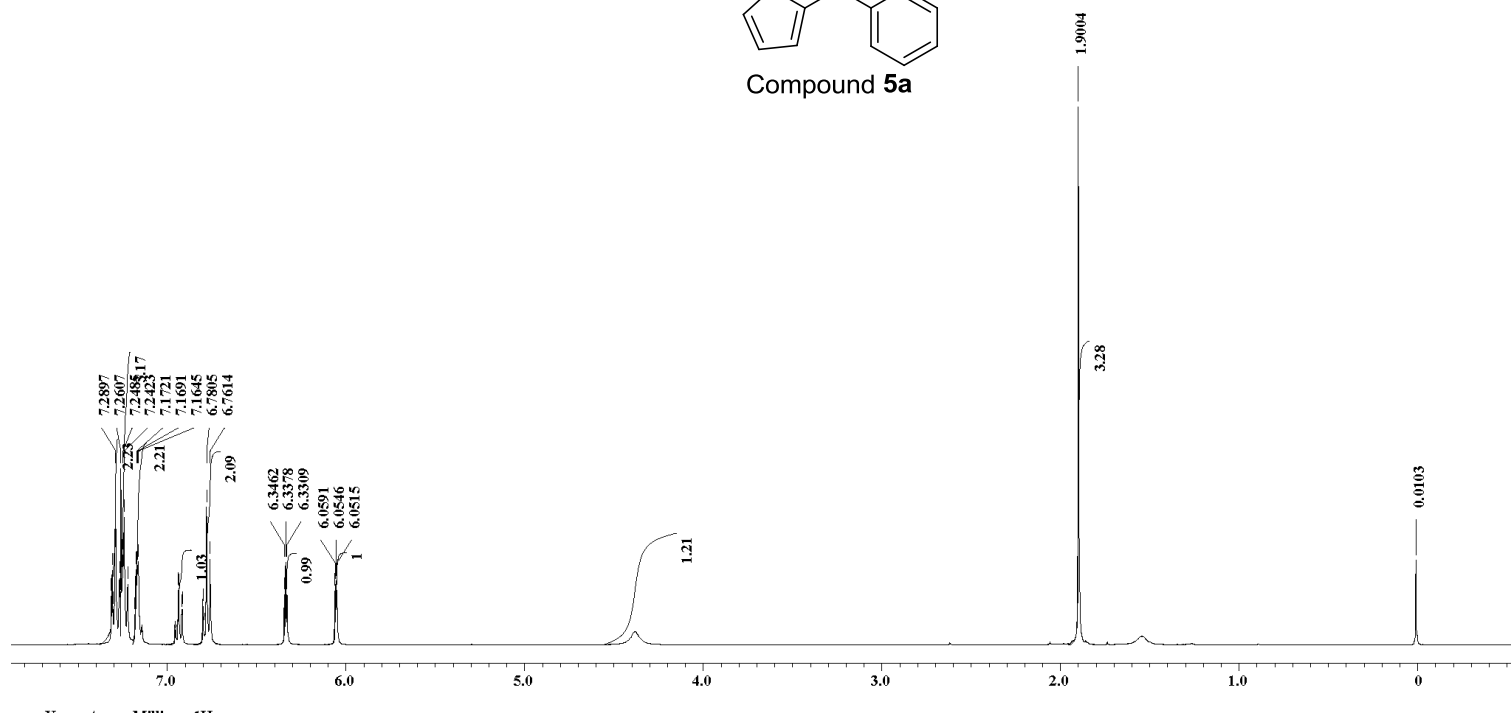
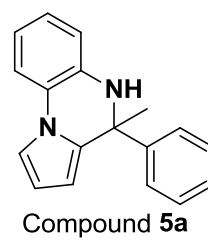


Figure 31: ¹H NMR spectrum of **5a**

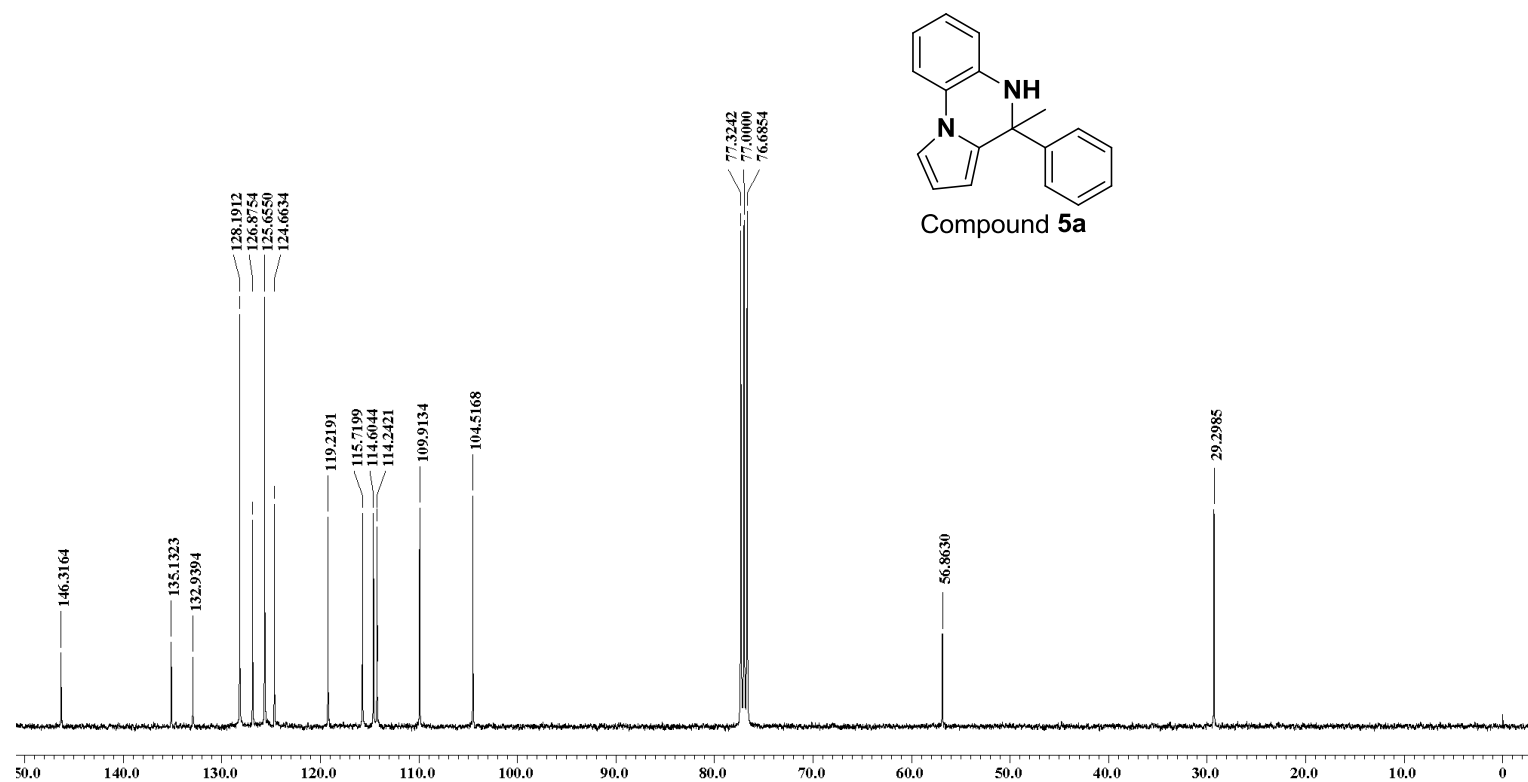


Figure 32: ^{13}C NMR spectrum of 5a

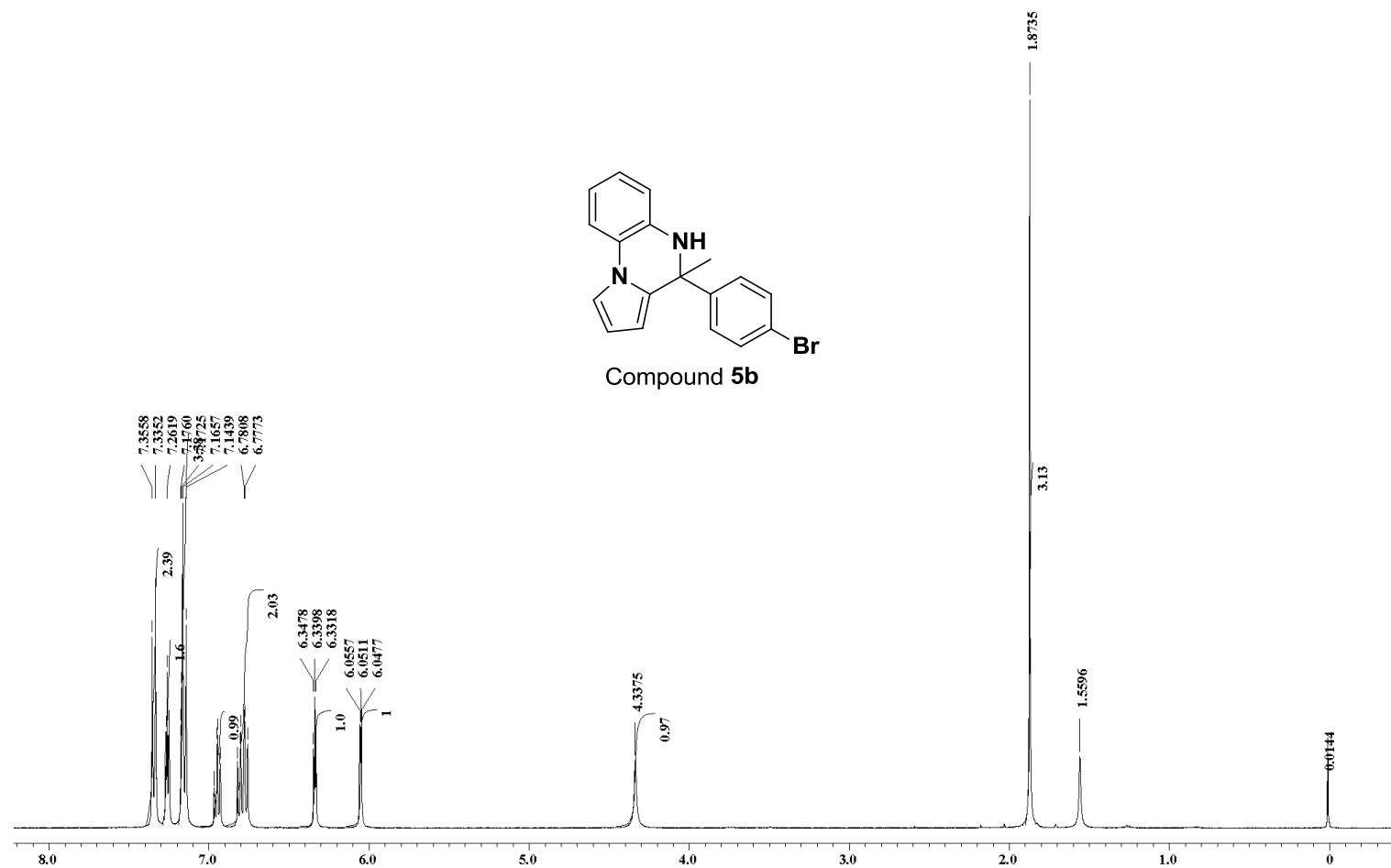


Figure 33: ¹H NMR spectrum of **5b**

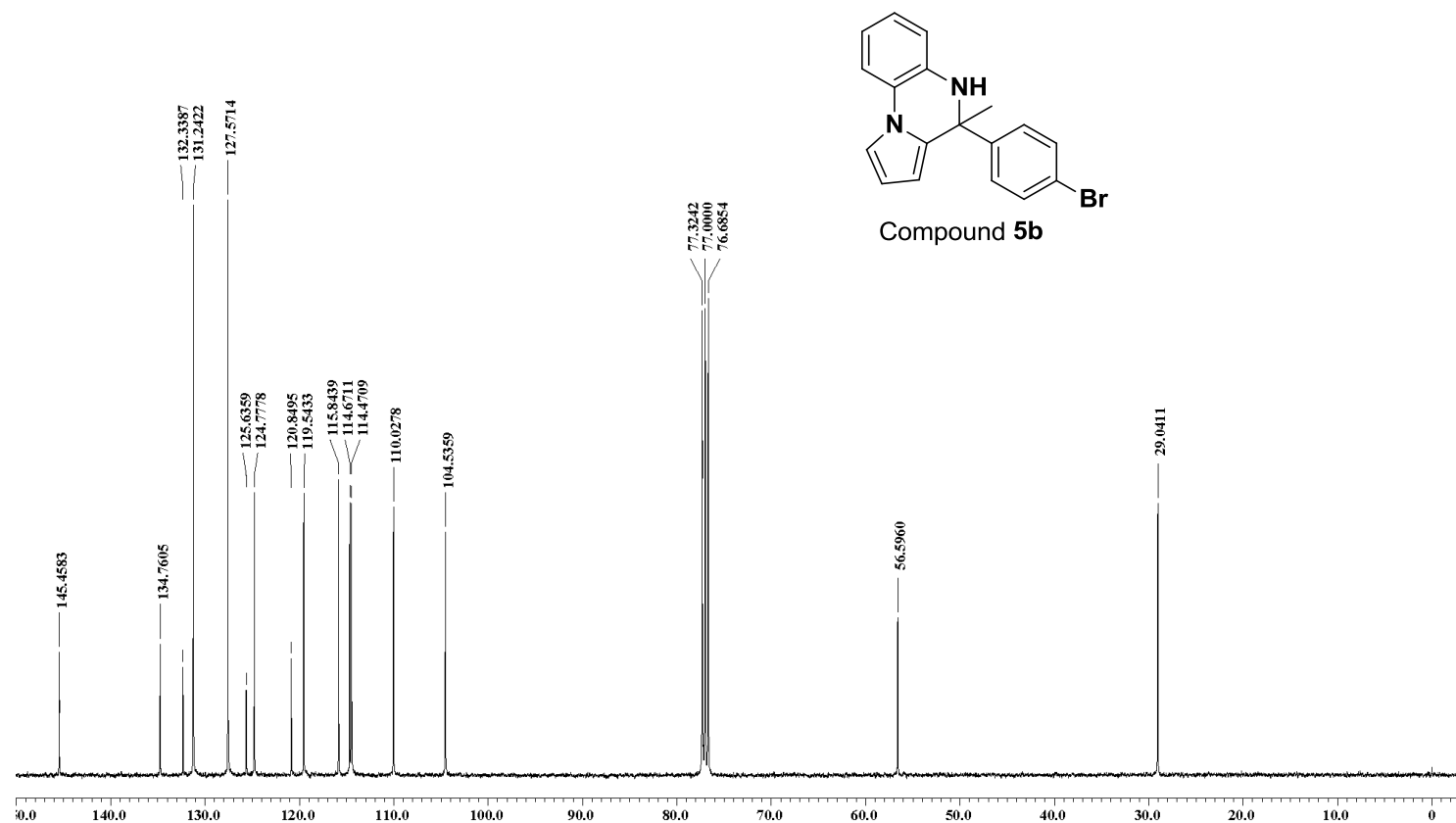


Figure 34: ¹³C NMR spectrum of 5b

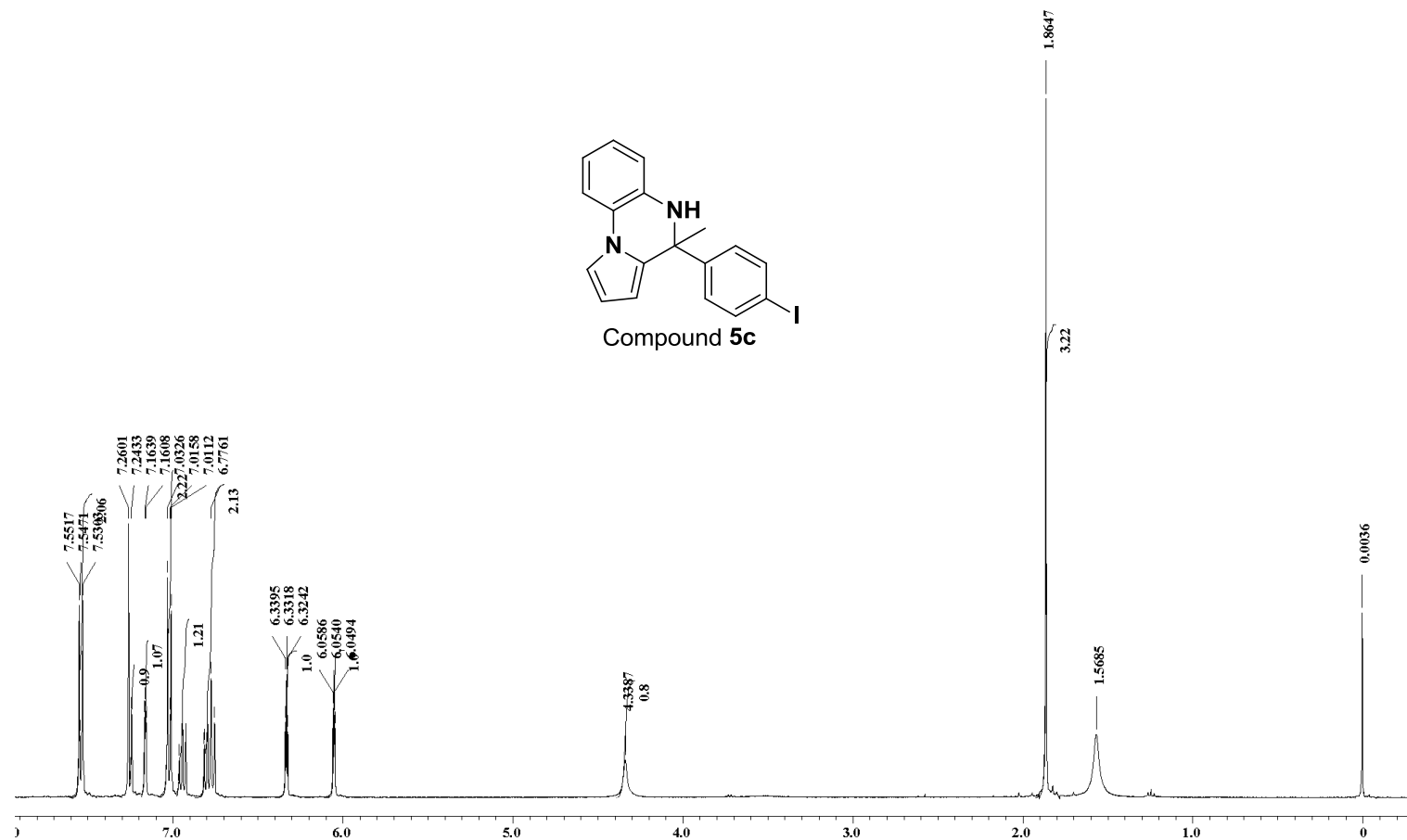


Figure 35: ¹H NMR spectrum of **5c**

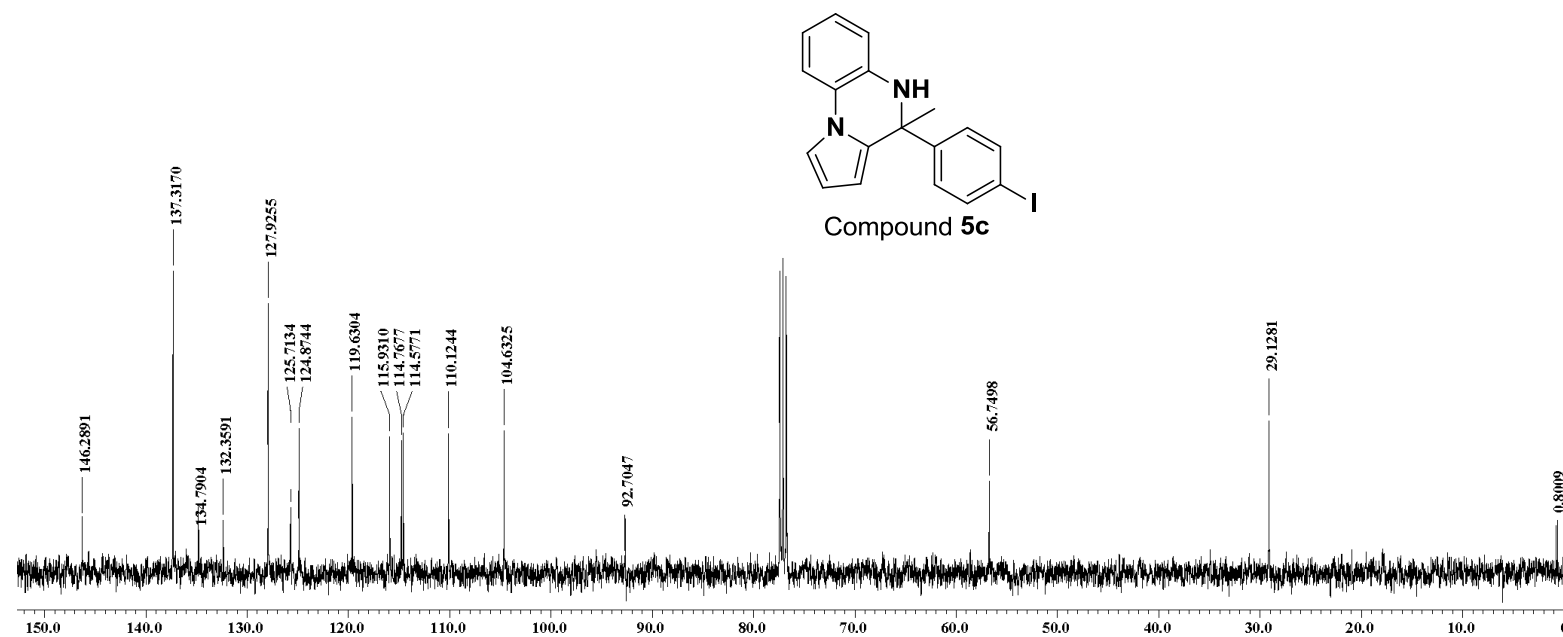


Figure 36: ^{13}C NMR spectrum of **5c**

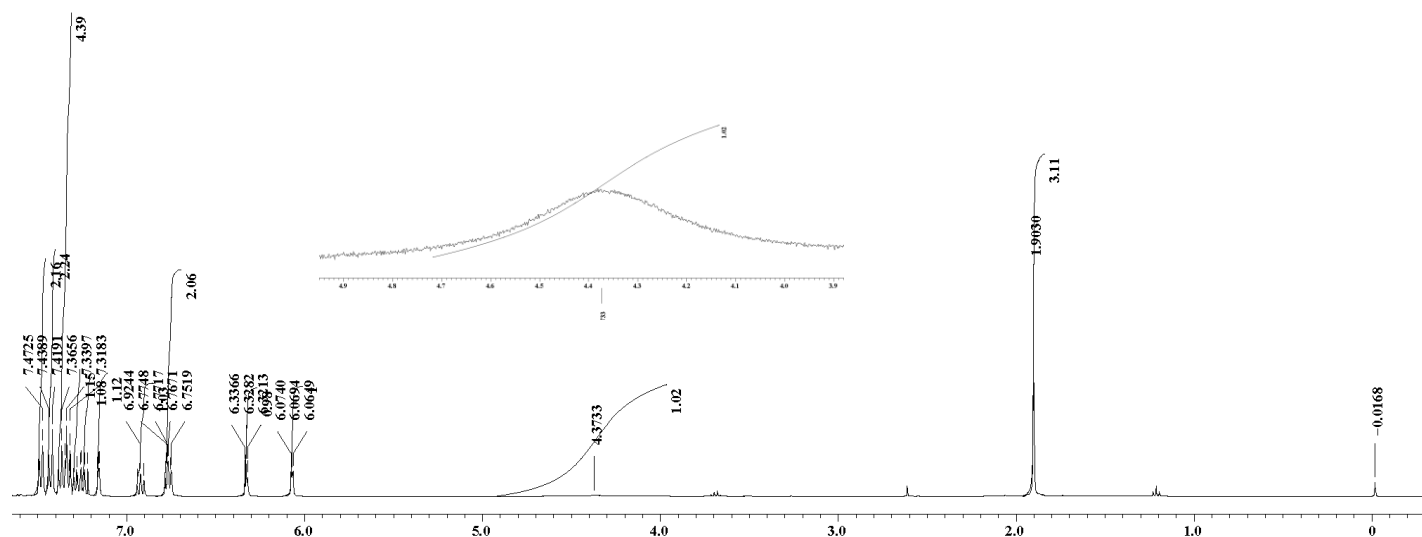
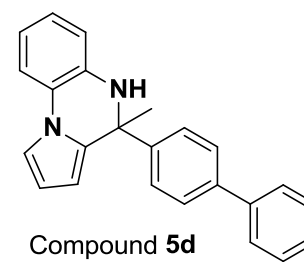


Figure 37: ¹H NMR spectrum of **5d**

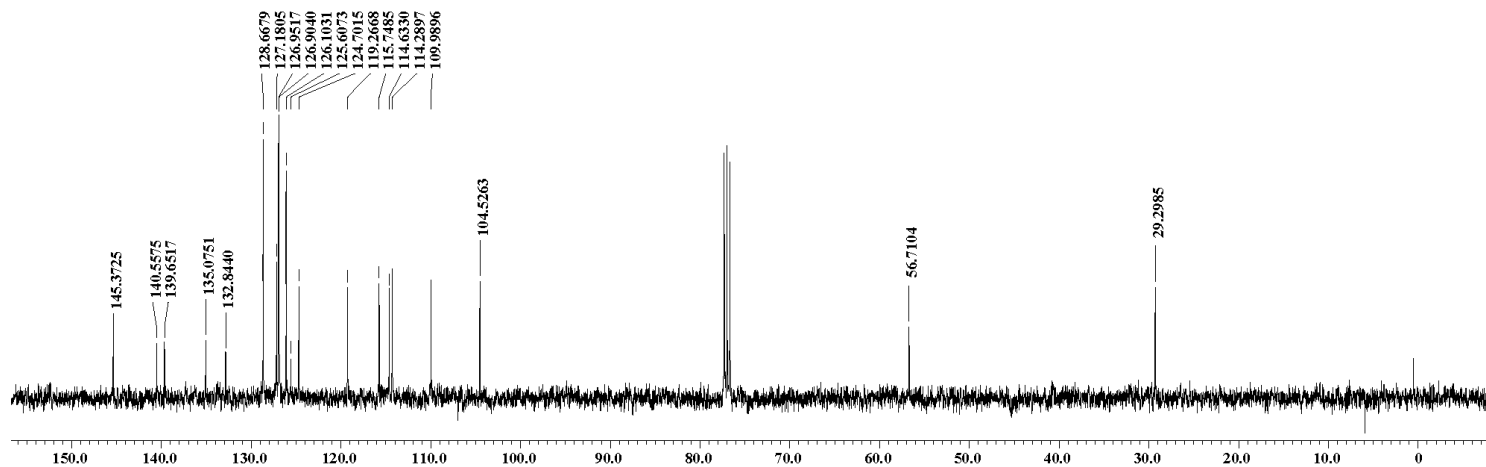
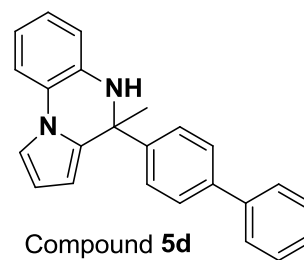


Figure 38: ¹³C NMR spectrum of **5d**

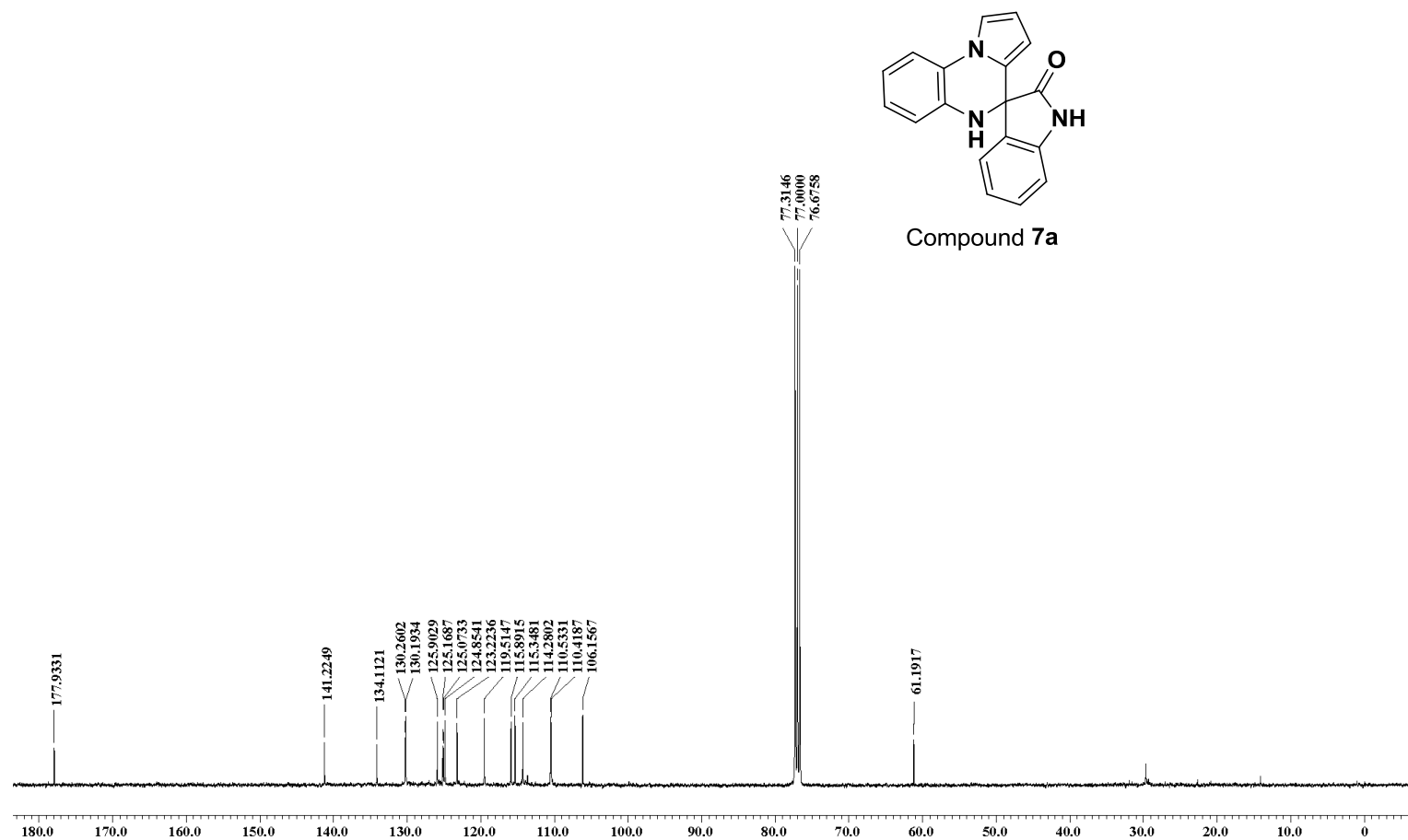


Figure 40: ^{13}C NMR spectrum of 7a

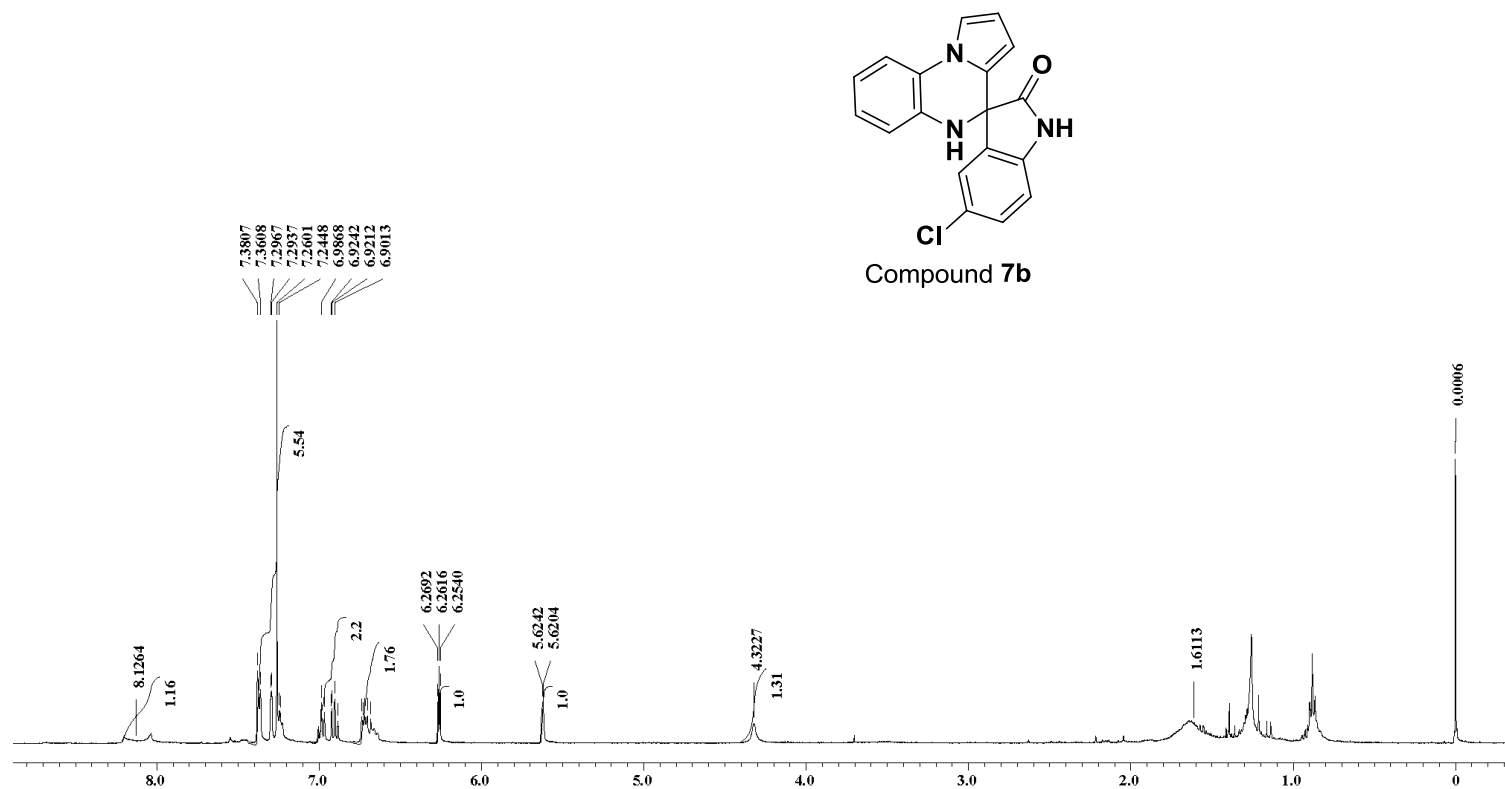
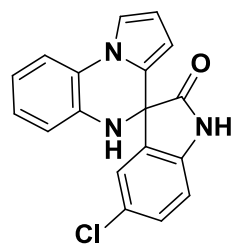


Figure 41: ^1H NMR spectrum of **7b**



Compound **7b**

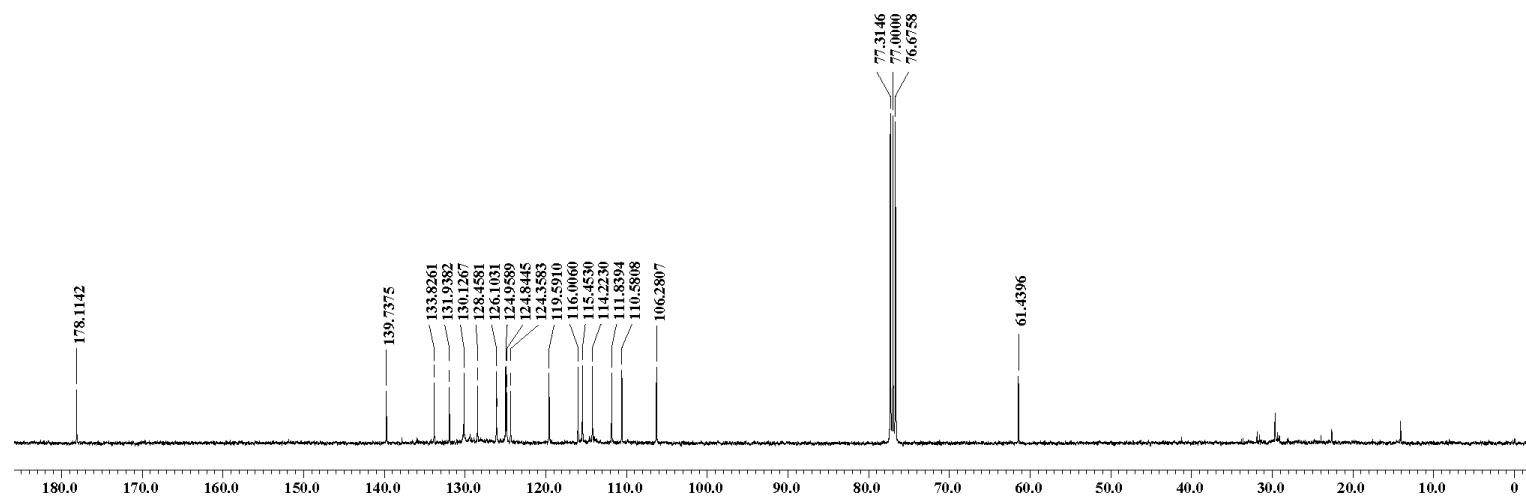
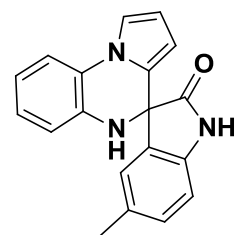


Figure 42: ^{13}C NMR spectrum of **7b**



Compound **7c**

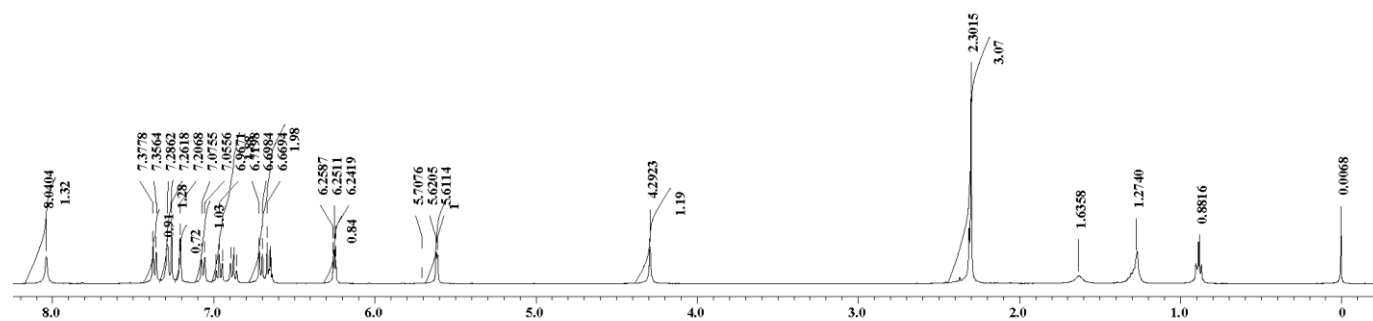


Figure 43: ¹H NMR spectrum of **7c**

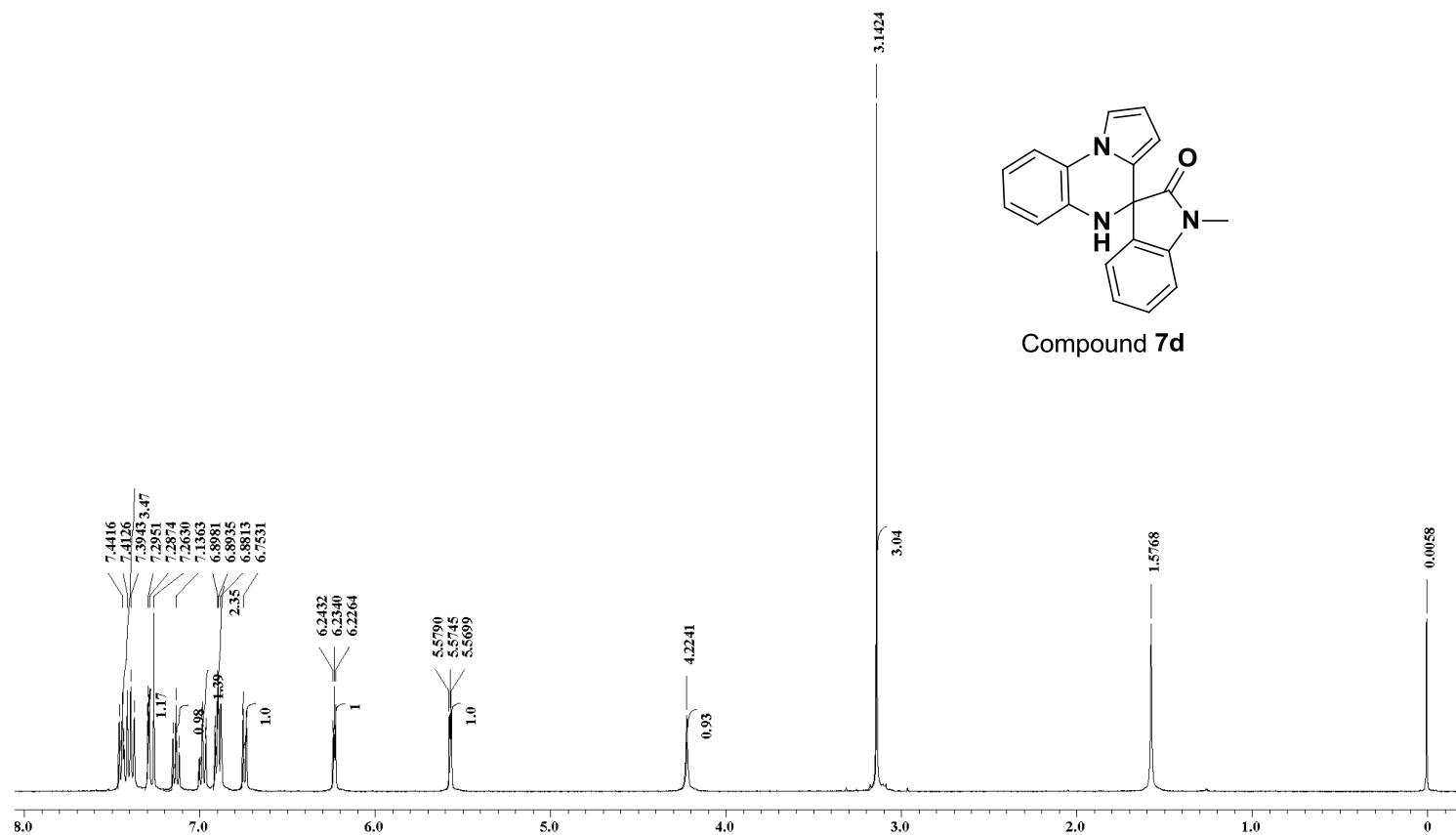


Figure 44: ¹H NMR spectrum of 7d

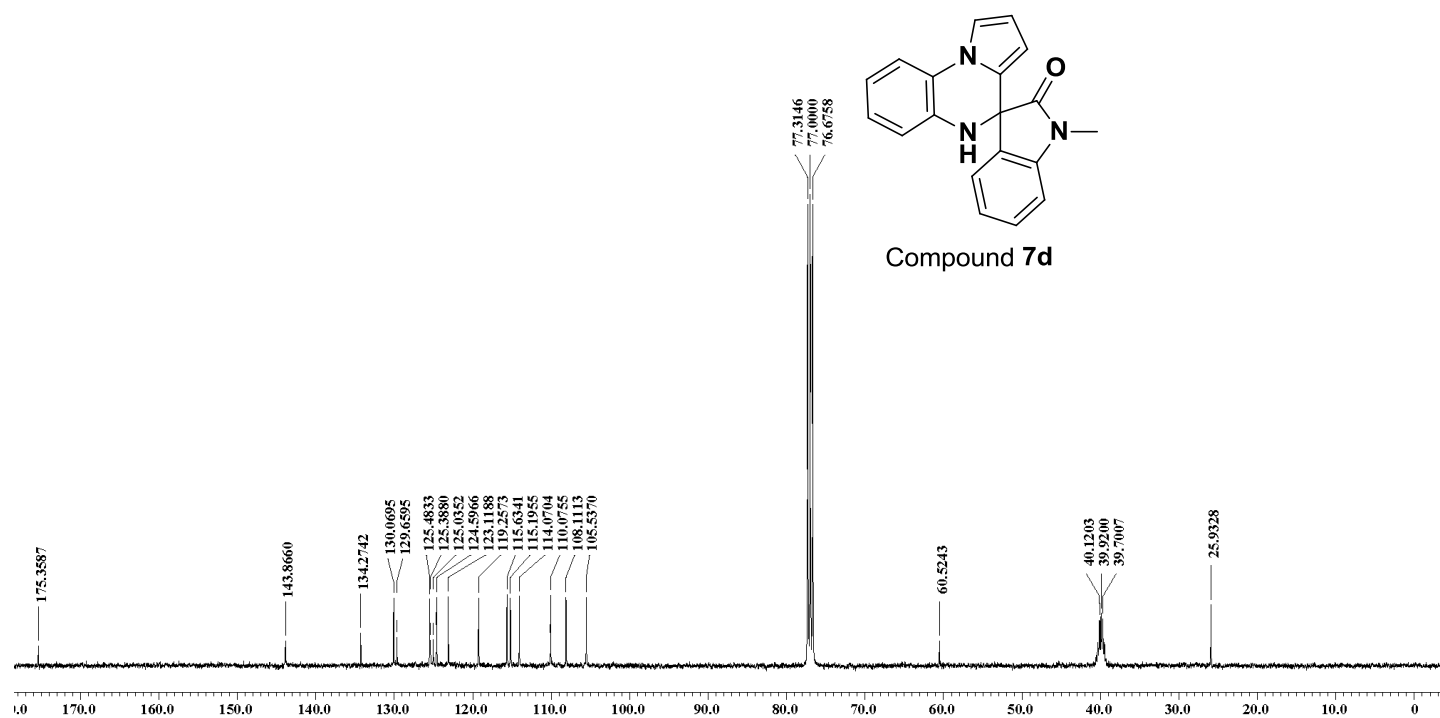
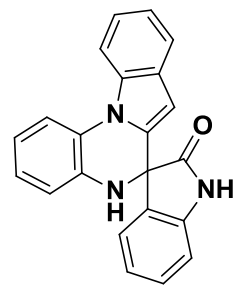


Figure 45: ¹³C NMR spectrum of 7d



Compound 7e

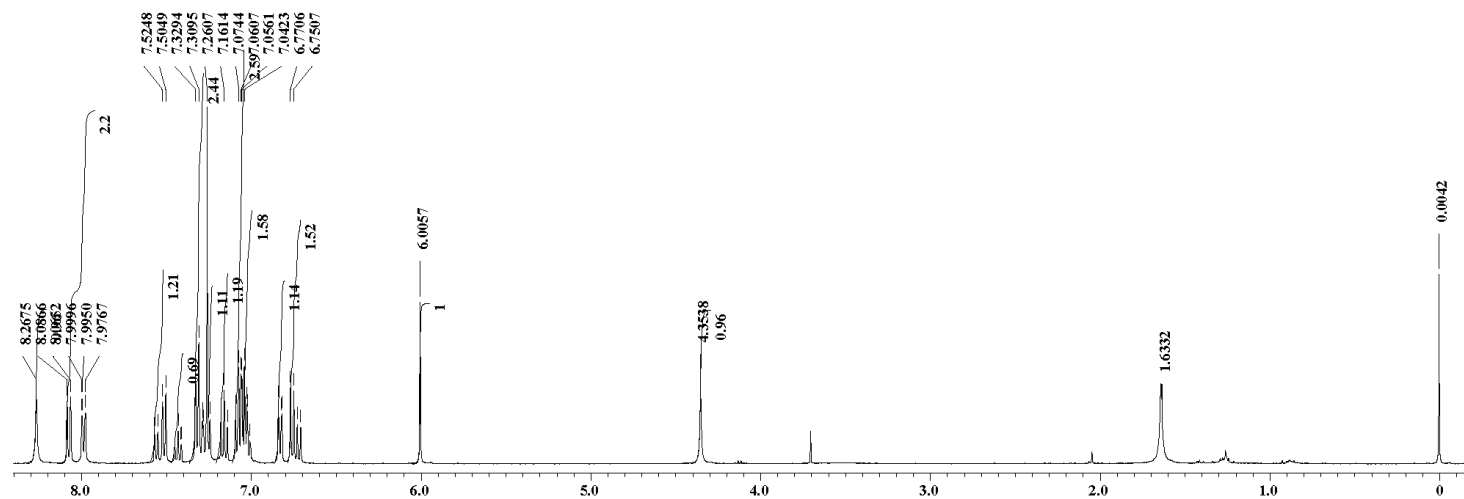


Figure 46: ¹H NMR spectrum of 7e

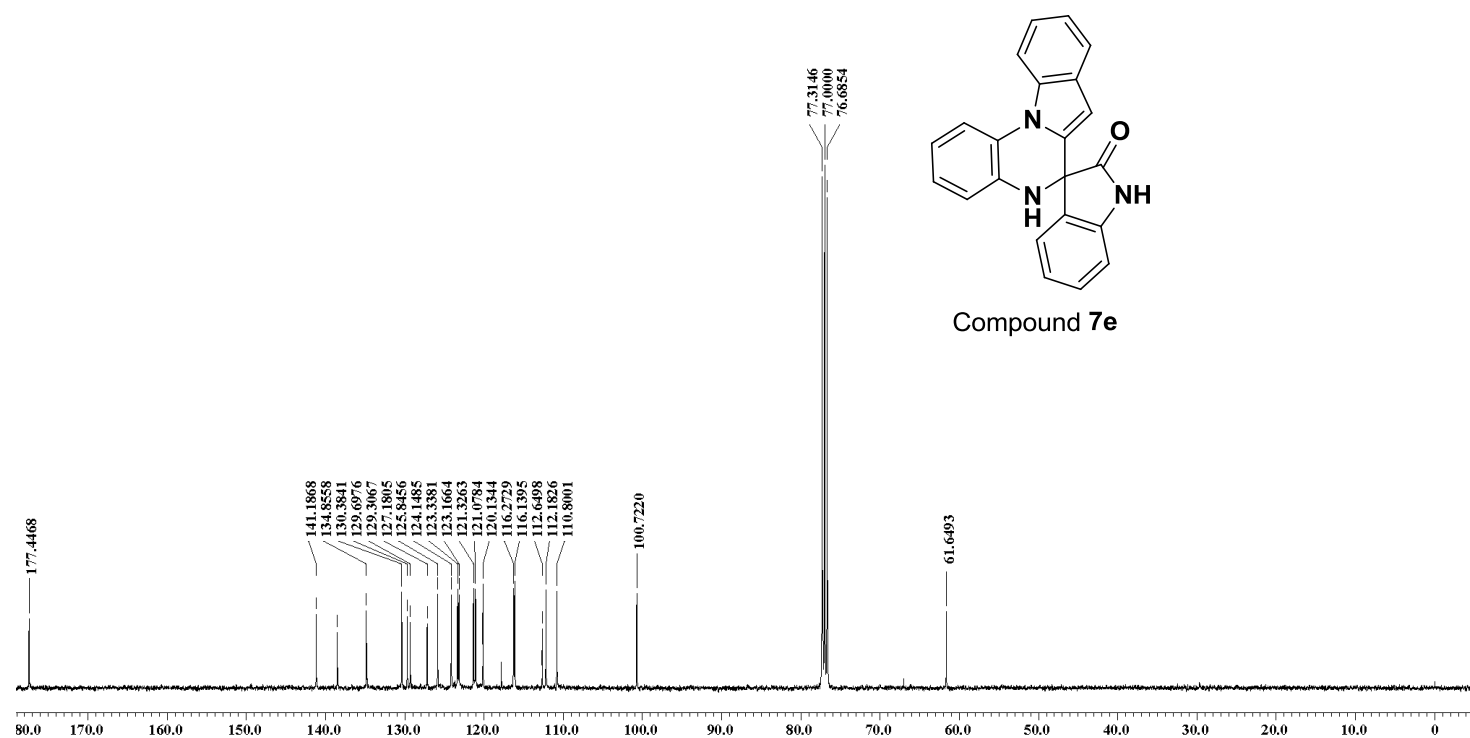
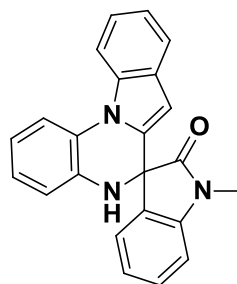


Figure 47: ^{13}C NMR spectrum of 7e



Compound 7f

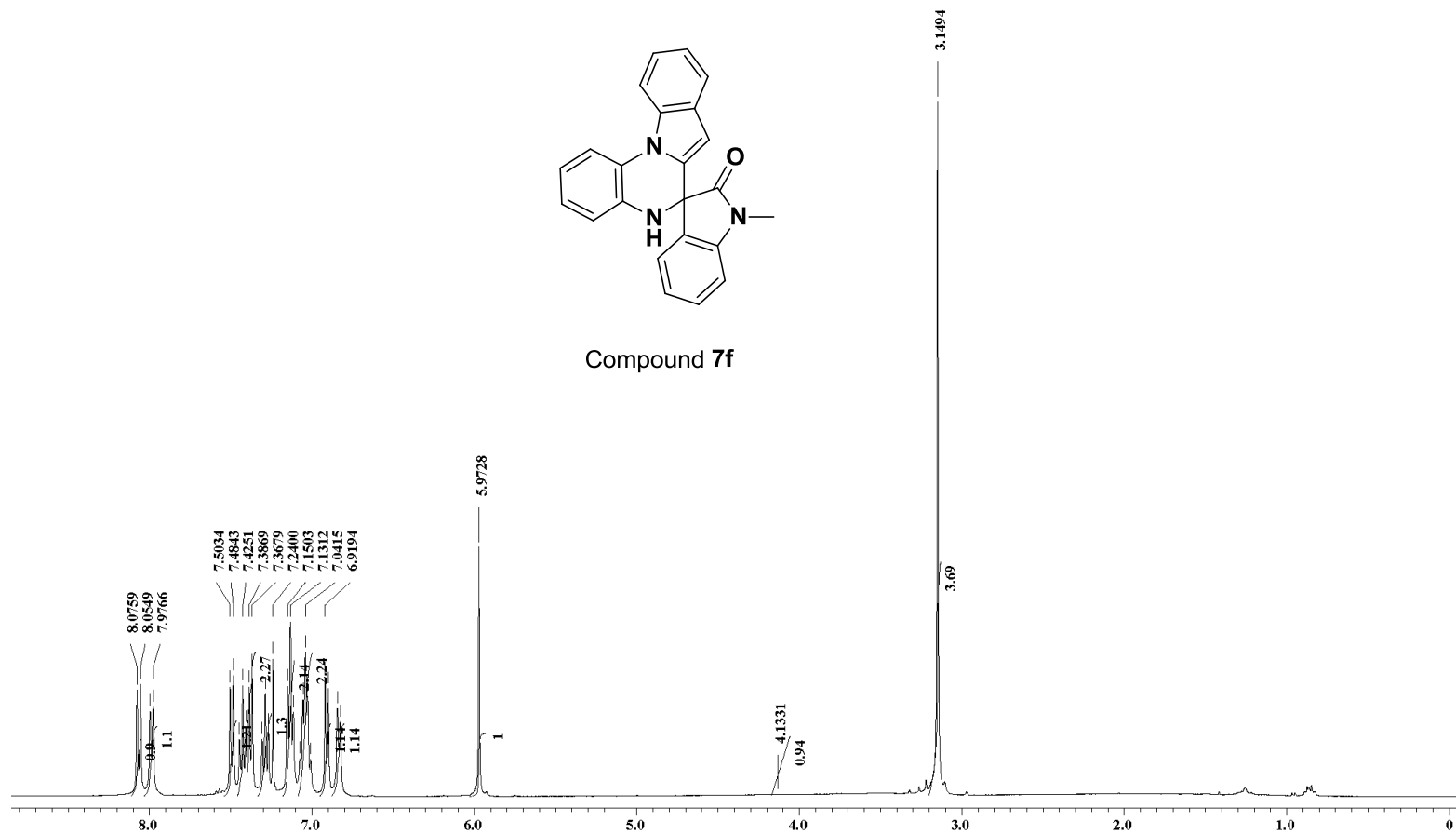


Figure 48: ^1H NMR spectrum of 7f

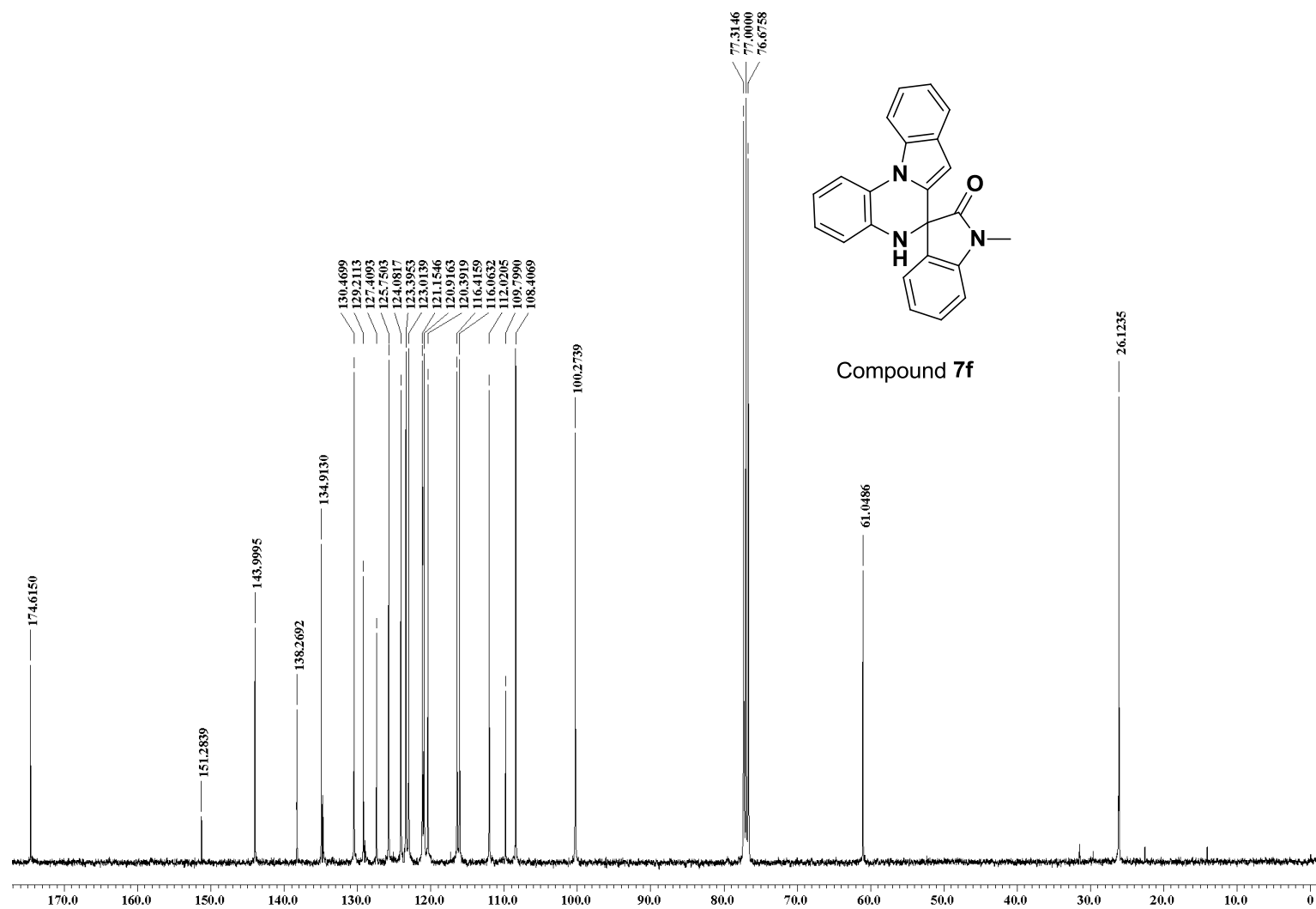


Figure 49: ¹³C NMR spectrum of **7f**

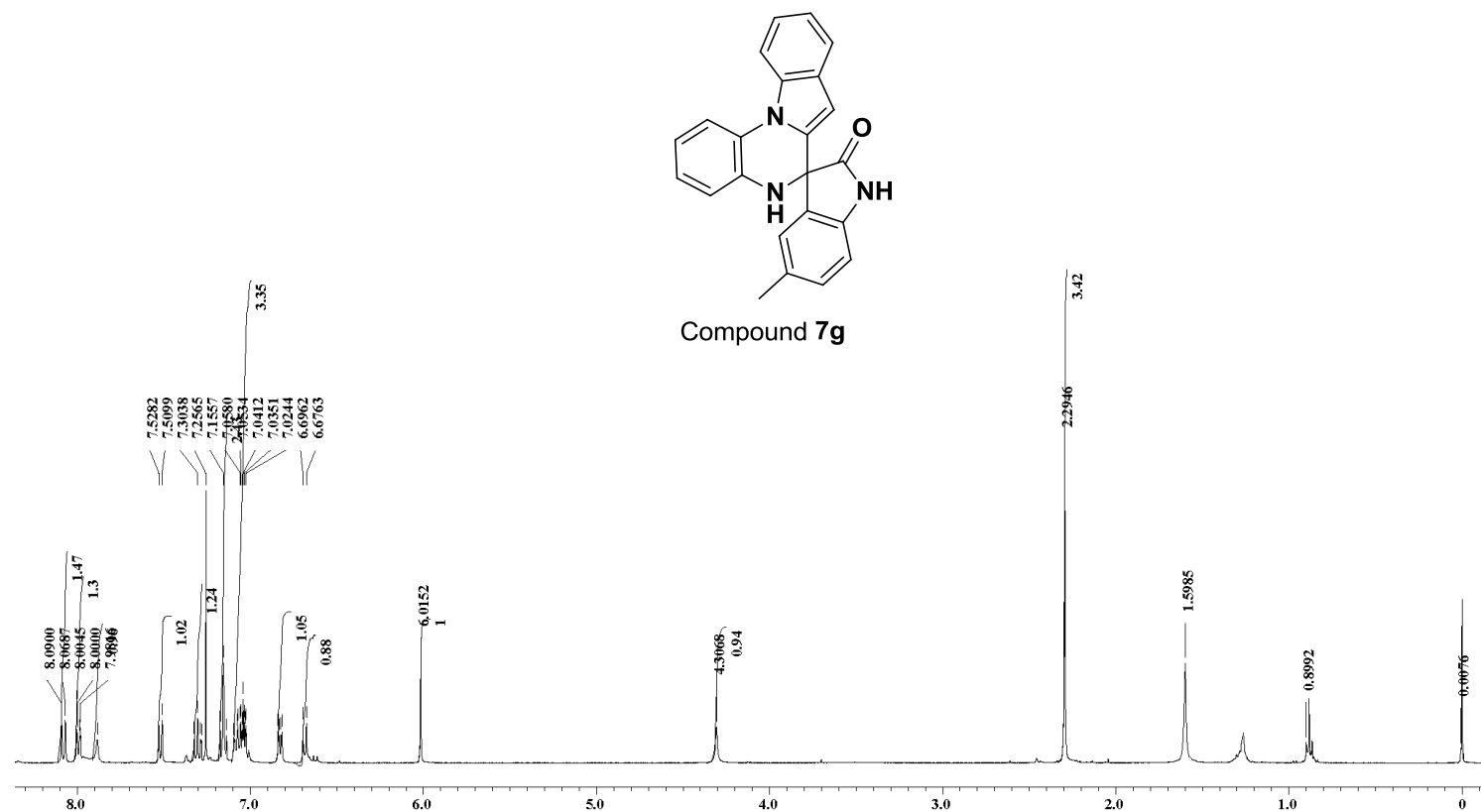
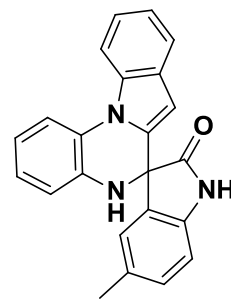


Figure 50: ^1H NMR spectrum of 7g



Compound **7g**

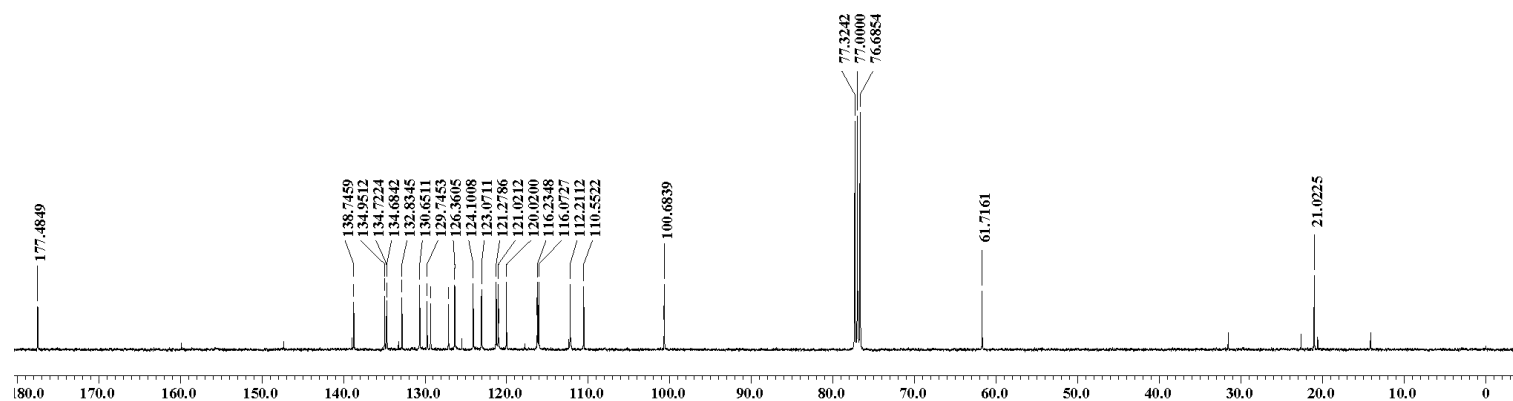


Figure 51: ^{13}C NMR spectrum of 7g

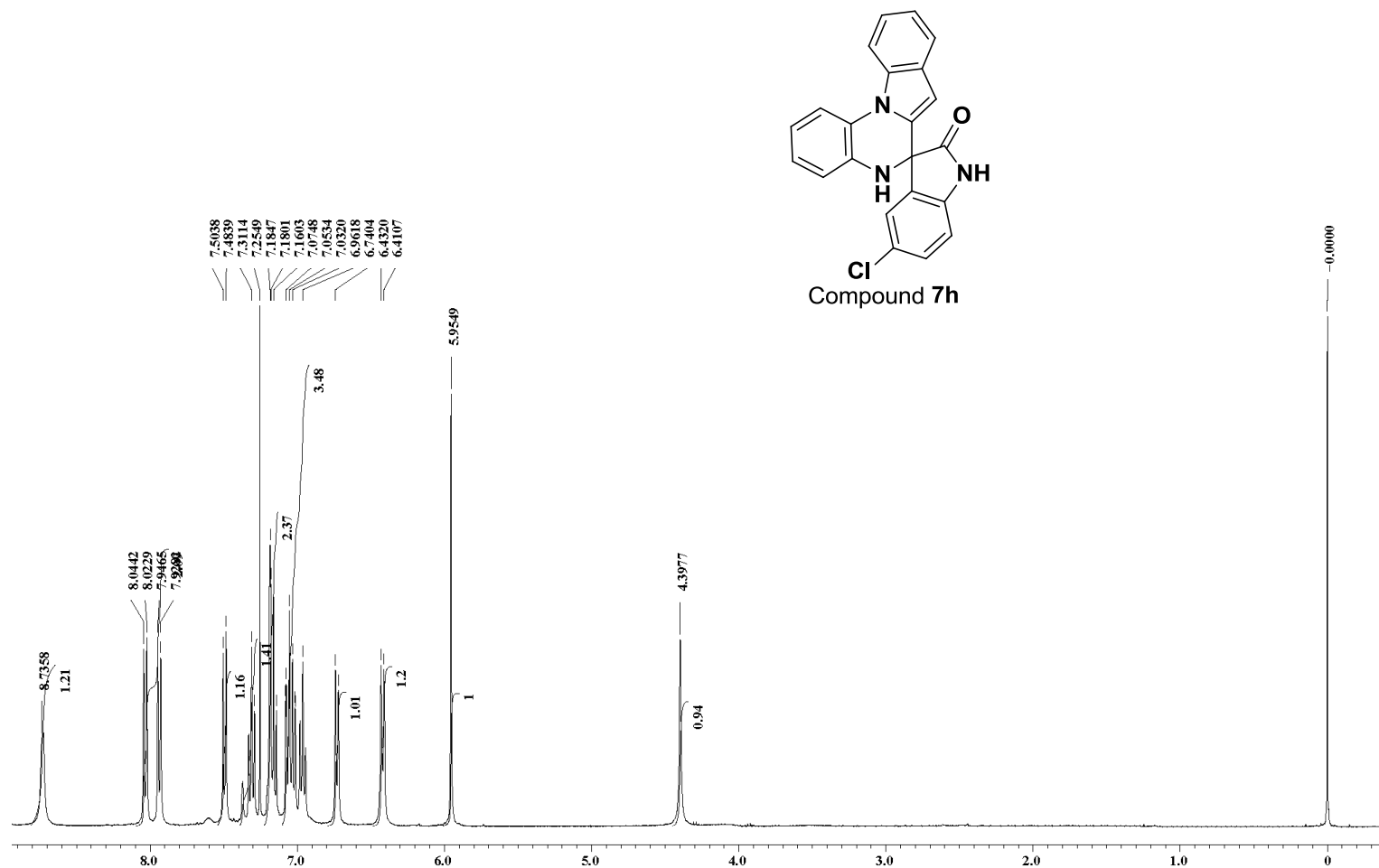


Figure 52: ¹H NMR spectrum of 7h

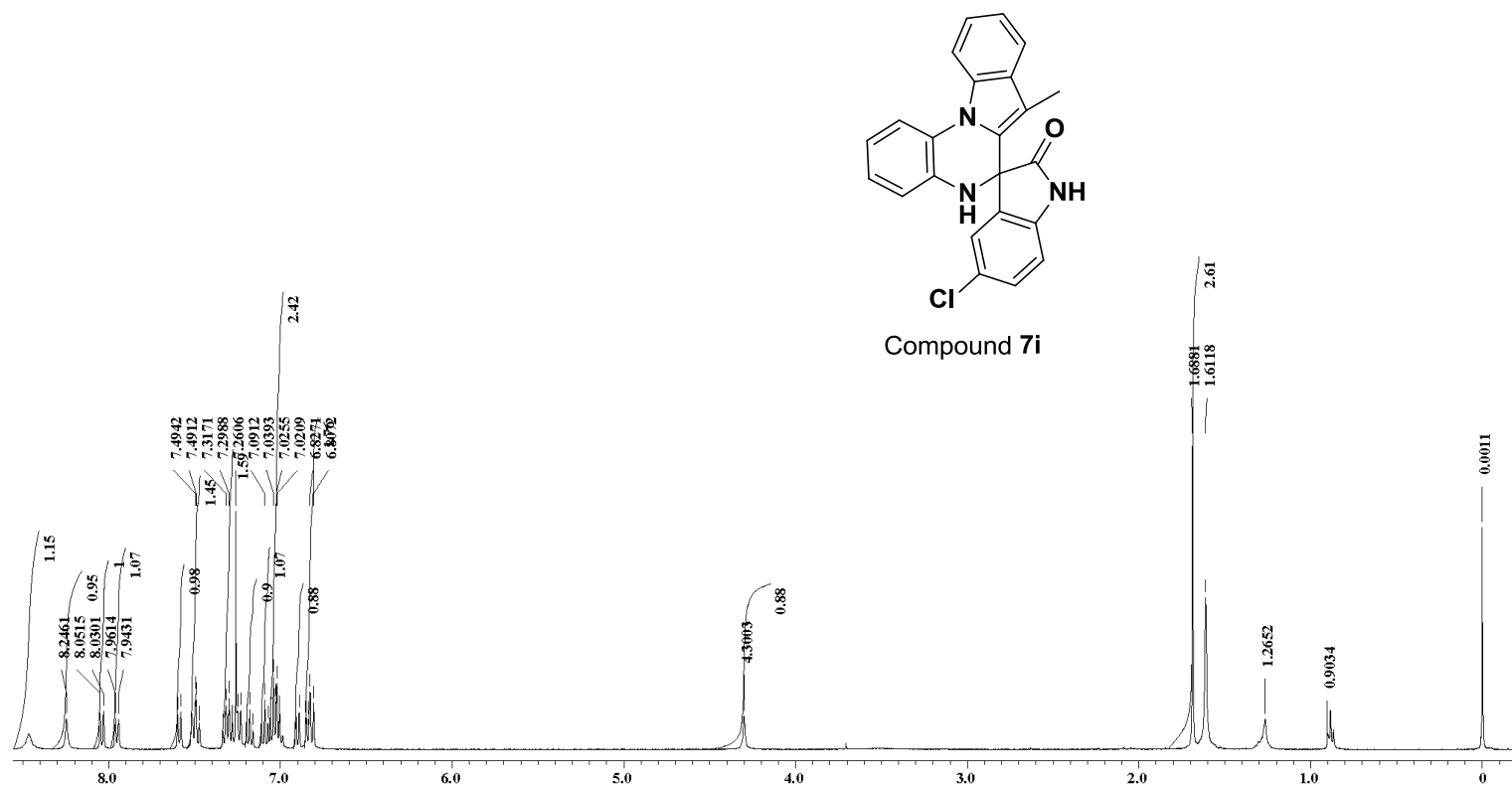
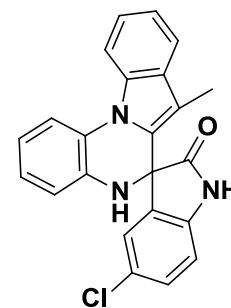


Figure 53: ^1H NMR spectrum of 7i



Compound 7i

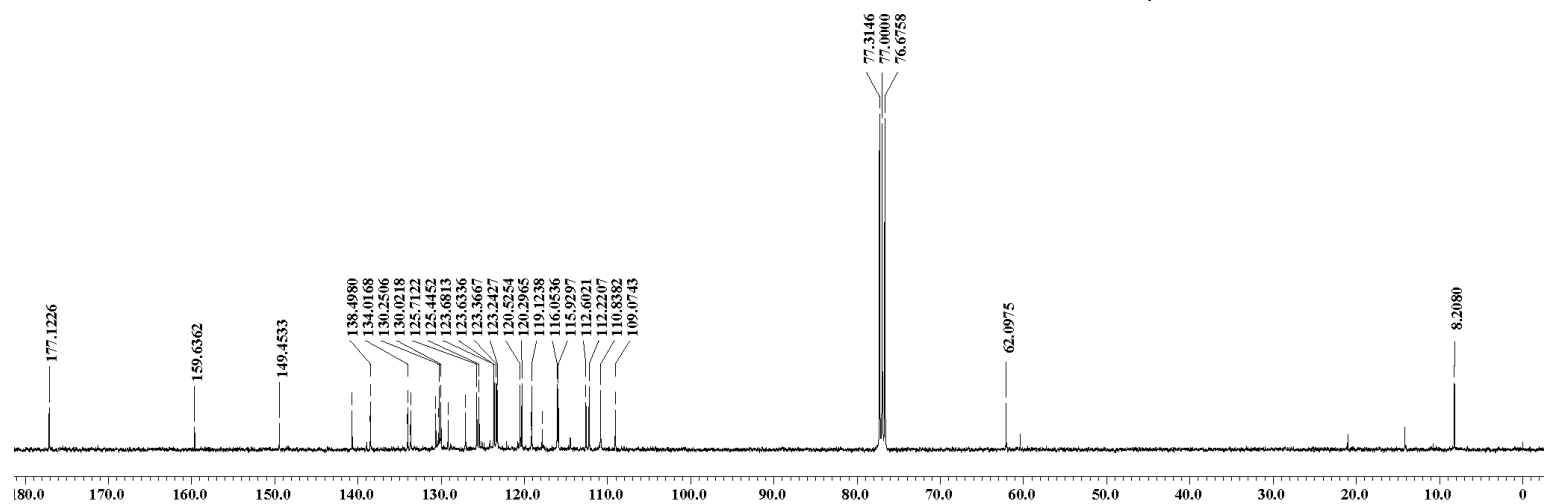
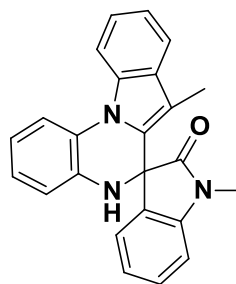


Figure 54: ^{13}C NMR spectrum of 7i



Compound **7j**

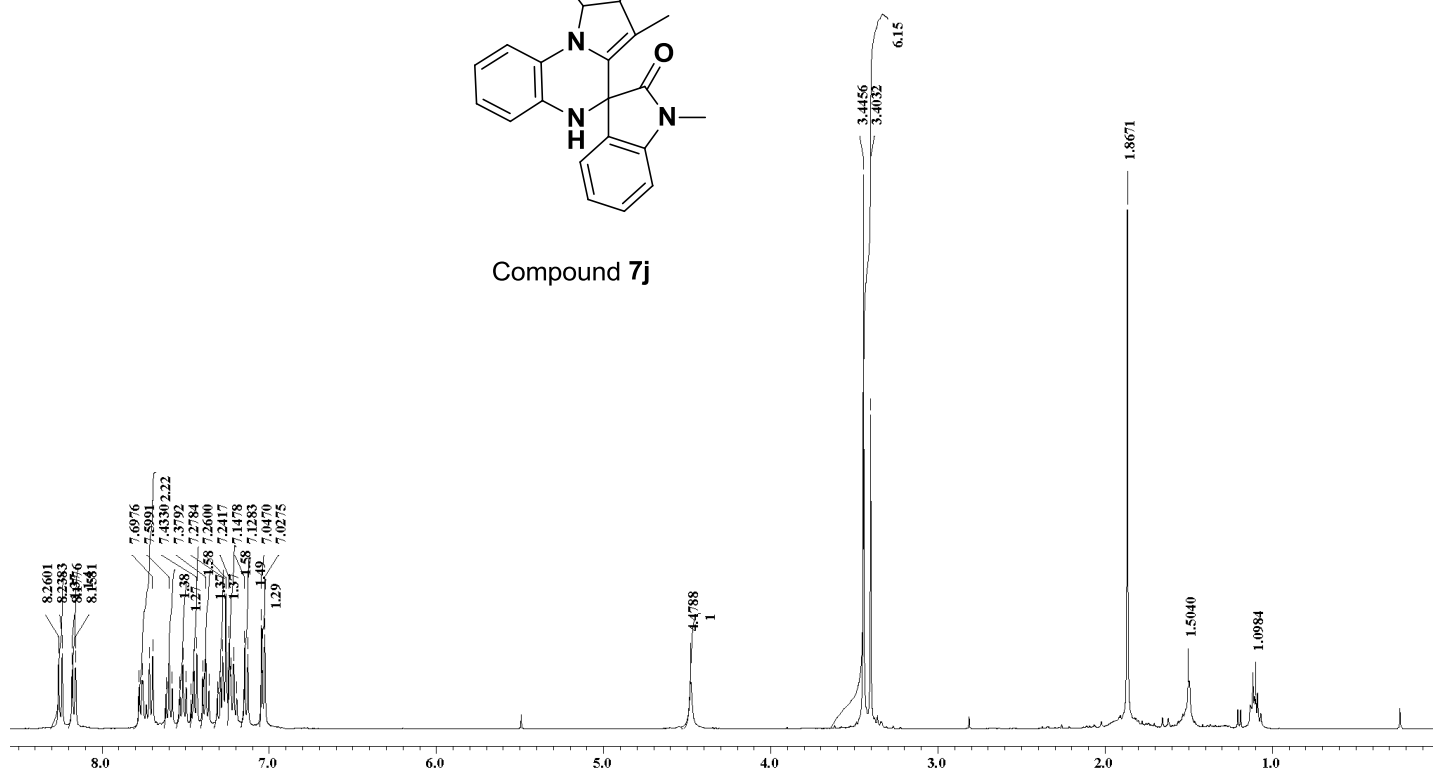
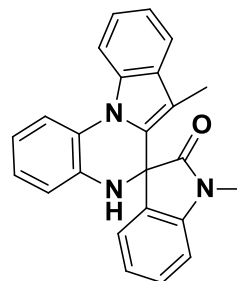


Figure 55: ¹H NMR spectrum of **7j**



Compound **7j**

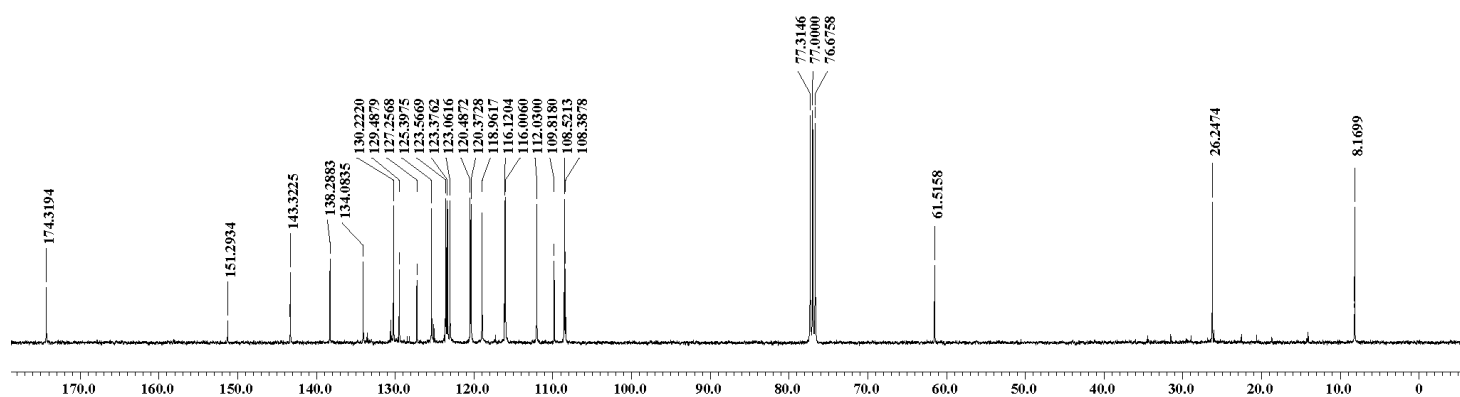


Figure 56: ^{13}C NMR spectrum of **7j**

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-K α radiation ($\lambda = 0.71073 \text{ \AA}$) 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).

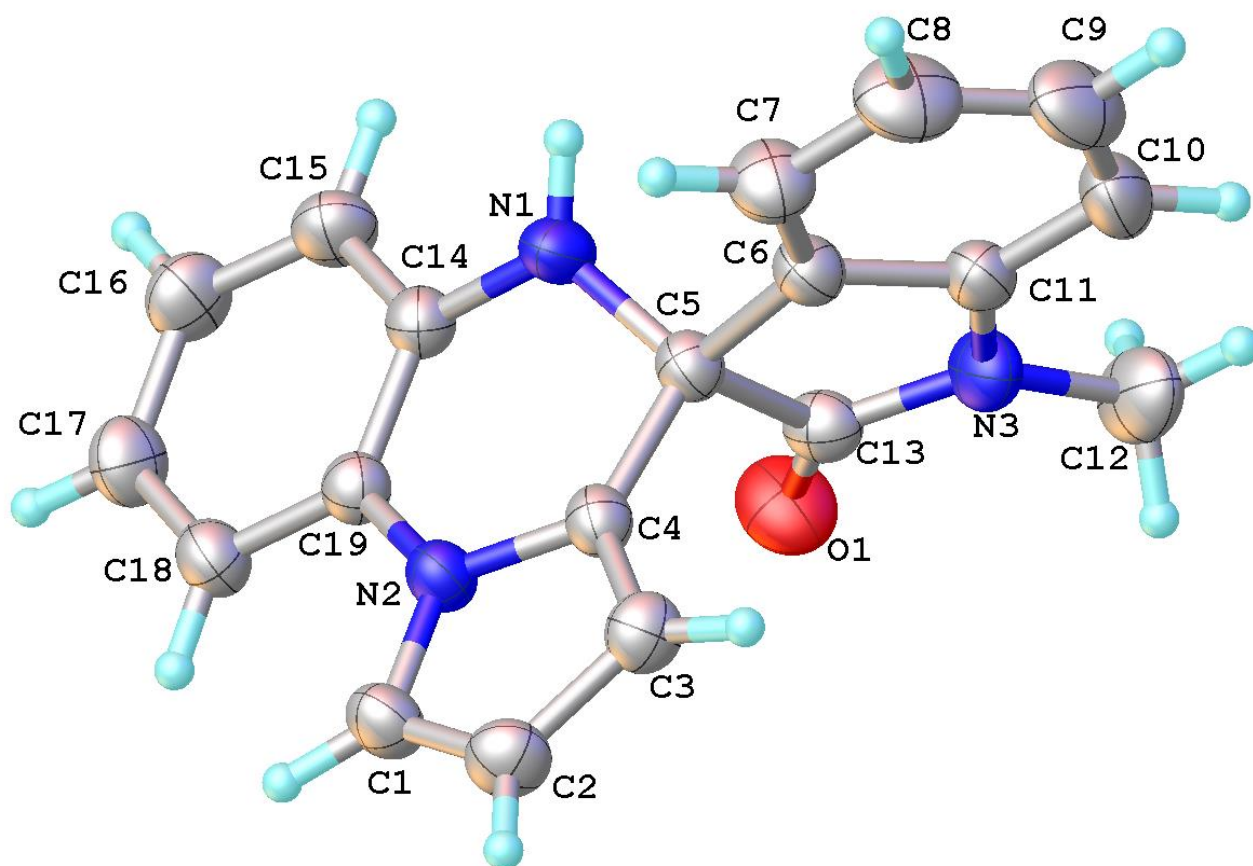


Figure 57: Molecular structure for compound **7d** (thermal ellipsoids are drawn at 30% probability level).

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

Empirical formula	C ₁₉ H ₁₅ N ₃ O
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 ≤ h ≤ 10, -12 ≤ k ≤ 13, -22 ≤ l ≤ 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