

Supplementary Information for

**Late-Stage Diversification of Biologically Active Pyridazinones via
Direct C-H Functionalization Strategy**

Wei Li,^{‡,a} Zhoulong Fan,^{‡,b} Kaijun Geng,^b Youjun Xu^{*,a} and Ao Zhang^{*,b}

^a School of Pharmaceutical Engineering, Shenyang Pharmaceutical University, Shenyang 110016, China

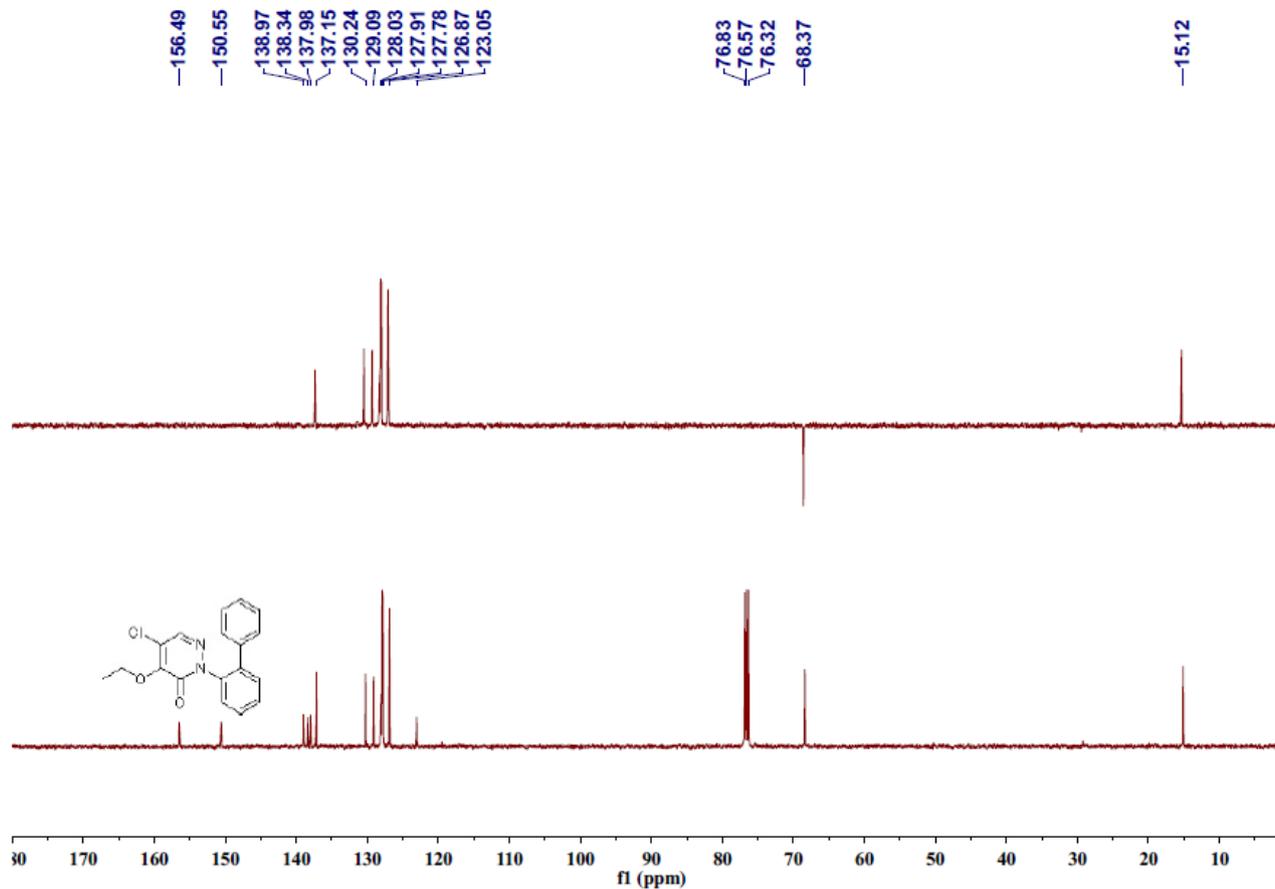
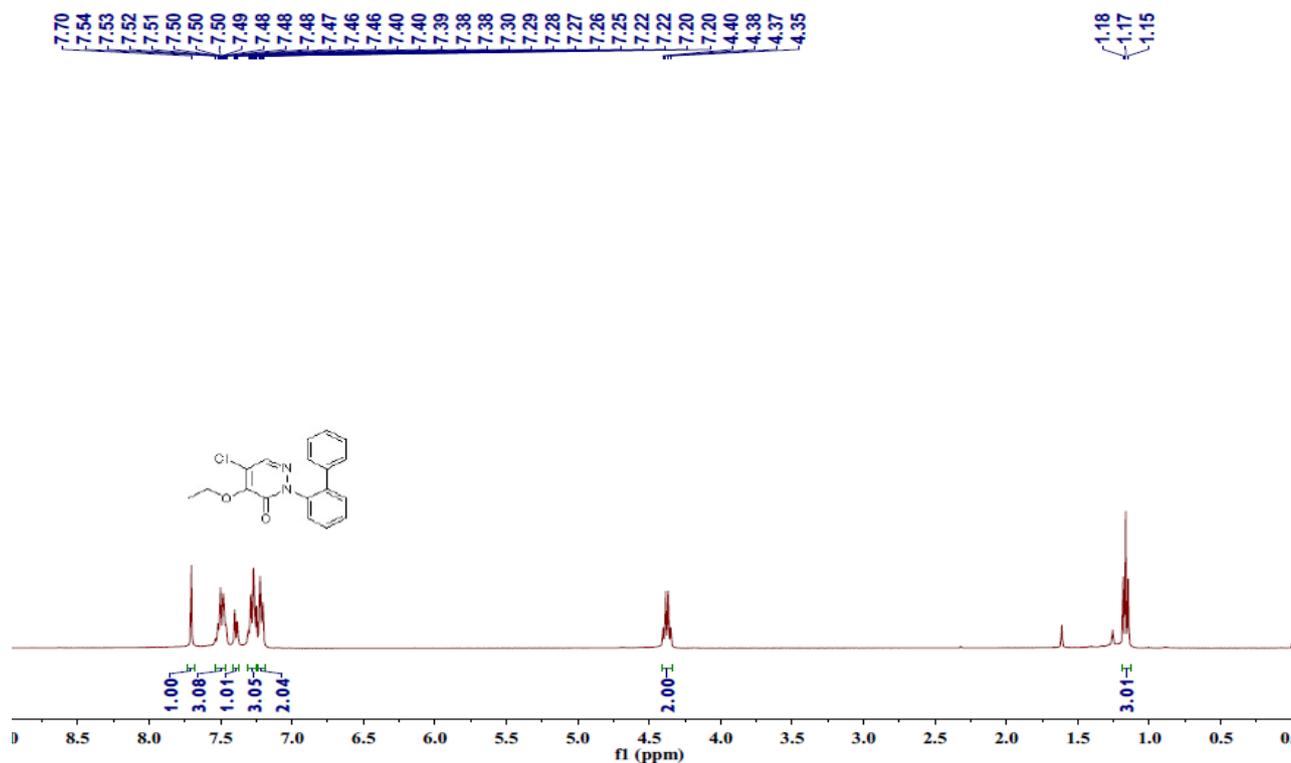
^b CAS Key Laboratory of Receptor Research, and Synthetic Organic & Medicinal Chemistry Laboratory (SOMCL),
Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences, Shanghai 201203, China;

Table of Contents

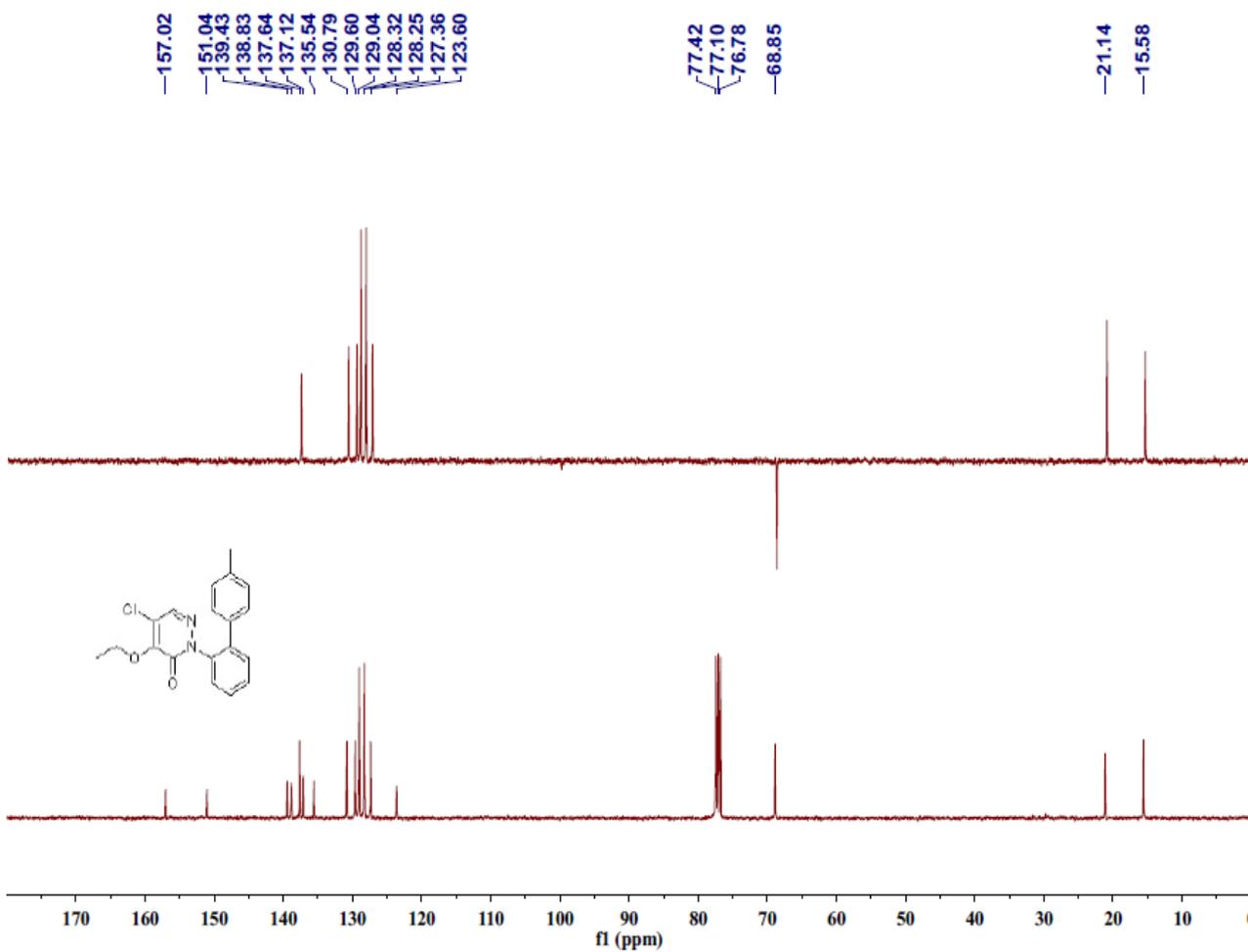
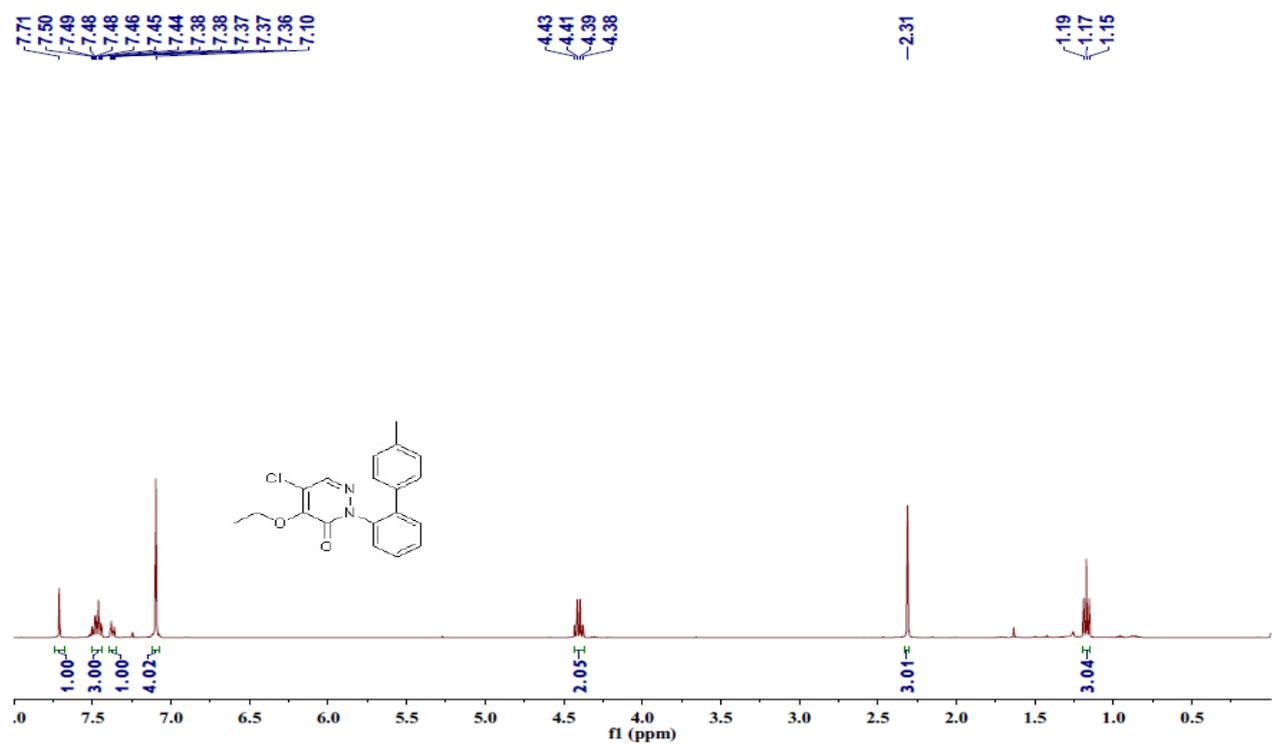
1. Copies of NMR Data for All Compounds.....	S2
2. X-ray Data of Compound 12	S44

1. Copies of NMR Data for All Compounds.

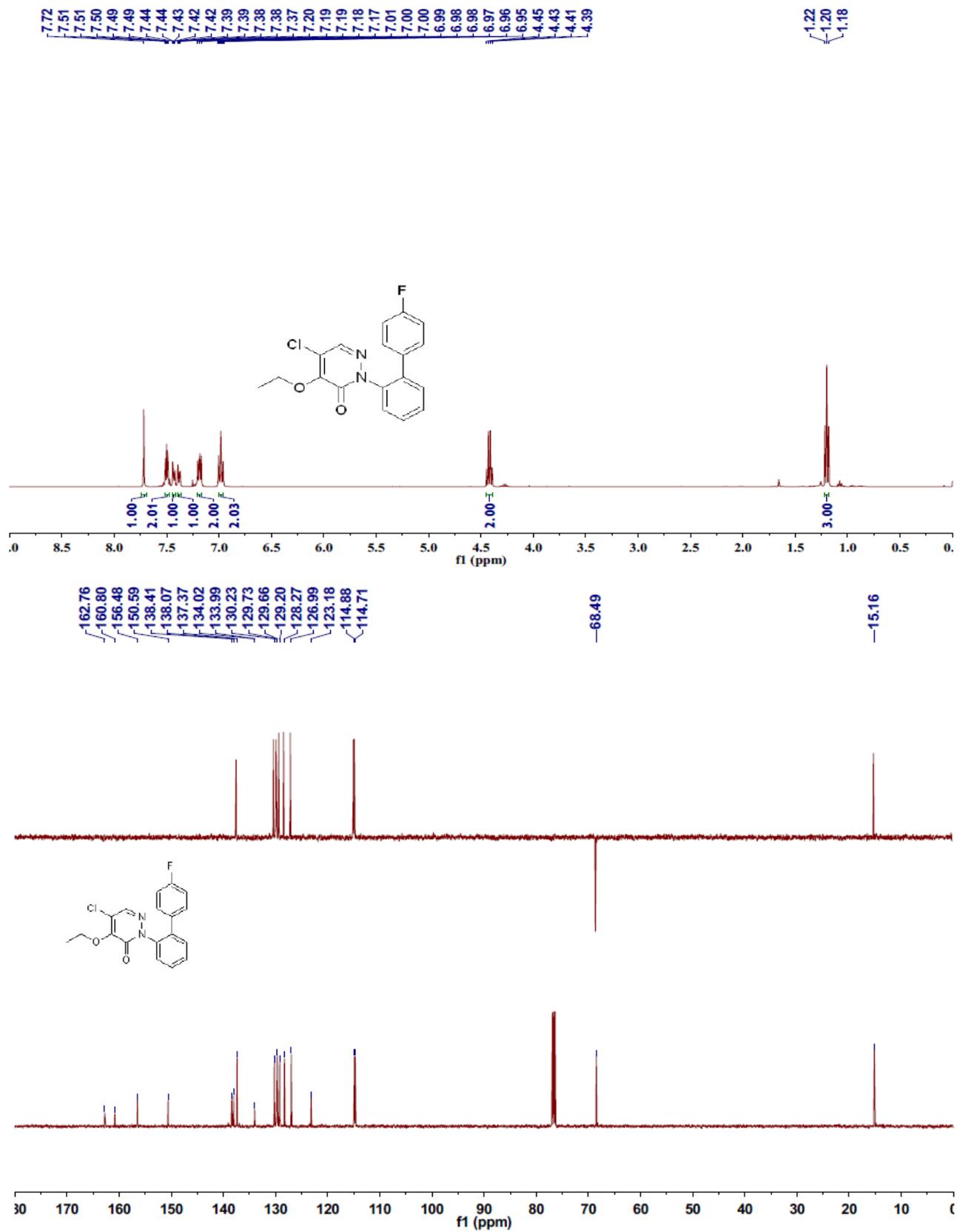
^1H and ^{13}C NMR spectra of compound **3a**.



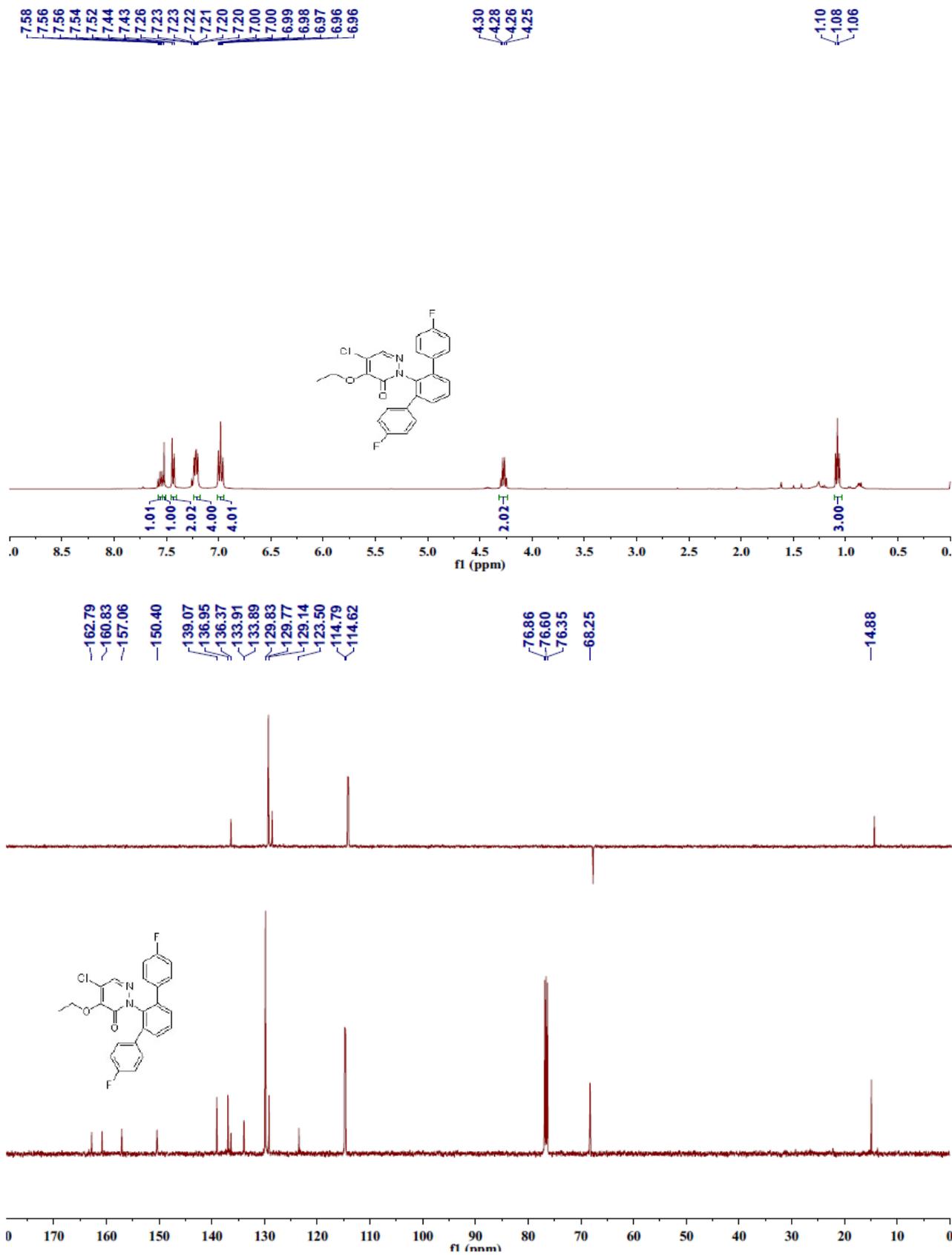
^1H and ^{13}C NMR spectra of compound **3b**.



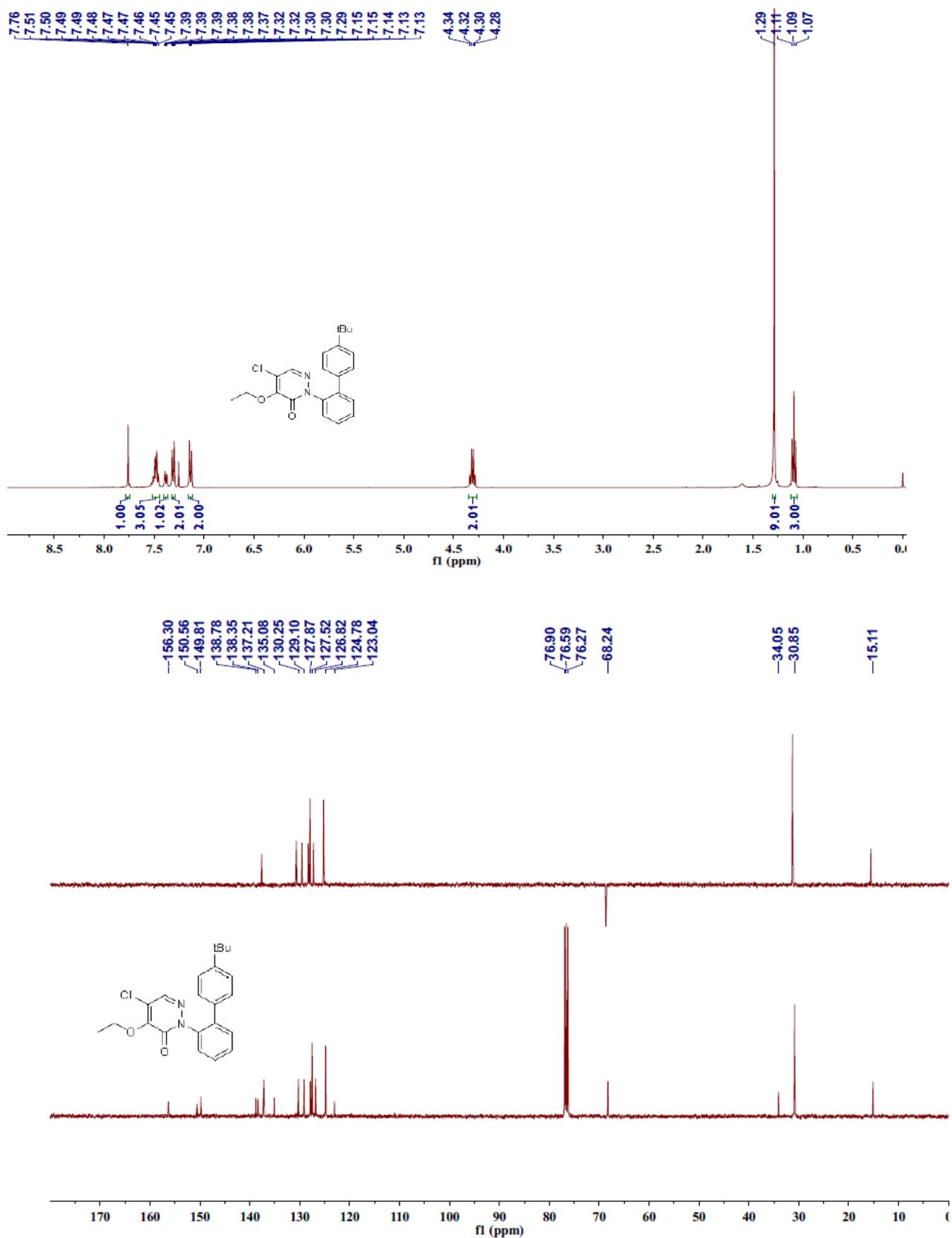
^1H and ^{13}C NMR spectra of compound **3c**.



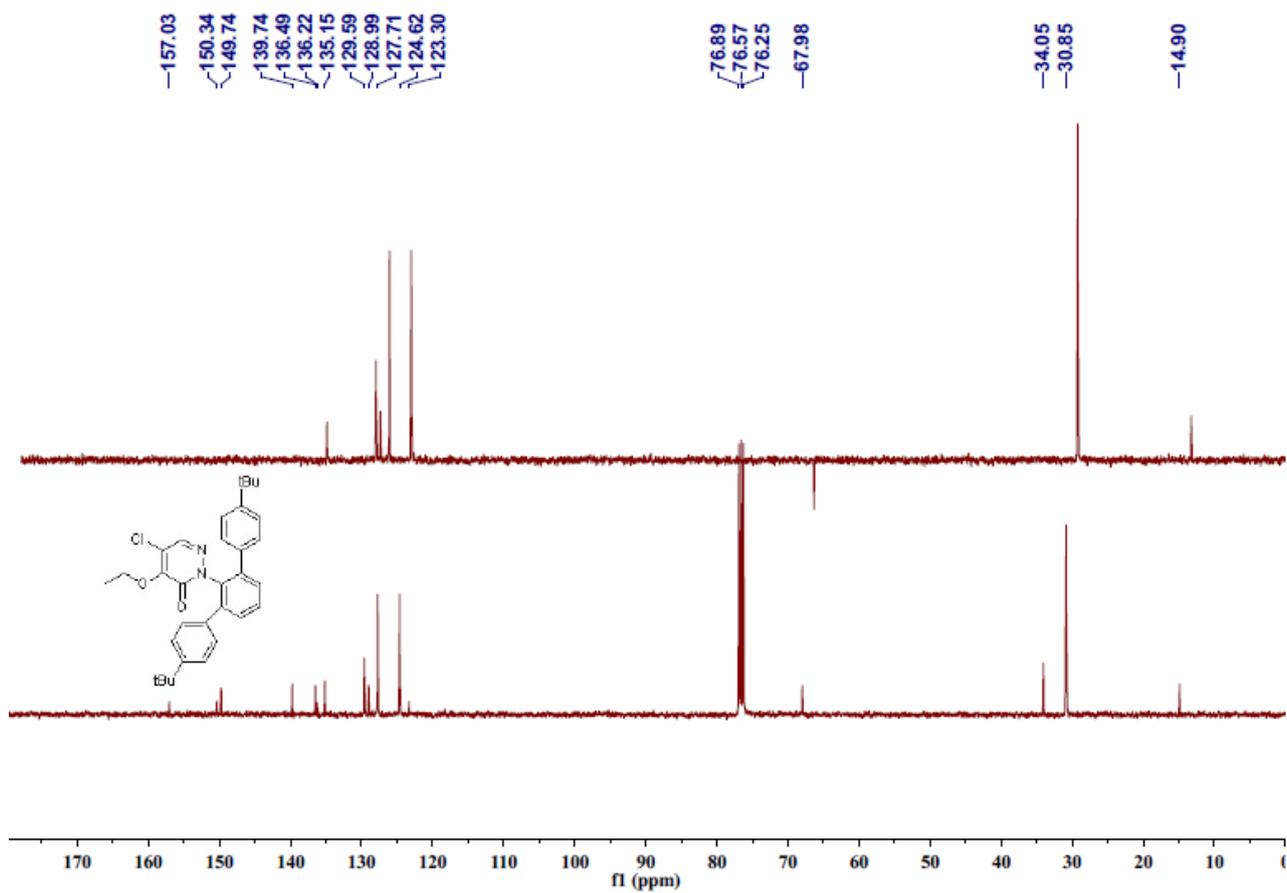
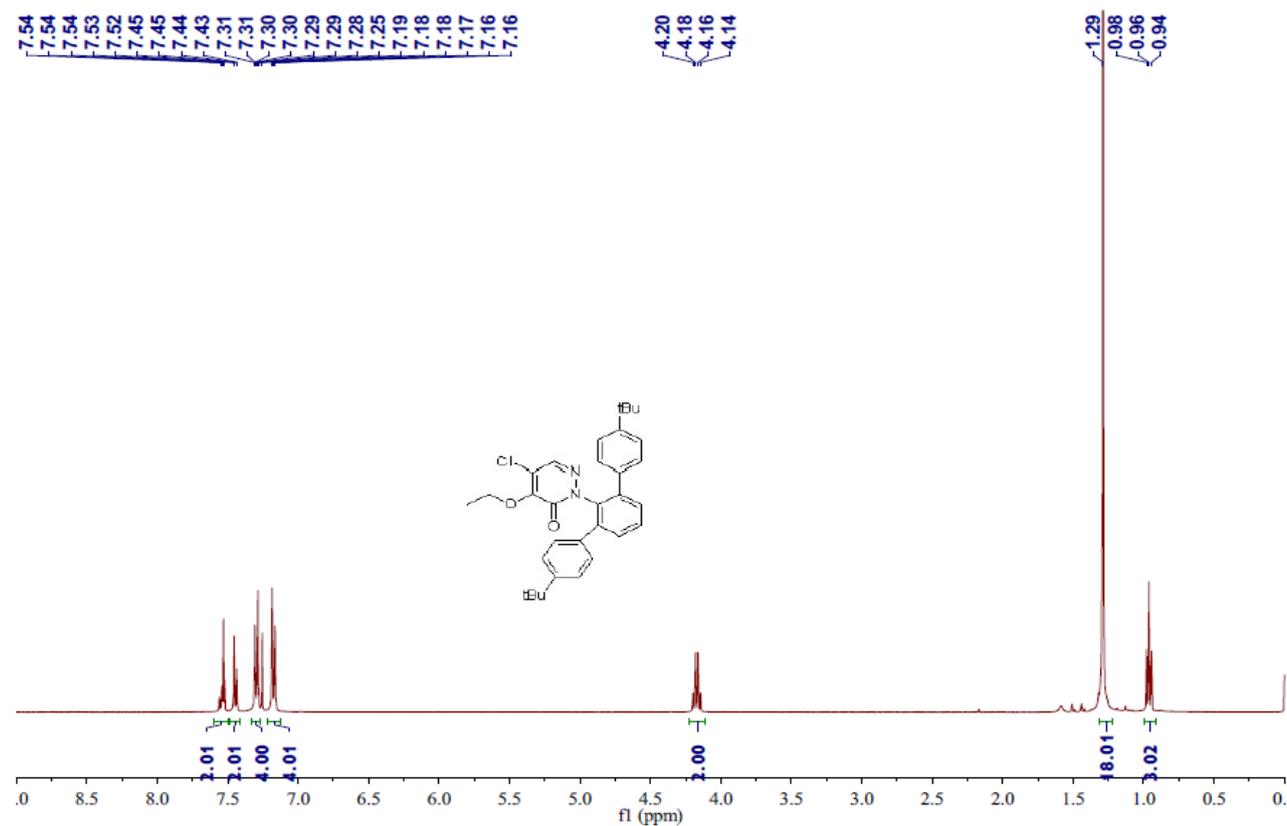
^1H and ^{13}C NMR spectra of compound **3c'**.



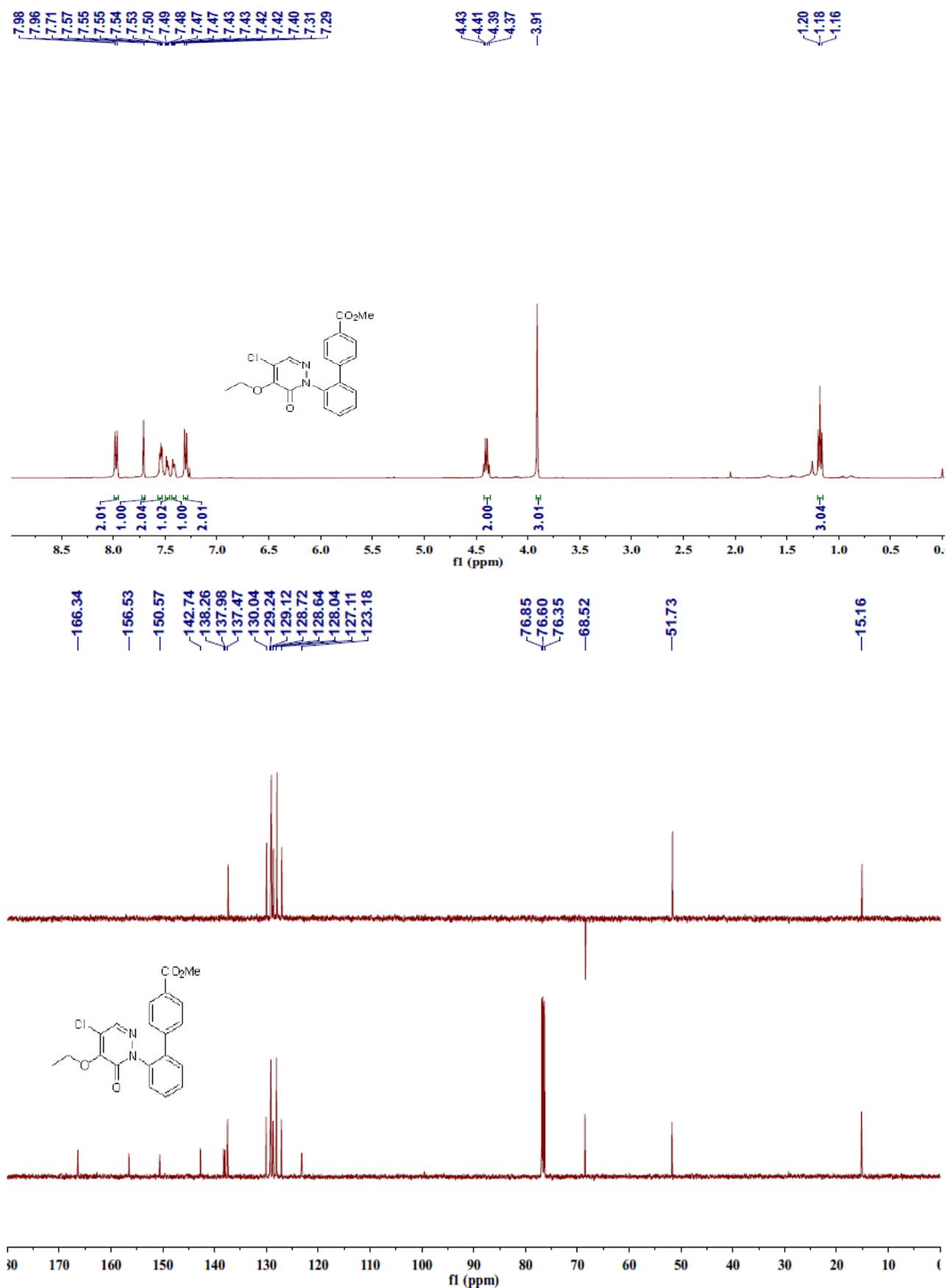
^1H and ^{13}C NMR spectra of compound **3d**.



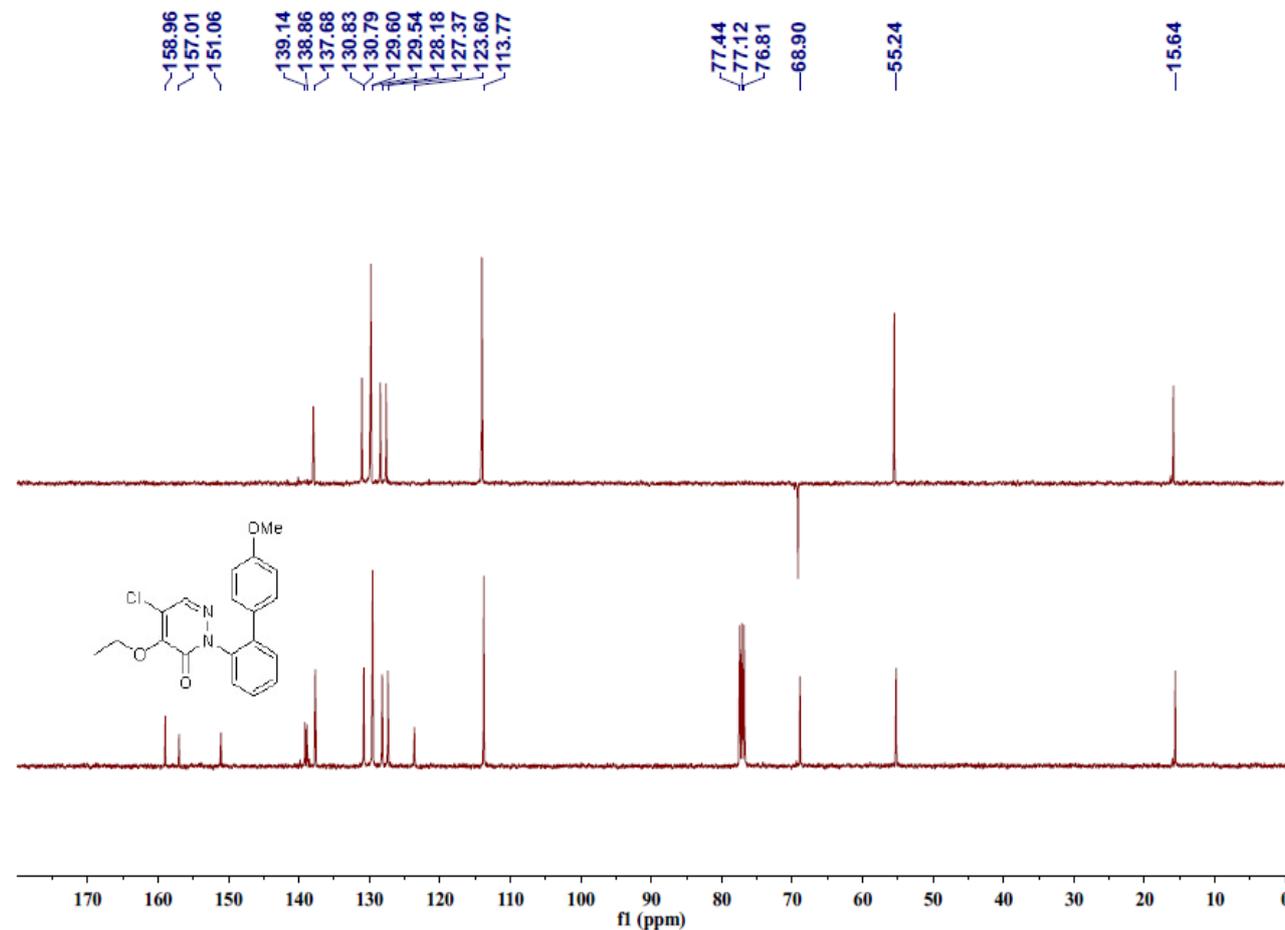
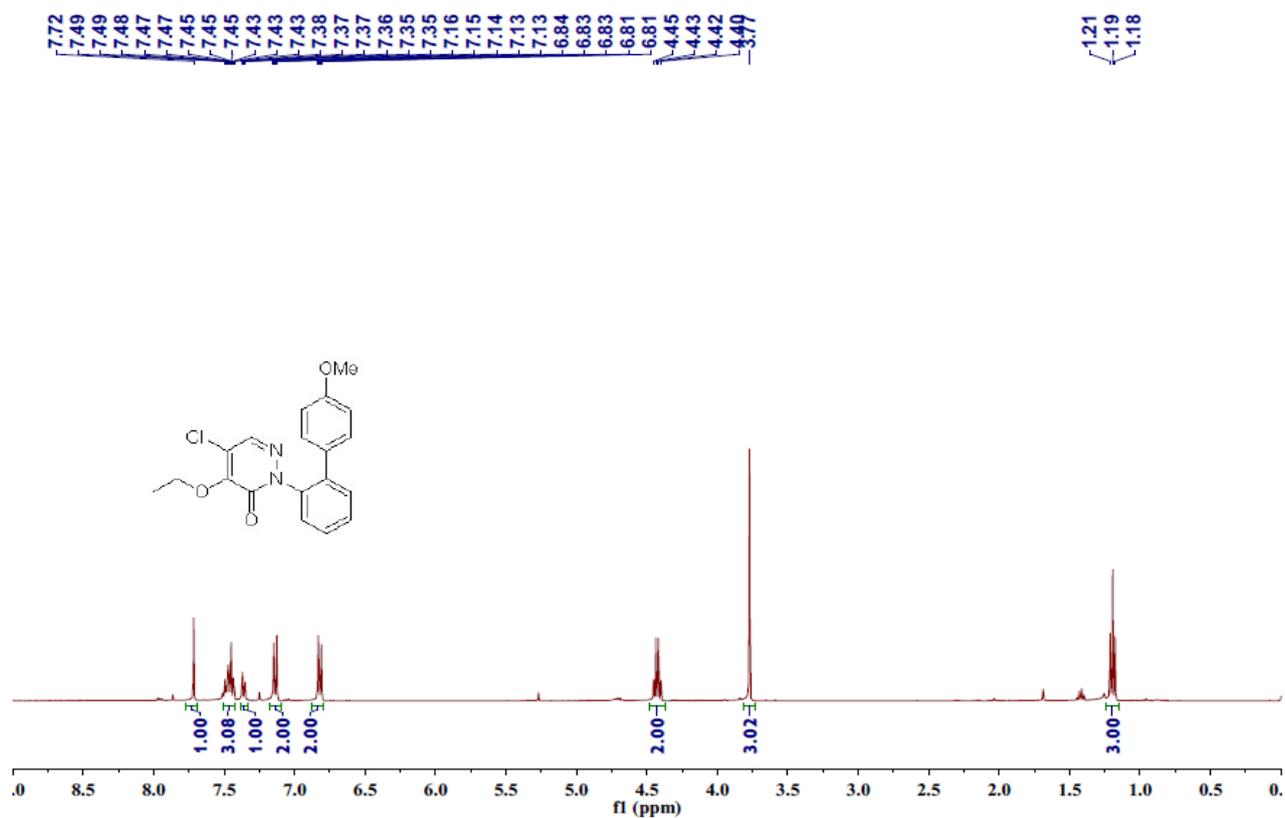
^1H and ^{13}C NMR spectra of compound **3d'**.



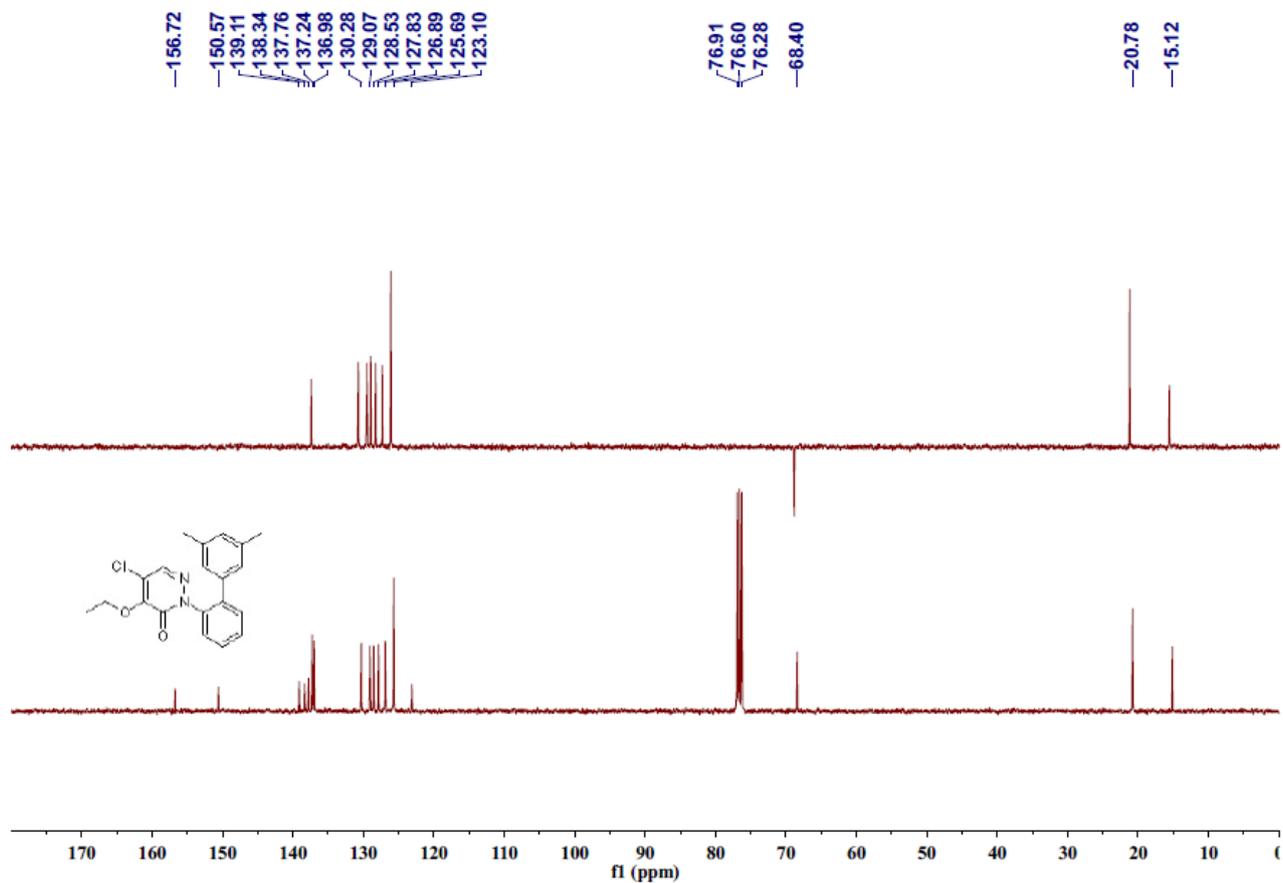
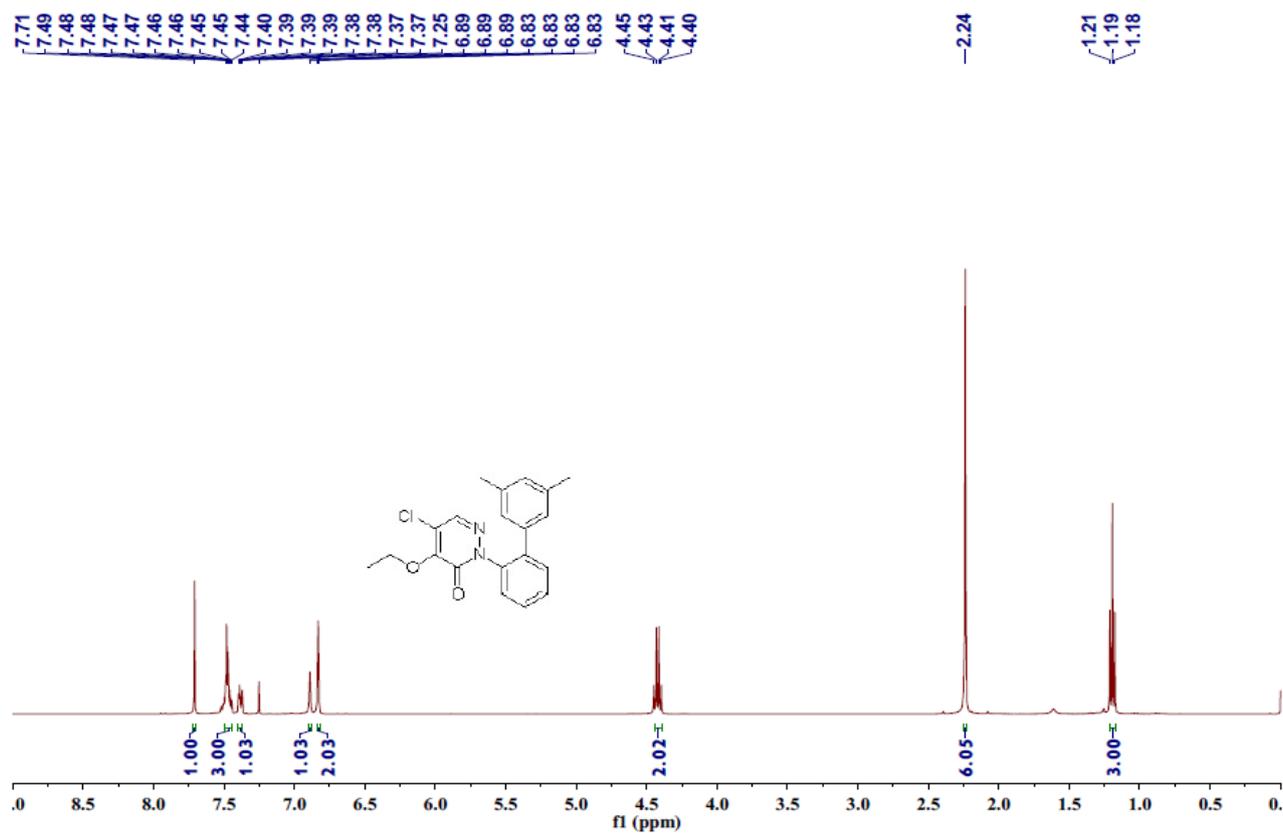
^1H and ^{13}C NMR spectra of compound **3e**.



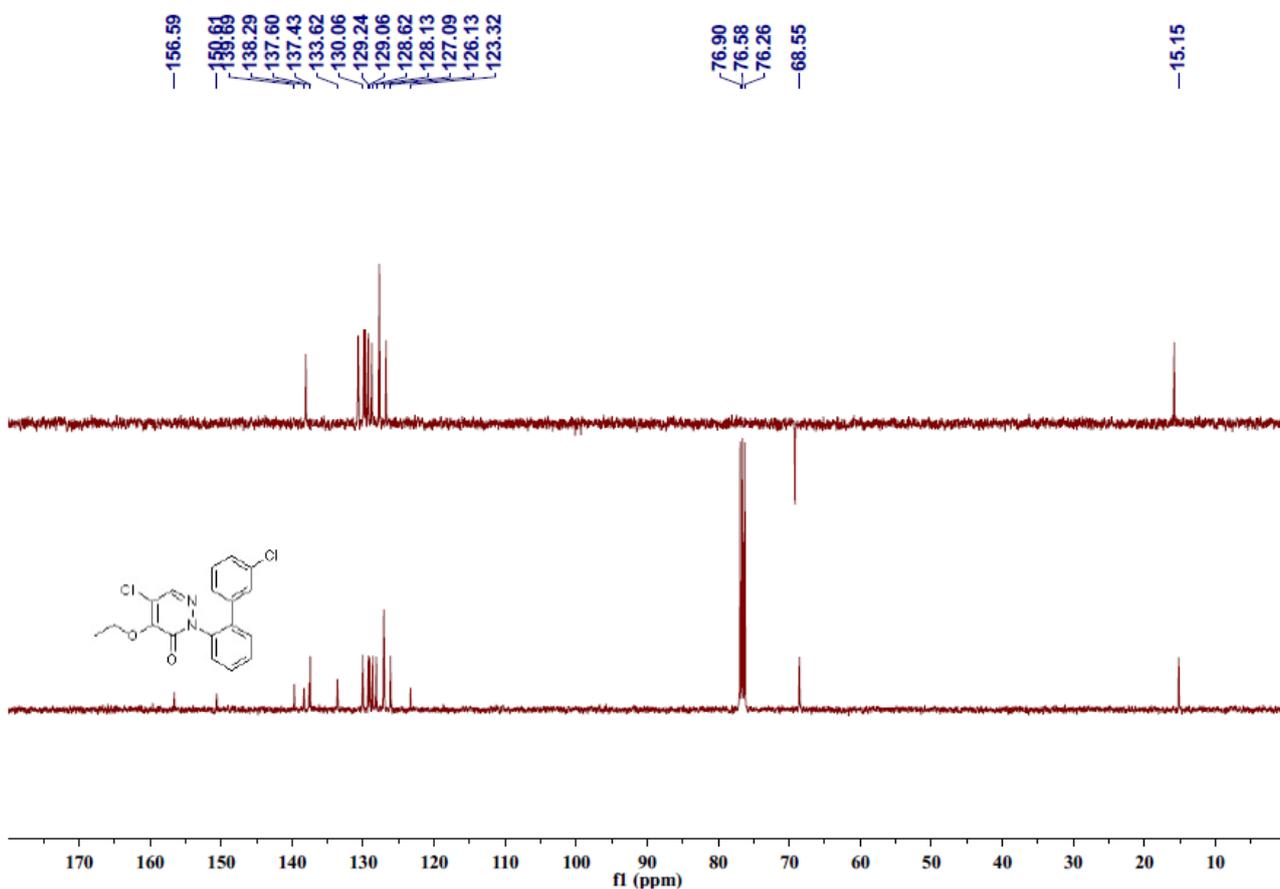
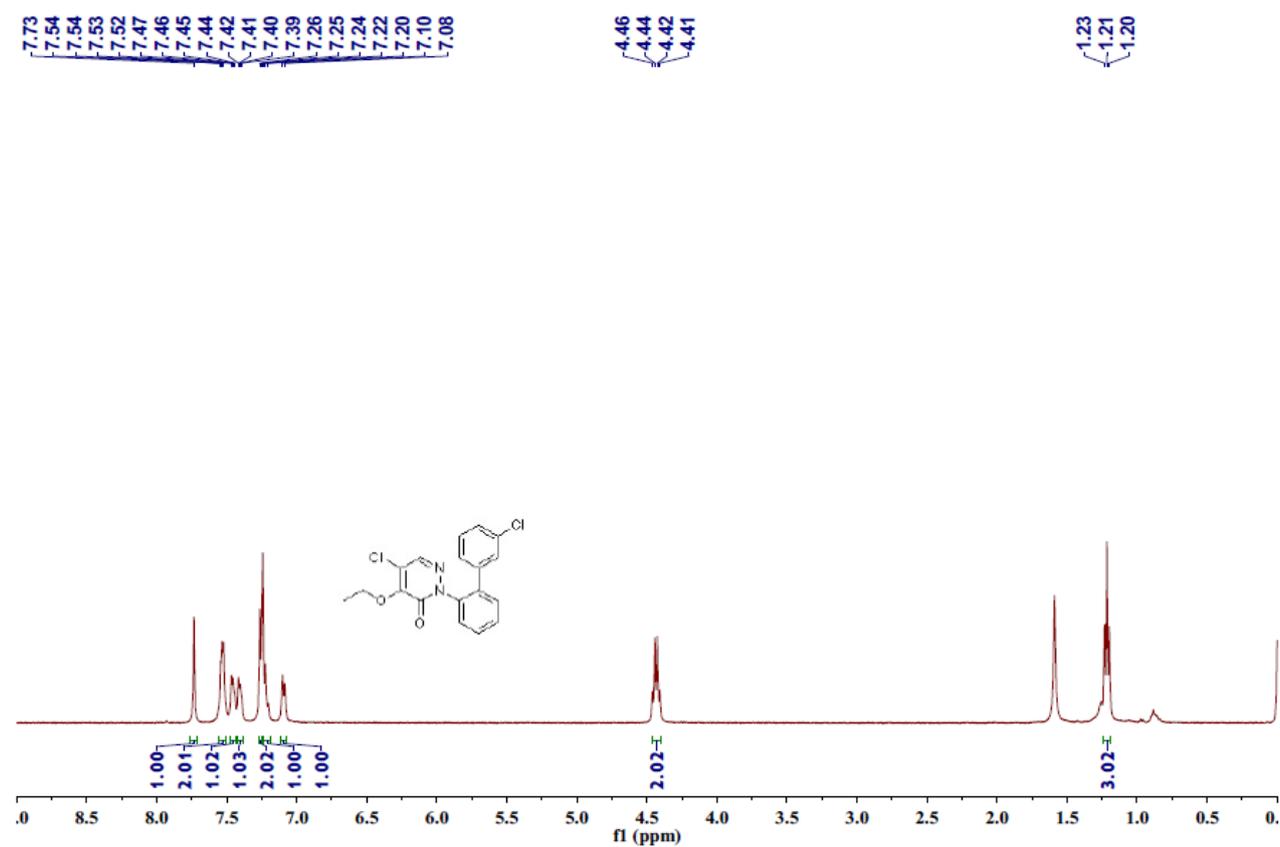
^1H and ^{13}C NMR spectra of compound **3f**.



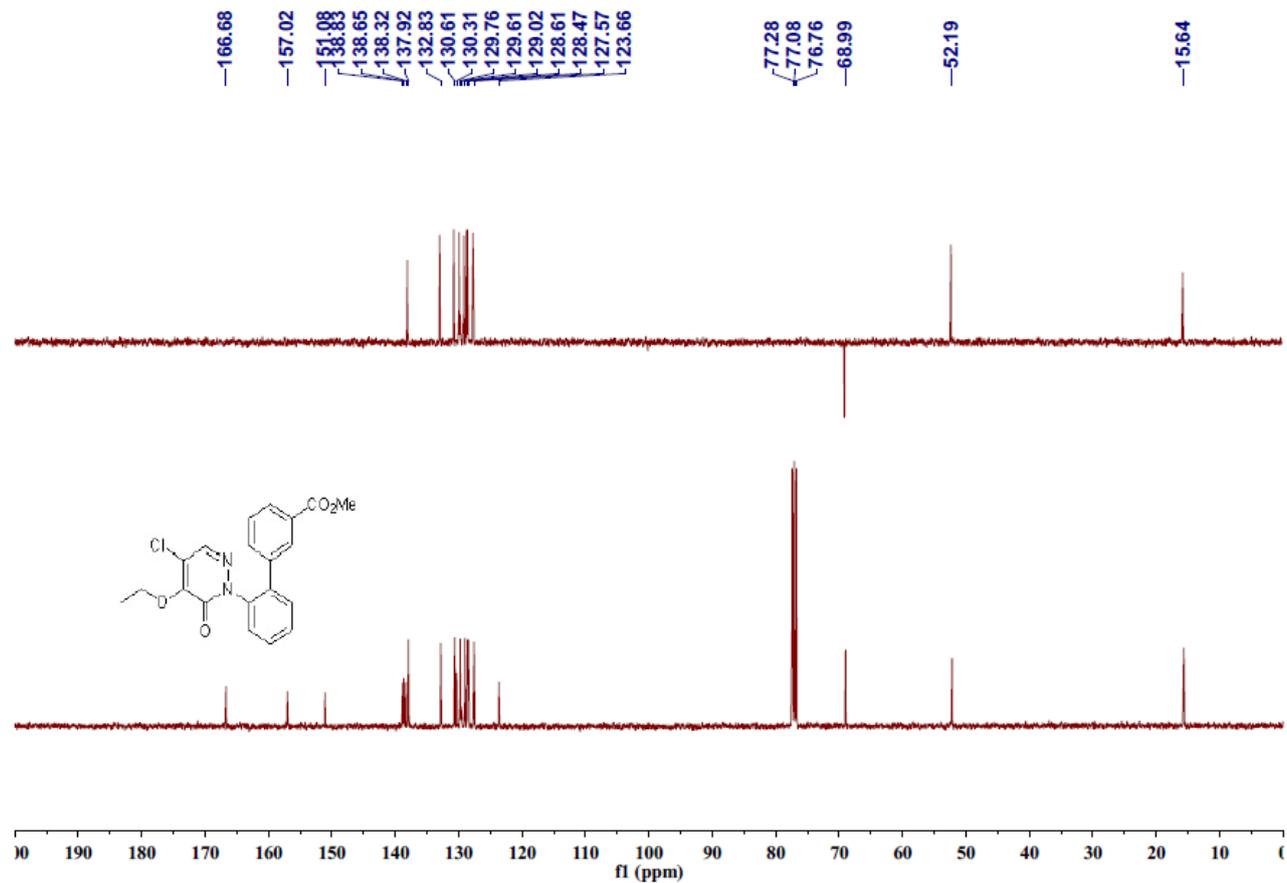
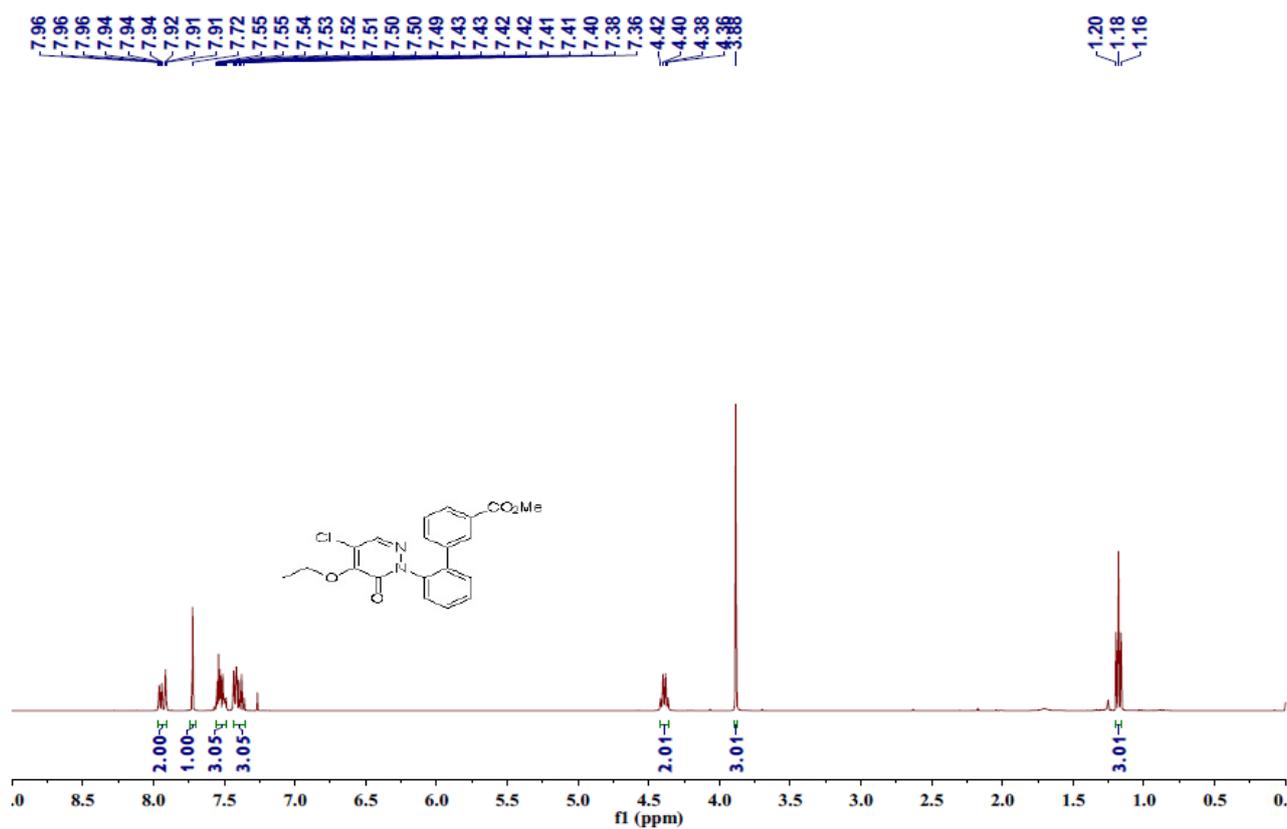
^1H and ^{13}C NMR spectra of compound **3g**.



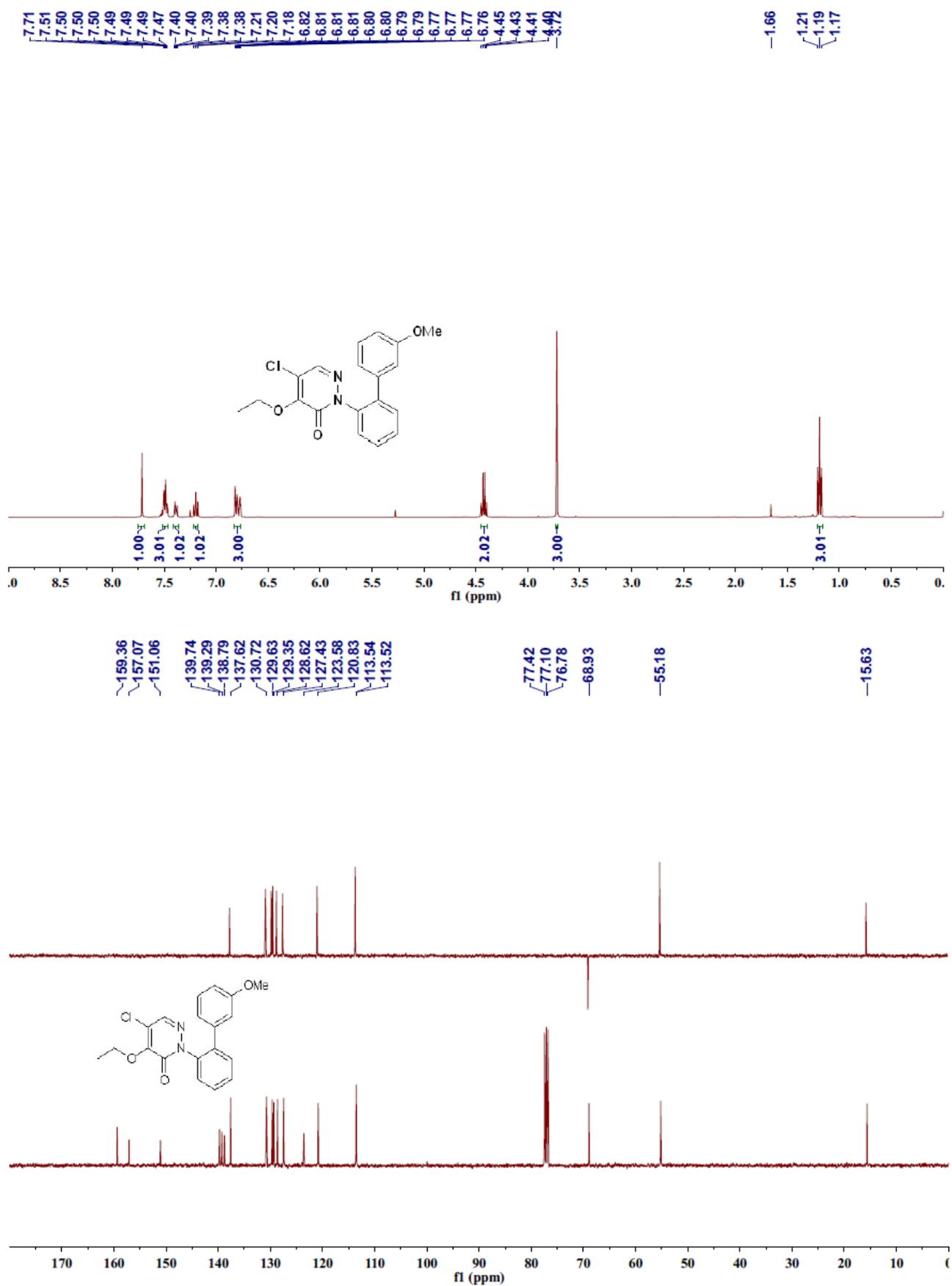
¹H and ¹³C NMR spectra of compound **3h**.



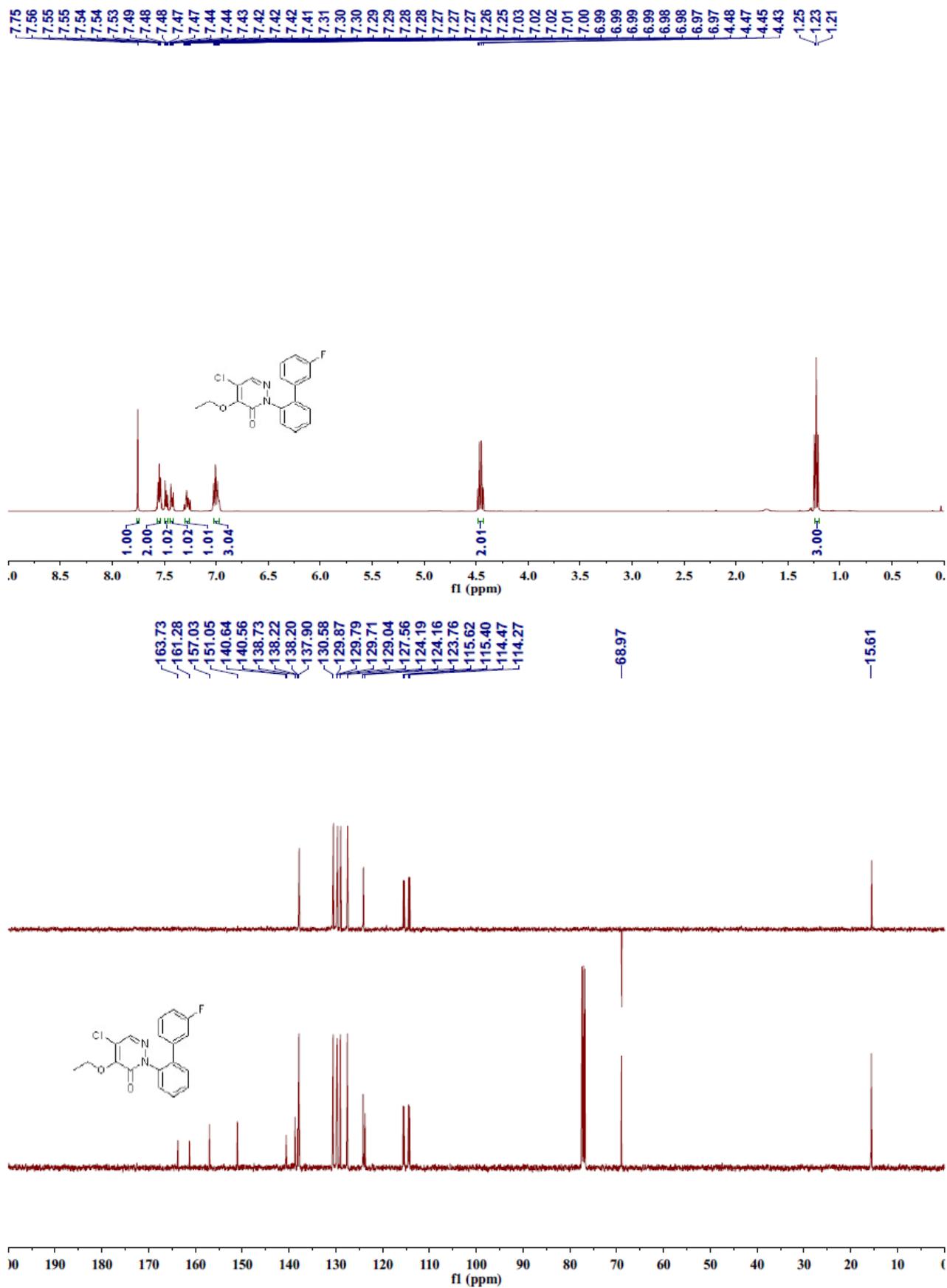
^1H and ^{13}C NMR spectra of compound **3i**.



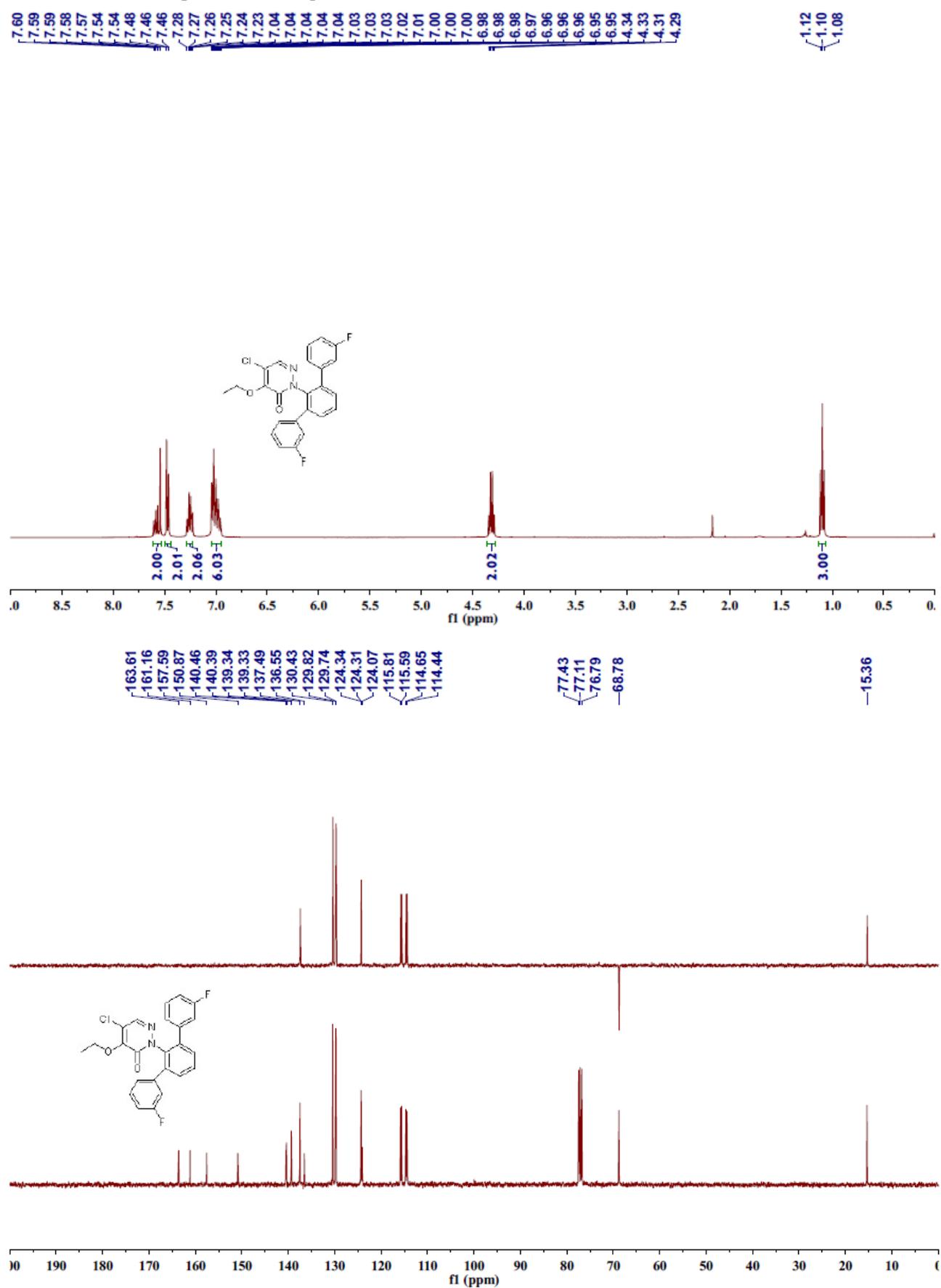
^1H and ^{13}C NMR spectra of compound **3j**.



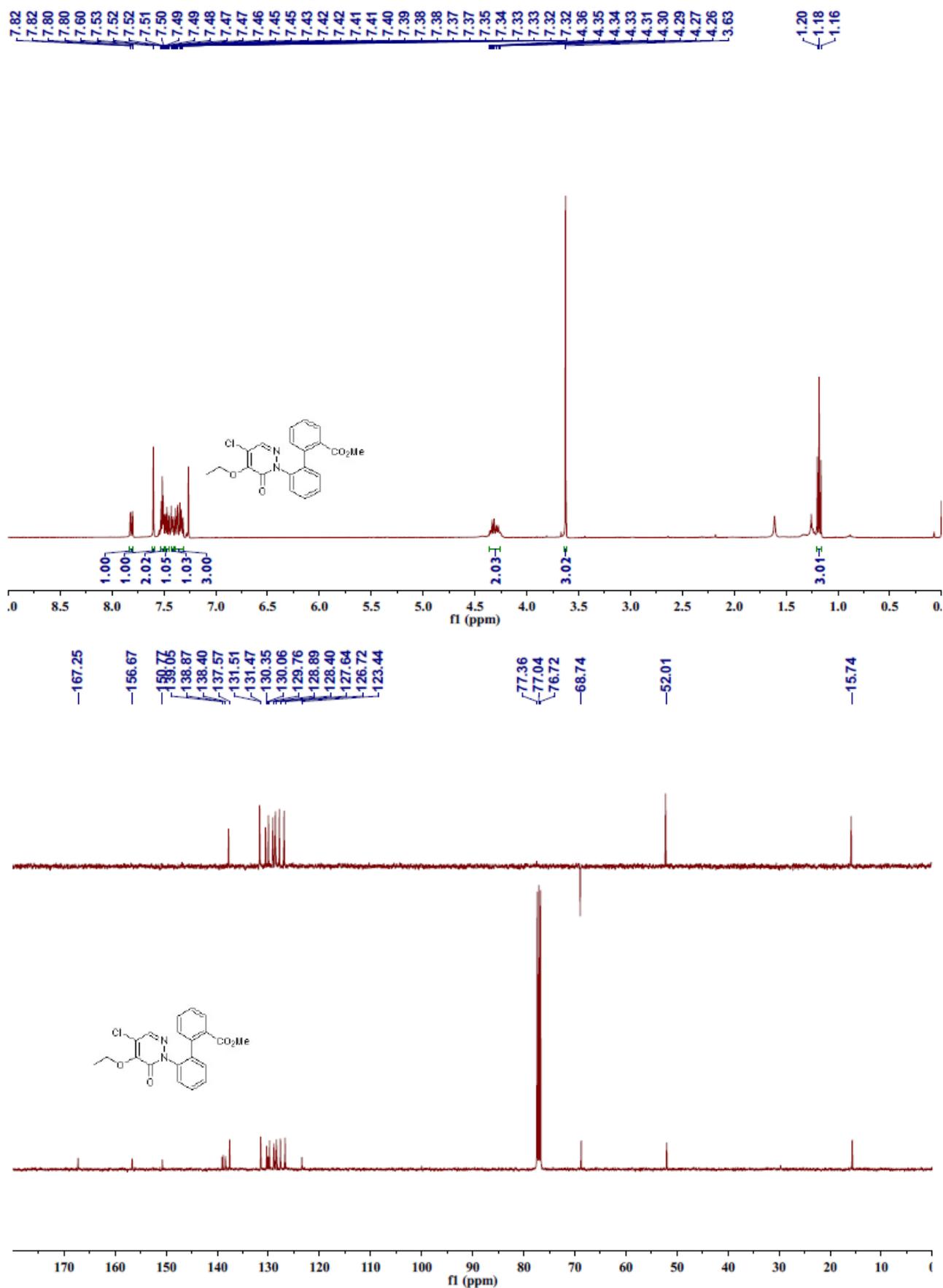
¹H and ¹³C NMR spectra of compound **3k**.



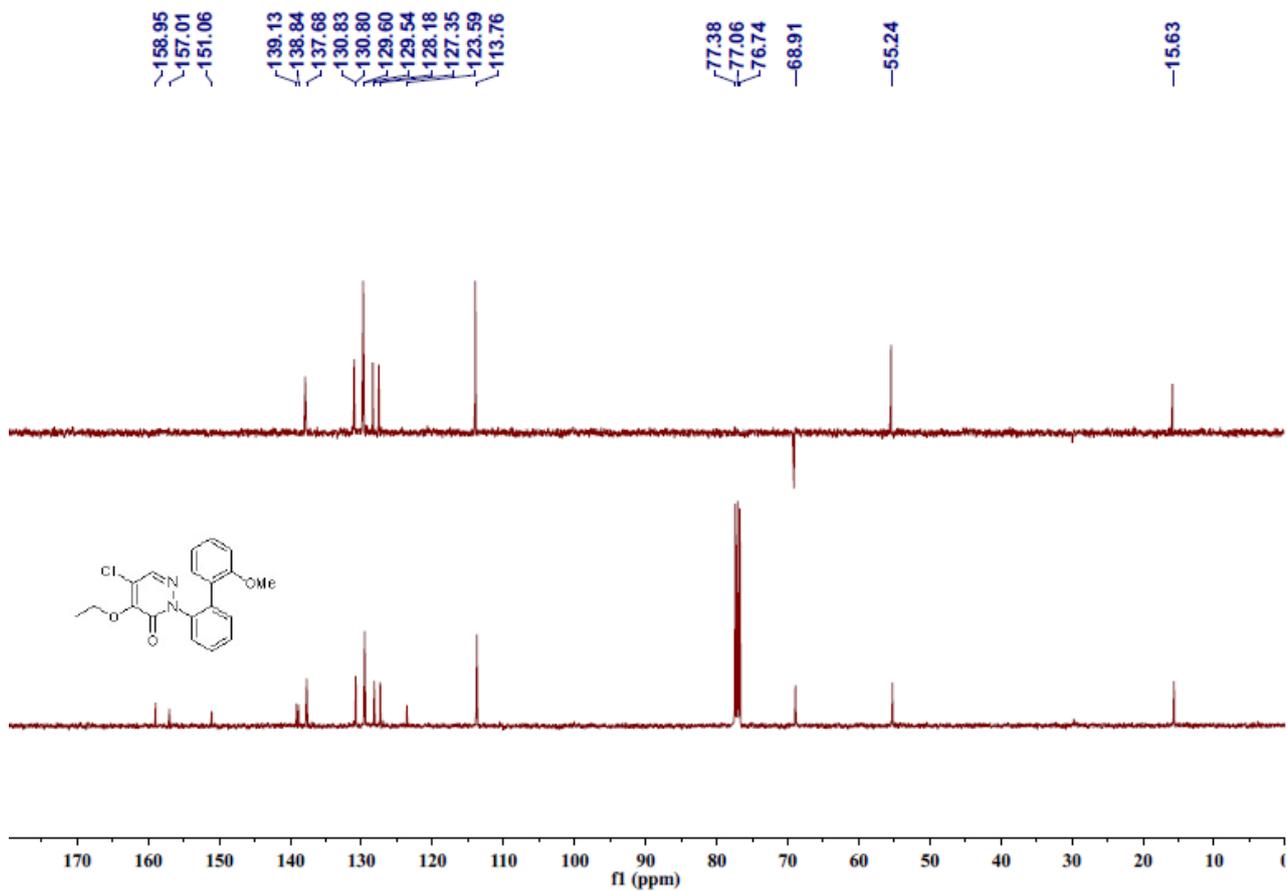
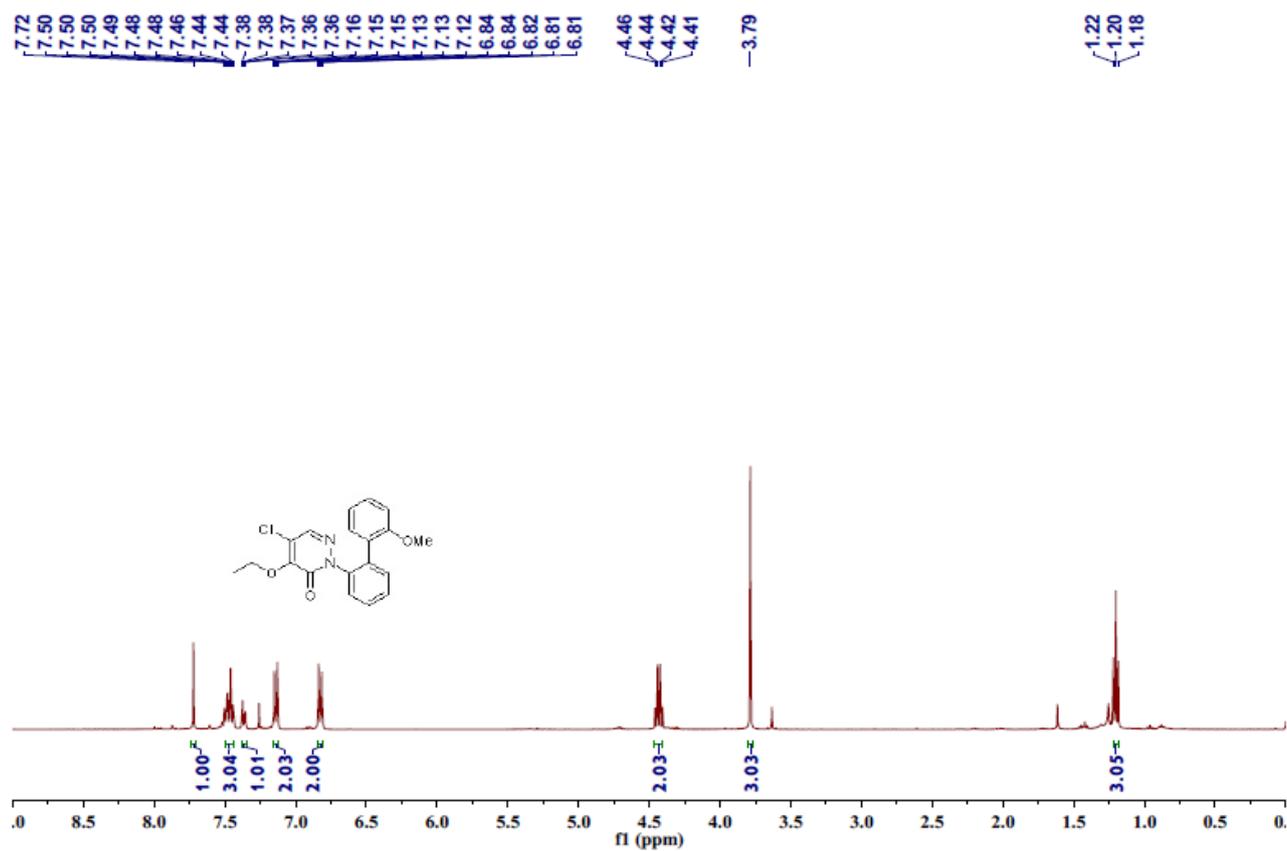
^1H and ^{13}C NMR spectra of compound **3k'**.



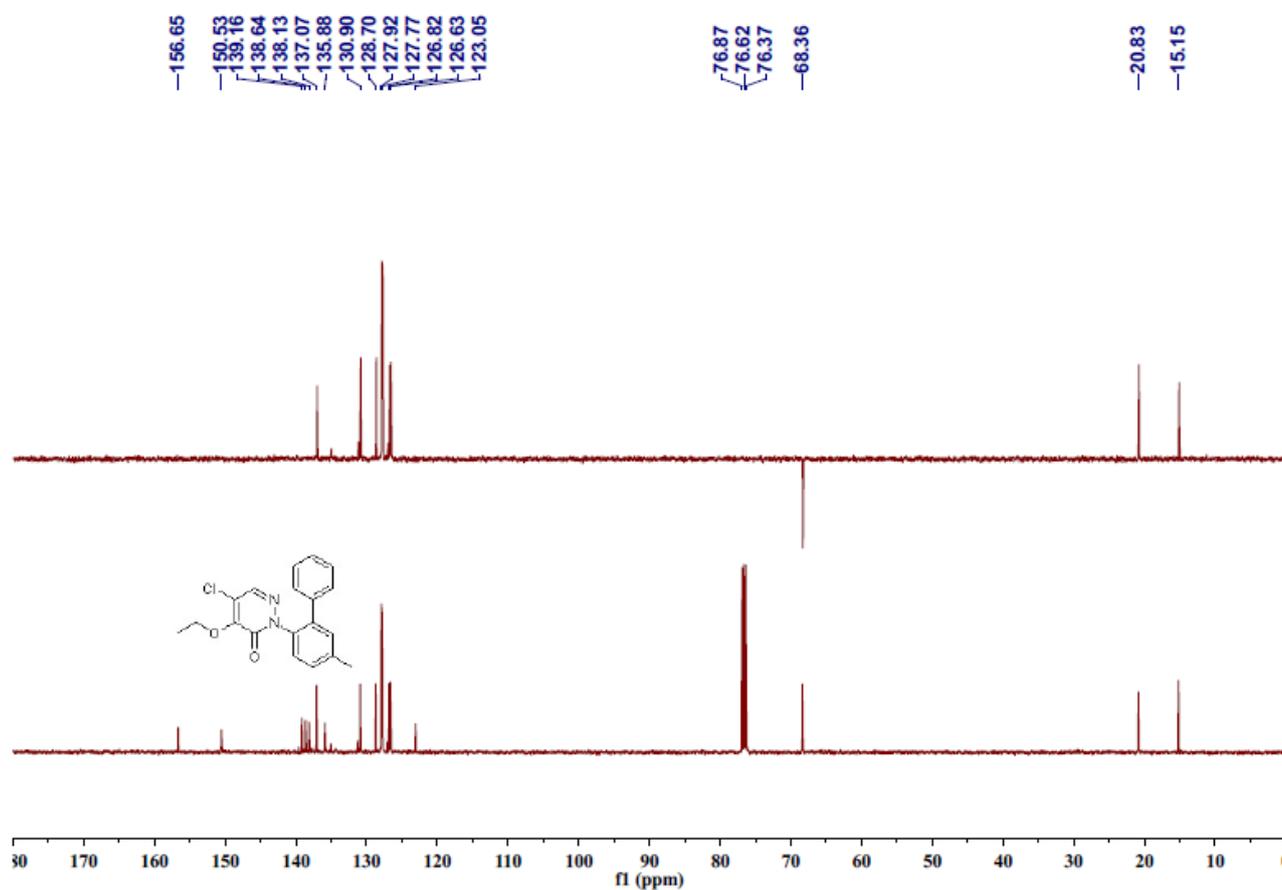
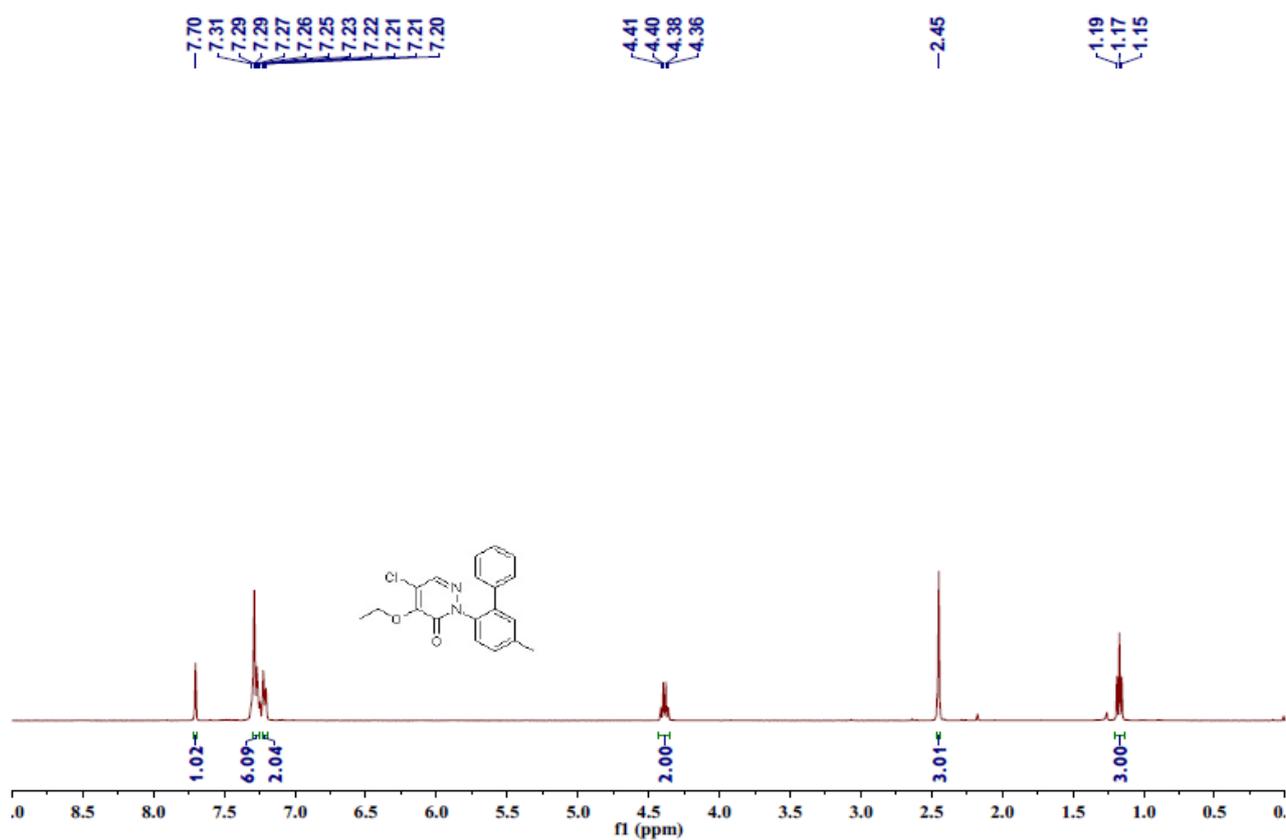
^1H and ^{13}C NMR spectra of compound **31**.



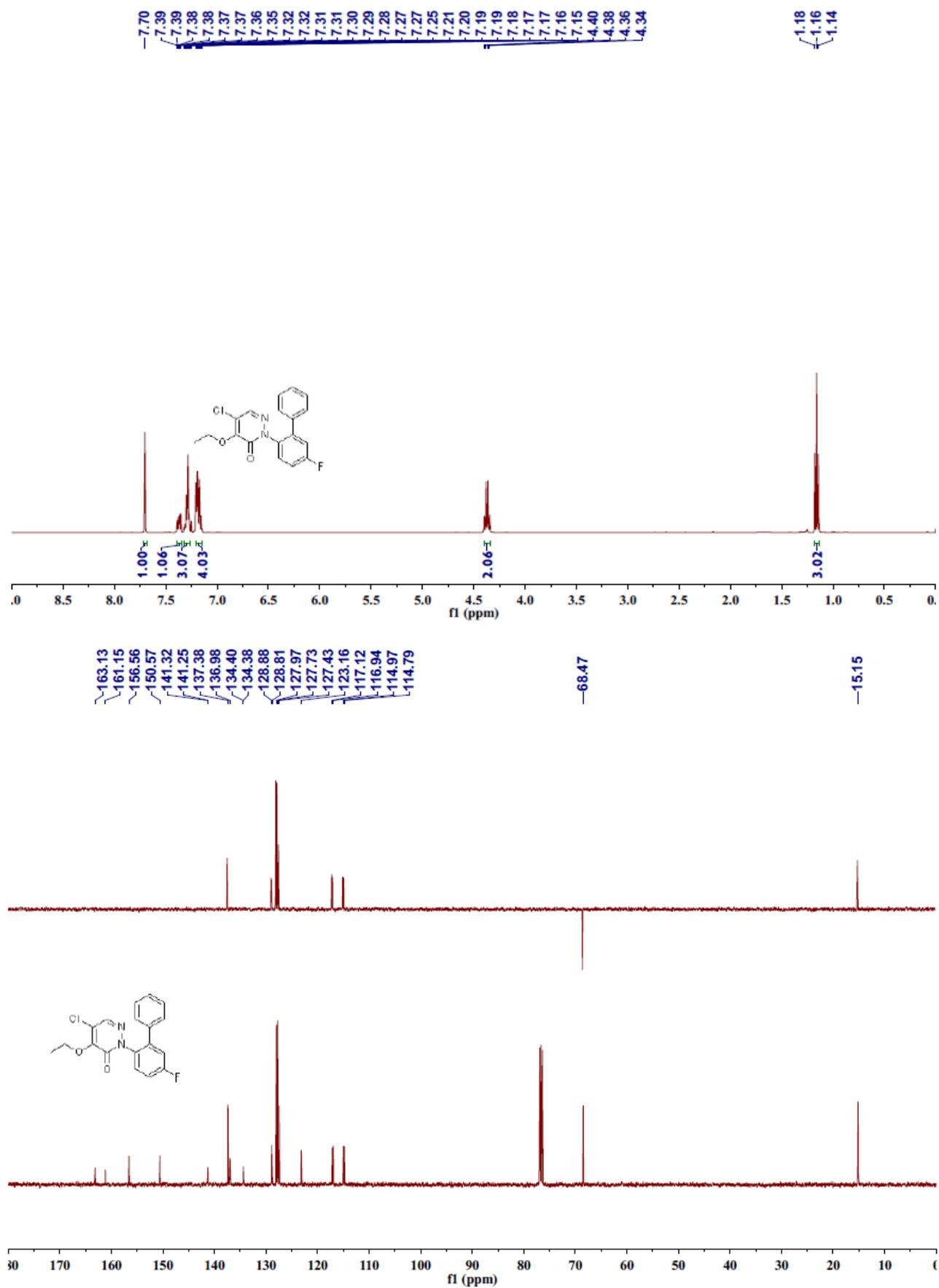
^1H and ^{13}C NMR spectra of compound **3m**.



^1H and ^{13}C NMR spectra of compound **3n**.

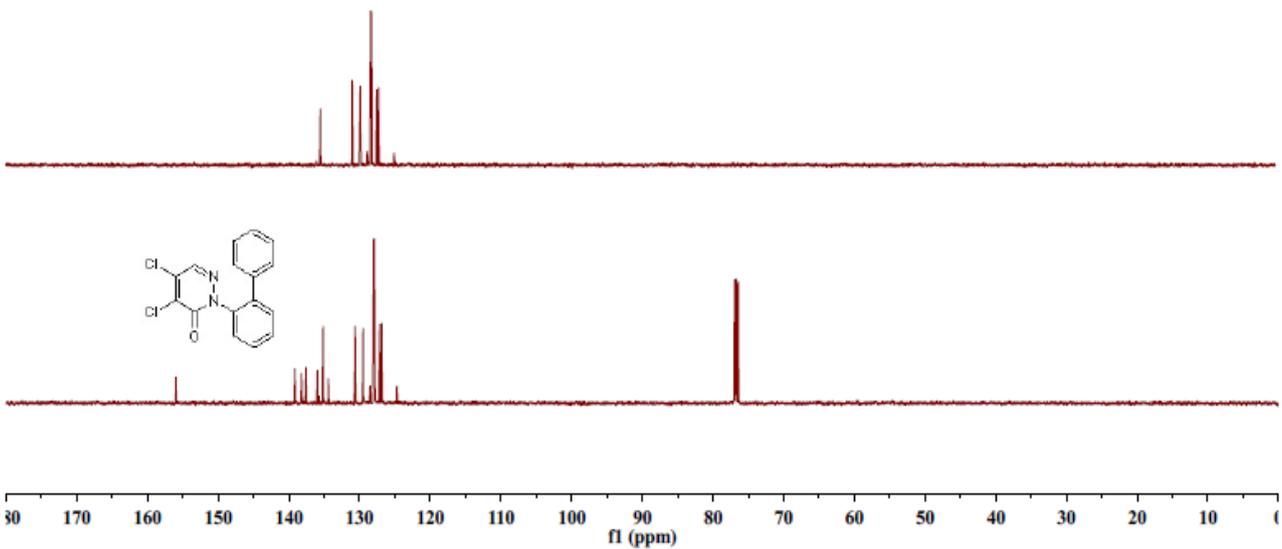
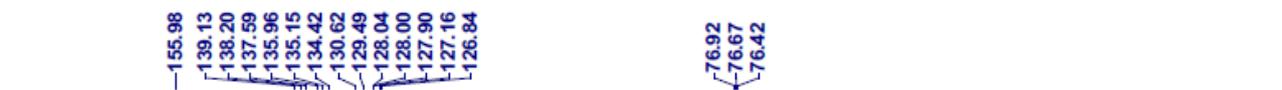
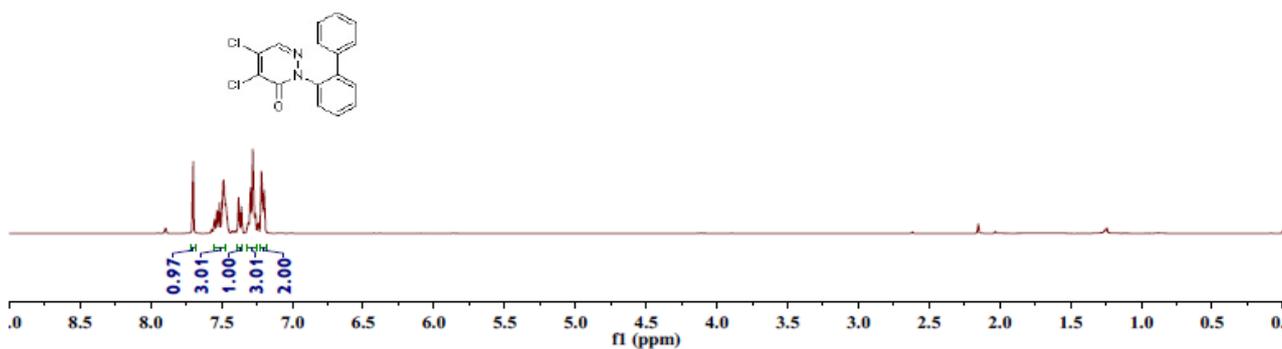


^1H and ^{13}C NMR spectra of compound **30**.

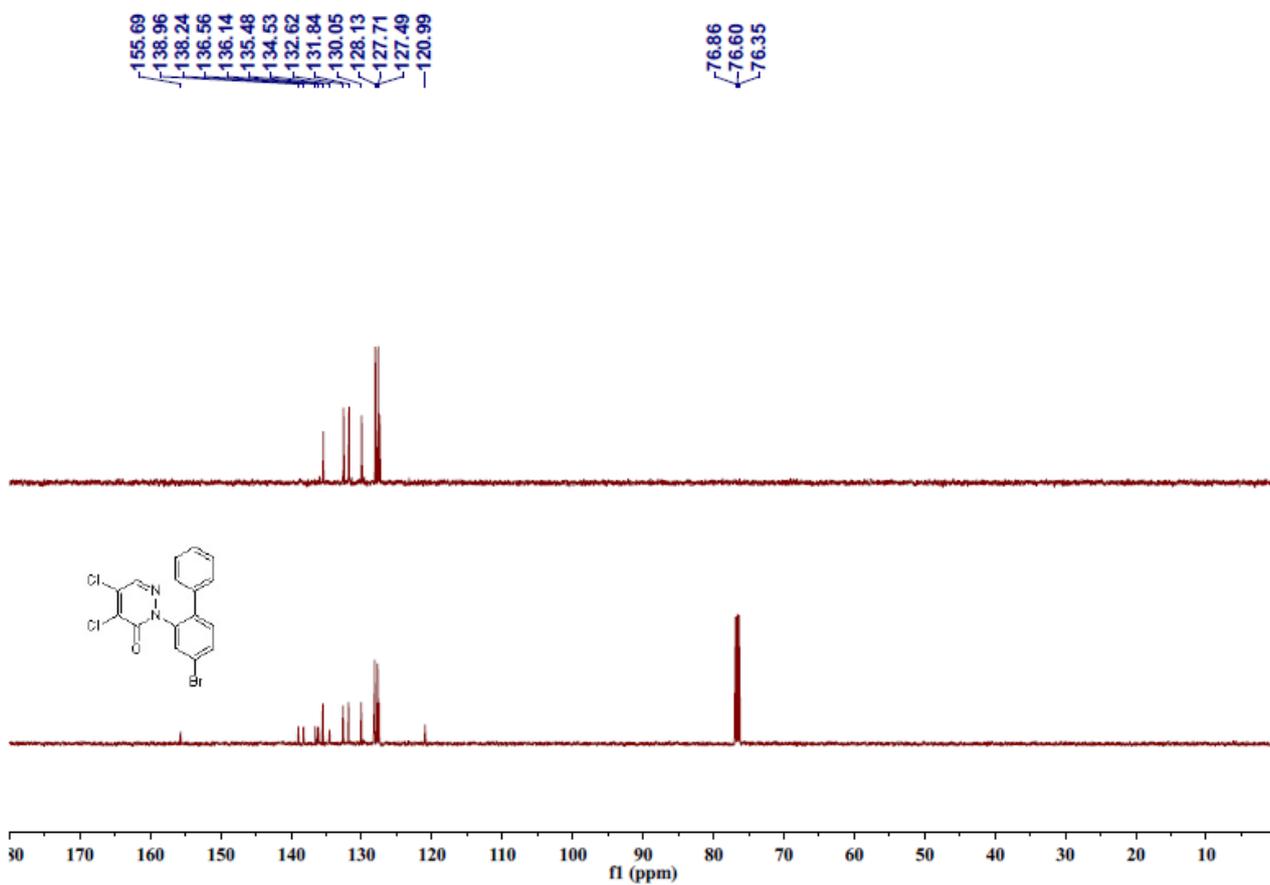
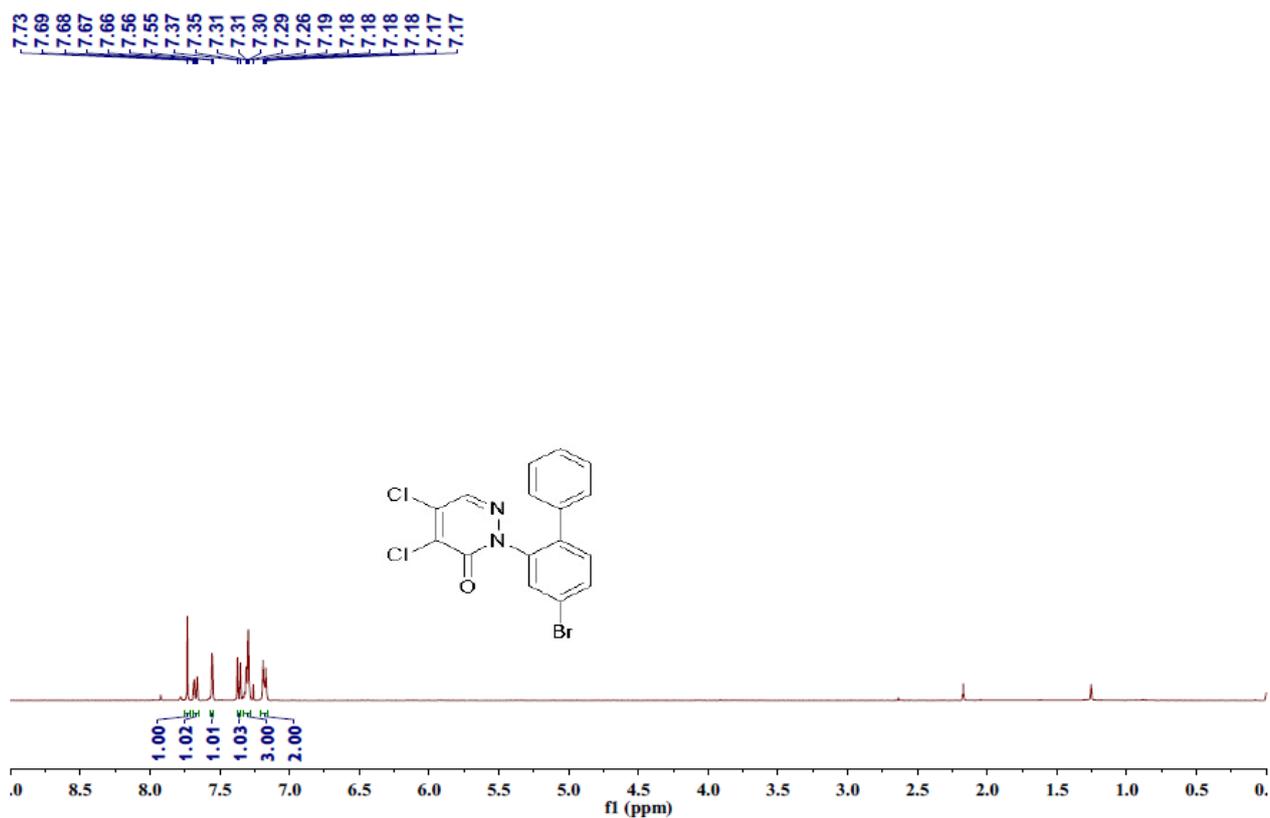


¹H and ¹³C NMR spectra of compound **3p**.

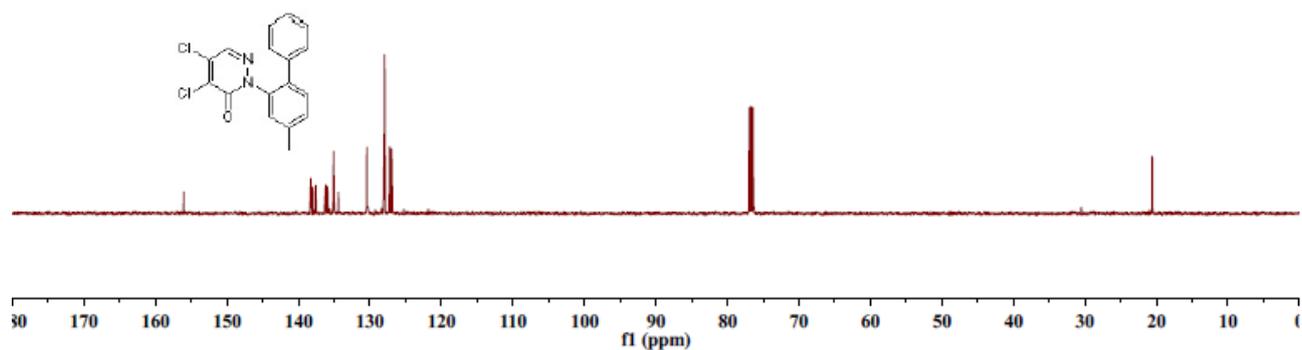
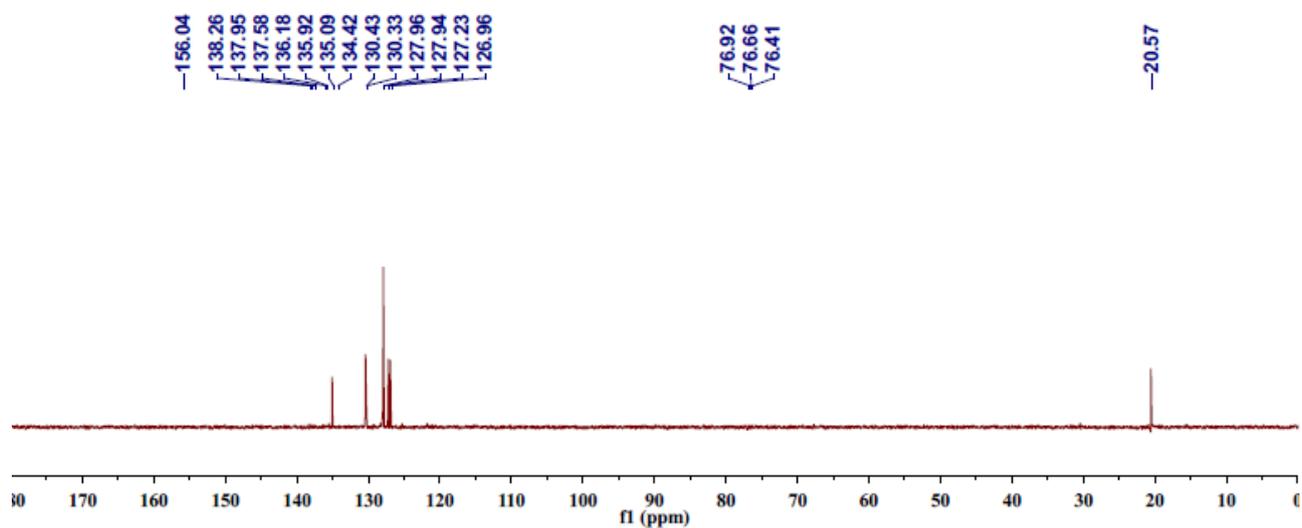
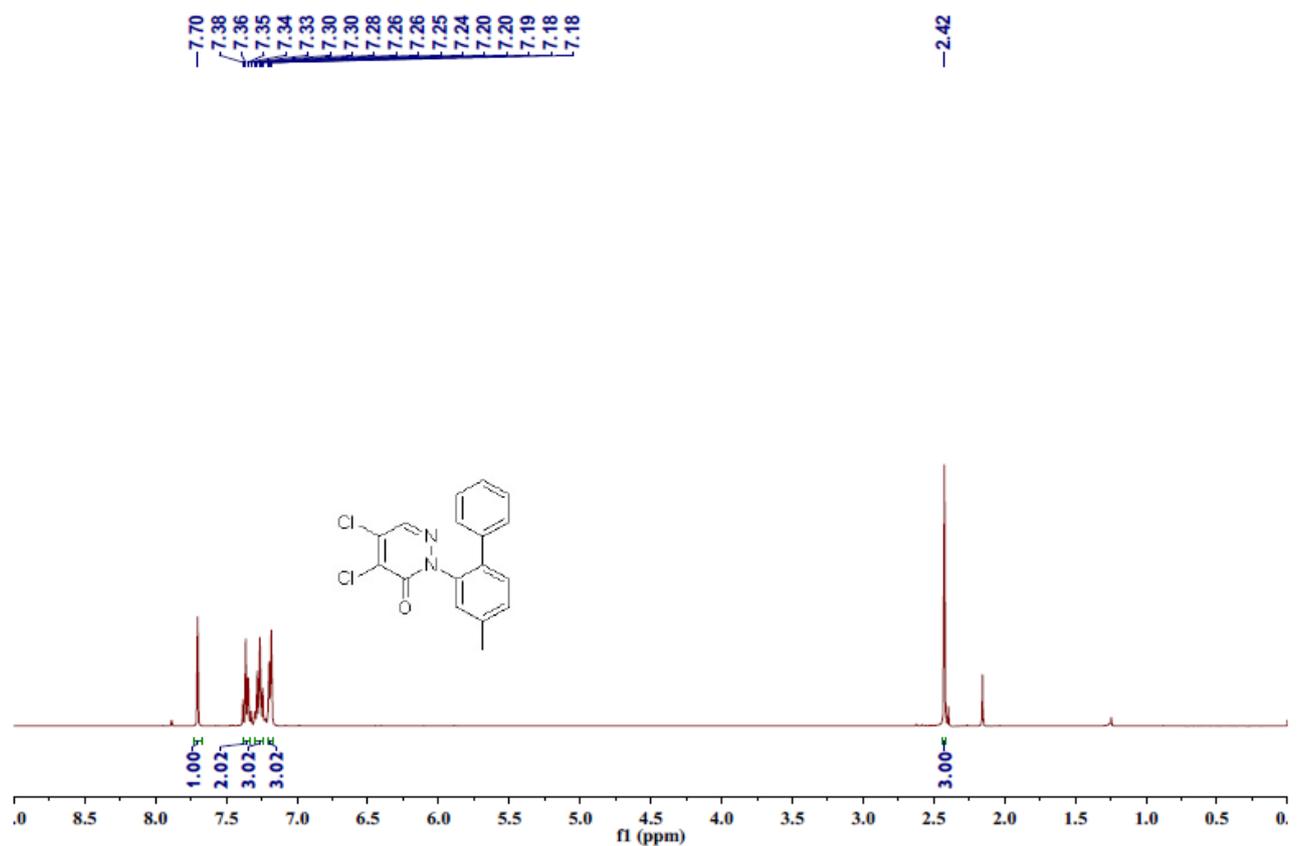
7.70
7.55
7.55
7.53
7.51
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.38
7.38
7.37
7.36
7.31
7.31
7.30
7.28
7.28
7.27
7.26
7.24
7.22
7.22
7.22
7.21
7.20
7.20



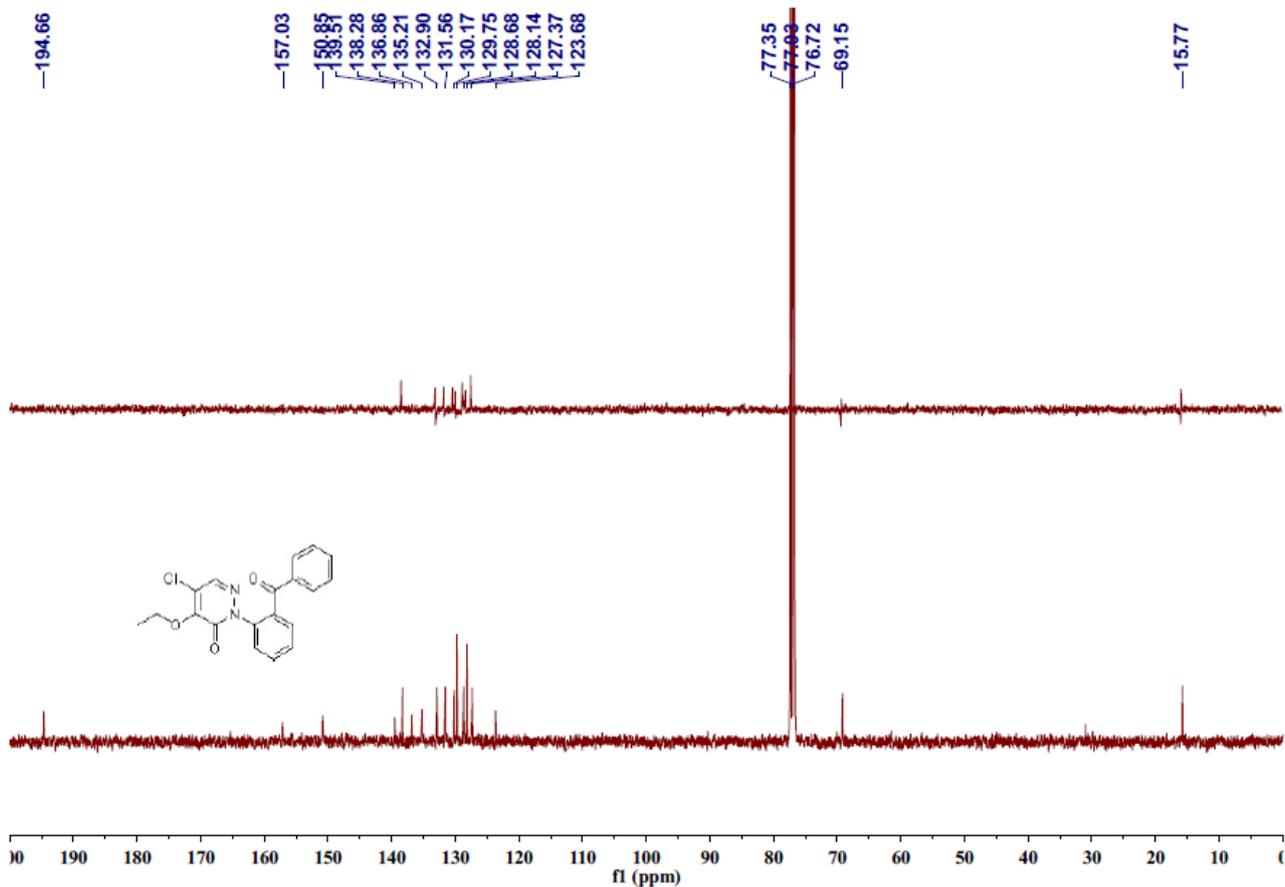
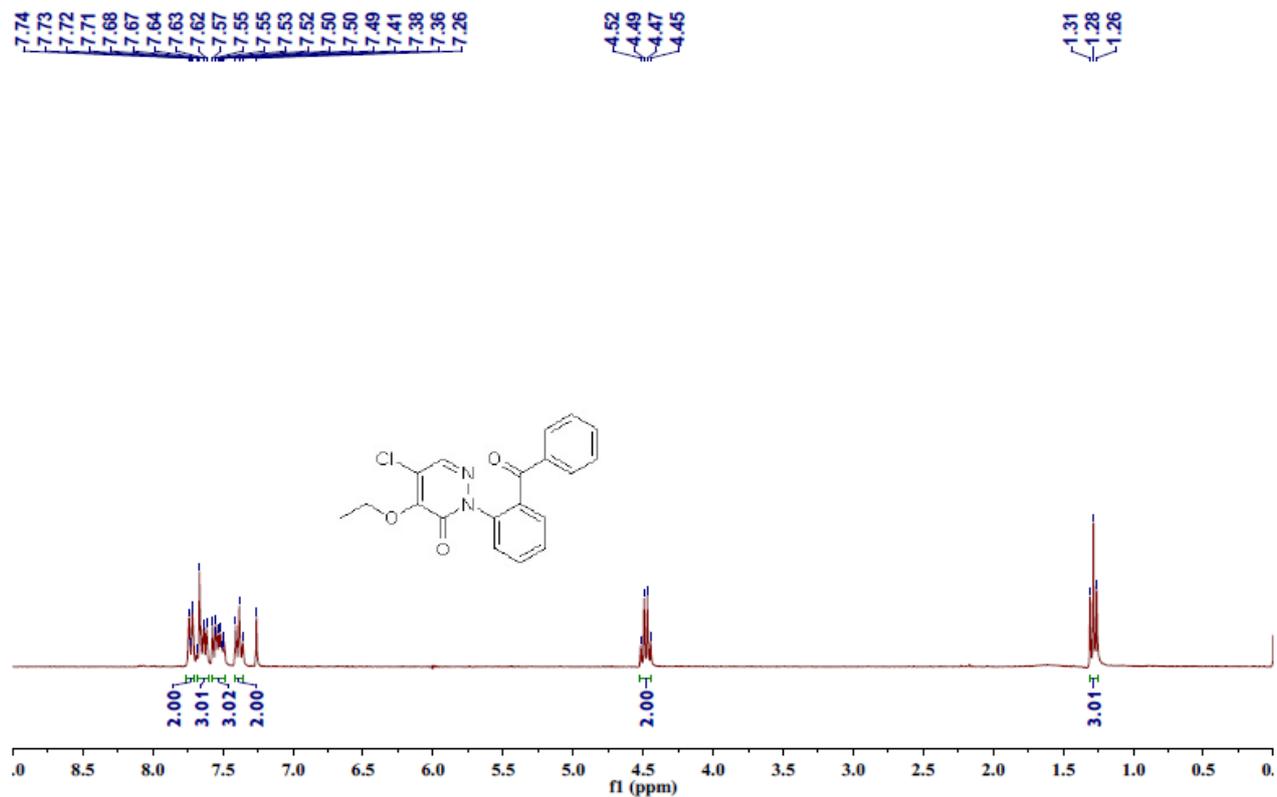
^1H and ^{13}C NMR spectra of compound **3q**.



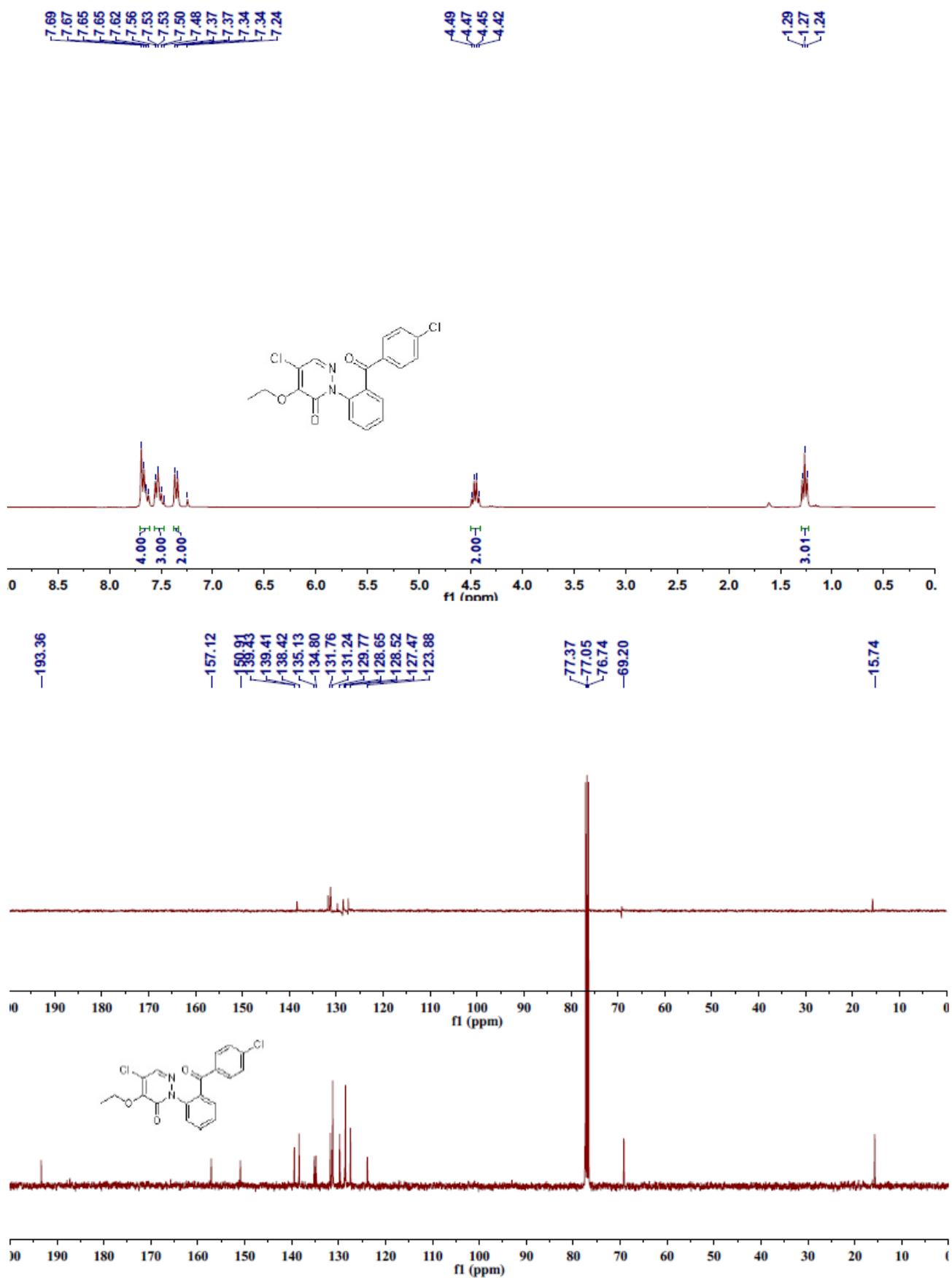
^1H and ^{13}C NMR spectra of compound **3r**.



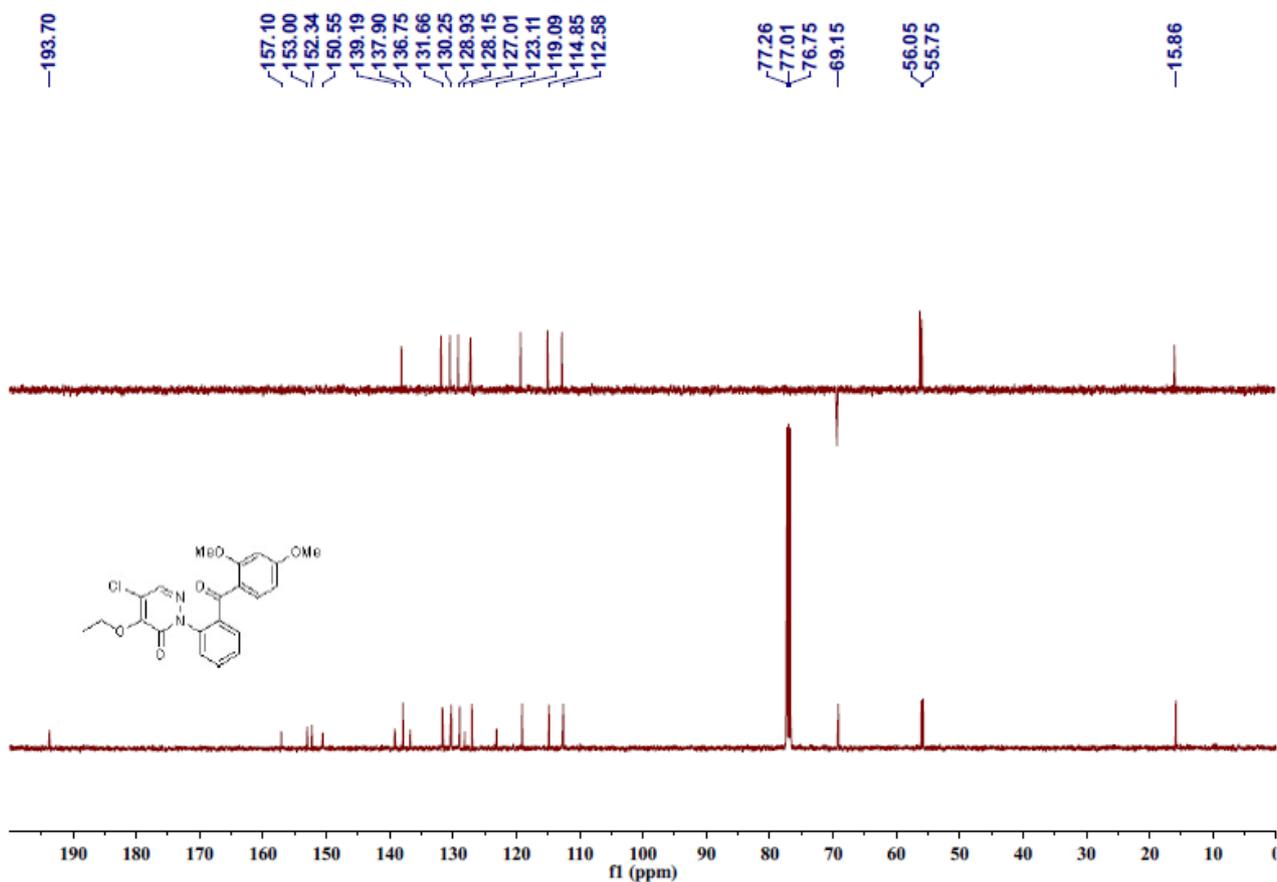
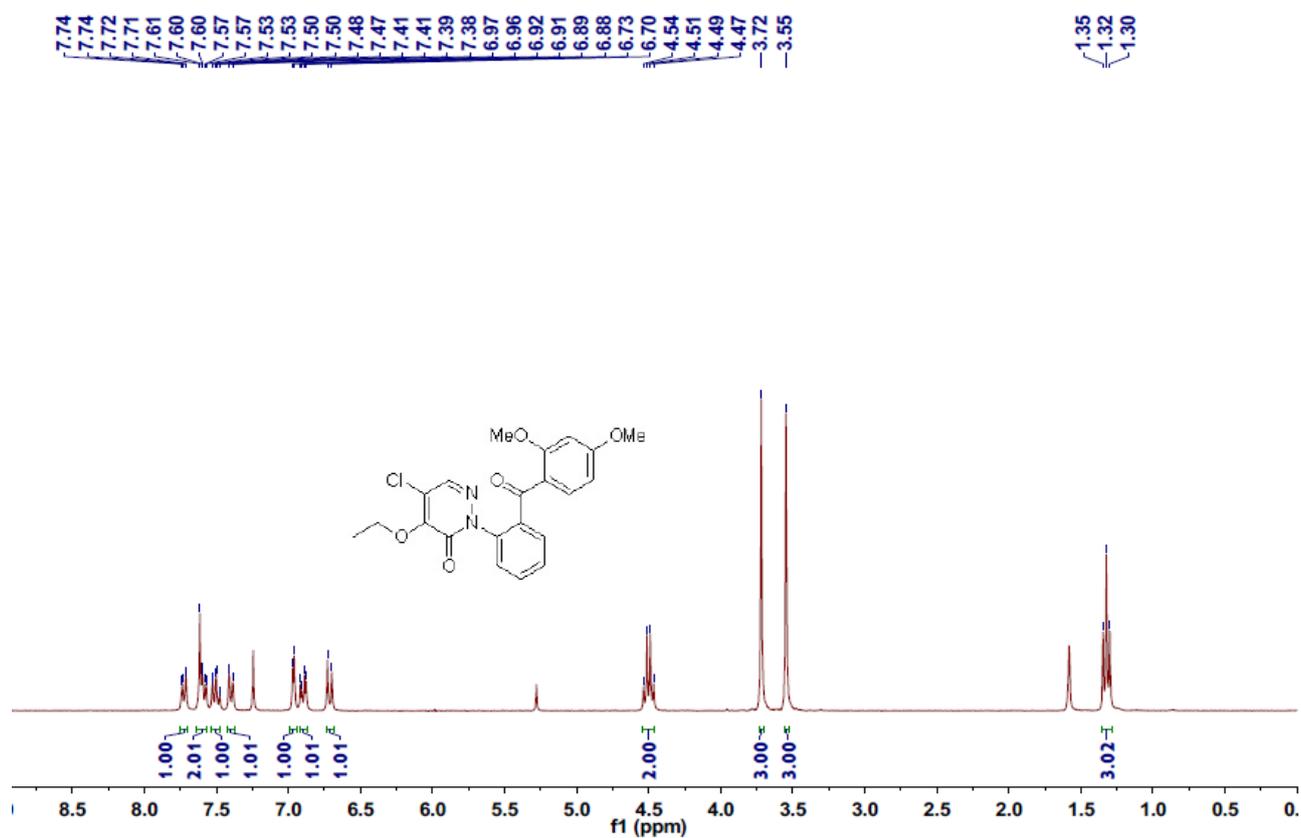
^1H and ^{13}C NMR spectra of compound **5a**.



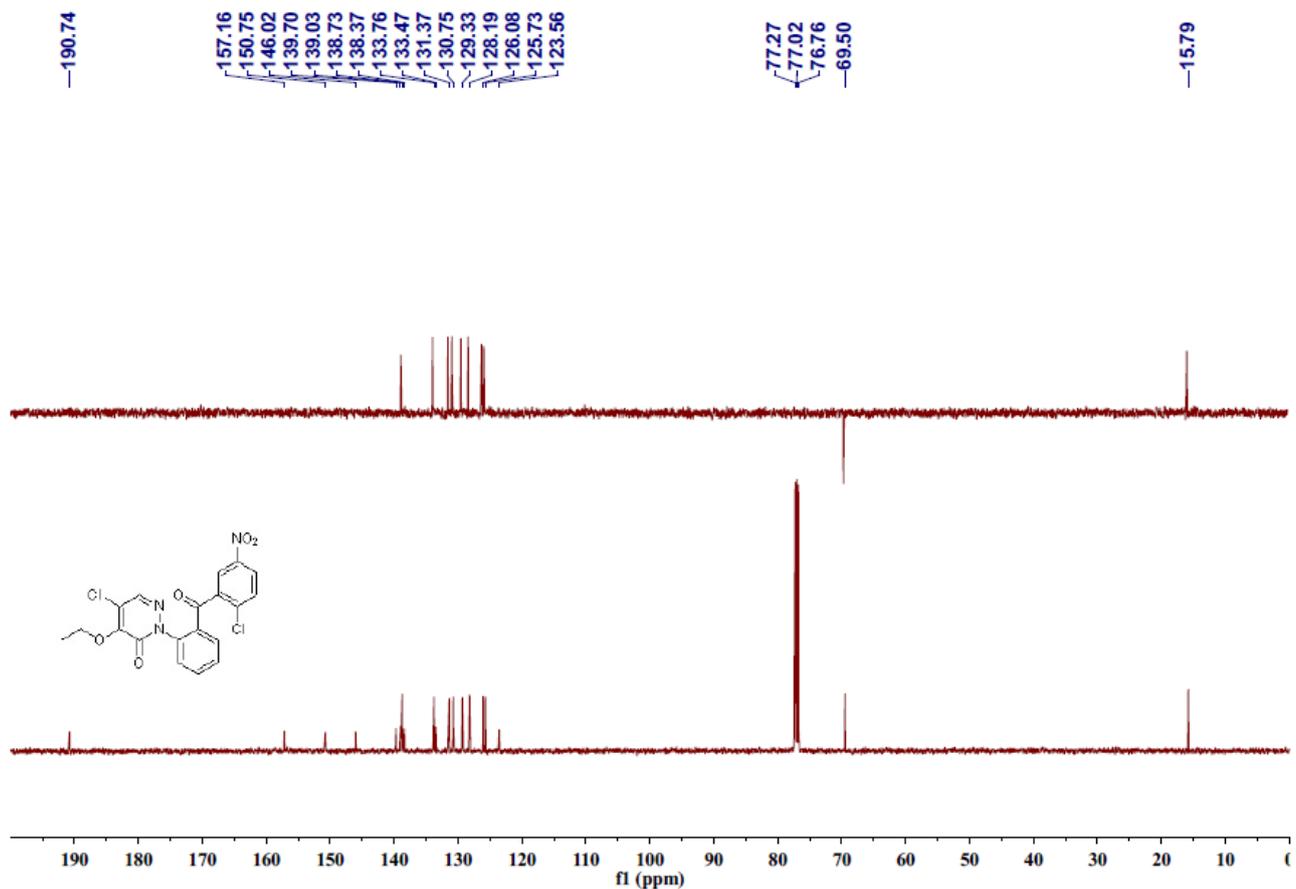
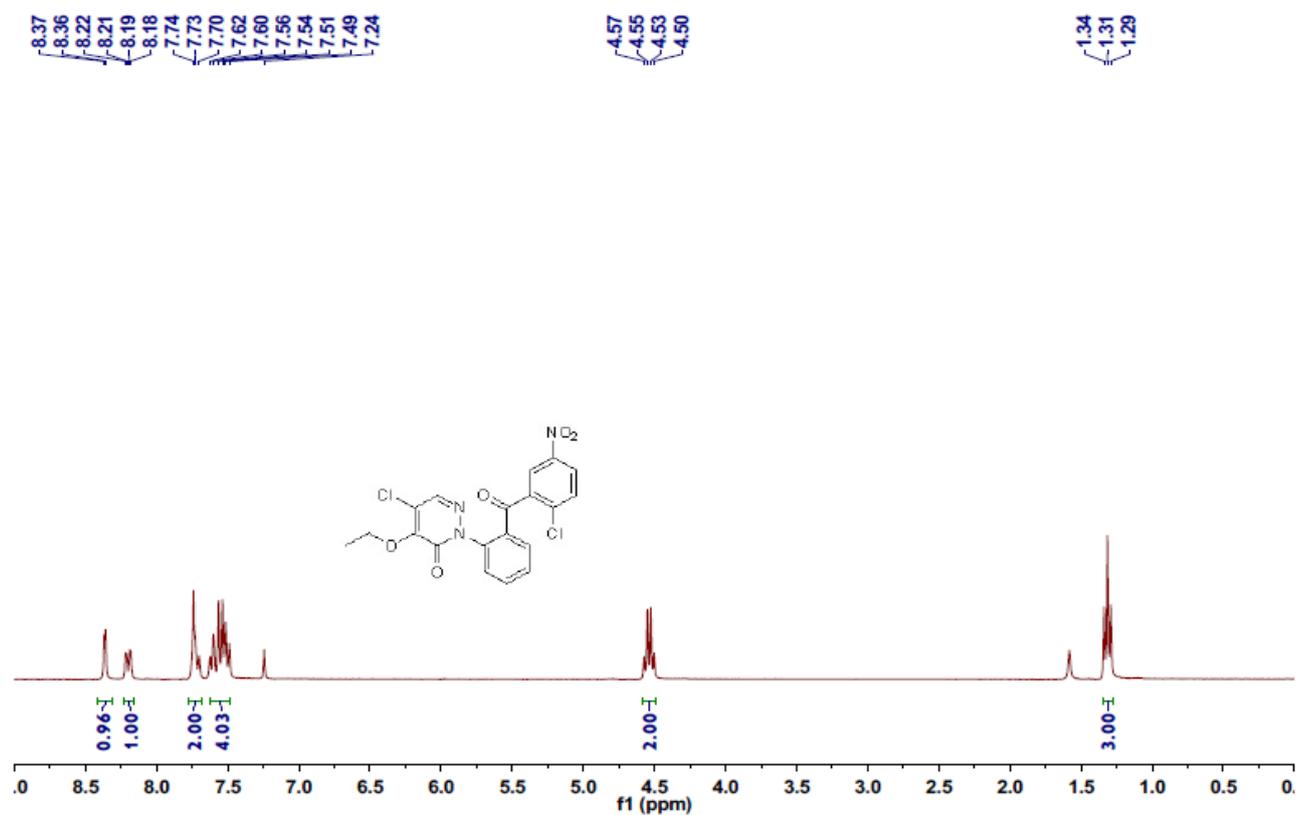
^1H and ^{13}C NMR spectra of compound **5b**.



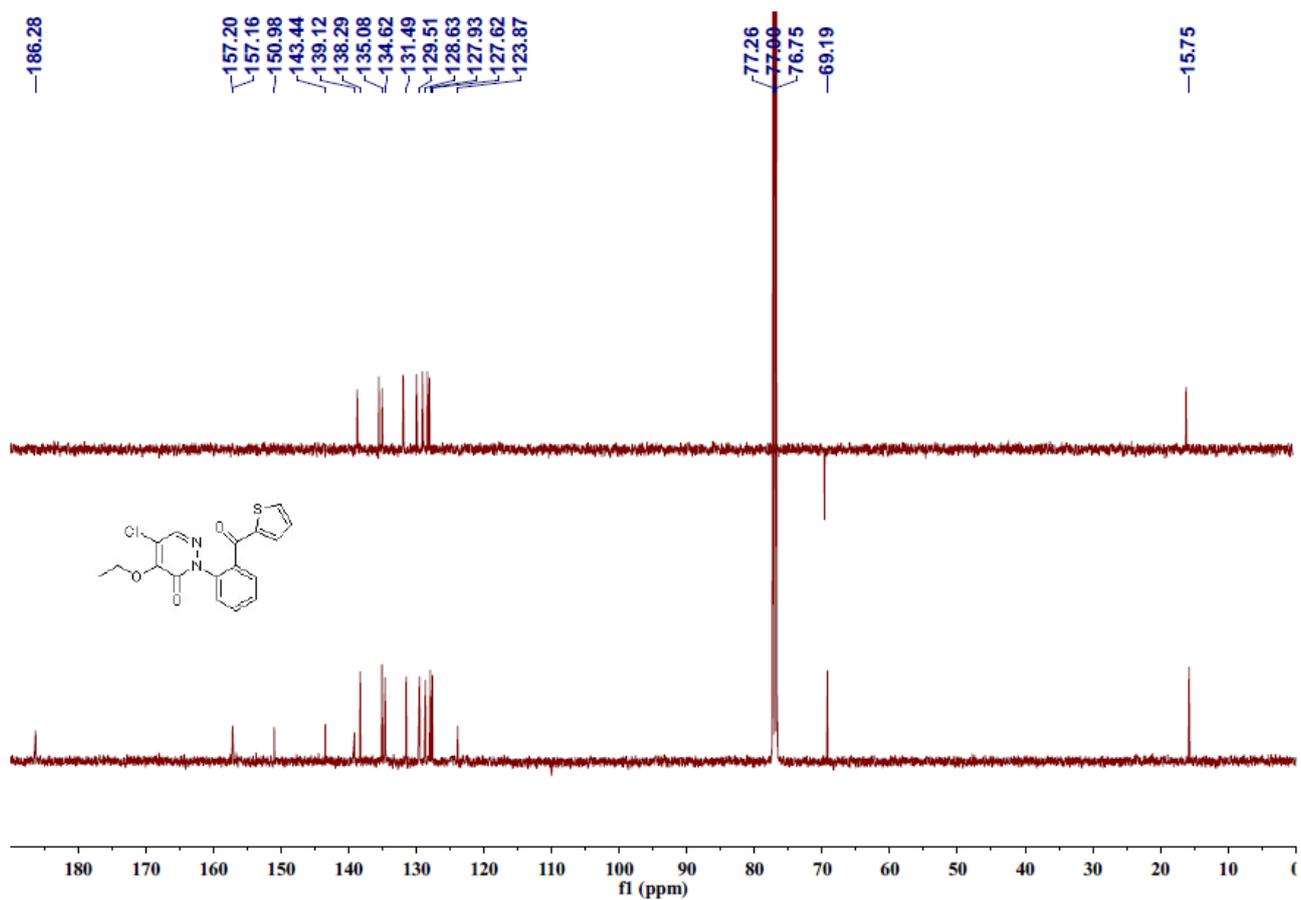
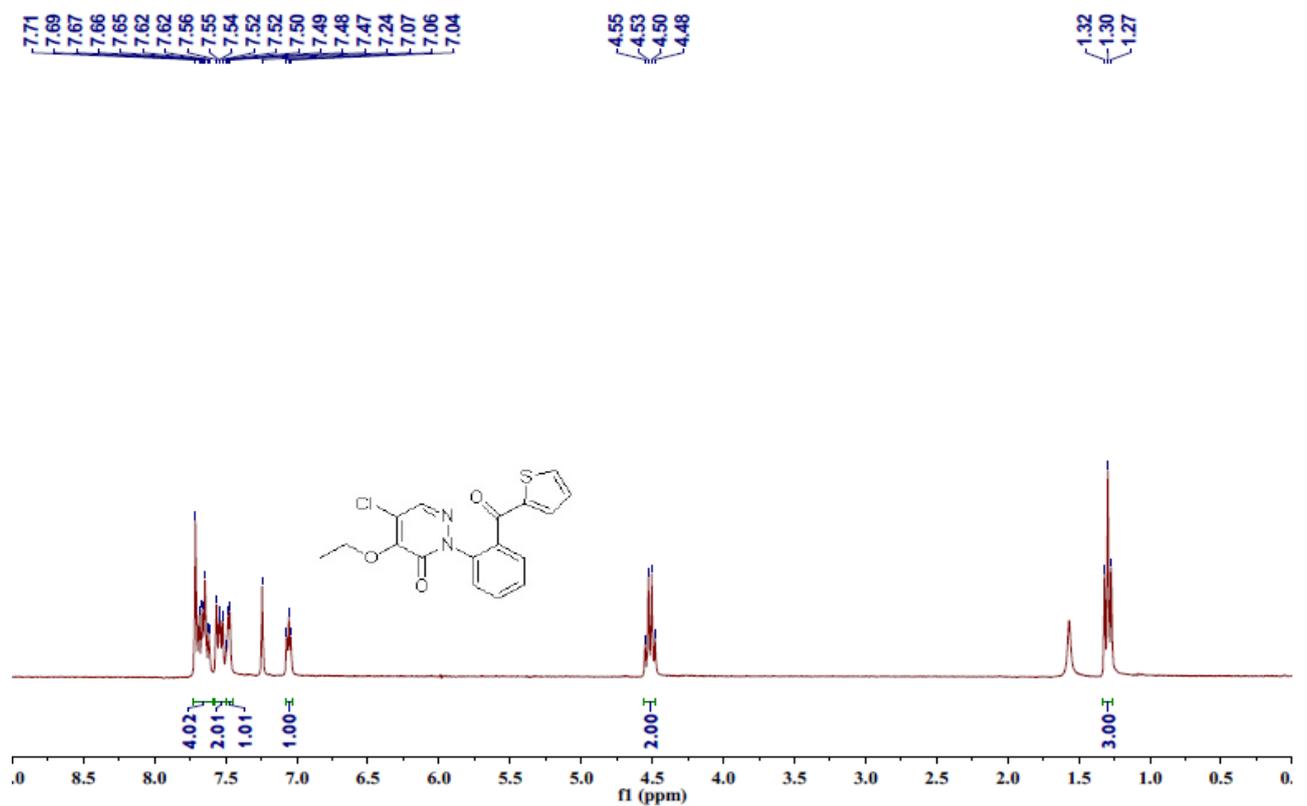
^1H and ^{13}C NMR spectra of compound **5c**.



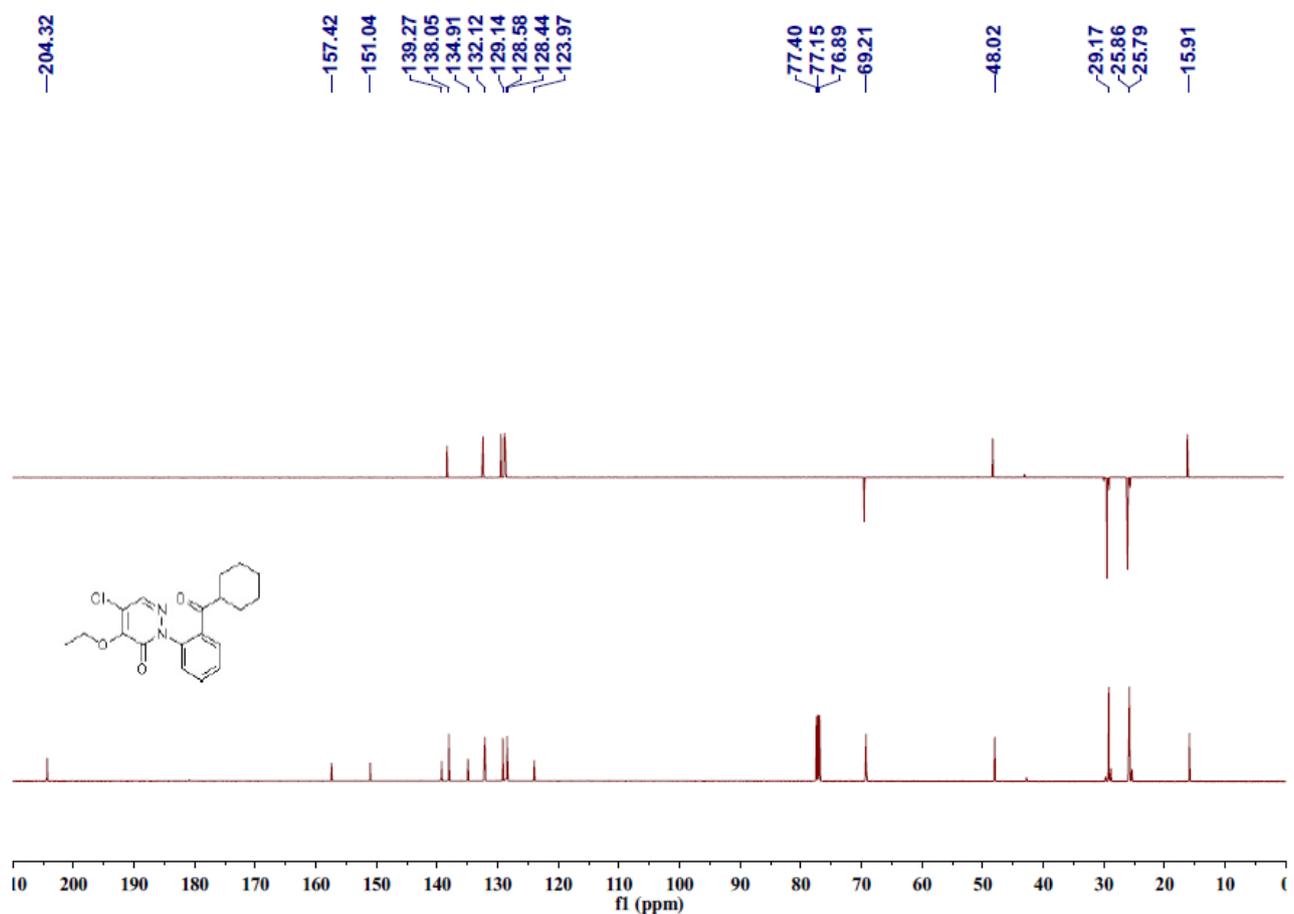
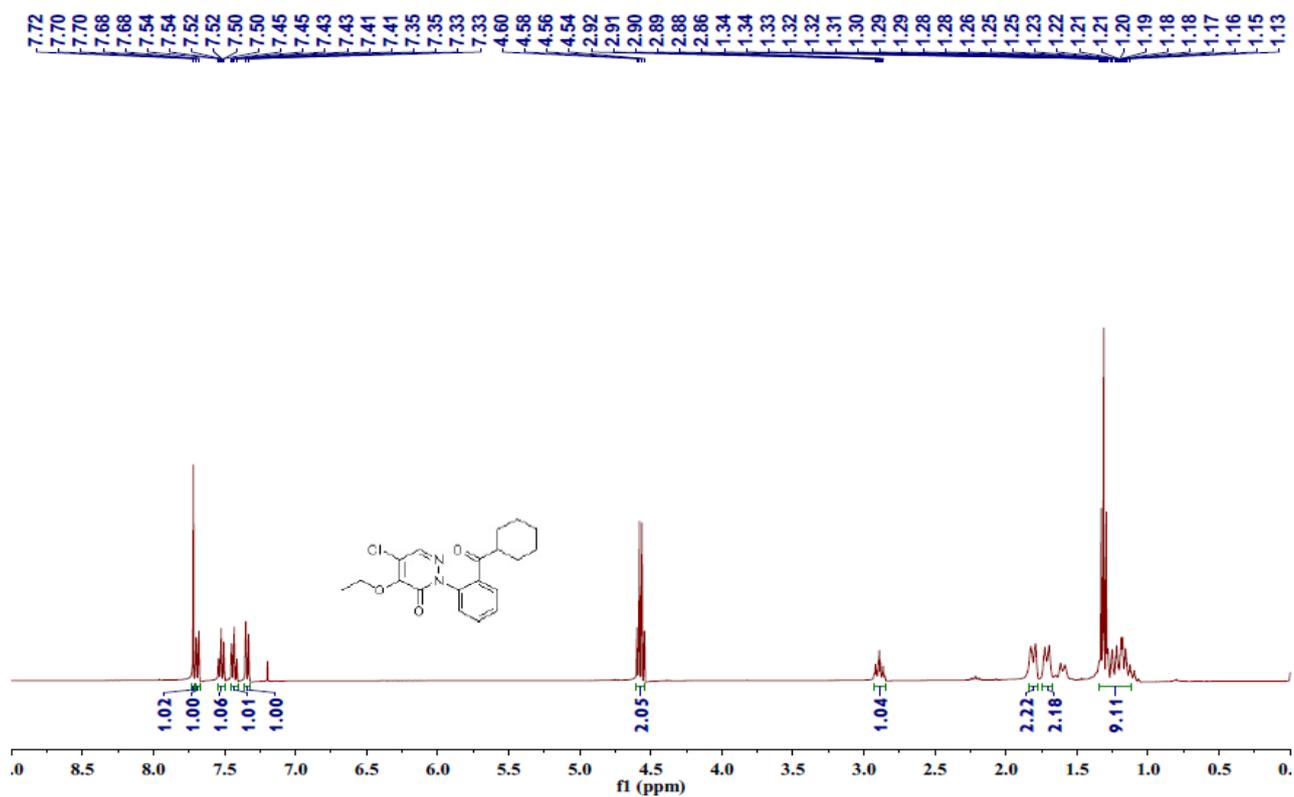
^1H and ^{13}C NMR spectra of compound **5d**.



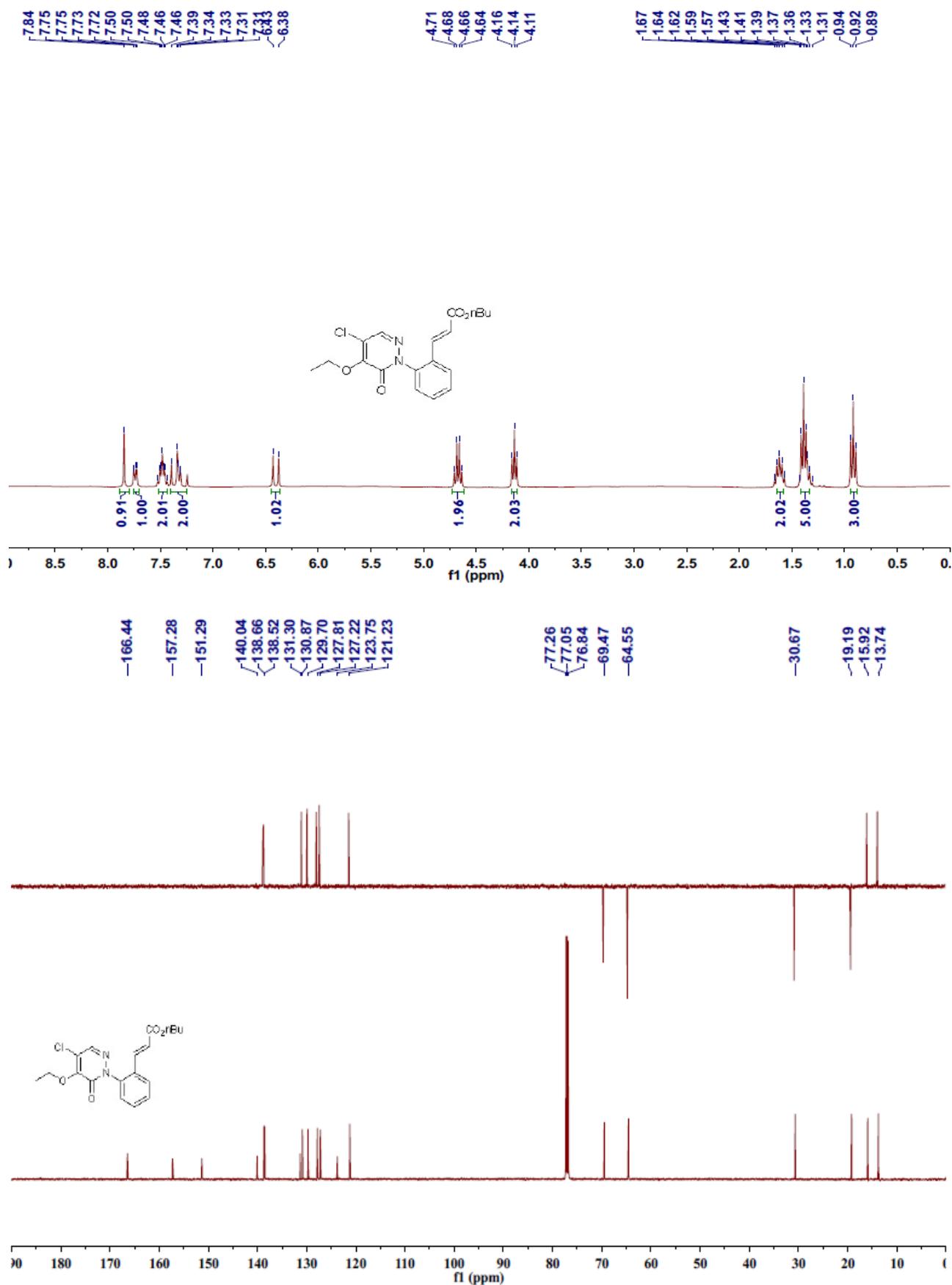
^1H and ^{13}C NMR spectra of compound **5e**.



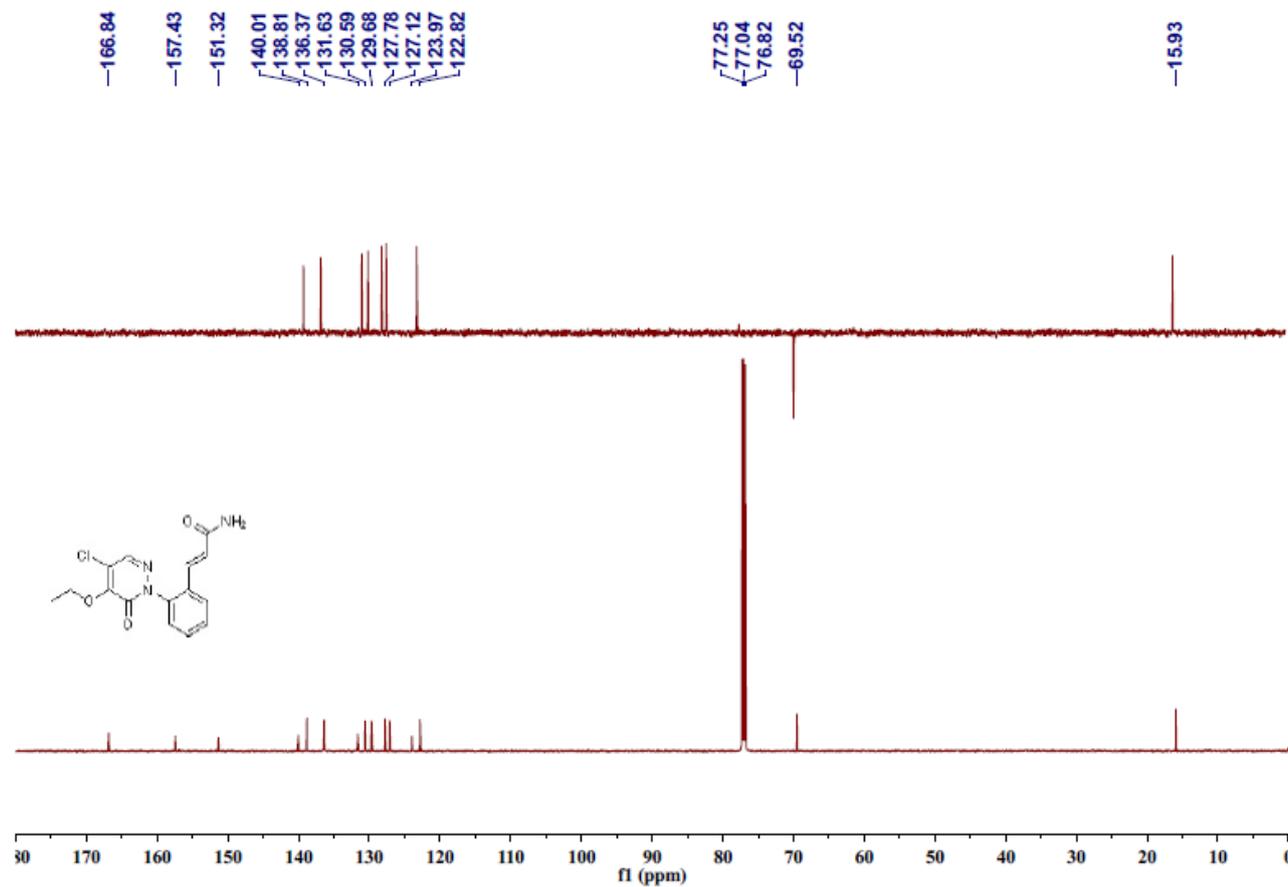
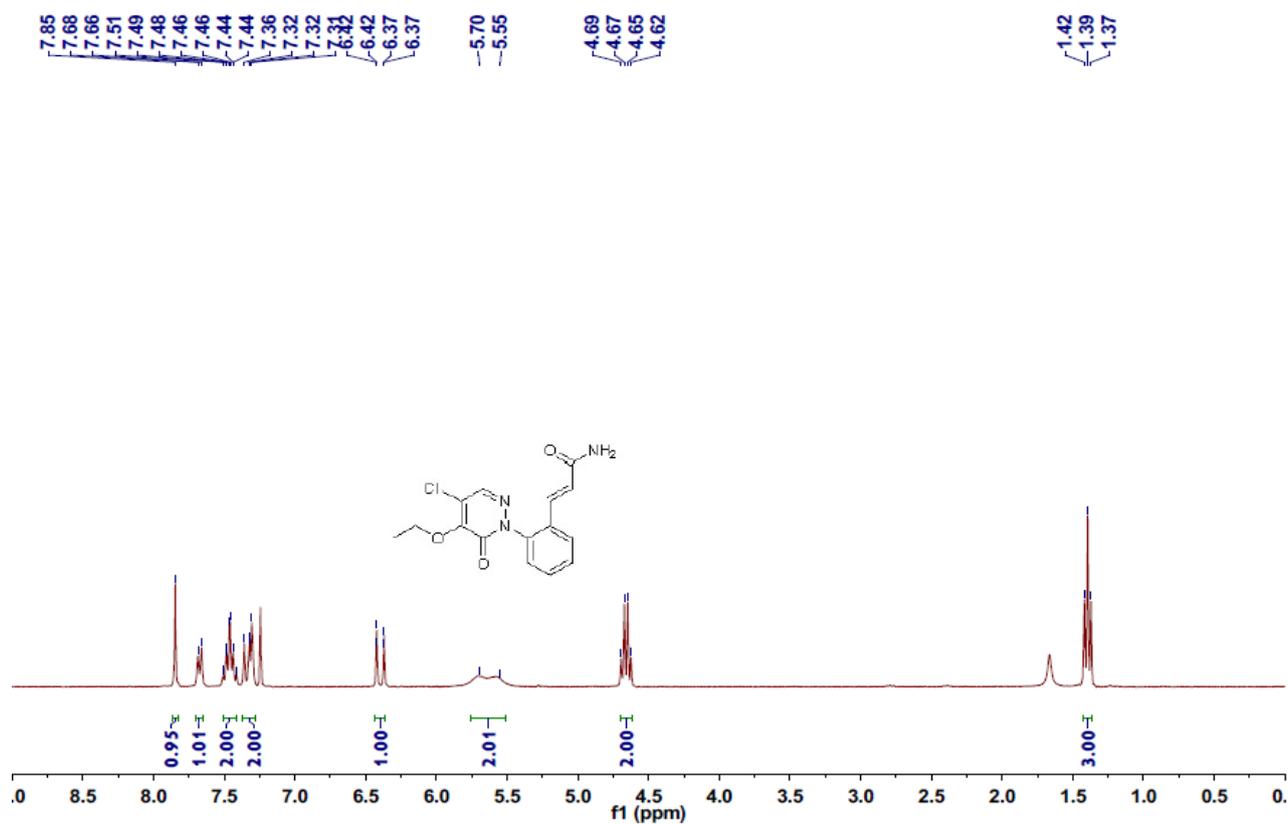
^1H and ^{13}C NMR spectra of compound **5f**.



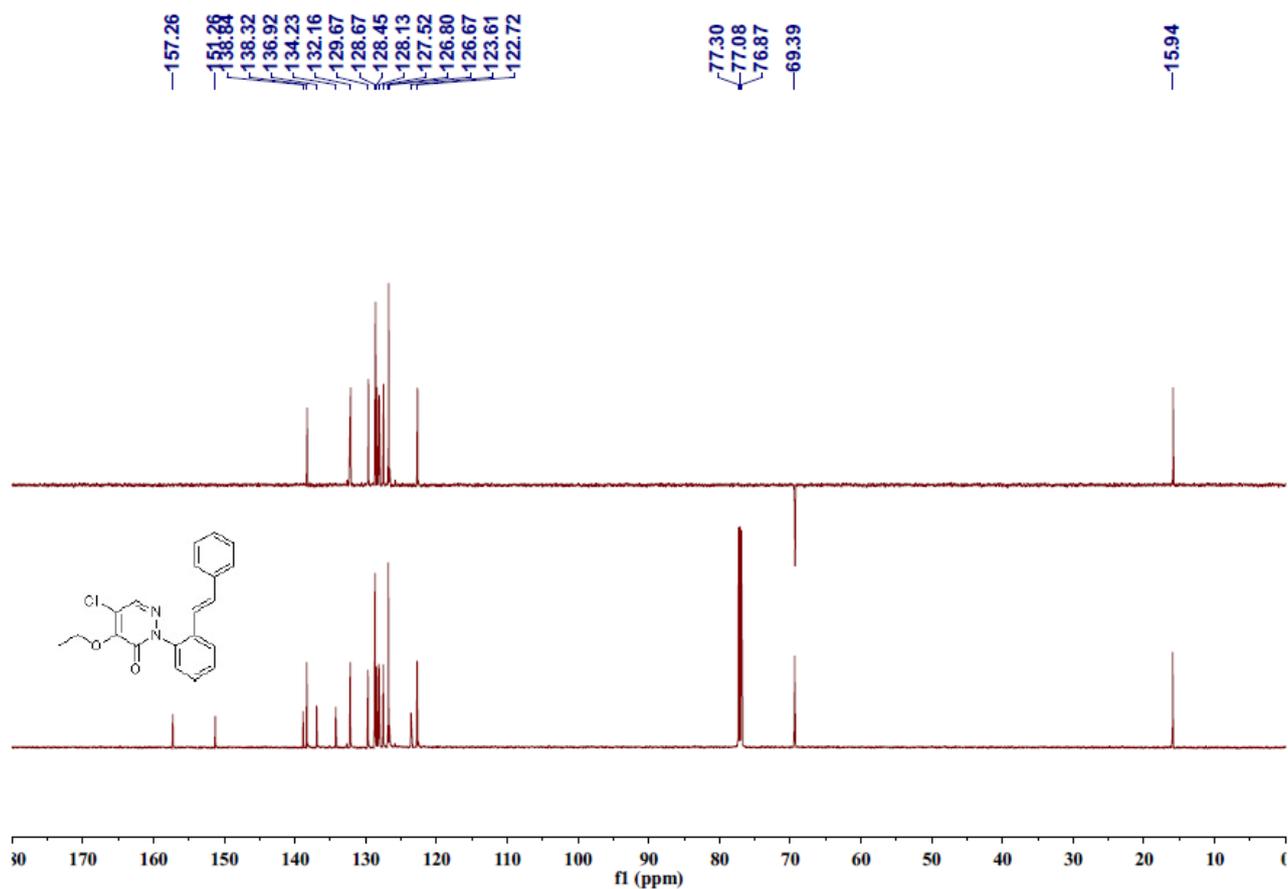
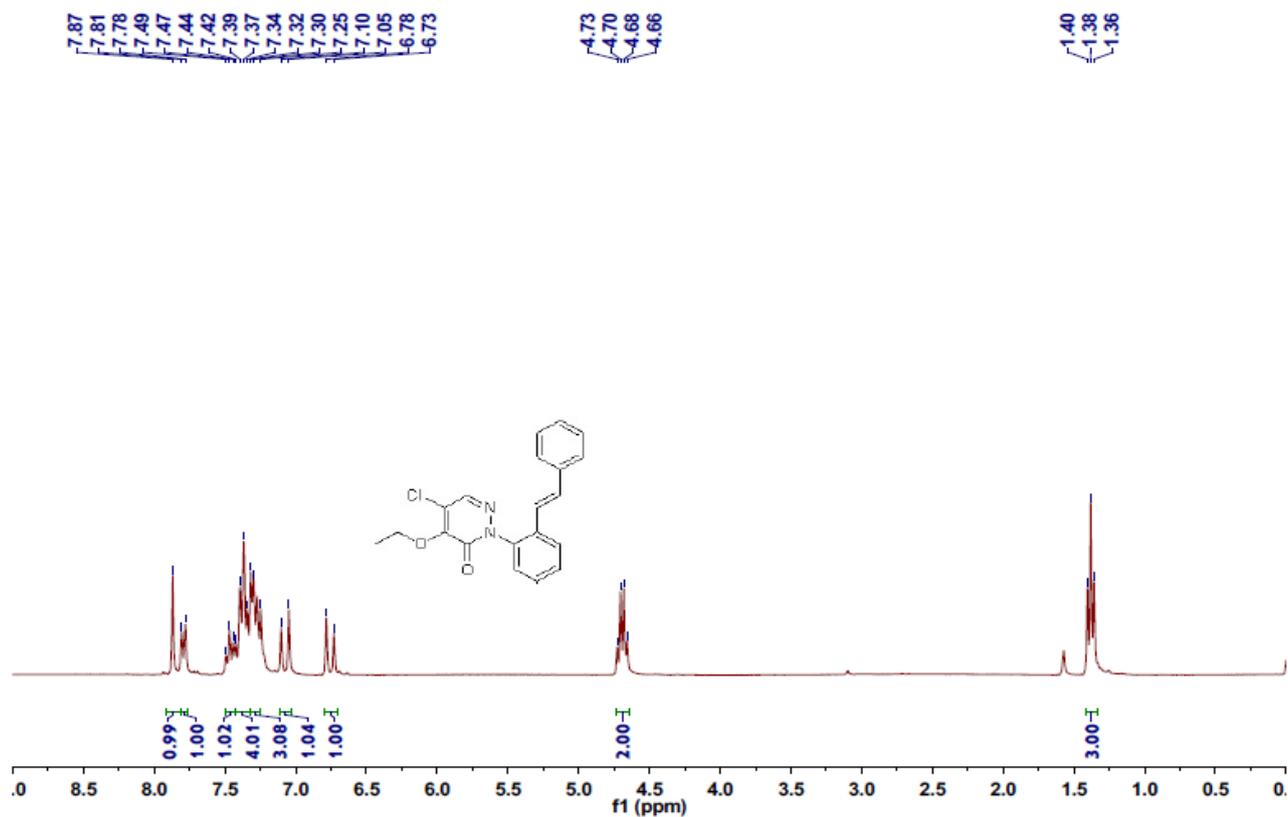
^1H and ^{13}C NMR spectra of compound **7a**.



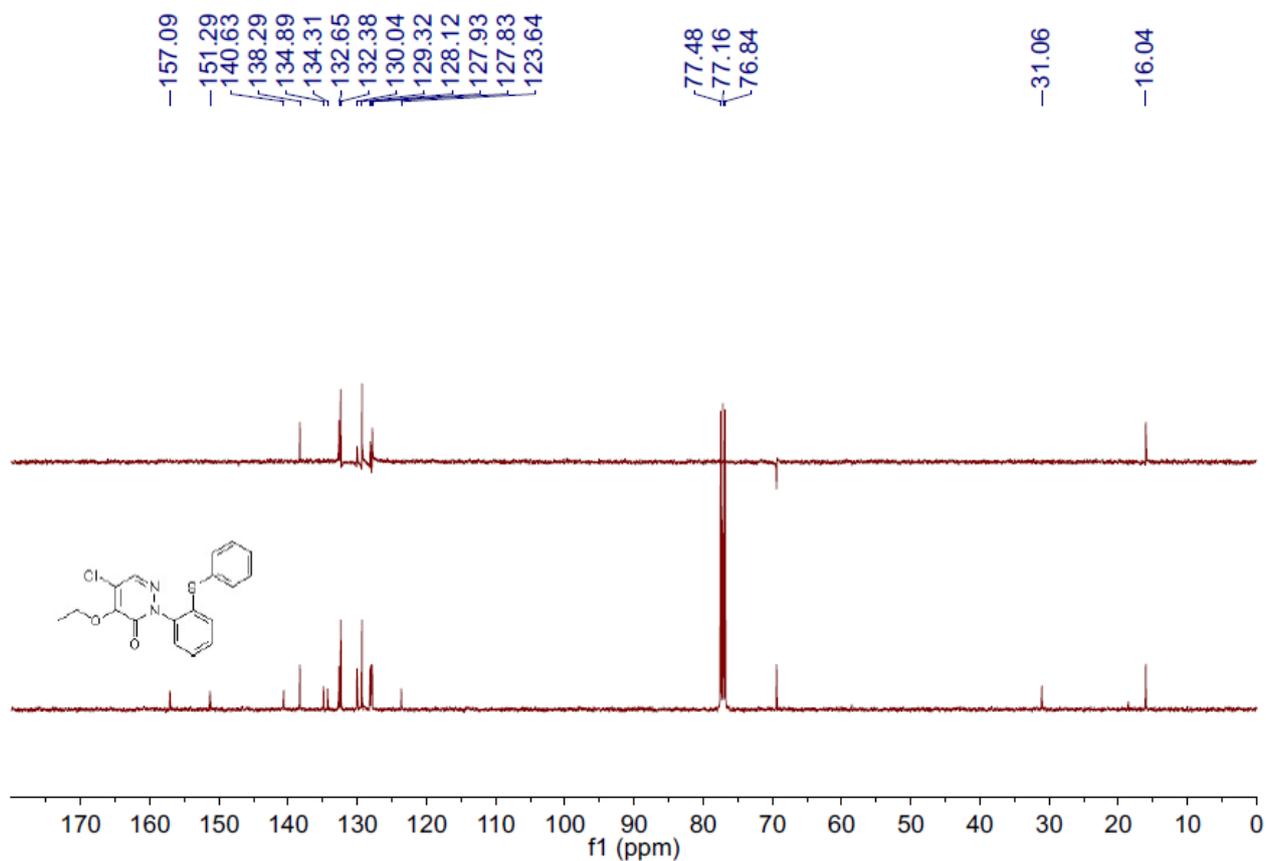
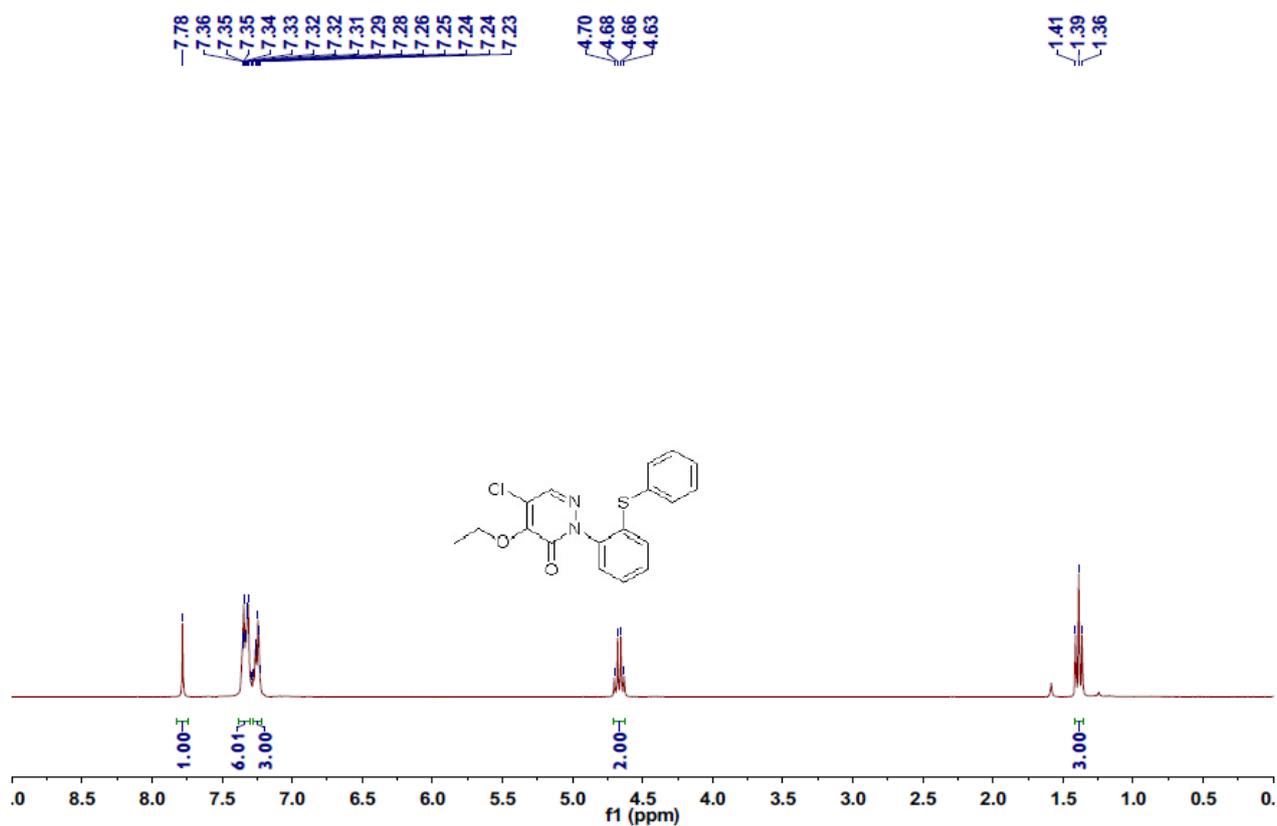
^1H and ^{13}C NMR spectra of compound **7b**.



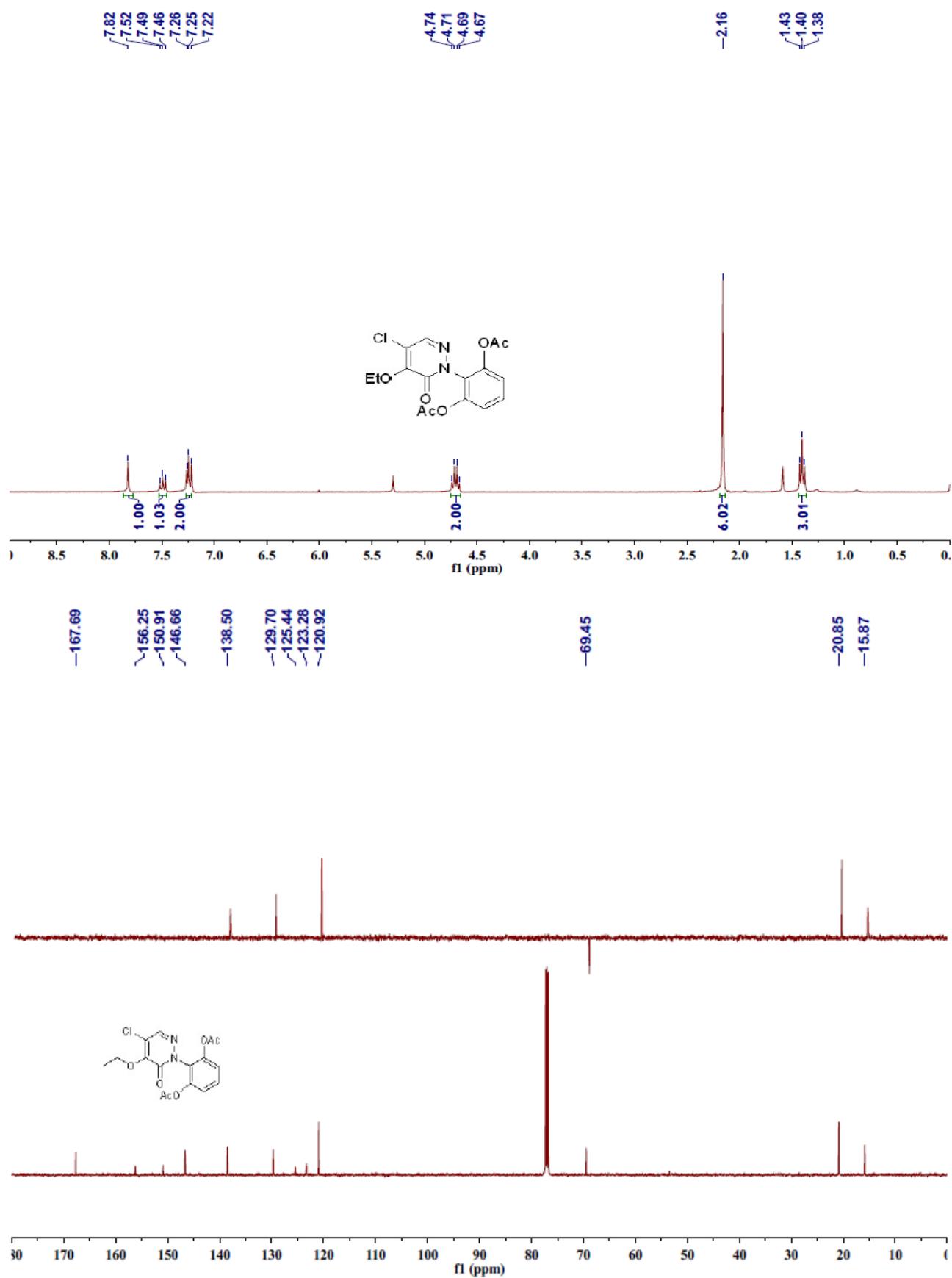
^1H and ^{13}C NMR spectra of compound **7c**.



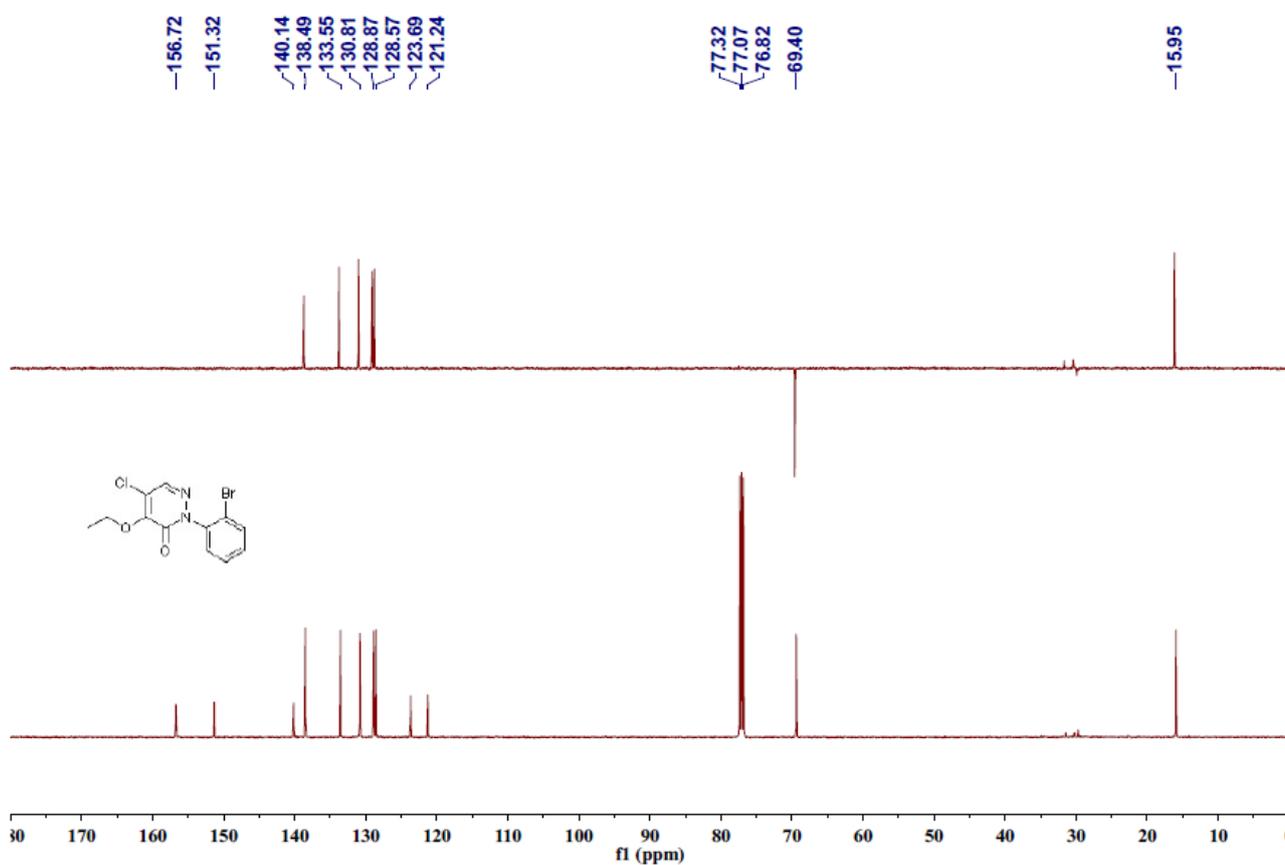
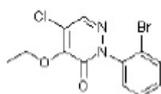
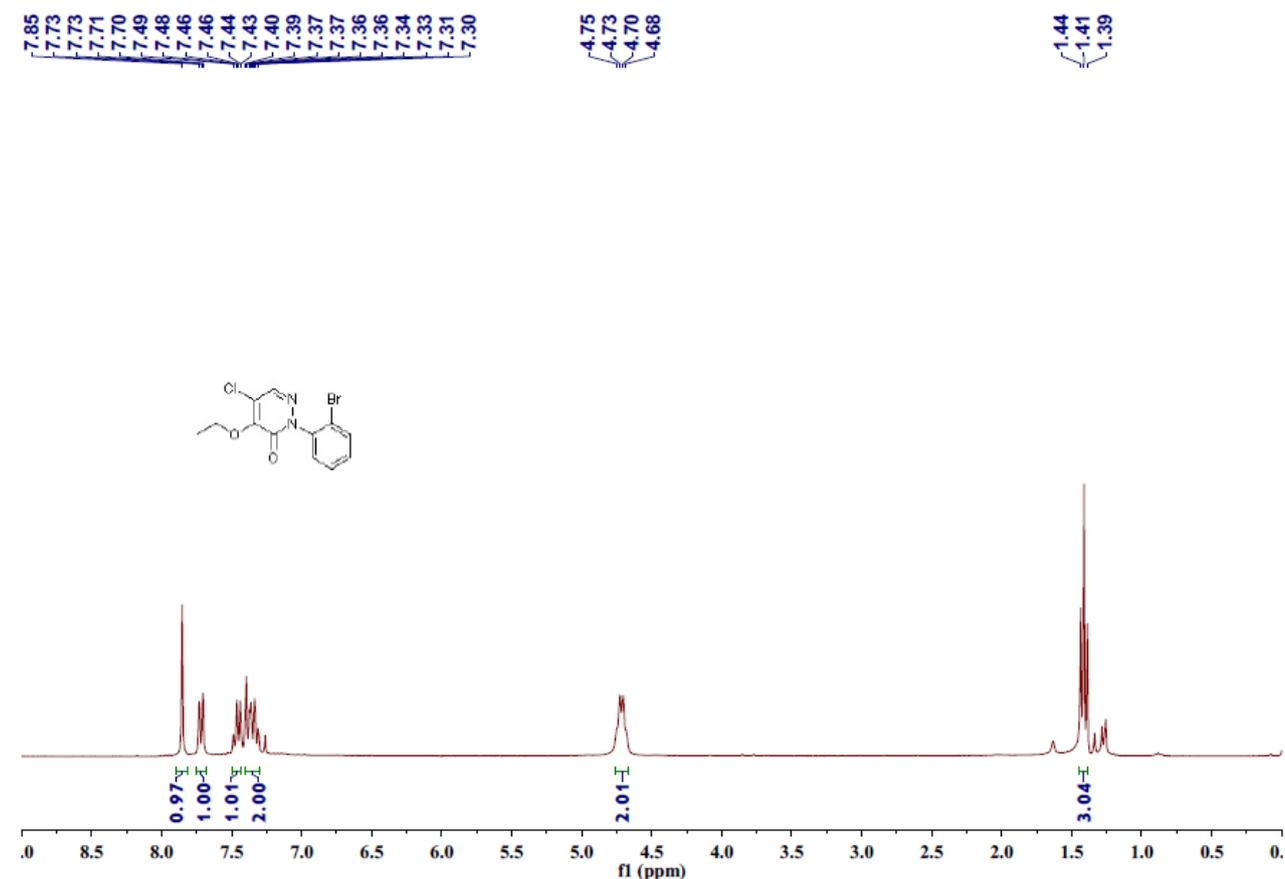
^1H and ^{13}C NMR spectra of compound **8**.



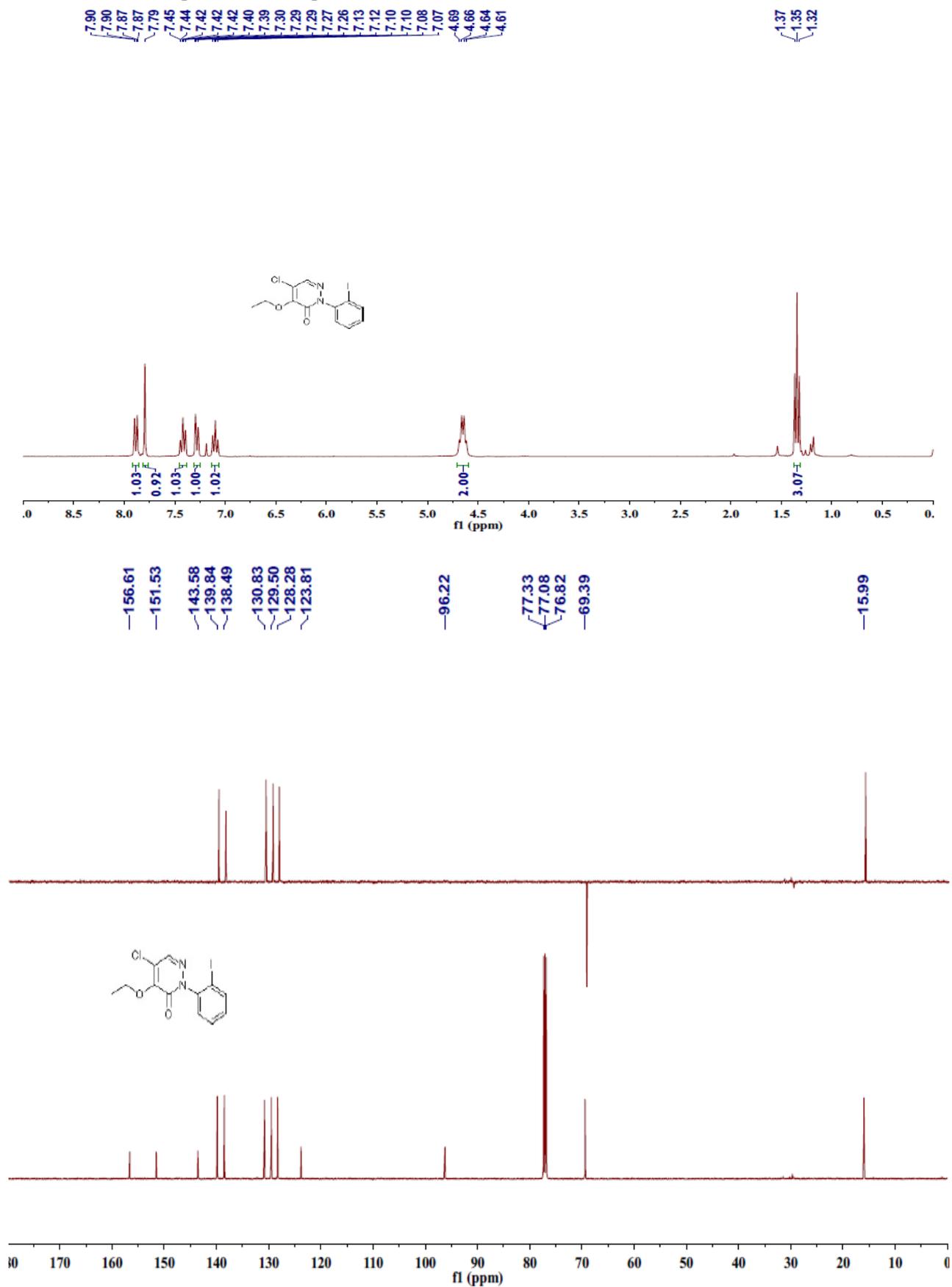
^1H and ^{13}C NMR spectra of compound 9.



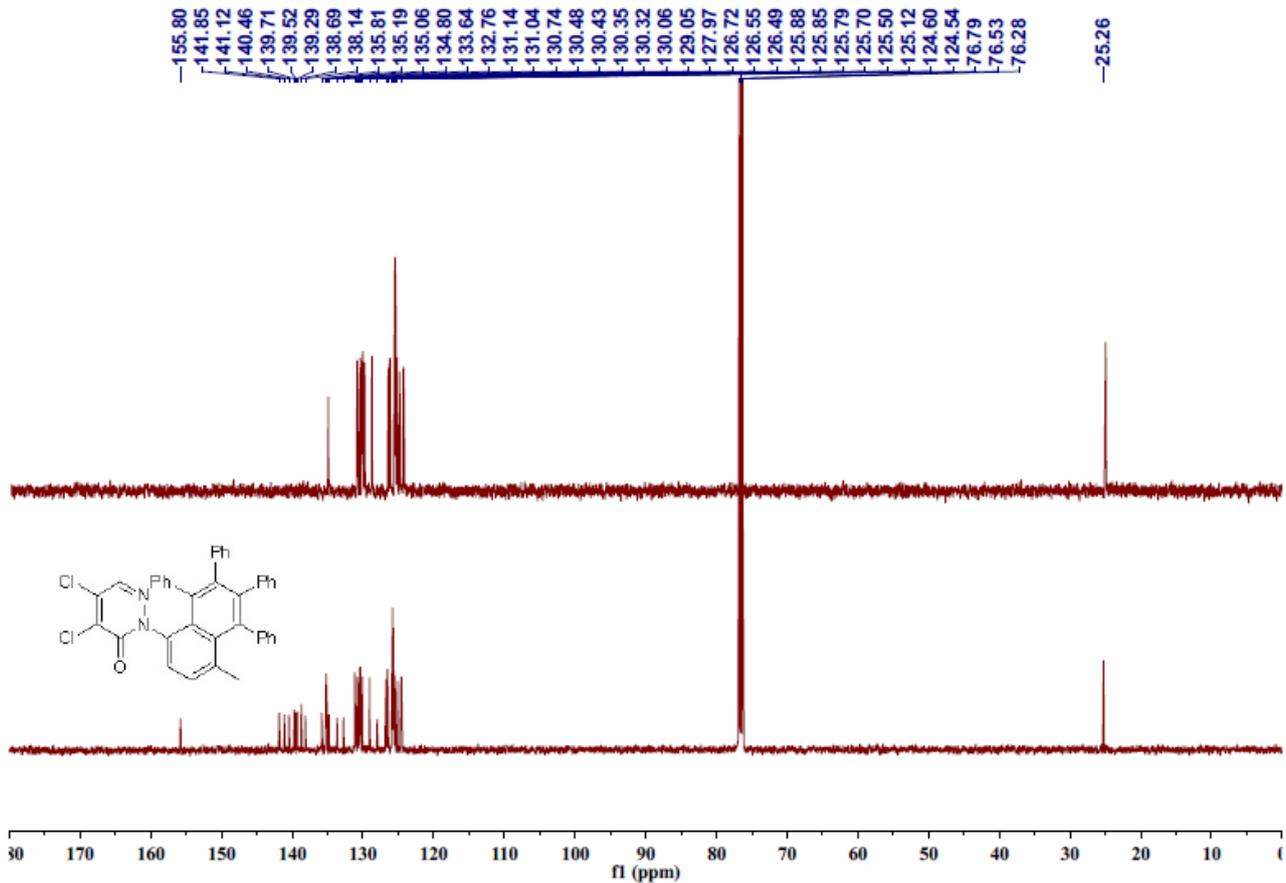
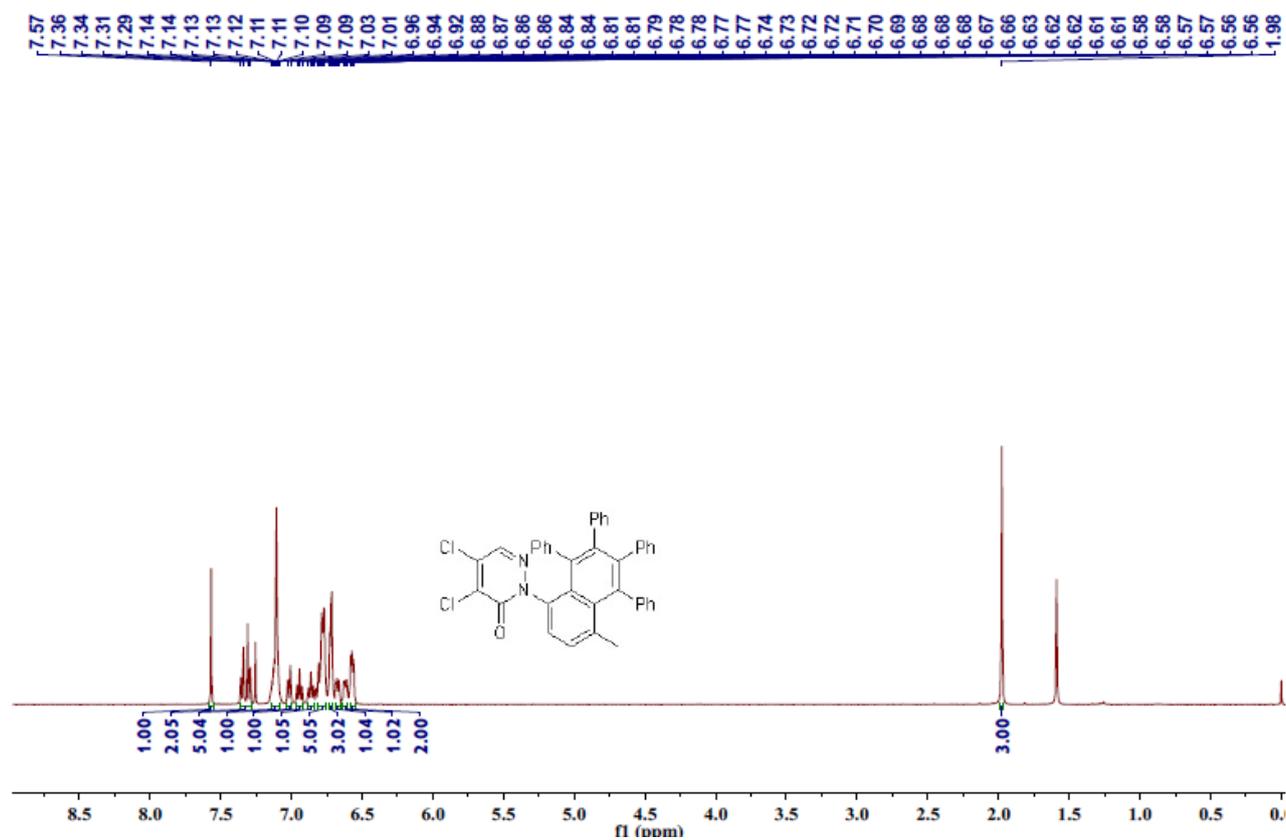
^1H and ^{13}C NMR spectra of compound **10**.



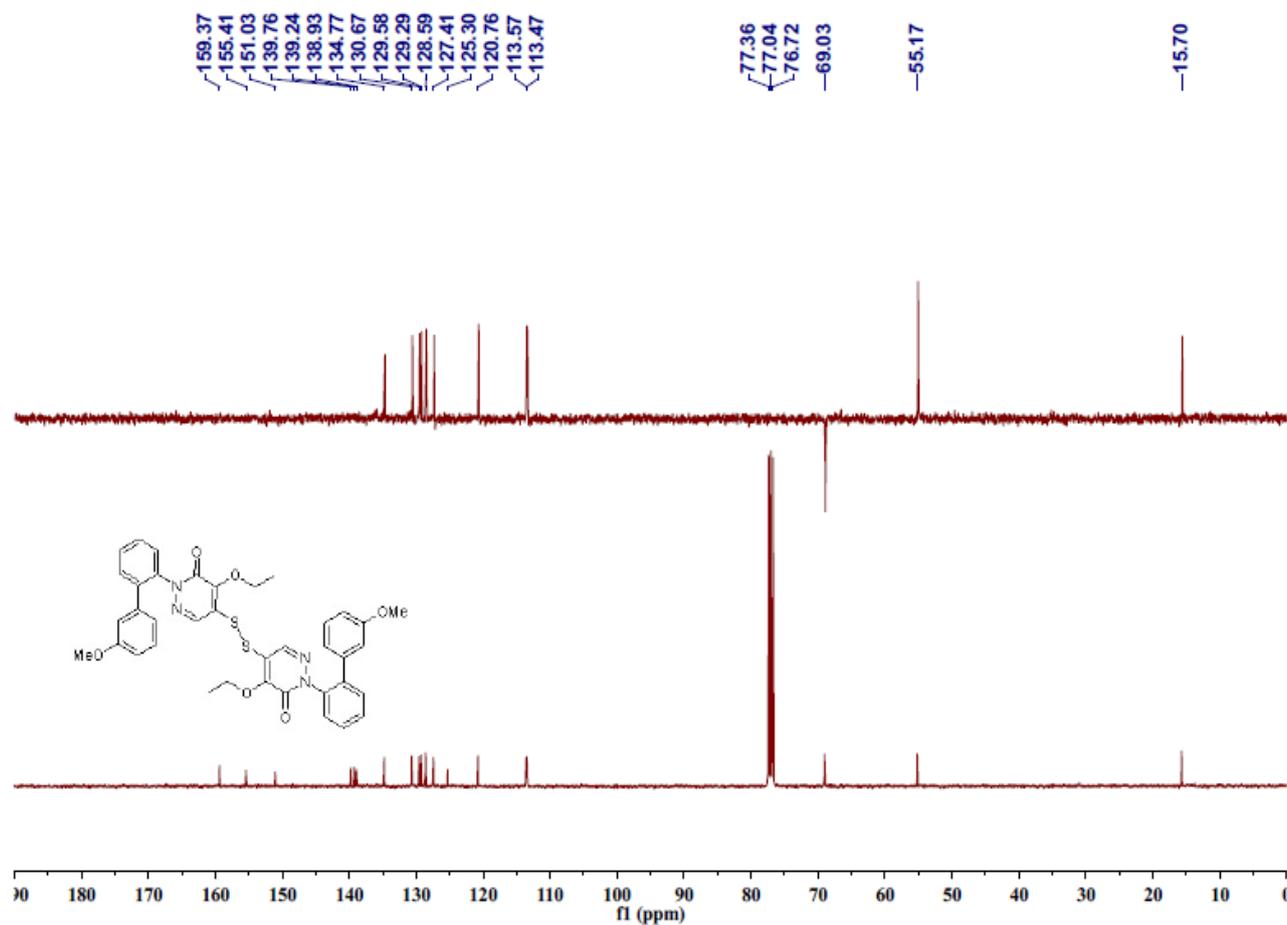
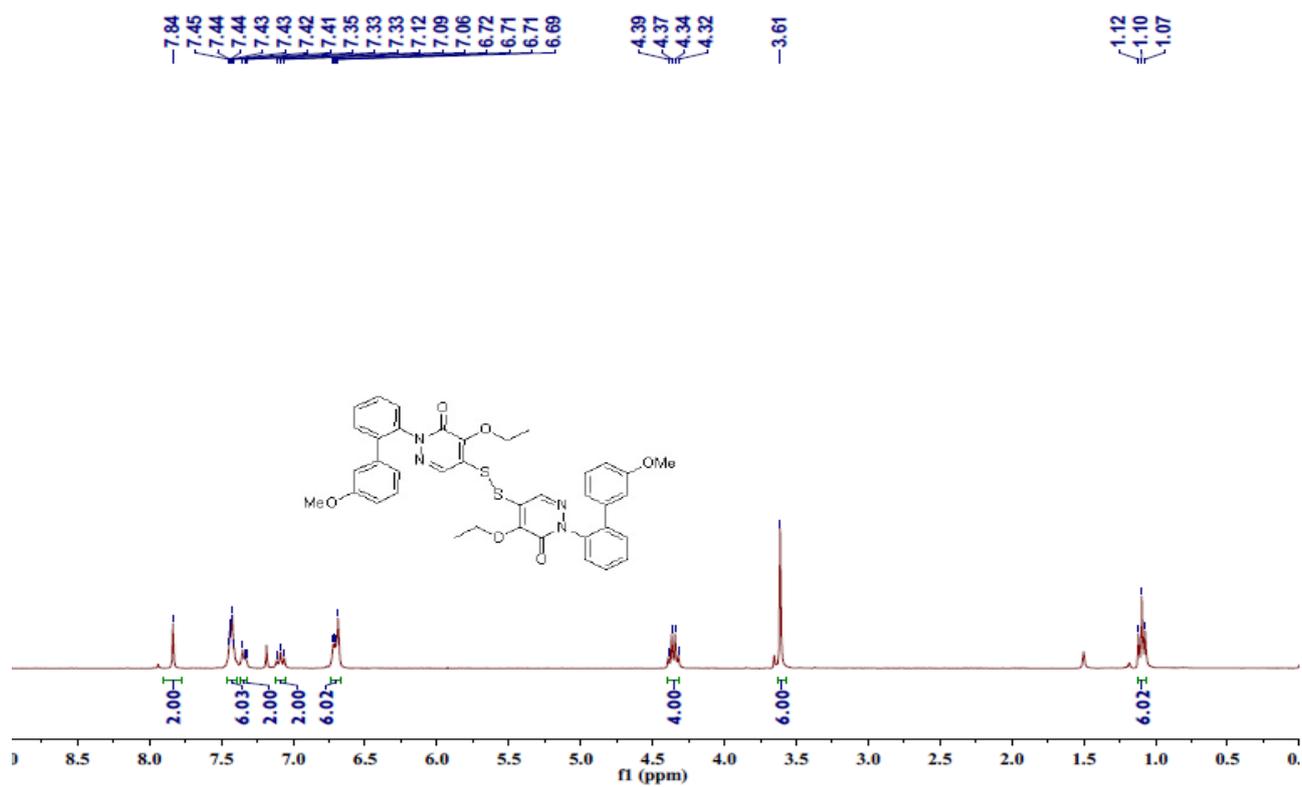
¹H and ¹³C NMR spectra of compound 11.



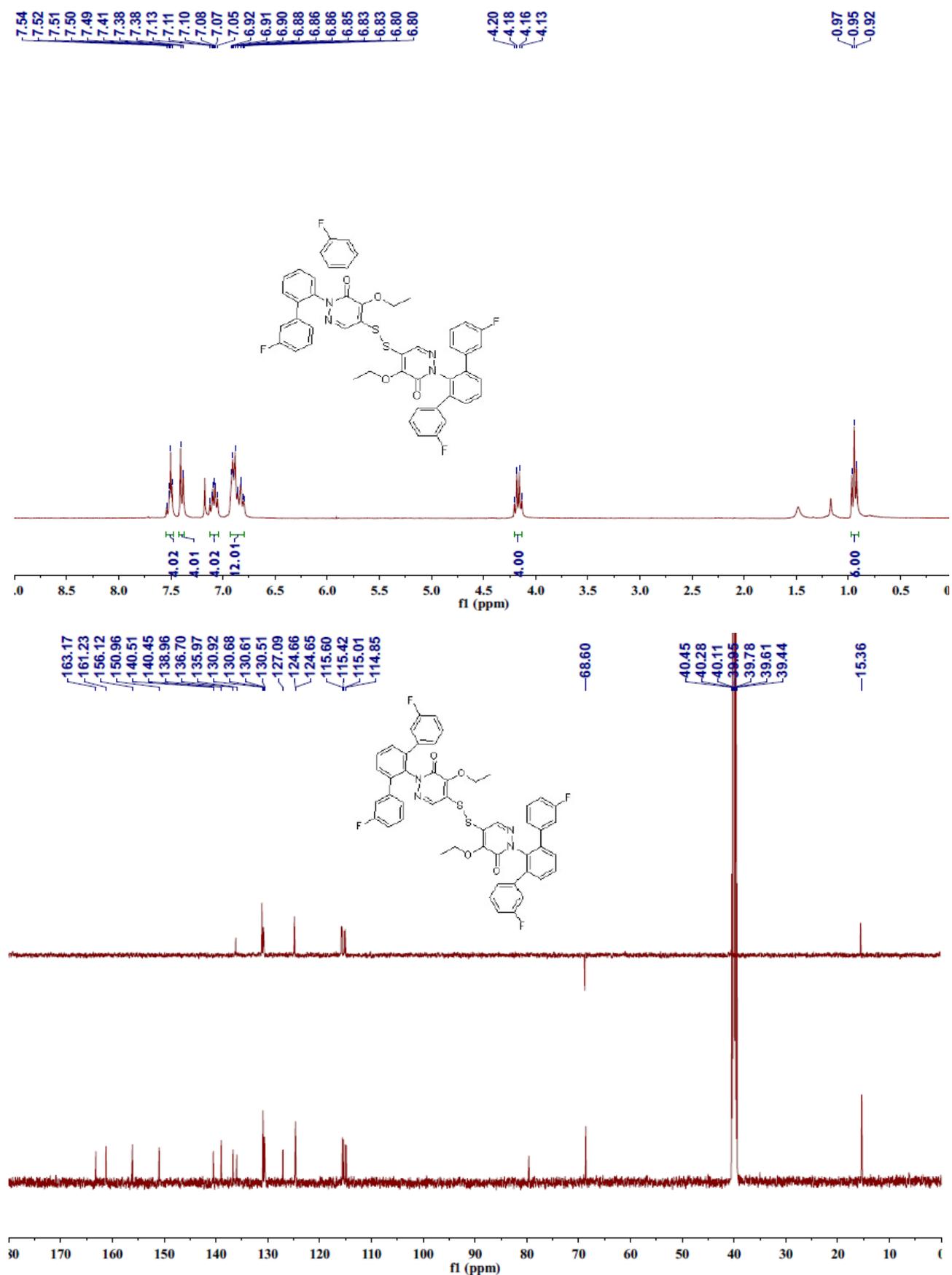
^1H and ^{13}C NMR spectra of compound 12.



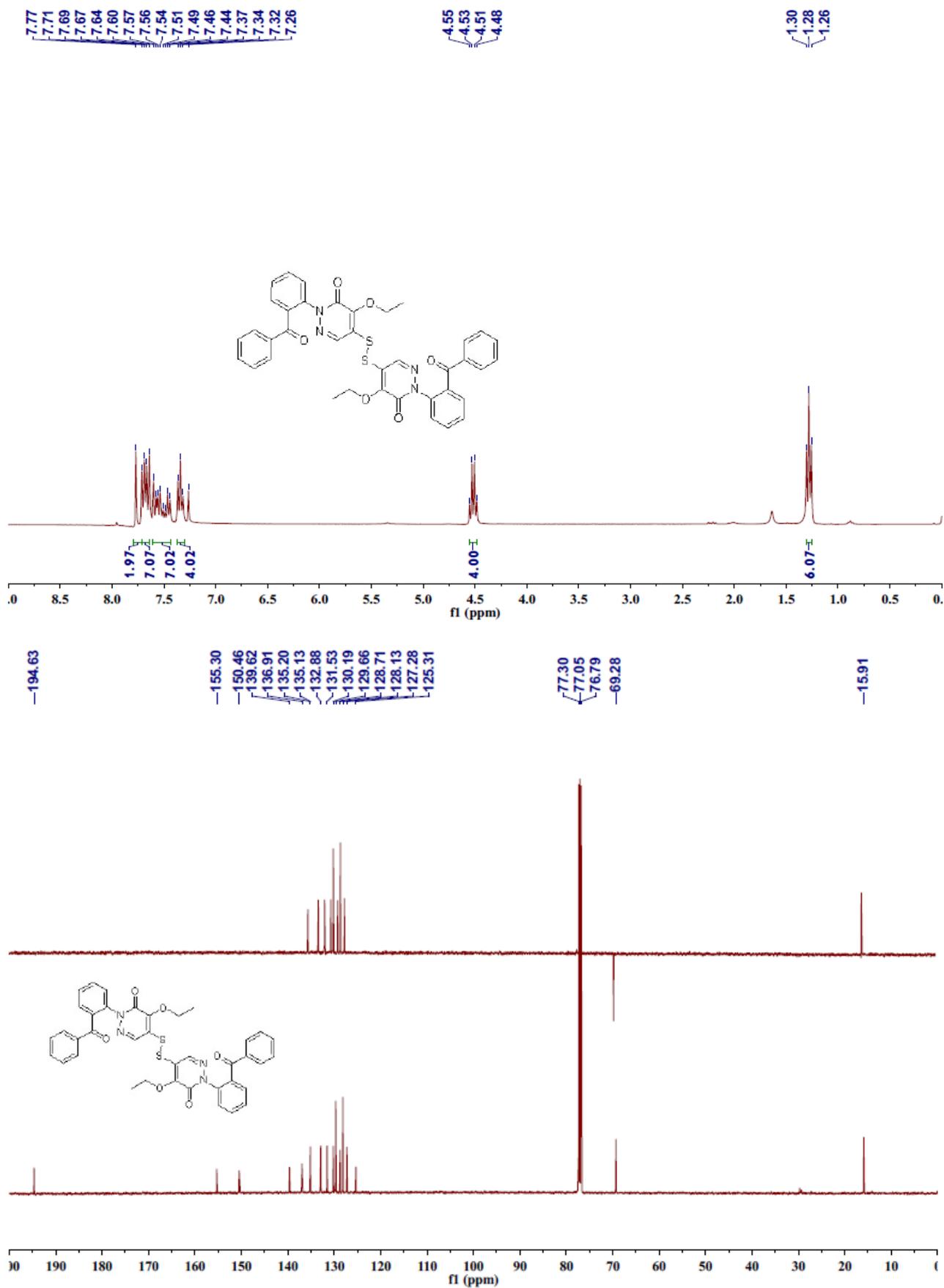
^1H and ^{13}C NMR spectra of compound **14a**.



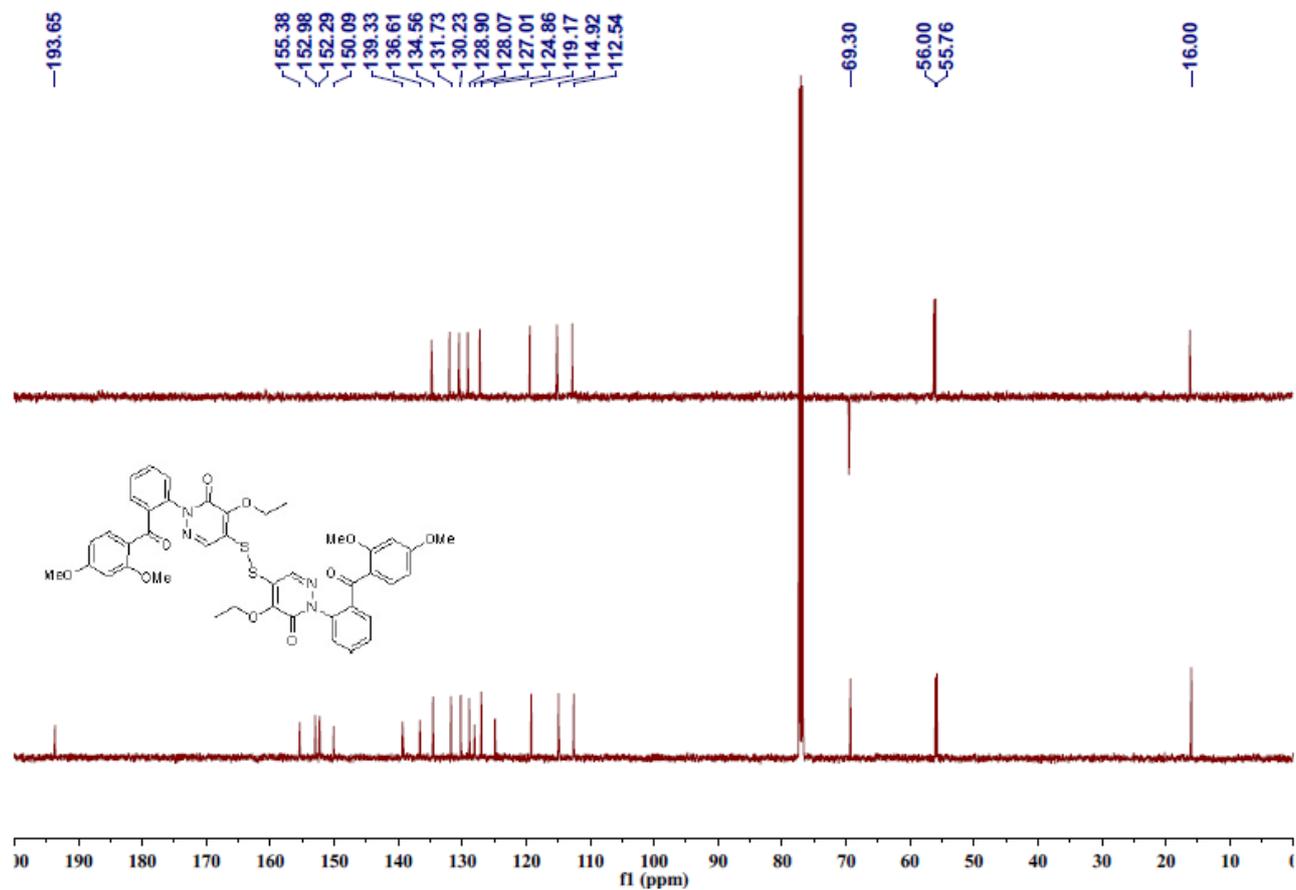
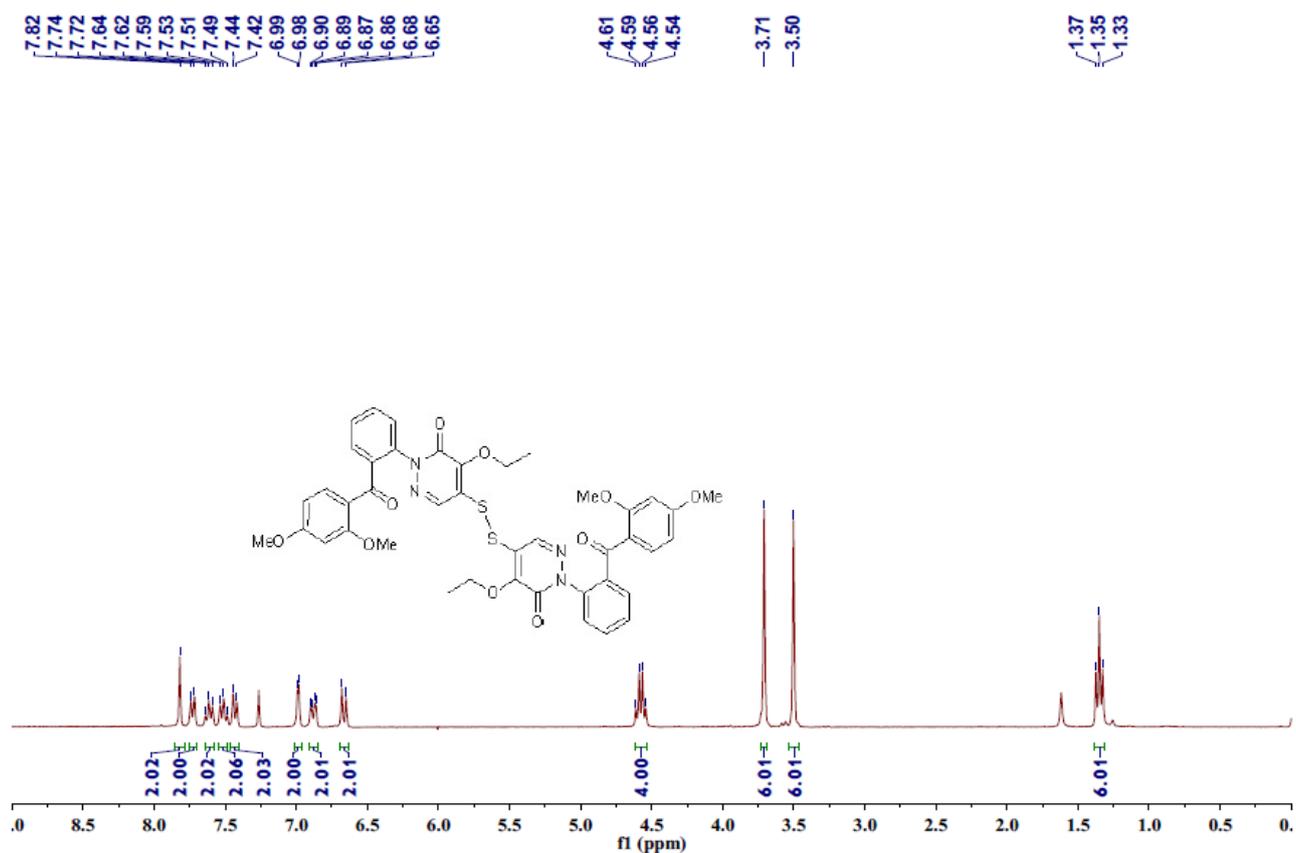
^1H and ^{13}C NMR spectra of compound **14c**.



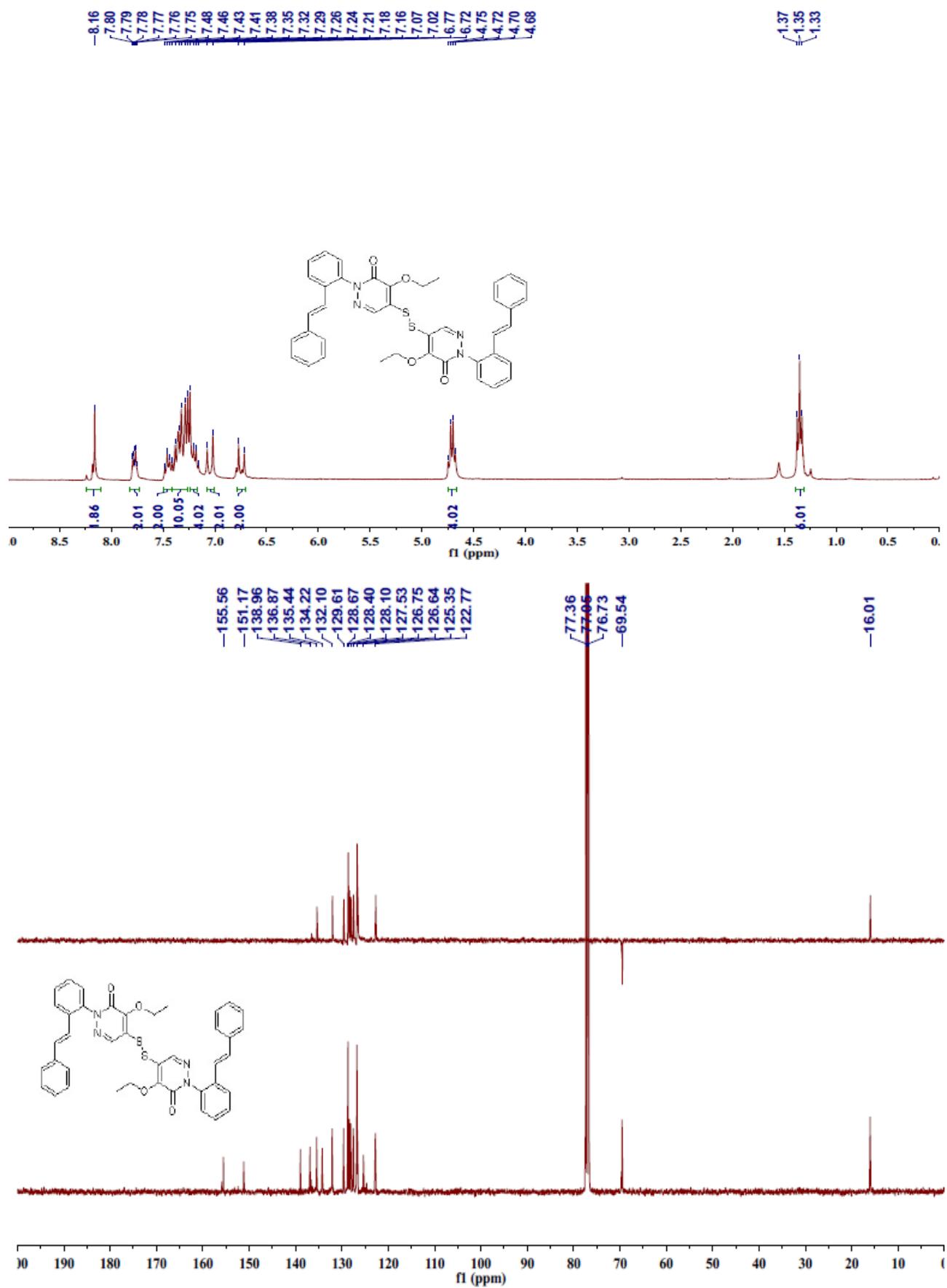
^1H and ^{13}C NMR spectra of compound **14d**.



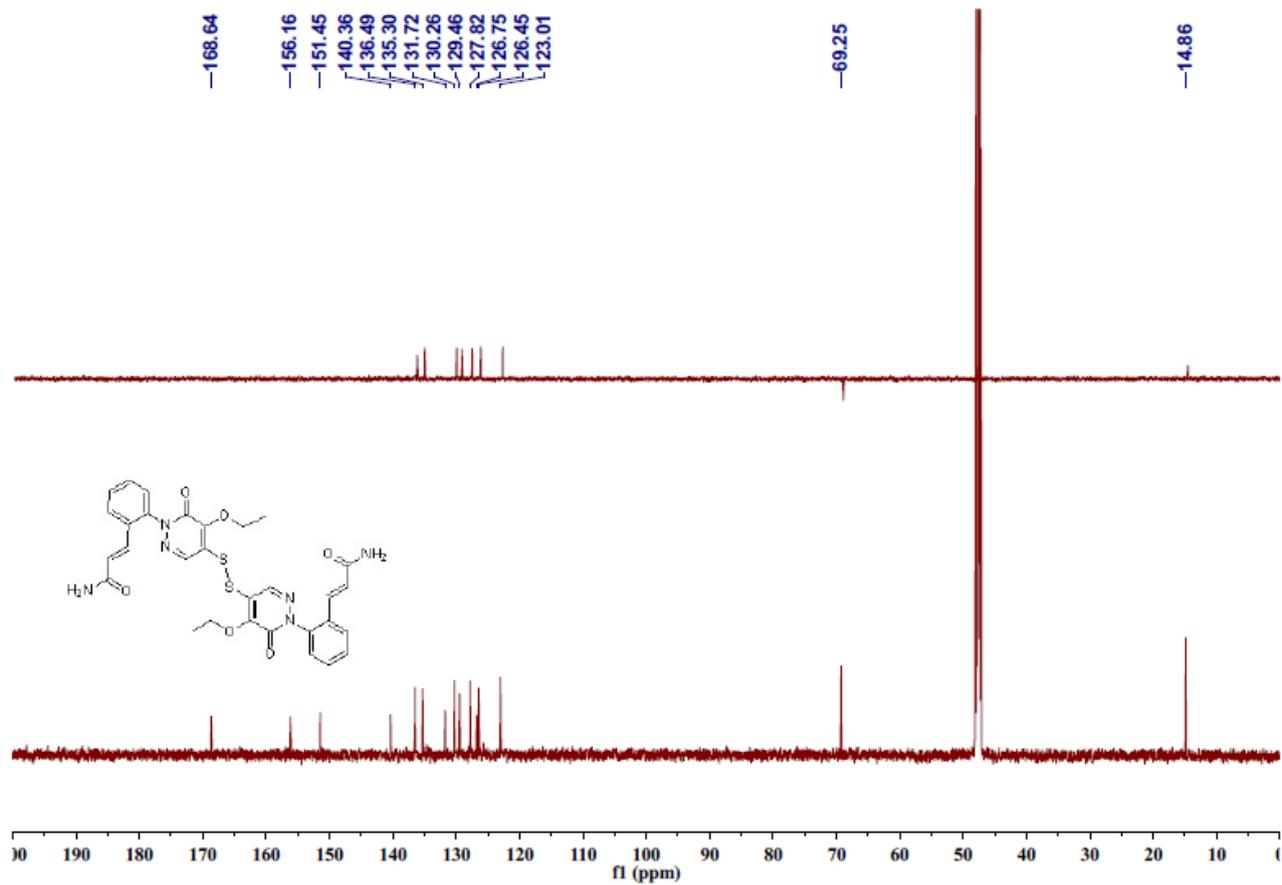
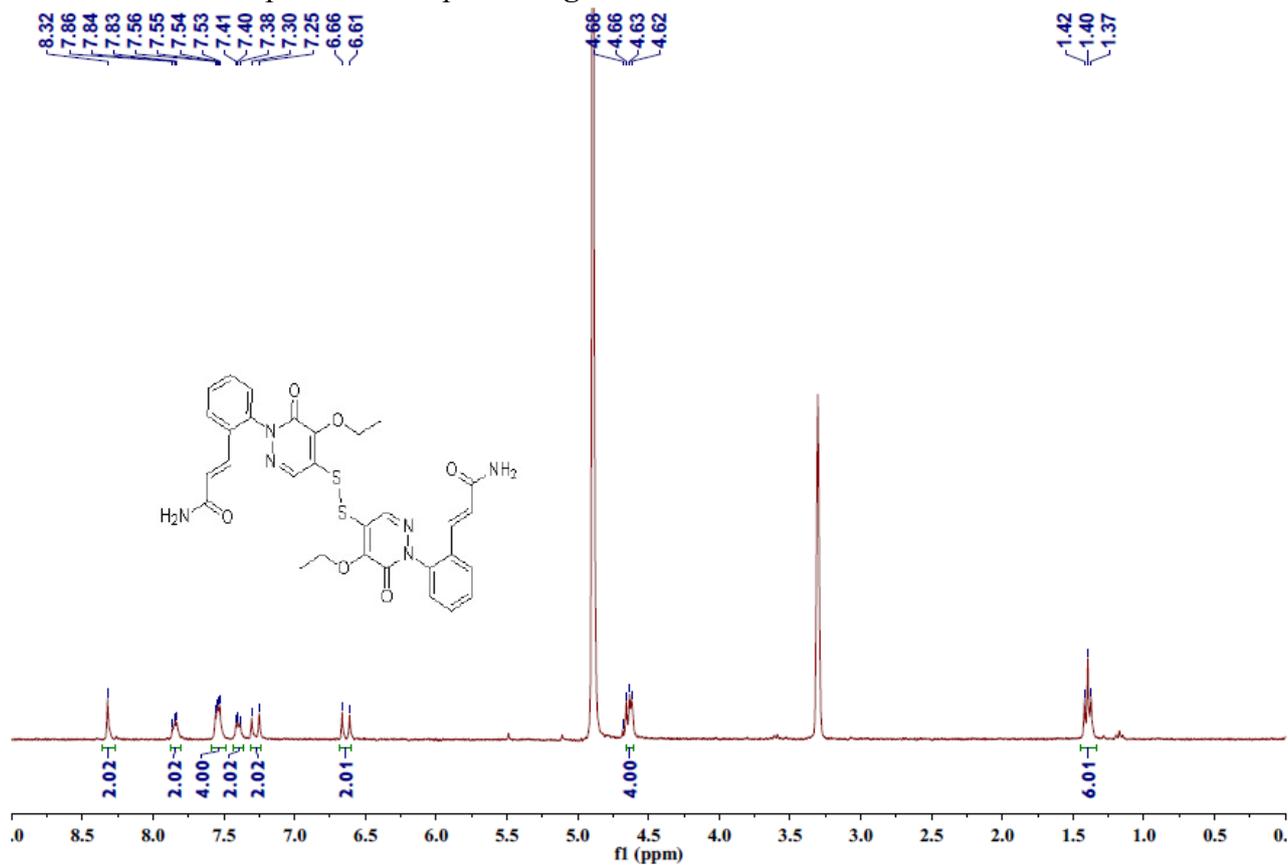
^1H and ^{13}C NMR spectra of compound **14e**.



^1H and ^{13}C NMR spectra of compound **14f**.



^1H and ^{13}C NMR spectra of compound **14g**.



2. X-ray Data of Compound 12.

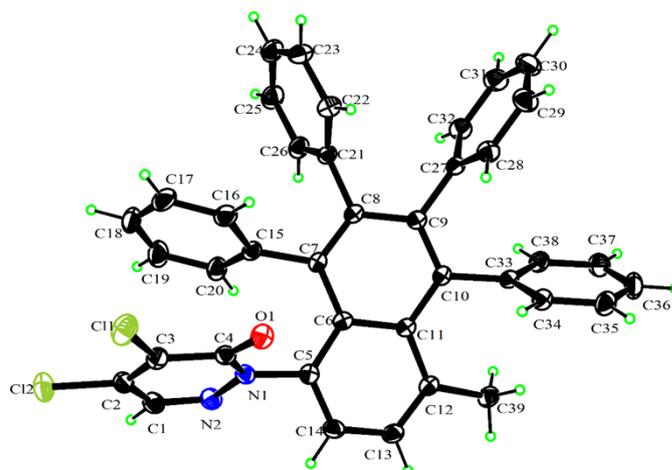


Table 1 Crystal data and structure refinement details for compound **12**.

Identification code	2014283	
Chemical formula	C ₃₉ H ₂₆ Cl ₂ N ₂ O	
Formula weight	609.52	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.200 x 0.300 x 0.700 mm	
Crystal system	orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.1928(3) Å	α = 90°
	b = 13.3215(6) Å	β = 90°
	c = 32.7007(16) Å	γ = 90°
Volume	3133.3(2) Å ³	
Z	4	
Density (calculated)	1.292 Mg/cm ³	
Absorption coefficient	0.242 mm ⁻¹	
F(000)	1264	
Theta range for data collection	1.65 to 27.65°	
Index ranges	-9 ≤ h ≤ 8, -17 ≤ k ≤ 16, -33 ≤ l ≤ 42	
Reflections collected	16279	
Independent reflections	7109 [R(int) = 0.0221]	
Coverage of independent reflections	99.6%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9522 and 0.8459	
Structure solution technique	direct methods	

Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F ²	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	7109 / 0 / 399	
Goodness-of-fit on F²	1.023	
Final R indices	5579 data; I>2 σ (I)	R1 = 0.0596, wR2 = 0.1151
	all data	R1 = 0.0418, wR2 = 0.1051
Weighting scheme	w=1/[$\sigma^2(F_o^2)+(0.0600P)^2+0.2800P$] where P=(F _o ² +2F _c ²)/3	
Extinction coefficient	0.0018(6)	
Largest diff. peak and hole	0.242 and -0.221 eÅ ⁻³	
R.M.S. deviation from mean	0.037 eÅ ⁻³	
CCDC	1023268	
