Supplementary Material

New efficient synthesis of bis-1,2,4-oxadiazole derivatives via subsequent Staudinger/aza-Wittig reaction

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Table Crystal data and structure refinement for compound 4a.

Identification code	4a
Empirical formula	C16 H10 N4 O2
Formula weight	290.28
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.6846(8) A alpha = 90 deg.
	b = 5.5361(5) A beta = 90.409(2) deg.
	c = 13.9324(12) A gamma = 90 deg.
Volume	669.84(10) A^3
Z, Calculated density	2, 1.439 Mg/m^3
Absorption coefficient	0.100 mm^-1
F(000)	300
Crystal size	0.35 x 0.23 x 0.10 mm
Theta range for data collection	2.35 to 25.00 deg.
Limiting indices	-10<=h<=9, -6<=k<=6, -12<=l<=16
Reflections collected / unique	3183 / 1180 [R(int) = 0.0438]
Completeness to theta = 25.00	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9901 and 0.9660
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1180 / 0 / 100
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1283
R indices (all data)	R1 = 0.0687, wR2 = 0.1377
Largest diff. peak and hole	0.187 and -0.214

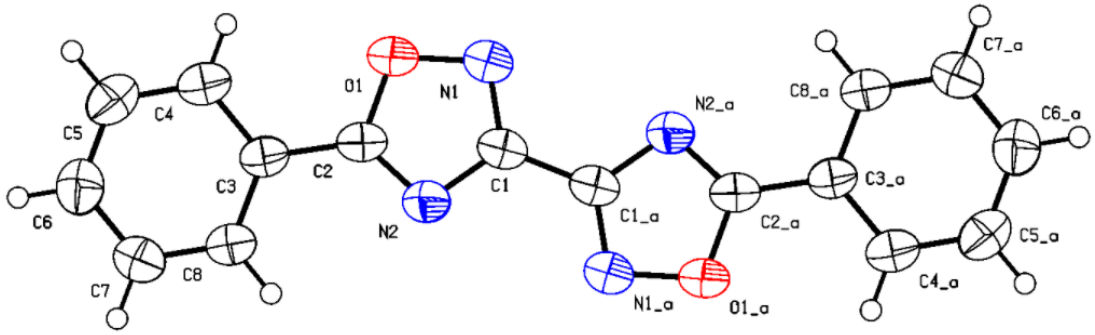
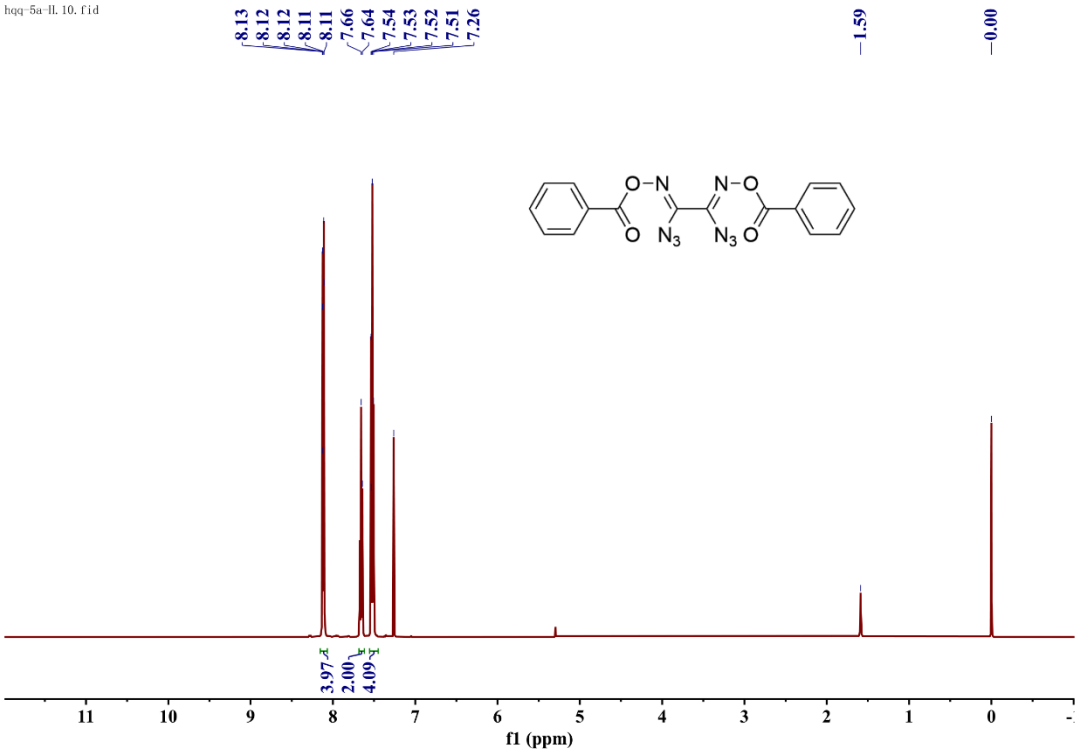
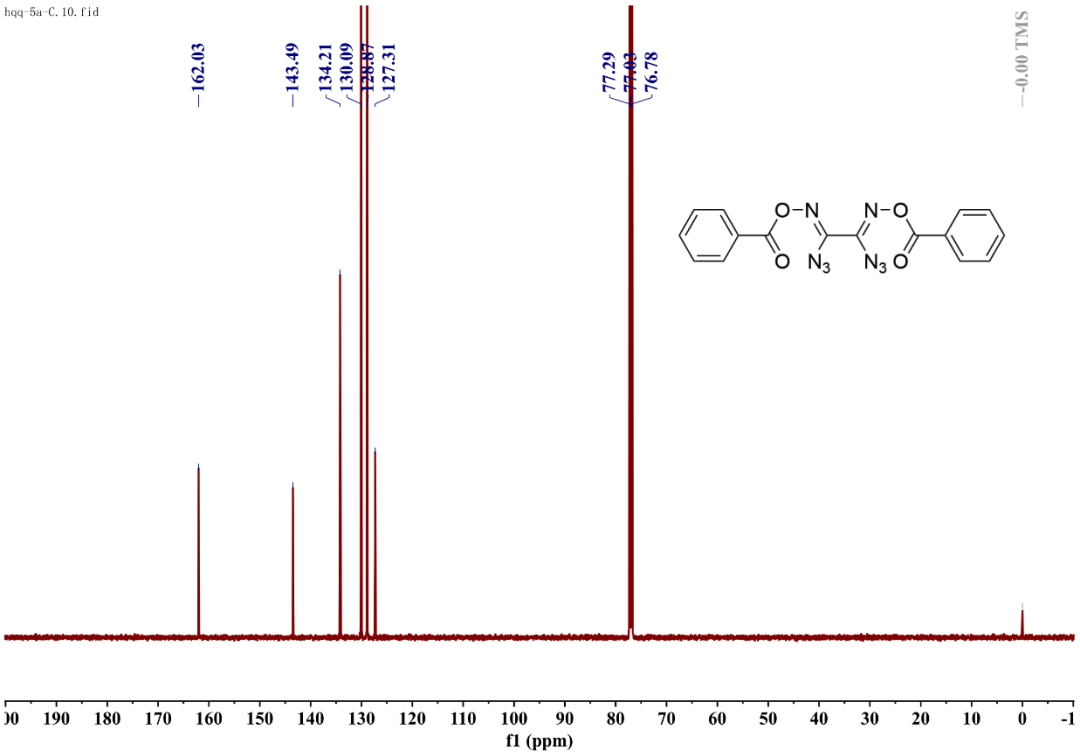


Figure 1. ORTEP diagram of the crystal structure of 6n (30% thermal ellipsoids).

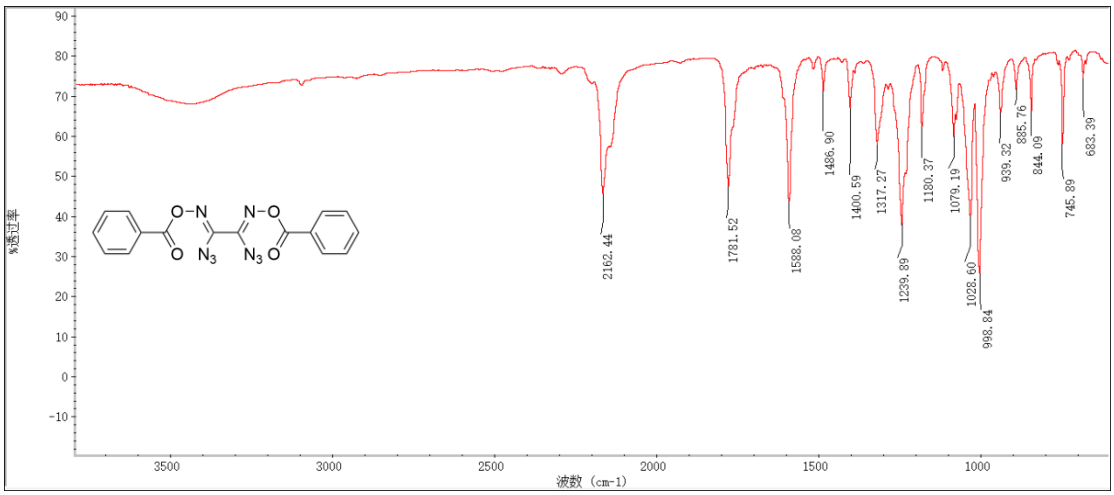
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **2a**:



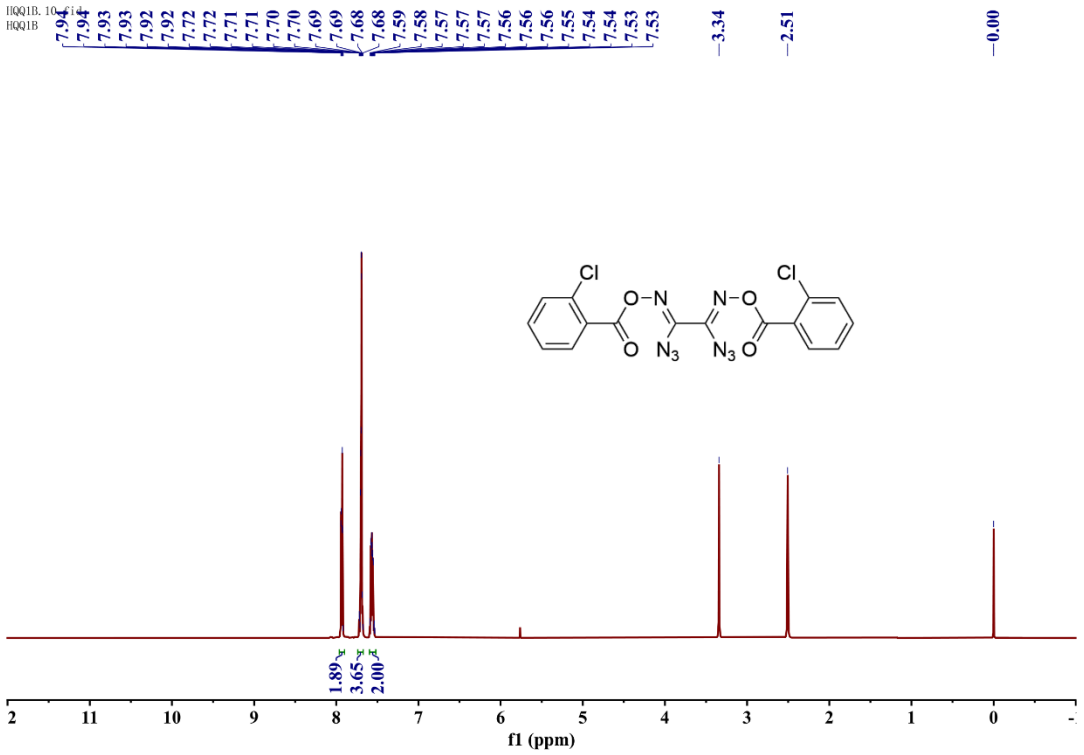
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **2a**:



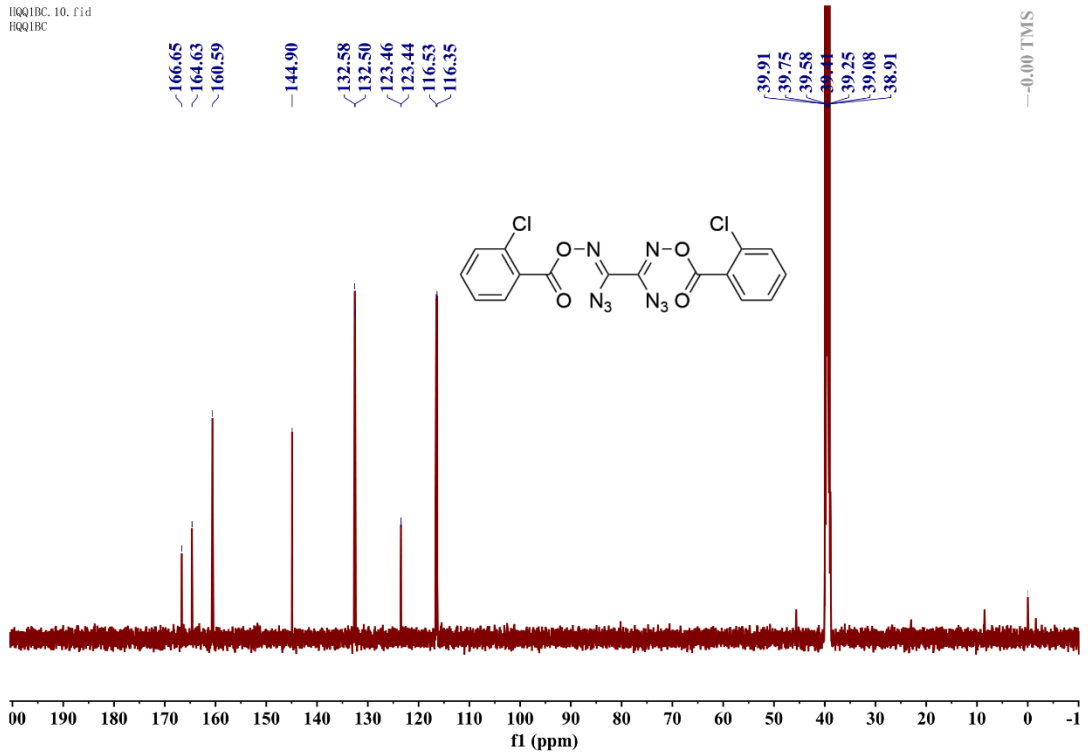
IR of compound **2a**:



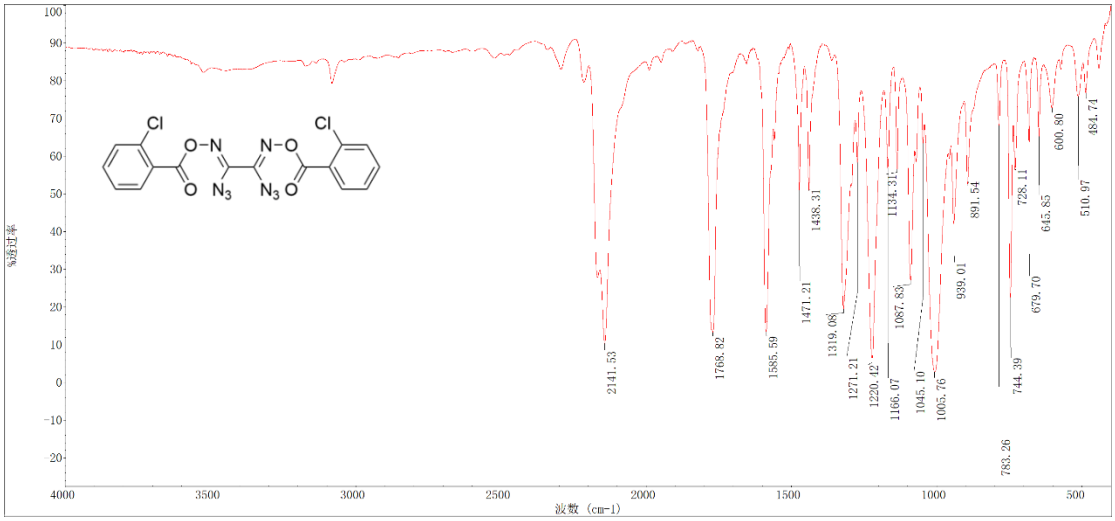
^{1}H NMR (500 MHz, DMSO) spectra of compound **2b**:



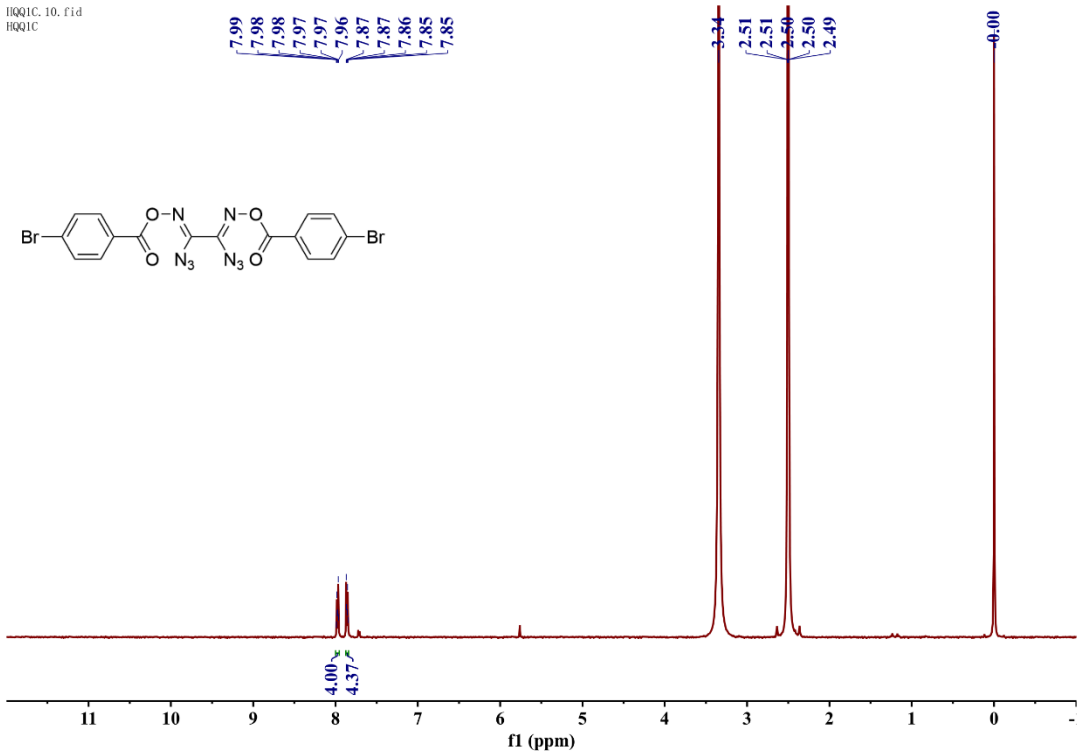
^{13}C NMR (125 MHz, DMSO) spectra of compound **2b**:



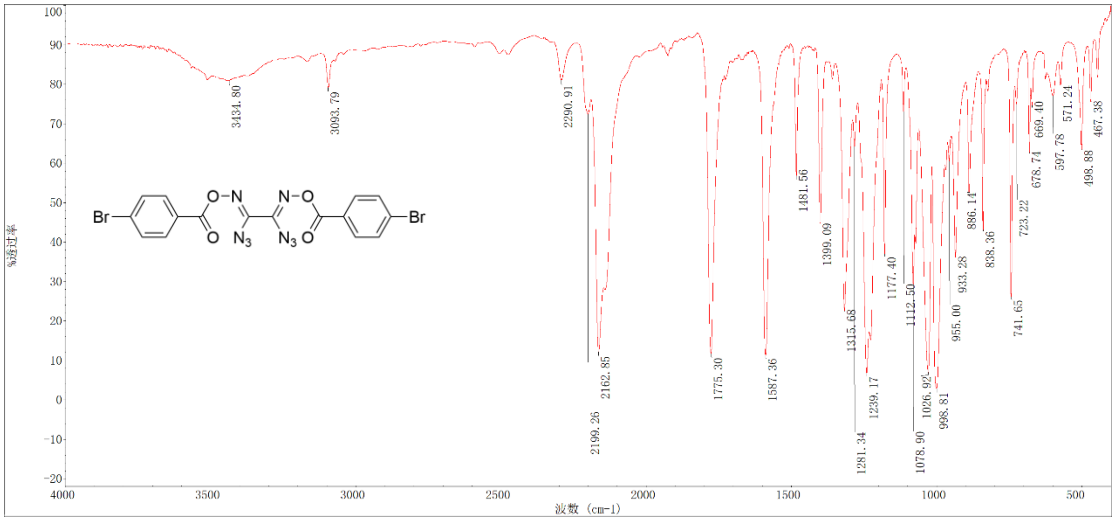
IR of compound **2b**:



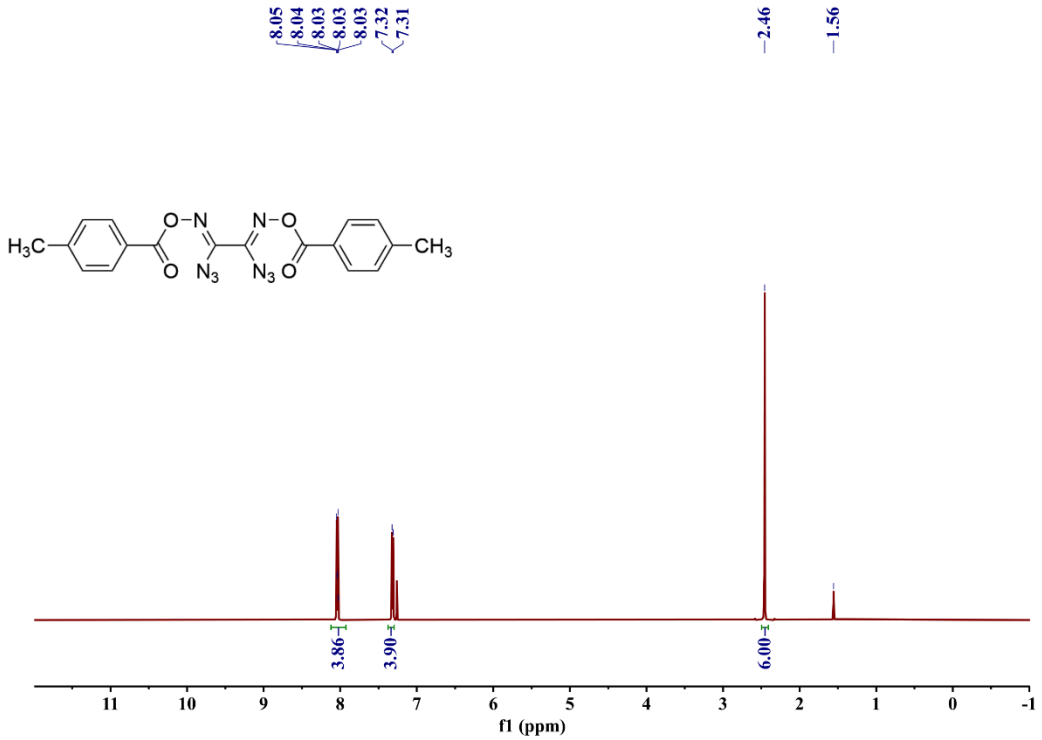
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **2c**:



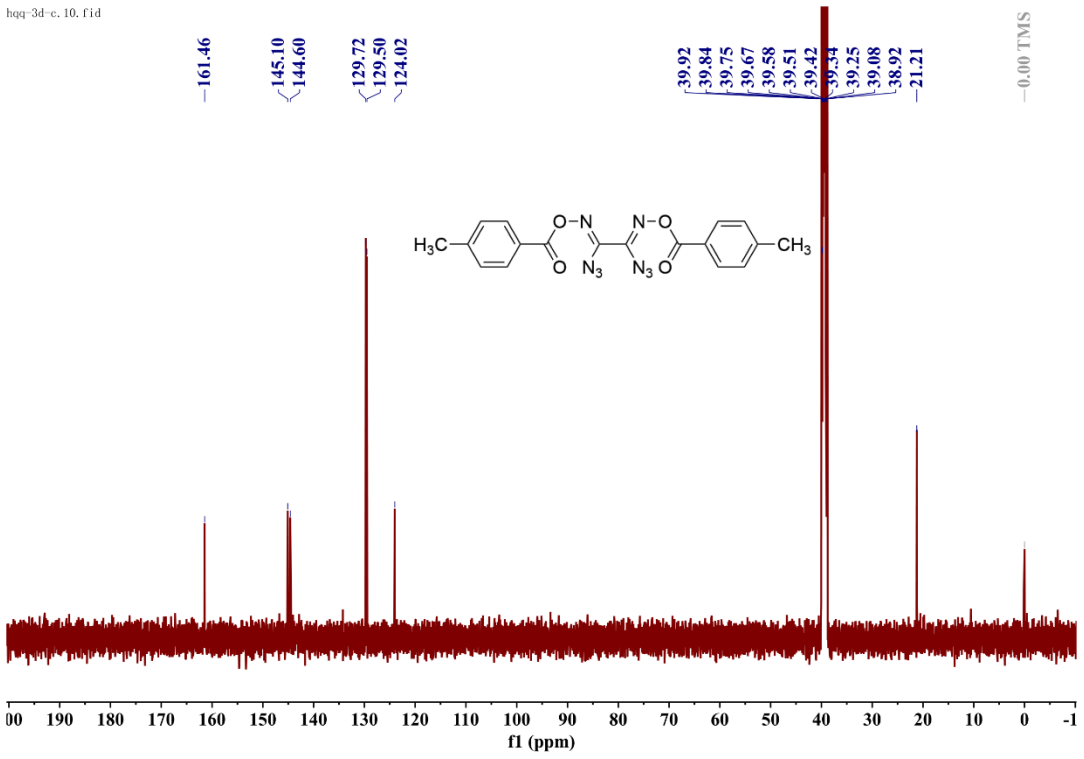
IR of compound **2c**:



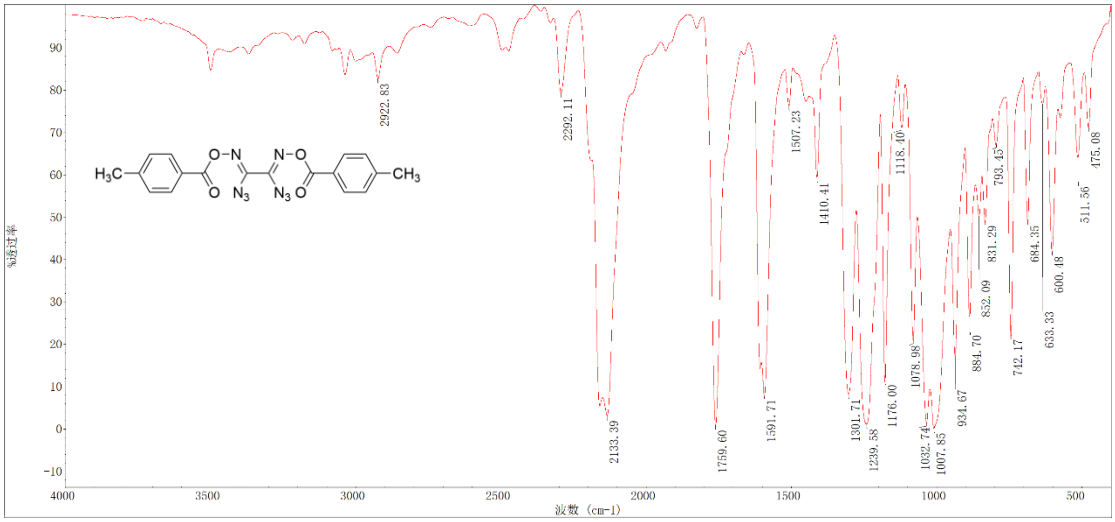
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **2d**:



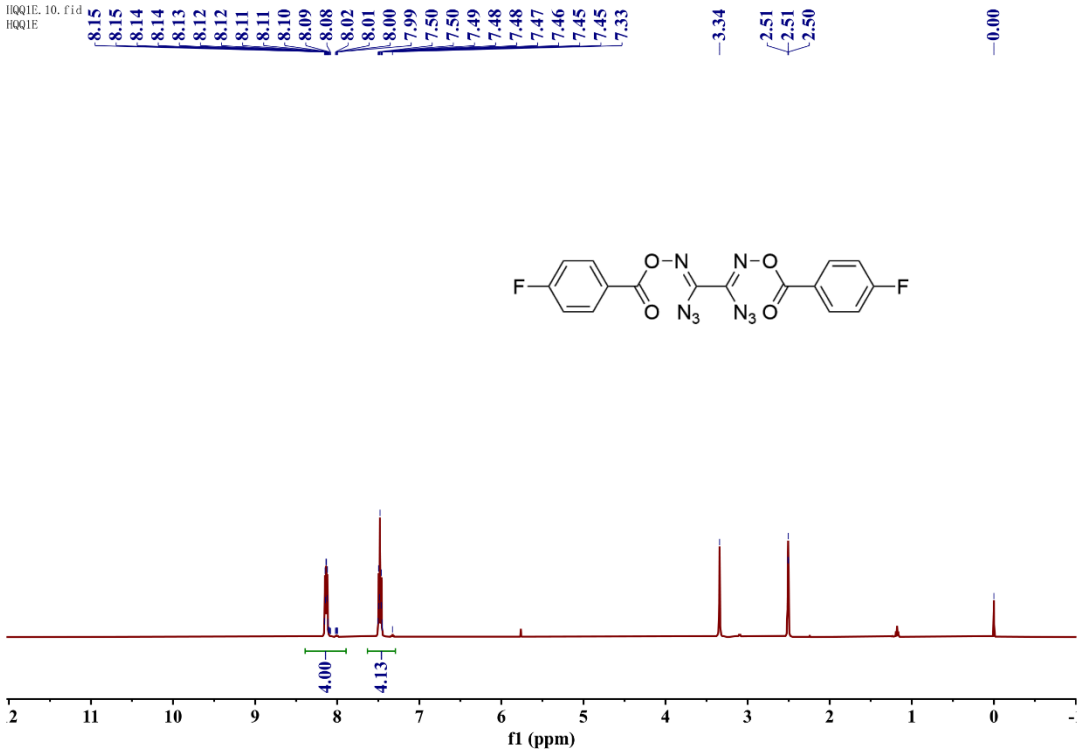
^{13}C NMR (125 MHz, DMSO) spectra of compound **2d**:



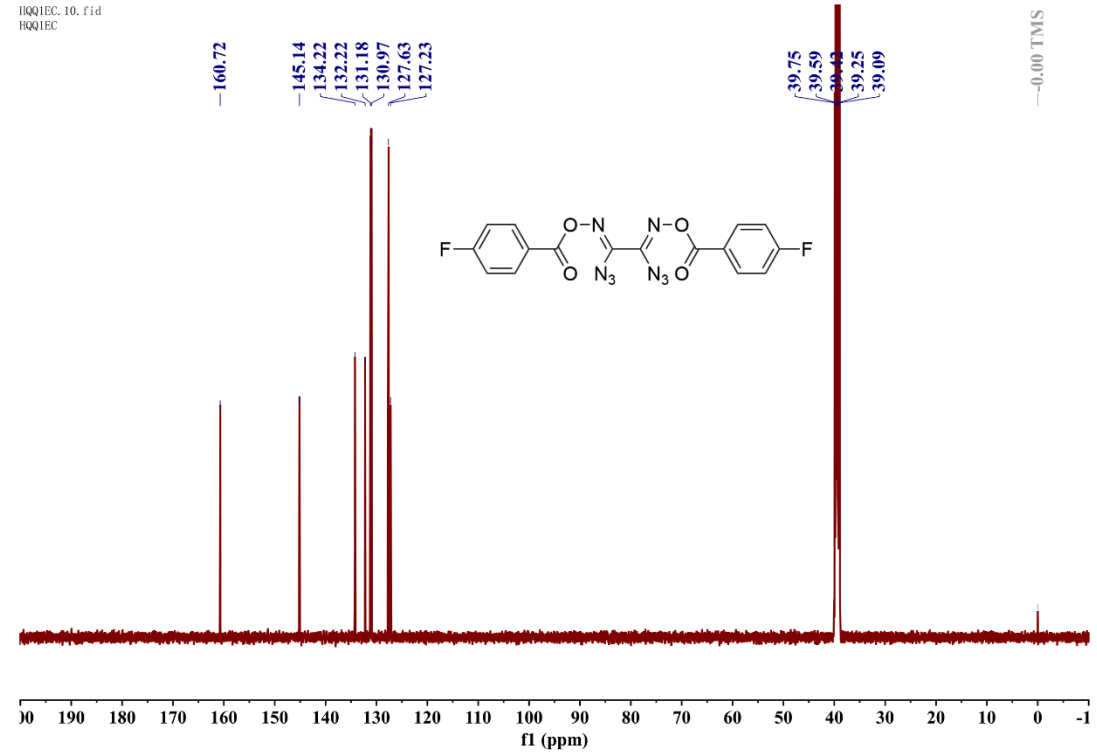
IR of compound **2d**:



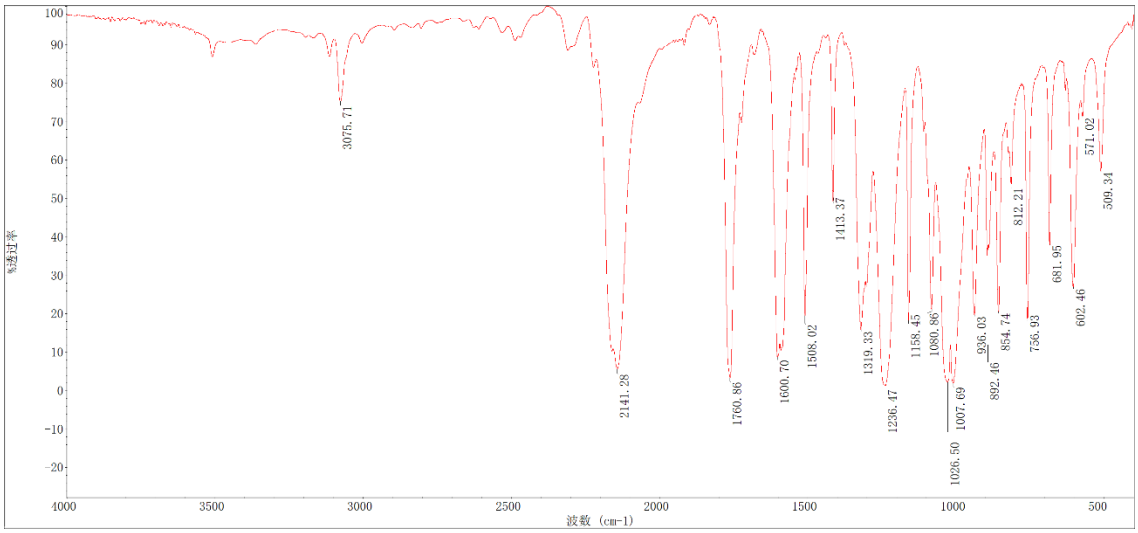
^{1}H NMR (500 MHz, DMSO) spectra of compound **2e**:



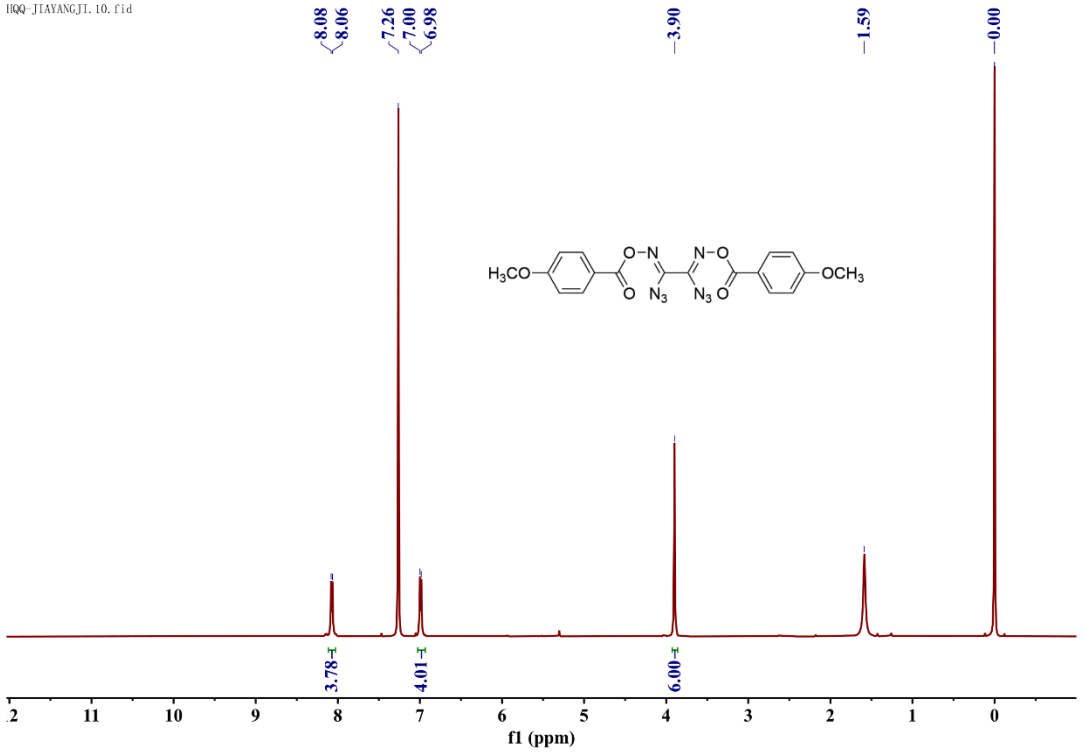
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **2e**:



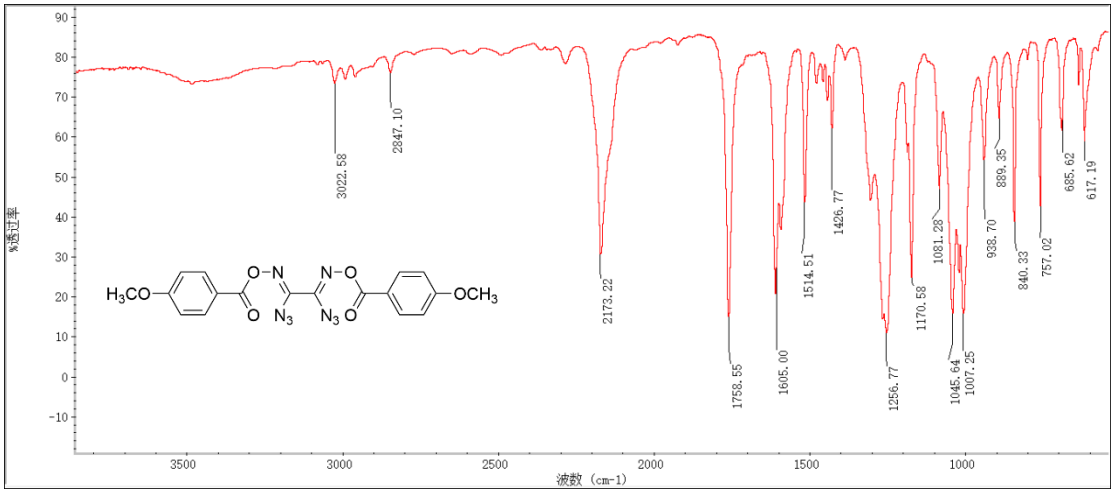
IR of compound **2e**:



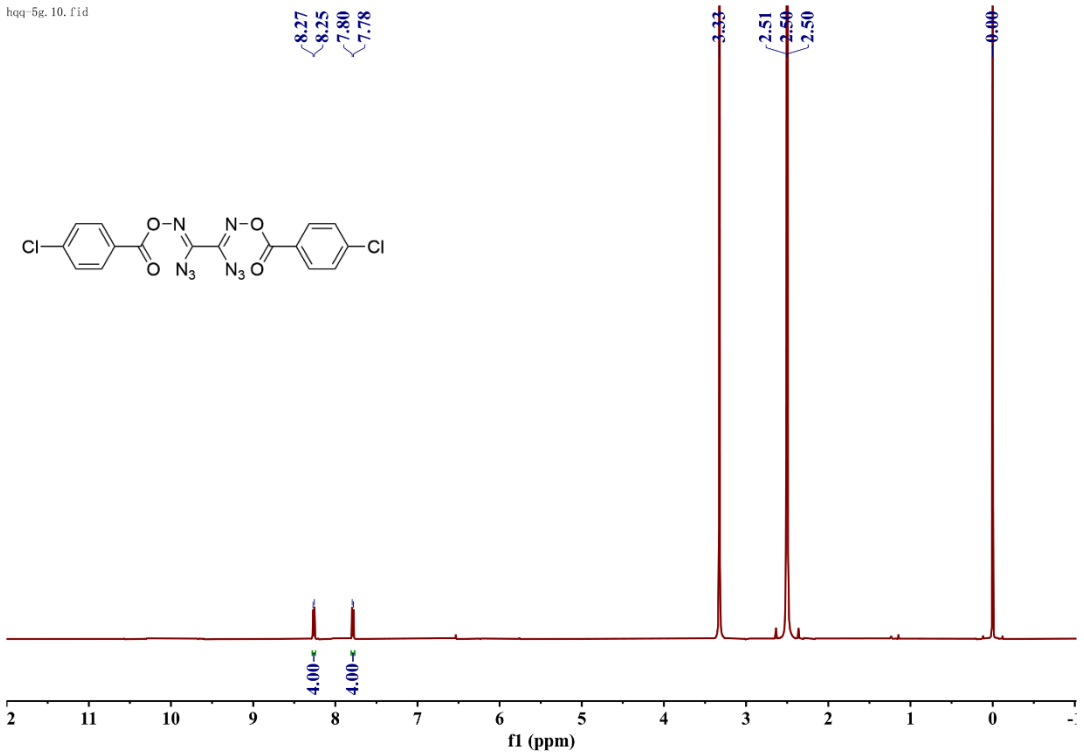
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **2f**



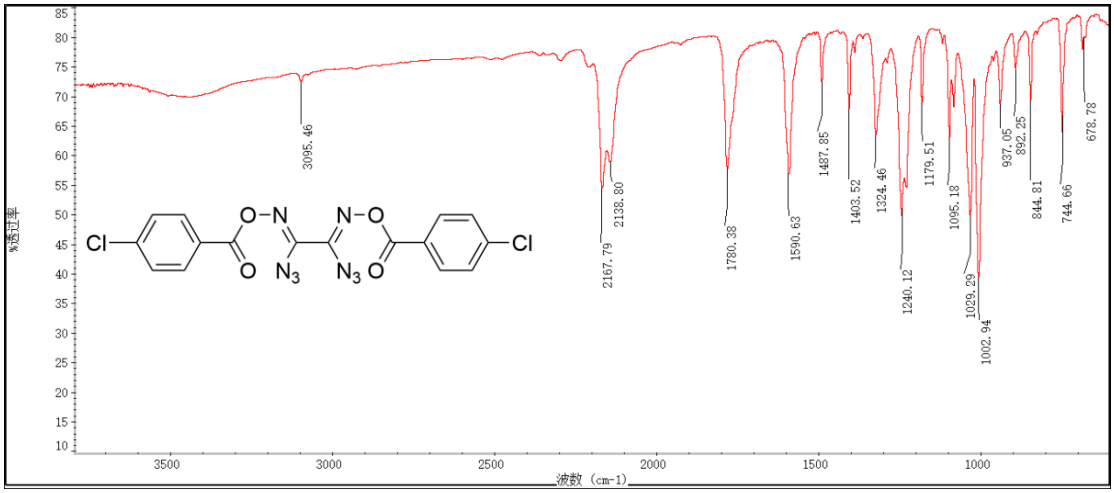
IR of compound **2f:**



^{1}H NMR (500 MHz, DMSO) spectra of compound **2g**:

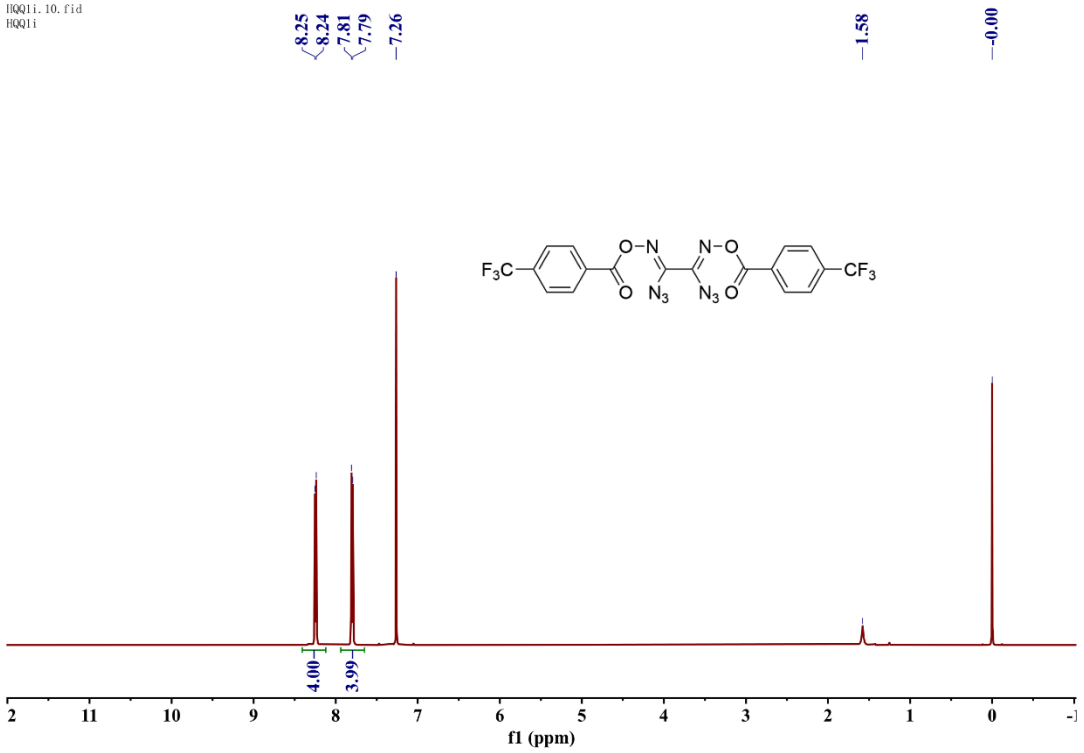


IR of compound **2g**:

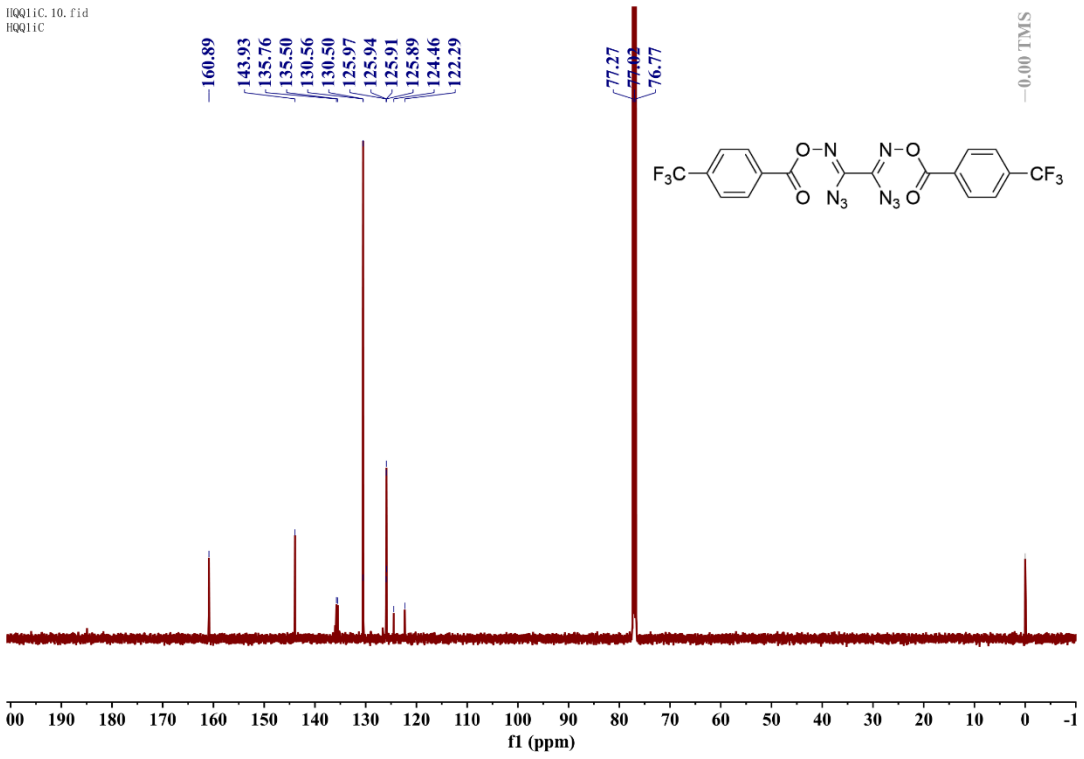


7.

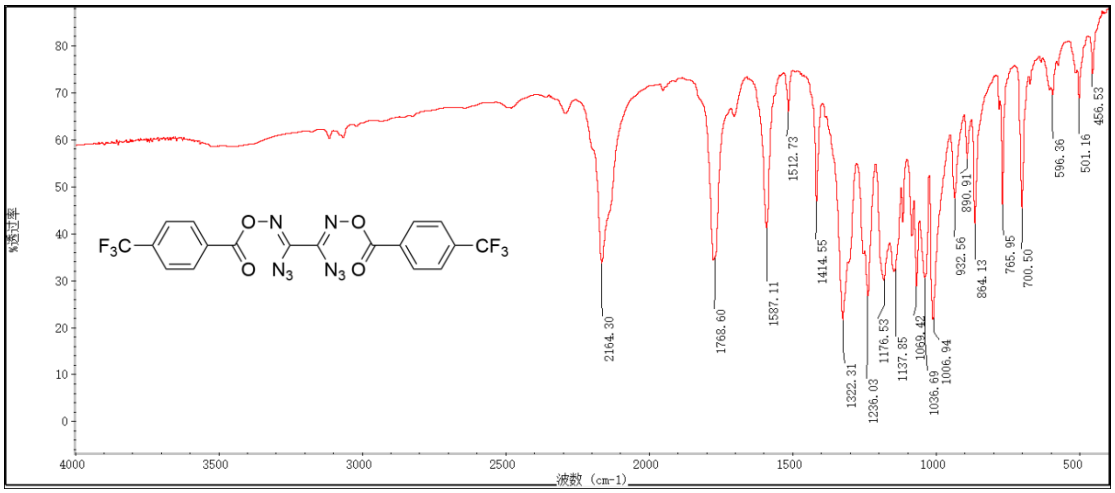
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **2h**:



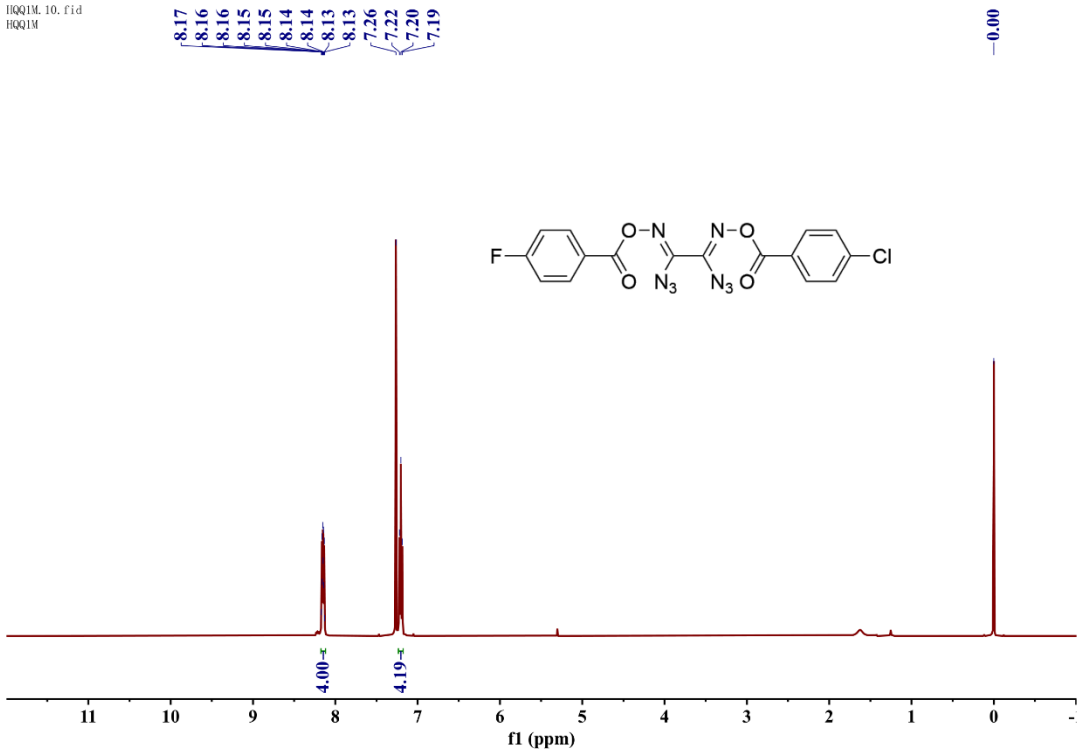
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **2h**:



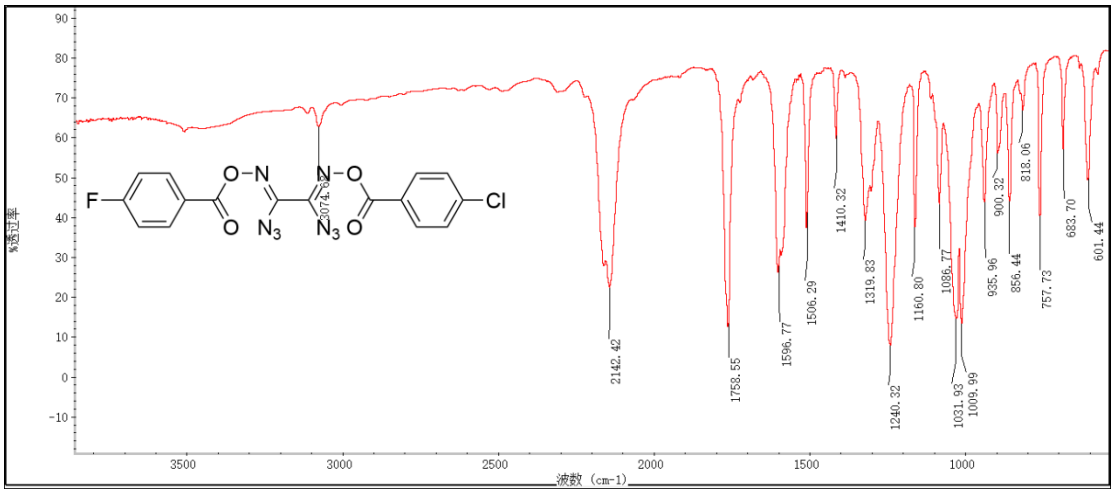
IR of compound **2h**:



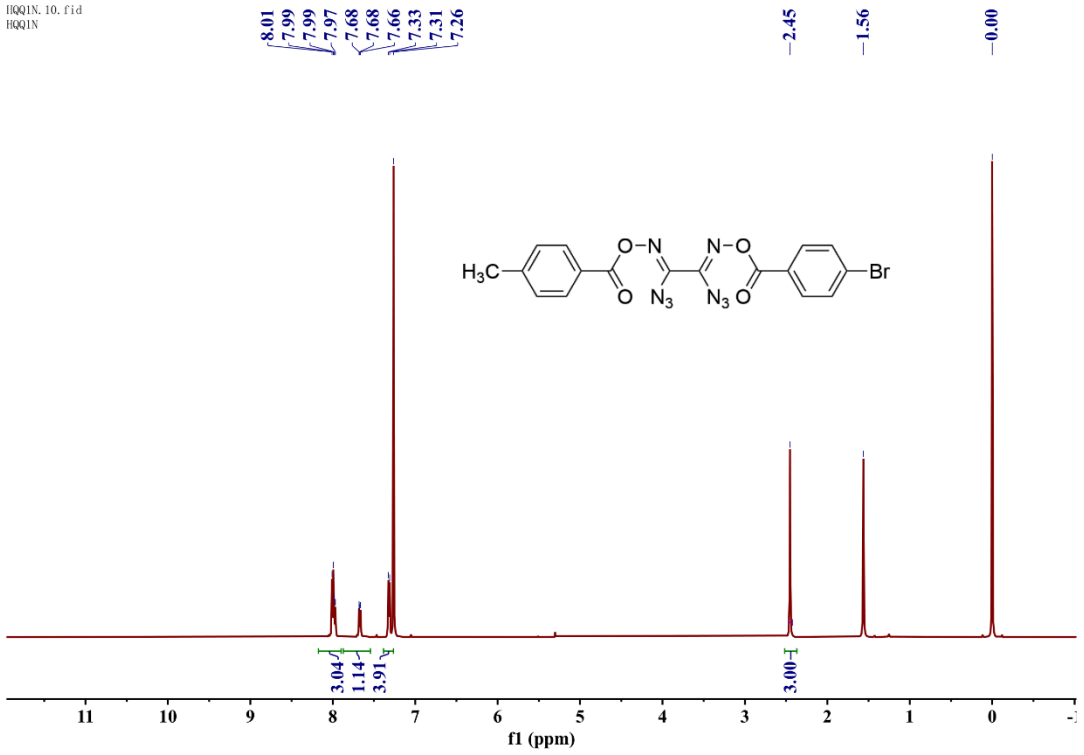
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **2i**:



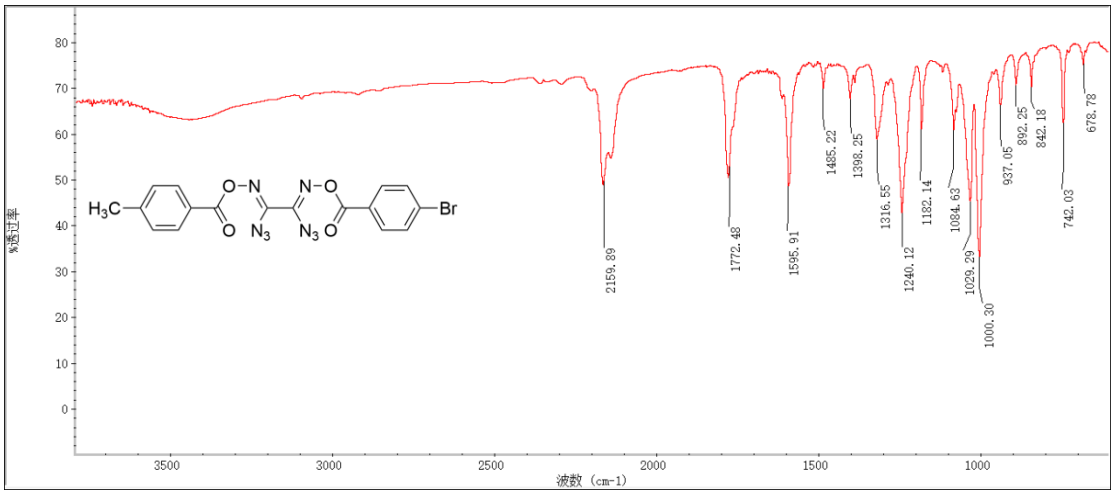
IR of compound **2i**:



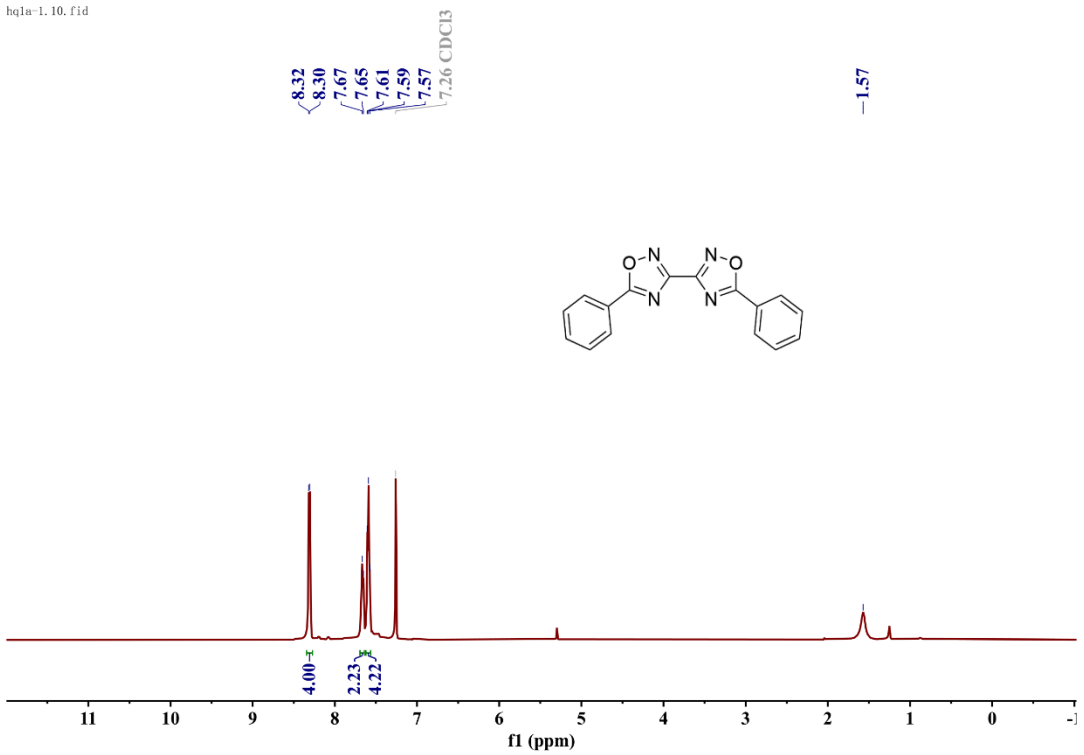
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **2j:**



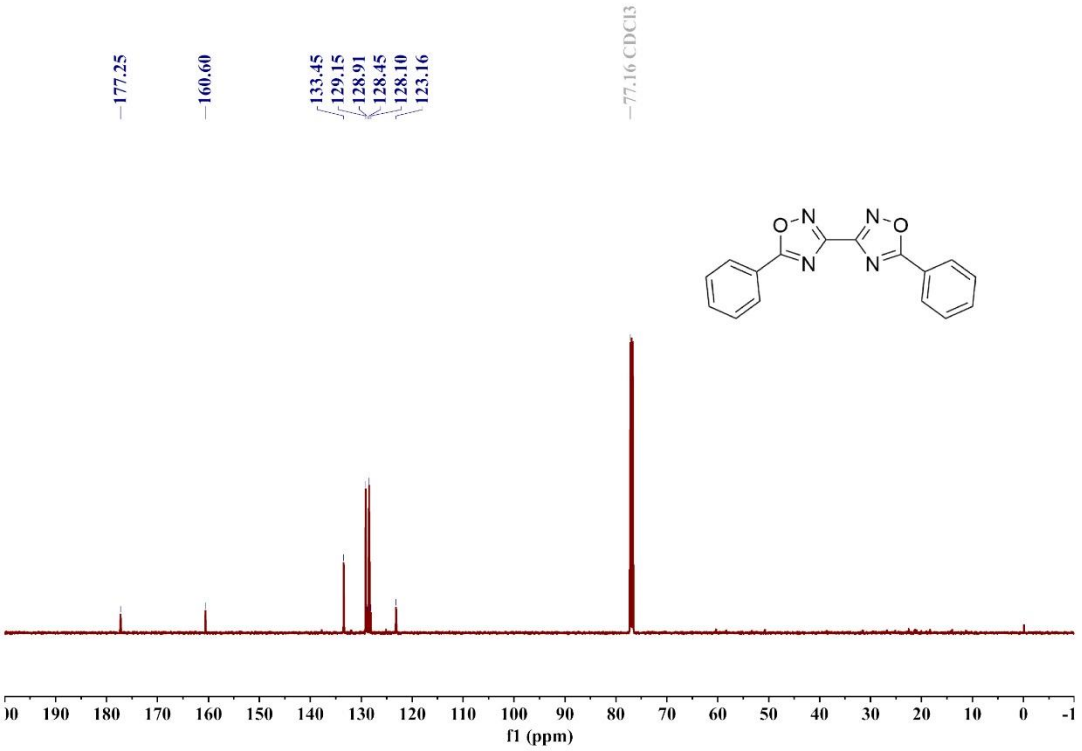
IR of compound **2j**:



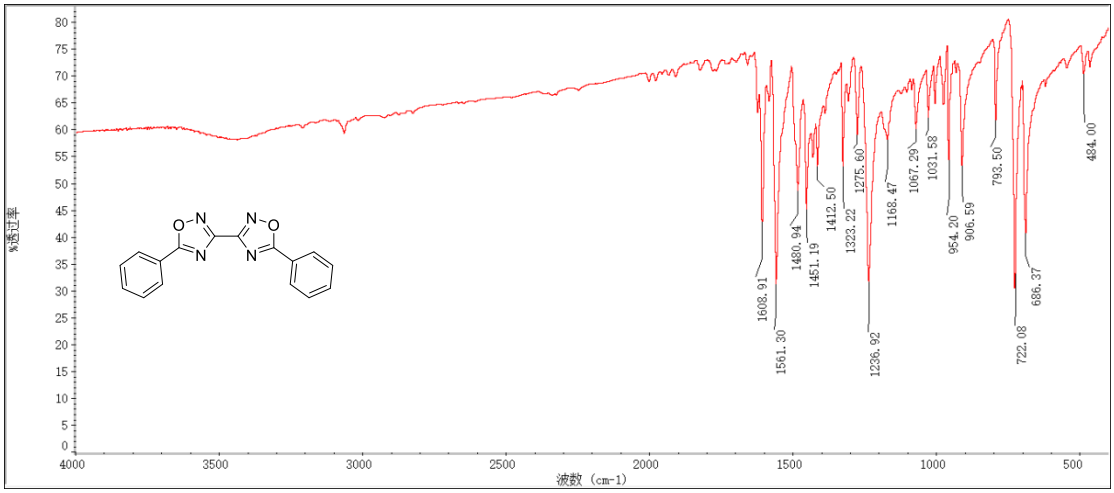
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4a**:



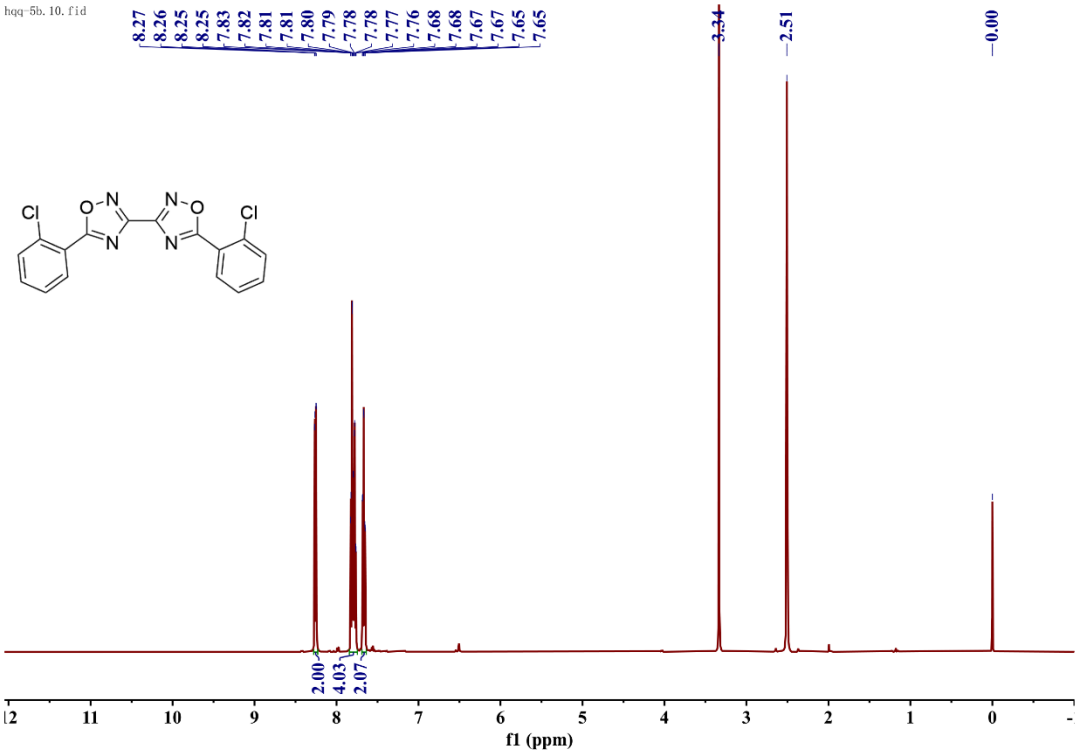
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4a**:



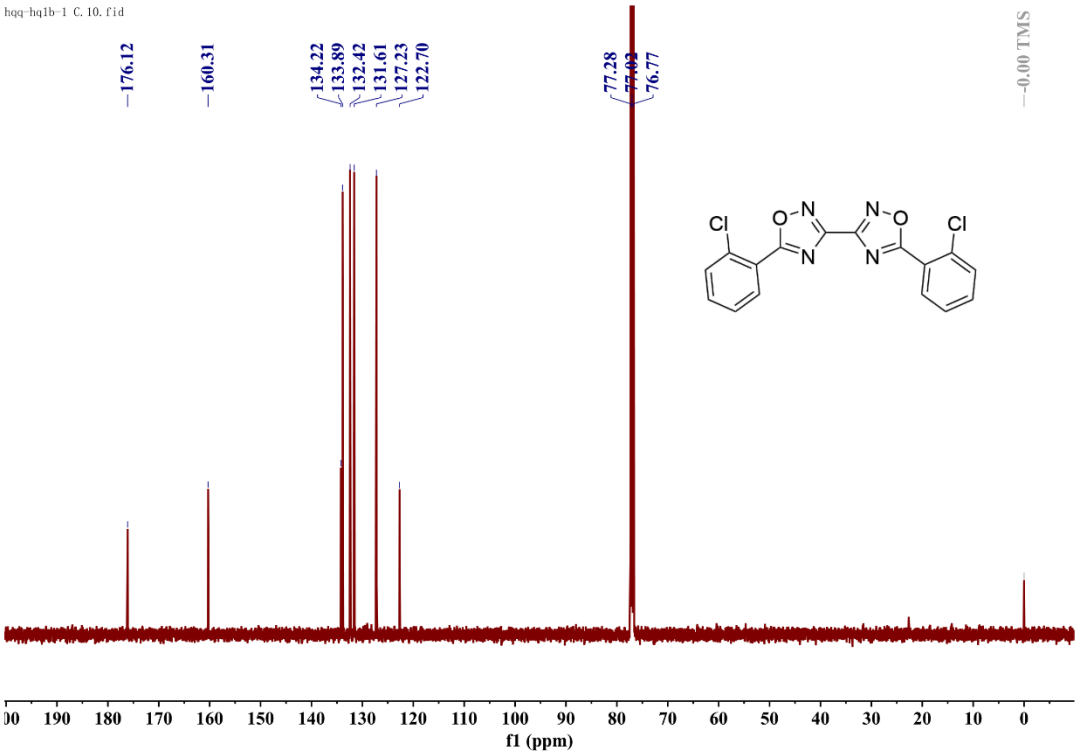
IR of compound **4a**:



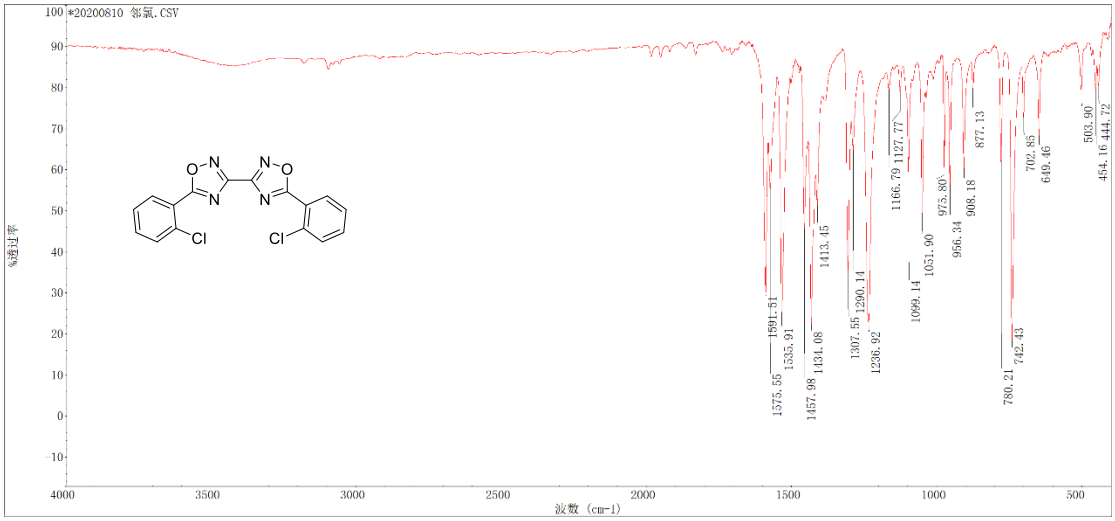
^{1}H NMR (500 MHz, DMSO) spectra of compound **4b**:



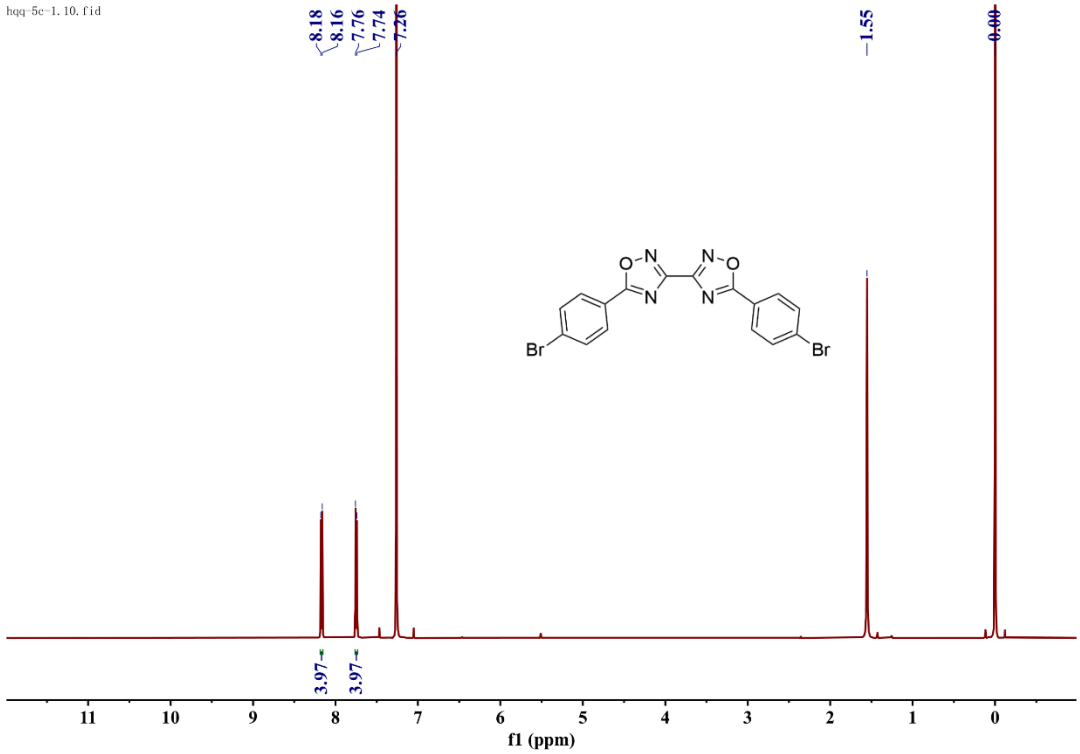
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4b**:



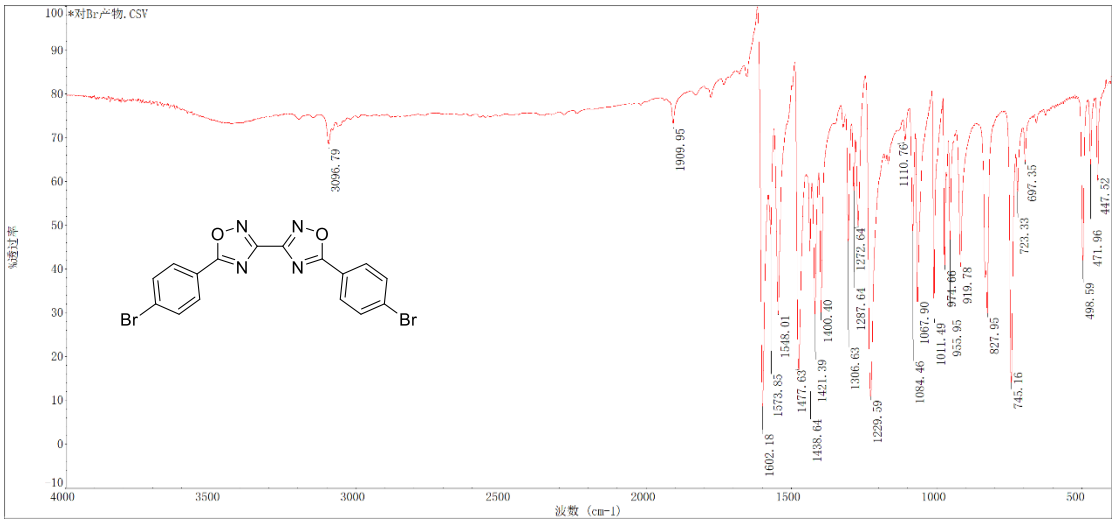
IR of compound **4b**:



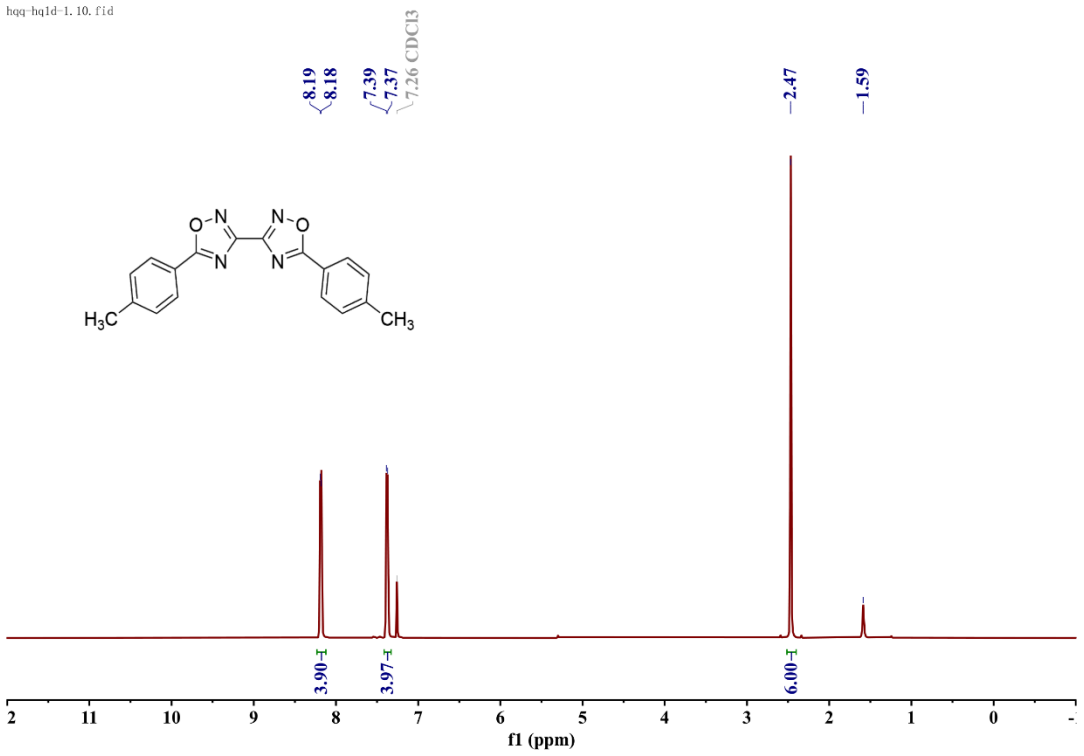
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4c**:



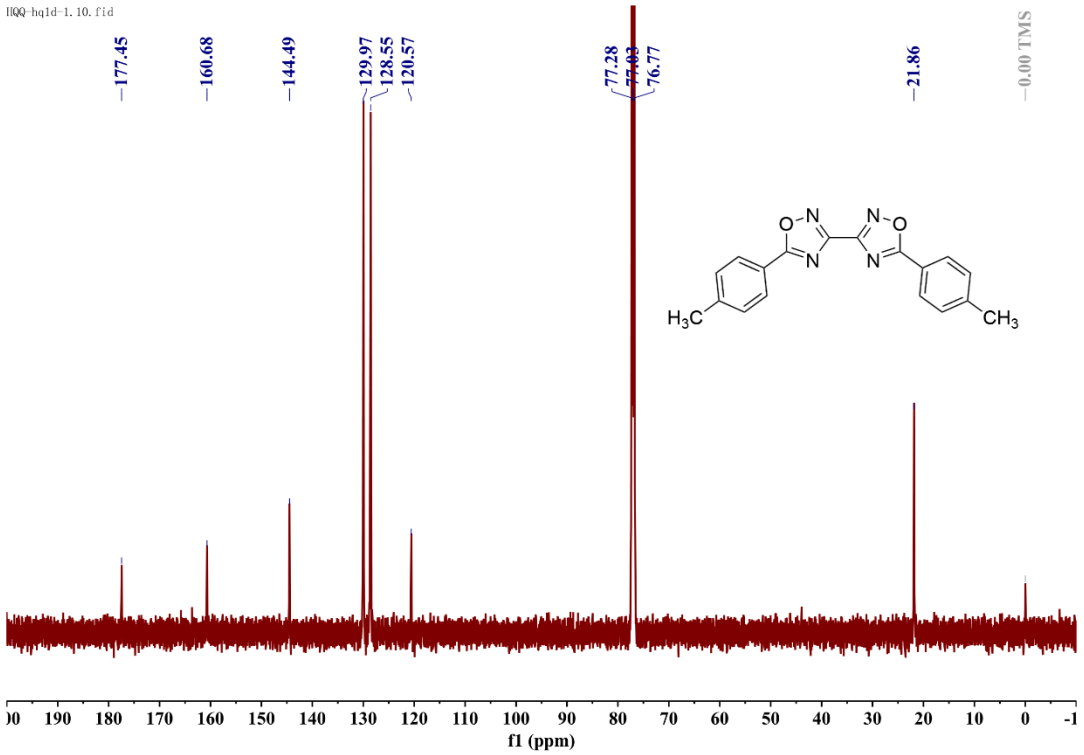
IR of compound **4c**:



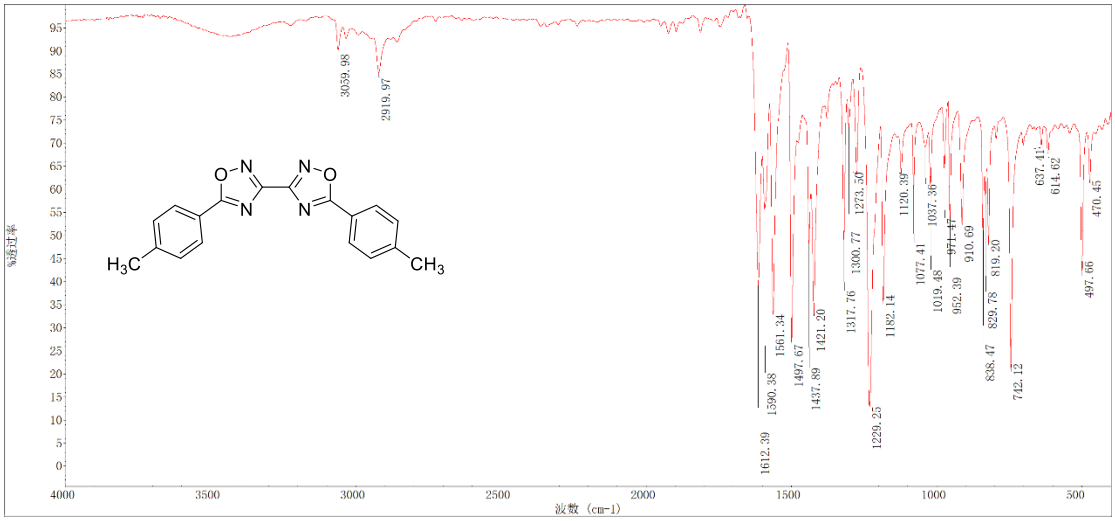
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4d**:



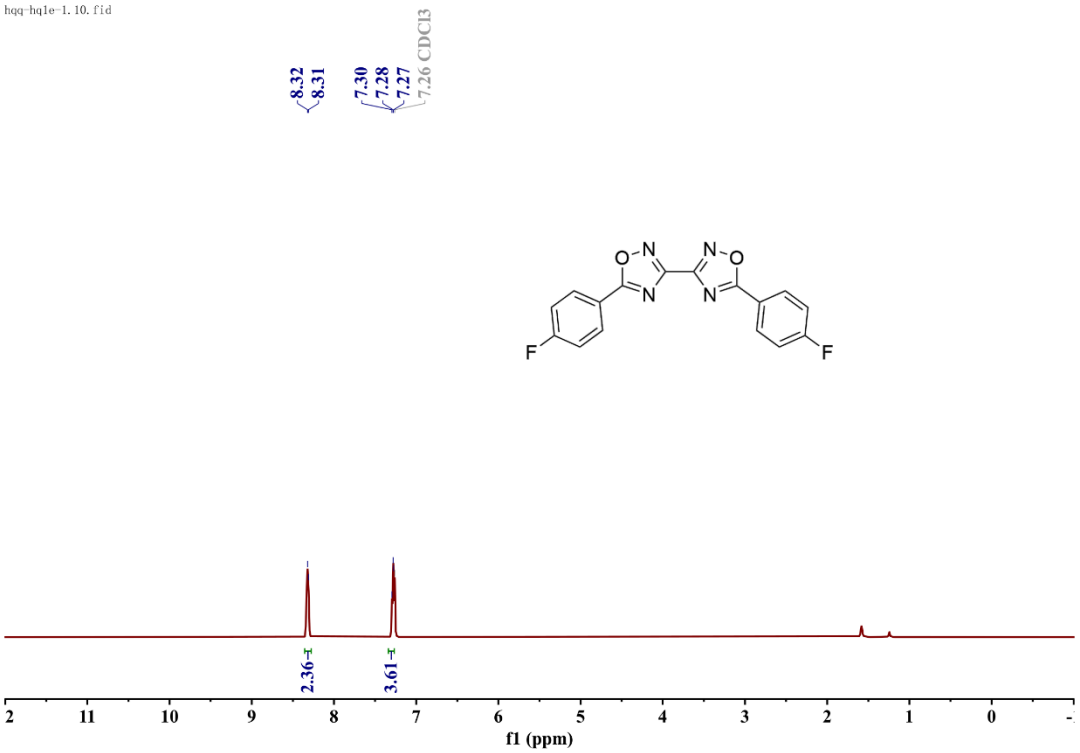
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4d**:



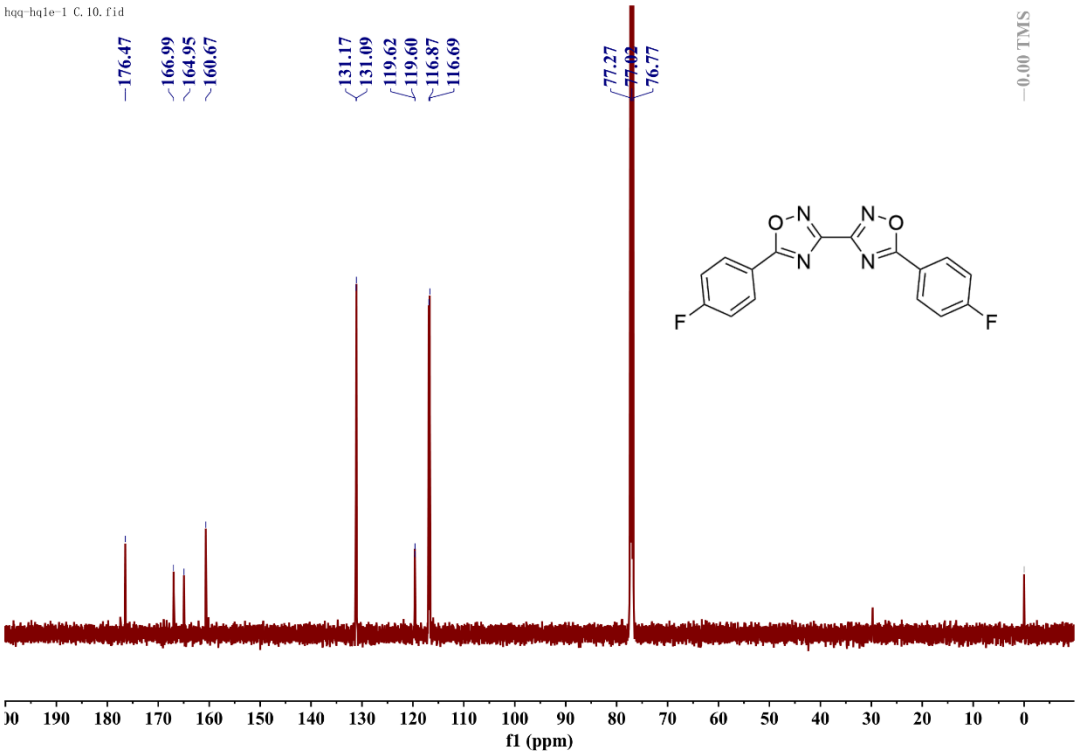
IR of compound **4d**:



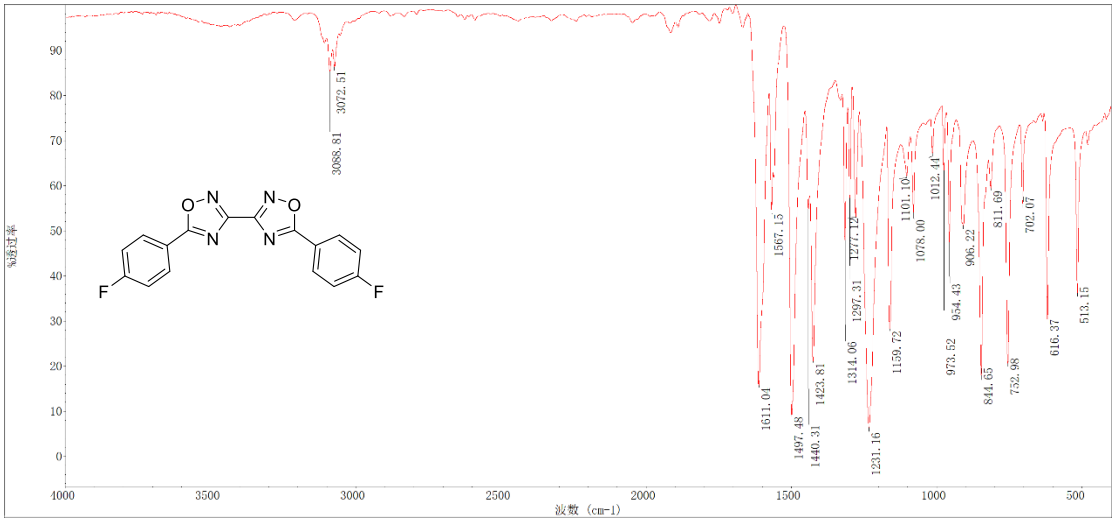
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4e**:



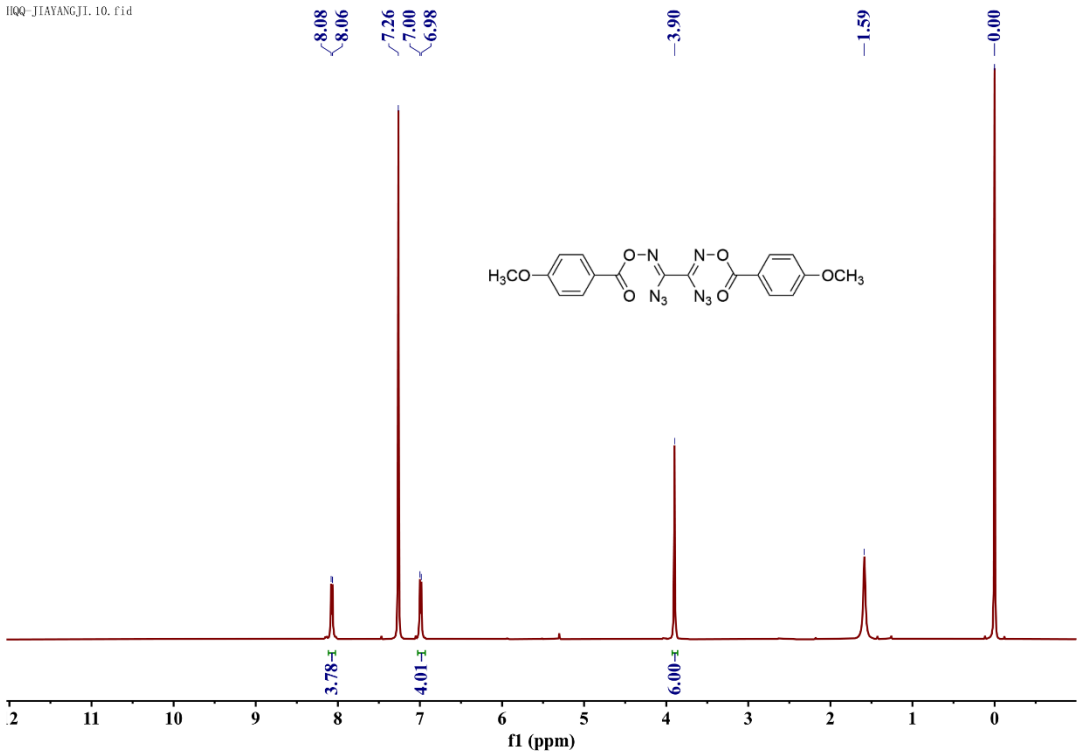
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4e**:



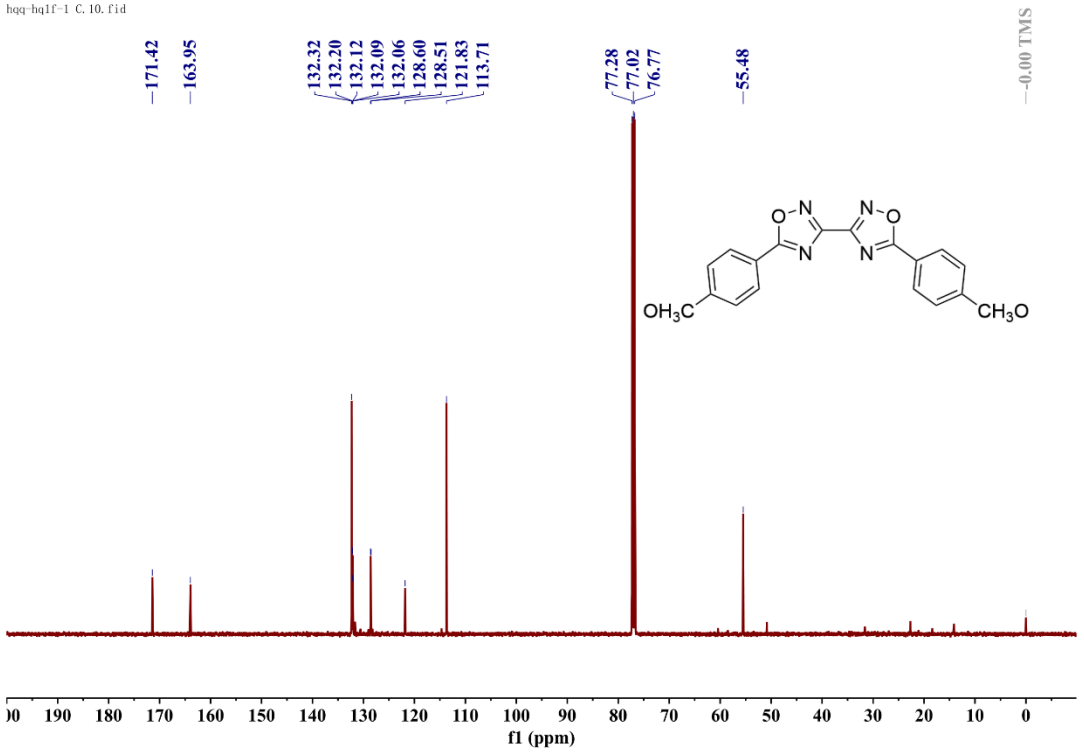
IR of compound **4e**:



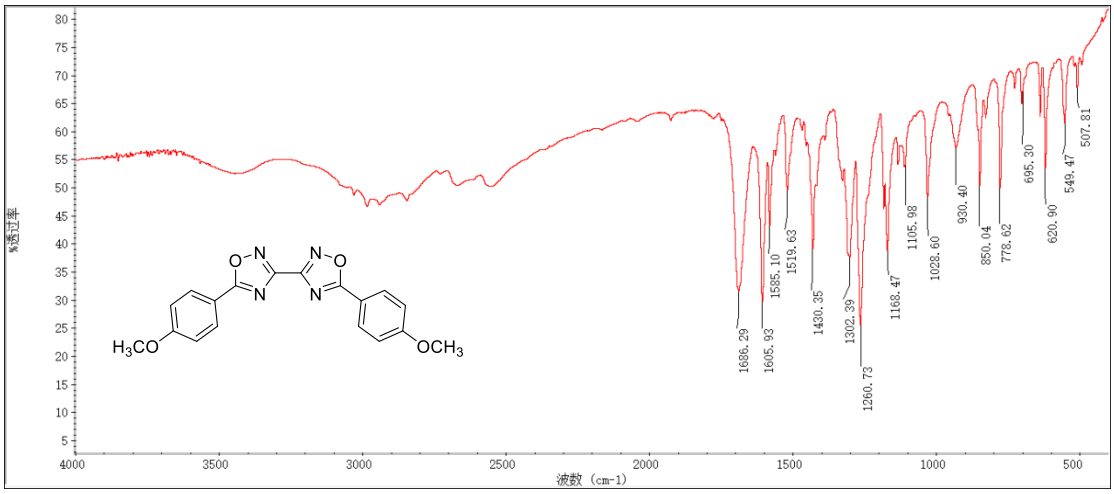
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4f**:



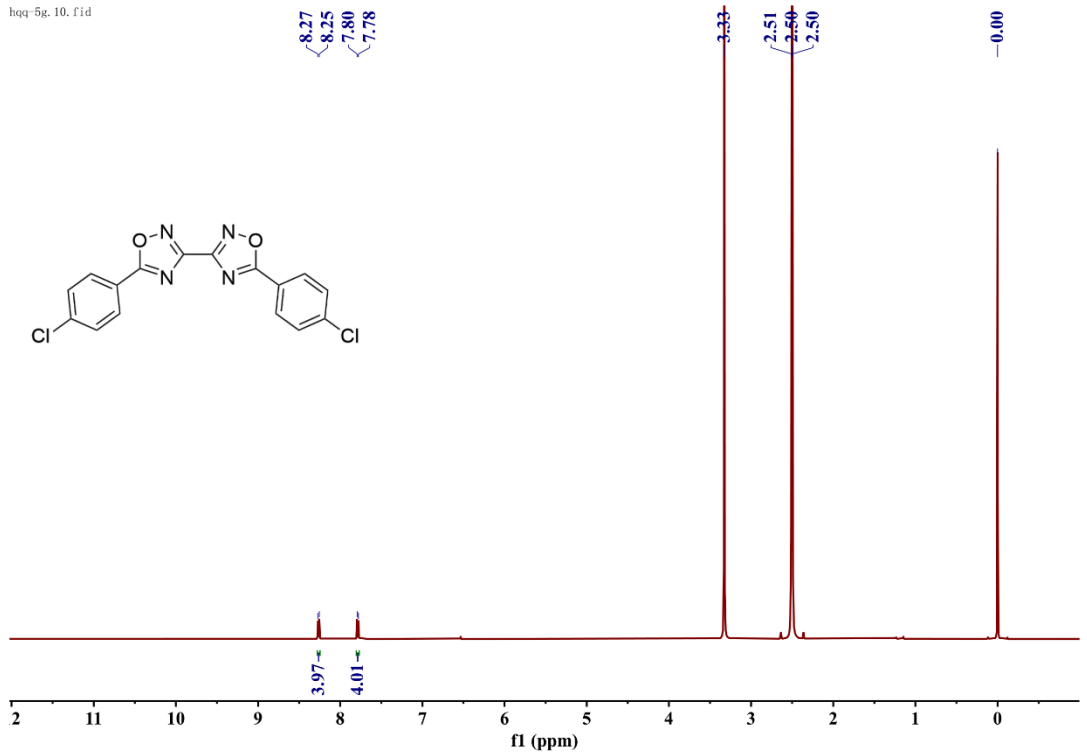
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4f**:



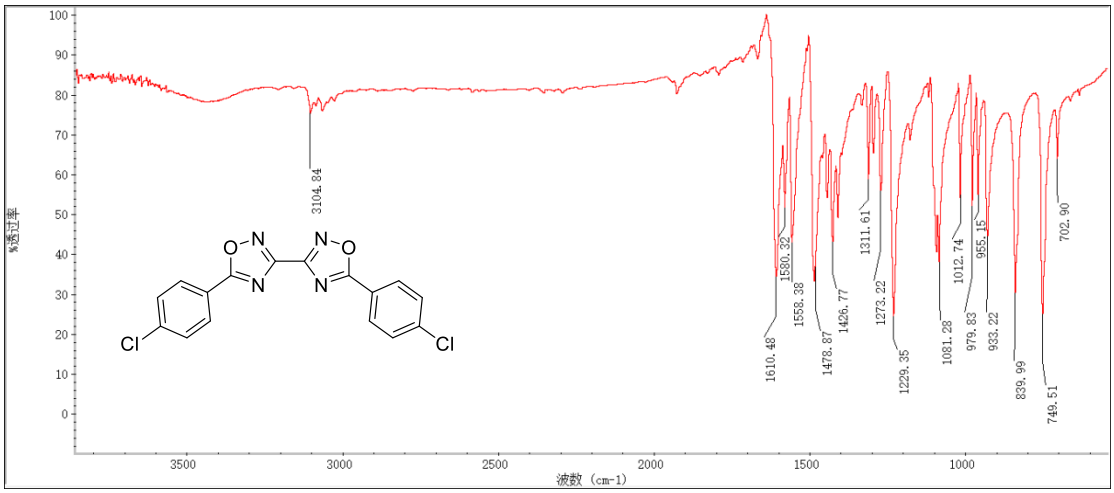
IR of compound **4f**:



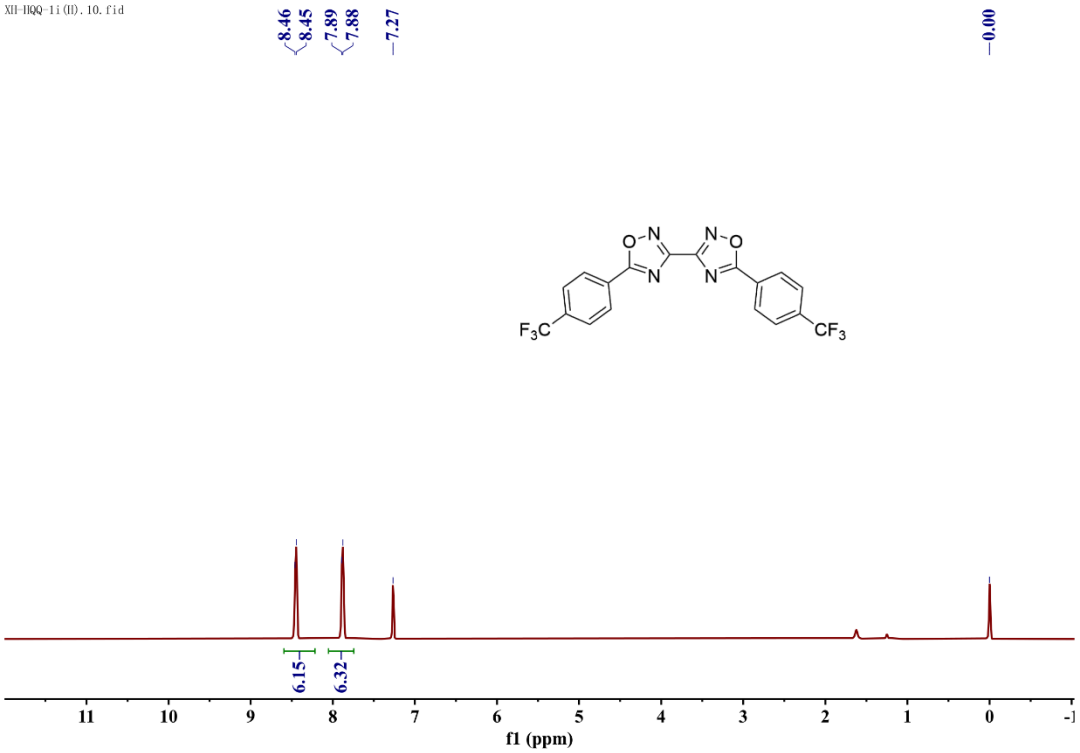
^{1}H NMR (500 MHz, DMSO) spectra of compound **4g**:



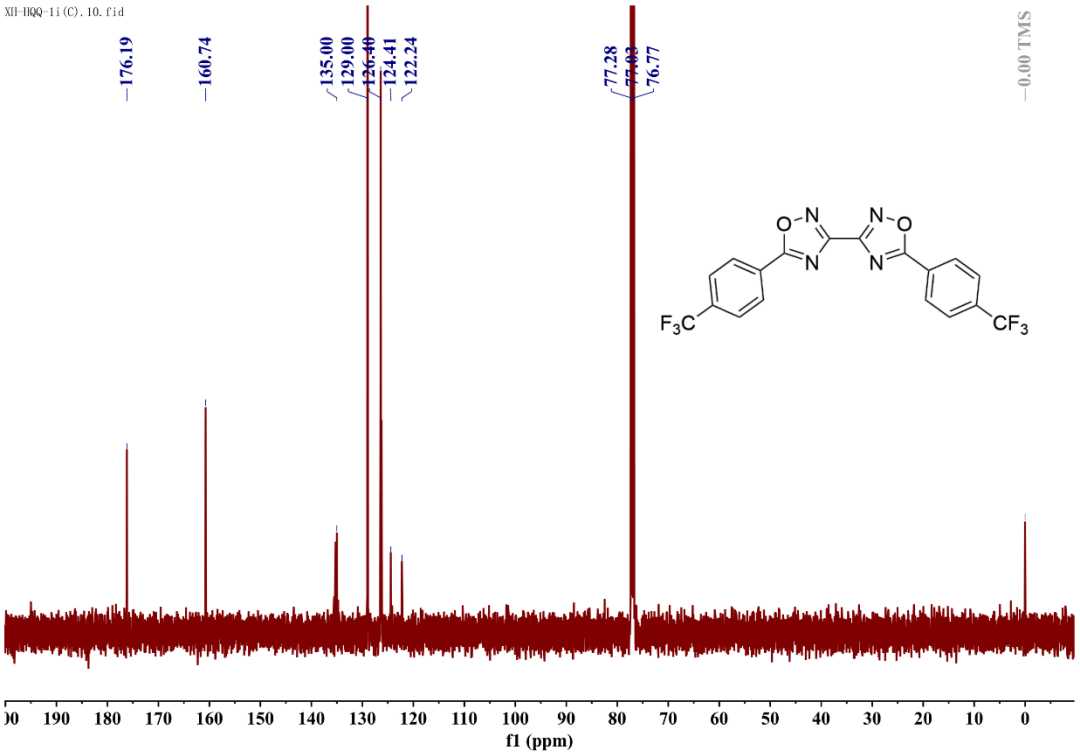
IR of compound **4g**:



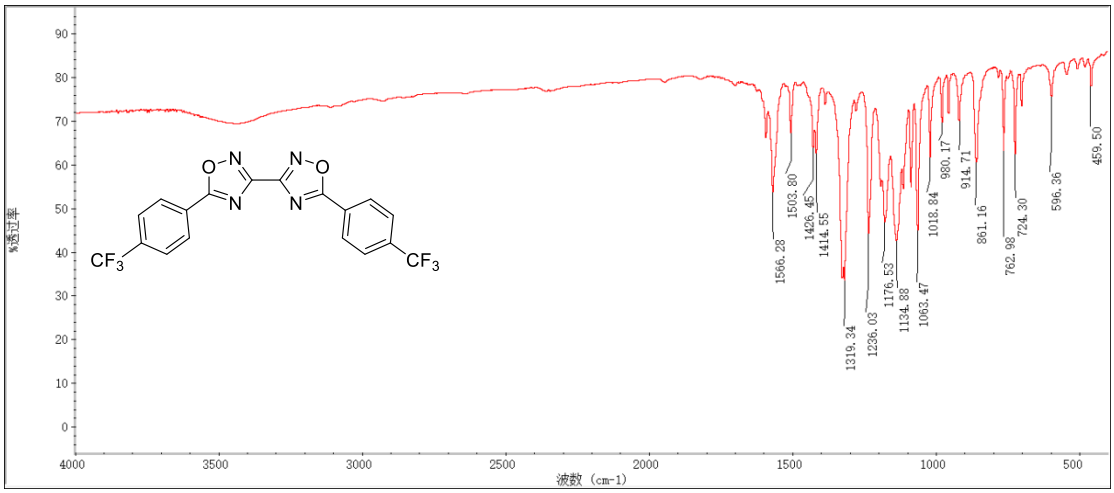
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4h**:



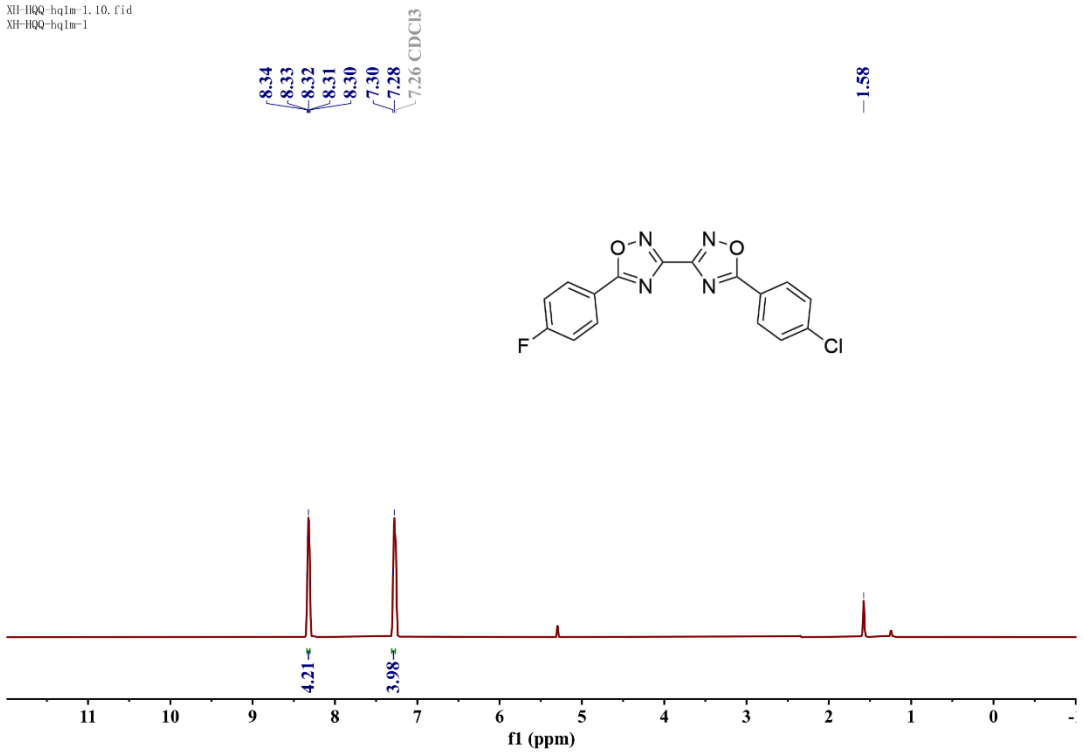
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4h**:



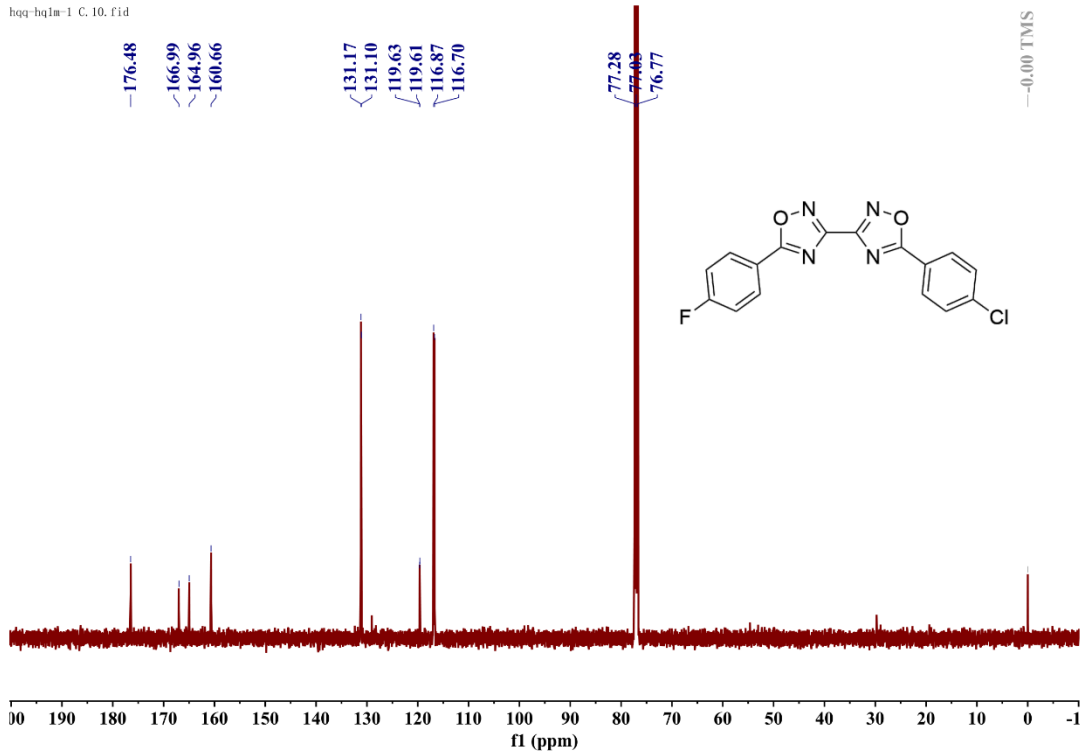
IR of compound **4h**:



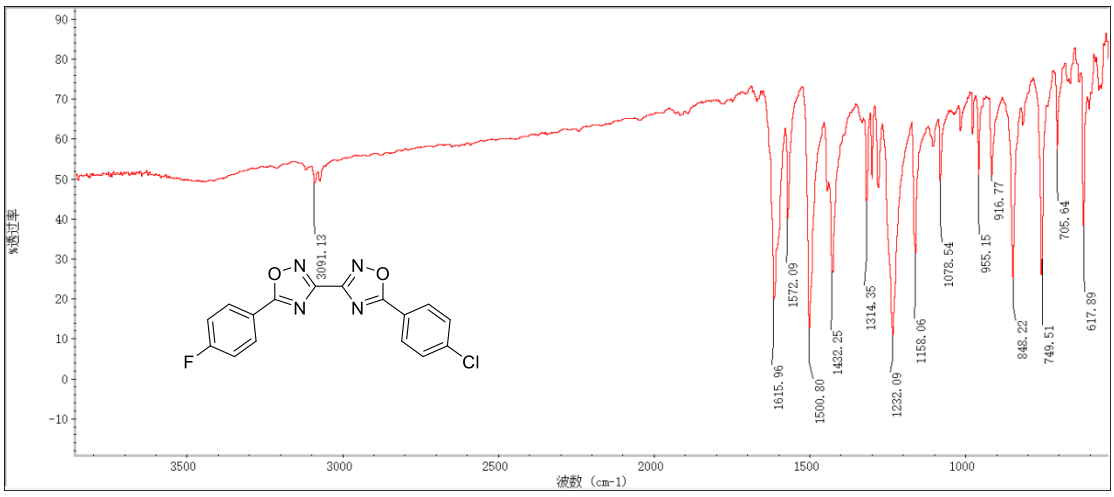
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4i**:



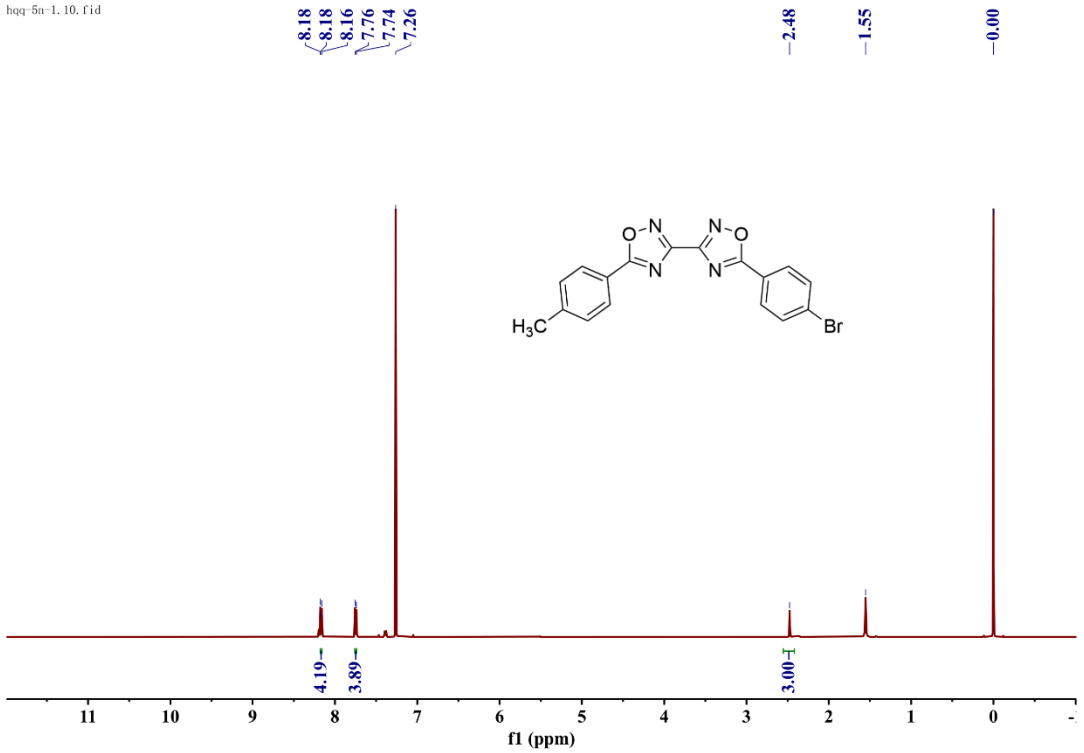
^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4i**:



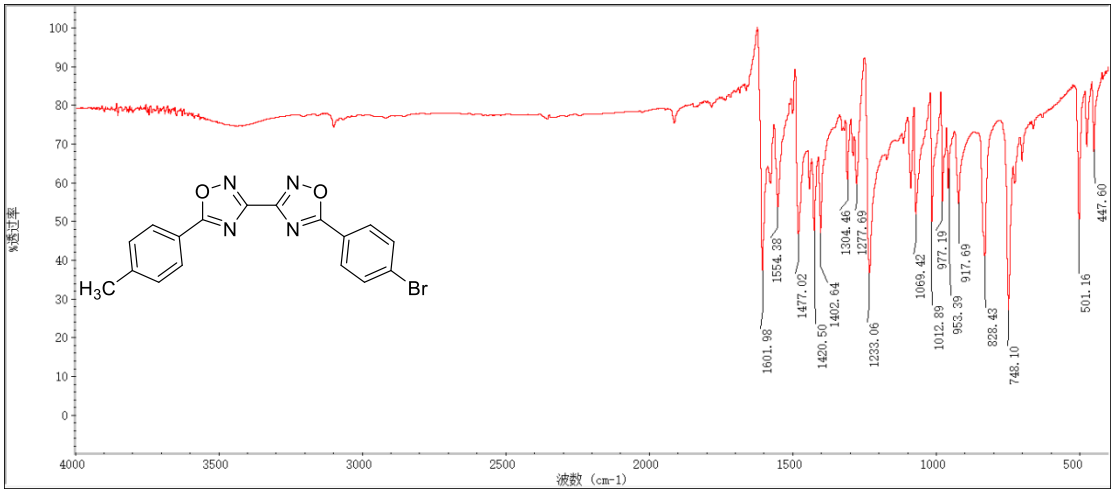
IR of compound **4i**:



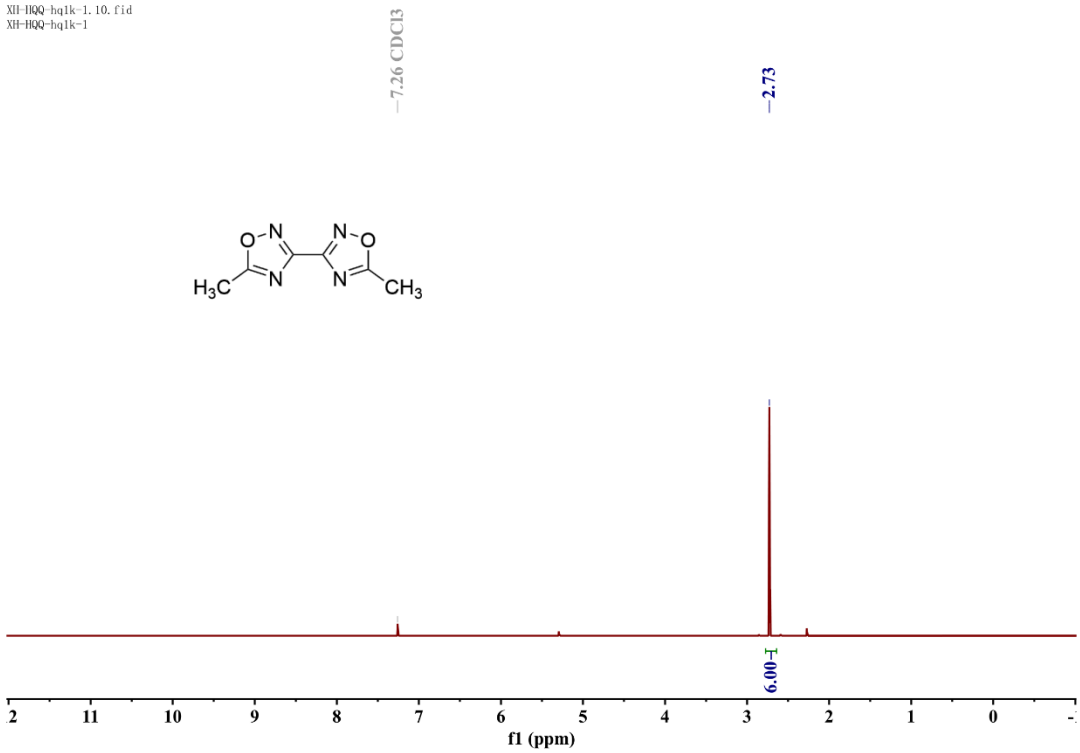
^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4j**:



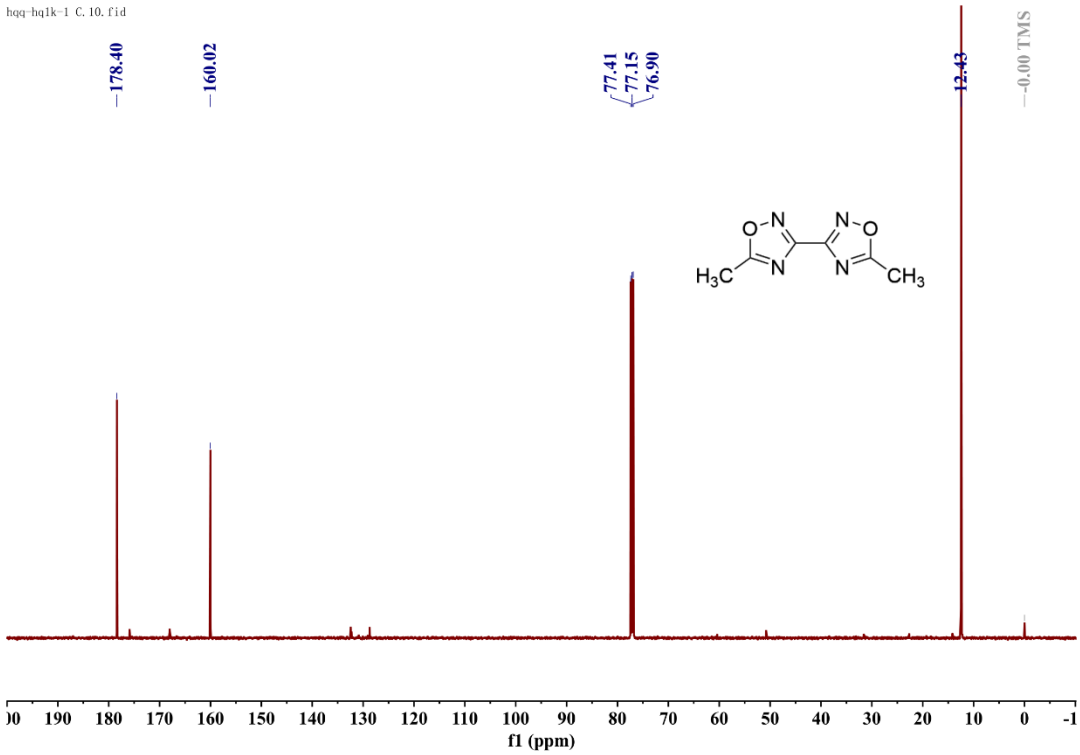
IR of compound **4j**:



^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **4k**:



^{13}C NMR (125 MHz, $CDCl_3$) spectra of compound **4k**:



IR of compound **4k**: