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RESEARCH ARTICLE

Novel 1,2,3-triazole-based compounds: Iodo effect on their gelation behavior and cation response

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Electronic supplementary material

Table S1. Crystal data and structure refinement for compound **1**

Empirical formula	C17H17N3O2
Formula weight	295.34
Temperature/K	113(2)
Wavelength/Å	0.71073
Crystal system	Orthorhombic
space group	*P*na2(1)
a/Å	9.159(4)
b/Å	5.693(3)
c/Å	27.591(12)
α/(°)	90
β/(°)	90
γ/(°)	90
Volume/Å^3, *Z*	1438.7(11), 2
Cald. density/(Mg·cm^{-3})	1.364
Abs. Coefficient/(mm^{-1})	0.092
F(000)	624
Crystal size/(mm)	0.22 × 0.22 × 0.06
θ range for data collection/(°)	1.48 to 27.87
Limiting indices	–12 ≤ h ≤ 11, –7 ≤ k ≤6, –36 ≤ l ≤3 6
Reflections collected / unique	11442 / 3348 [R_{int} = 0.0399]
Completeness to *θ* = 27.87	99.80%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9945, 0.9801

Refinement method	Full-matrix least-squares on F2
Data/restraints/parameters	3348 / 1 / 202
Goodness-of-fit on F2	1.005
Final R indices [$I > 2\delta(I)$]	$R_1 = 0.0380$, $wR_2 = 0.0892$
R indices (all data)	$R_1 = 0.0440$, $wR_2 = 0.0926$
Absolute structure parameter	1.2(11)
Extinction coefficient	0.0158(16)
Largest diff. peak and hole	0.190 and –0.187 eÅ^{-3}

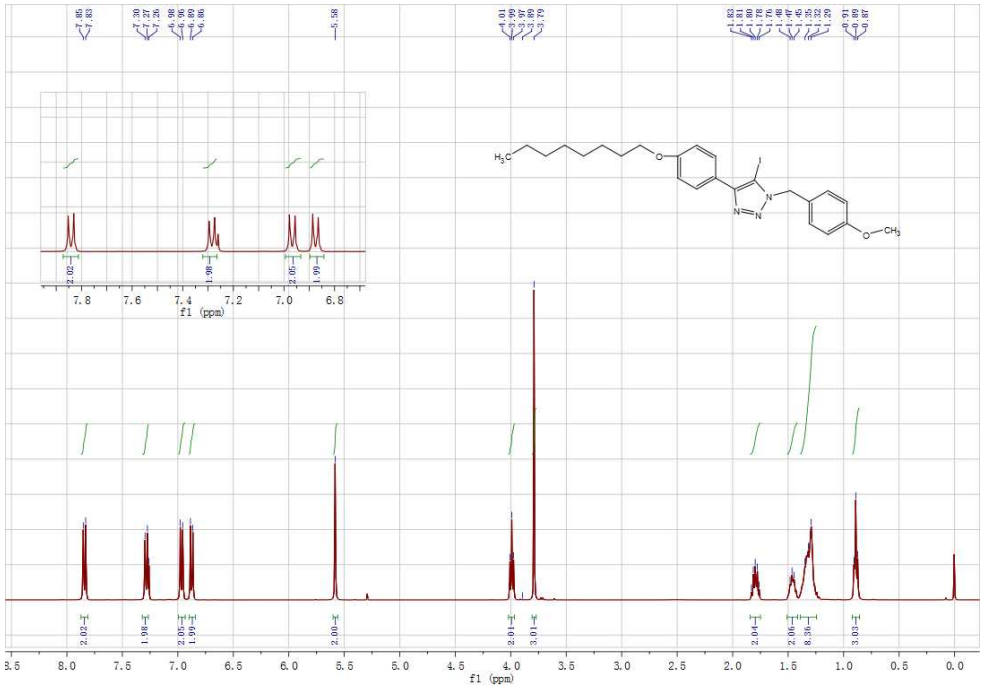

Fig. S1 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K) of compound **1**

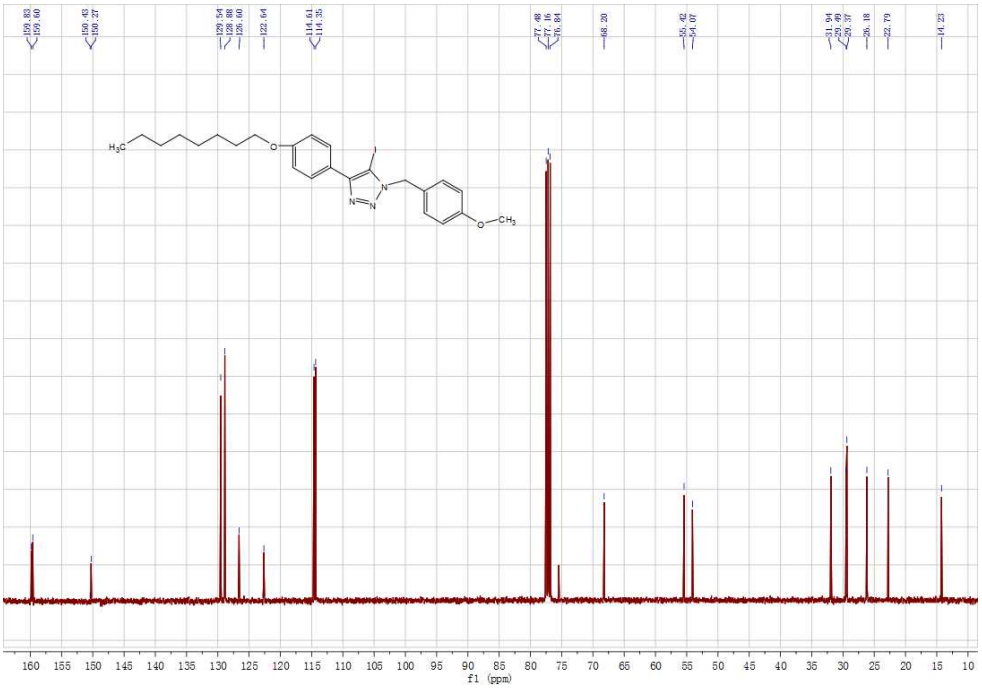

Fig. S2 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 293 K) of compound **1**

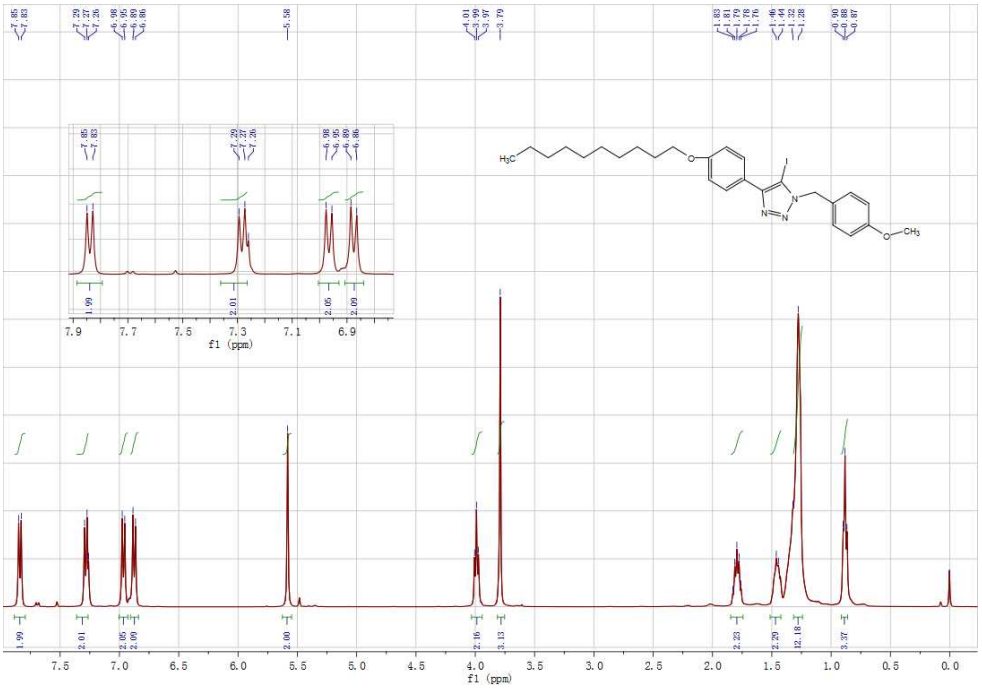

Fig. S3 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K) of compound **2**

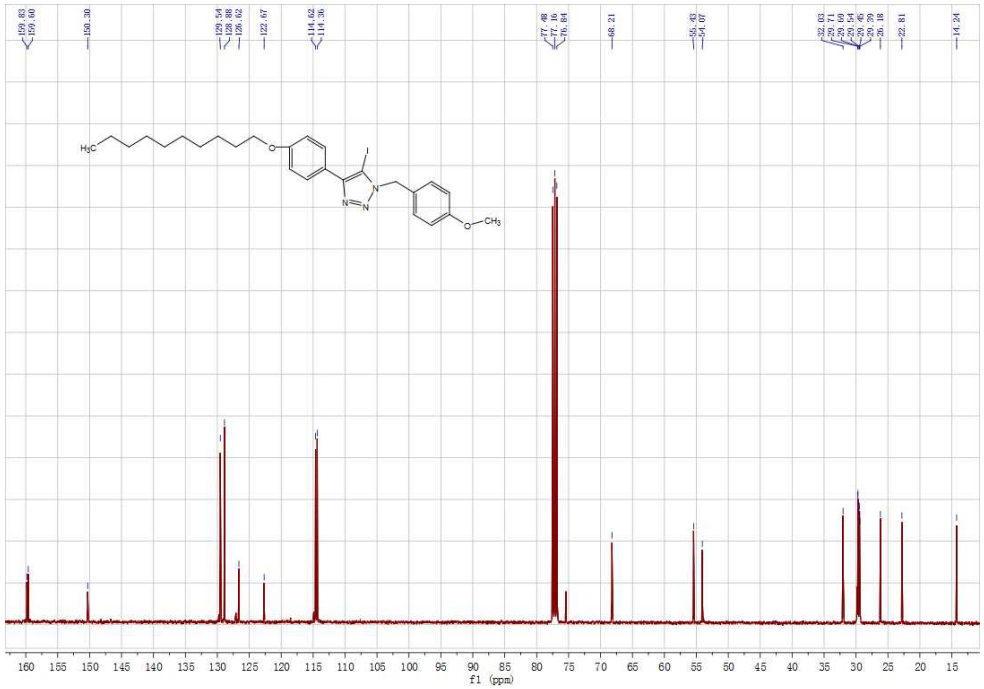

Fig. S4 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 293 K) of compound **2**

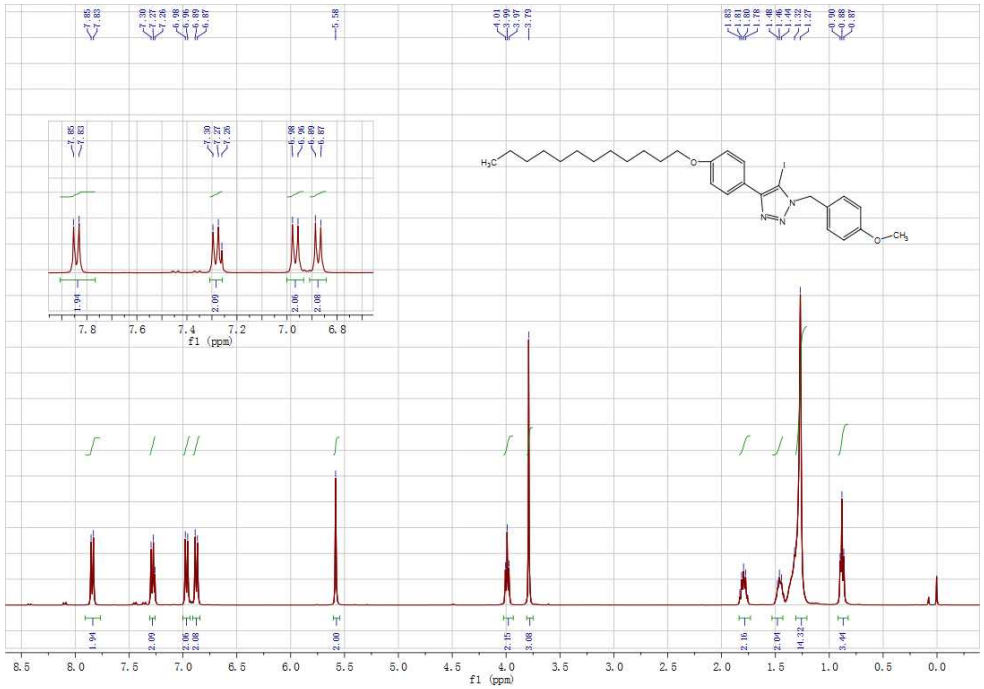

Fig. S5 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K) of compound **3**

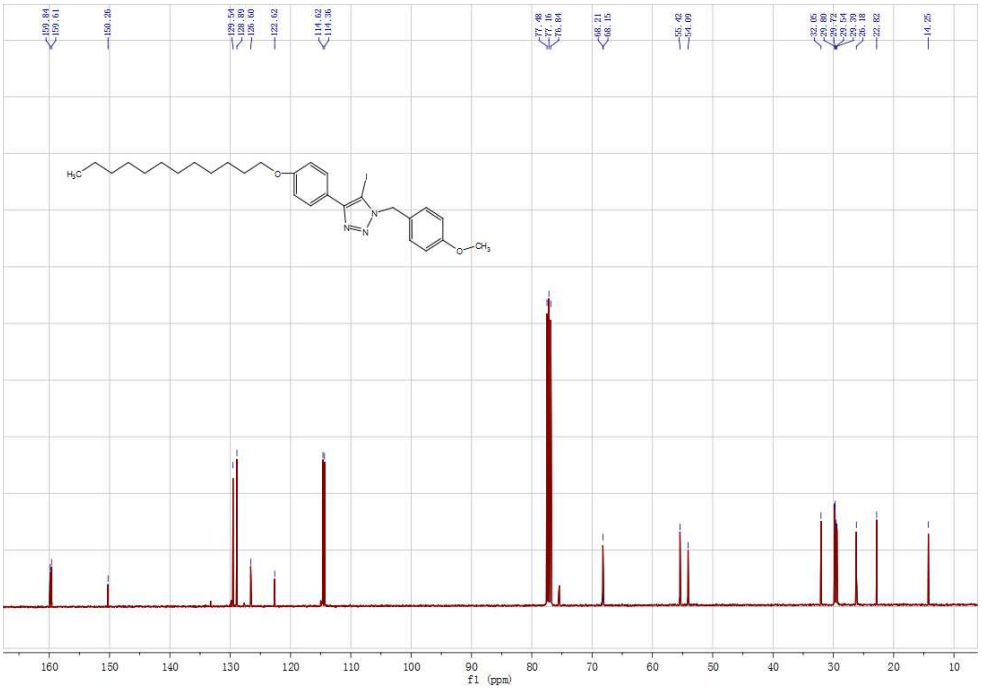

Fig. S6 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 293 K) of compound **3**

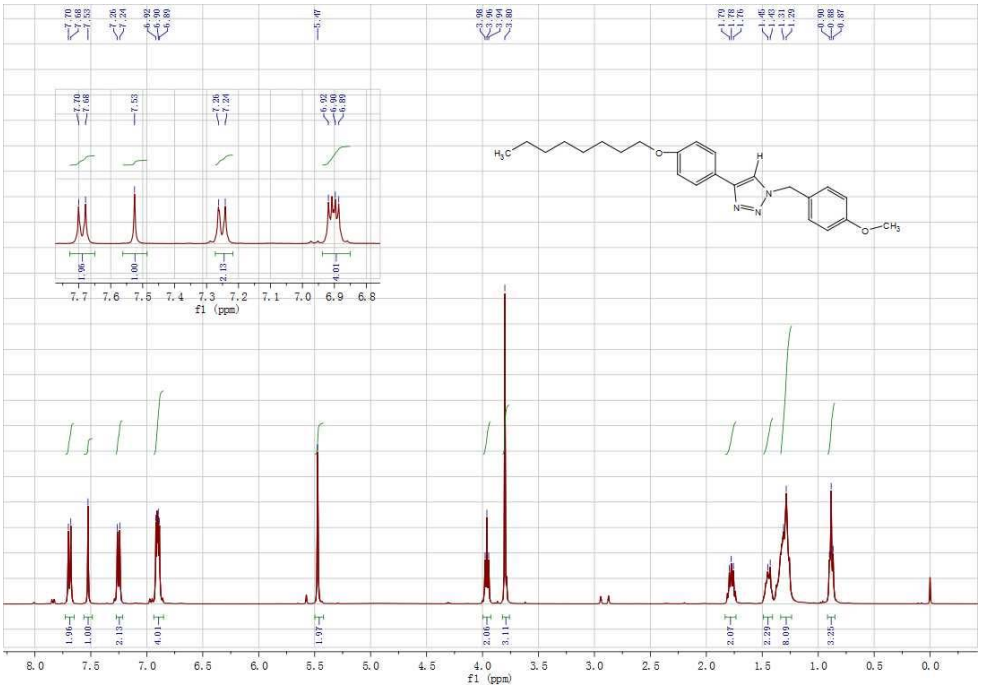

Fig. S7 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K) of compound **4**

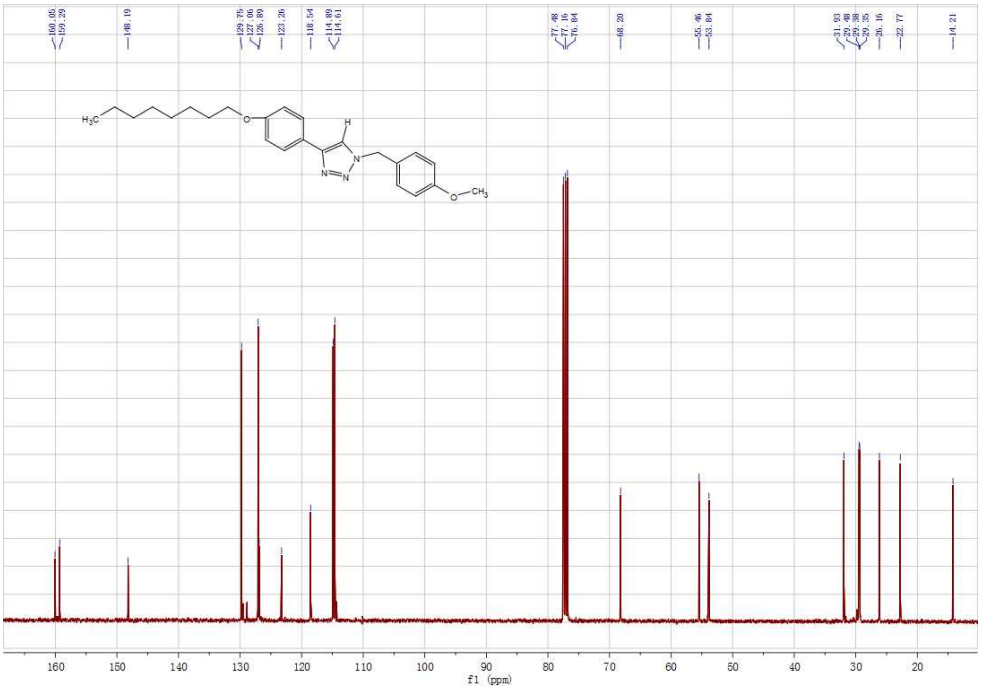

Fig. S8 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 293 K) of compound **4**

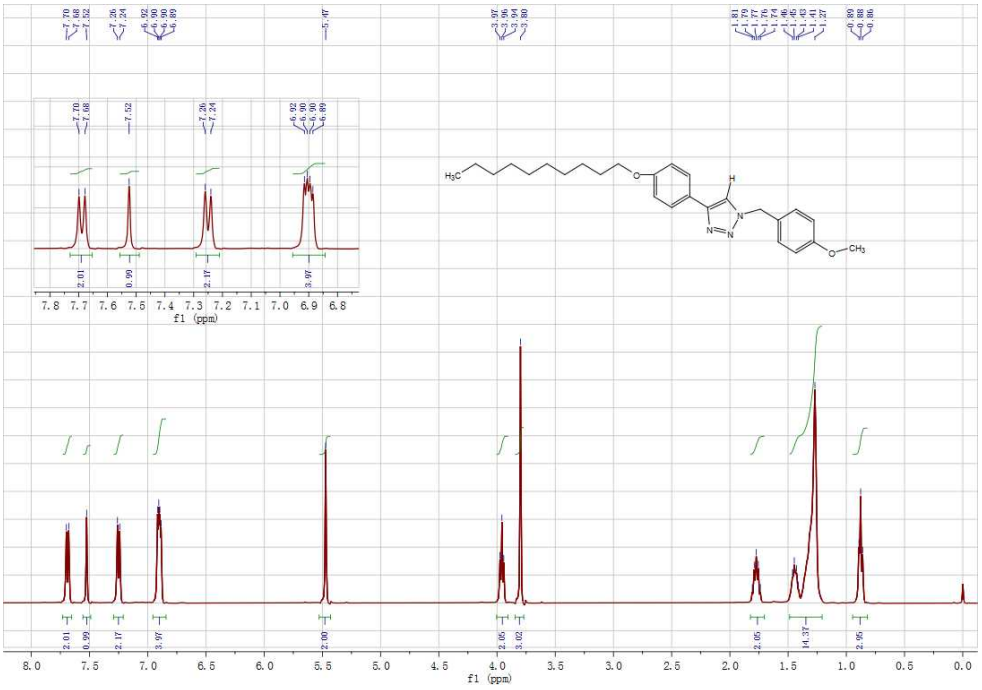

Fig. S9 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K) of compound **5**

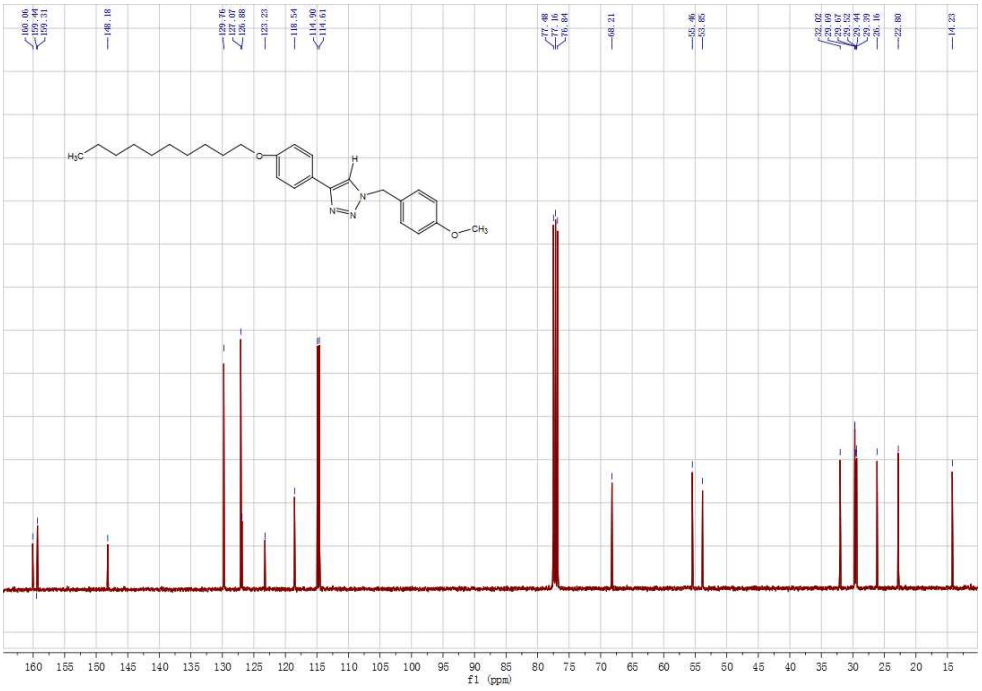

Fig. S10 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 293 K) of compound **5**

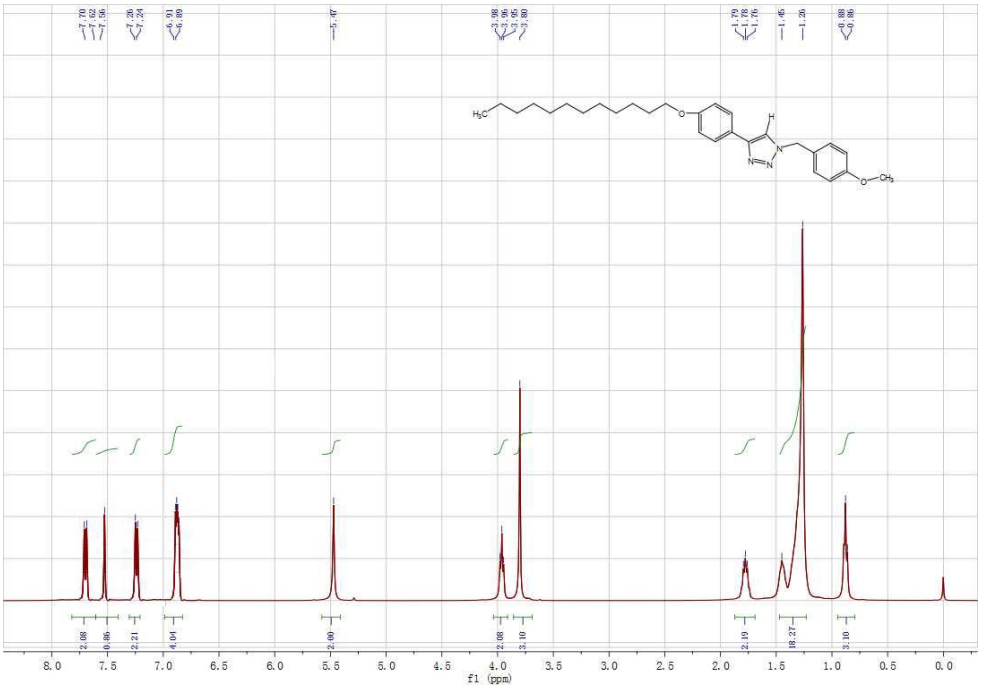

Fig. S11 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K) of compound **6**

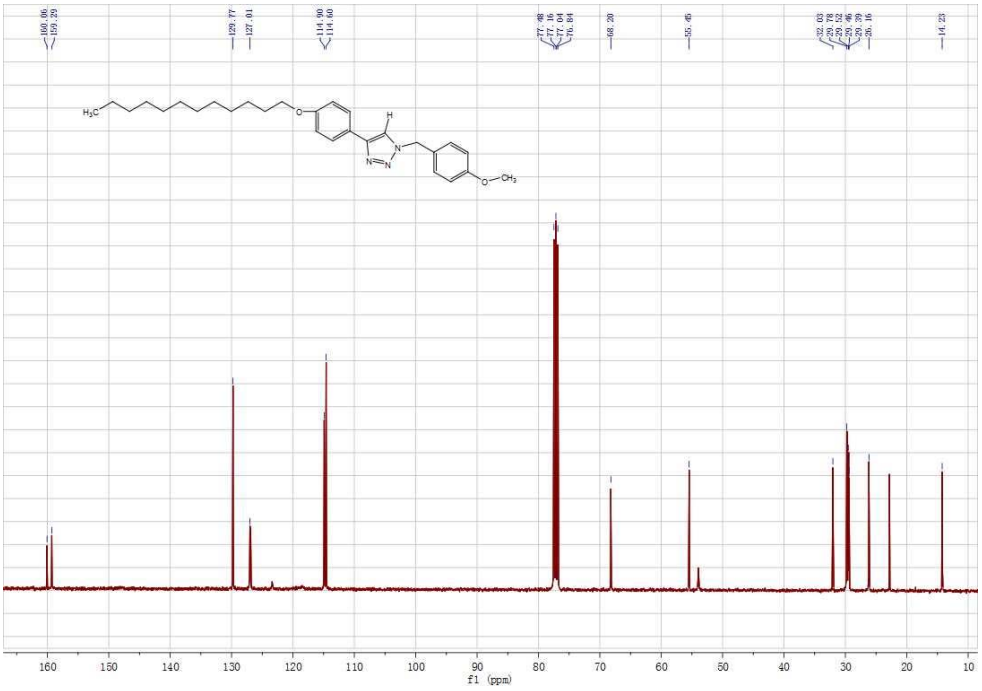

Fig. S12 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 293 K) of compound **6**