

Supporting information

Substituent and solvent effects on the fluorescent and photochromic properties of 2-(2-pyridyl) imidazole containing diarylethene derivatives

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1. Lippert-Mataga equations

$$\Delta\nu = \nu_{ab} - \nu_{fl} = \frac{2\Delta f(\mu_e - \mu_g)^2}{hca^3} + C \quad (1)$$

$$a = (3M/4N\pi d)^{1/3} \quad (2)$$

$$\Delta f = f - \frac{1}{2}f' = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{1}{2} \frac{n^2 - 1}{n^2 + 1} \quad (3)$$

Where, ν_{ab} and ν_{fl} are the wave numbers of the absorption and emission maxima, respectively, μ_e and μ_g is the excited state and ground state dipole moments of a solute, h is the Planck's constant, c is the velocity of light in vacuum, a (Å) is Onsager radius of solute, which can be derived from the Avogadro number N , molecular weight M , and density d of solute. C is a constant. The solvent polarity parameter Δf is a function of the dielectric constant ε and the refractive index n .¹

2. Absorption and fluorescence spectra

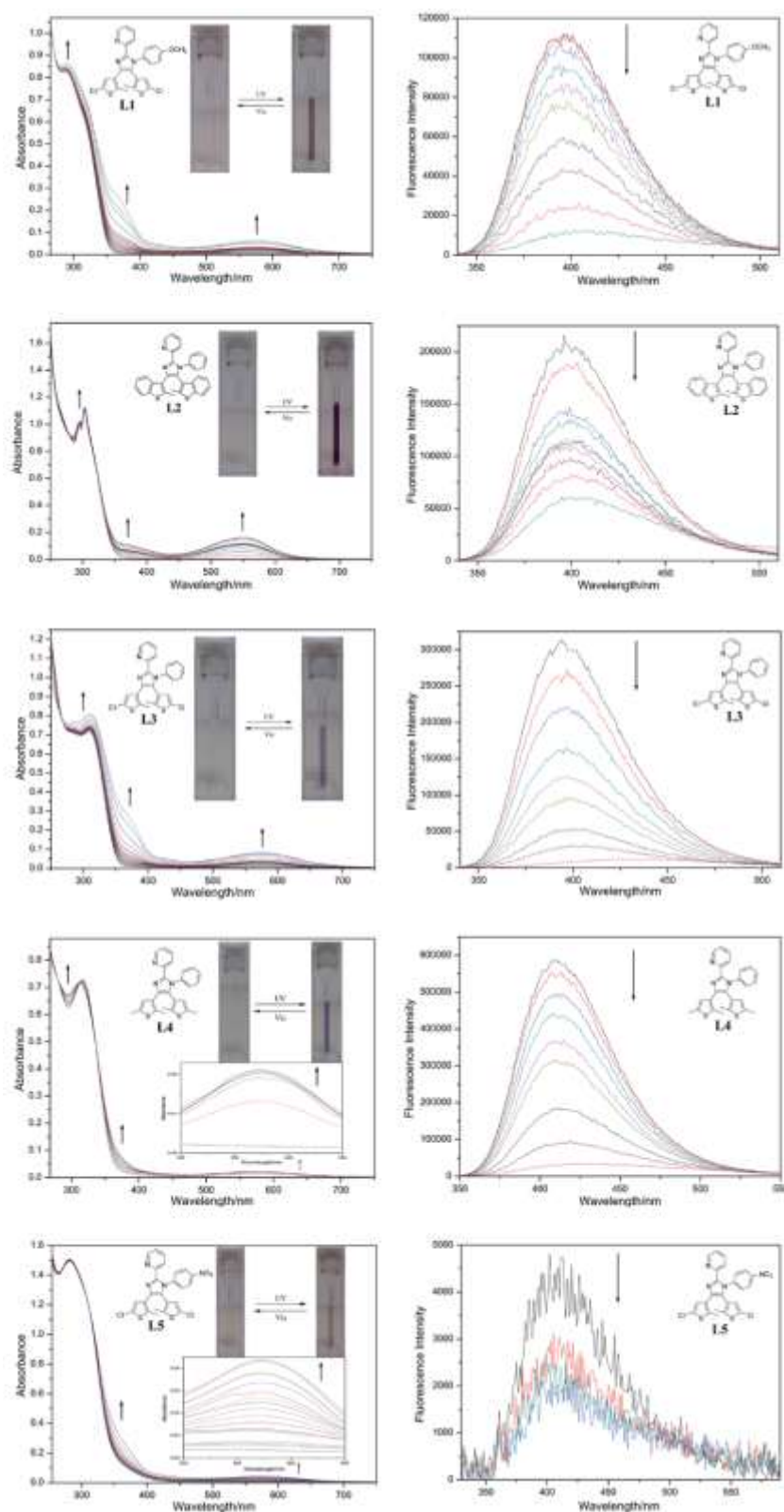


Figure S1. Absorption spectra (left, the insets show the reversible color changes between the open forms and photostationary states) and emission spectra ($\lambda_{\text{ex}} = 325$ nm, right) of **L1–L5** (5×10^{-5} mol/L) in CH_2Cl_2 upon irradiation with UV light.

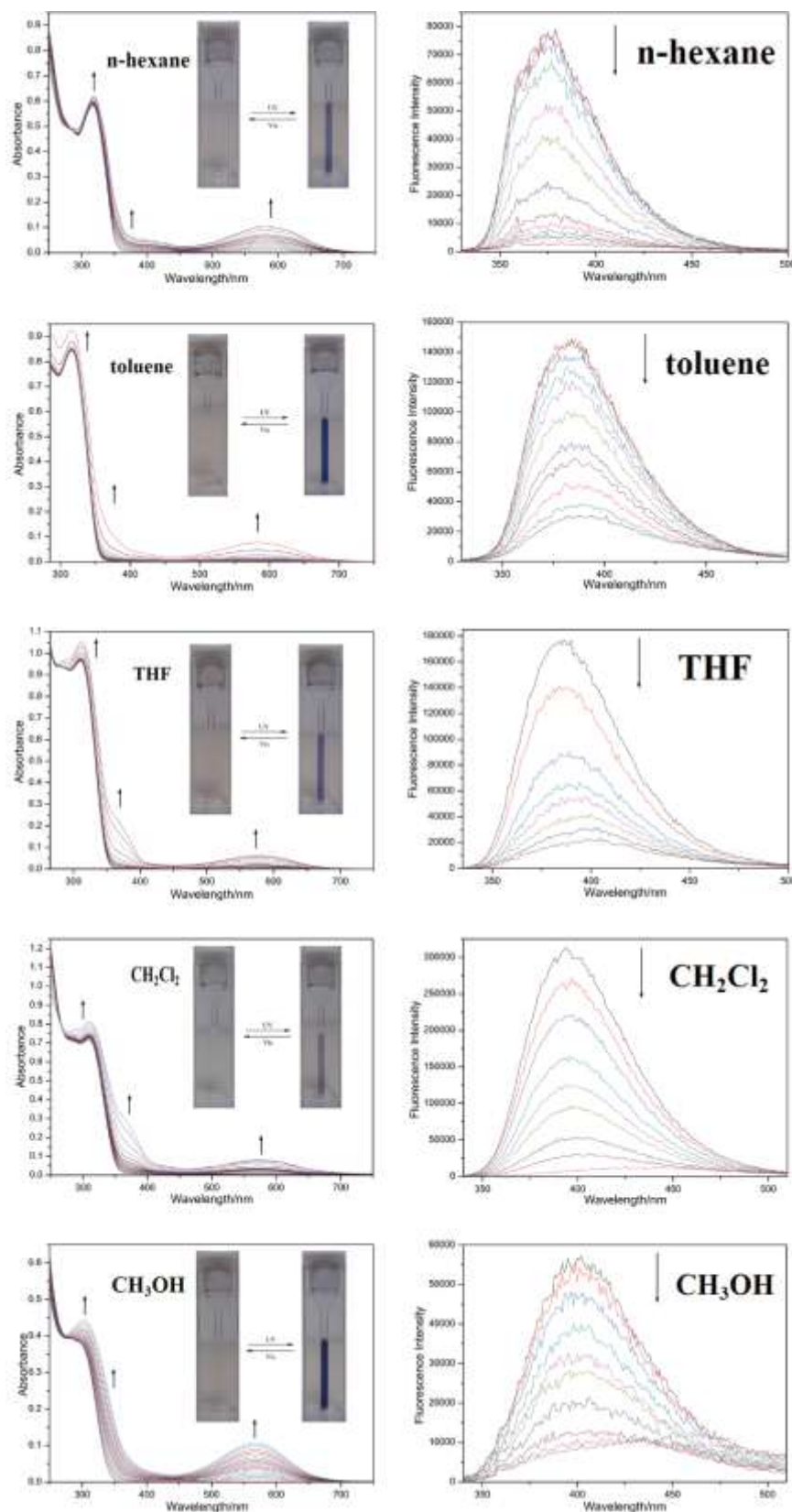


Figure S2. Absorption spectra (left, the insets show the reversible color changes between the open forms and photostationary states) and emission spectra ($\lambda_{\text{ex}} = 325$ nm, right) of **L3** (5×10^{-5} mol/L) in various solutions upon irradiation with UV light.

3. Fatigue resistance

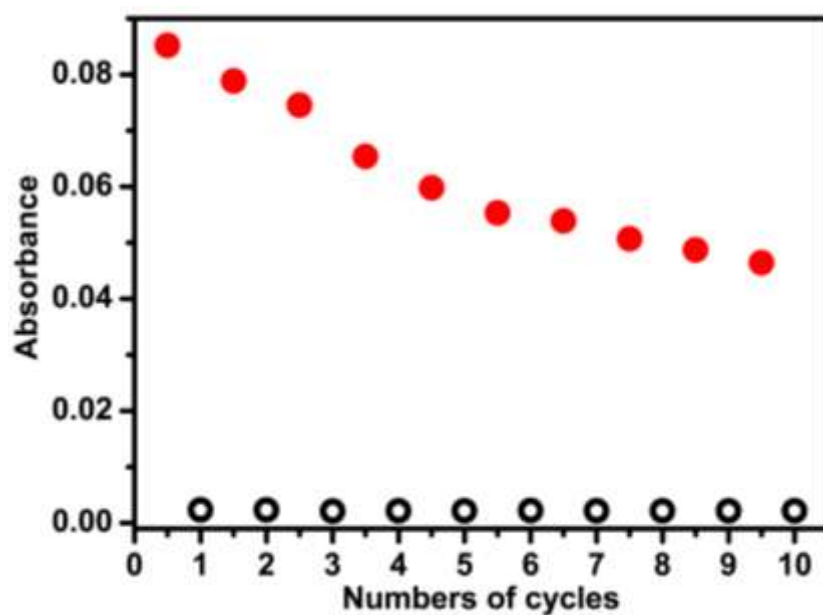


Figure S3. Fatigue resistance of **L3** (5×10^{-5} mol/L) was tested in degassed CH_2Cl_2 by alternatively irradiating with the UV ($\lambda = 302$ nm) and the visible light ($\lambda = 520$ nm) (open (○) and closed (●) form), monitored by the absorbance at 572 nm.

4. Solvent effect

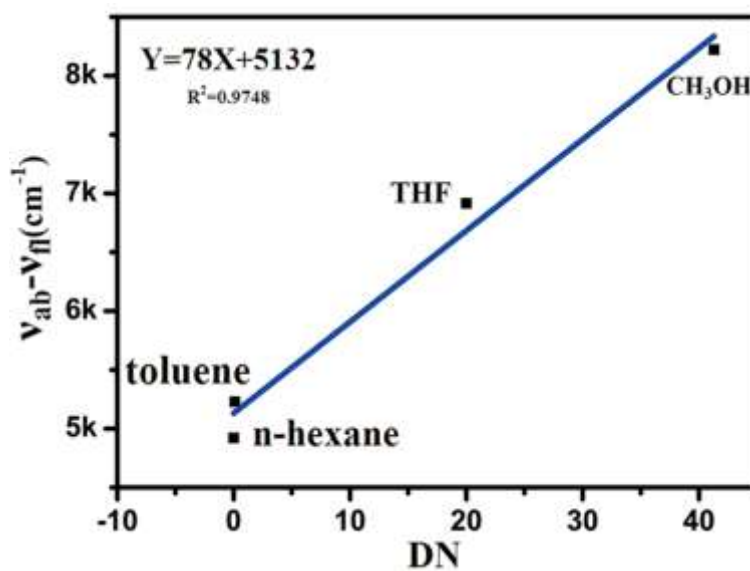


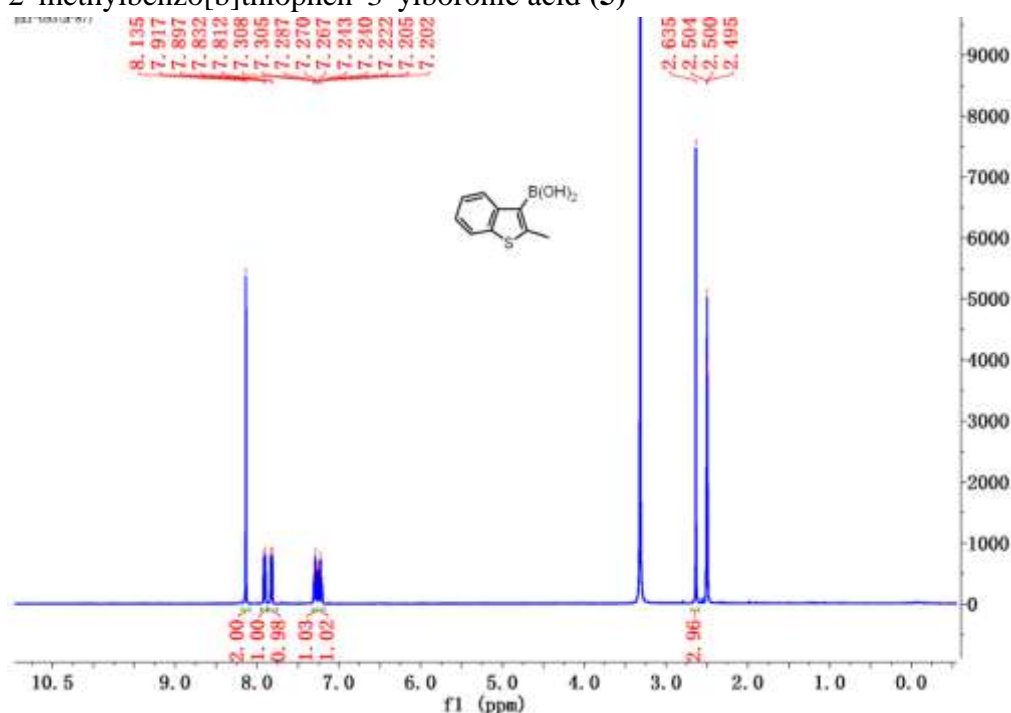
Figure S4. Linear relationship between the Stokes shift ($\Delta\nu$) values of **L3** in various solvents and the DN.

5.Reference

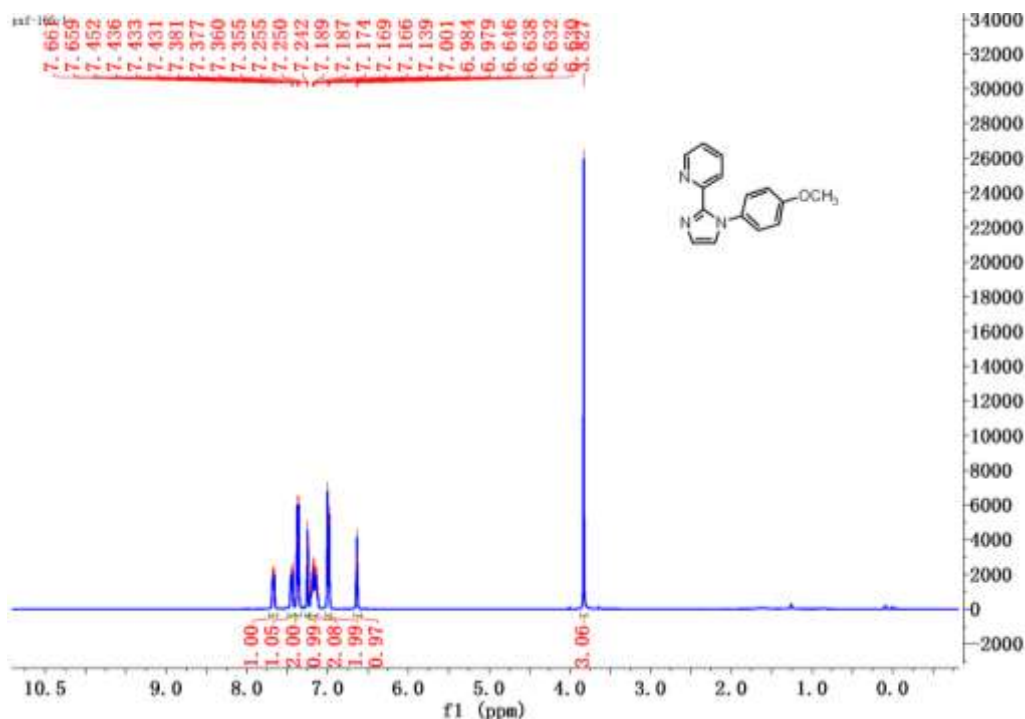
1. Reichardt, C.; Welton, T., *Solvents and Solvent Effects in Organic Chemistry 4rd Edition*. WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim: Germany, 2011.

6.Copies of ^1H NMR

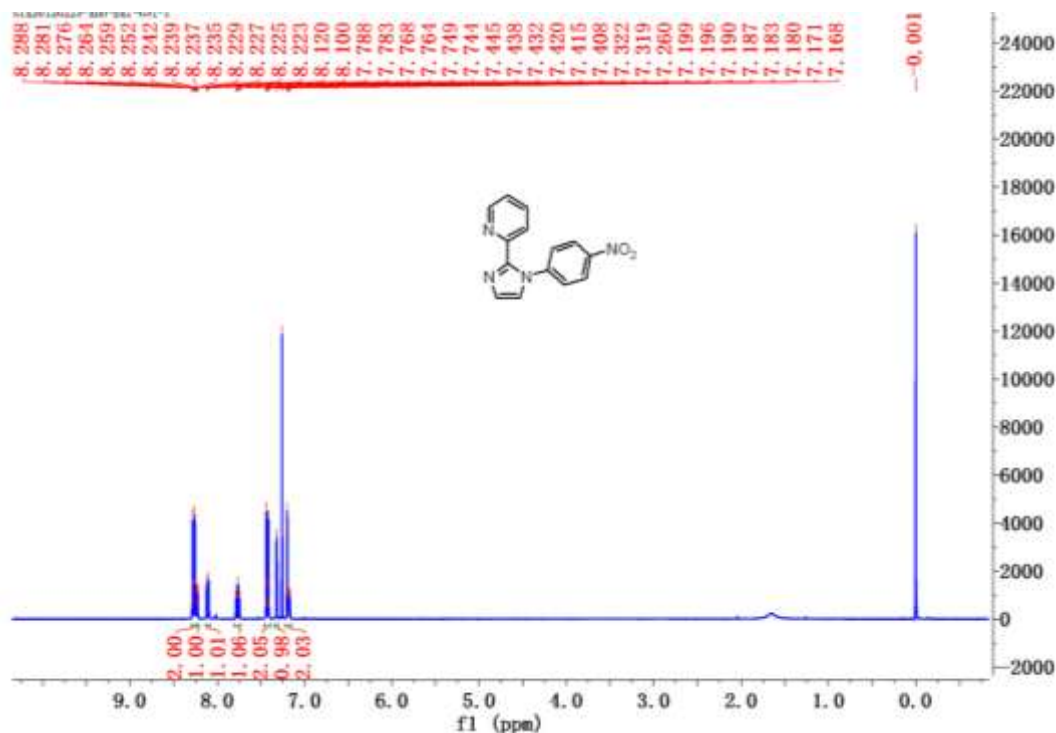
(1) 2-methylbenzo[b]thiophen-3-ylboronic acid (**5**)



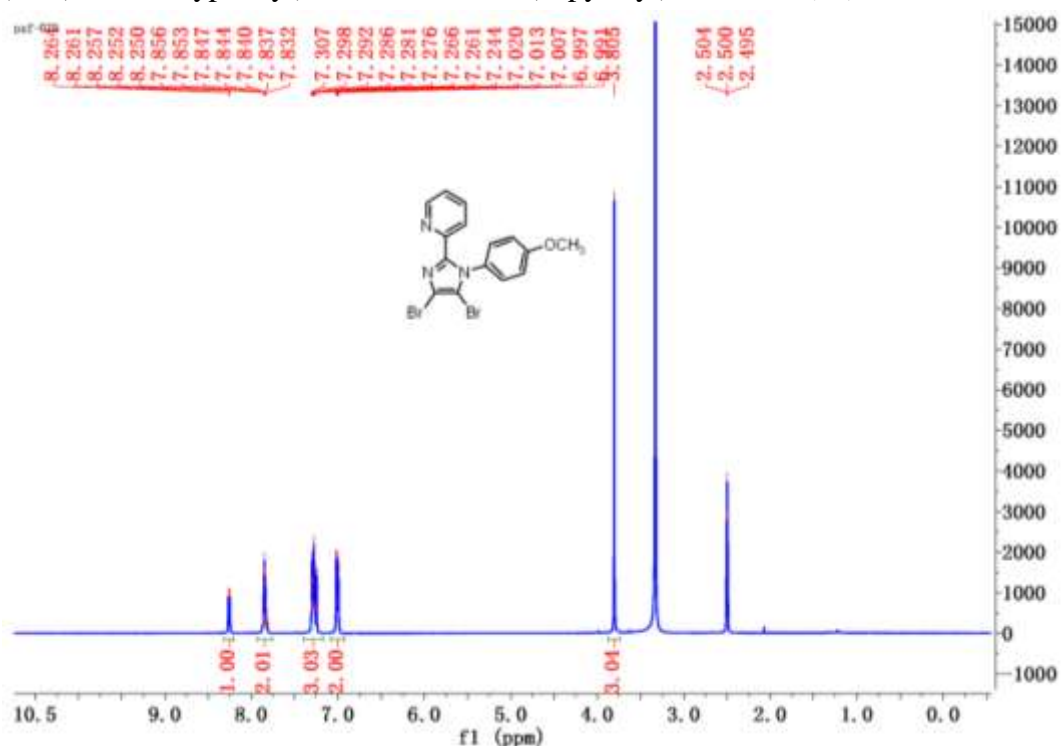
(2) 1-(4-methoxyphenyl)-2-(2-pyridyl)imidazole (**9**)



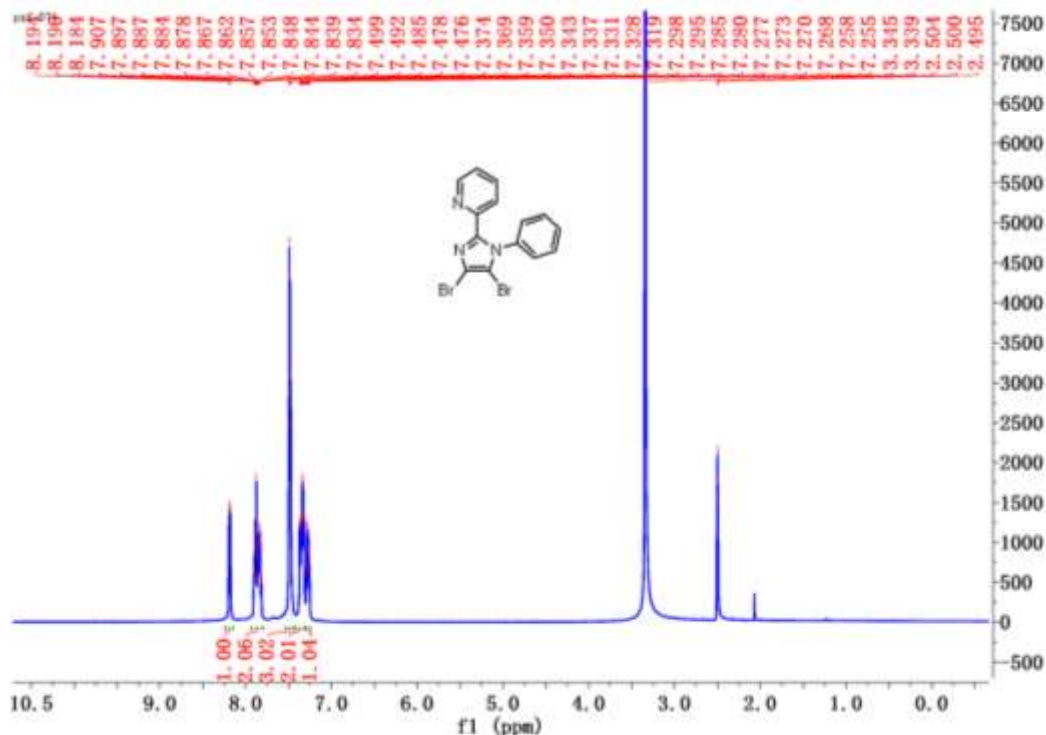
(3) 1-(4-nitrophenyl)-2-(2-pyridyl)imidazole (**11**)



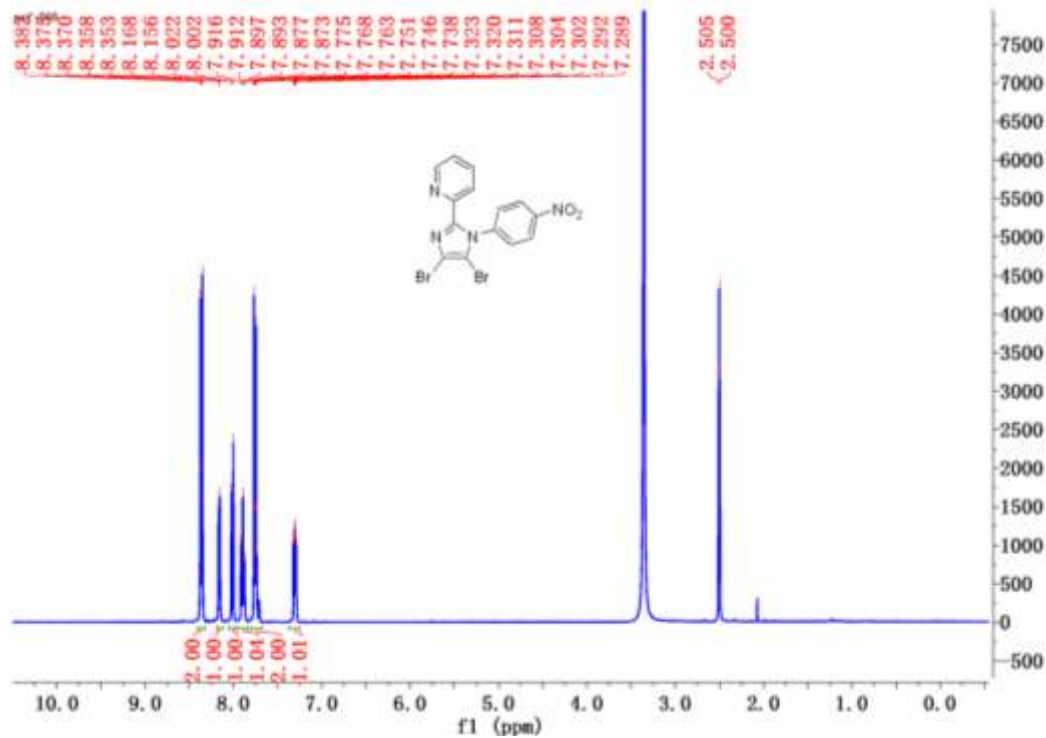
(4) 1-(4-methoxyphenyl)-4,5-dibromo-2-(2-pyridyl)imidazole (**12**)



(5) 1-phenyl-4,5-dibromo-2-(2-pyridyl)imidazole (**13**)

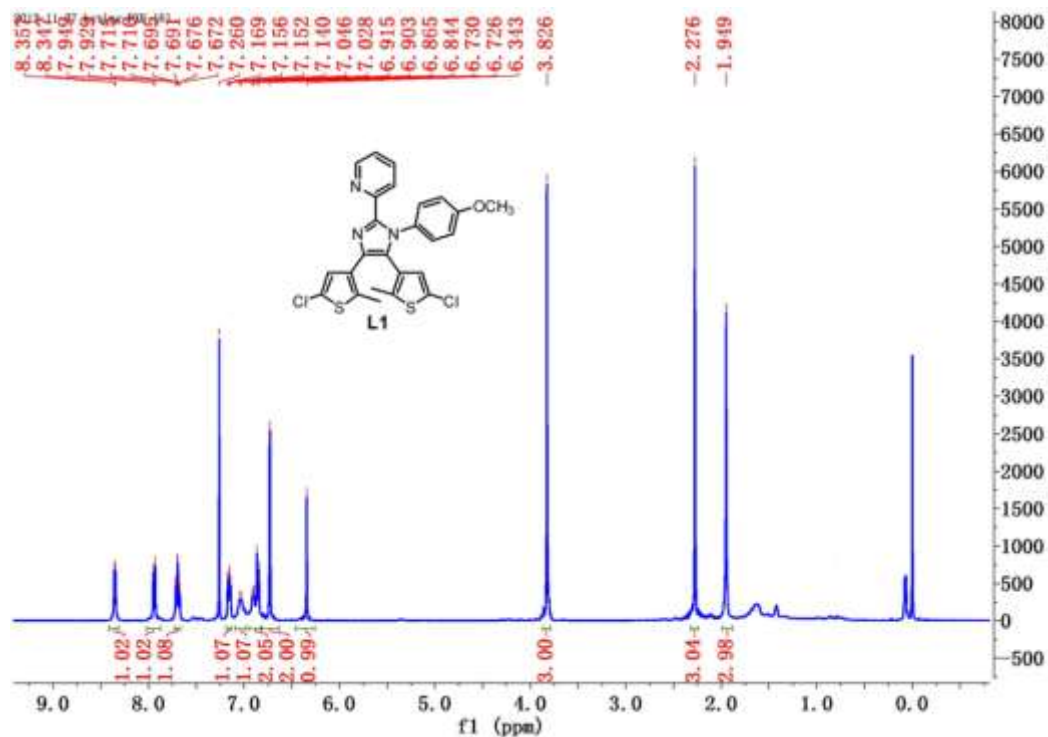


(6) 1-(4-nitrophenyl)-4,5-dibromo-2-(2-pyridyl)imidazole (**14**)

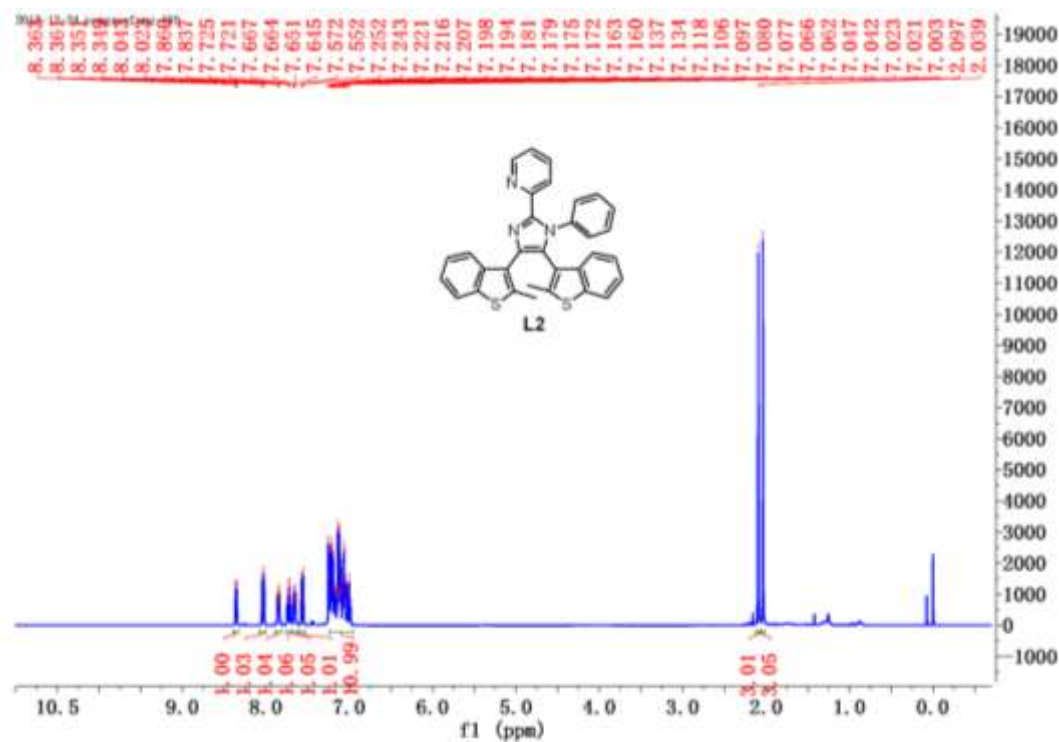


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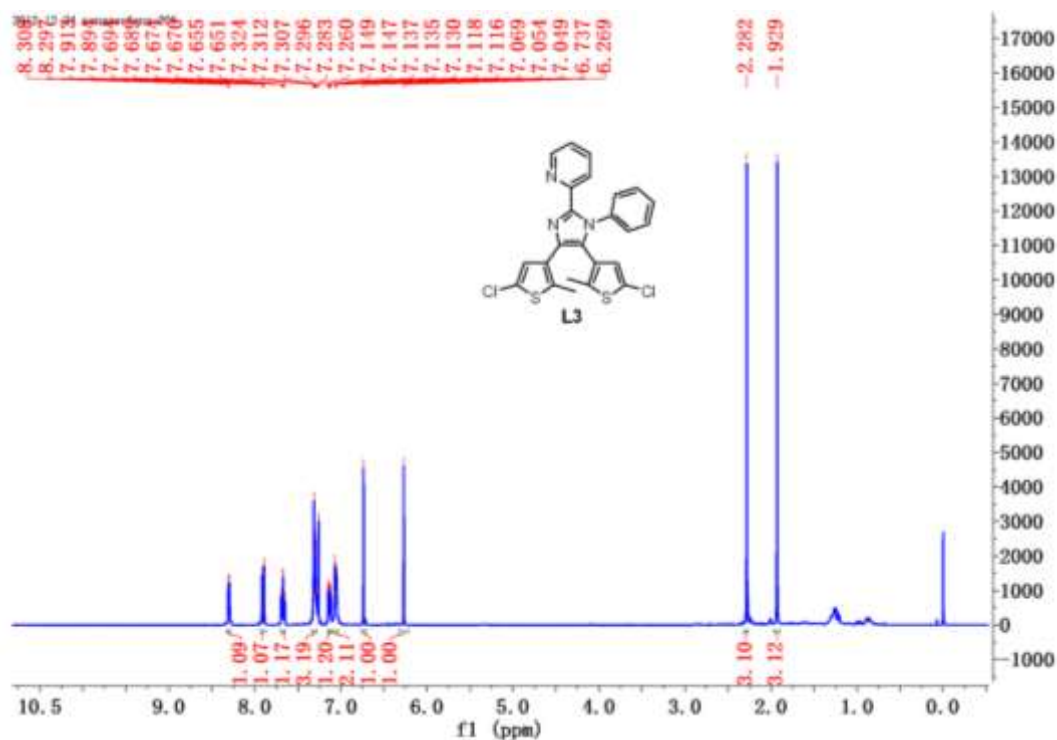
1-(4-methoxyphenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (**L1**)



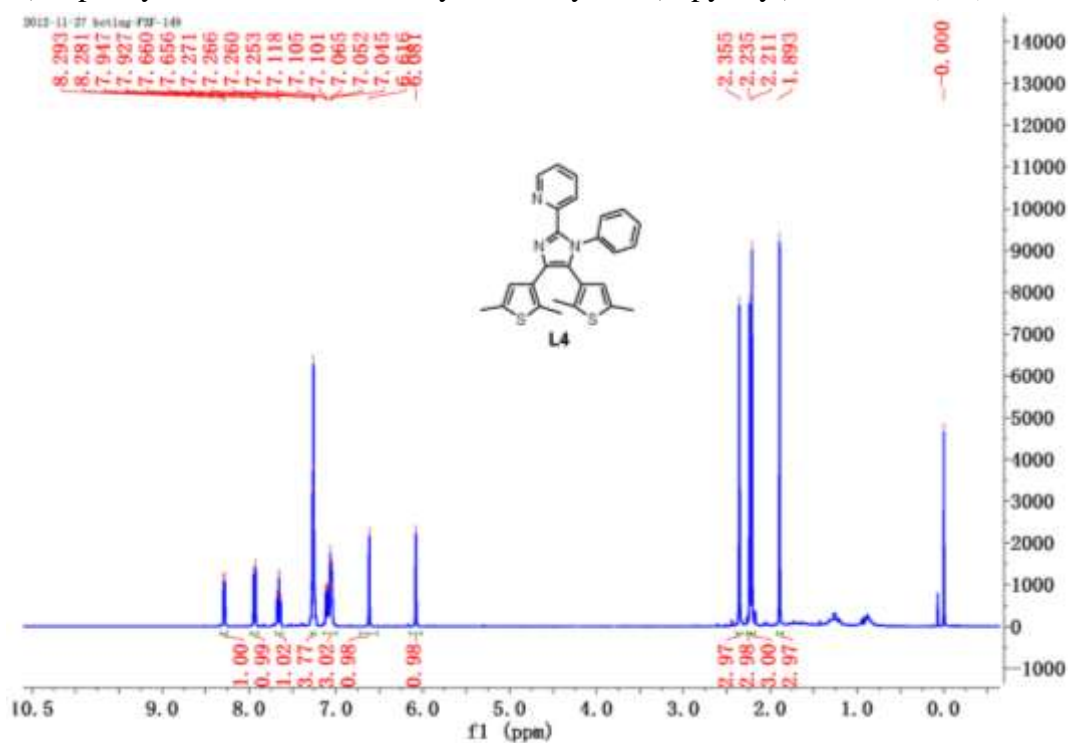
(8) 1-phenyl-4,5-bis-[2-methylbenzo[b]thiophen-3-yl]-2-(2-pyridyl)imidazole (**L2**)



(9) 1-phenyl-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (**L3**)



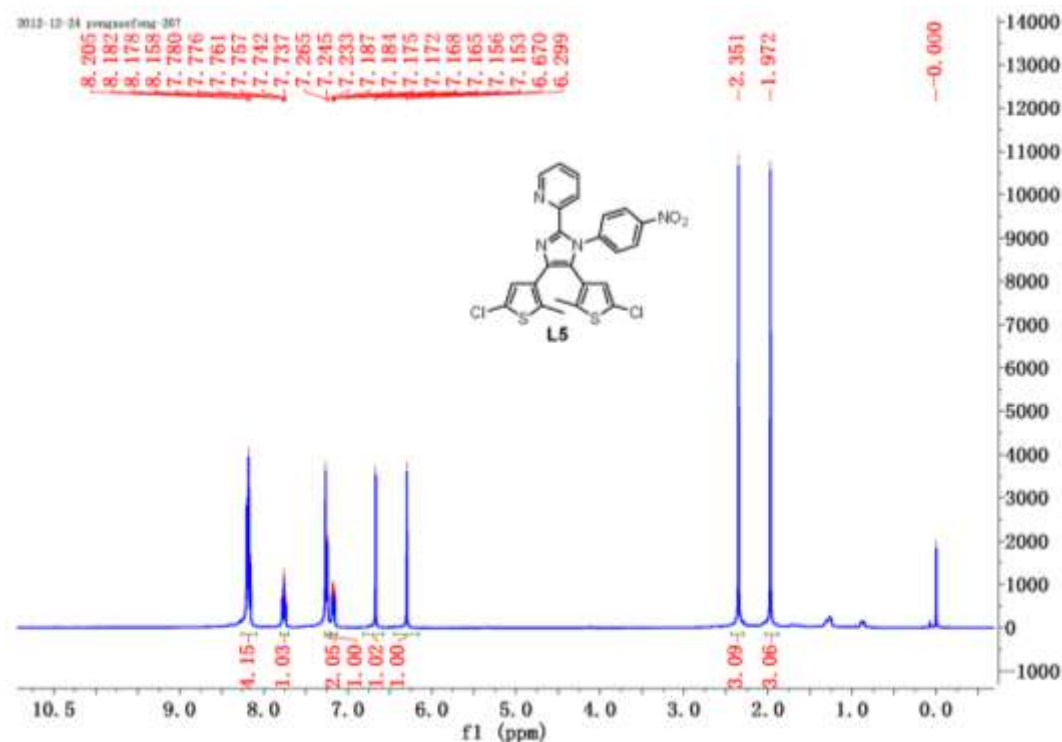
(10) 1-phenyl-4,5-bis-[2,5-dimethyl-3-thienyl]-2-(2-pyridyl)imidazole (**L4**)



(11)

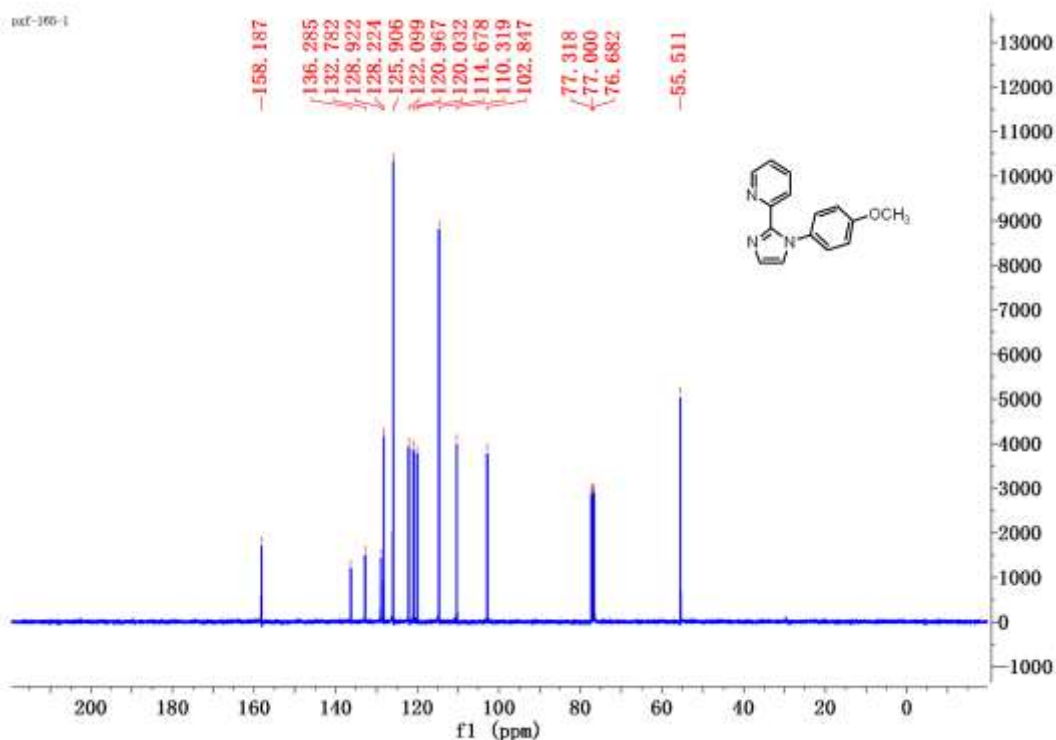
1-(4-nitrophenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole

(L5)

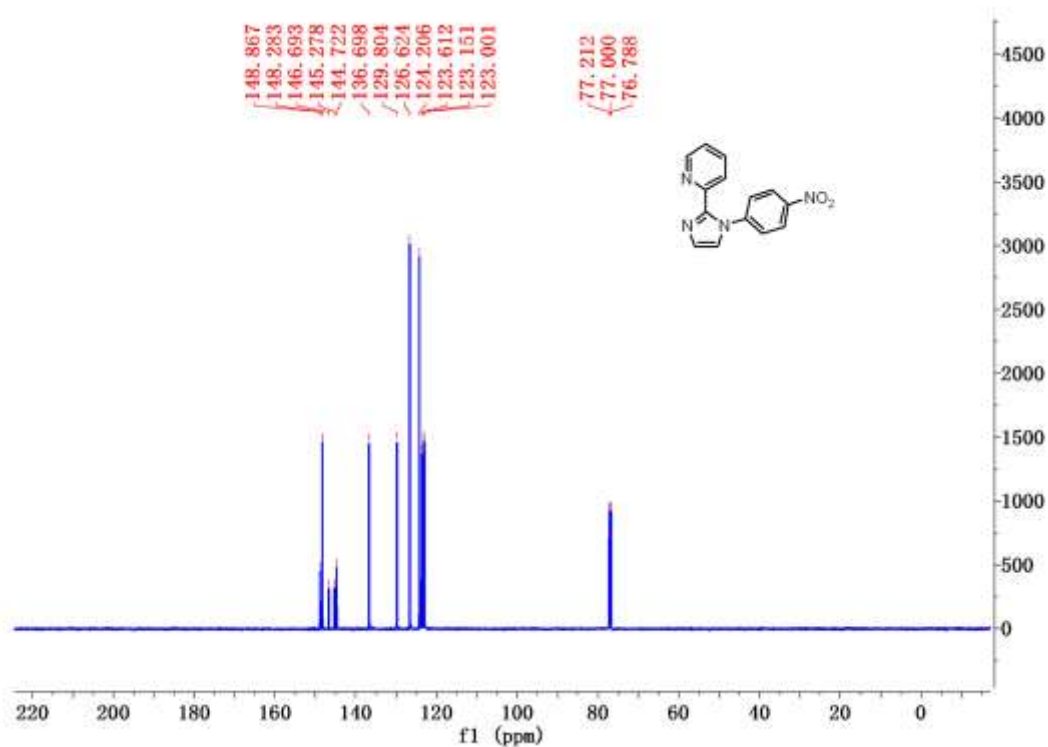


7. Copies of ¹³C NMR

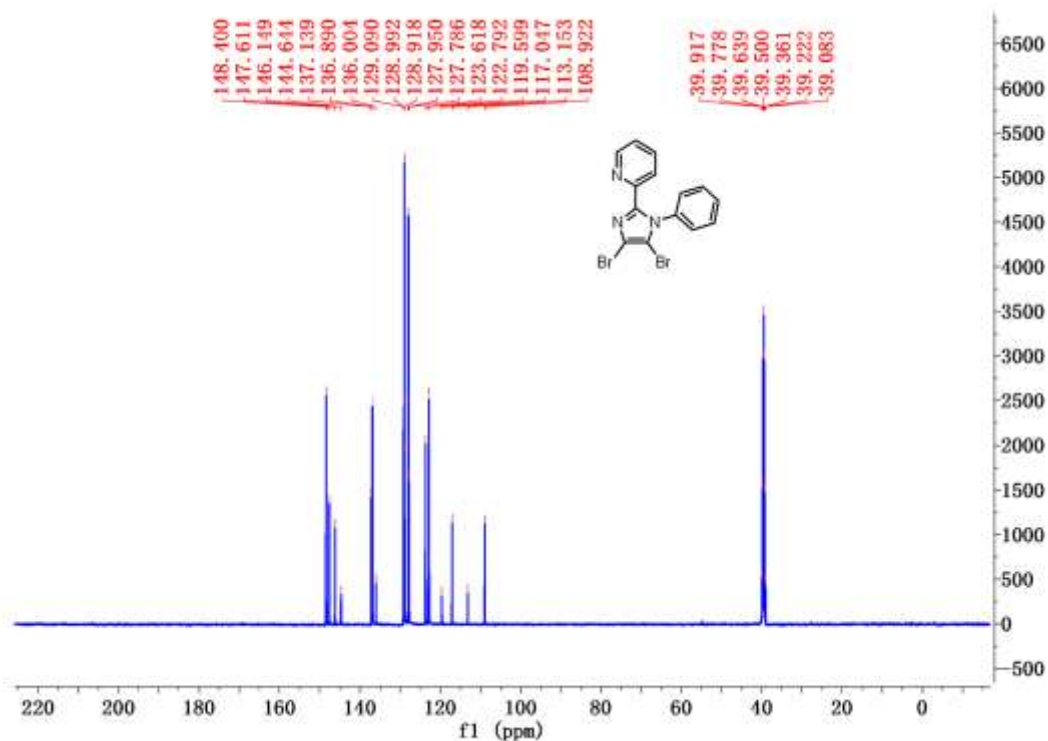
(1) 1-(4-methoxyphenyl)-2-(2-pyridyl)imidazole (9)



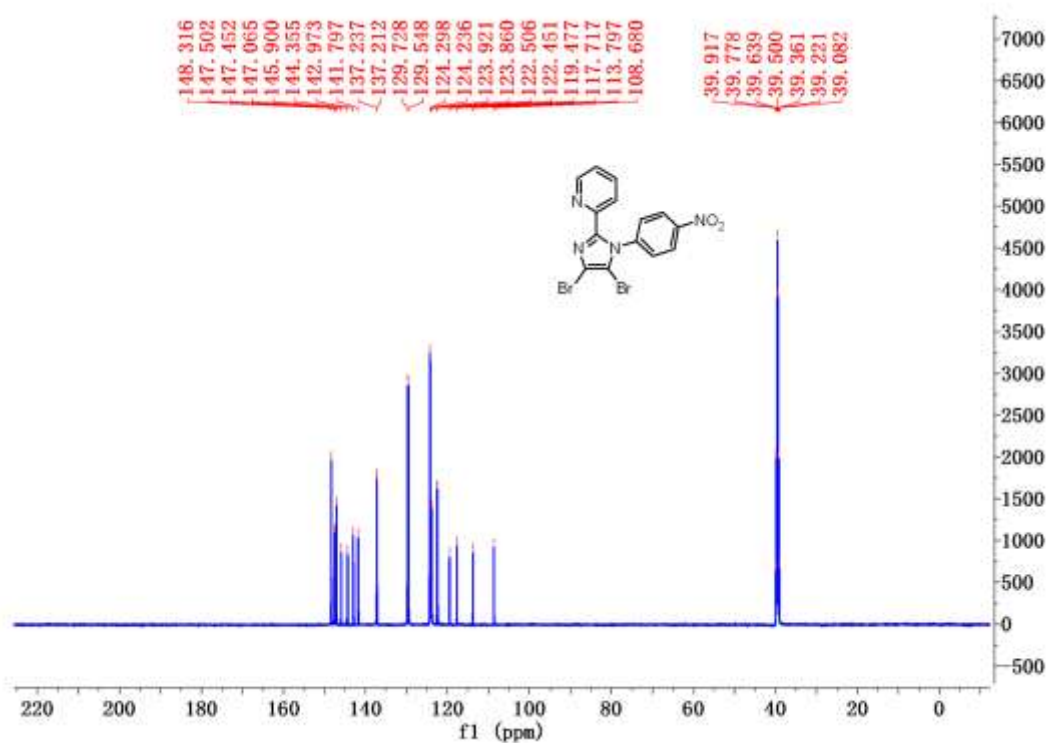
(2) 1-(4-nitrophenyl)-2-(2-pyridyl)imidazole (**11**)



(3) 1-phenyl-4,5-dibromo-2-(2-pyridyl)imidazole (**13**)

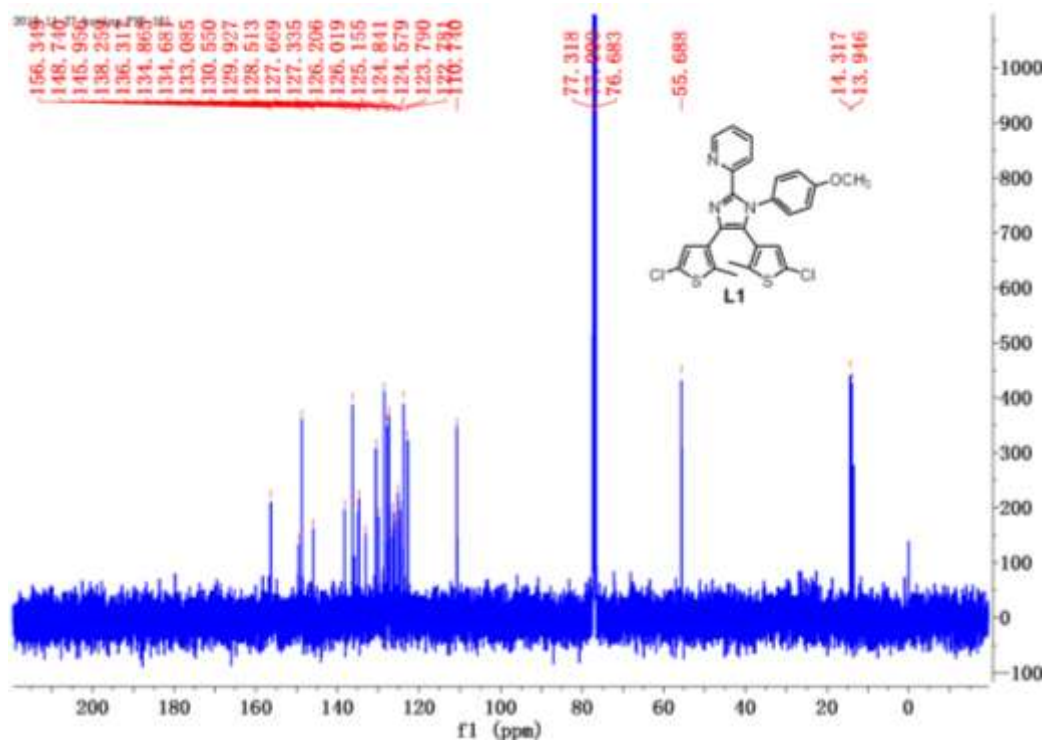


(4) 1-(4-nitrophenyl)-4,5-dibromo-2-(2-pyridyl)imidazole (**14**)

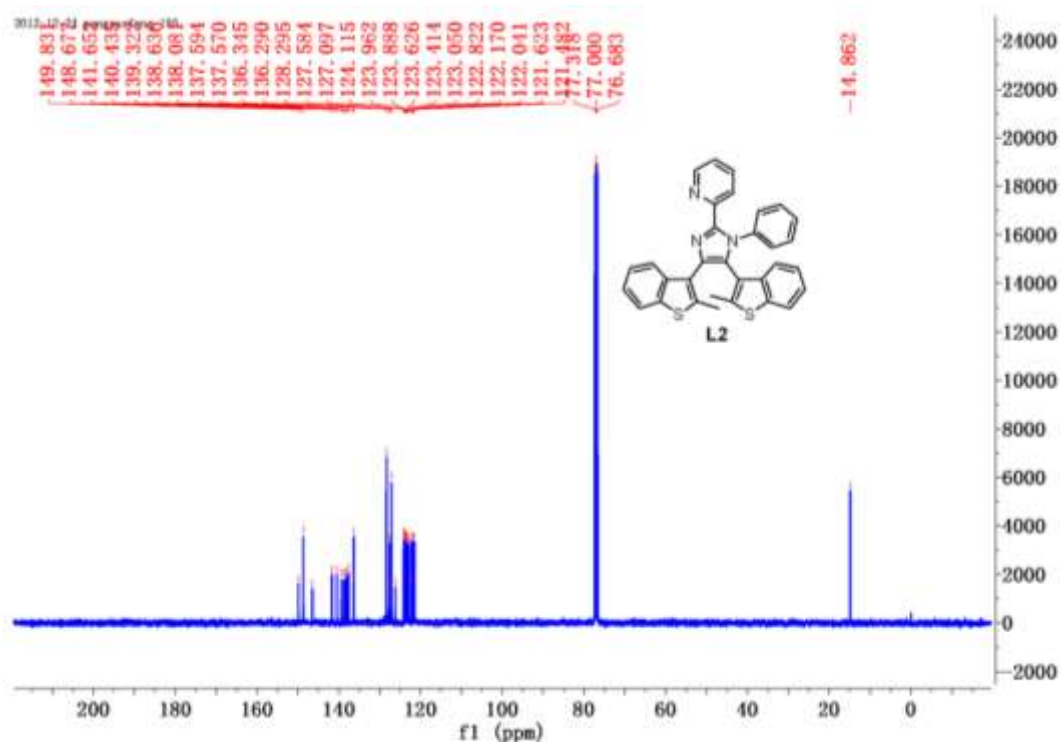


(5)

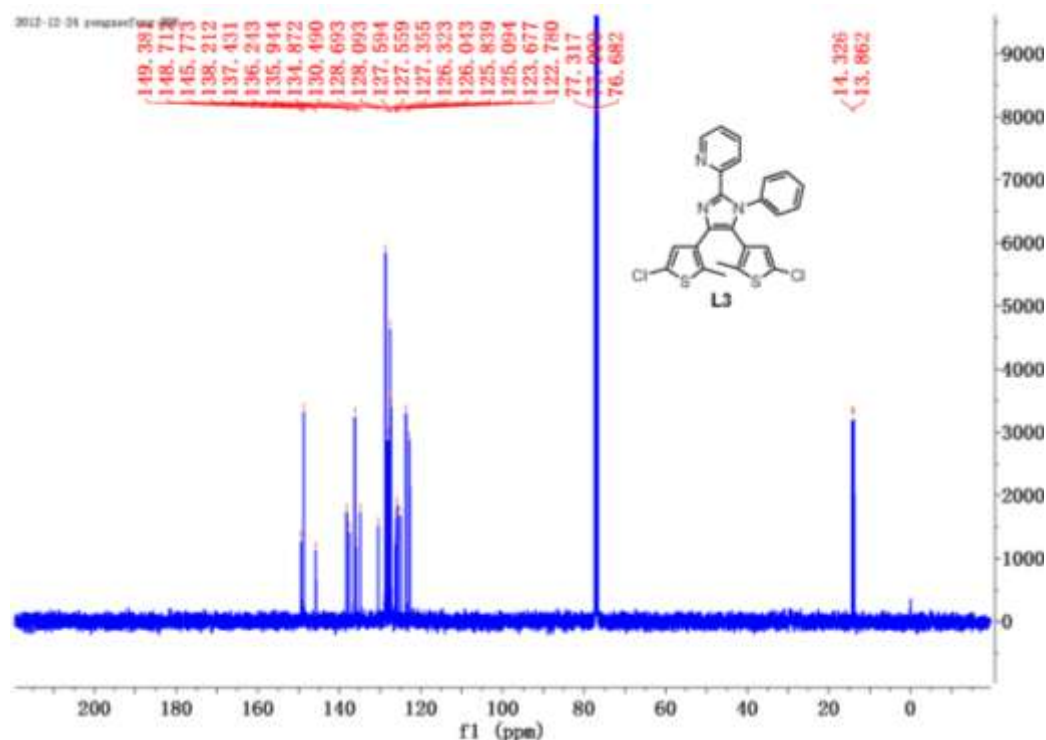
1-(4-methoxyphenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (**L1**)



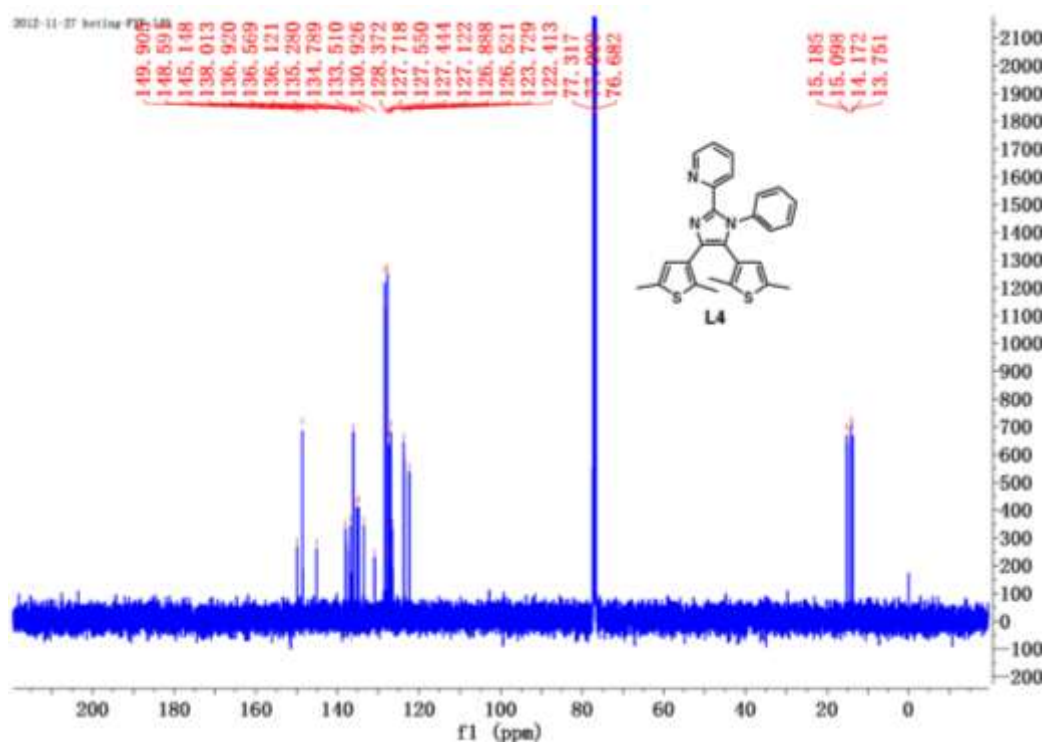
(6) 1-phenyl-4,5-bis-[2-methylbenzo[b]thiophen-3-yl]-2-(2-pyridyl)imidazole (**L2**)



(7) 1-phenyl-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (**L3**)



(8) 1-phenyl-4,5-bis-[2,5-dimethyl-3-thienyl]-2-(2-pyridyl)imidazole (**L4**)



(9) 1-(4-nitrophenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (**L5**)

