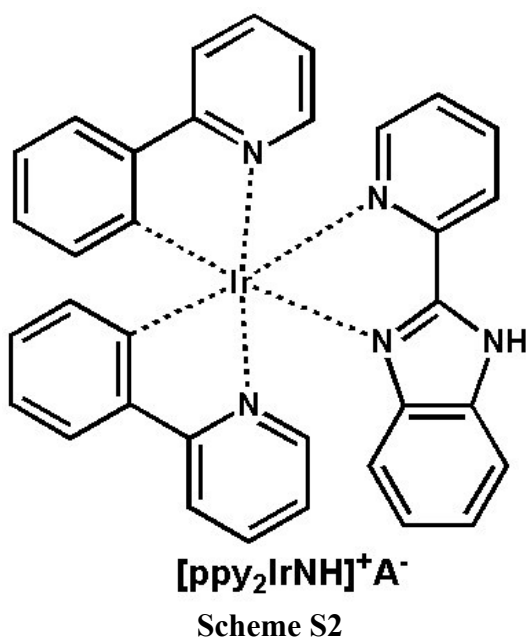
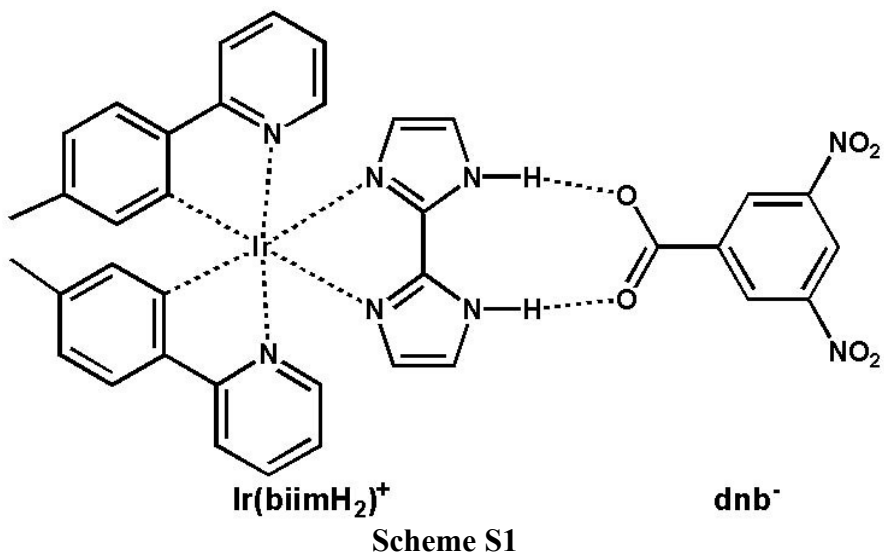
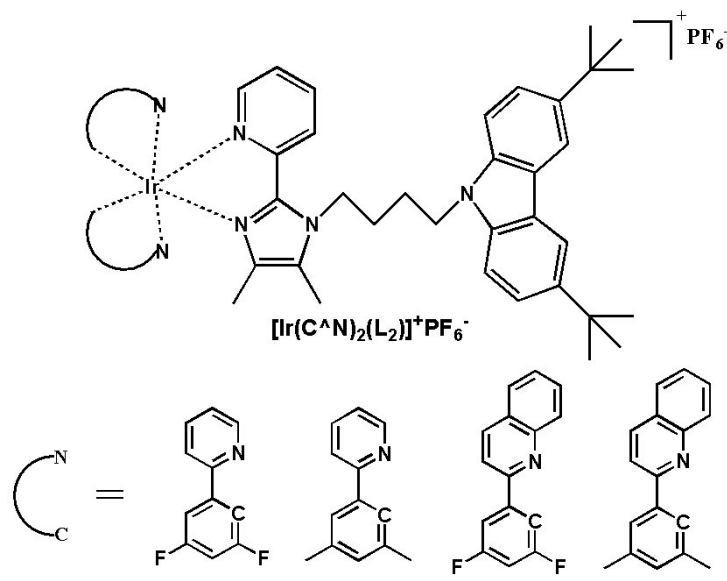
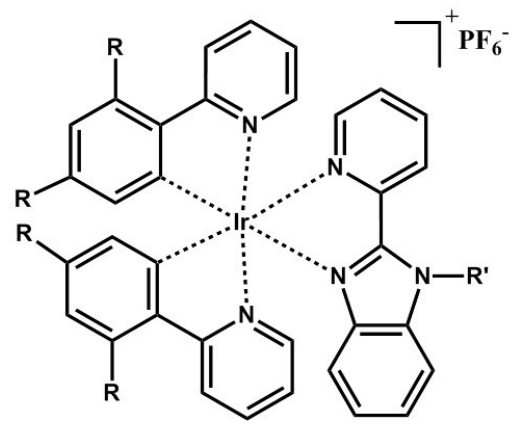


Supporting Information

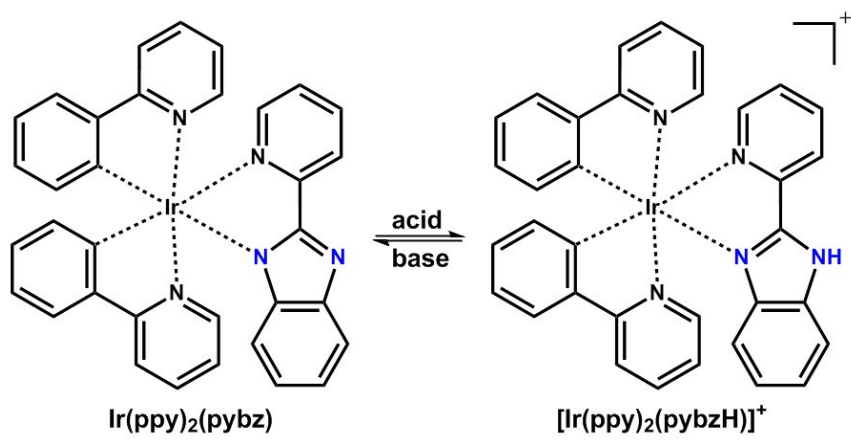




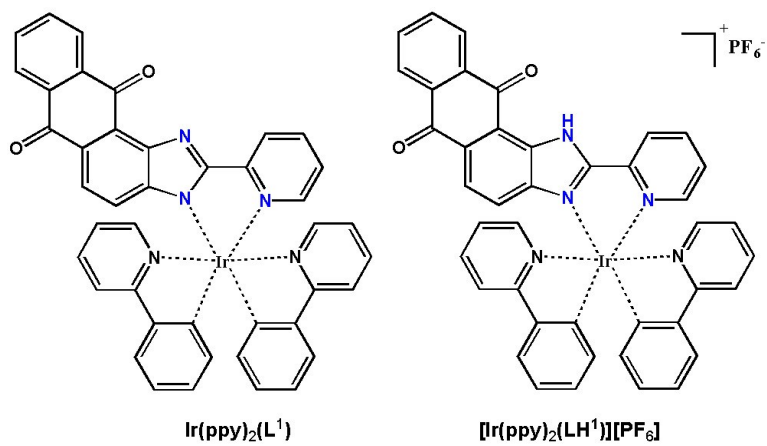
Scheme S3



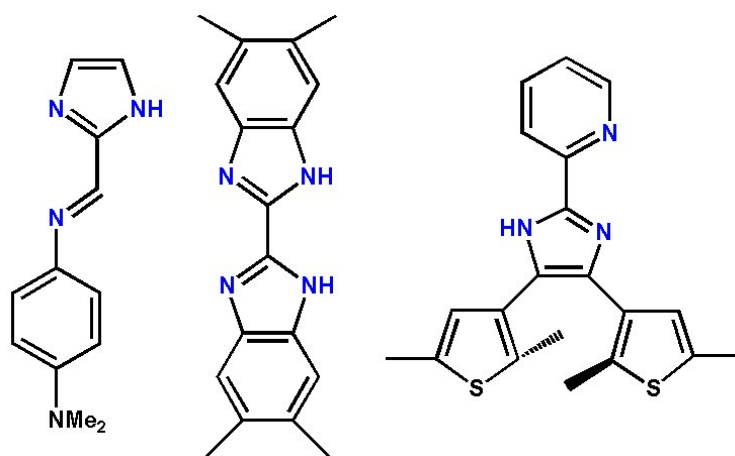
Scheme S4



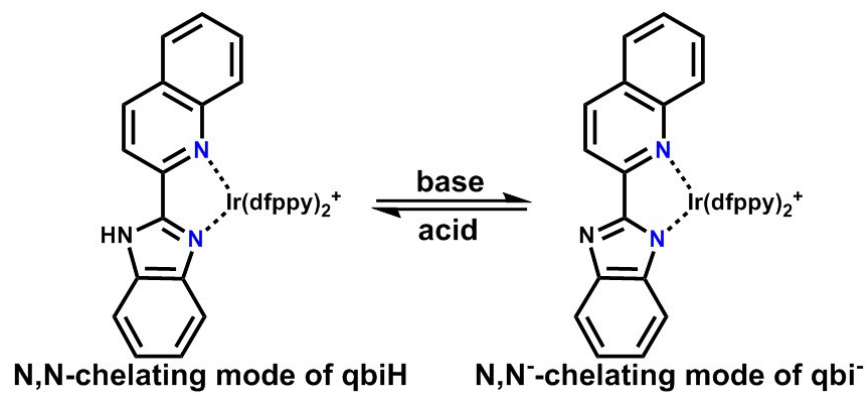
Scheme S5



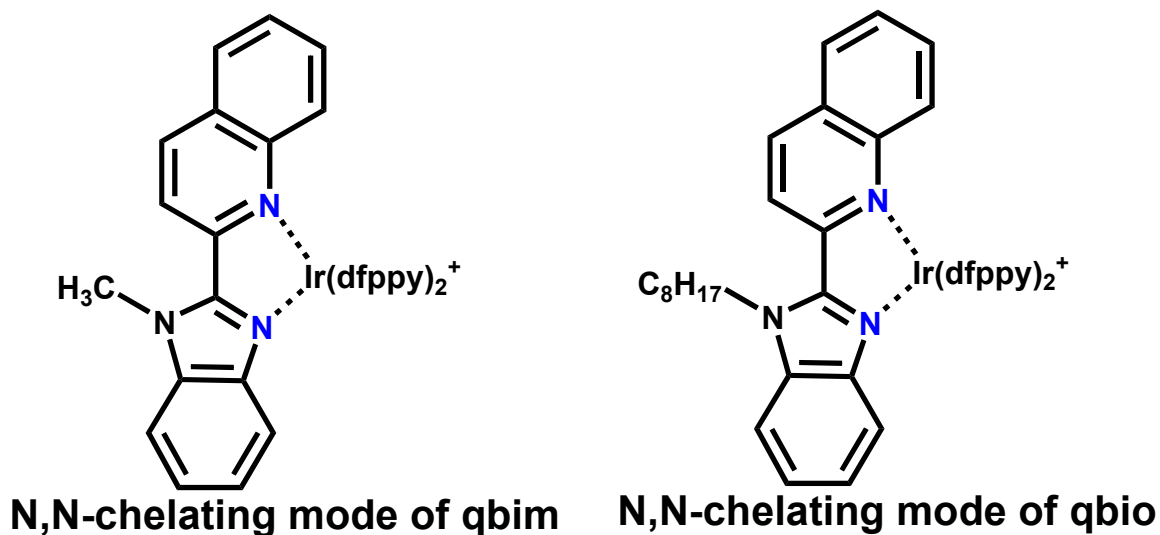
Scheme S6



Scheme S7



Scheme S8



Scheme S9

Table S1 UV-vis absorption bands of qbiH, qbim, qbio and compounds **1-4** in CH₂Cl₂ at room temperature.

Compound	absorption band (nm)
qbiH	245, 286, 336-350
qbim	243, 284, 336-348
qbio	243, 285, 336-348
1	251, 299, 362, a tail to 430
2	252, 302, 365, a tail to 430
3	252, 302, 365, a tail to 430
4	245, 298, 386, a tail to 454

Table S2 Emission data of qbiH, qbim, qbio and **1-4** in CH₂Cl₂ at room temperature.

Compound	emission wavelength (nm) at room temperature	quantum yield in CH ₂ Cl ₂	luminescence lifetimes (ns)
qbiH	389	-	-
qbim	386	-	-
qbio	386	-	-
1	558, 585	14%	1018
2	572, 600	16%	956
3	573, 600	18%	1002
4	546	3.2%	377

Table S3 Emission data of **1-4** C₂H₅OH-CH₃OH (v/v = 3/1) at 77 K.

Compound	emission wavelength (nm) at 77 K
1	528, 570
2	536, 578
3	537, 579
4	523, 563

Table S4 Emission data of the solid-state samples of **1-4** at room temperature ($\lambda_{\text{ex}} = 370$ nm for **1** and **4**, and $\lambda_{\text{ex}} = 380$ nm for **2** and **3**).

Compound	emission wavelength (nm)
1	542, 572, 611
2	553, 581, 612
3	544, 578, 630
4	595, 633

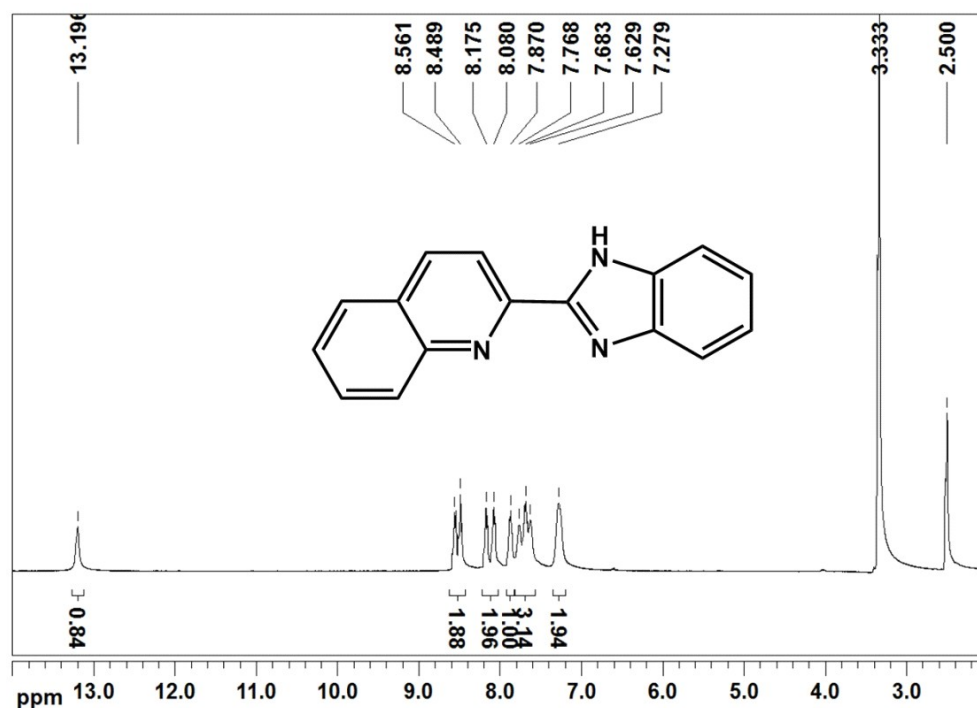


Fig. S1 ¹H NMR spectrum of qbiH (500 MHz, DMSO-*d*₆).

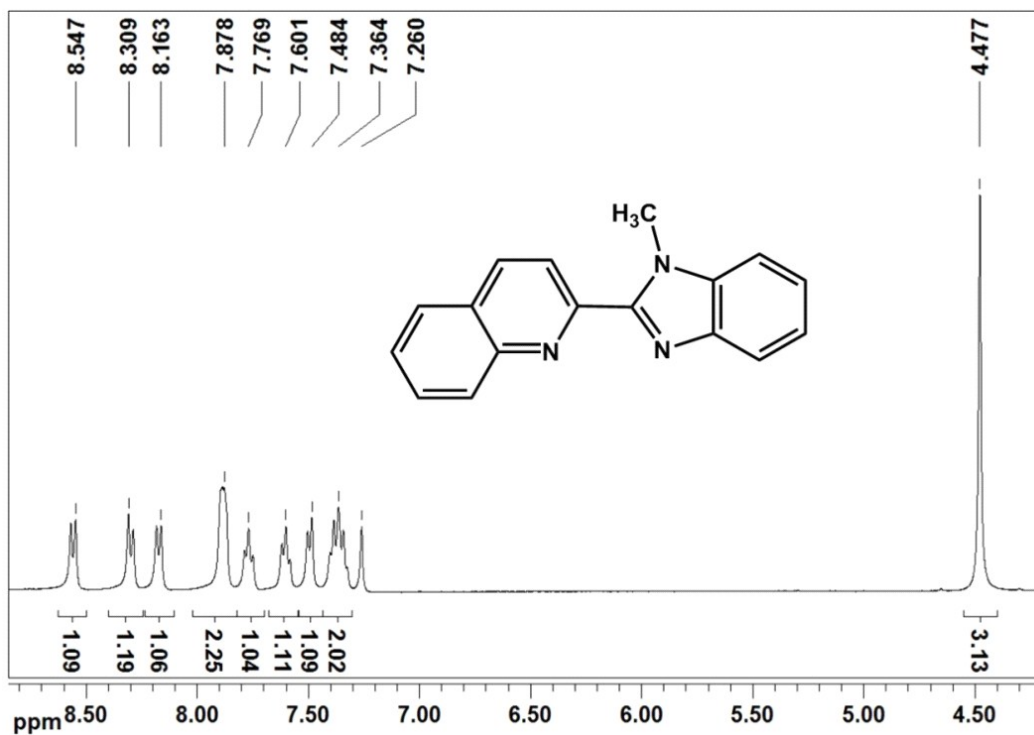


Fig. S2 ^1H NMR spectrum of qbim (300 MHz, CDCl_3).

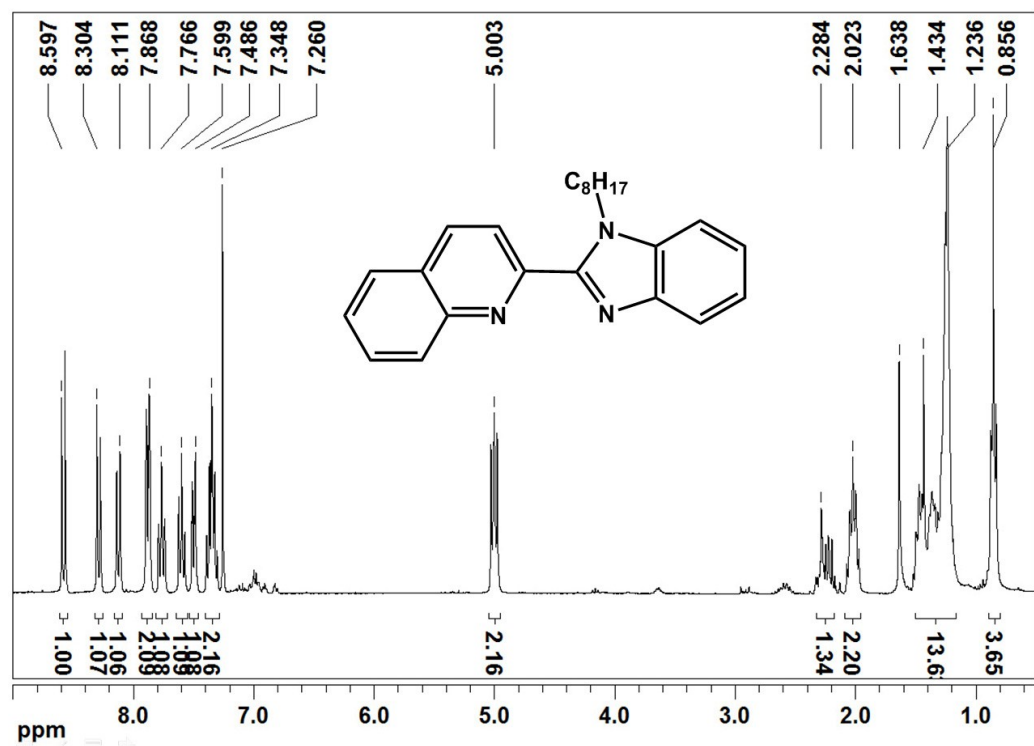


Fig. S3 ^1H NMR spectrum of qbio (300 MHz, CDCl_3).

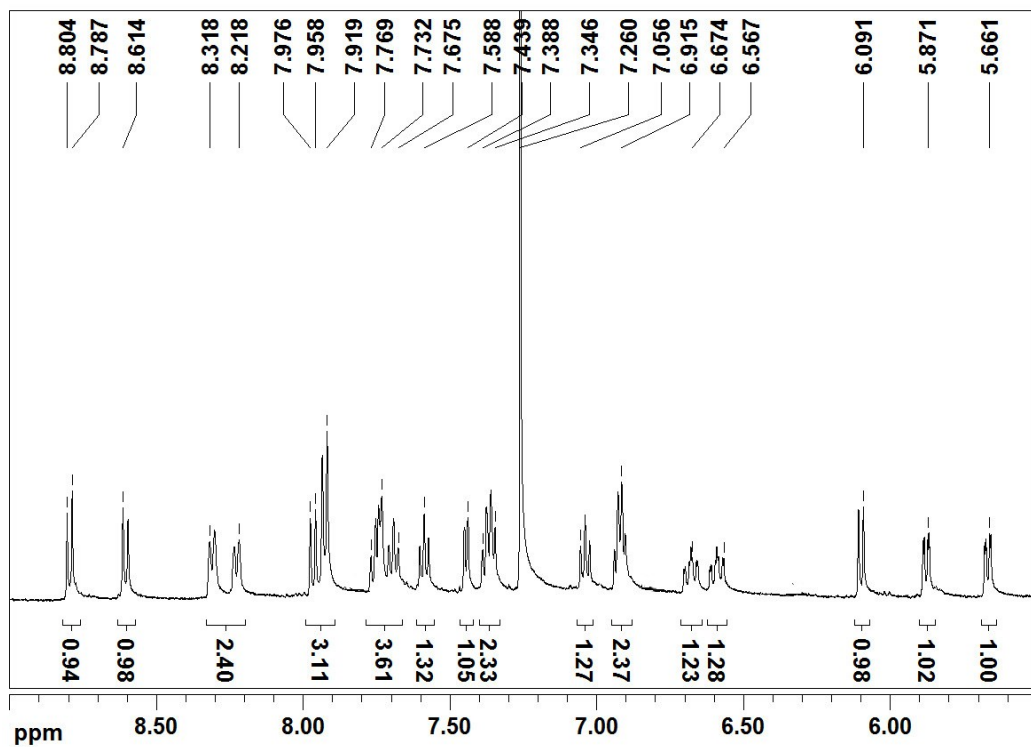


Fig. S4 ^1H NMR spectrum of **1** (500 MHz, CDCl_3).

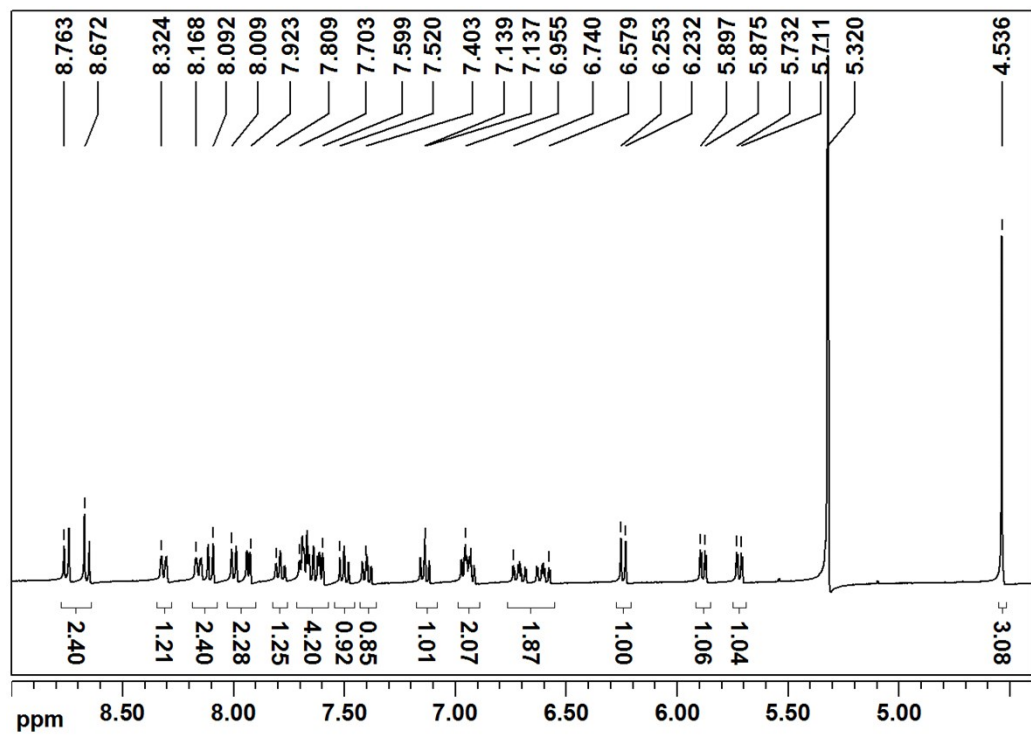


Fig. S5 ^1H NMR spectrum of **2** (300 MHz, CD_2Cl_2).

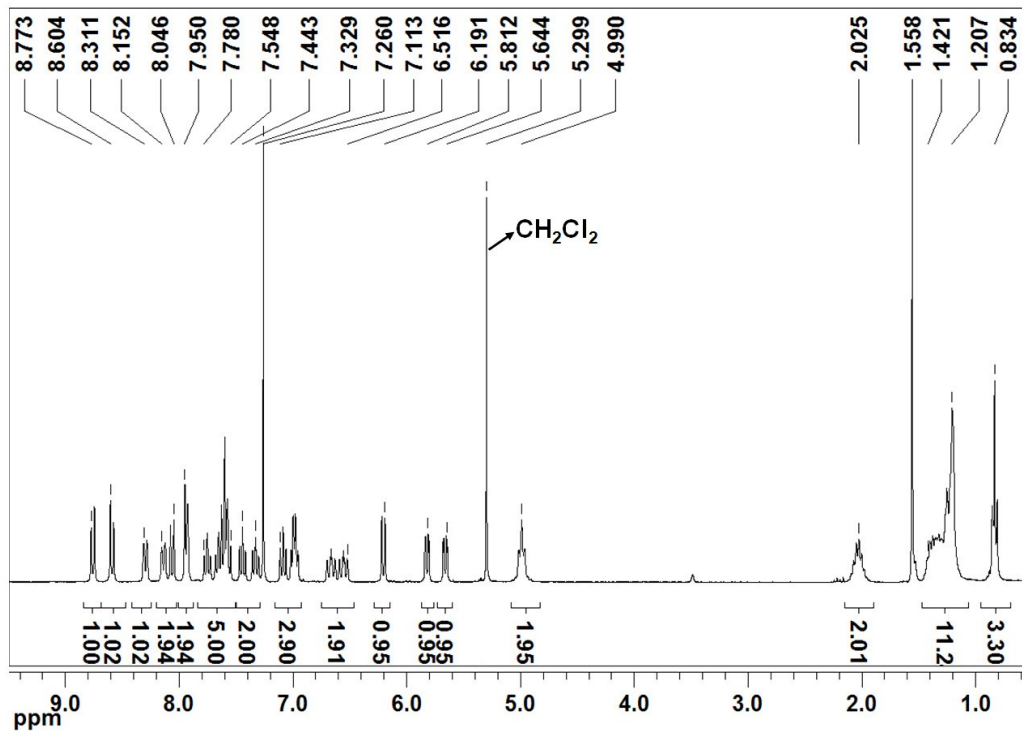


Fig. S6 ^1H NMR spectrum of **3** (300 MHz, CDCl_3).

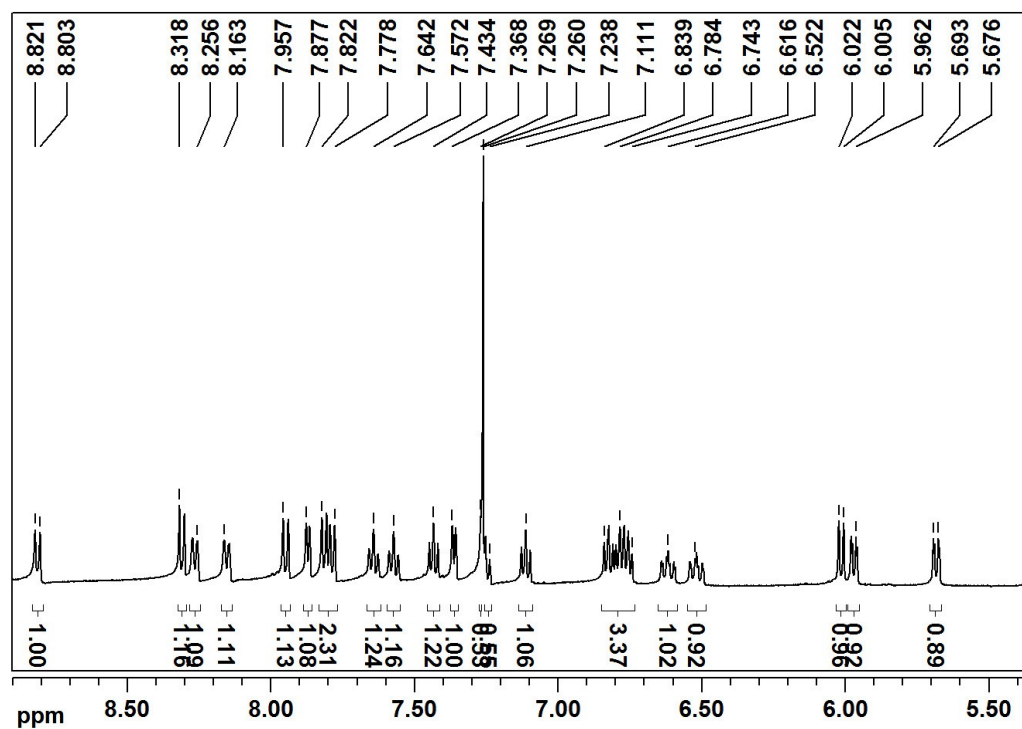


Fig. S7 ^1H NMR spectrum of **4** (500 MHz, CDCl_3).

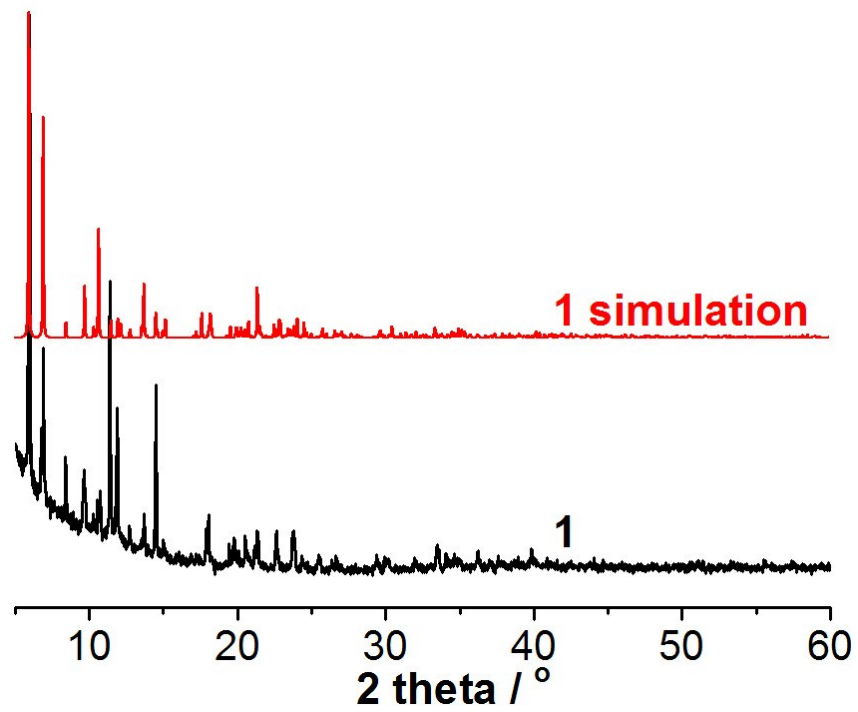


Fig. S8 Experimental and simulated XRD patterns of 1.

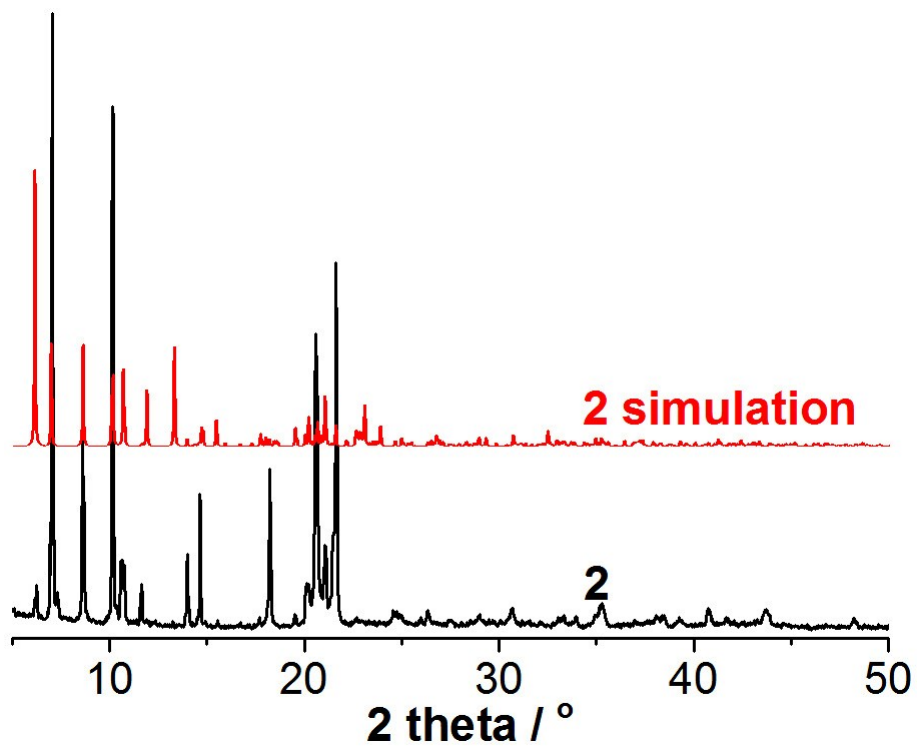


Fig. S9 Experimental and simulated XRD patterns of 2.

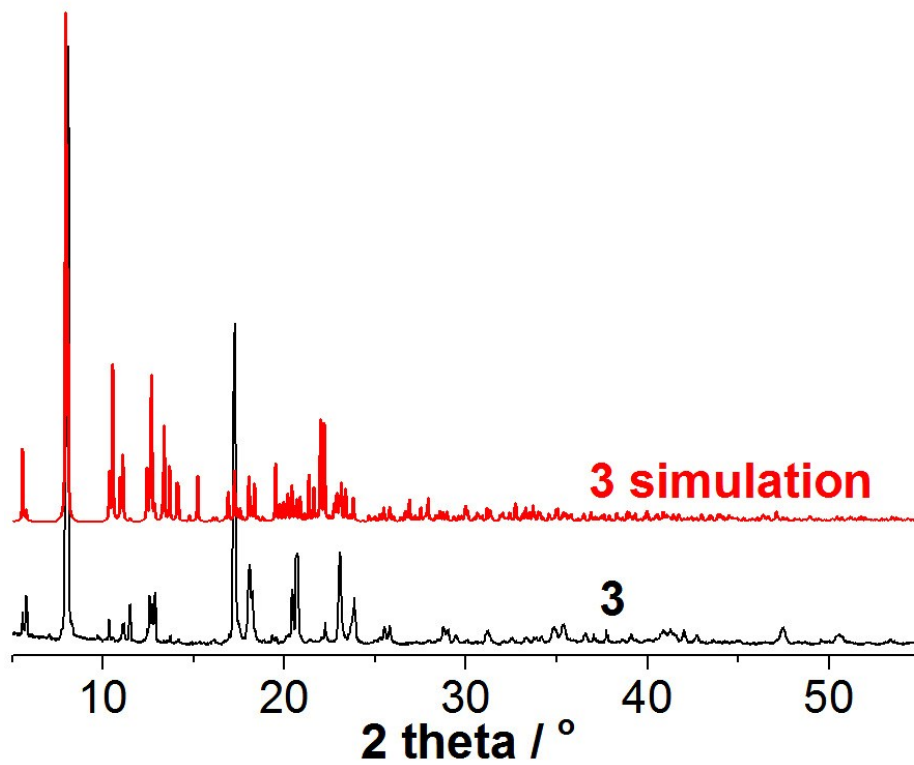


Fig. S10 Experimental and simulated XRD patterns of 3.

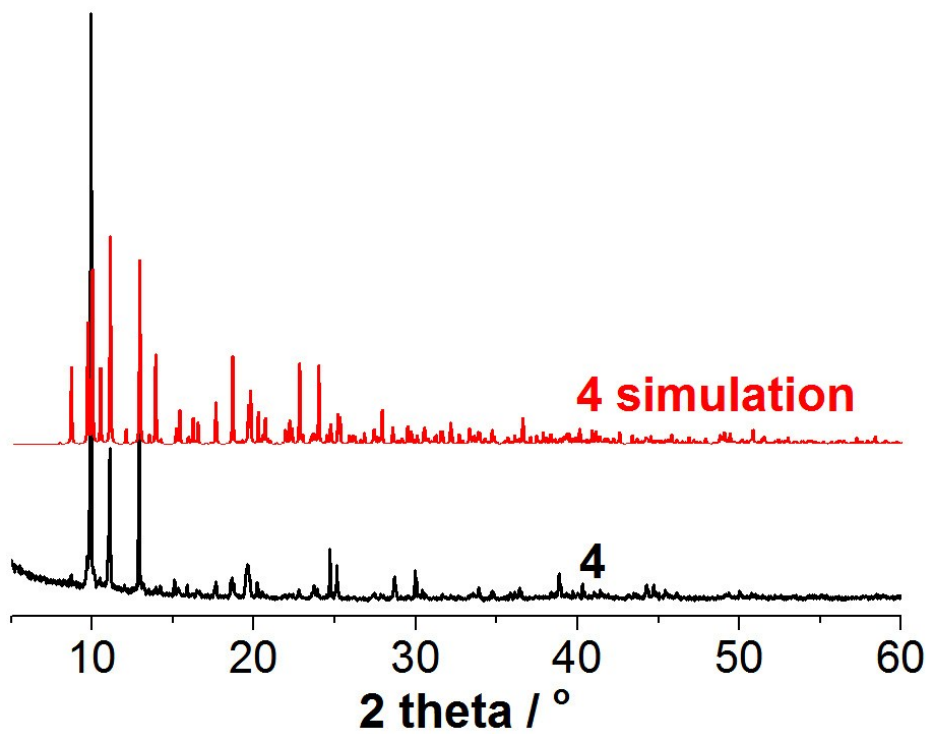


Fig. S11 Experimental and simulated XRD patterns of 4.

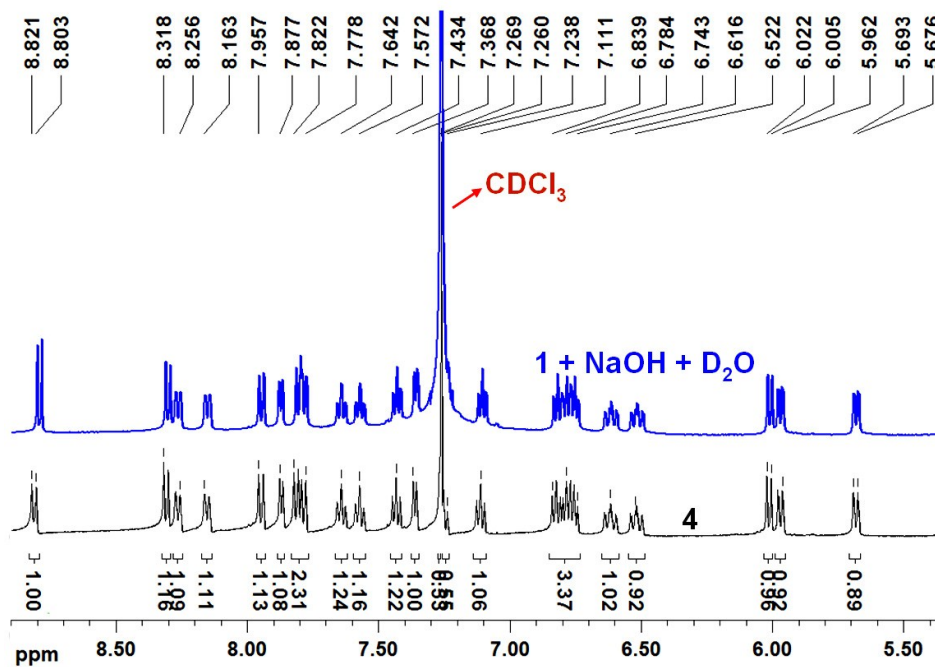


Fig. S12 ¹H NMR spectrum of **1** (500 MHz, CDCl₃) after adding a D₂O solution of NaOH, and ¹H NMR spectrum of **4** (500 MHz, CDCl₃).

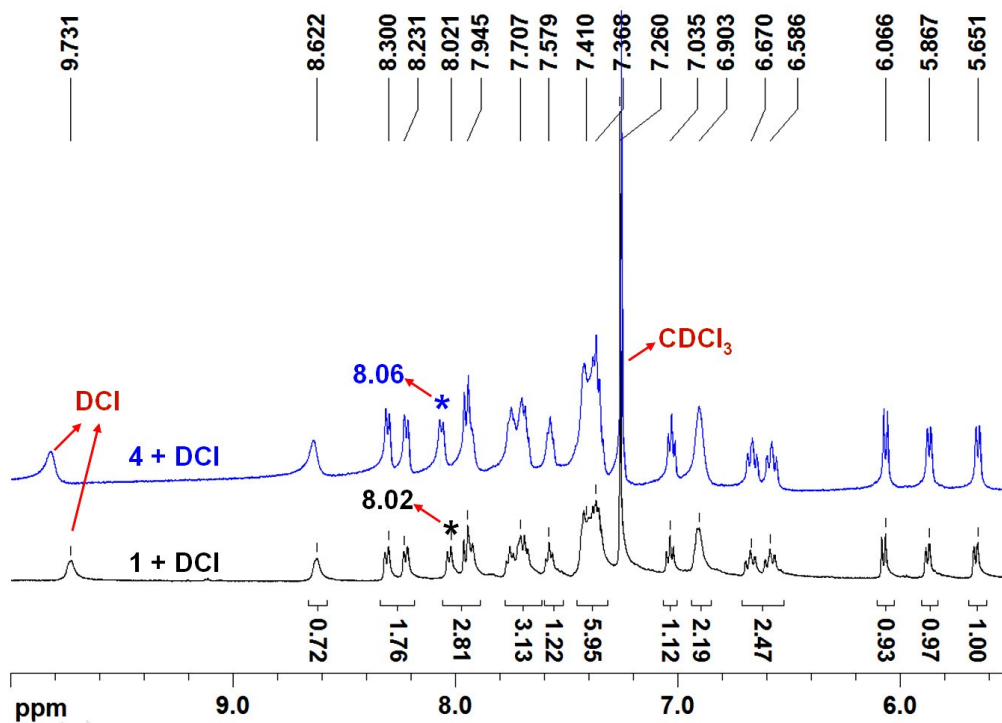


Fig. S13 ¹H NMR spectra of **1** and **4** (500 MHz, CDCl₃) after adding DCl.

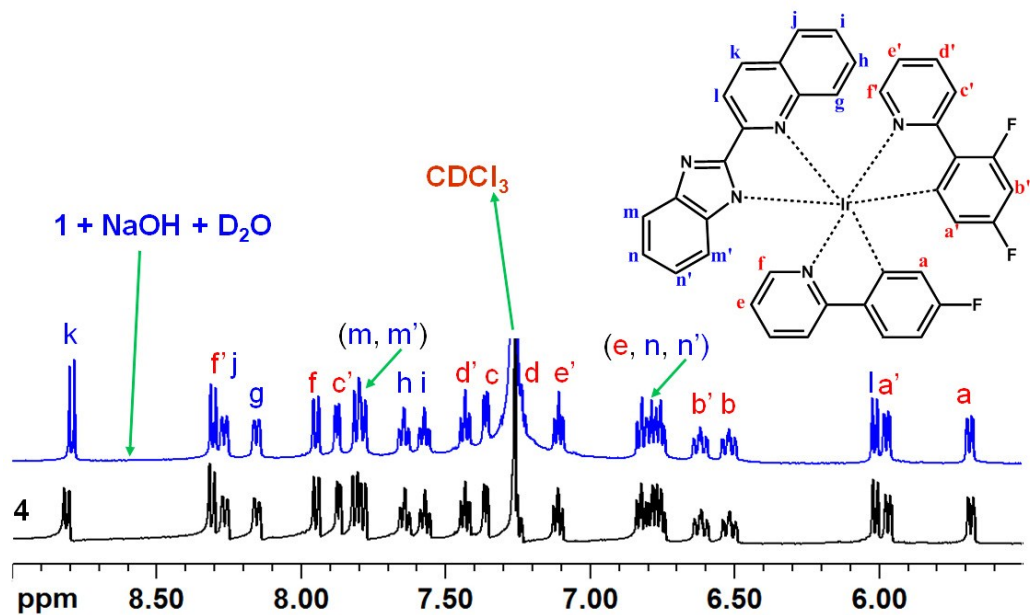


Fig. S14 The tentative assignment of different proton resonances in the ^1H NMR spectra of **1** and **1+NaOH+D₂O** (Letters a-n are used to indicate different H atoms).

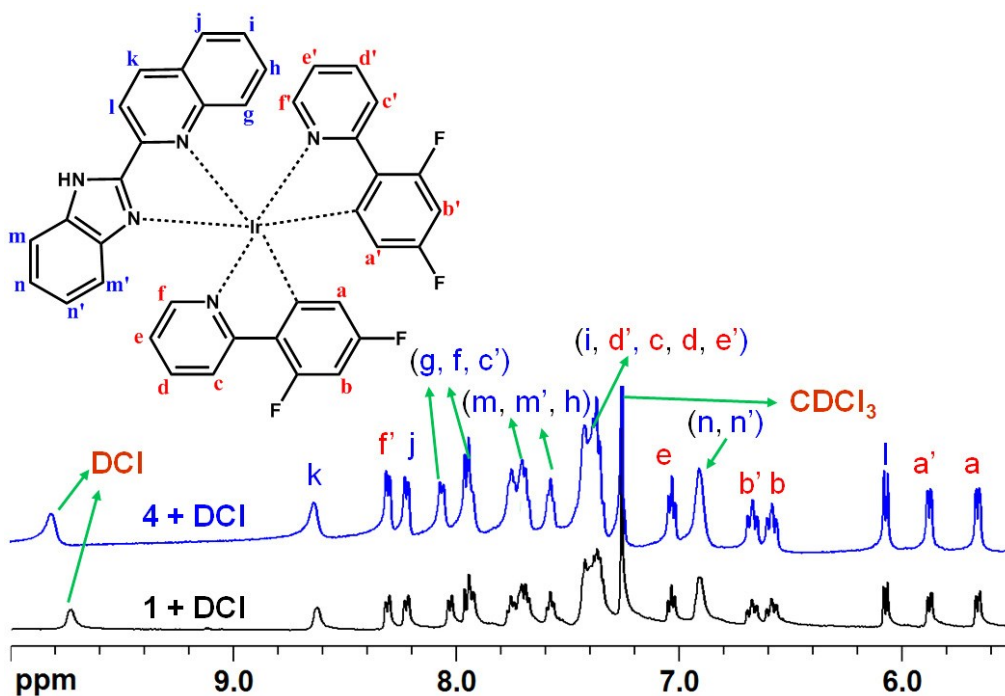


Fig. S15 The tentative assignment of different proton resonances in the ^1H NMR spectra of **4+DCI** and **1+DCI** (a-n are used to indicate different H atoms).

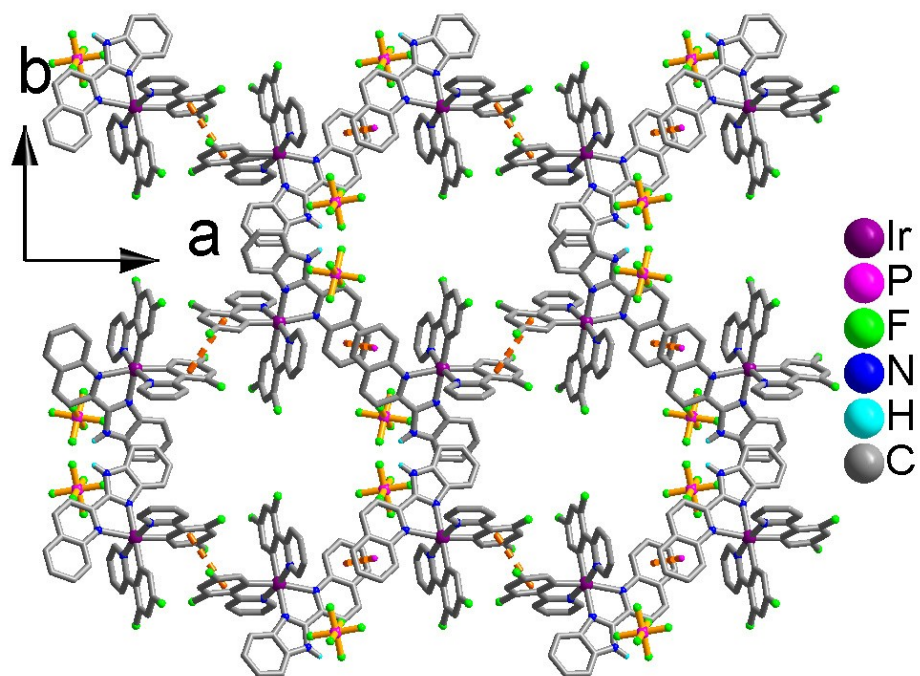


Fig. S16 Packing structure of 1.

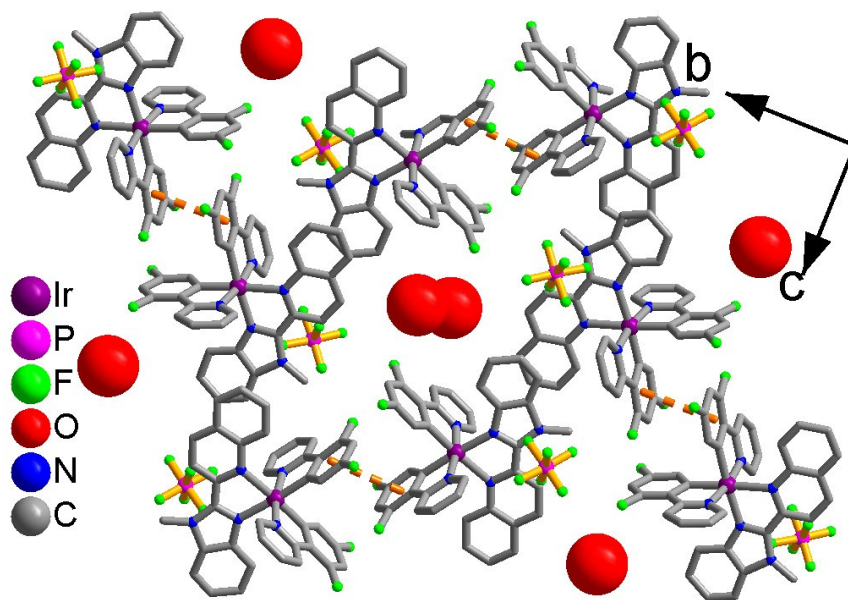


Fig. S17 Packing structure of 2. Big red balls are O atoms from H₂O molecules.

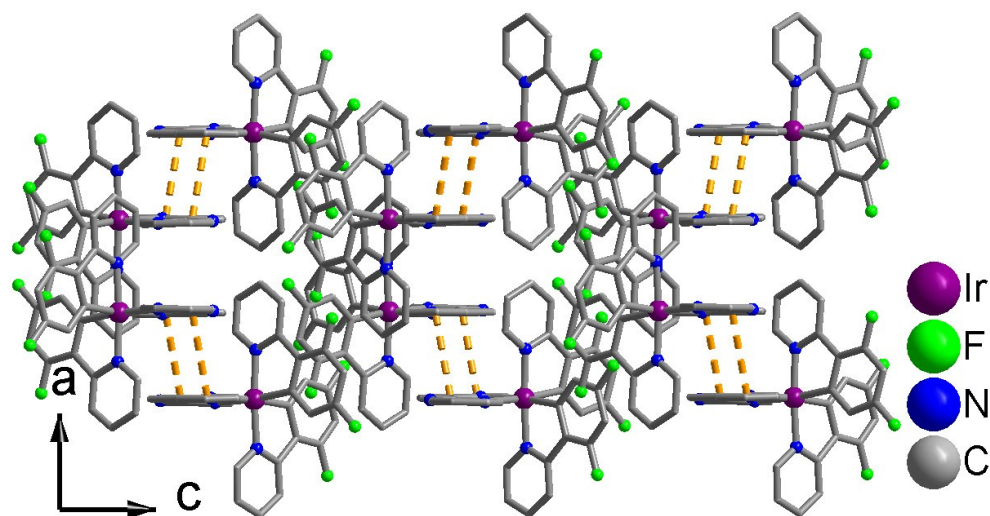


Fig. S18 The supramolecular dimers in 4 stacking through van der Waals interactions.

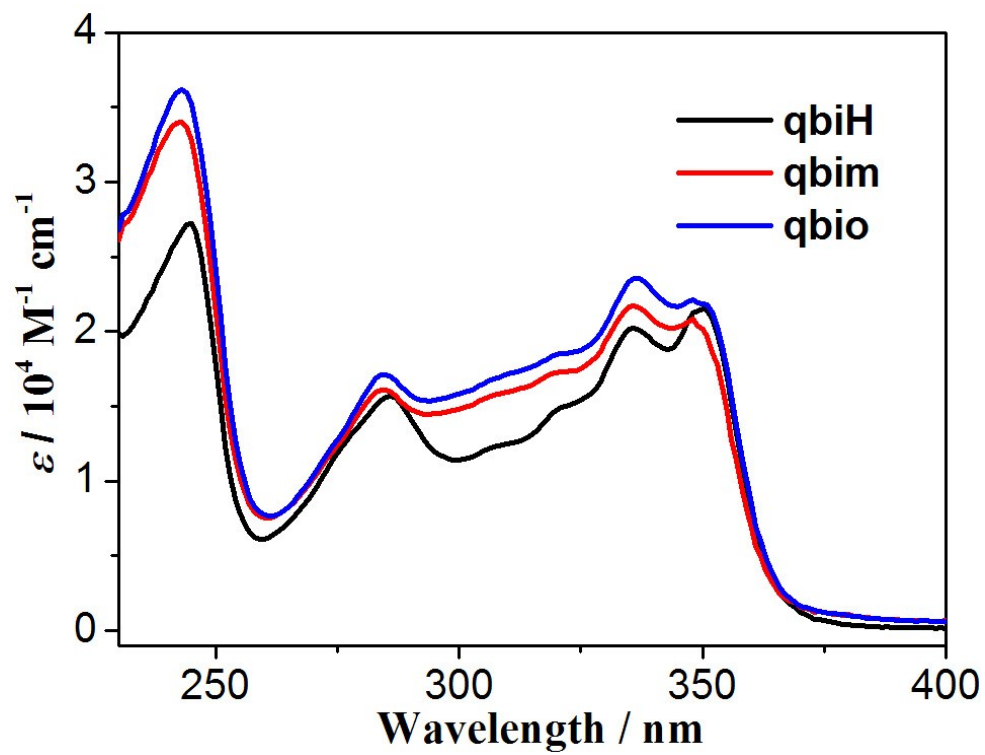


Fig. S19 UV-vis absorption spectra of qbiH, qbim and qbio in CH_2Cl_2 .

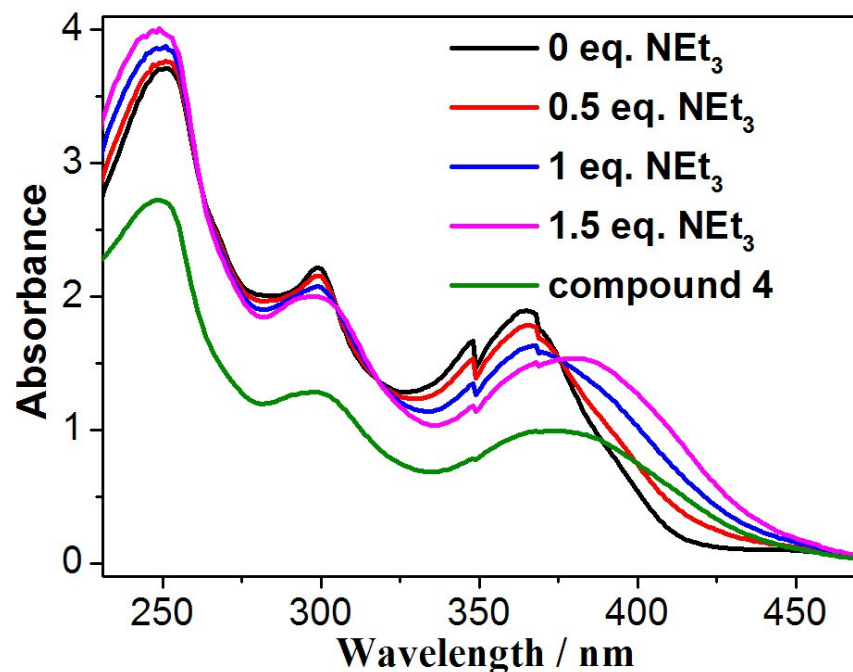


Fig. S20 UV-vis absorption spectra changes of **1** in CH₂Cl₂ ($c = 4 \times 10^{-5}$ M) upon adding NEt₃, and UV-vis absorption spectrum of compound **4** in CH₂Cl₂ ($c = 4 \times 10^{-5}$ M).

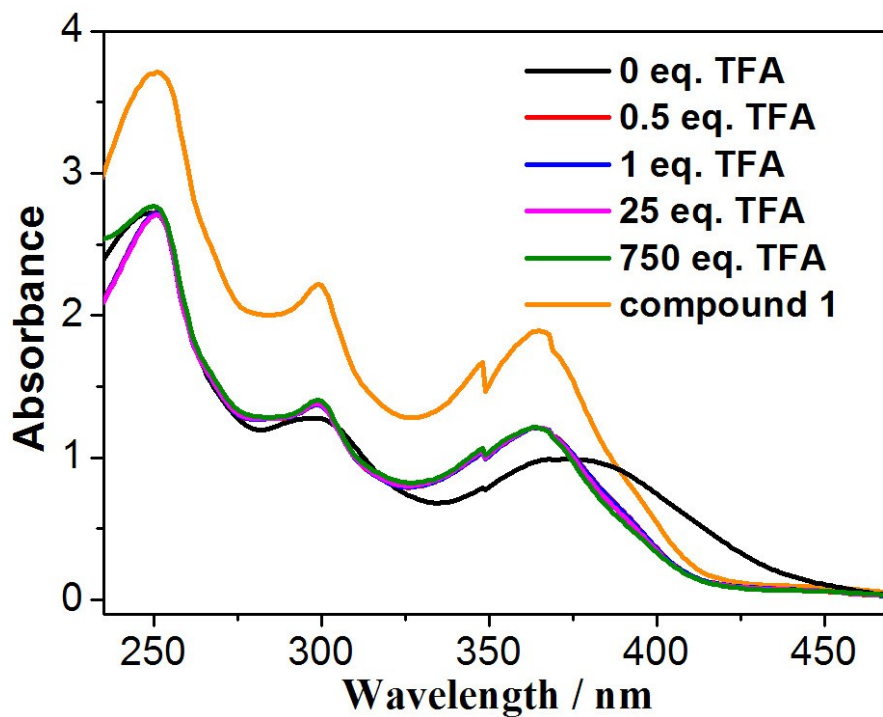


Fig. S21 UV-vis absorption spectra changes of **4** in CH₂Cl₂ ($c = 4 \times 10^{-5}$ M) upon adding TFA, and UV-vis absorption spectrum of compound **1** in CH₂Cl₂ ($c = 4 \times 10^{-5}$ M).

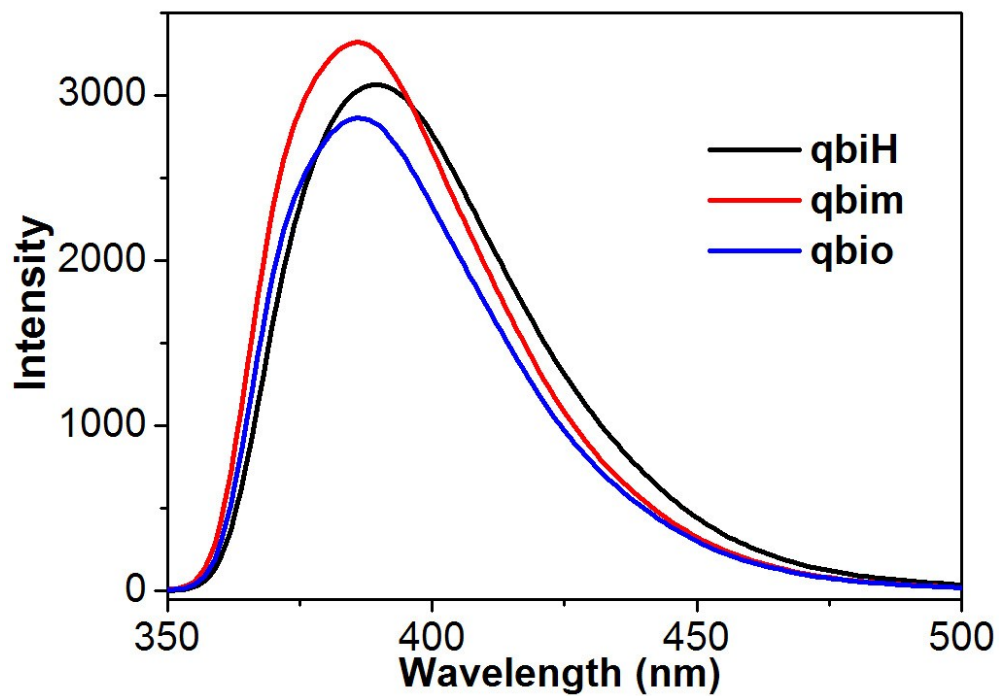


Fig. S22 Luminescence spectra of qbiH, qbim and qbio in CH_2Cl_2 ($c = 1.0 \times 10^{-4} \text{ M}$, $\lambda_{\text{ex}} = 345 \text{ nm}$) at room temperature.

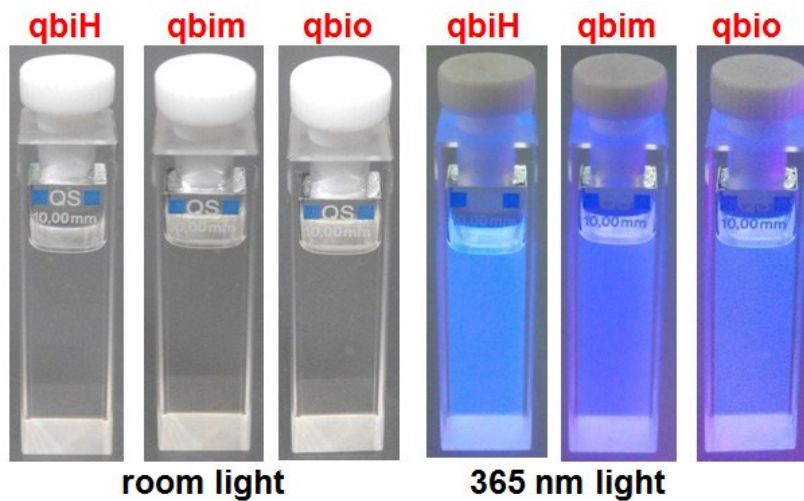


Fig. S23 The photographs of qbiH, qbim and qbio in CH_2Cl_2 under room light or 365 nm light.

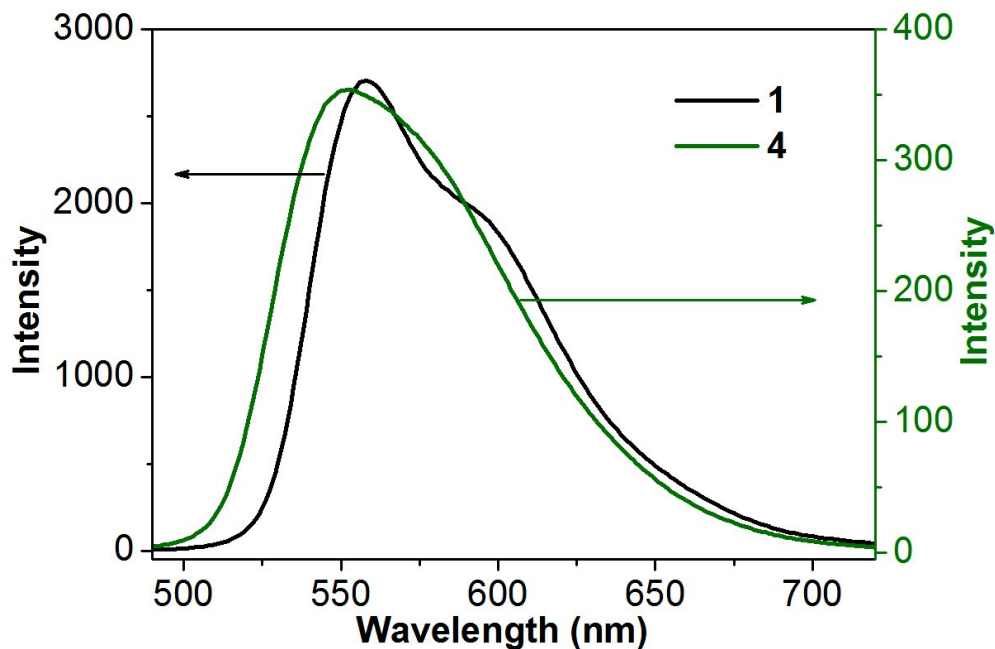


Fig. S24 Luminescence spectra of **1** and **4** in CH_2Cl_2 ($c = 4 \times 10^{-5}$ M) at room temperature.

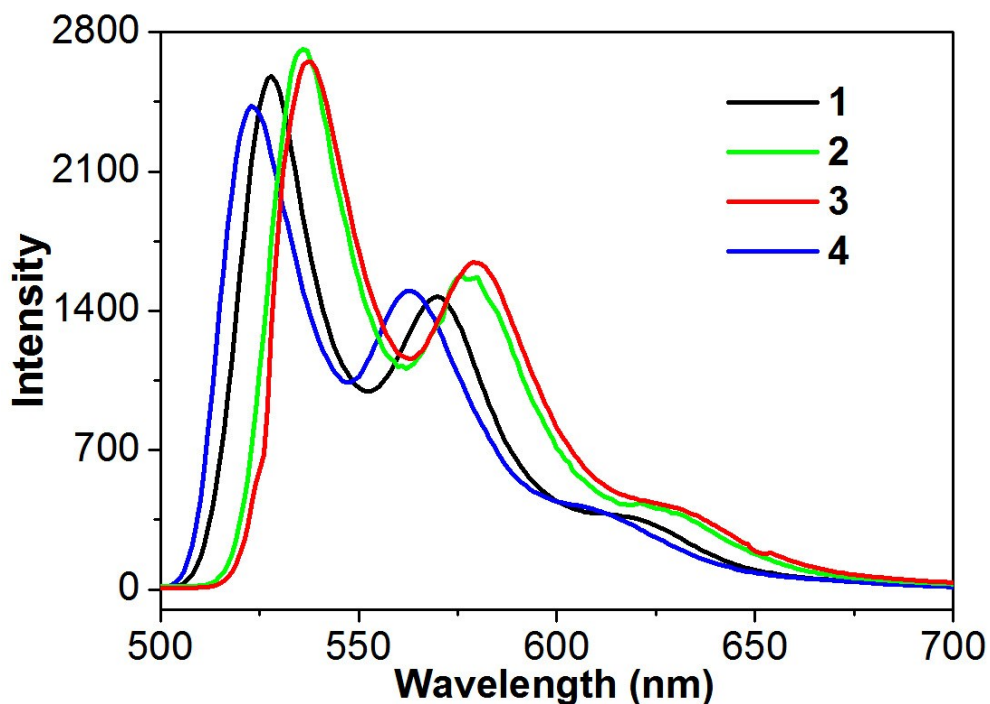


Fig. S25 Phosphorescence spectra of **1-4** in $\text{C}_2\text{H}_5\text{OH}-\text{CH}_3\text{OH}$ ($v/v = 3/1$) at 77 K ($c = 1.0 \times 10^{-4}$ M, $\lambda_{\text{ex}} = 370$ nm).

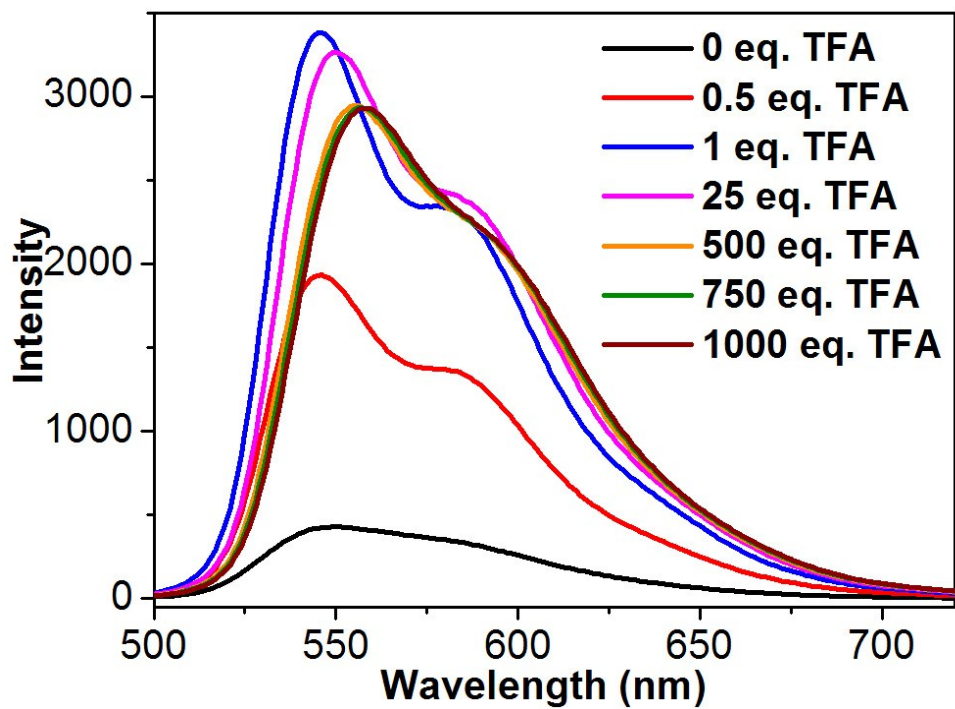


Fig. S26 Luminescence spectra changes of **4** in CH₂Cl₂ ($c = 4 \times 10^{-5}$ M, $\lambda_{\text{ex}} = 370$ nm) upon adding TFA.

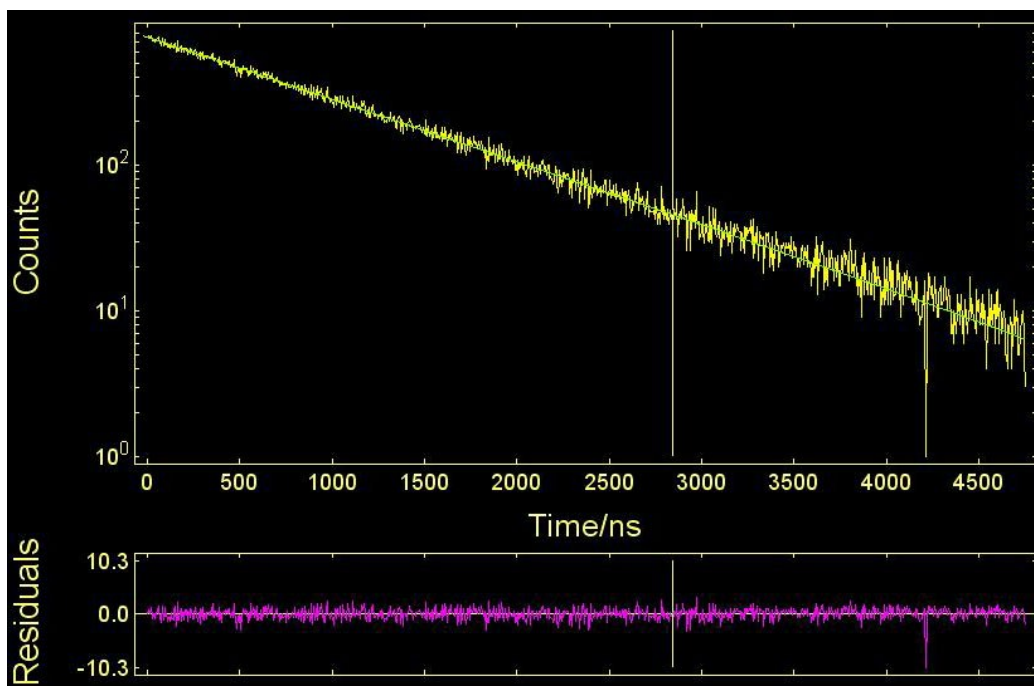


Fig. S27 The emission decay of compound **1** in CH₂Cl₂.

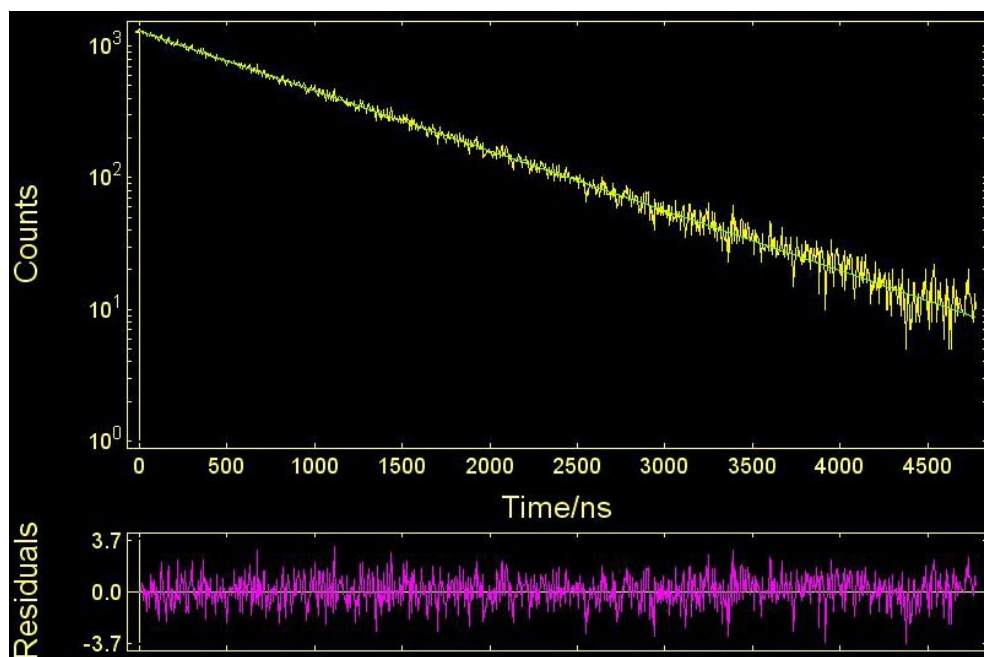


Fig. S28 The emission decay of compound **2** in CH₂Cl₂.

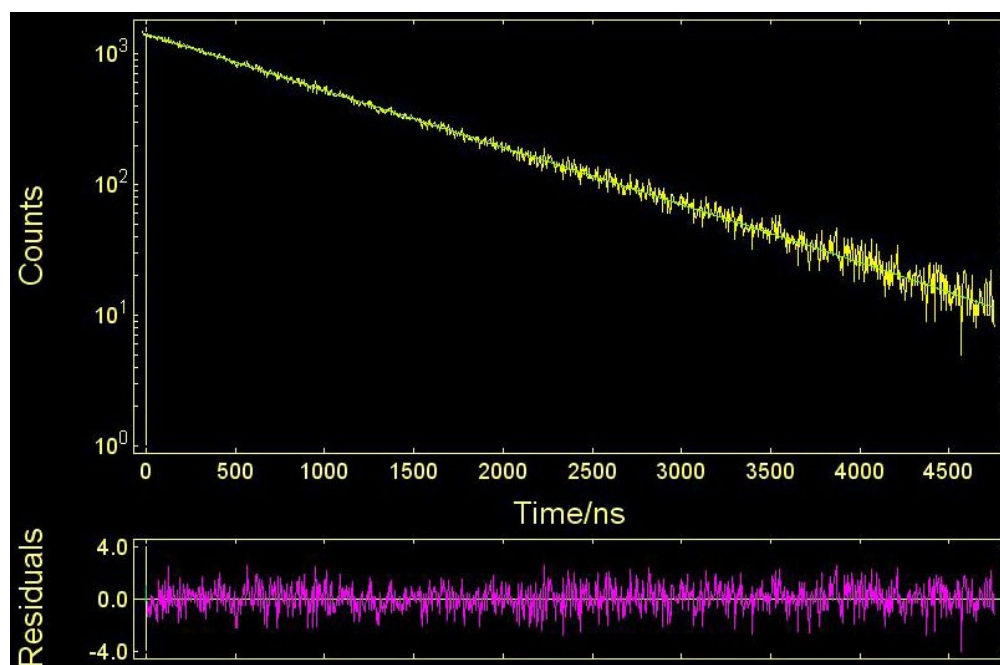


Fig. S29 The emission decay of compound **3** in CH₂Cl₂.

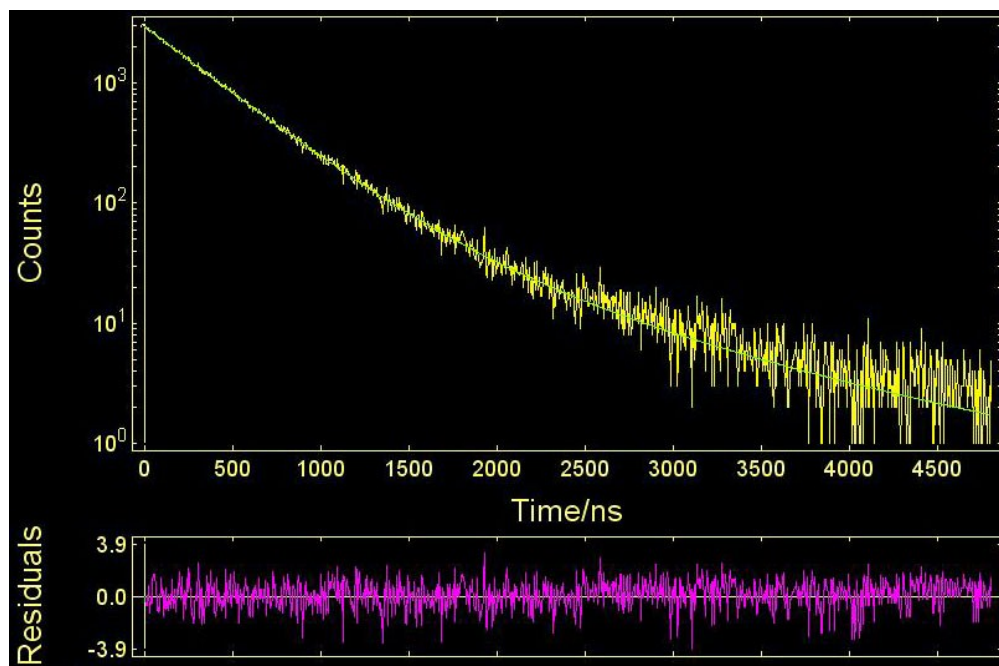


Fig. S30 The emission decay of compound **4** in CH_2Cl_2 .