Electronic Supplementary Information

Effect of Connecting Unit on Aggregation-Induced Emission and Mechanofluorochromic Properties of Isoquinoline Derivatives with Malononitrile as Terminal Group

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Contents:

Solvatochromic Property of IQ-BM Based on Lippert-Mataga Equation in Different Solvents

The relationship between solvent polarity and photophysical property of **IQ-BM** is investigate by the Lippert-Mataga equation listed as follows: $\Delta\nu = 2(\mu_e-\mu_g)^2\Delta f/hca^3+C$. Herein, $\Delta\nu$ is the Stokes shifts of the molecule determined by the following equation: $\Delta\nu = \nu_{abs}-\nu_{em}$. μ_g and μ_e are the dipole moments in the ground and the excited states, respectively. The constants h and c are the Planck constant and the speed of light, respectively, and a represents the radius of the fluorescent molecule. Δf is the solvent

polarity parameter of solvent, which is determined by the following equation: $(\varepsilon\text{-}1)/(2\varepsilon+1)\text{-}(n^2\text{-}1)/(2n^2+1)$, herein, ε and n are the dielectric constant and refractive index of the solvent, respectively. Δf values for the various solvents can be calculated from known values of ε and n. In this work, the Δf values of hexane, dioxane, $CHCl_3$, THF, dimethyl sulfoxide, acetonitrile, and methanol were obtained from the previous literatures.[1]

Time-Resolved Emission Decay Parameters of Solid-State IQ-BM

The solid-state fluorescence decay parameters of **IQ-BM** are determined by the following equation: $I = A_1\exp(-t/\tau_1)+A_2\exp(-t/\tau_2)$.[2] In this equation, τ_1 and τ_2 represent the lifetimes of the shorter-lived and longer-lived species, and A_1 and A_2 are their respective amplitudes, respectively. The weighted mean lifetime $<\tau>$ is calculated from the following equation: $<\tau> = (A_1\tau_1+A_2\tau_2)/(A_1+A_2)$. The radiative rate constant k_f and non-radiative rate constant k_{nr} are calculated from the equations of $k_f = \Phi_F/<\tau>$ and $k_{nr} = (1\text{-}\Phi_F)/<\tau>$, respectively.[3]

References

1. (a) S. Y. Fung, J. Duhamel and P. Chen, *J. Phys. Chem. A*, 2006, **110**, 11446-11454; (b) H. Li, Y. Guo, Y. Lei, W. Gao, M. Liu, J. Chen, Y. Hu, X. Huang and H. Wu, *Dyes Pigm.*, 2015, **112**, 105–115.

2. X. Zhang, Z. Chi, B. Xu, C. Chen, X. Zhou, Y. Zhang, S. Liu and J. Xu, *J. Mater. Chem.*, 2012, **22**, 18505–18513.

3. B. Fang, M. Chu, Z. Wu, Y. Shi, Y. S. Zhao and M. Yin, *J. Mater. Chem. C*, 2019, **7**, 4434–4440.

2. Figures and Tables

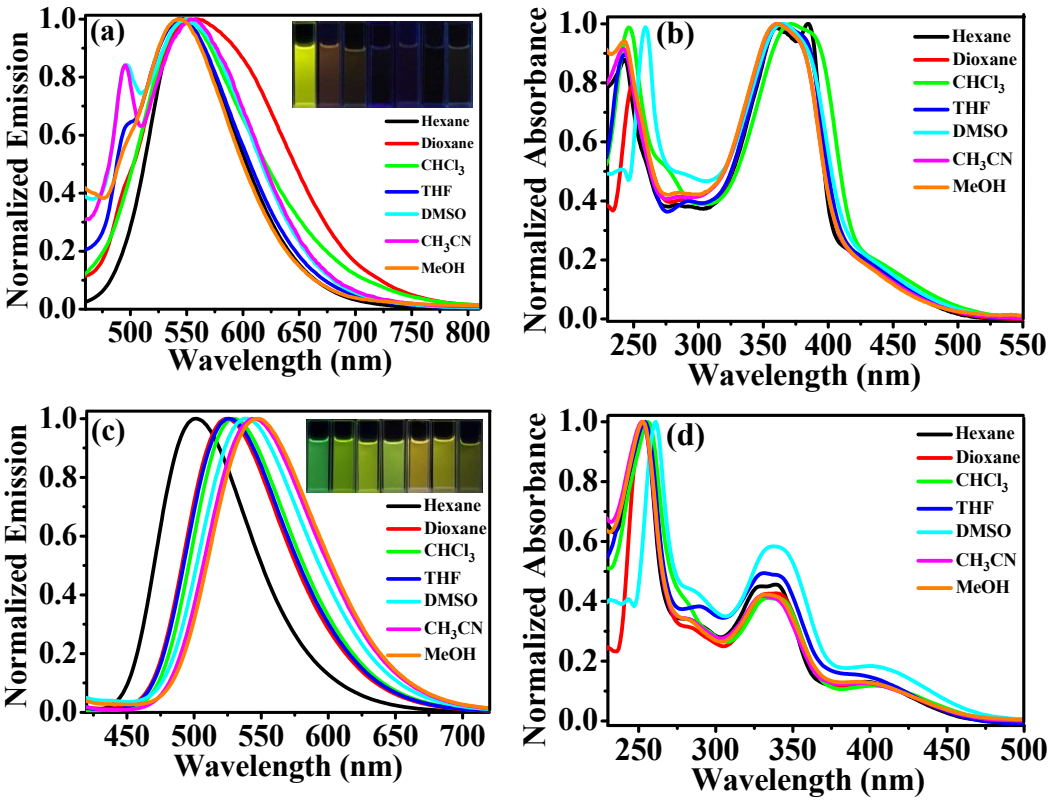

Figure S1. Normalized fluorescence and absorption spectra of **IQ-BIM** (a, b) and **IQ-BM** (c, d) in different solvents (Ex: 440 nm for **IQ-BIM** and 420 nm for **IQ-BM**). Concentration: 1×10^{-5} mol/L.

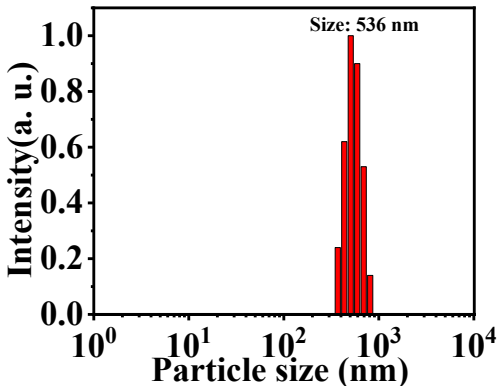

Figure S2. Size distribution of the aggregates of **IQ-BIM** in pure hexane at a concentration of 1×10^{-5} mol/L.

Table S1. UV-vis Absorption Maxima and Fluorescence Emission Maxima of IQ-BM and Solvent Polarity Parameter in Different Solvents

	Hexane	Dioxane	$CHCl_3$	THF	DMSO	CH_3CN	CH_3OH
λ_{abs}/nm	338	342	336	330	331	330	333
ν_{abs}/cm^{-1}	29586	29240	29762	30303	30211	30303	30030
λ_{em}/nm	501	525	529	526	537	543	547
ν_{em}/cm^{-1}	19960	19048	18904	19011	18622	18416	18282
$\Delta\nu$/cm^{-1}	9626	10192	10858	11292	11589	11887	11748
Δf	0.002	0.021	0.155	0.210	0.263	0.305	0.308

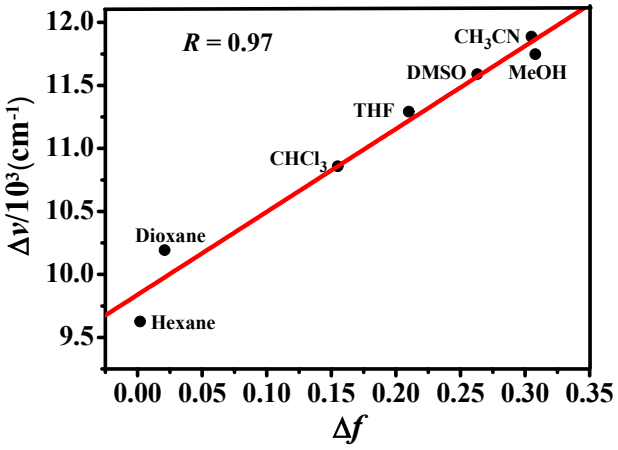

Figure S3. Linear fitting of Stokes shifts ($\Delta\nu$) of **IQ-BM** with orientation polarizability (Δf) in various solvents.

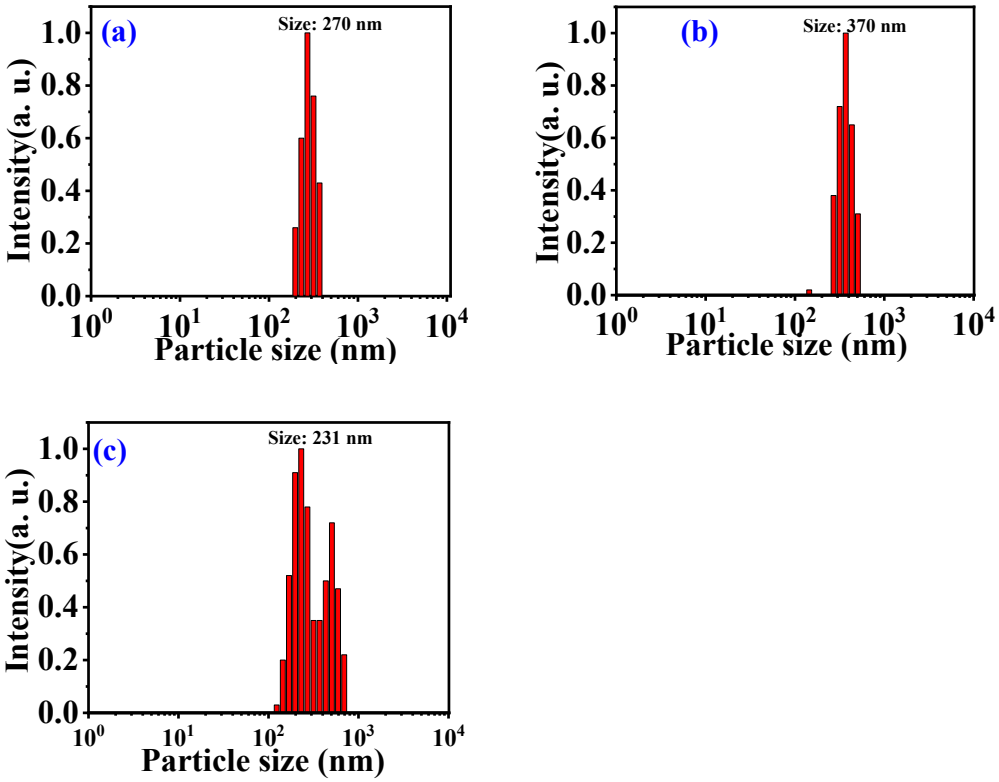

Figure S4. Size distributions of the aggregates of **IQ-BIM** in THF-water mixtures with f_w = 80% (a), 90% (b), and 99% (c), respectively. Concentration: 1 × 10^{-5} mol/L.

Table S2. Crystal Data and Details of Collection and Refinement of IQ-BIM and IQ-BM

	IQ-BIM	**IQ-BM**
CCDC (No.)	2097239	2097240
Empirical formula	$C_{29}H_{23}N_5$	$C_{29}H_{25}N_5$
Formula weight	441.52	443.54
Temperature (K)	293(2)	293(2)
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
Z	2	2
D_{calcd} [Mg/m^3]	1.254	1.035
F (000)	464	468
θ range [°]	2.774-25.495	2.359-25.498
R_1 [I>2σ(I)]	0.0480	0.0605
wR_2 [I>2σ(I)]	0.1081	0.1539
a [Å]	6.1532(3)	6.1207(18)
b [Å]	13.1141(6)	14.099(4)
c [Å]	15.5713(8)	18.263(6)
α [deg]	109.057(2)	112.610(9)
β [deg]	90.519(2)	91.088(9)
γ [deg]	99.450(2)	100.540(9)
V [Å^3]	1168.87(10)	1423.3(8)

GOF	1.050	1.095
R (int)	0.0451	0.0673
No. of reflcns collected	17080	20886
No. of unique reflcns	4348	5293
R_1 (all data)	0.0725	0.1135
wR_2 (all data)	0.1240	0.1819

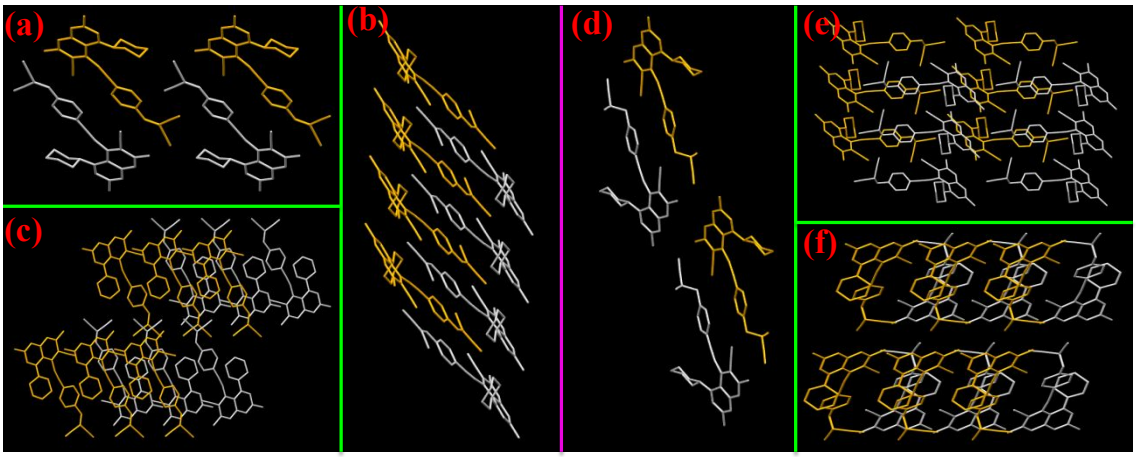

Figure S5. Stacking arrangements in the crystals of **IQ-BIM** and **IQ-BM**: (a, d) viewed along the *a*-axis; (b, e) viewed along the *b*-axis; (c, f) viewed along the *c*-axis. The hydrogen atoms have been omitted for clarity.

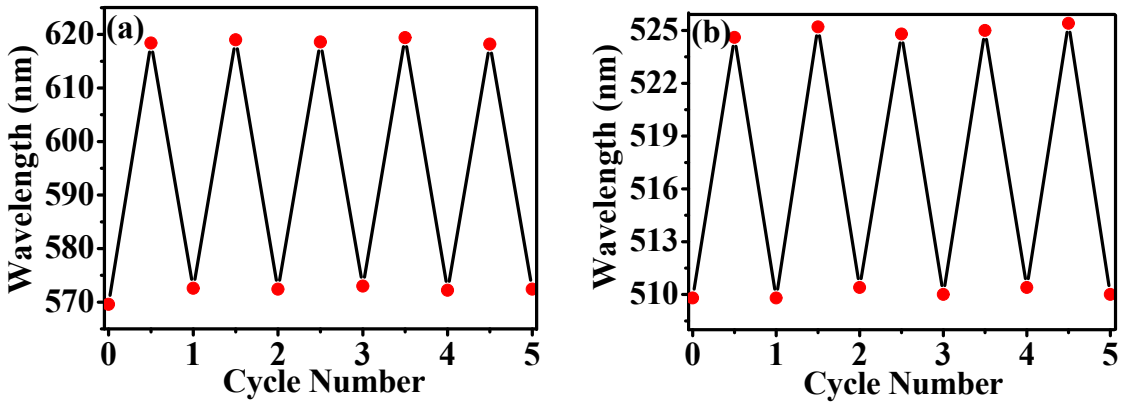

Figure S6. Recycling of grinding and fuming processes of **IQ-BIM** (a) and **IQ-BM** (b).

3. Spectra of NMR

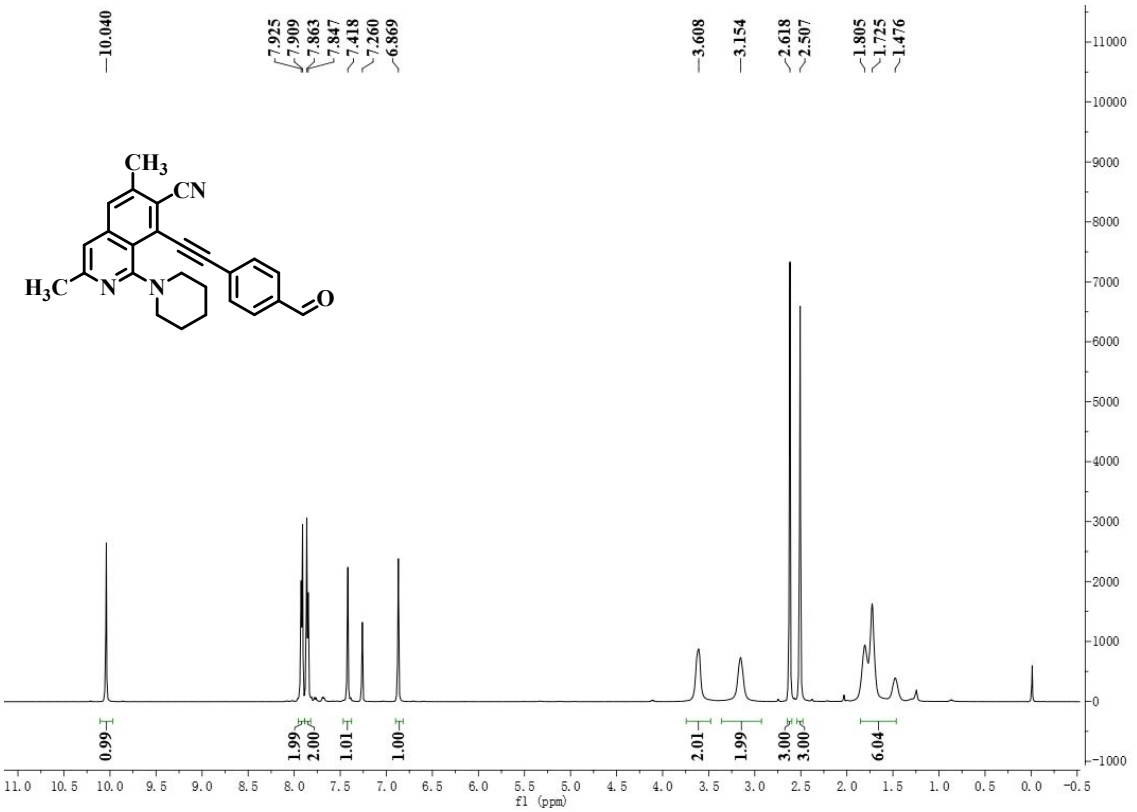

Figure S7. ^{1}H NMR of compound **5** ($CDCl_3$, 500 MHz).

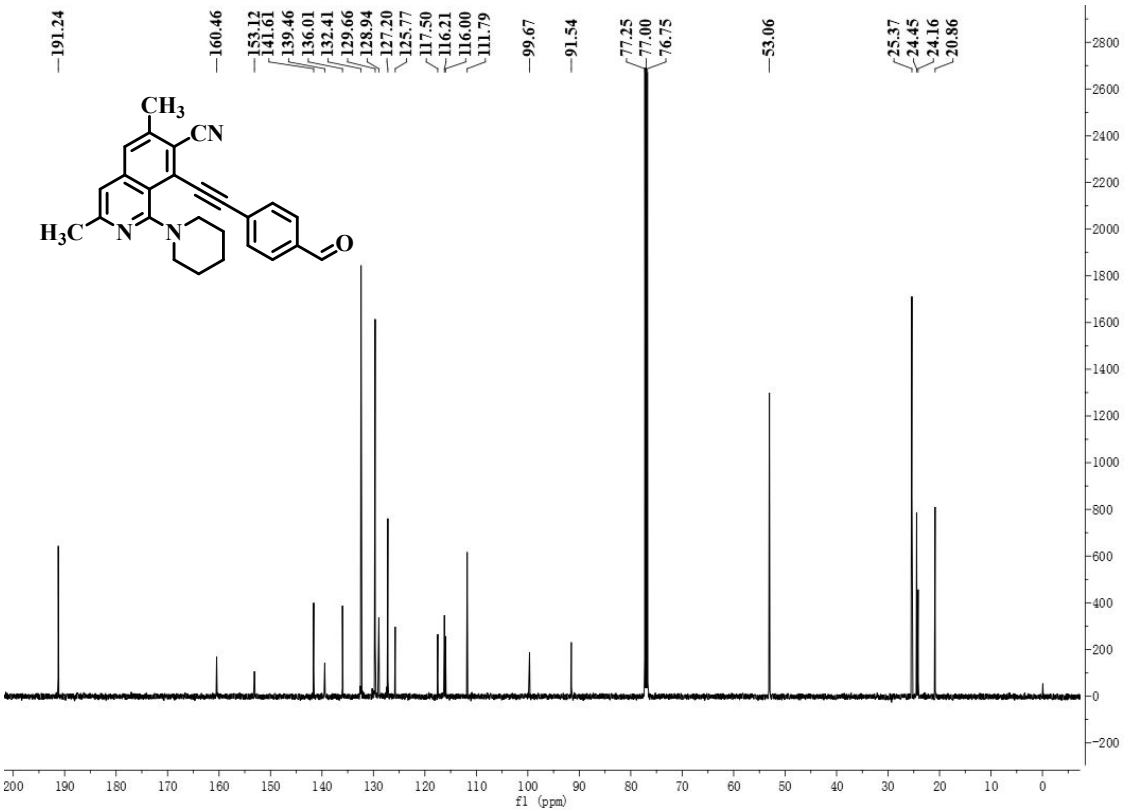

Figure S8. ^{13}C NMR of compound **5** ($CDCl_3$, 125 MHz).

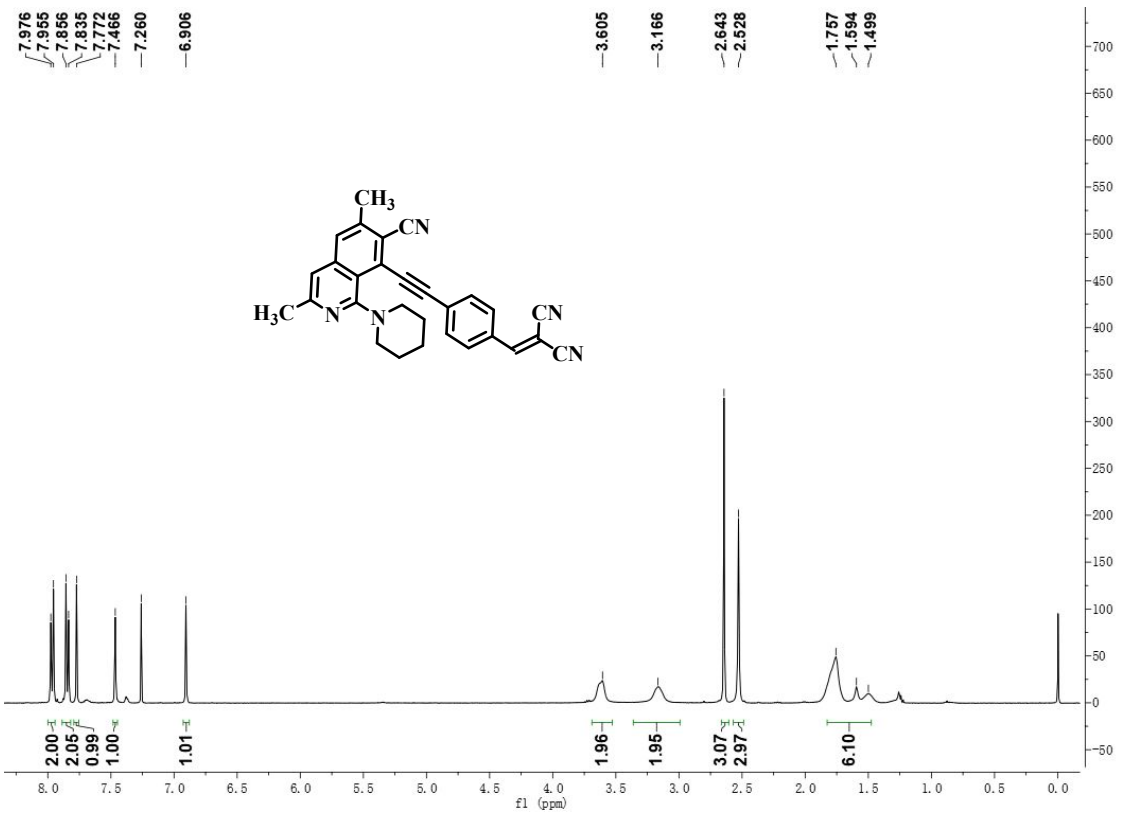

Figure S9. ^{1}H NMR of **IQ-BIM** ($CDCl_3$, 400 MHz).

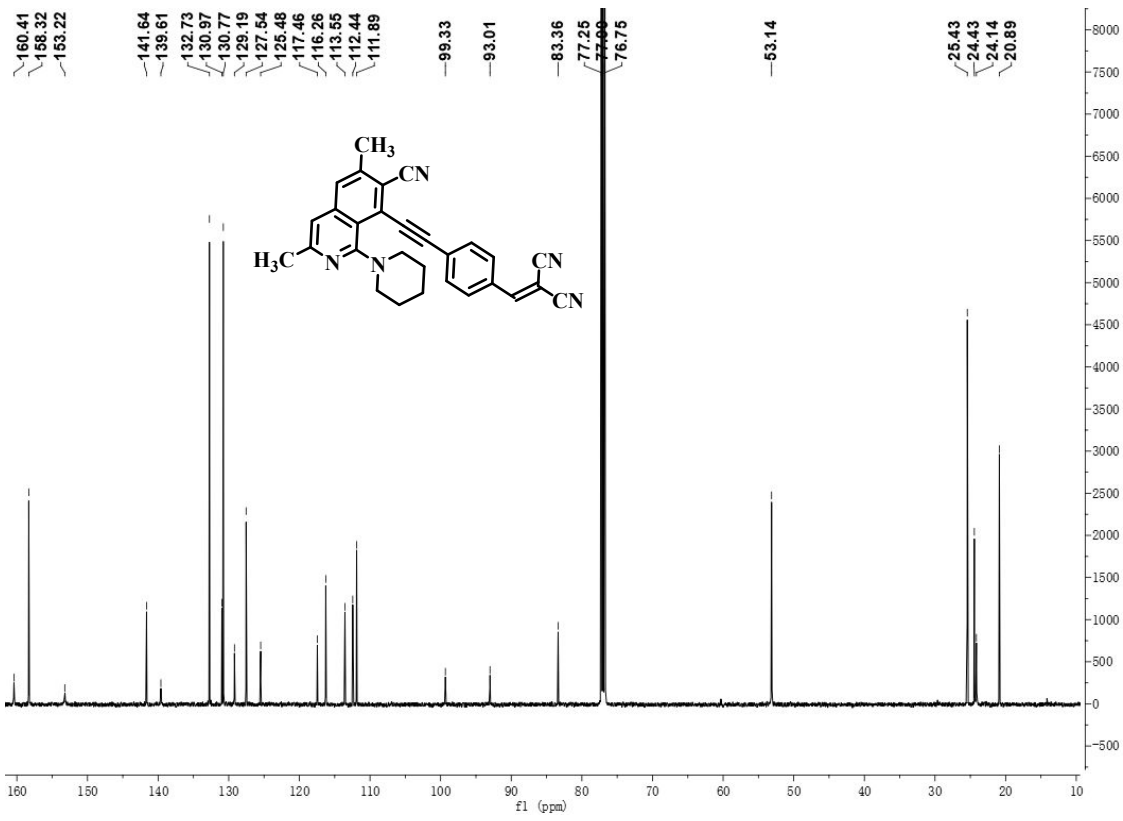

Figure S10. ^{13}C NMR of **IQ-BIM** ($CDCl_3$, 125 MHz).

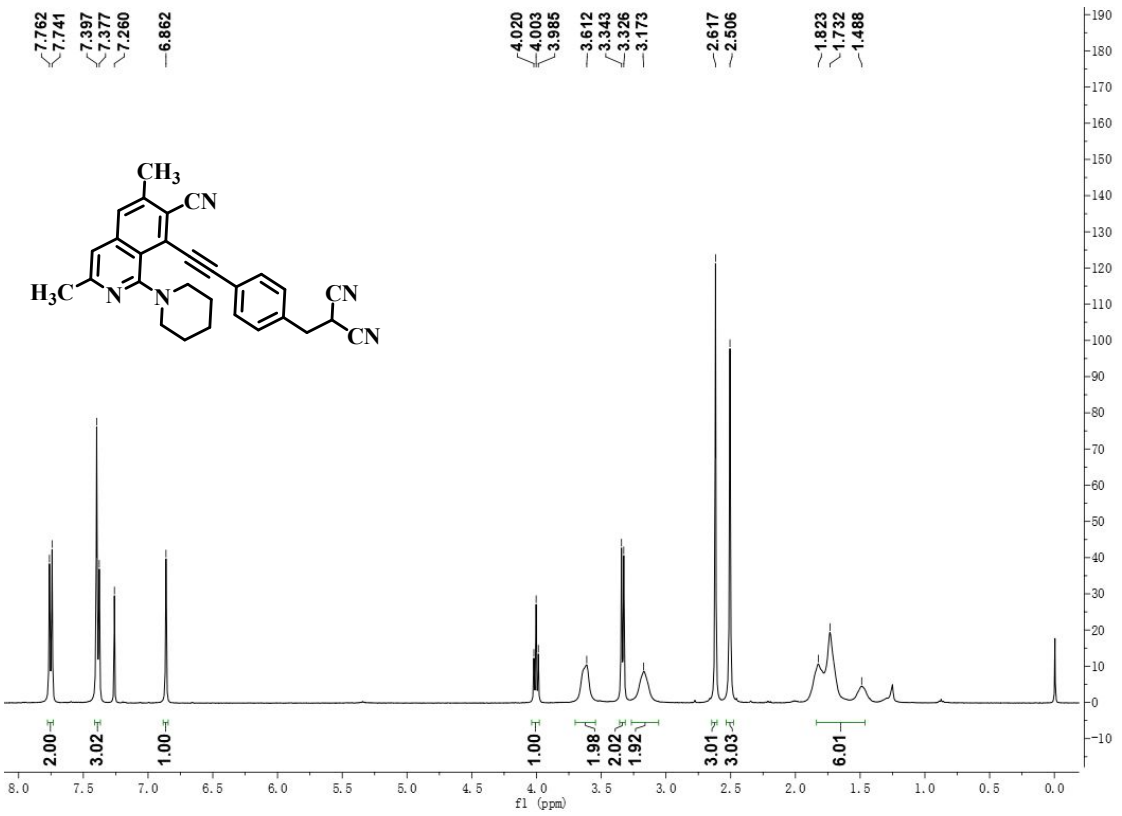

Figure S11. ^{1}H NMR of **IQ-BM** ($CDCl_3$, 400 MHz).

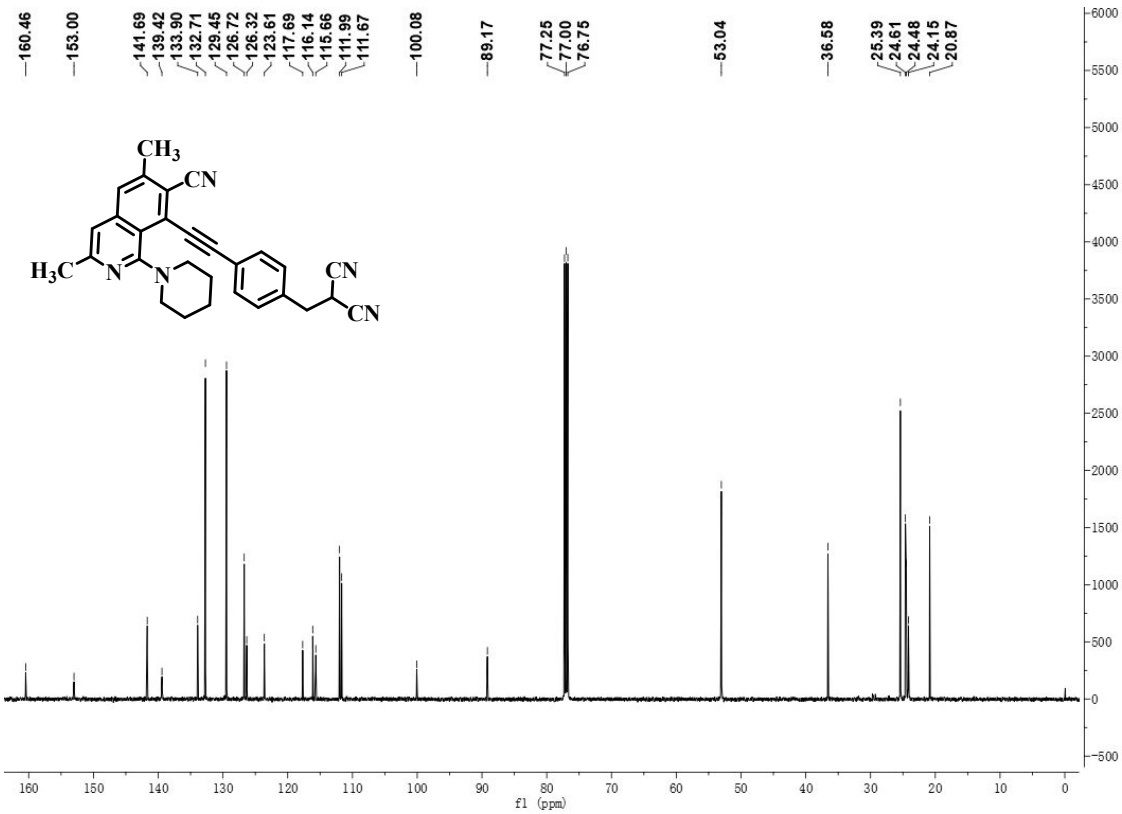

Figure S12. ^{13}C NMR of **IQ-BM** ($CDCl_3$, 125 MHz).