

Synthesis, Physical Properties, and Light-Emitting Diode Performance of Phenazine-Based Derivatives with Three, Five and Nine Fused Six-Membered Rings

Pei-Yang Gu,¹ Yongbiao Zhao,² Jing-Hui He,³ Jing Zhang,¹ Chengyuan Wang,¹ Qing-Feng Xu,³ Jian-Mei Lu,³ Xiaowei Sun,^{2*} and Qichun Zhang^{1,4*}

¹ School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore.

* Correspondence to Q. Zhang, E-mail: qc Zhang@ntu.edu.sg.

² School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798, Singapore.

* Correspondence to X. Sun, E-mail: EXWSun@ntu.edu.sg.

³ College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou, 215123, China.

⁴ Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore

Contents

General Information.....	S2
Figure S1 ¹ H NMR spectrum of 2a in CDCl ₃	S2
Figure S2 ¹³ C NMR spectrum of 2a in CDCl ₃	S3
Figure S3 HRMS spectrum of 2a	S3
Figure S4 ¹ H NMR spectrum of 2b in CDCl ₃	S4
Figure S5 ¹³ C NMR spectrum of 2b in CDCl ₃	S4
Figure S6 HRMS spectrum of 2b	S5
Figure S7 ¹ H NMR spectrum of 2c in CDCl ₃	S5
Figure S8 ¹³ C NMR spectrum of 2c in CDCl ₃	S6
Figure S9 MS spectrum of 2c	S6
Figure S10 Normalized absorption spectra of 2a recorded in different solvents.....	S6
Figure S11 Normalized absorption spectra of 2b recorded in different solvents.....	S7
Figure S12 Normalized absorption spectra of 2c recorded in different solvents.....	S7
Figure S13 Normalized PL spectra of 2a recorded in different solvents.....	S7
Figure S14 Normalized PL spectra of 2b recorded in different solvents.....	S8
Figure S15 TGA curves of 2a , 2b , and 2c with a heating rate of 20 °C min ⁻¹ under N ₂	S8
Figure S16 Cyclic voltammogram of the Ferrocene standard in CH ₂ Cl ₂ solution at the scan rate of 100 mV S ⁻¹	S8
Figure S17 The crystals images of compound 2a (A), 2b (B), and 2c (C).....	S9

General Information

The fluorescent quantum yields (QYs) in the solution were determined using quinine bisulfate ($\Phi_F = 0.54$ in $0.1 \text{ mol L}^{-1} \text{ H}_2\text{SO}_4$) using the equation:

$$\phi_r = \frac{F_r}{F_s} \frac{A_s}{A_r} \phi_s \quad (1)$$

In this equation, subscripts s and r represent the sample and reference, respectively. F is the integral area of the fluorescence spectra, A is the absorbance, ϕ is the fluorescence quantum yield.

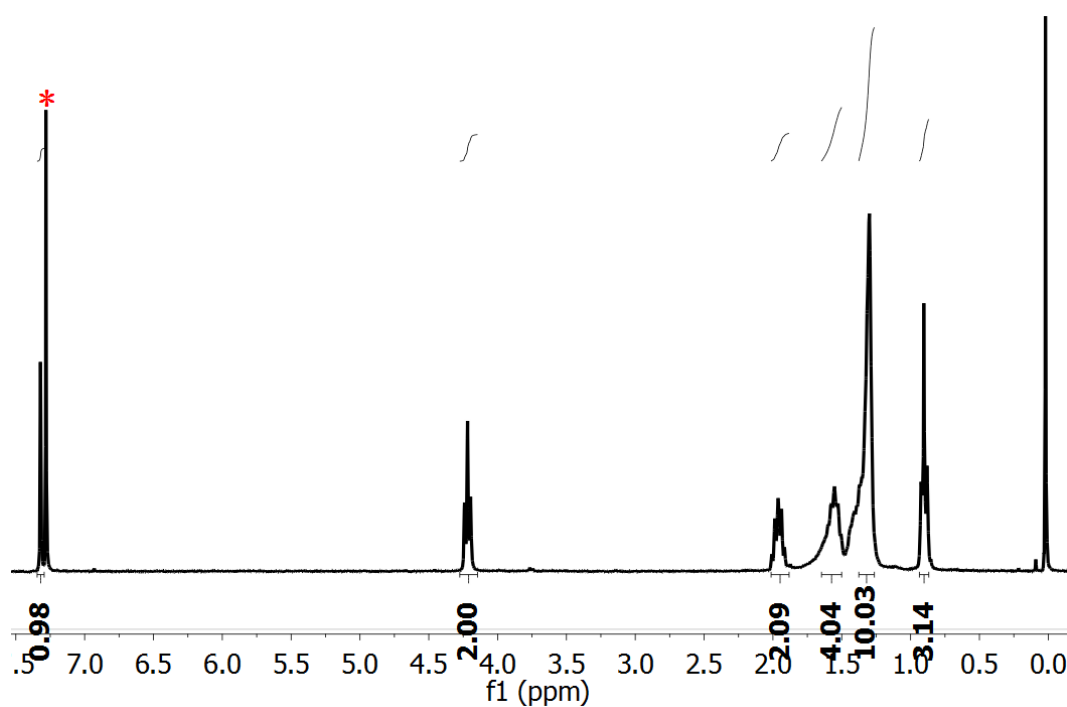


Figure S1 ^1H NMR spectrum of **2a** in CDCl_3 .

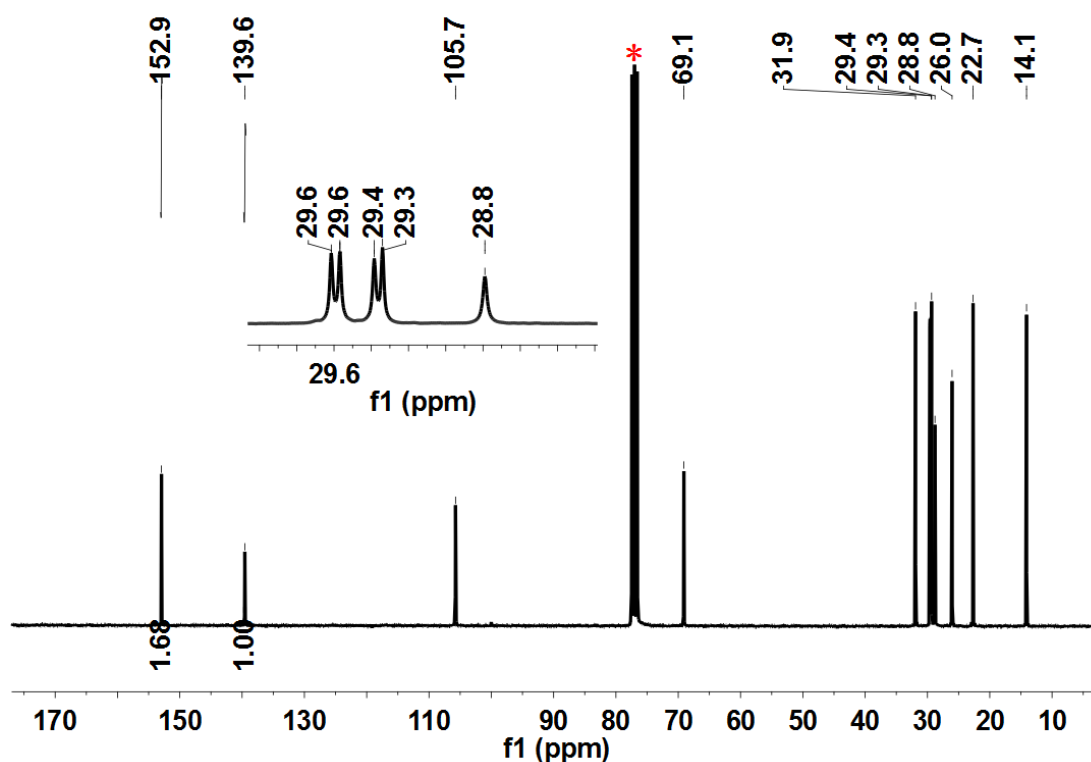


Figure S2 ^{13}C NMR spectrum of **2a** in CDCl_3 .

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 51-53 H: 87-89 N: 1-3 O: 3-4

C52H88N2O4

zyl-py-5 26 (0.591)

1: TOF MS ES+
2.03e+000

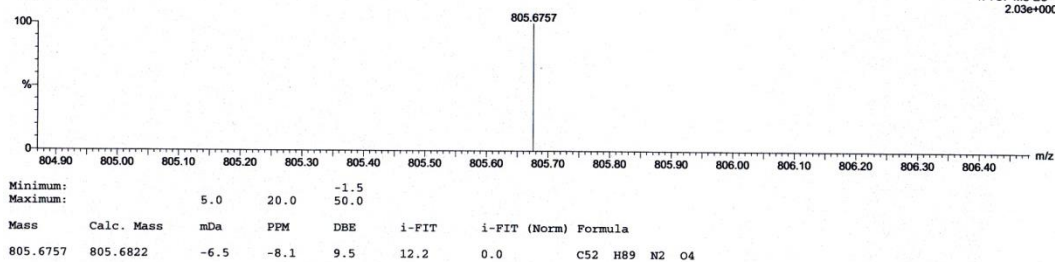


Figure S3 HRMS spectrum of **2a**

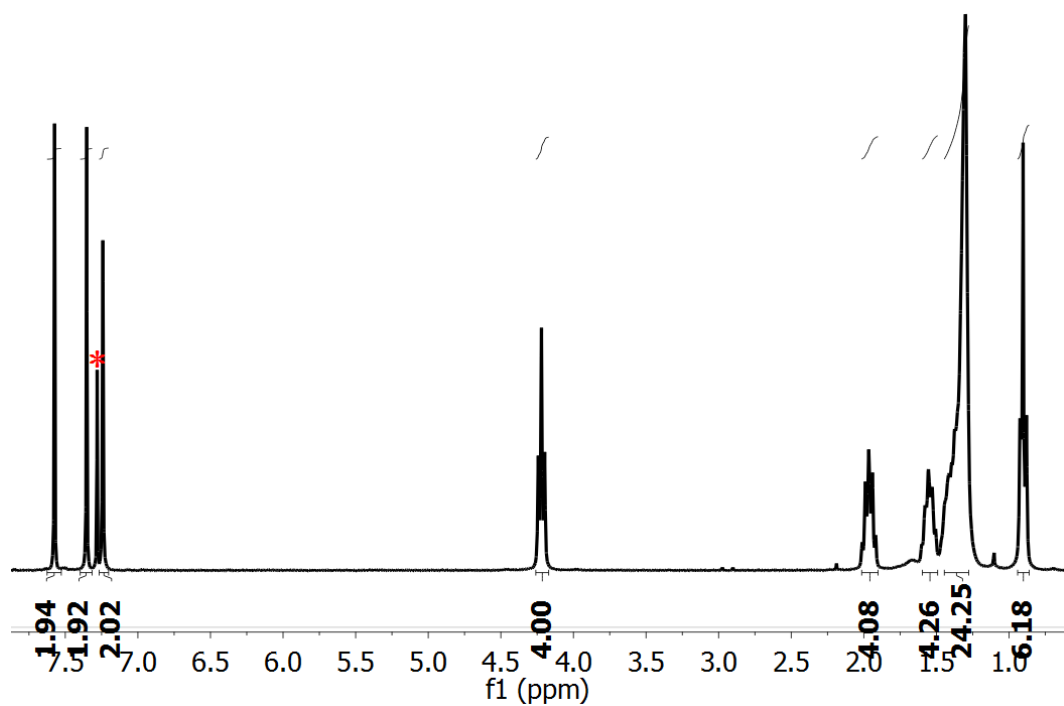


Figure S4 ¹H NMR spectrum of **2b** in CDCl₃.

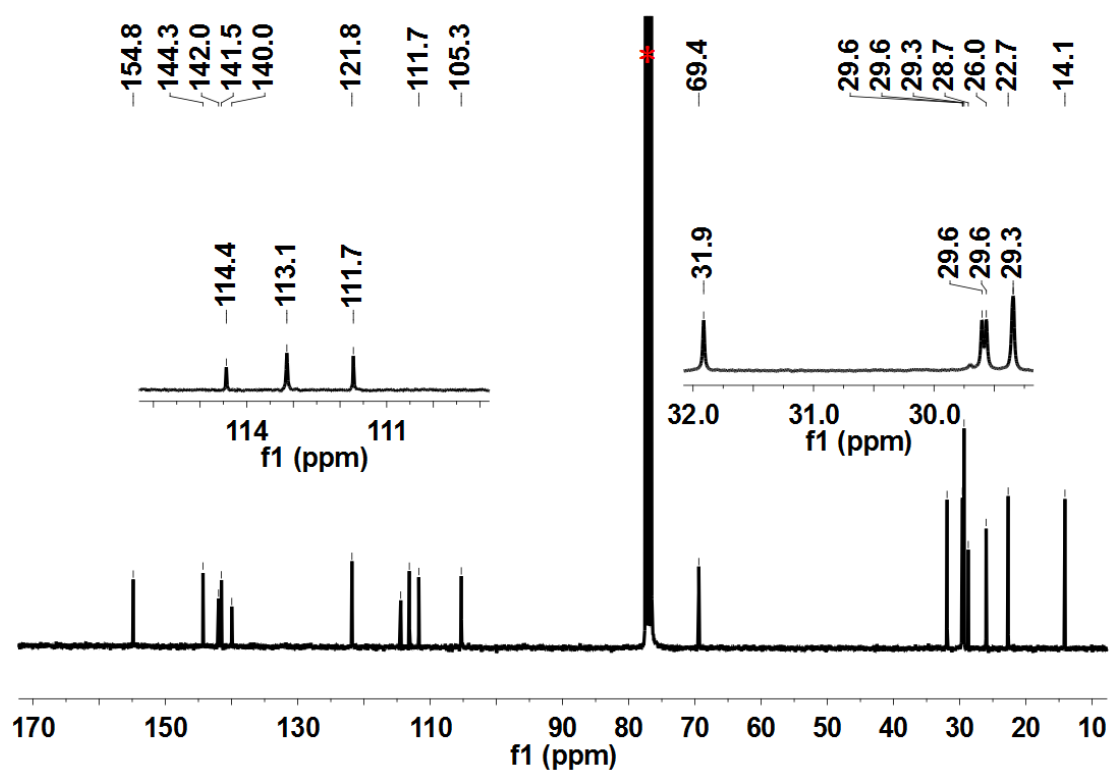


Figure S5 ¹³C NMR spectrum of **2b** in CDCl₃.

Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 39-40 H: 48-49 N: 3-4 O: 3-4

C40H49N4O4

G-43 (0.082)

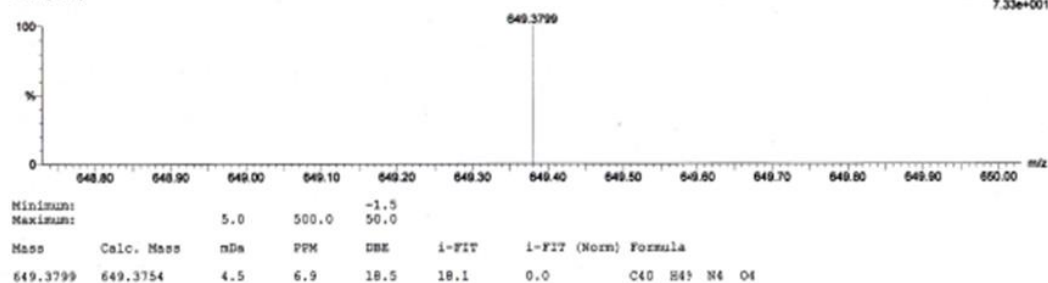
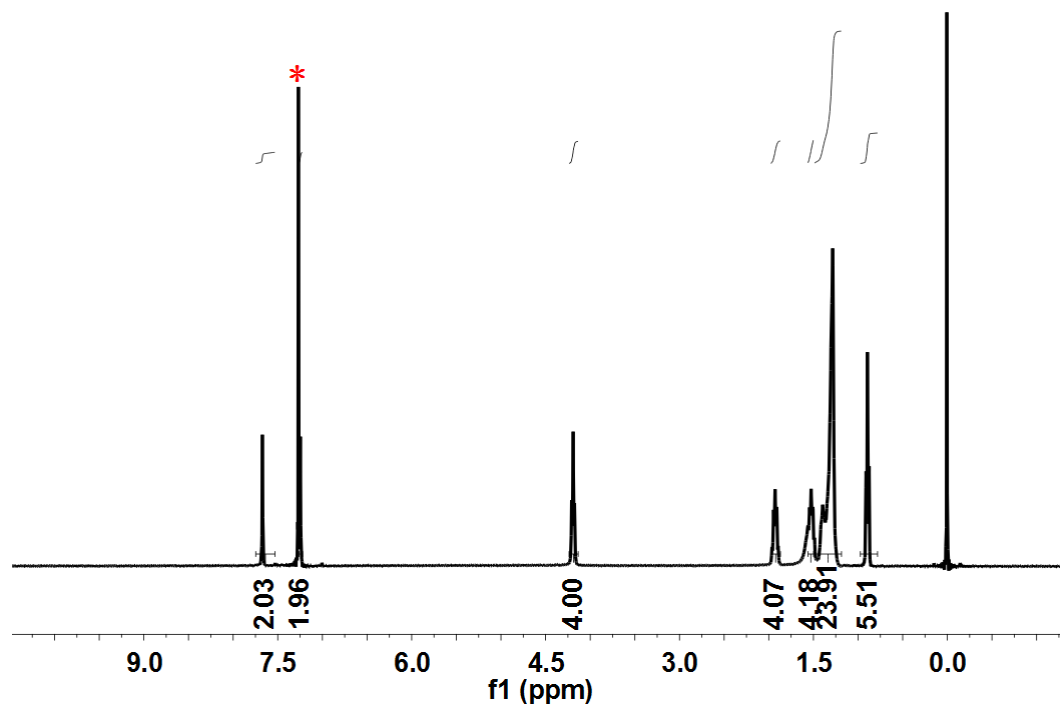
1: TOF MS ES+
7.33e+001

Figure S6 HRMS spectrum of 2b.

Figure S7 ¹H NMR spectrum of 2c in CDCl₃.

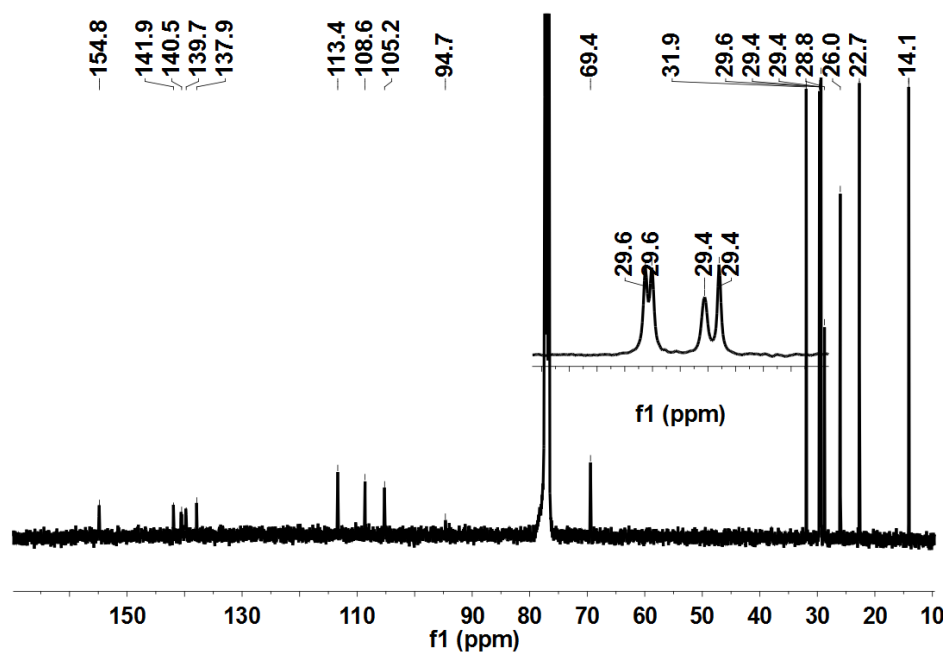


Figure S8 ^{13}C NMR spectrum of **2c** in CDCl_3

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

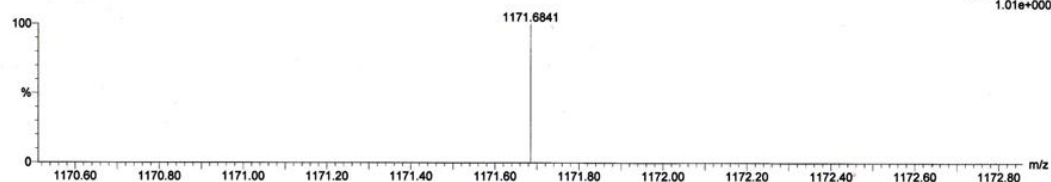
Elements Used:

C: 71-72 H: 92-94 O: 7-8 14N: 1-4 15N: 1-2

C72H93N8O8

G-1 11 (0.259)

1: TOF MS ES+
1.01e+000



Minimum:									
Maximum:	5.0	500.0	-1.5	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula		
1171.6841	1171.6996	-15.5	-13.2	29.5	11.1	0.0	C72 H93 O8 14N4 15N2		

Figure S9 MS spectrum of **2c**.

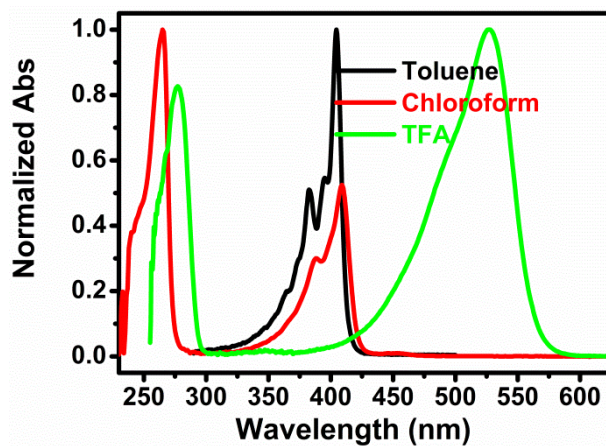


Figure S10 Normalized absorption spectra of **2a** recorded in different solvents.

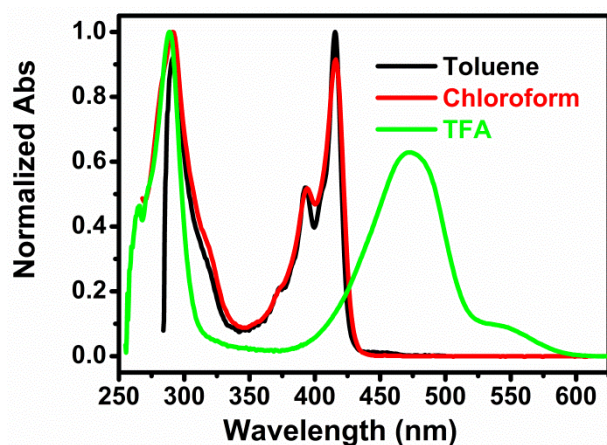


Figure S11 Normalized absorption spectra of **2b** recorded in different solvents.

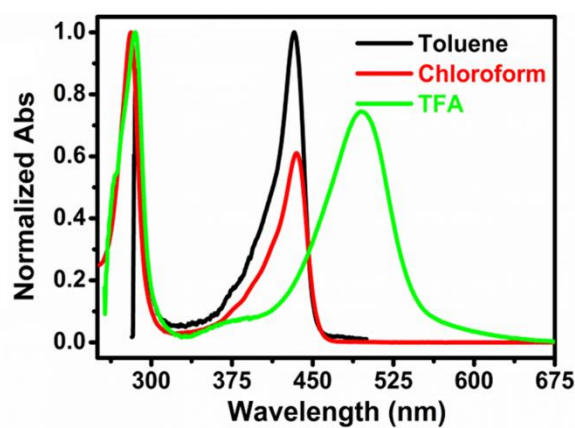


Figure S12 Normalized absorption spectra of **2c** recorded in different solvents.

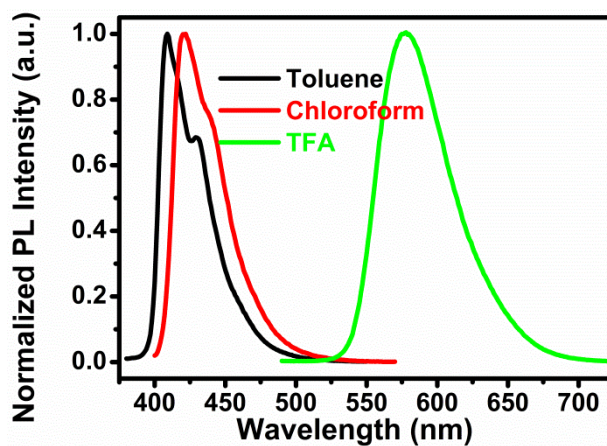


Figure S13 Normalized PL spectra of **2a** recorded in different solvents.

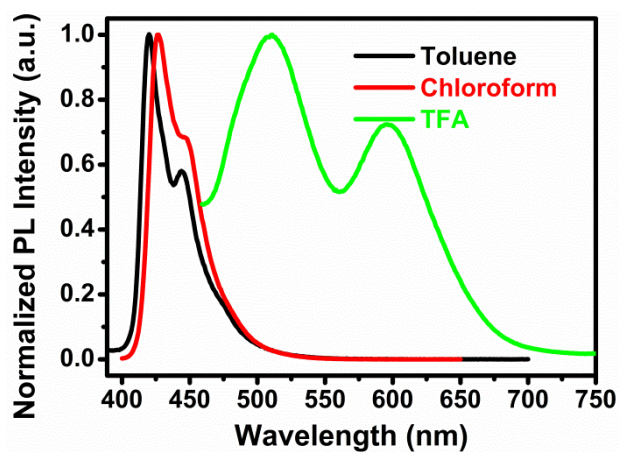


Figure S14 Normalized PL spectra of **2b** recorded in different solvents.

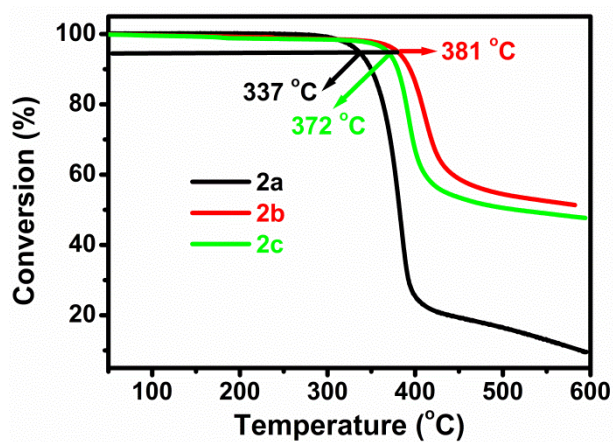


Figure S15 TGA curves of **2a**, **2b**, and **2c** with a heating rate of $20\text{ }^{\circ}\text{C min}^{-1}$ under N_2

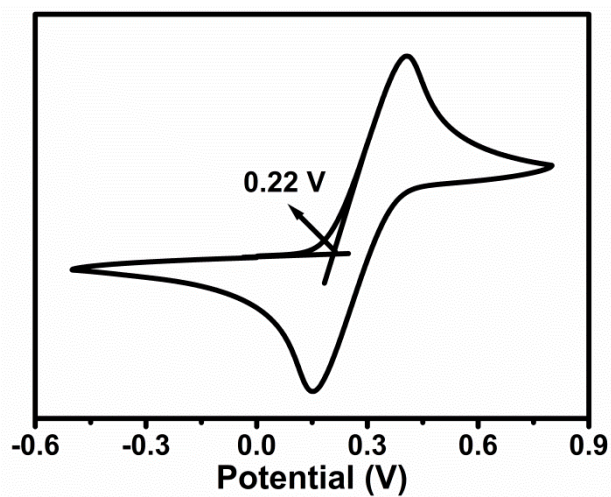


Figure S16 Cyclic voltammogram of the ferrocene standard in CH_2Cl_2 solution at the scan rate of 100 mV S^{-1} .



(A)



(B)



(C)

Figure S17 The crystal images of compounds **2a** (A), **2b** (B), and **2c** (C)