

Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022 Supporting Information

Supplementary Information

Novel Carbazole- and dioxino[2,3-b]pyrazine-based bipolar hosts for red PhOLEDs with a high brightness

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Content

Experimental section	1
General information	2
Fig. S1 The whole DSC analysis spectra of HF1 (a) and HF2 (b).	3
Fig. S2 The ^1H NMR spectrum of IM1.	4
Fig. S3 The ^{13}C NMR spectrum of IM1.	5
Fig. S4 The MS spectrum of IM1.	5
Fig. S5 The ^1H NMR spectrum of IM2.	6
Fig. S6 The ^{13}C NMR spectrum of IM2.	6
Fig. S7 The MS spectrum of IM2.	7
Fig. S8 The ^1H NMR spectrum of IM3.	7
Fig. S9 The ^{13}C NMR spectrum of IM3.	8
Fig. S10 The MS spectrum of IM3.	8
Fig. S11 The ^1H NMR spectrum of HF1.	9
Fig. S12 The ^{13}C NMR spectrum of HF1.	10
Fig. S13 The MS spectrum of HF1.	10
Fig. S14 The ^1H NMR spectrum of HF2.	11
Fig. S15 The ^{13}C NMR spectrum of HF2.	12
Fig. S16 The MS spectrum of HF2.	12

Experimental section

General information

Chemicals and solvents used in the process were reagent grades and purchased from J&K Chemical Co. and Shanghai Taoe Chemical Co. without further purification. All reactions and manipulations were carried out under N₂ atmosphere. The ¹H and ¹³C NMR spectra were measured using a Bruker Ascend 600 spectrometer. Mass spectra were obtained on a Waters LCT Premier XE spectrometer. The ultraviolet-visible (UV-Vis) absorption spectra of the samples were characterized using a Varian Cary 500 spectrophotometer. Photoluminescence (PL) measurements were conducted by a Varian-Cary fluorescence spectrophotometer at room temperature. The cyclic voltammetry experiments were performed by a Versastat II electrochemical workstation (Princeton applied research) using a conventional three-electrode configuration with a glassy carbon working electrode, a Pt wire counter electrode, and a regular calomel reference electrode in saturated KCl solution, 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF₆) in dichloromethane solution as the supporting electrolyte with a scan rate of 100 mV/s. The differential scanning calorimetry (DSC) analysis was performed under a nitrogen atmosphere using a NETZSCH STA 409 PC/PG instrument with a heating scan rate of 10 °C/min. Thermogravimetric analysis (TGA) was carried out using a TGA instrument under a nitrogen atmosphere with a heating scan rate of 10 °C/min.

All OLEDs were fabricated on the pre-patterned indium tin oxide (ITO) glass substrate with sheet resistance of 10Ω/□. OLEDs have an active area of 3.0×3.0 mm², defined by the overlap between the ITO anode and Al cathode. The ITO substrates were cleaned first with acetone, deionized water and acetone, and then dried in drying cabinet, and treated with ultraviolet-ozone for 15 min. After these processes, the cleaned ITO glass substrates were loaded in a vacuum chamber, a base pressure of ≤ 5×10⁻⁴ Pa, for film deposition using thermal evaporation technology. The deposition

rate and film thickness were monitored and controlled by the calibrated crystal quartz sensors, e.g., the deposition rates of organic materials, MoO₃, LiF, and cathode Al were controlled at about 1 Å/s, 0.3 Å/s, 0.1 Å/s, and 3–6 Å/s, respectively.

The EL spectra and CIE coordinates of all OLEDs were measured by a computer controlled PR-655 spectra scan spectrometer. The current density-voltage-luminance characteristics, current efficiency, and power efficiency were recorded by a computer-controlled Keithley 2400 source integrated with a BM-70A luminance meter. The EQE was calculated from the current density-voltage-luminance curve and spectra data. All samples were immediately characterized after thin films deposition without encapsulation in ambient atmosphere at room temperature.

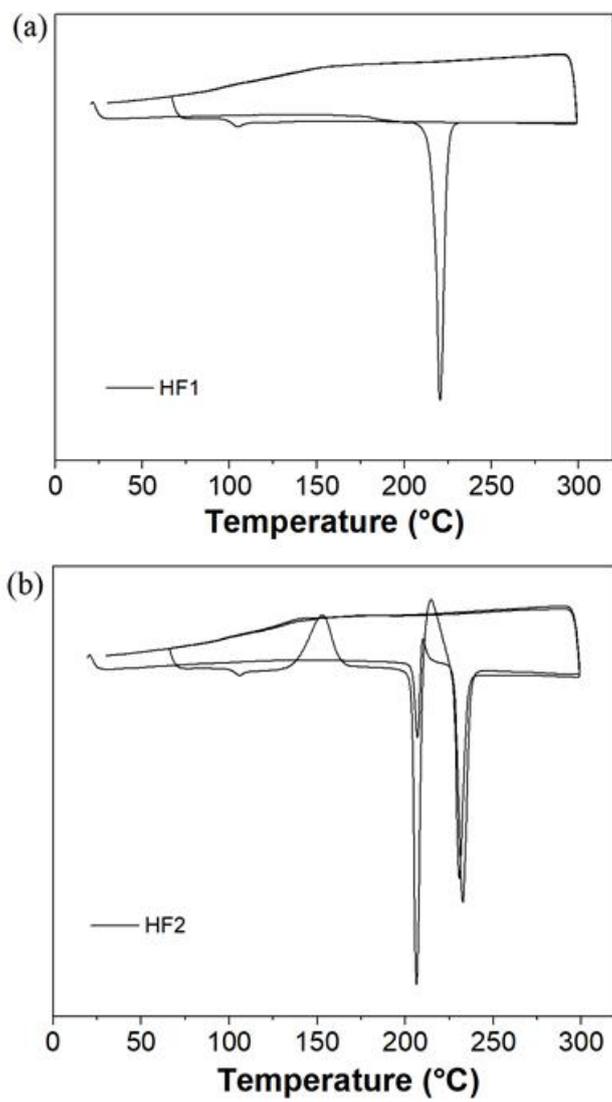


Fig. S1 The whole DSC analysis spectra of **HF1** (a) and **HF2** (b).

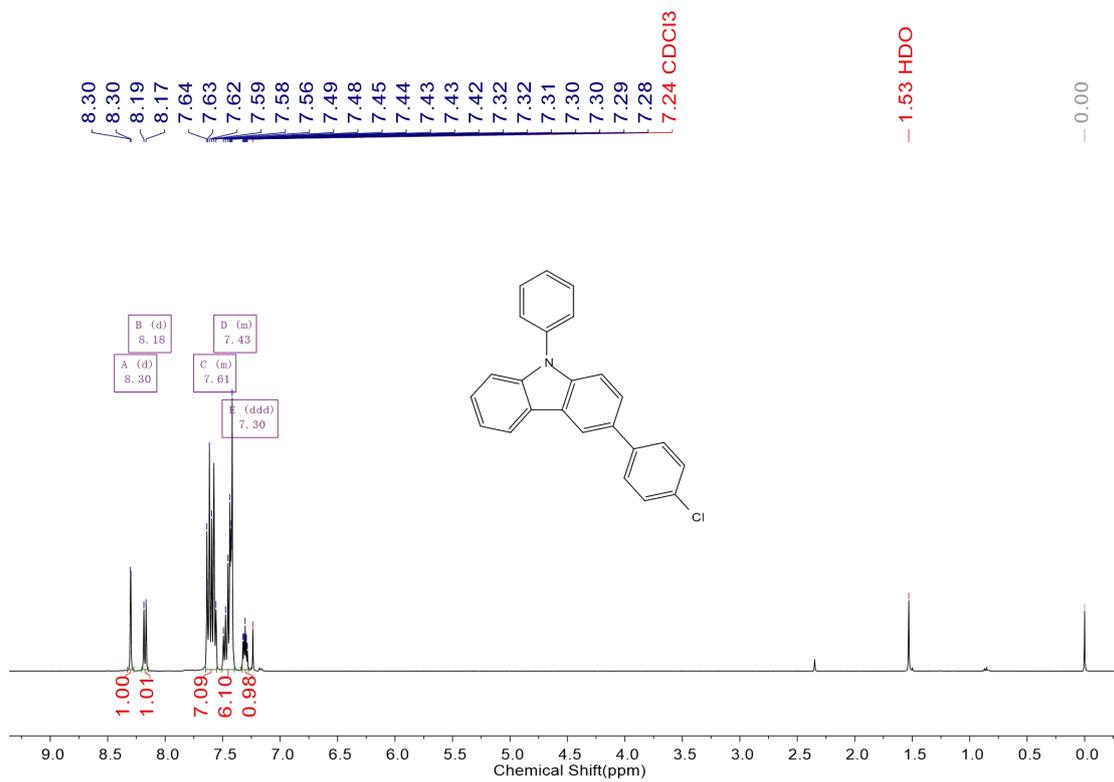


Fig. S2 The ^1H NMR spectrum of IM1.

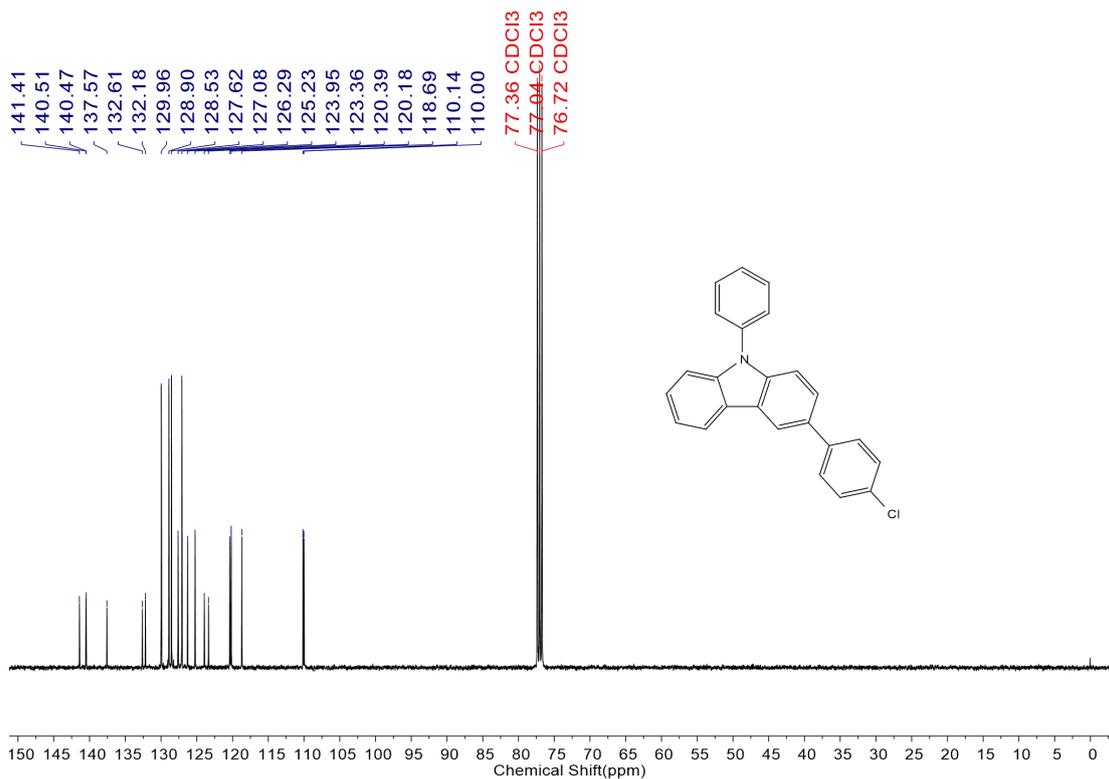


Fig. S3 The ^{13}C NMR spectrum of **IM1**.

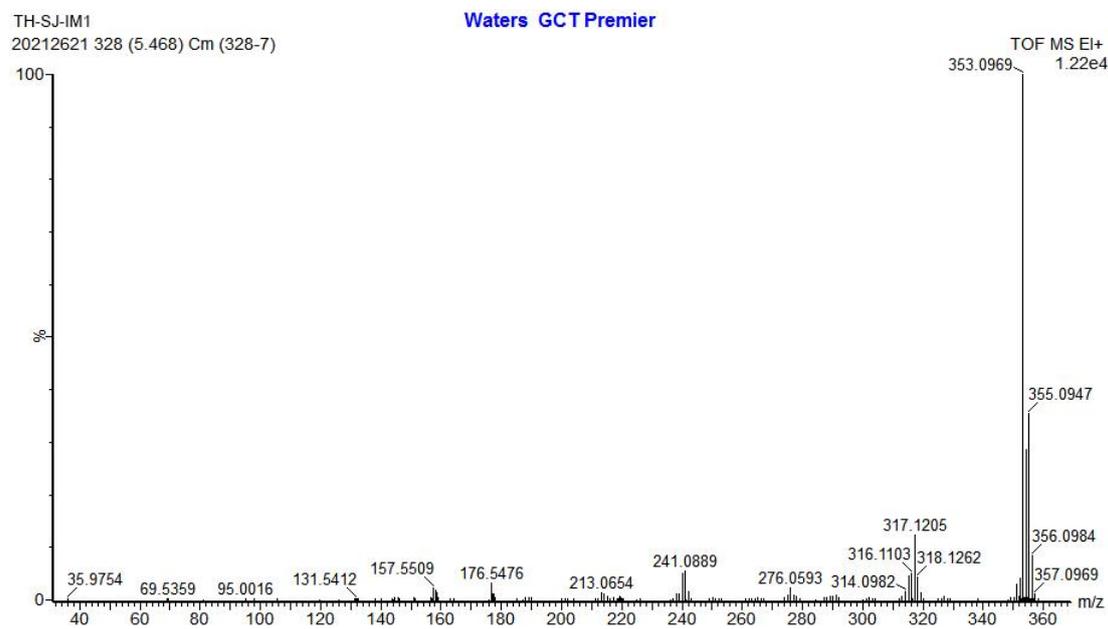


Fig. S4 The MS spectrum of **IM1**.

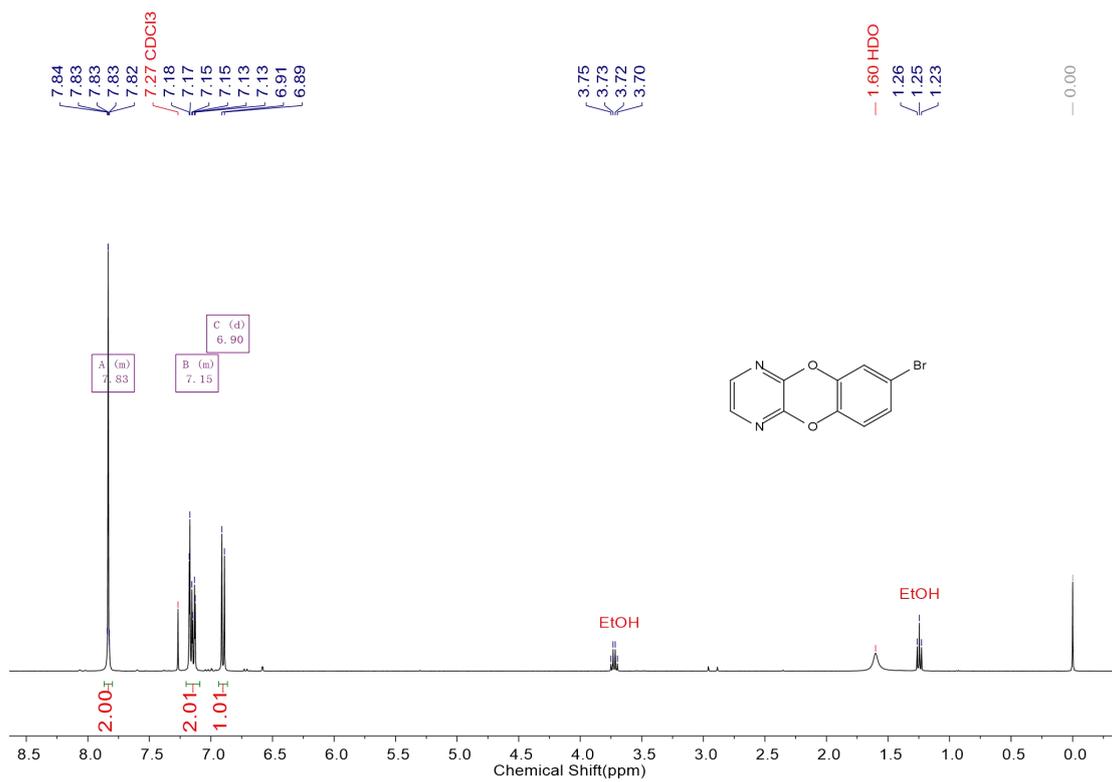


Fig. S5 The ¹H NMR spectrum of IM2.

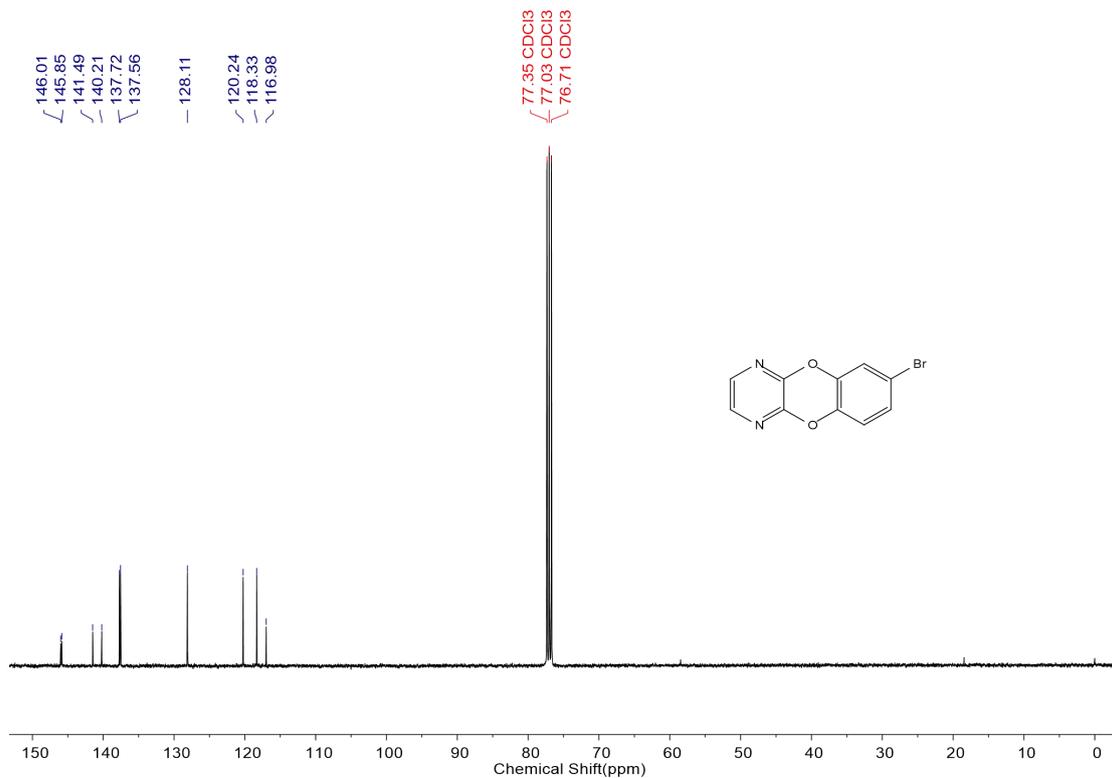


Fig. S6 The ^{13}C NMR spectrum of **IM2**.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

16 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-10 H: 0-7 N: 0-2 O: 0-2 Br: 0-1

TH-SJ-IM2 38 (0.446) Cm (38.39)

1: TOF MS ES+
9.94e+001

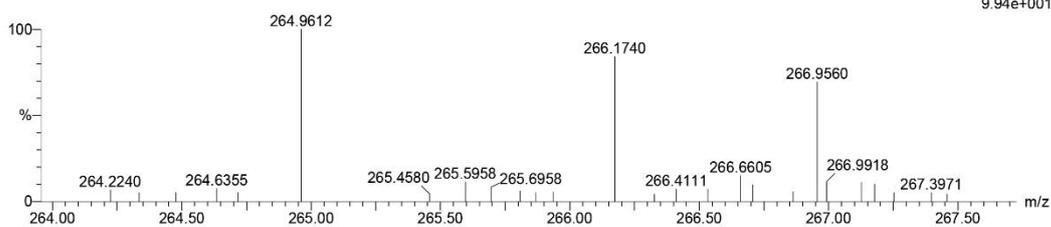


Fig. S7 The MS spectrum of **IM2**.

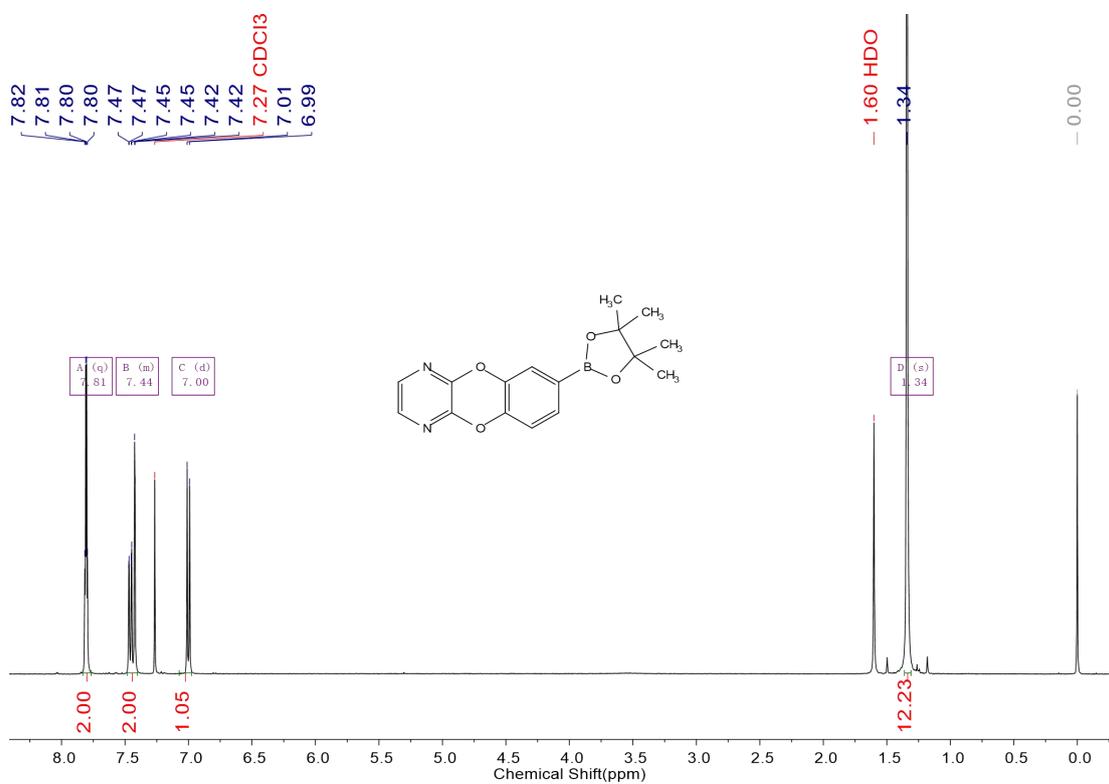


Fig. S8 The ^1H NMR spectrum of **IM3**.

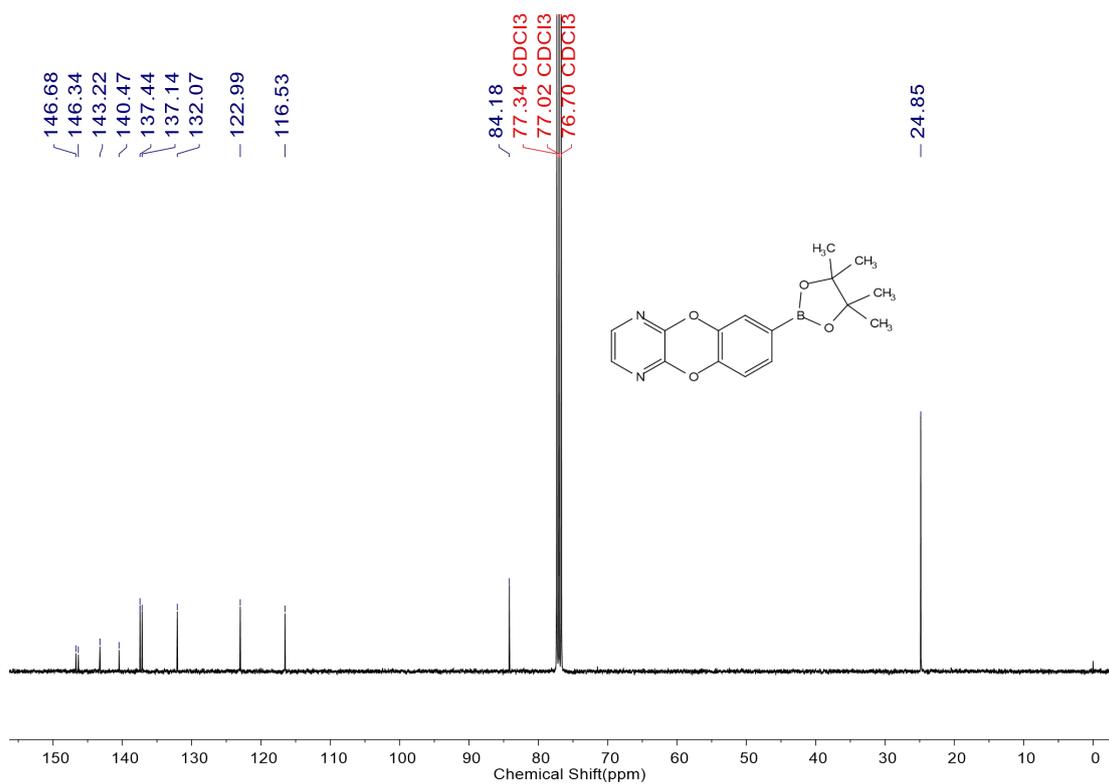


Fig. S9 The ^{13}C NMR spectrum of **IM3**.

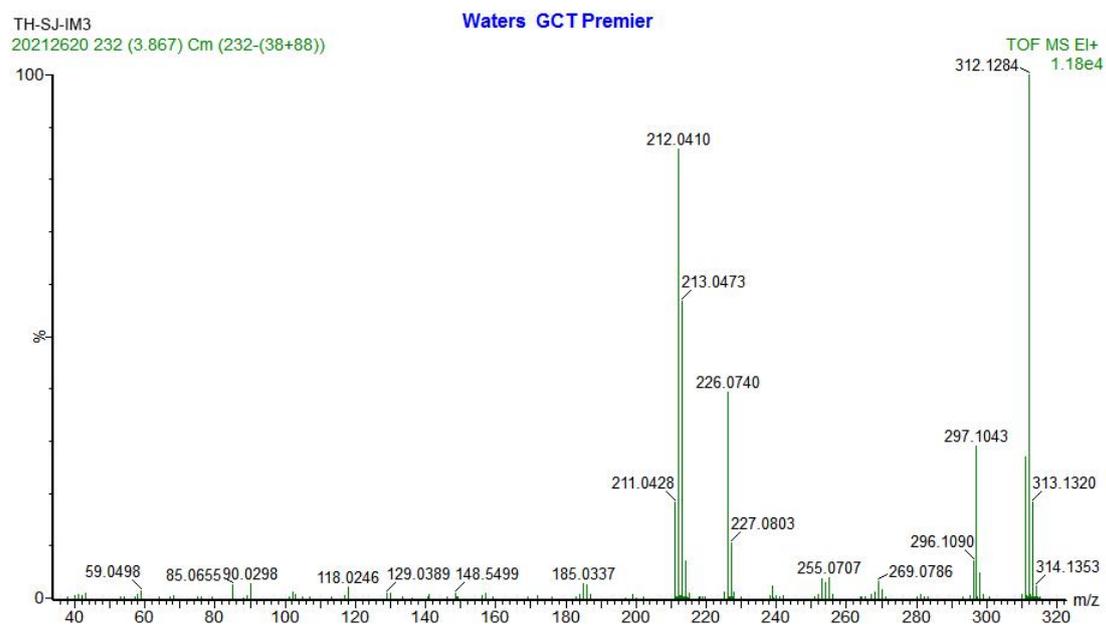


Fig. S10 The MS spectrum of **IM3**.

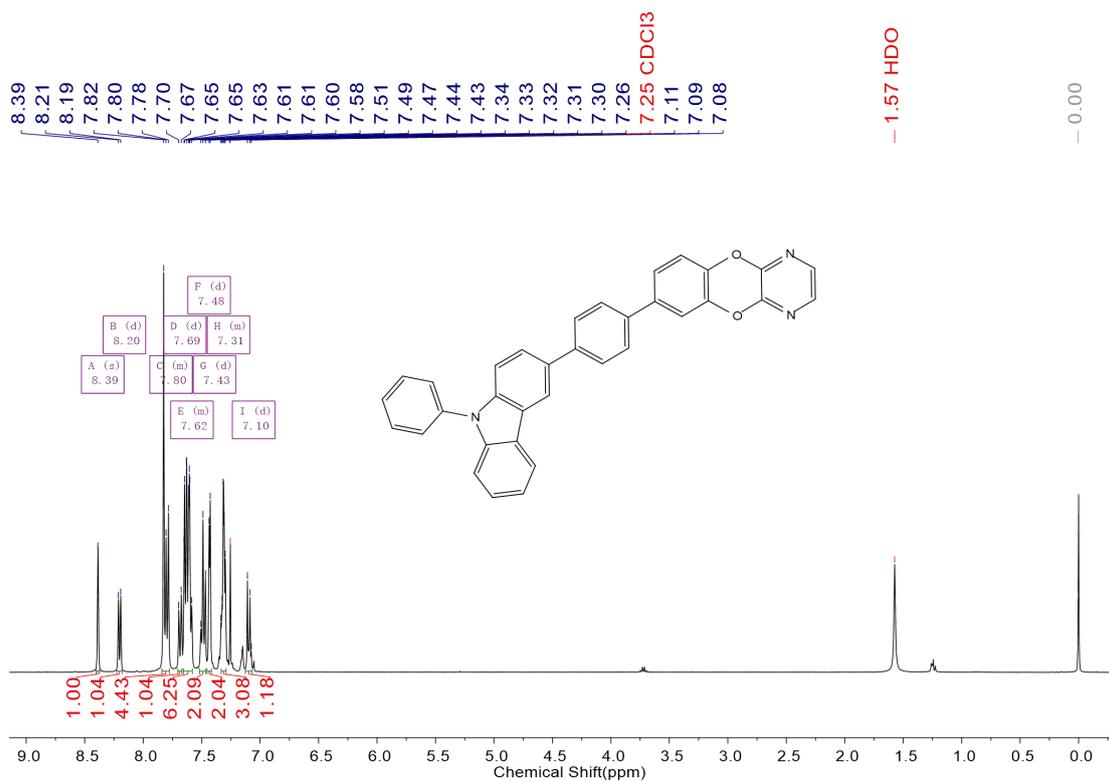


Fig. S11 The ¹H NMR spectrum of **HF1**.

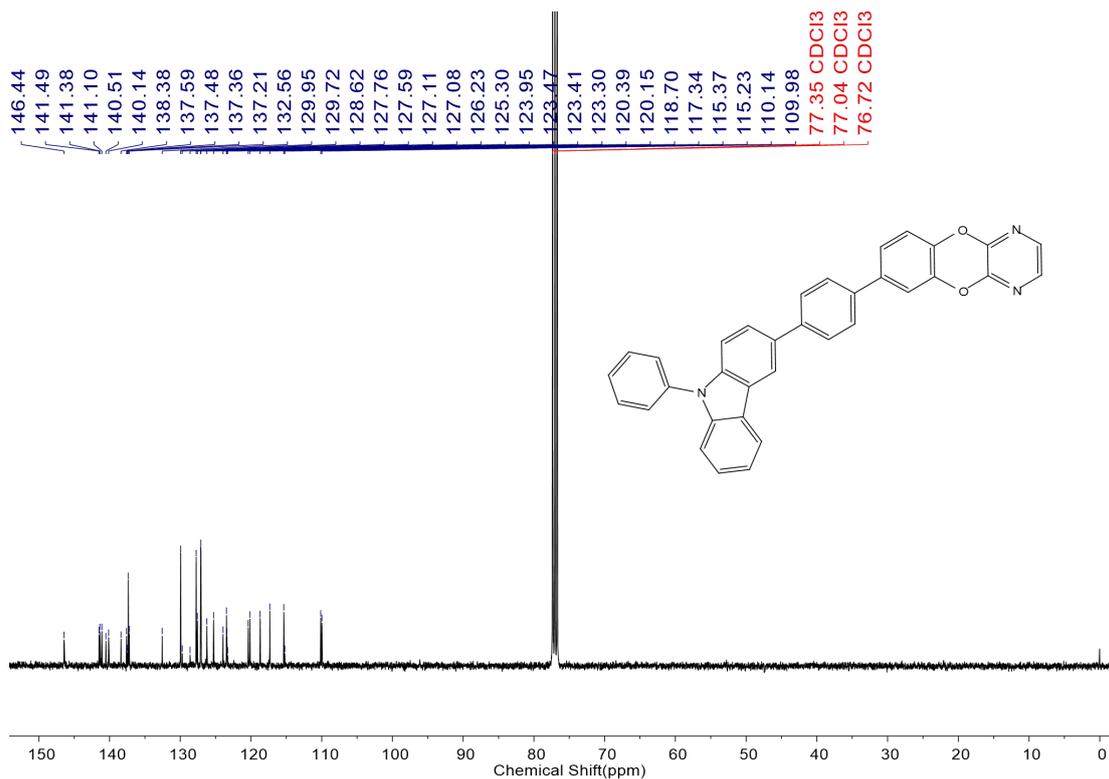


Fig. S12 The ^{13}C NMR spectrum of **HF1**.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

26 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-34 H: 0-22 N: 0-3 O: 0-2 Br: 0-1

TH-SJ-HF1 103 (1.172) Cm (98:107)

1: TOF MS ES+
4.04e+002

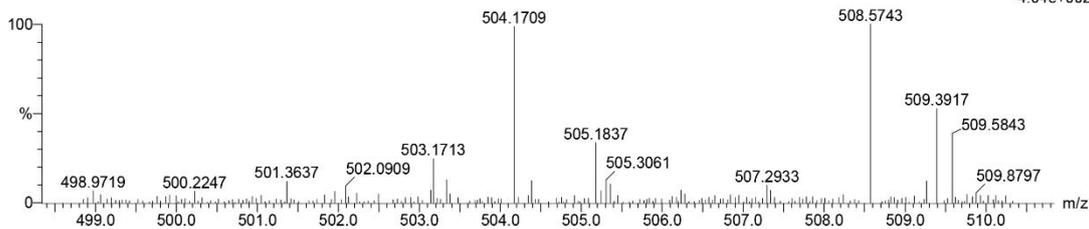


Fig. S13 The MS spectrum of **HF1**.

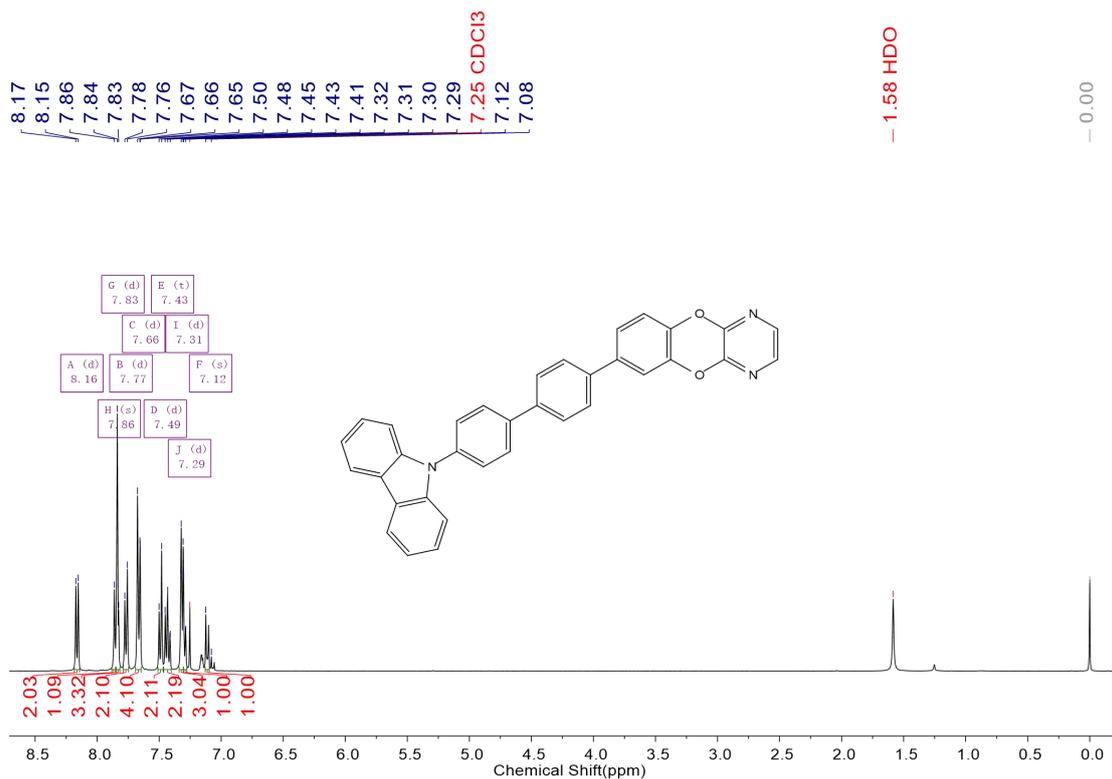


Fig. S14 The ¹H NMR spectrum of HF2.

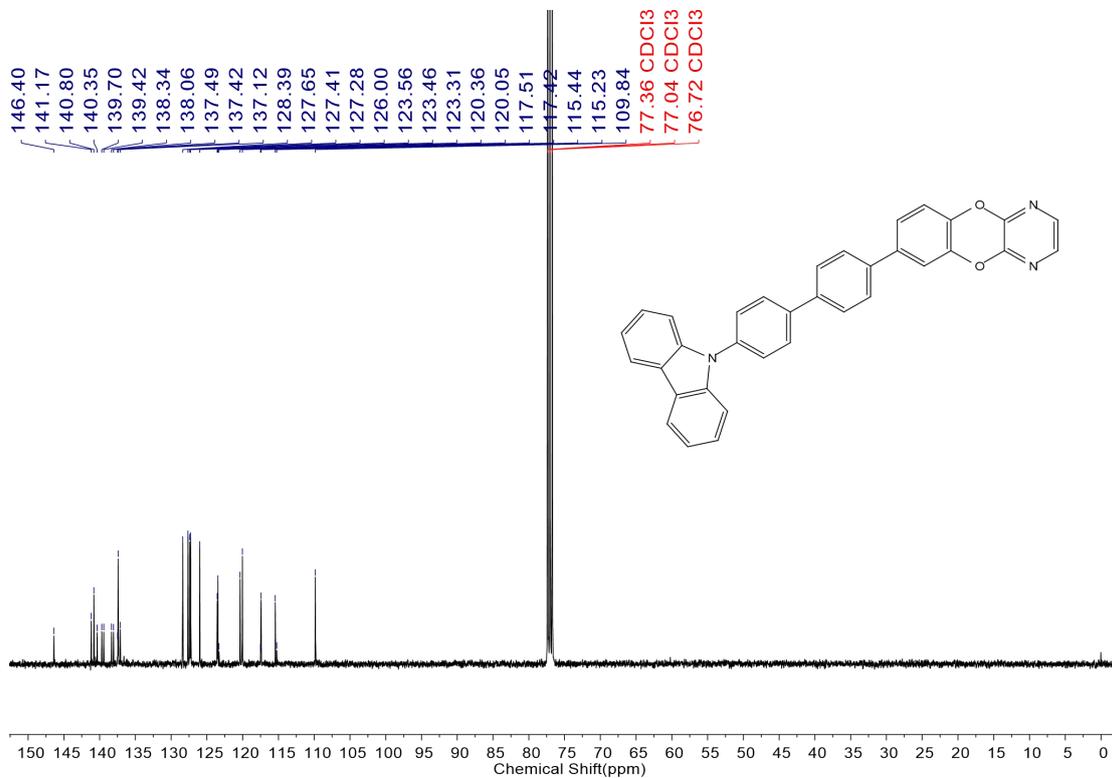


Fig. S15 The ^{13}C NMR spectrum of **HF2**.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

26 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-34 H: 0-22 N: 0-3 O: 0-2 Br: 0-1

TH-SJ-HF2 52 (0.581) Cm (52:56)

1: TOF MS ES+
1.28e+002

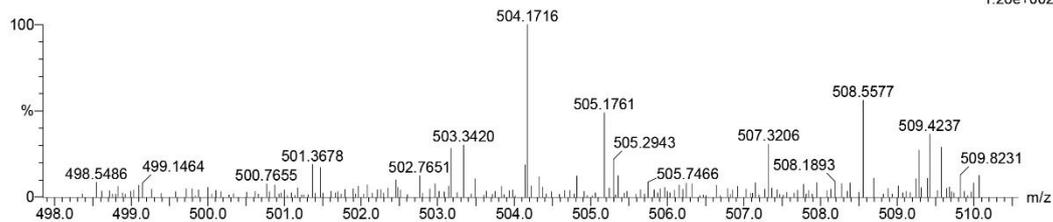


Fig. S16 The MS spectrum of **HF2**.