

Small organic molecules based on oxazole/thiazole with
excellent performances for green and red phosphorescent
organic light-emitting diodes

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Fig. S1-S4. The normalized emission spectra of 2a-2d in different solvents at the concentration of 1.0×10^{-5} .

Fig. S5-S16. The ¹H NMR, ¹³C NMR and HRMS spectra of 2a-2d.

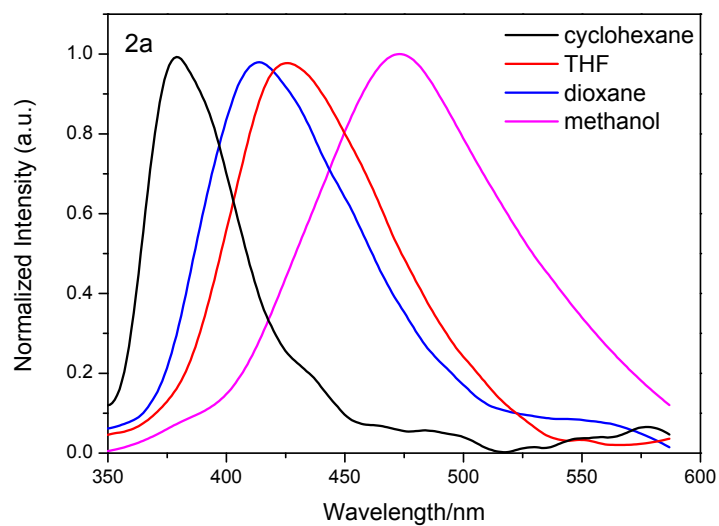


Fig. S1. The normalized emission spectra of 2a in different solvents at the concentration of 1.0×10^{-5} .

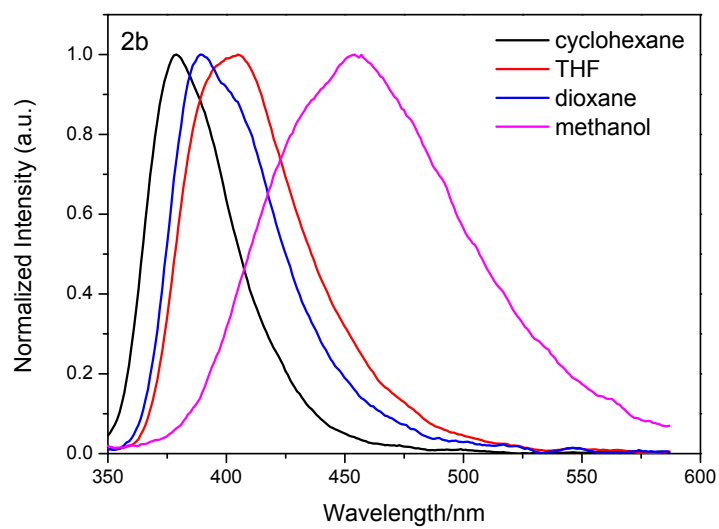


Fig. S2. The normalized emission spectra of 2b in different solvents at the concentration of 1.0×10^{-5} .

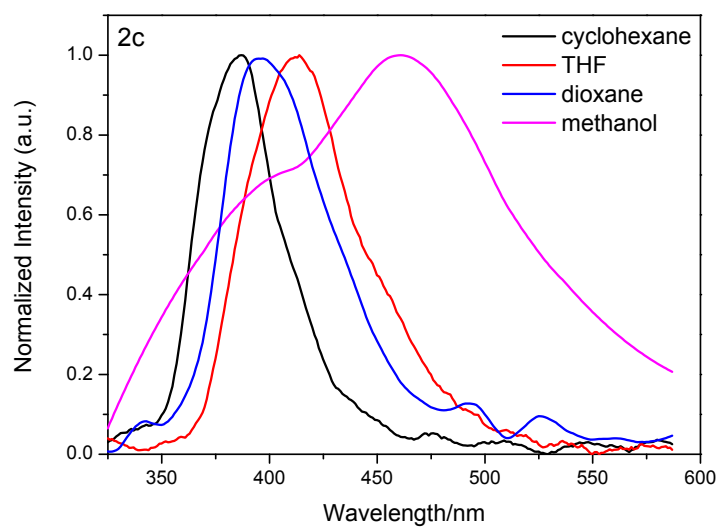


Fig. S3. The normalized emission spectra of 2c in different solvents at the concentration of 1.0×10^{-5} .

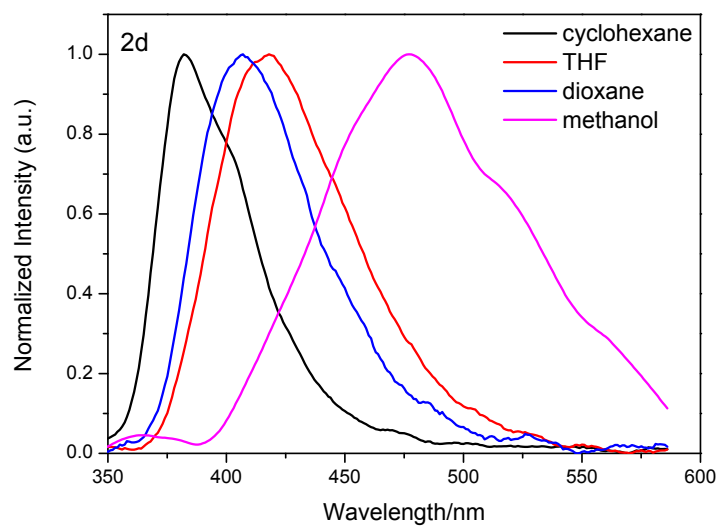


Fig. S4. The normalized emission spectra of 2d in different solvents at the concentration of 1.0×10^{-5} .

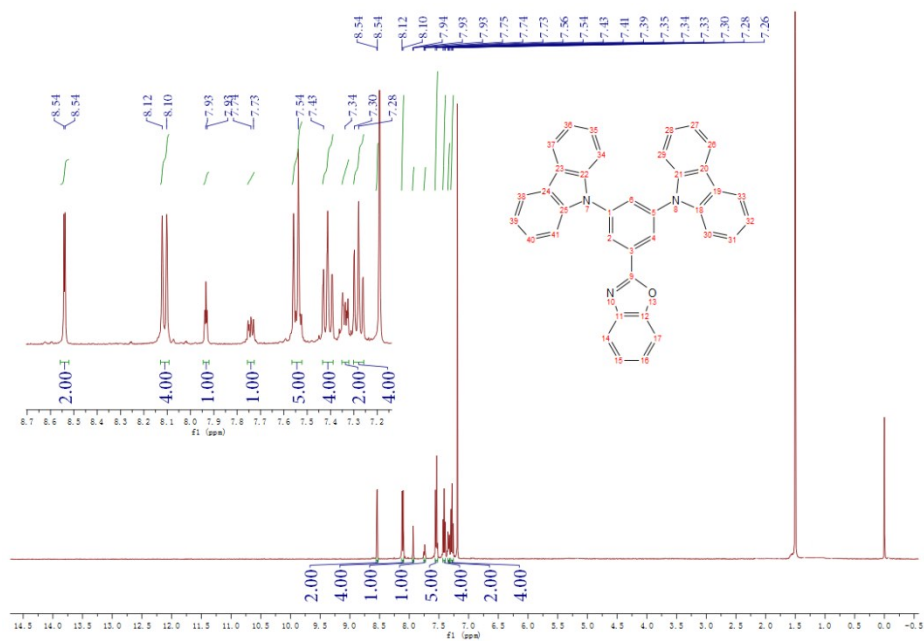


Fig.S5. The ¹H NMR spectra of 2a.

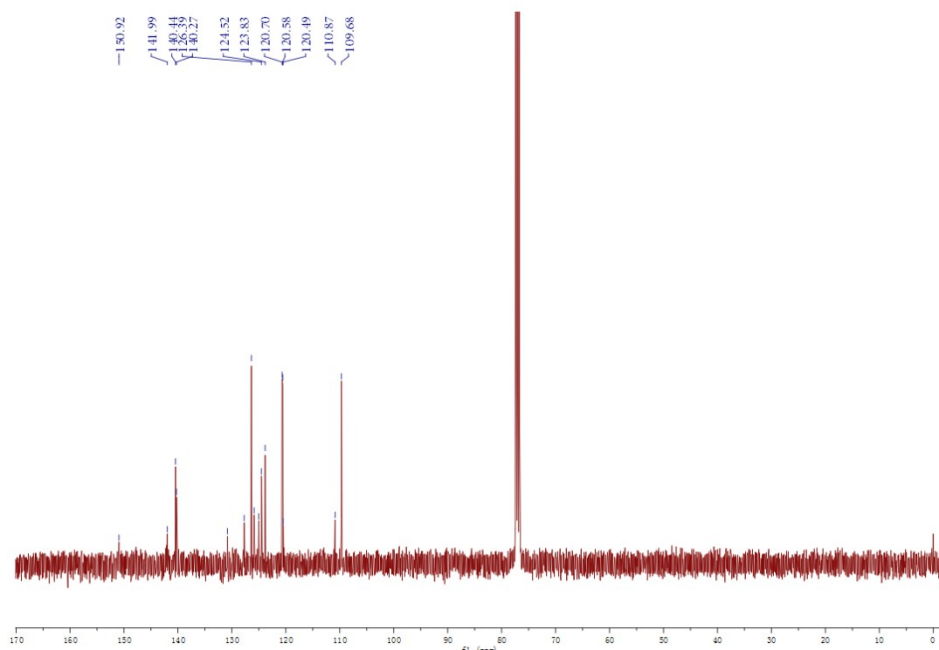


Fig.S6. The ¹³C NMR spectra of 2a.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 0-49 H: 0-32 N: 0-3 S: 0-1

H-TIAN

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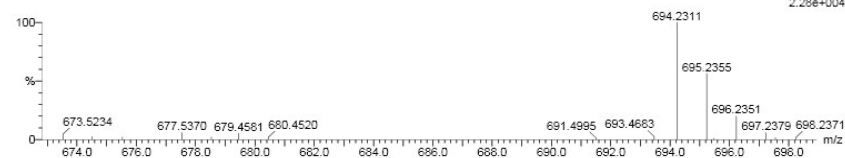
29-Oct-2015

19:58:27

1: TOF MS ES+

2.28e+004

TH-TGJ-3 198 (1.313) Cm (186.201)



Minimum:								
Maximum:								
Mass	Calc. Mass	mDa	PFM	DBE	i-FIT	i-FIT (Norm)	Formula	
694.2311	694.2317	-0.6	-0.9	35.5	20.1	0.0	C49 H32 N3 S	

Fig.S7. The HRMS spectra of 2a.

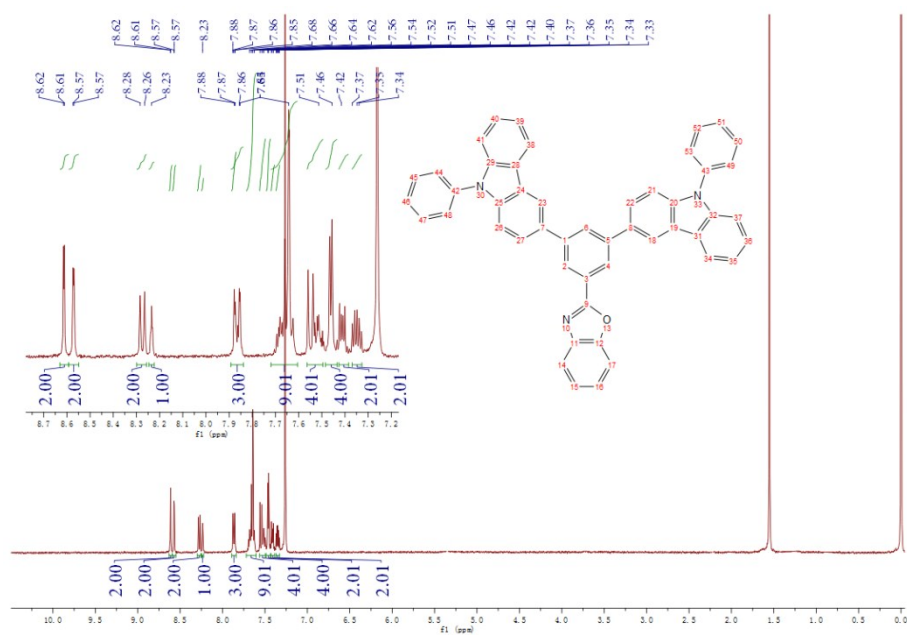


Fig.S8. The ¹H NMR spectra of 2b.

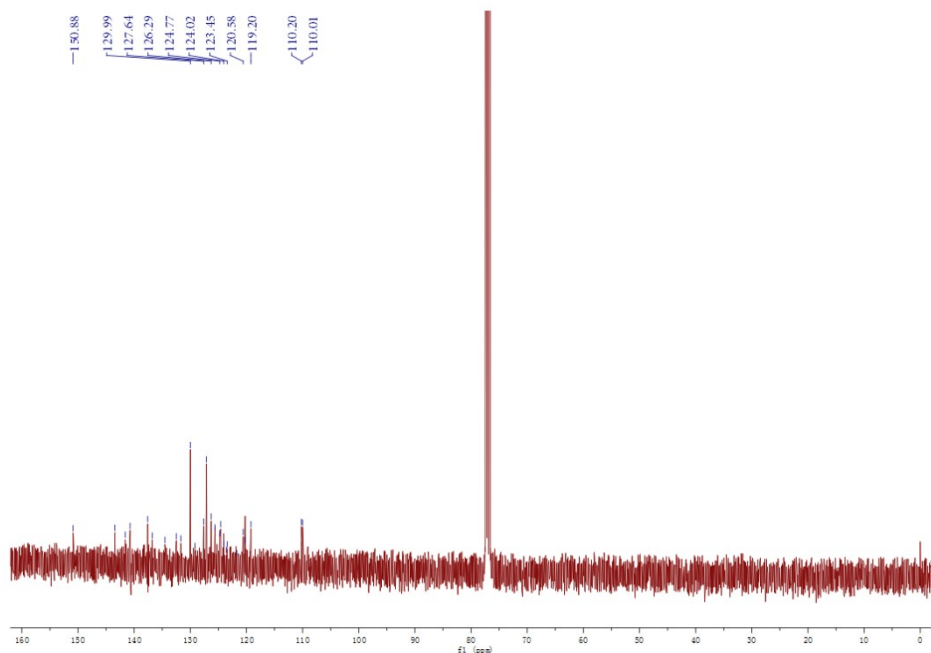


Fig.S9. The ^{13}C NMR spectra of 2b.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 0-49 H: 0-32 N: 0-3 O: 0-1

H-TIAN

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TH-TGJ-1 43 (0.354) Cm (38.46)

29-Oct-2015

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1: TOF MS ES+

6.51e+003

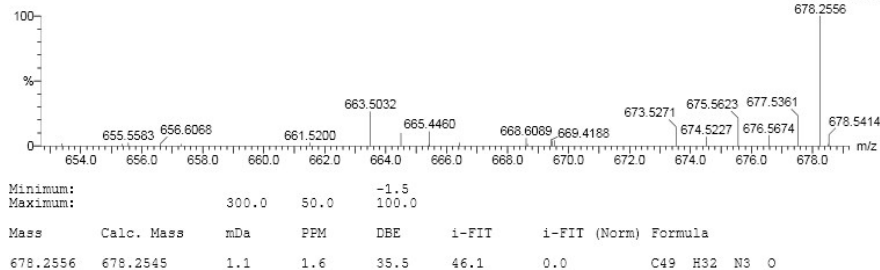


Fig.S10. The HRMS spectra of 2b.

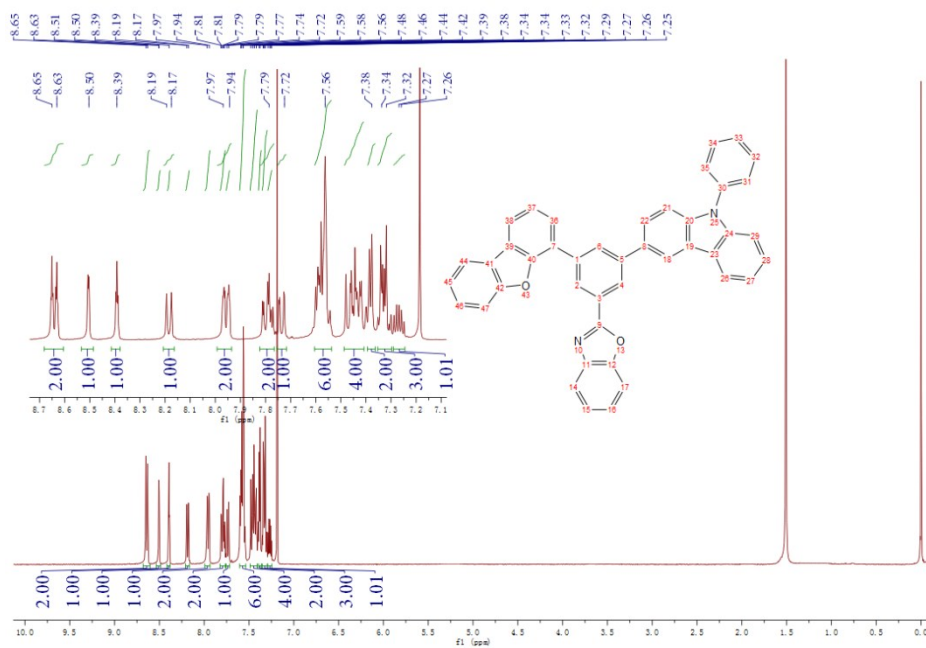


Fig.S11. The ¹H NMR spectra of 2c.

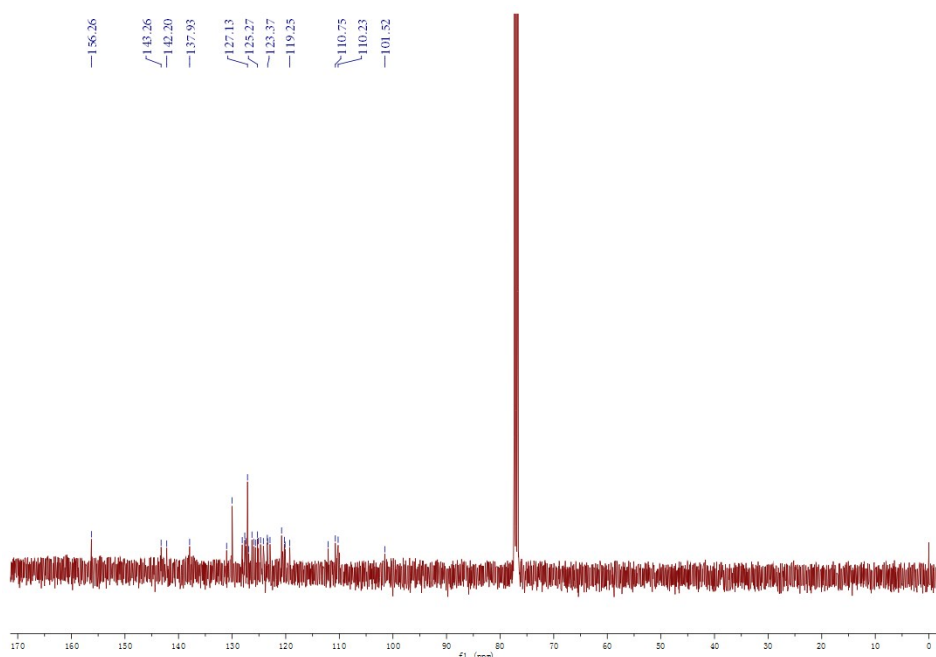


Fig.S12. The ¹³C NMR spectra of 2c.

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 0-43 H: 0-27 N: 0-2 O: 0-2

H-TIAN

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29-Oct-2015

20:18:55

1: TOF MS ES+

5.34e+003

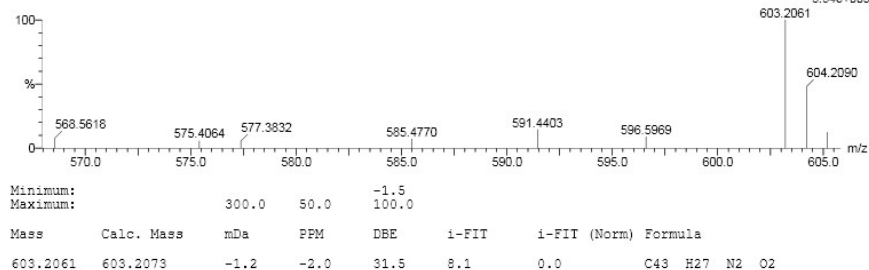
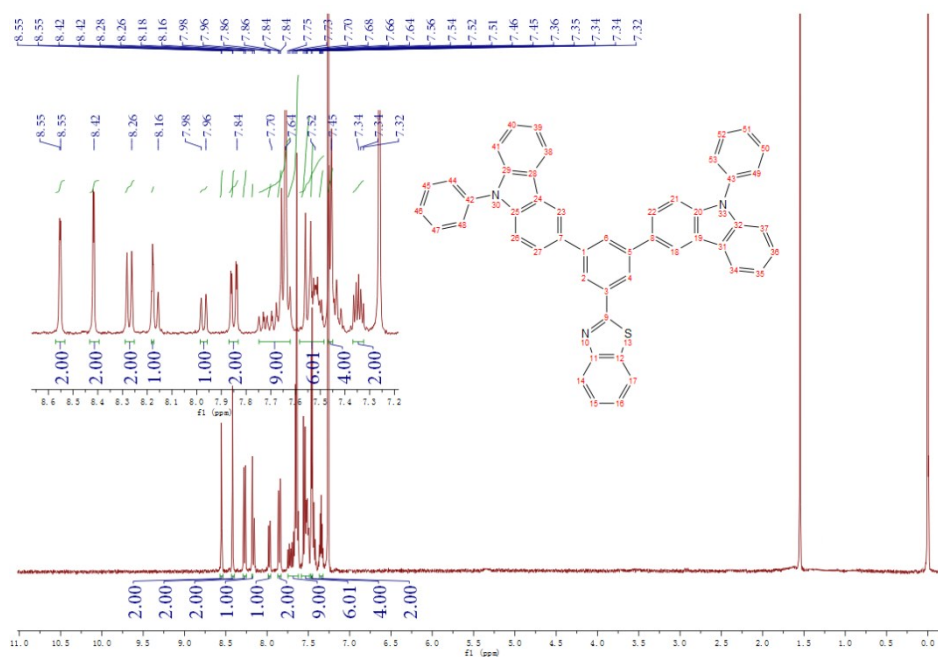


Fig.S13. The HRMS spectra of 2c.

Fig.S14. The ^1H NMR spectra of 2d.

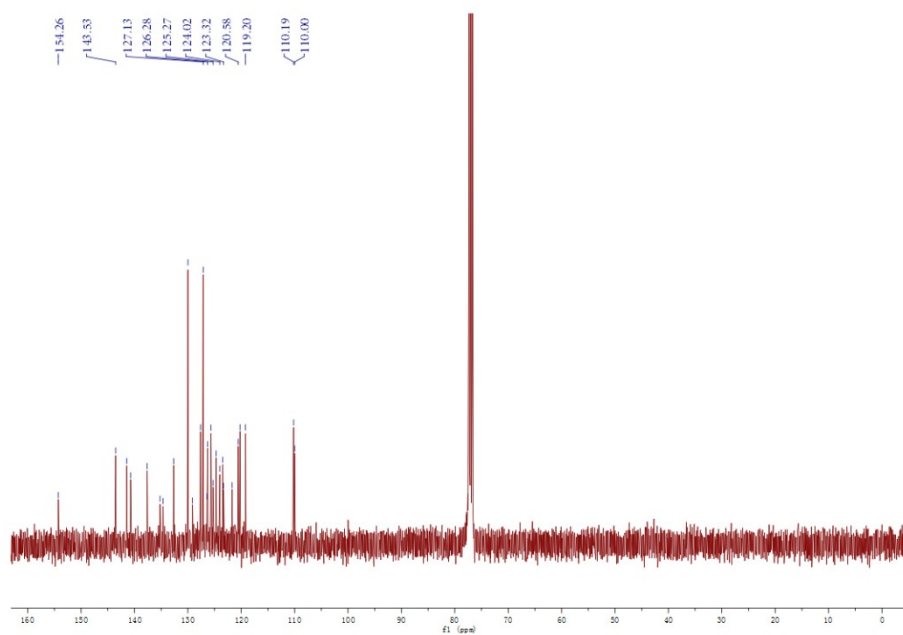


Fig.S15. The ^{13}C NMR spectra of 2d.

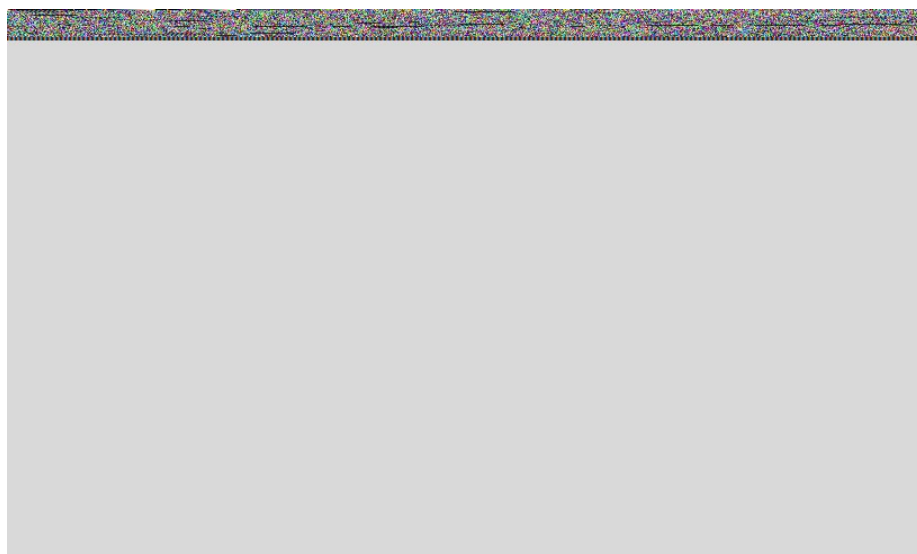


Fig.S16. The HRMS spectra of 2d.