

Supporting information

Synthesis and Bioimaging of Mitochondria Targeted Nitroreductase-Responsive Fluorescent Probe

Yixuan Li ^a, Wenjun Bai ^b, Yating Bao ^c, Jinhui Wang ^b, Jingbo Hu ^{a,*}, Jing Huang ^{c,*}

^a Faculty of Materials Science and Chemical Engineering, Ningbo University, Ningbo 315211, China.

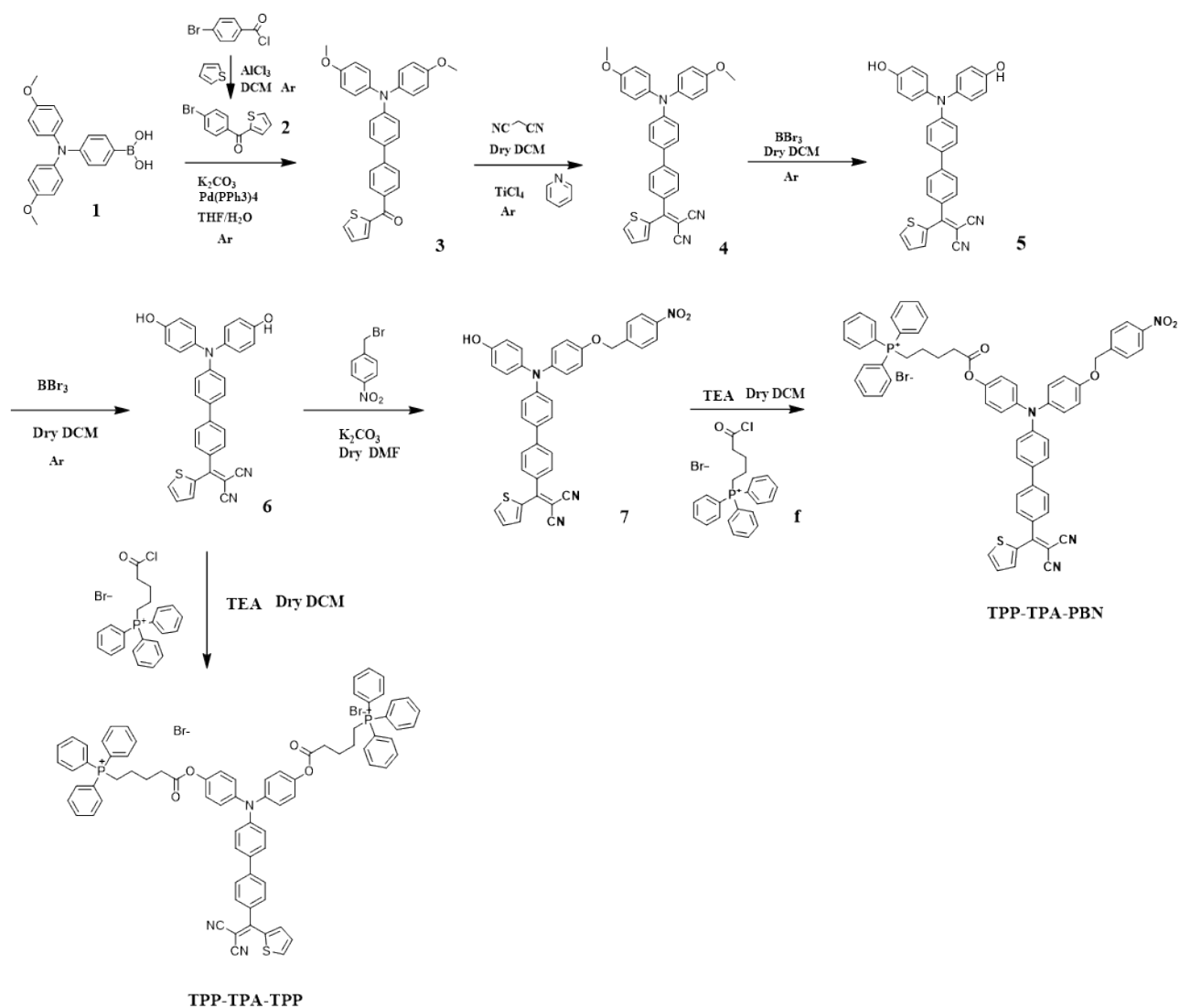
^b Institute of Drug Discovery Technology, Ningbo University, Ningbo 315211, China.

^c Department of Hepato-Pancreato-Biliary Surgery, Ningbo Medical Center Lihuili Hospital, The Affiliated Hospital of Ningbo University, Ningbo 315211, China.

* Corresponding authors: Jing Huang, Department of Hepato-Pancreato-Biliary Surgery, Ningbo Medical Center Lihuili Hospital, The Affiliated Hospital of Ningbo University, Ningbo 315211, China. E-mail: Huangjingonline@163.com

Jing-Bo Hu, School of Materials Science and Chemical Engineering, Ningbo University, Ningbo 315211, China. E-mail: hujingbo@nbu.edu.cn

1. synthesis routine



Scheme 1. The synthesis routine of the probe TPP-TPA-PBN and control molecule was showed.

2. ^1H NMR, ^{13}C NMR and mass spectrum (HR-MS)

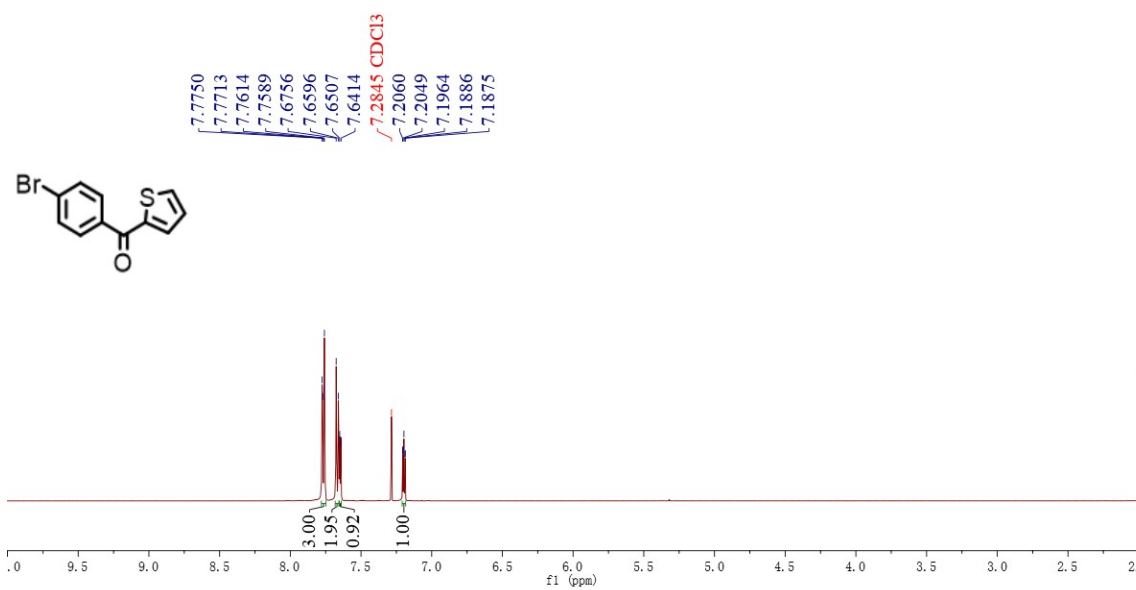


Fig. S1 ¹H NMR spectrum of compound 2 (500 MHz, Chloroform-d).

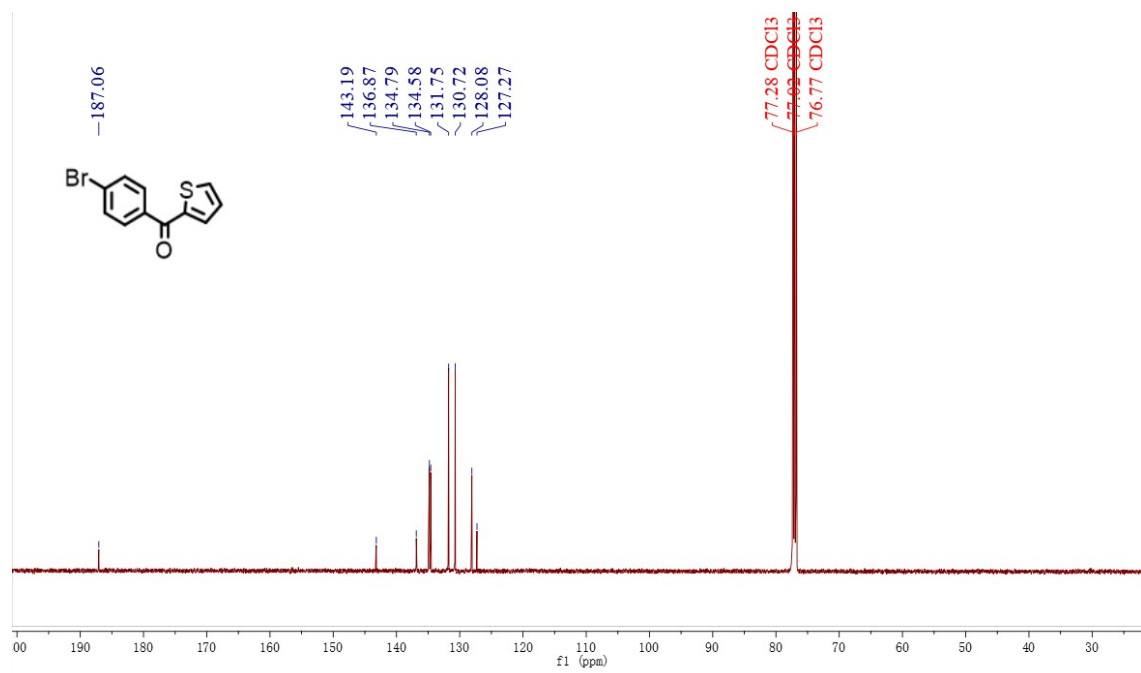


Fig. S2 ¹³C NMR spectrum of compound 2 (126 MHz, Chloroform-d).

BWJ-T-1-2+ #196-278 RT: 1.07-1.49 AV: 83 NL: 1.36E8
T: FTMS + p ESI Full ms [100.0000-1200.0000]

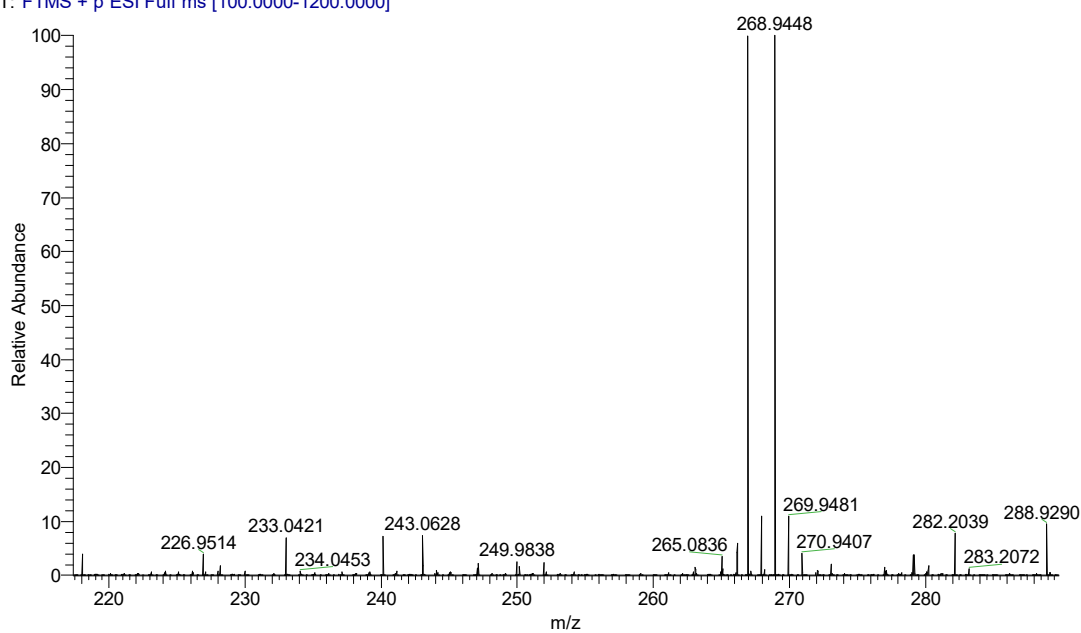


Fig. S3 High resolution mass spectrum (HR-MS) of compound 2.

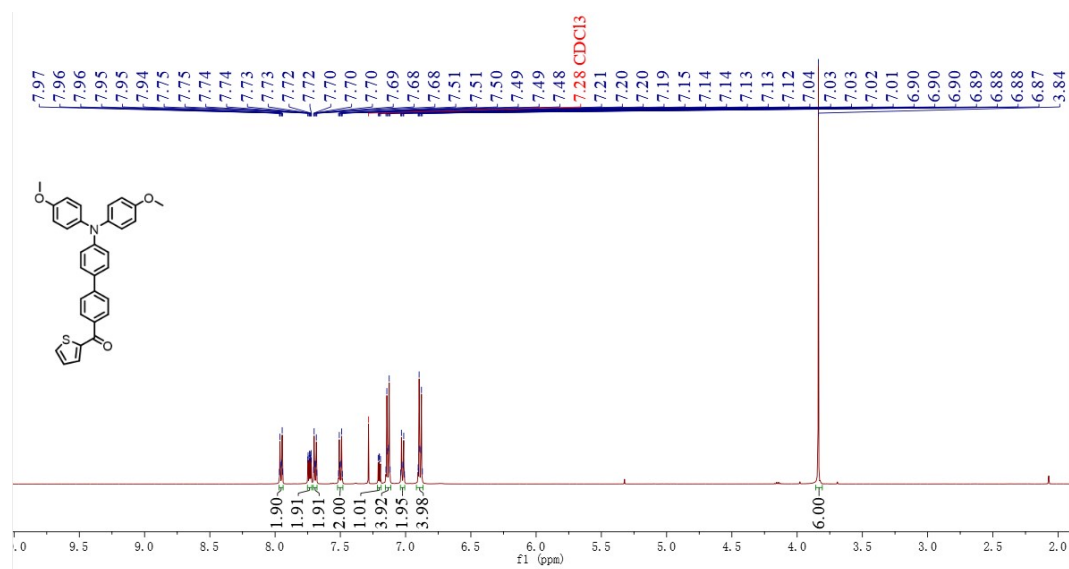


Fig. S4 ¹H NMR spectrum of compound 3 (500 MHz, Chloroform-d).

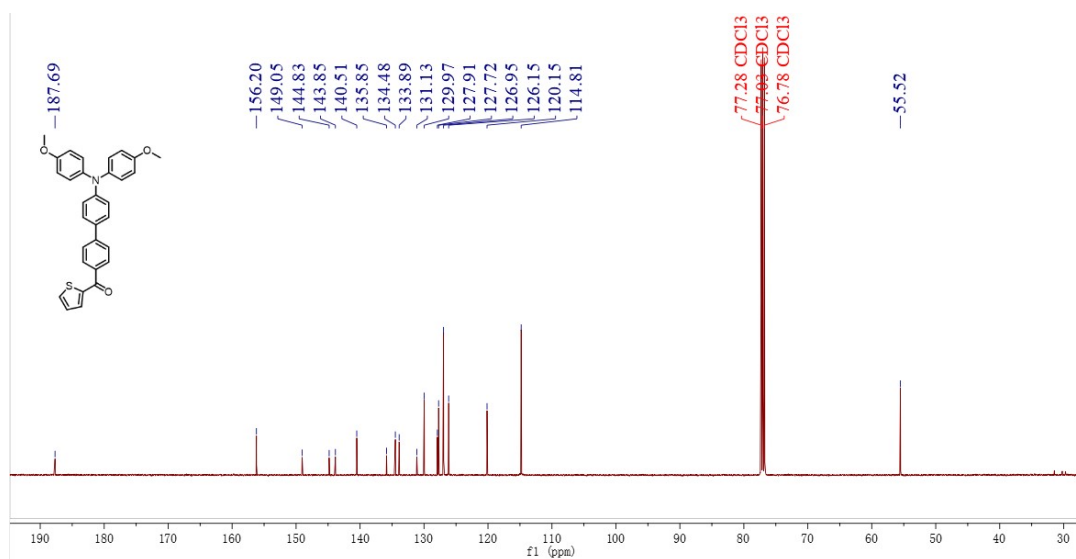


Fig. S5 ¹³C NMR spectrum of compound 3 (126 MHz, Chloroform-d).

BWJ-s-b #239-320 RT: 1.47-1.89 AV: 82 NL: 2.27E8
T: FTMS + p ESI Full ms [400.0000-1150.0000]

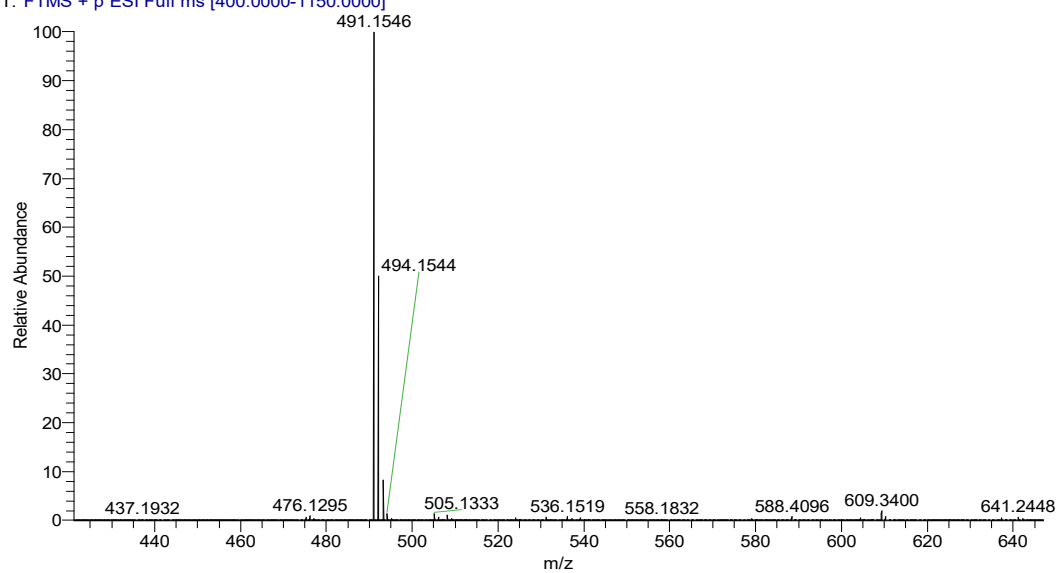


Fig. S6 High resolution mass spectrum (HR-MS) of compound 3.

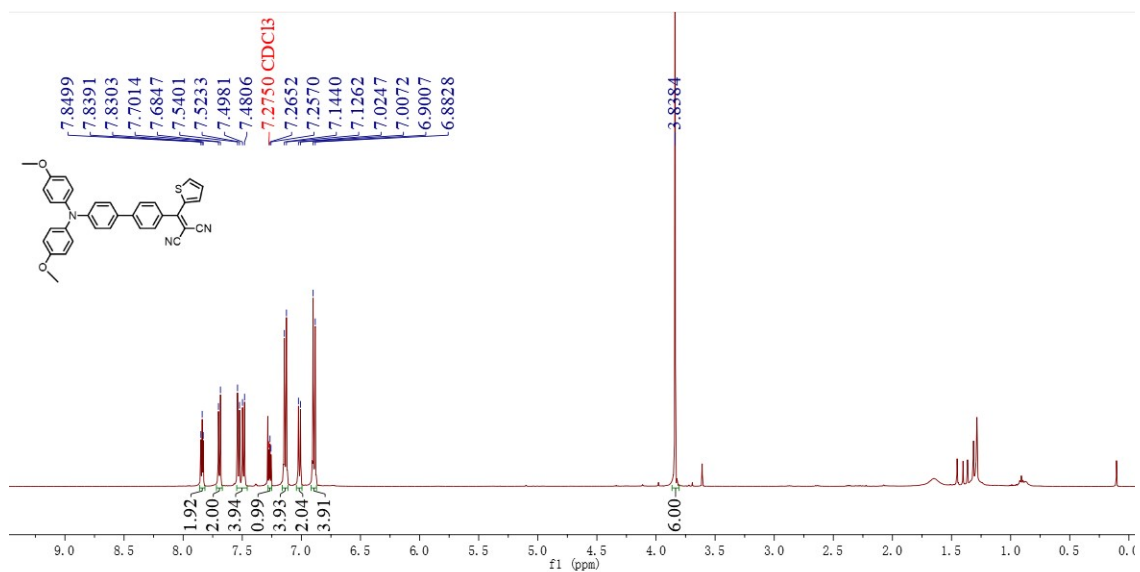


Fig. S7 ¹H NMR spectrum of compound 4 (500 MHz, Chloroform-d).

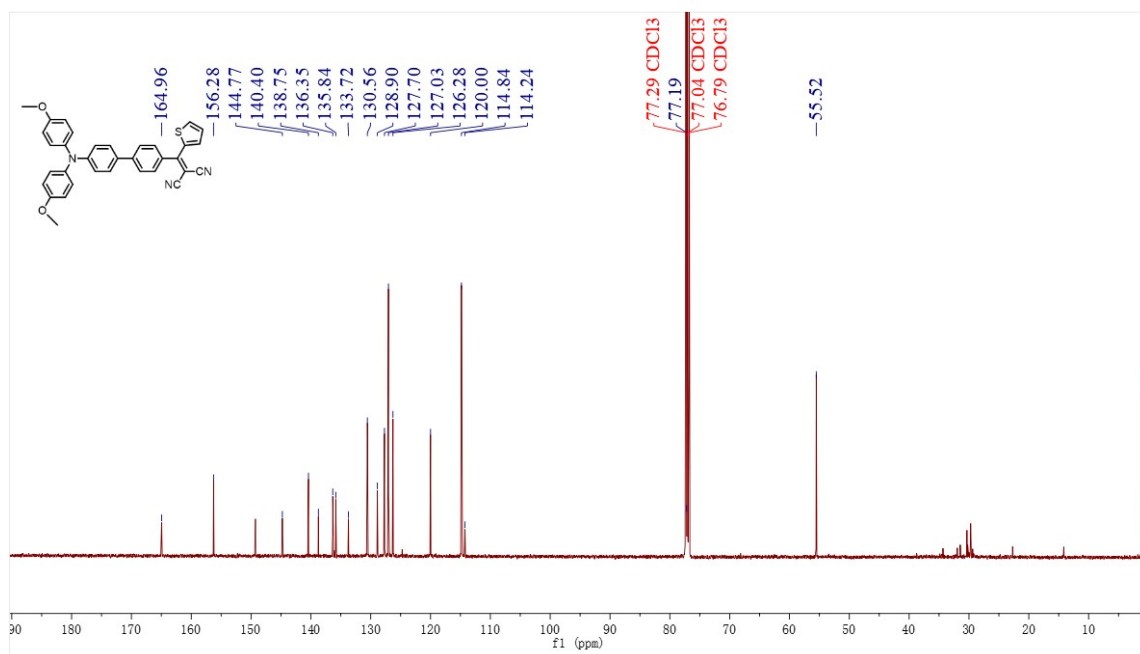


Fig. S8 ¹³C NMR spectrum of compound 4 (126 MHz, Chloroform-d).

BWJ-S-C #243-447 RT: 1.06-1.96 AV: 205 NL: 8.84E7
T: FTMS + p ESI Full ms [400.0000-700.0000]

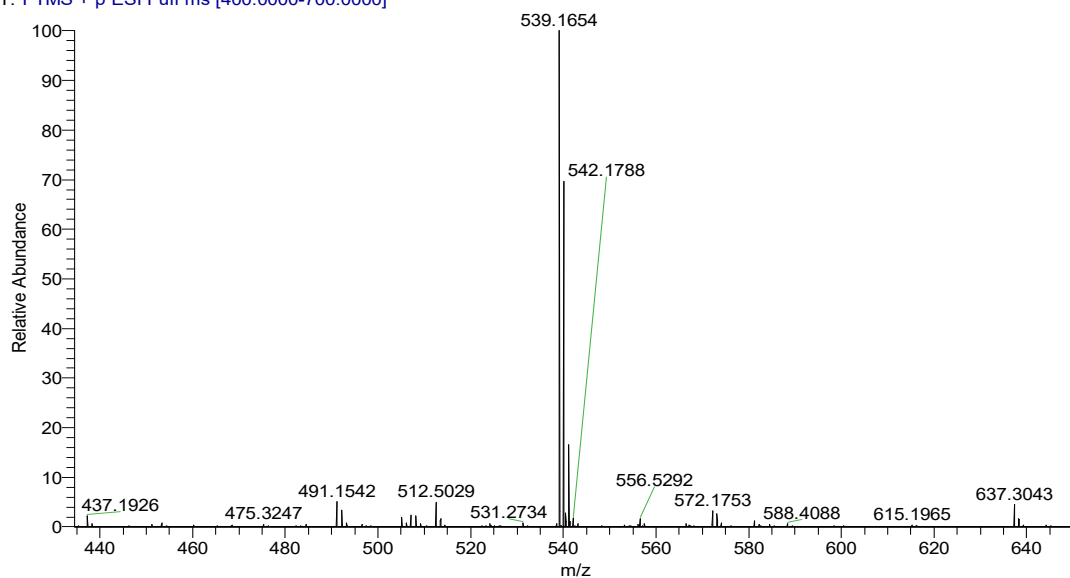


Fig. S9 High resolution mass spectrum (HR-MS) of compound 4.

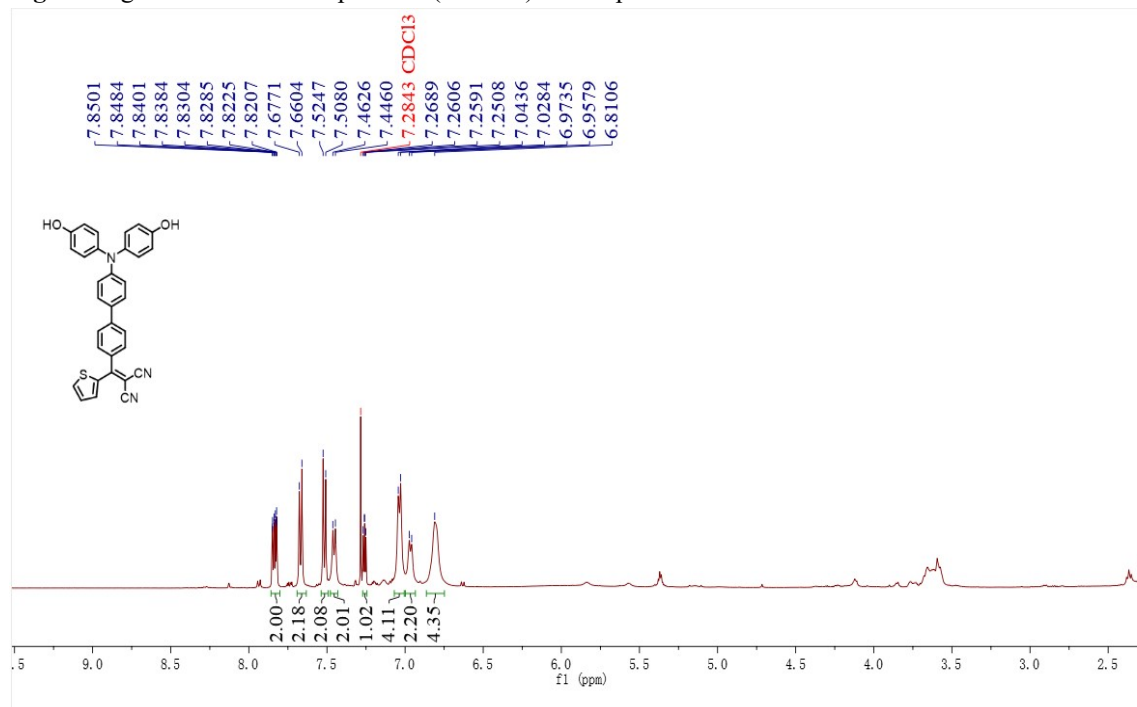


Fig. S10 ^1H NMR spectrum of compound 5 (500 MHz, Chloroform-d).

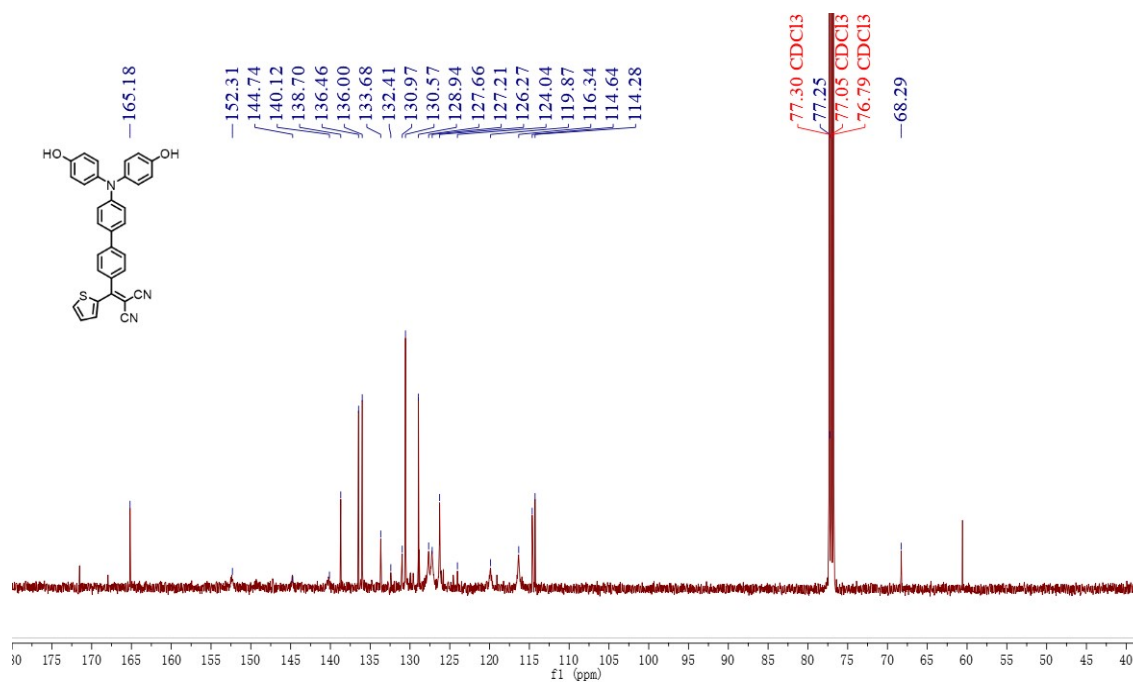


Fig. S11 ^{13}C NMR spectrum of compound 5 (126 MHz, Chloroform-d).

BWJ-S-d #123-177 RT: 0.81-1.12 AV: 55 NL: 5.52E7
T: FTMS - p ESI Full ms [200.0000-600.0000]

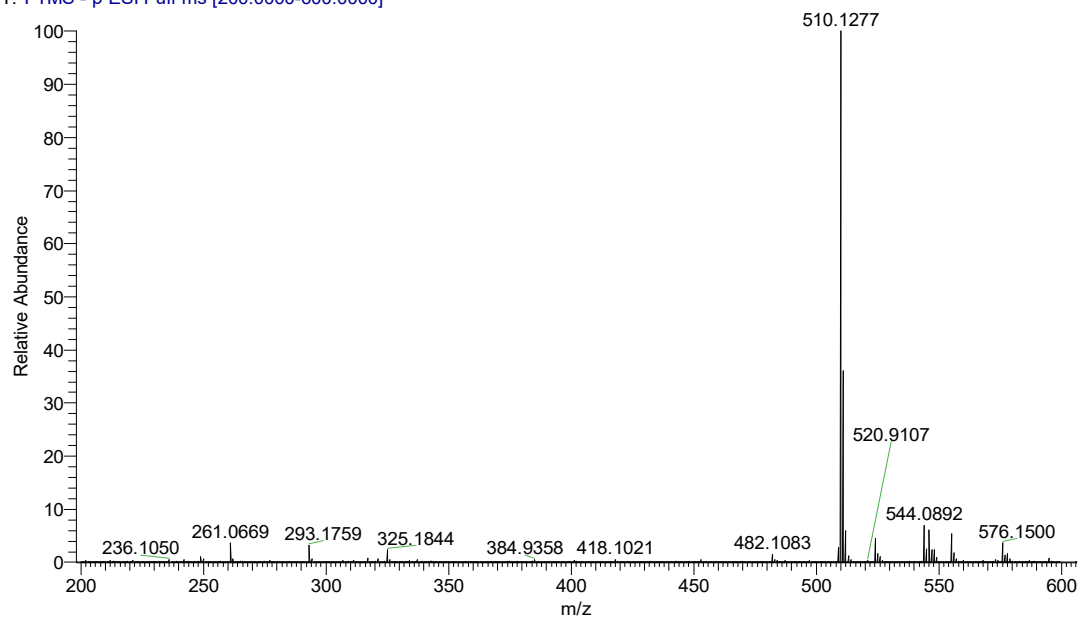


Fig. S12 High resolution mass spectrum (HR-MS) of compound 5.

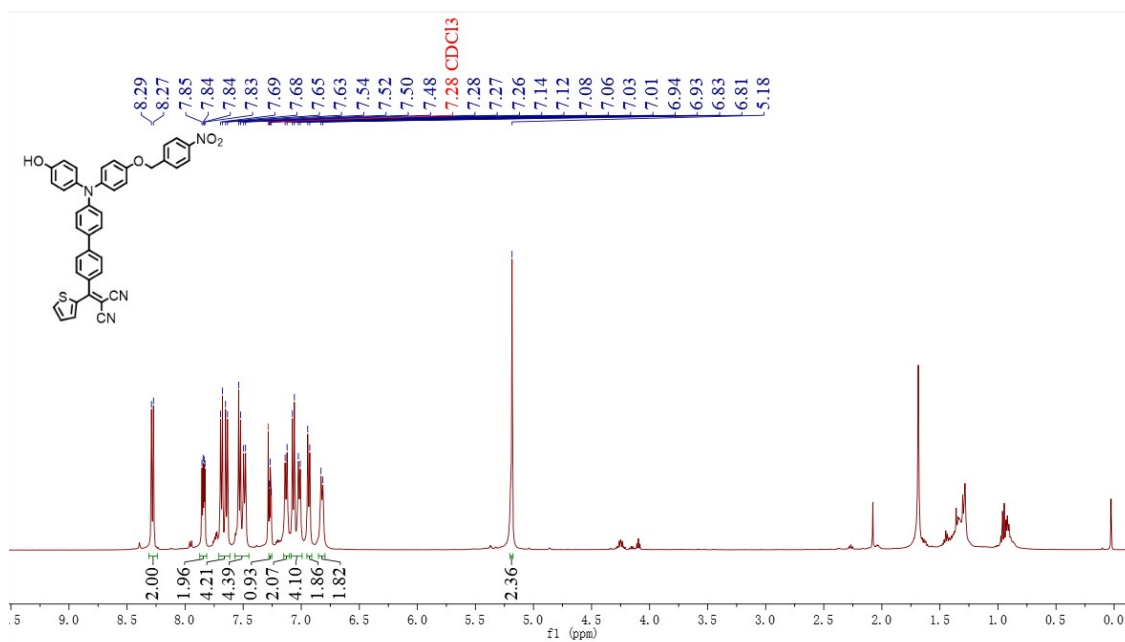


Fig. S13 ¹H NMR spectrum of compound 6 (500 MHz, Chloroform-d).

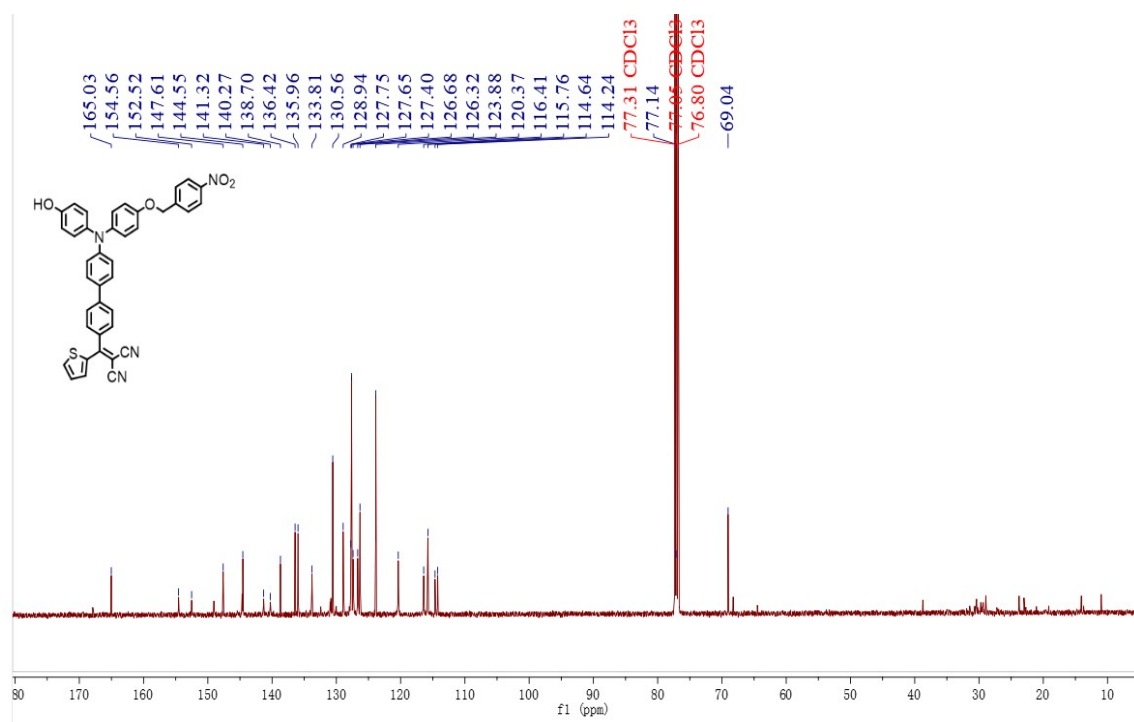


Fig. S14 ¹³C NMR spectrum of compound 6 (126 MHz, Chloroform-d).

BWJ-S-5-2 #141-201 RT: 0.93-1.27 AV: 61 NL: 3.90E7
T: FTMS - p ESI Full ms [400.0000-900.0000]

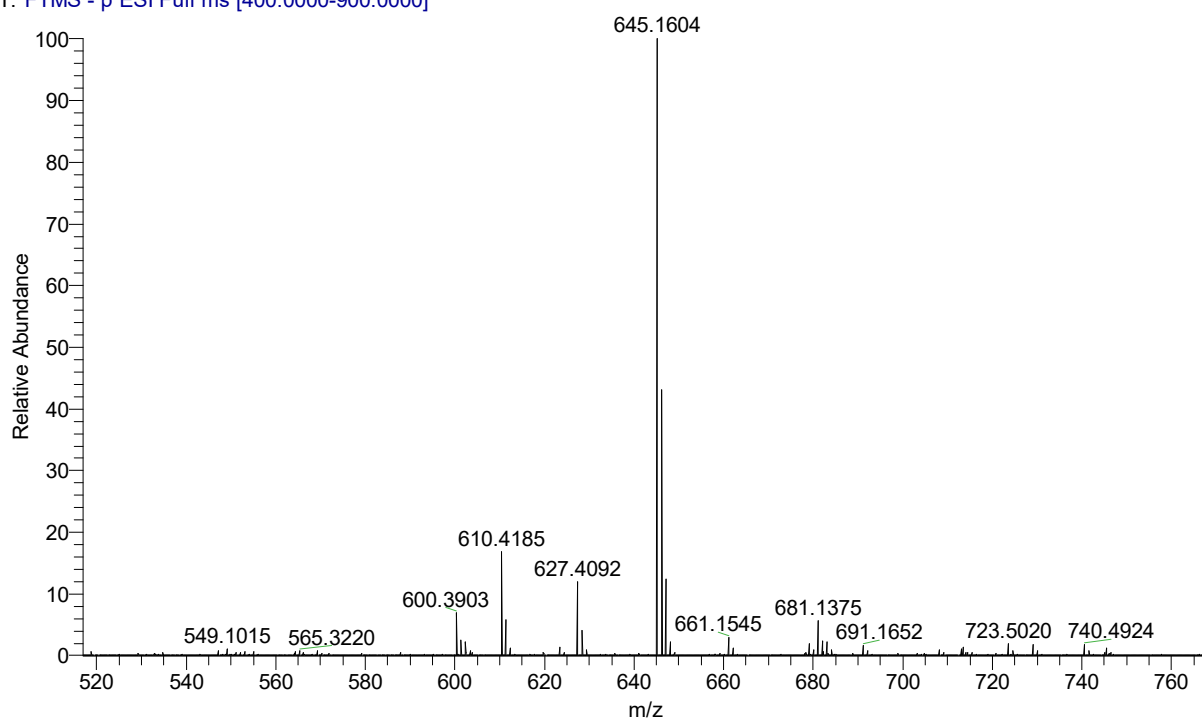


Fig. S15 High resolution mass spectrum (HR-MS) of compound 6.

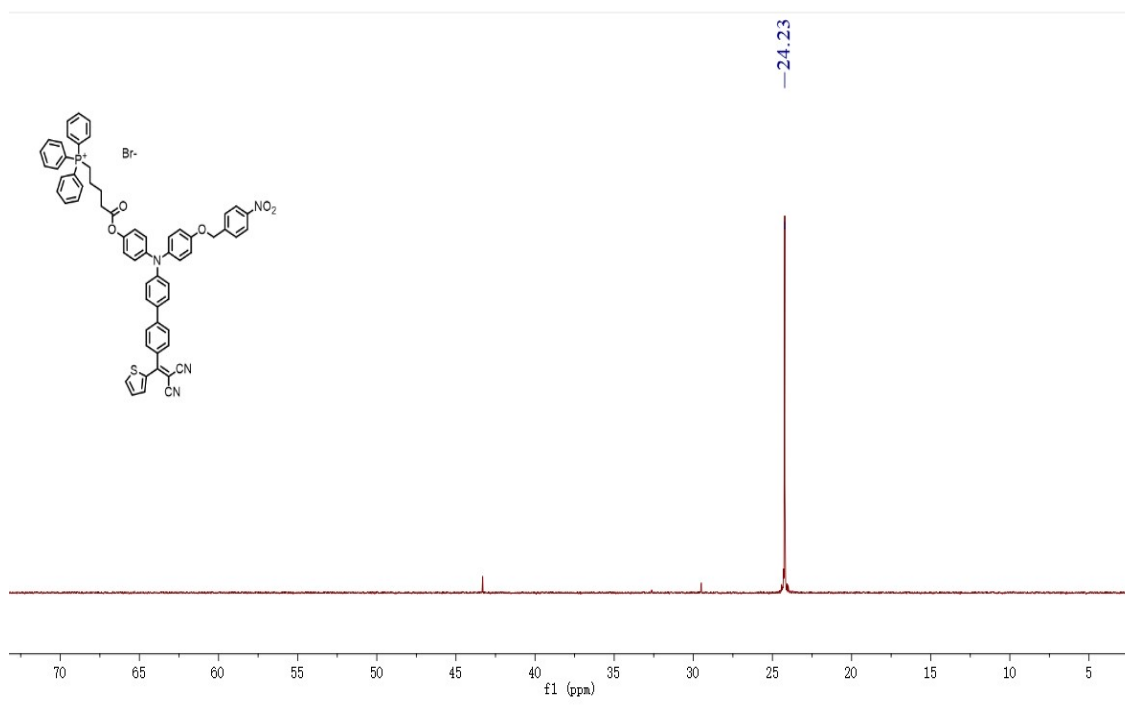


Fig. S16 ^{31}P CPD NMR spectrum of compound TPP-TPA-PBN(500 MHz, Chloroform-d).

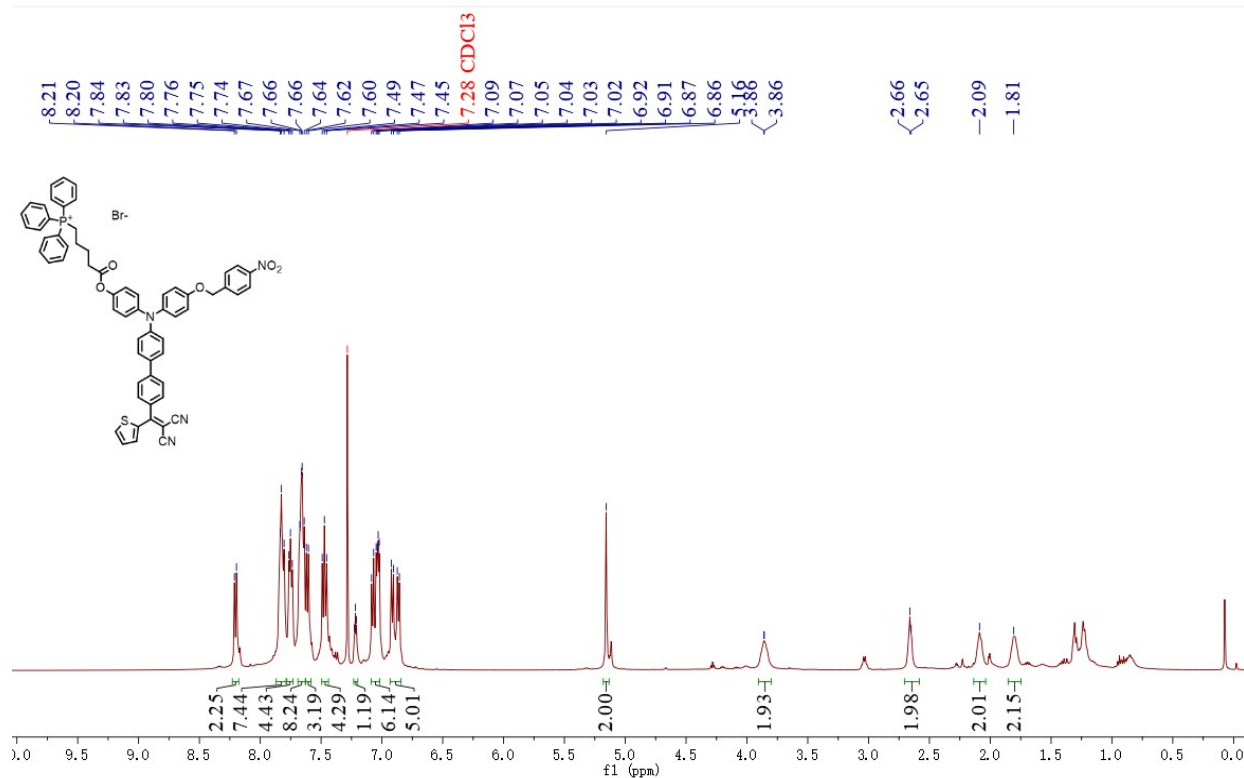


Fig. S17 ¹H NMR spectrum of compound TPP-TPA-PBN (500 MHz, Chloroform-d).

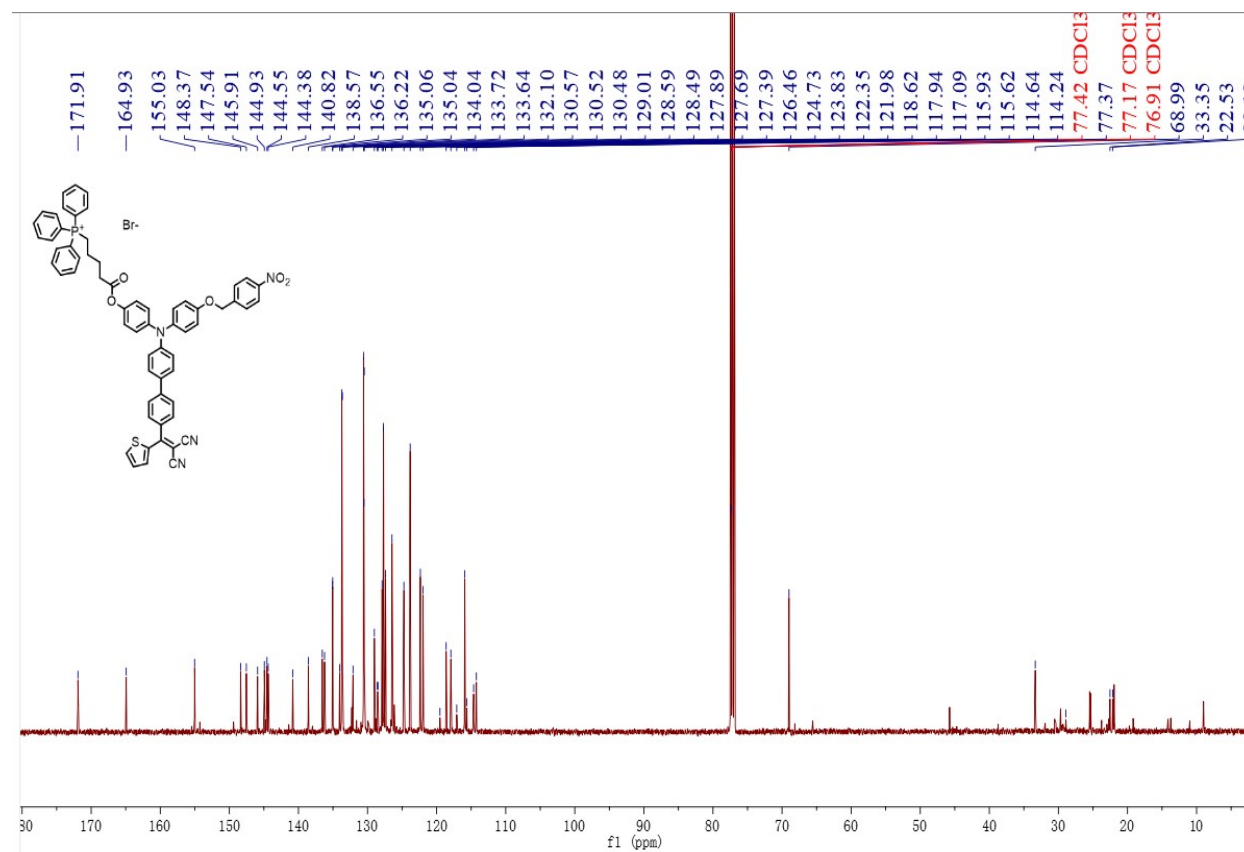


Fig. S18 ¹³C NMR spectrum of compound TPP-TPA-PBN (126 MHz, Chloroform-d).

TPA-TPP-PBN #157 RT: 0.82 AV: 1 NL: 6.57E8
T: FTMS + p ESI Full ms [100.0000-1200.0000]

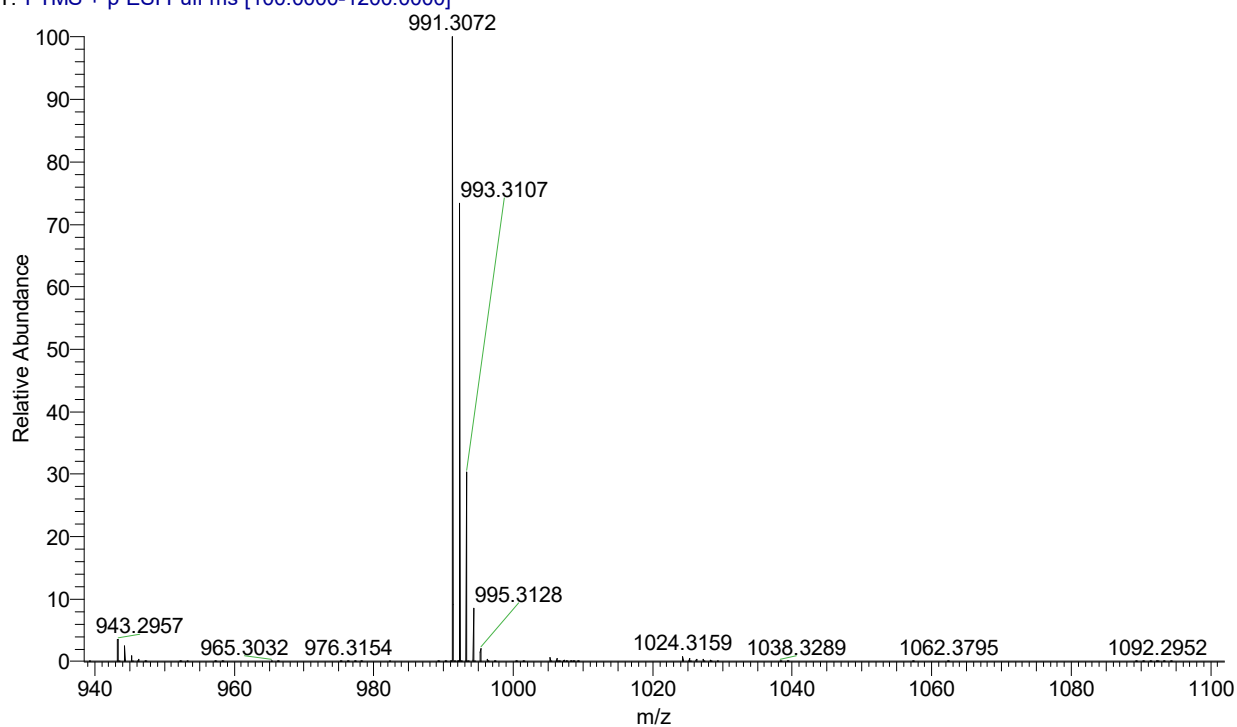


Fig. S19 High resolution mass spectrum (HR-MS) of compound TPP-TPA-PBN.

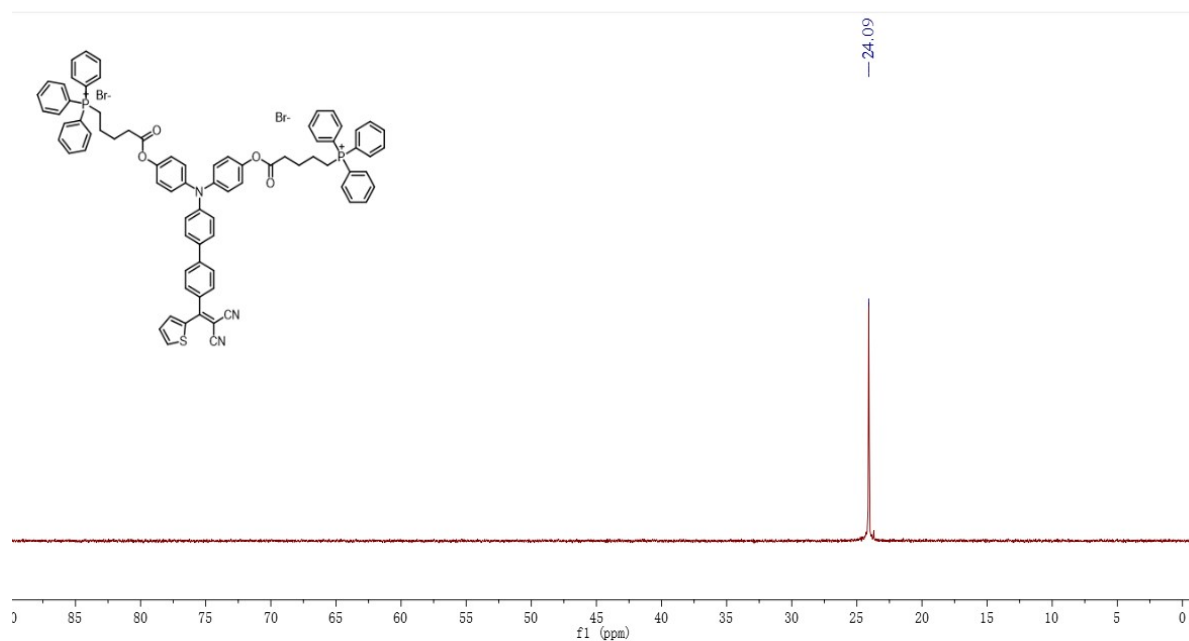


Fig. S20 ³¹P CPD NMR spectrum of compound TPA-TPP-TPP(500 MHz, Chloroform-d).

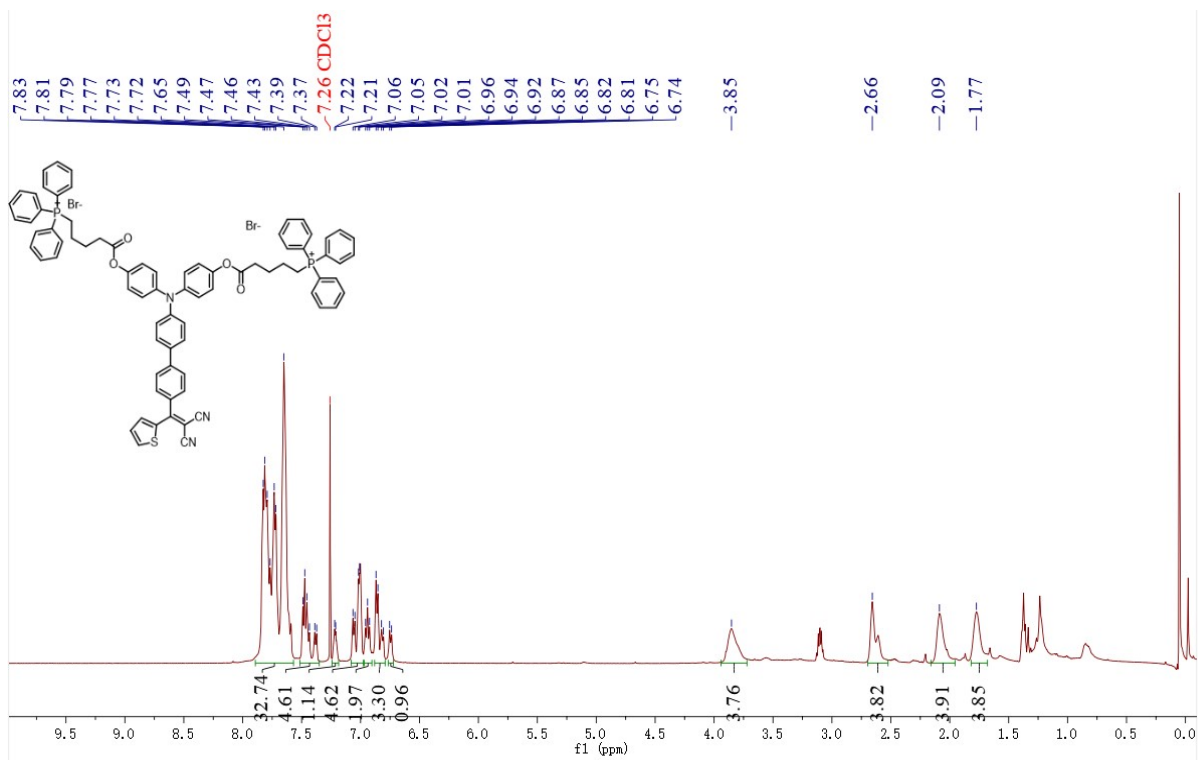


Fig. S21 ¹H NMR spectrum of compound TPA-TPP-TPP(500 MHz, Chloroform-d).

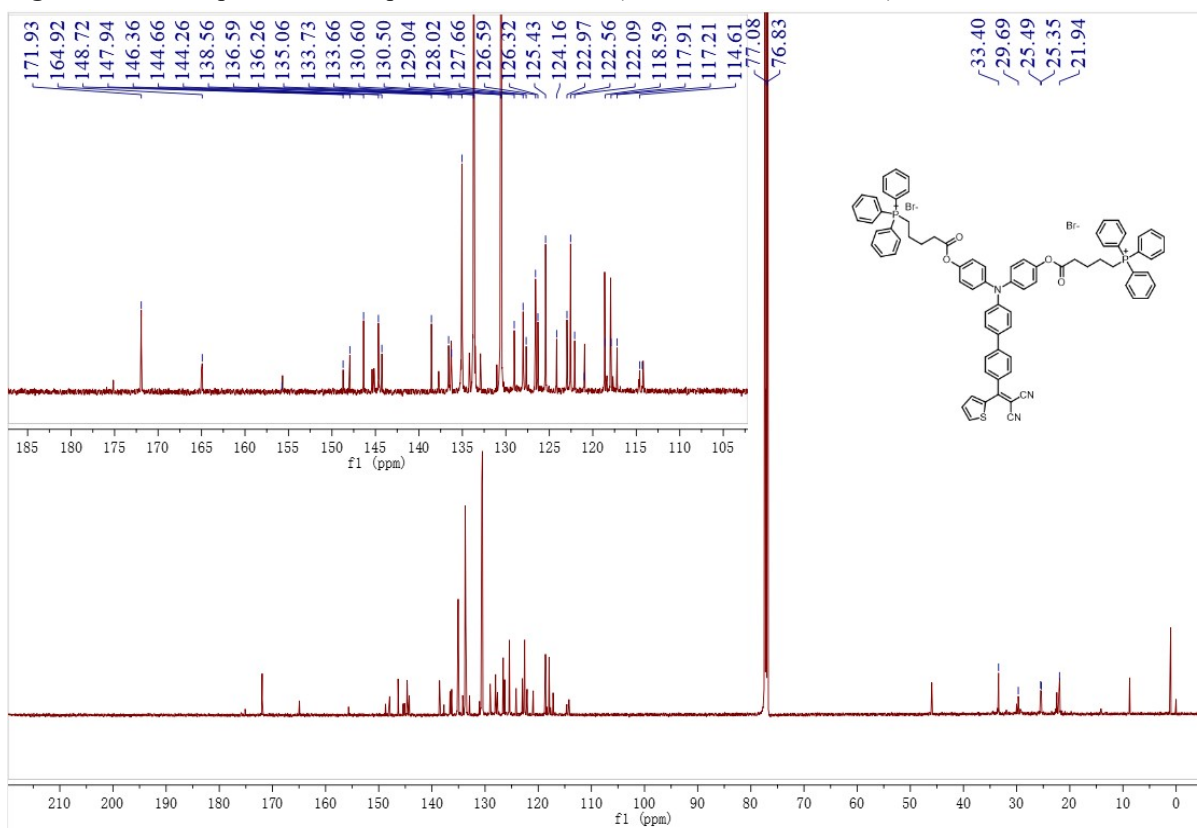


Fig. S22 ¹³C NMR spectrum of compound TPA-TPP-TPP(126 MHz, Chloroform-d).

TPA-TPP-TPP #30 RT: 0.13 AV: 1 NL: 7.20E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

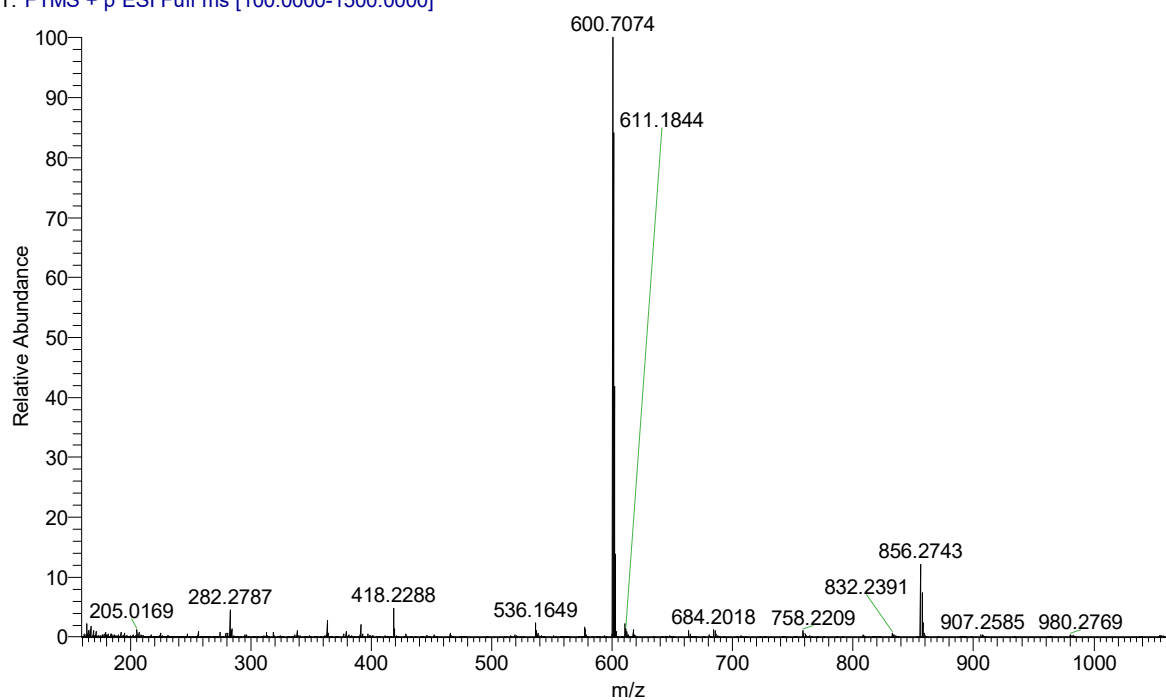


Fig. S23 High resolution mass spectrum (HR-MS) of compound TPA-TPP-TPP.

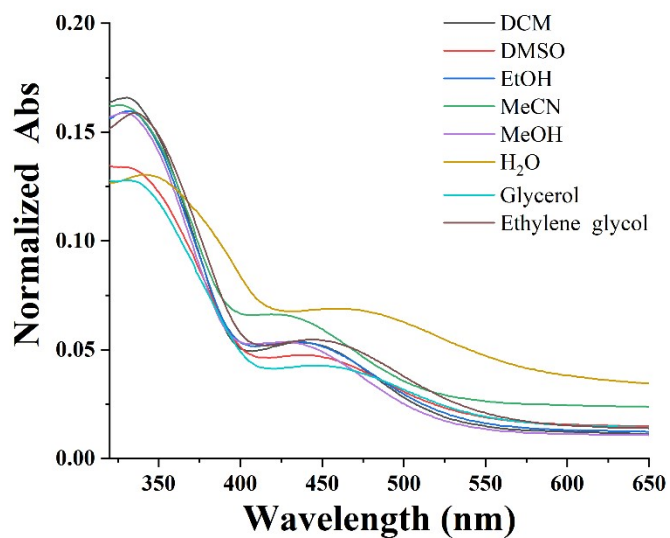


Fig. S24 UV absorption of probes in different solvents.

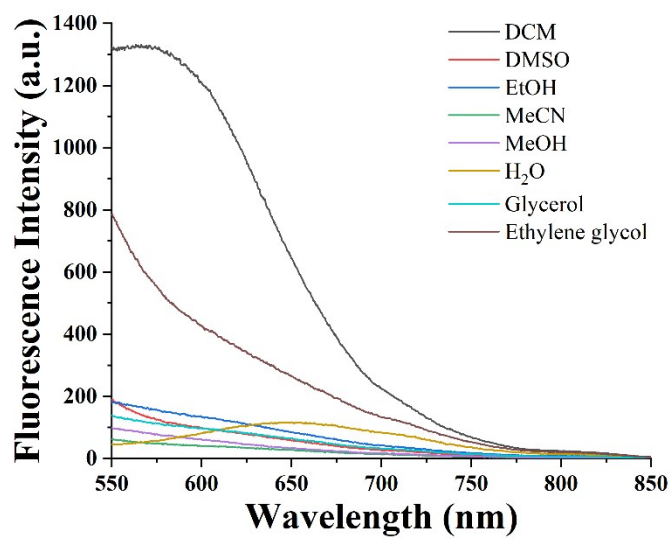


Fig. S25 Fluorescence emission intensity spectra of probes in different solvents.

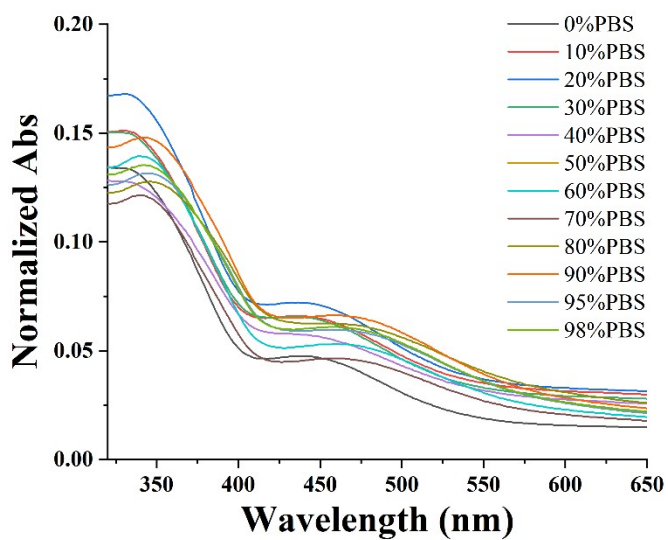


Fig. S26 UV absorption of probe in different water proportion.

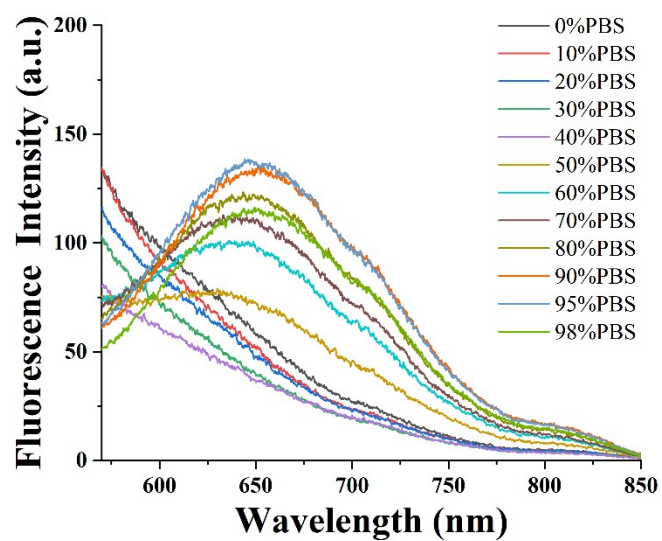


Fig. S27 Fluorescence emission intensity spectra of probe in different water proportion.

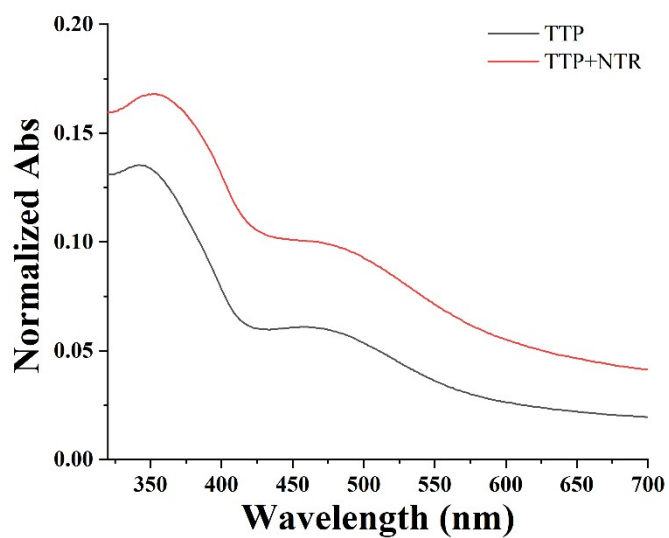


Fig. S28 UV absorption of the probe before and after adding NTR.

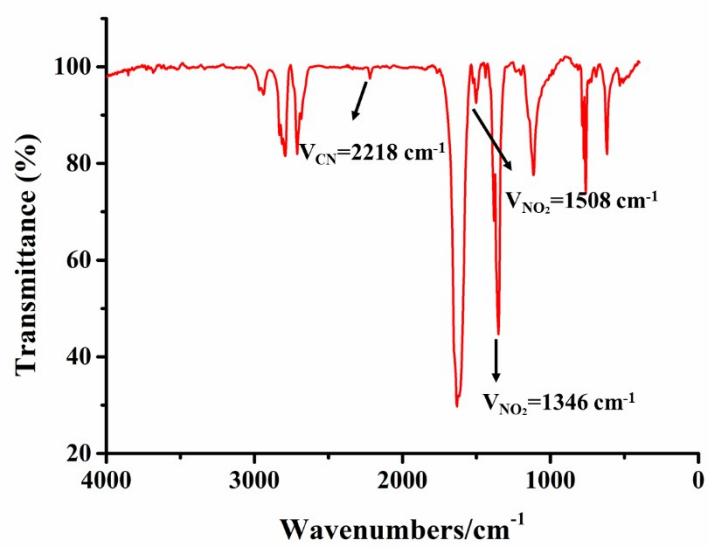


Fig. S29 FTIR spectrum of the TPP-TPA-PBN.