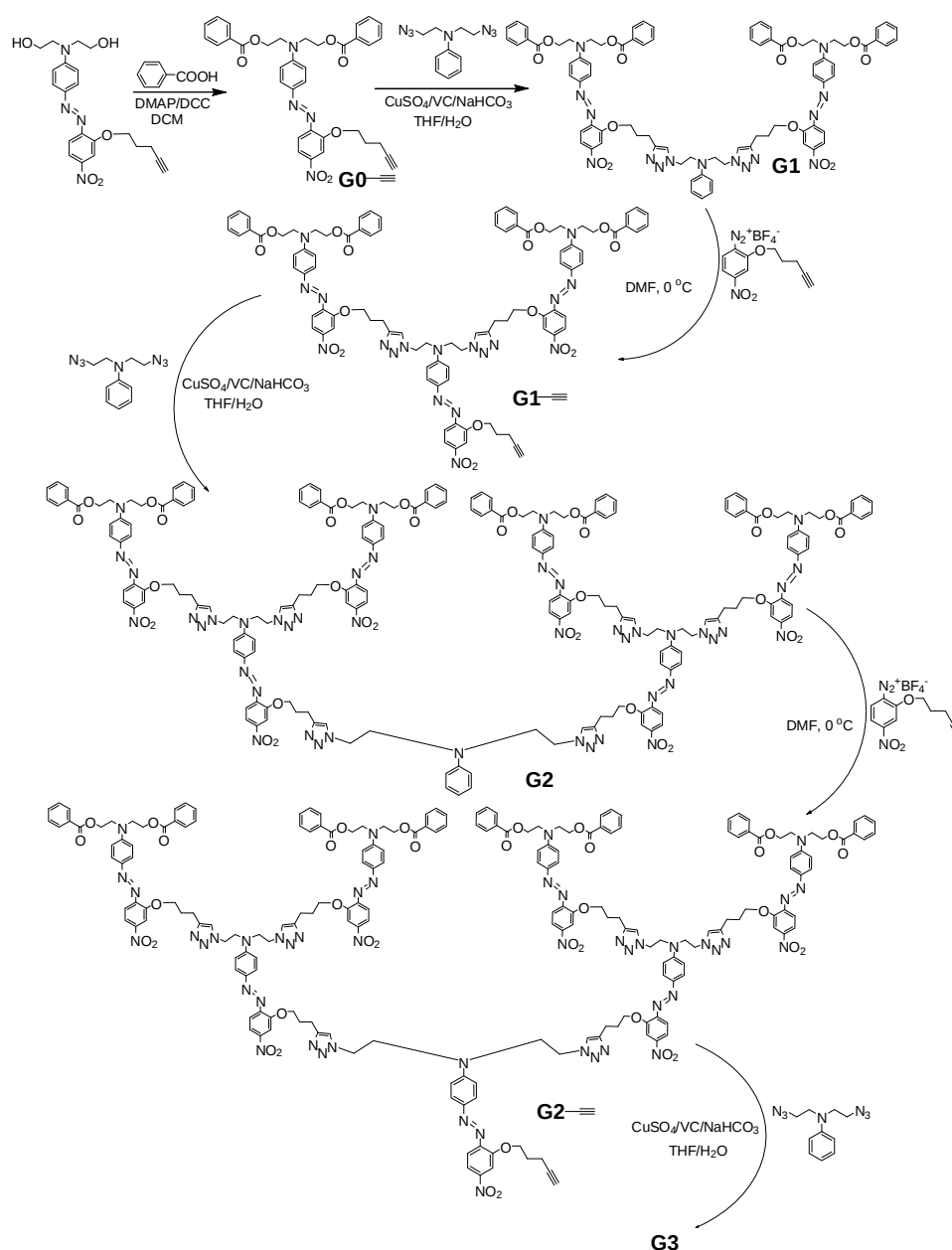


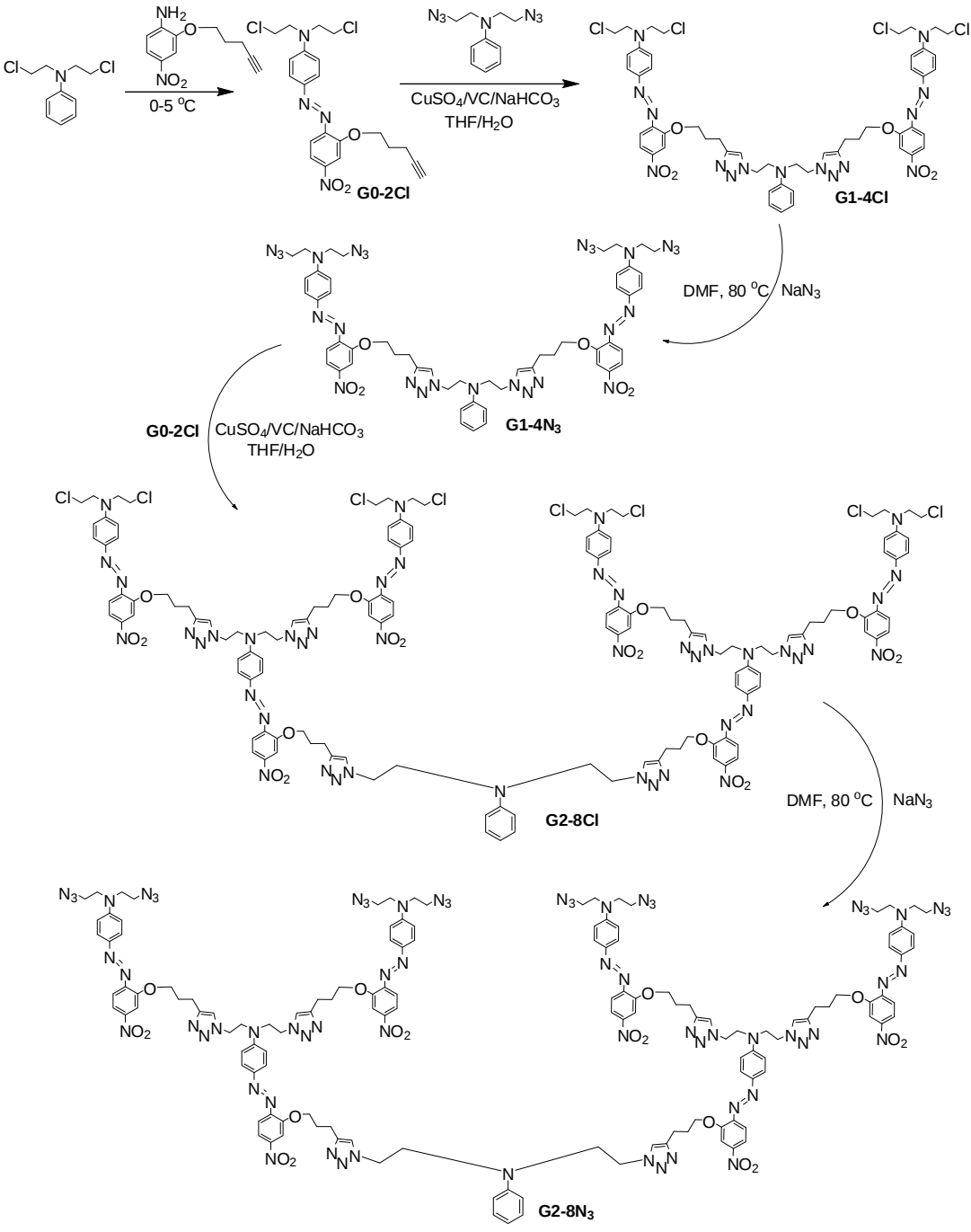
Electronic Supplementary Information:

Second-order nonlinear optical dendrimers containing different type of isolation groups: convenient synthesis through powerful “click chemistry” and large NLO effects †

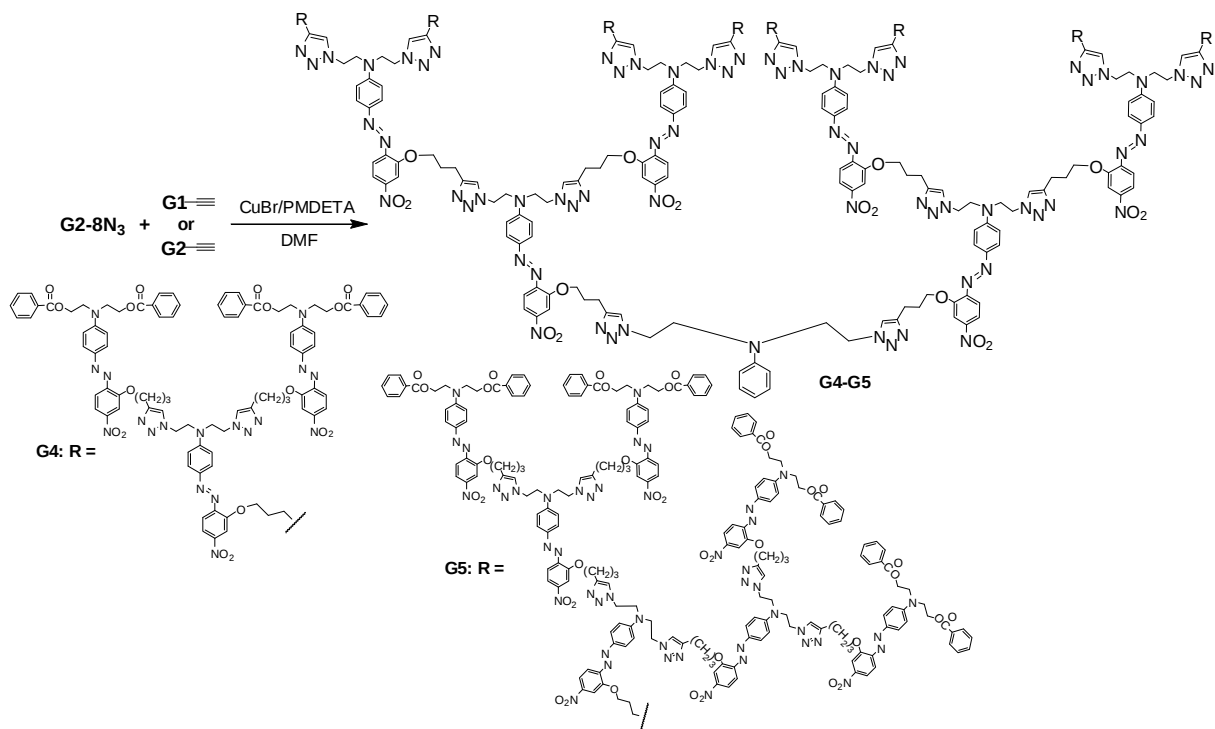
Wenbo Wu,^a Can Wang,^a Runli Tang,^a Yingjie Fu,^a Cheng Ye,^b Jingui Qin,^a and Zhen Li^{*a}



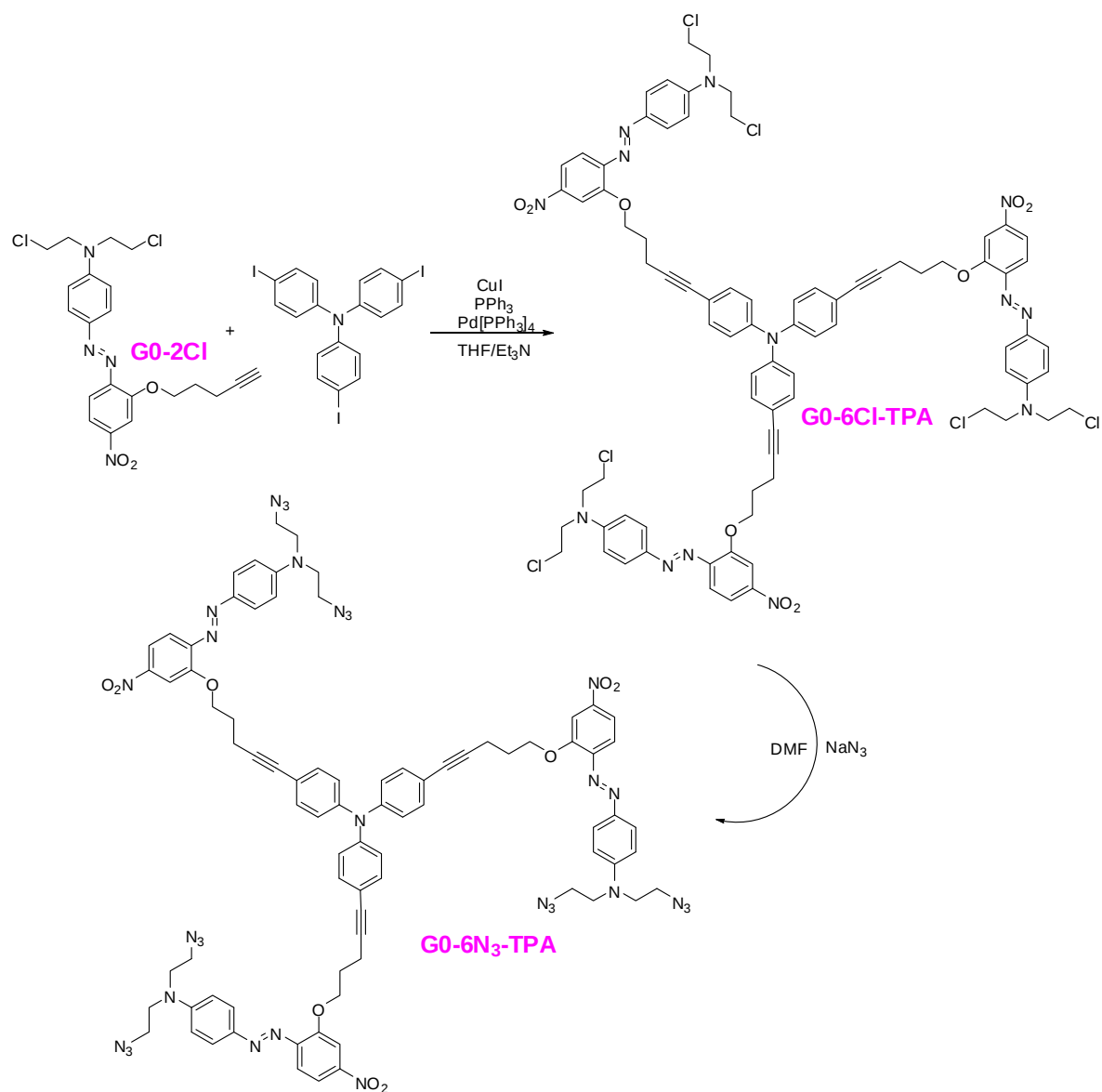
Scheme S1



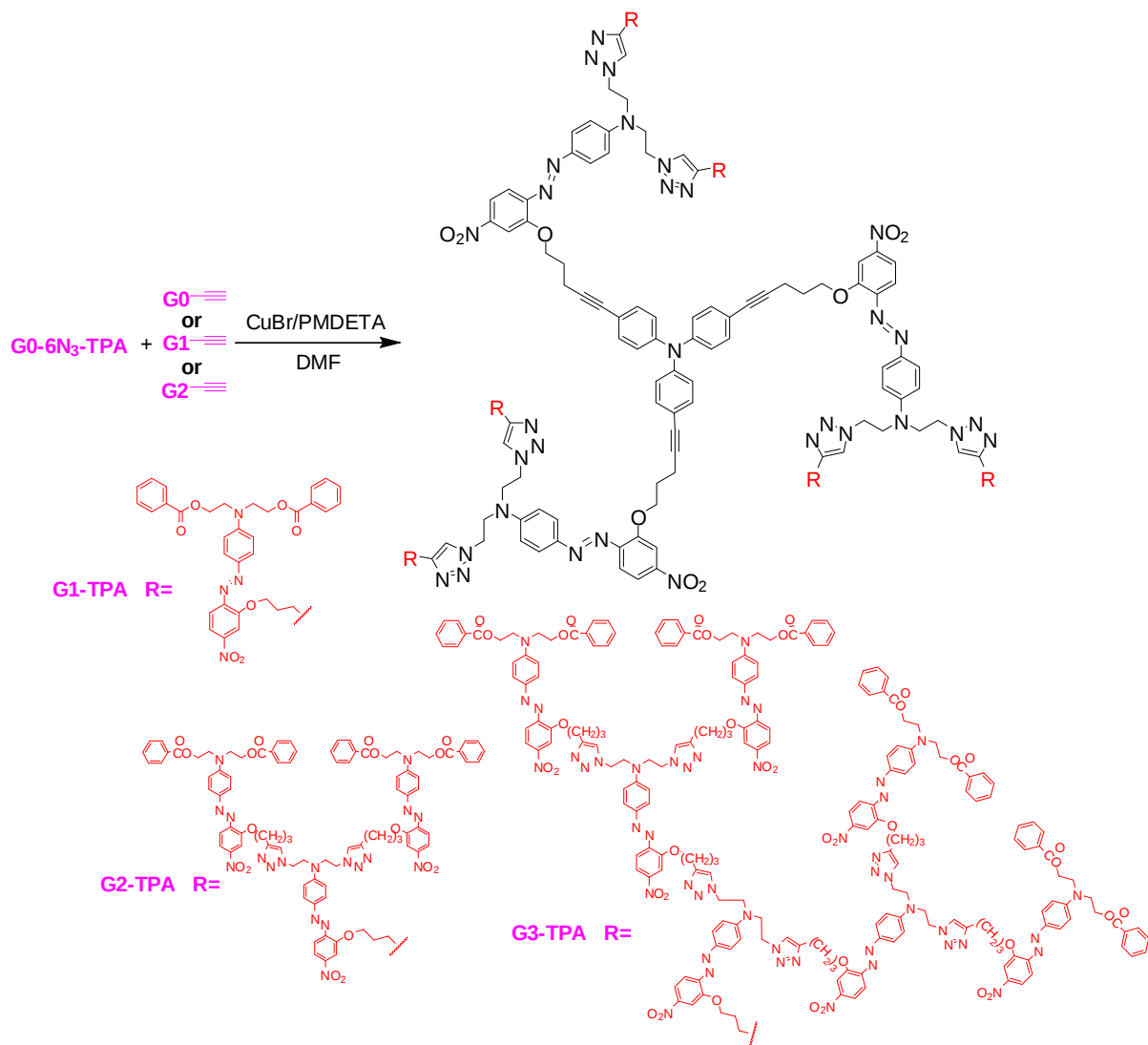
Scheme S2



Scheme S3



Scheme S4 The synthetic route to the core (**G0-6N₃-TPA**) of dendrimers.



Scheme S5 The synthetic route to the TBobal-like dendrimers **G1-TPA-G3-TPA**.

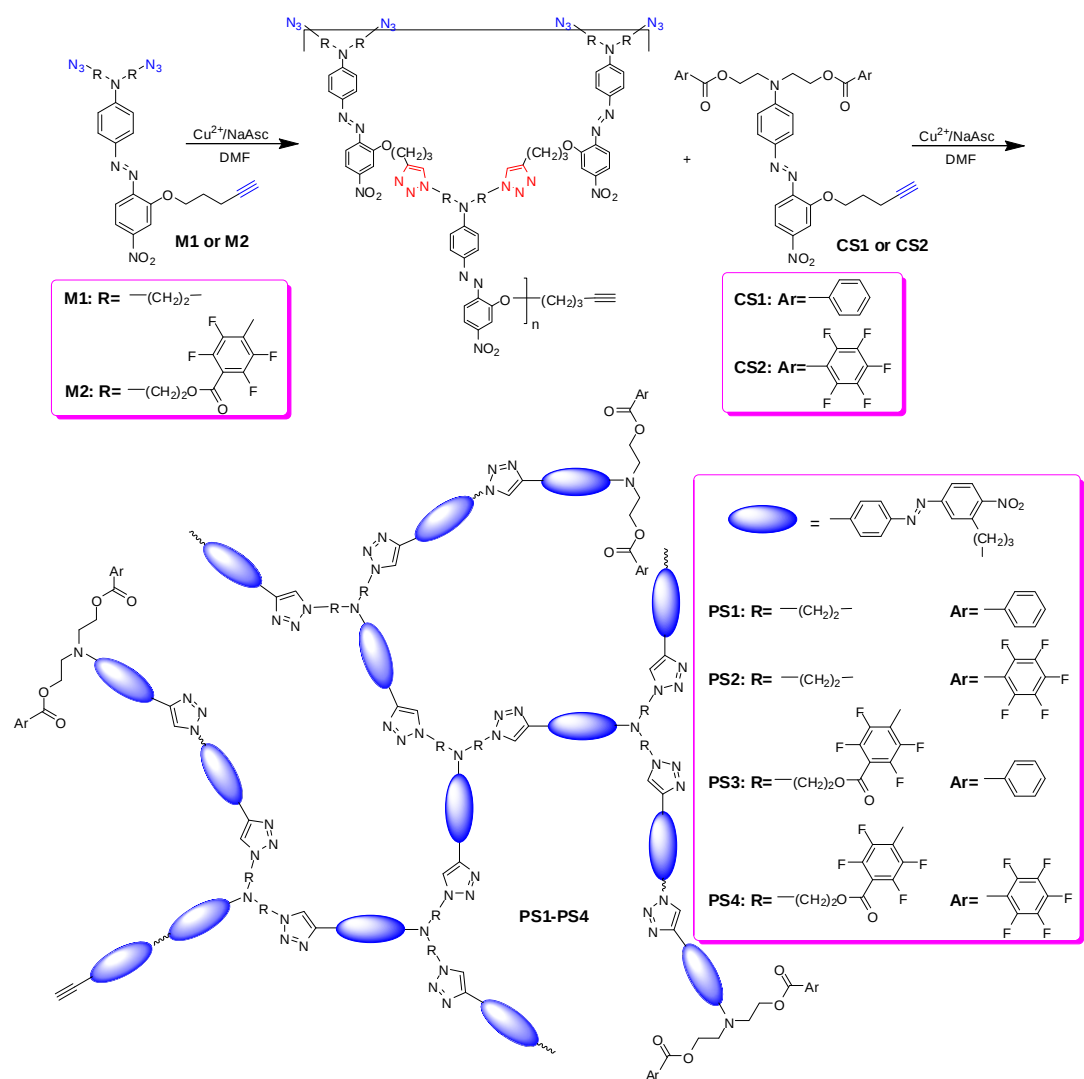


Chart S1 The structure of PS1-PS4 containing perfluoroaromatic rings.

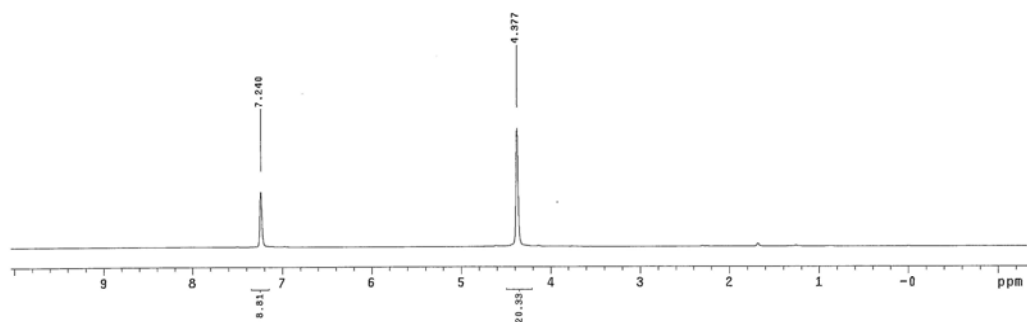


Fig. S1 ¹H NMR spectrum of G0-3N₃ in chloroform-*d*.

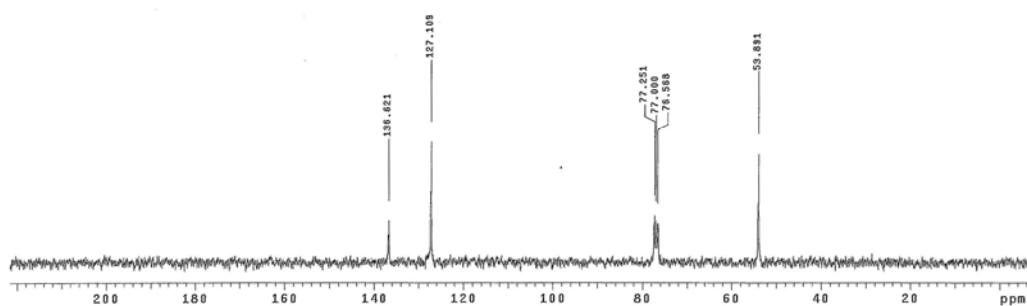


Fig. S2 ¹³C NMR spectrum of G0-3N₃ in chloroform-*d*.

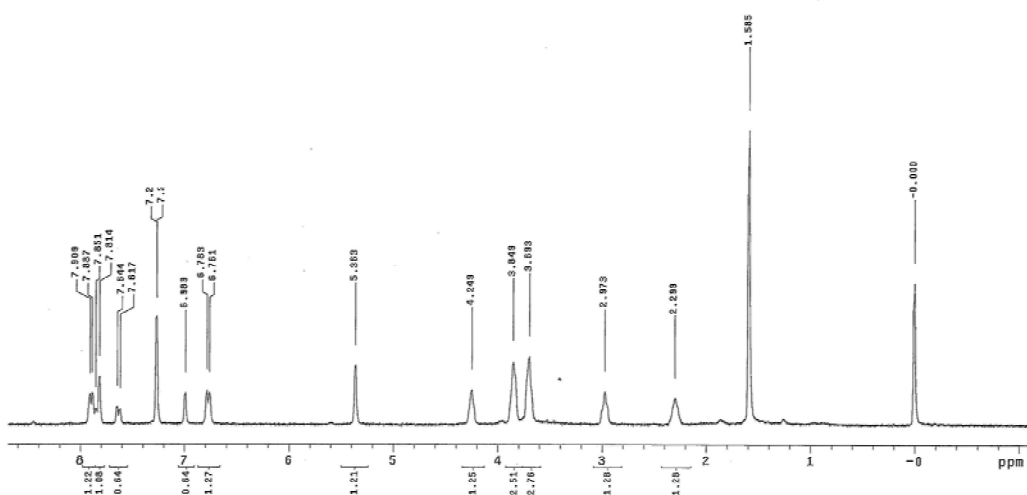


Fig. S3 ¹H NMR spectrum of G1-6Cl-TB in chloroform-*d*.

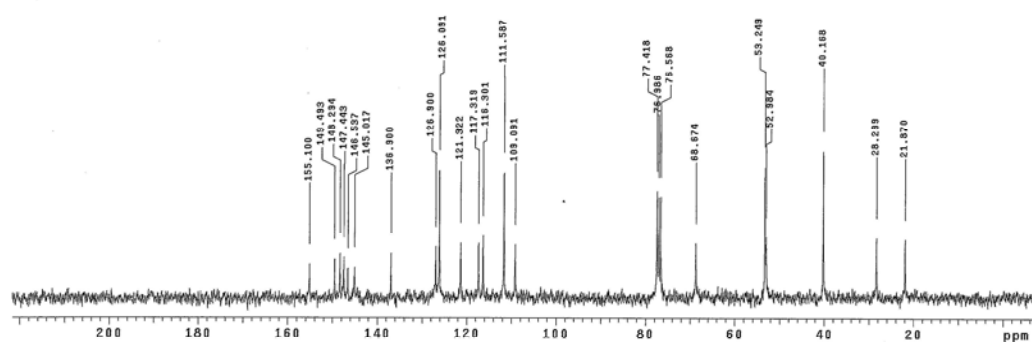


Fig. S4 ^{13}C NMR spectrum of **G1-6Cl-TB** in chloroform-*d*.

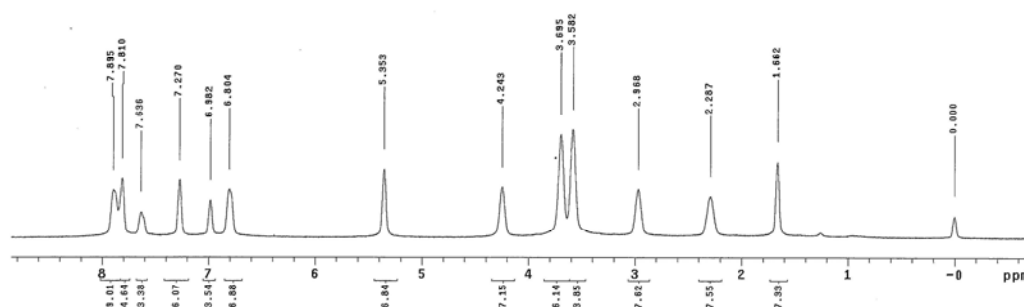


Fig. S5 ^1H NMR spectrum of **G1-6N₃-TB** in chloroform-*d*.

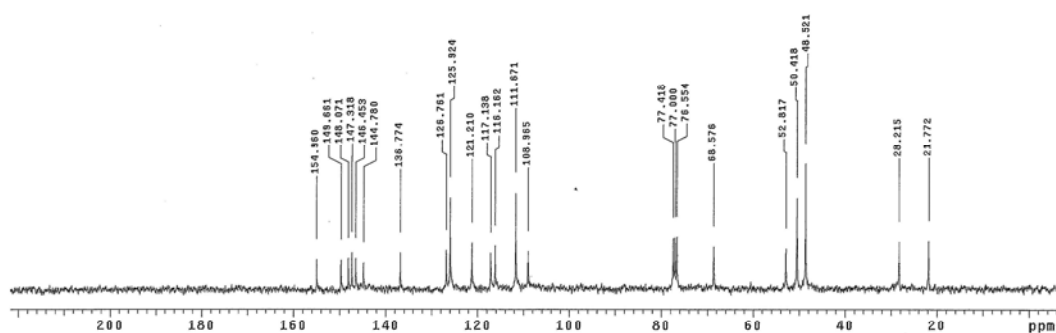


Fig. S6 ^{13}C NMR spectrum of **G1-6N₃-TB** in chloroform-*d*.

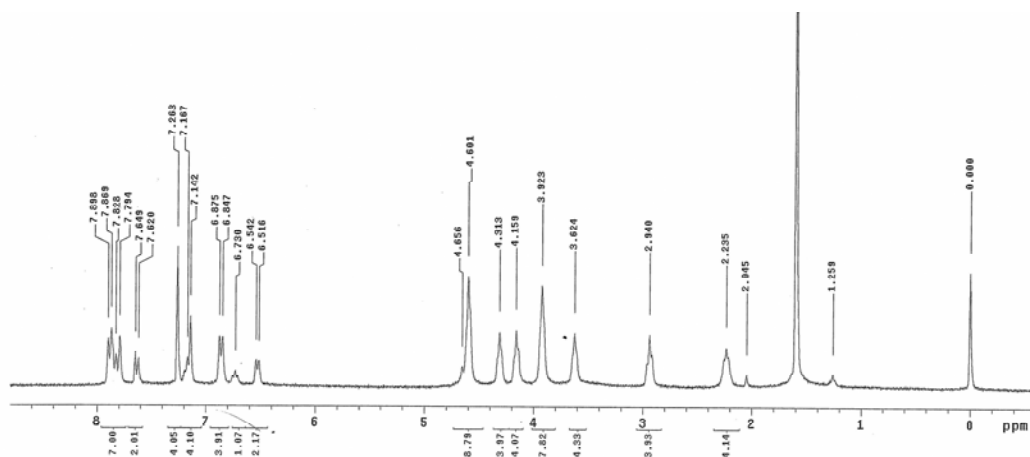


Fig. S7 ^1H NMR spectrum of **G1-PFPh** in chloroform-*d*.

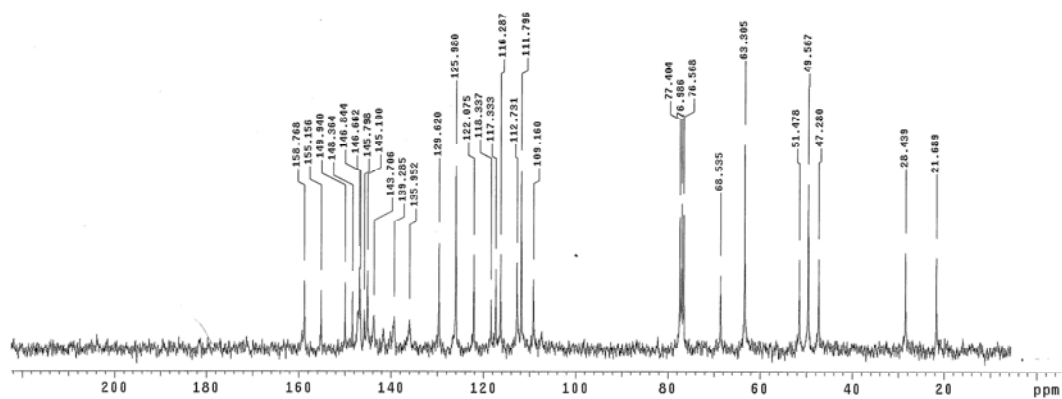


Fig. S8 ^{13}C NMR spectrum of **G1-PFPh** in chloroform-*d*.

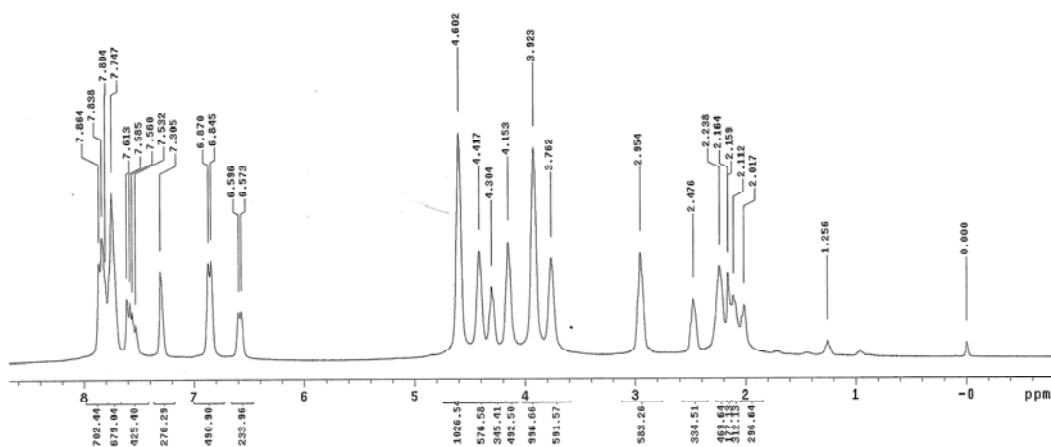


Fig. S9 ^1H NMR spectrum of **G1≡-PFPh** in chloroform-*d*.

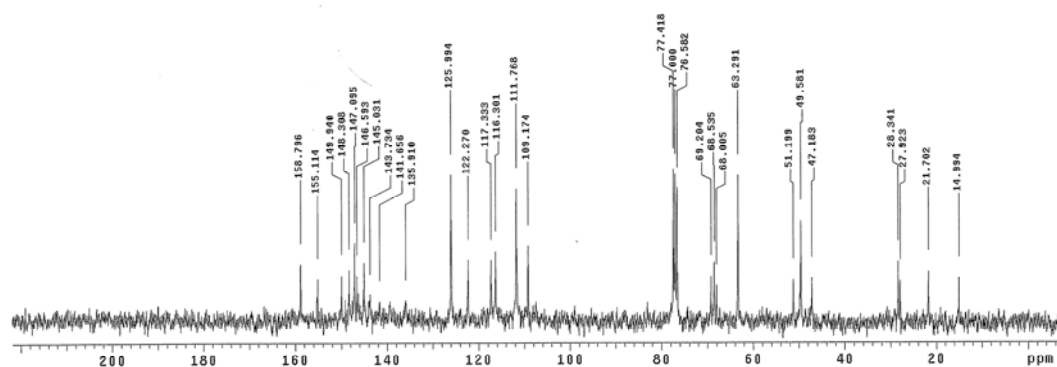


Fig. S10 ^{13}C NMR spectrum of **G1**- $\equiv$ -**PFPh** in chloroform-*d*.

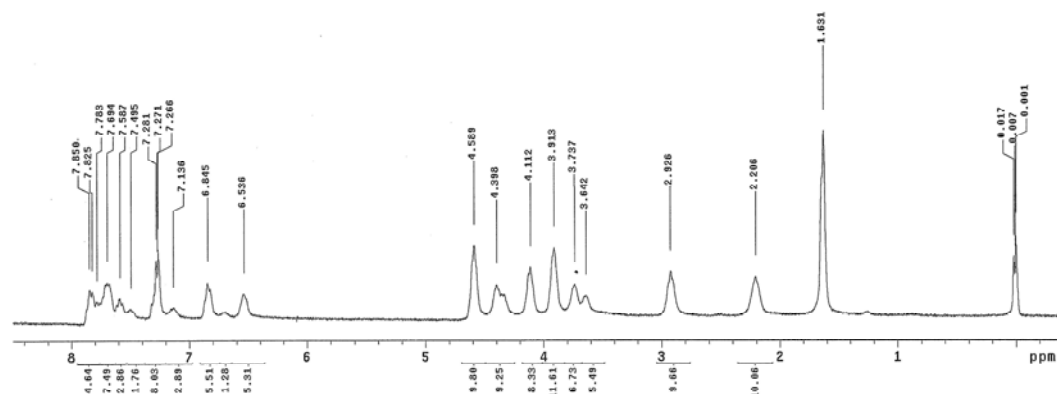


Fig. S11 ^1H NMR spectrum of **G2-PFPh** in chloroform-*d*.

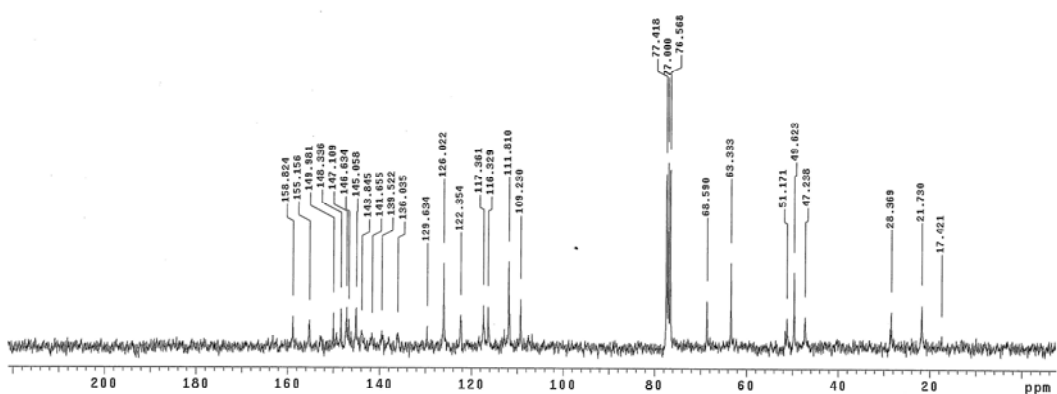


Fig. S12 ^{13}C NMR spectrum of **G2-PFPh** in chloroform-*d*.

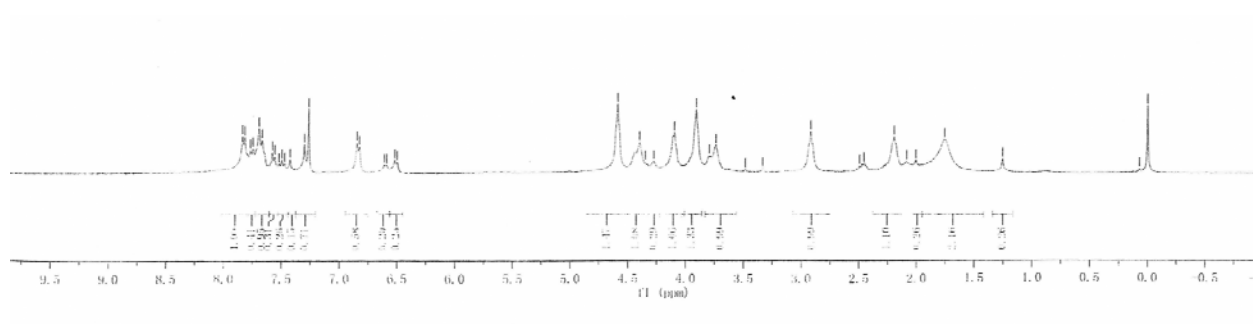


Fig. S13 ¹H NMR spectrum of G2≡-PFPh in chloroform-d.

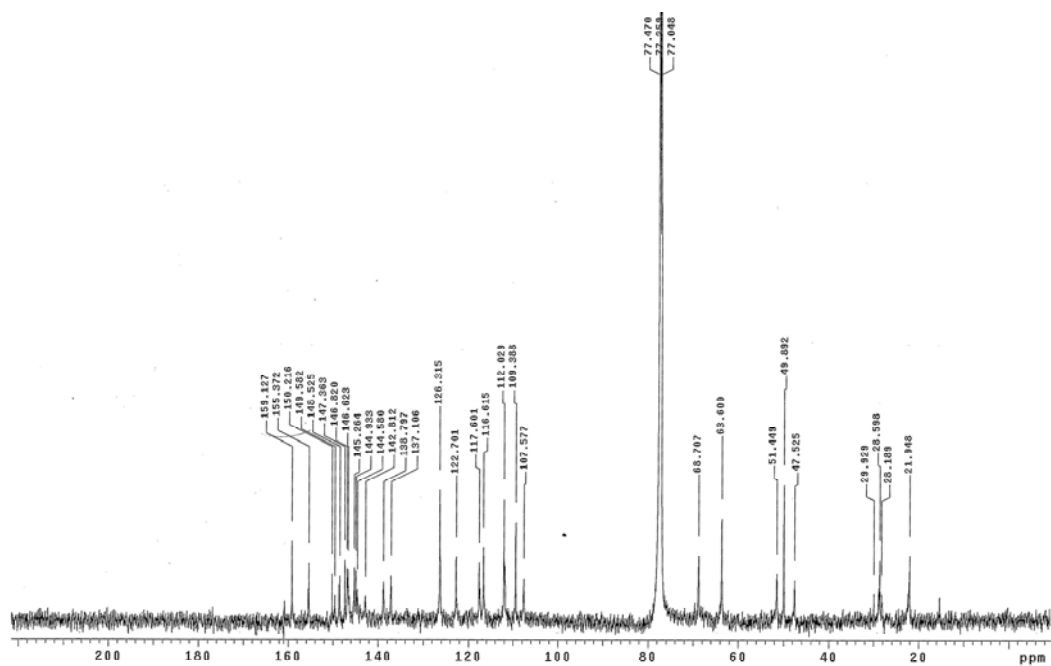


Fig. S14 ¹³C NMR spectrum of G2≡-PFPh in chloroform-d.

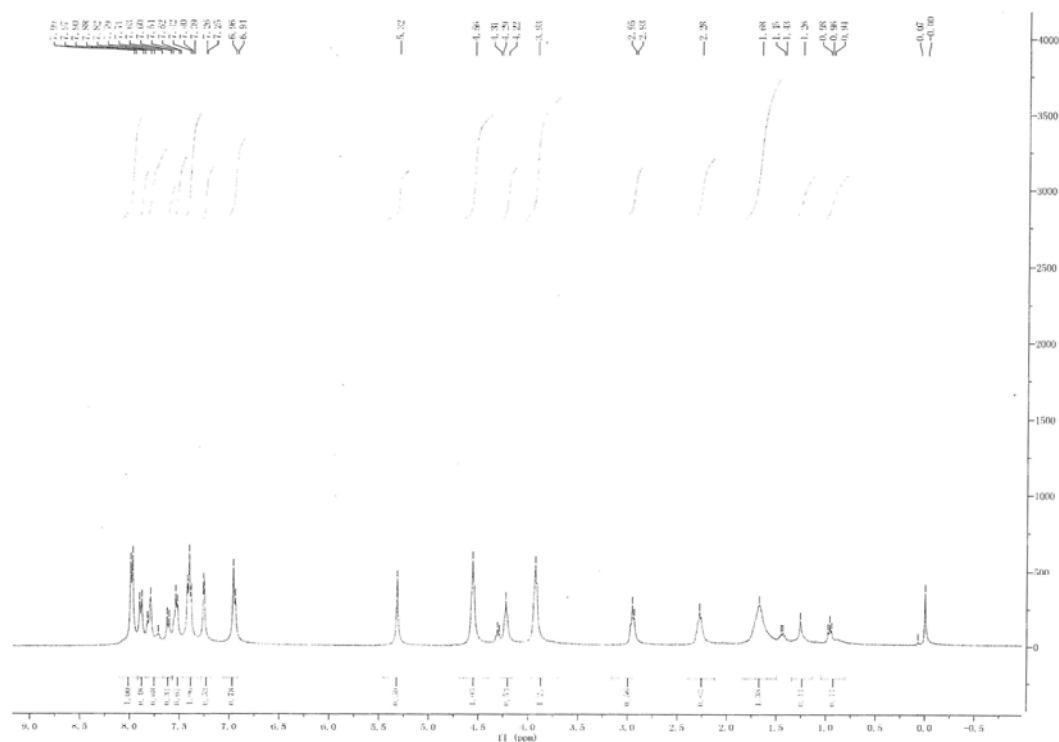


Fig. S15 ¹H NMR spectrum of G1-Ph-TB in chloroform-*d*.

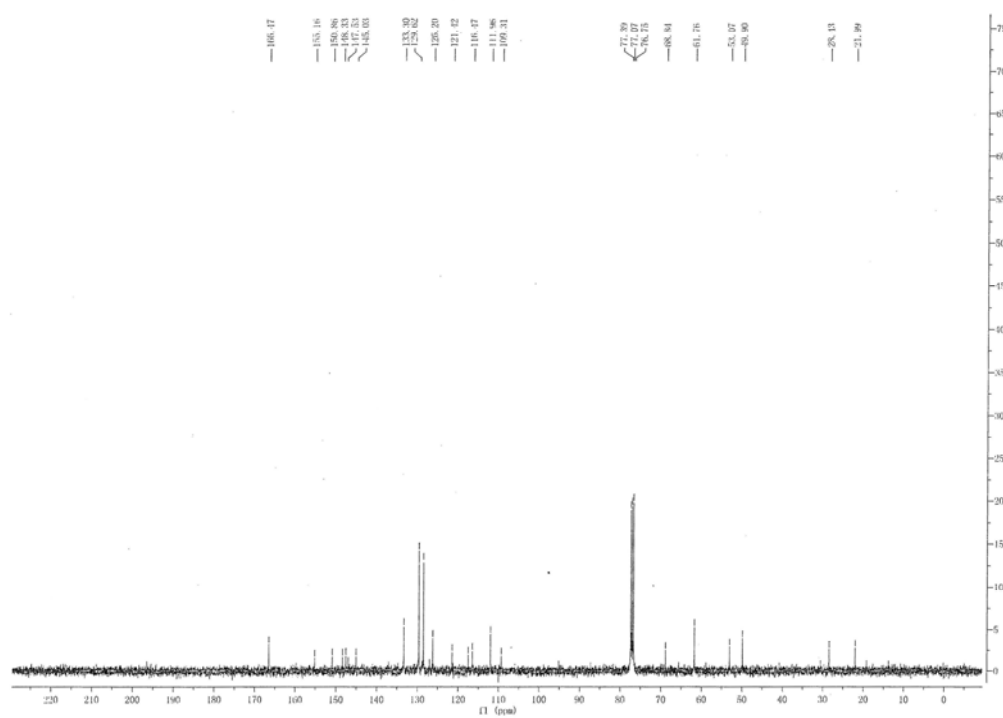


Fig. S16 ¹³C NMR spectrum of G1-Ph-TB in chloroform-*d*.

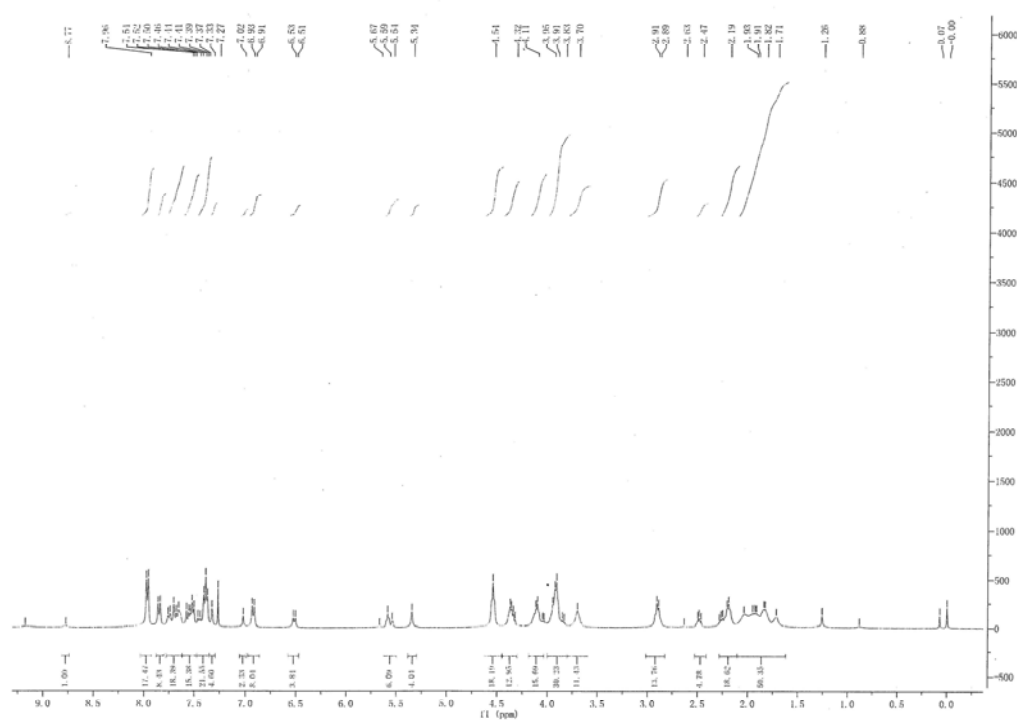


Fig. S17 ¹H NMR spectrum of G2-Ph-TB in chloroform-*d*.

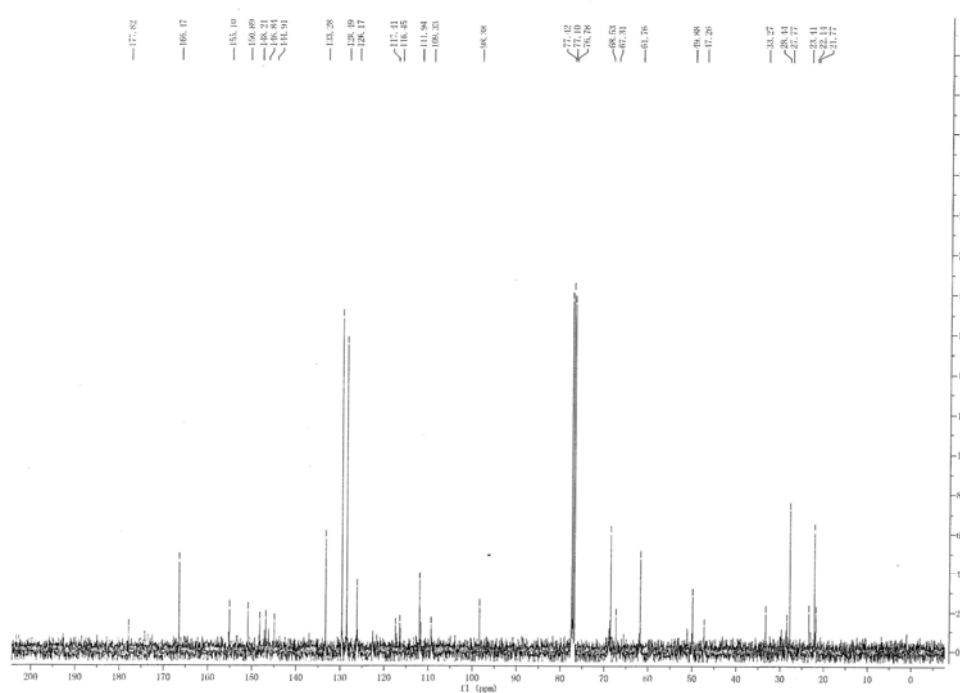


Fig. S18 ¹³C NMR spectrum of G2-Ph-TB in chloroform-*d*.

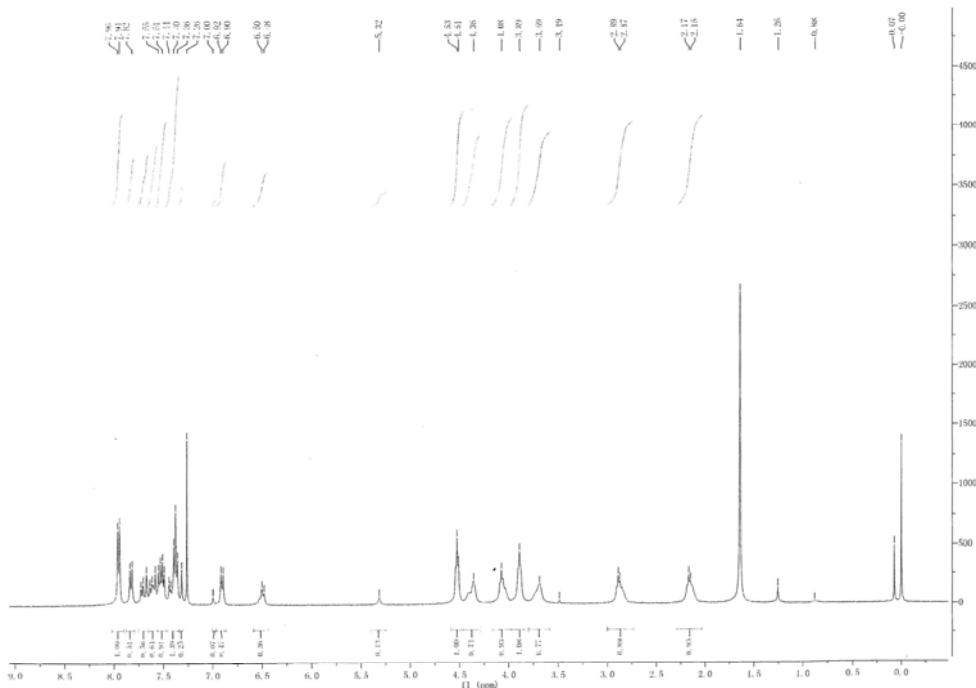


Fig. S19 ^1H NMR spectrum of **G3-Ph-TB** in chloroform-*d*.

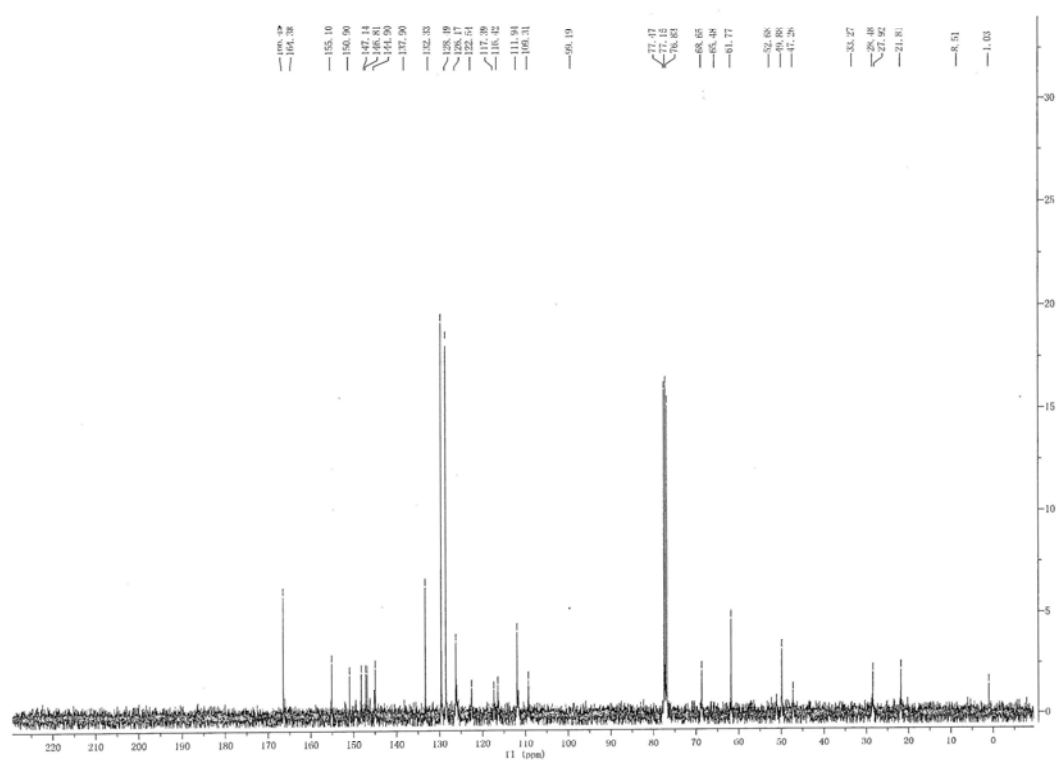


Fig. S20 ^{13}C NMR spectrum of **G3-Ph-TB** in chloroform-*d*.

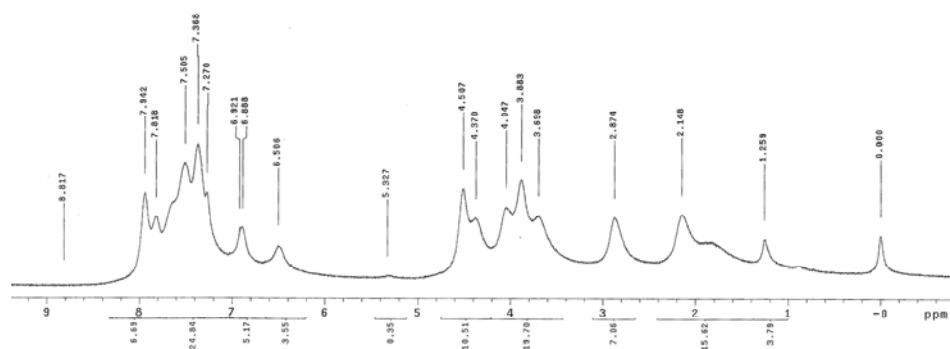


Fig. S21 ^1H NMR spectrum of **G4-Ph-TB** in chloroform-*d*.

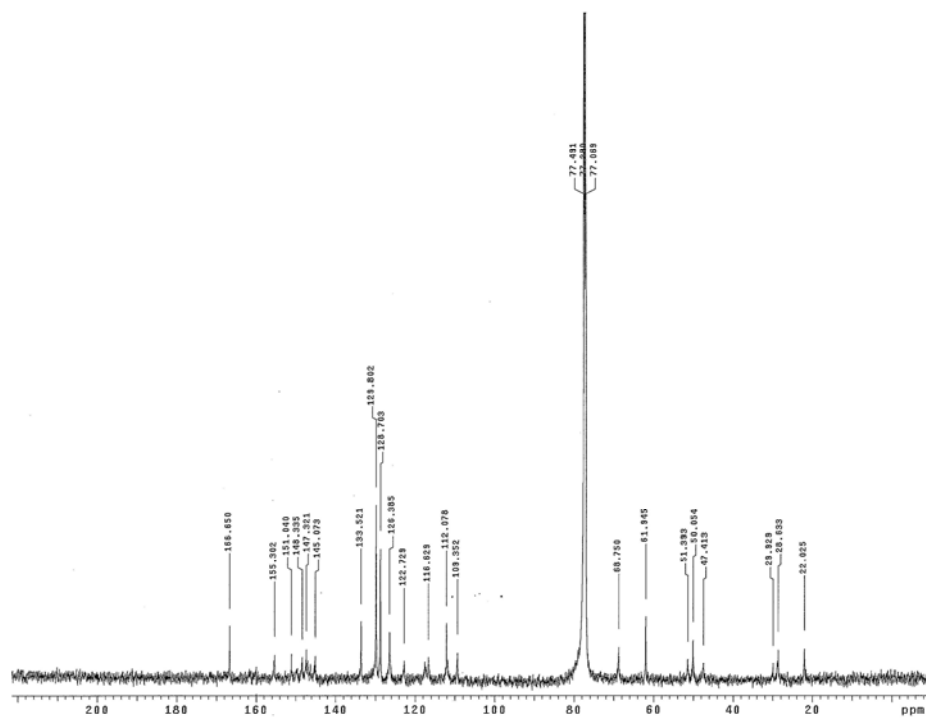


Fig. S22 ^{13}C NMR spectrum of **G4-Ph-TB** in chloroform-*d*.

158.86
155.27
150.07
148.46
147.52
146.72
145.14
141.40
137.07
135.56
130.99
128.07
125.88
121.29
117.99
116.31
111.88
109.76
107.11
102.11
77.81
77.12
76.86
68.85
63.41
51.05
49.68
28.42
27.77
21.91

Fig. S24 ^{13}C NMR spectrum of **G1-PFPh-TB** in chloroform-*d*.

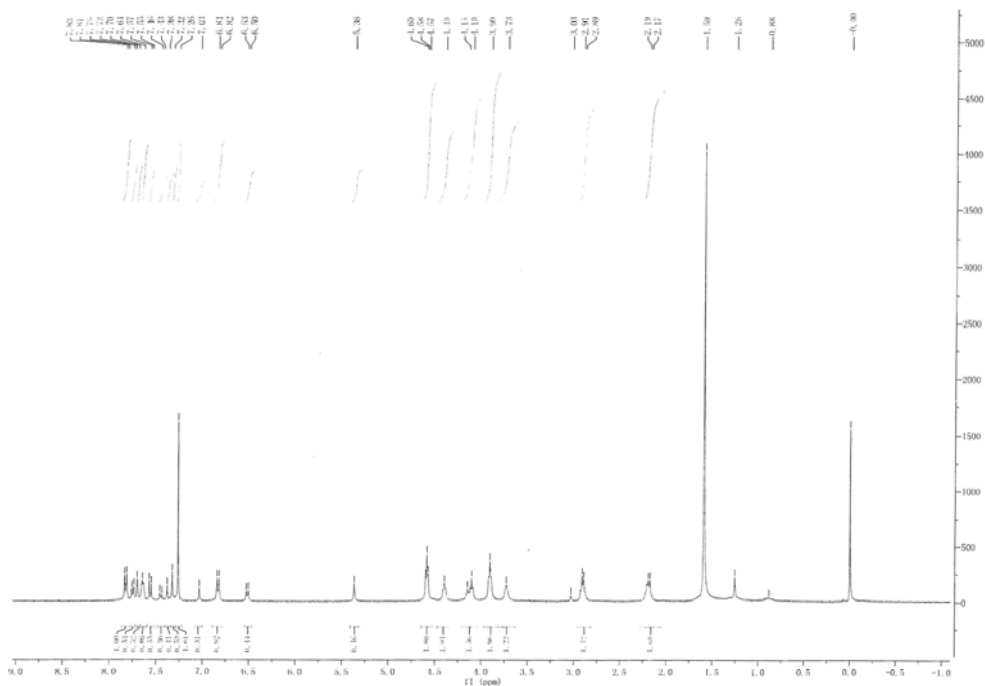


Fig. S25 ^1H NMR spectrum of G2-PFPh-TB in chloroform-*d*.

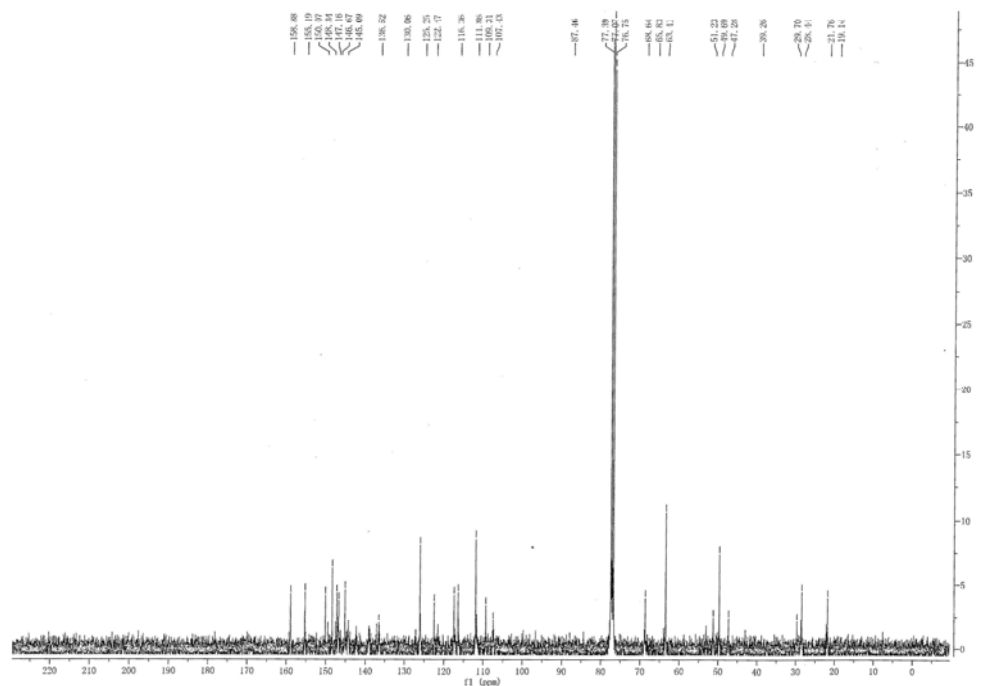


Fig. S26 ^{13}C NMR spectrum of G2-PFPh-TB in chloroform-*d*.

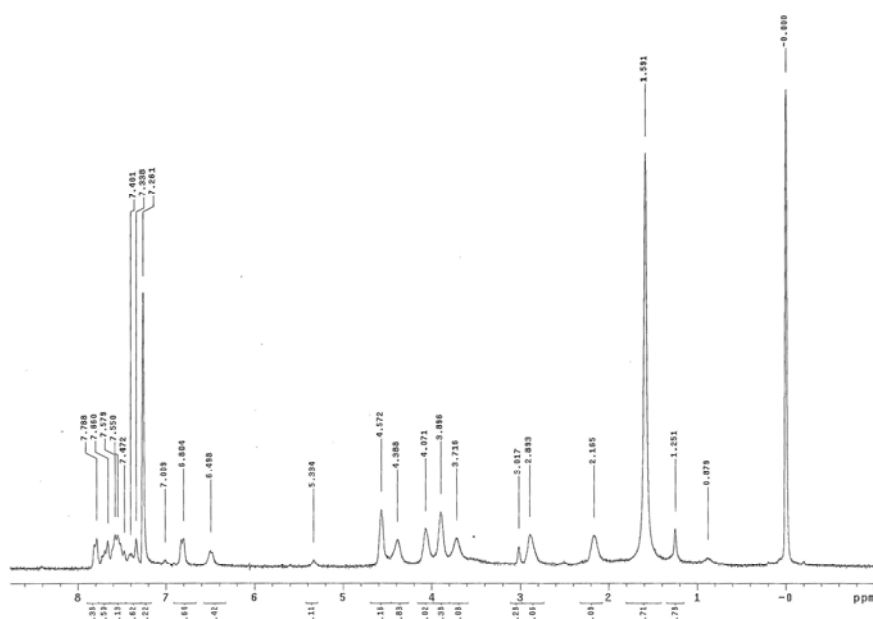


Fig. S27 ¹H NMR spectrum of G3-PFPh-TB in chloroform-*d*.

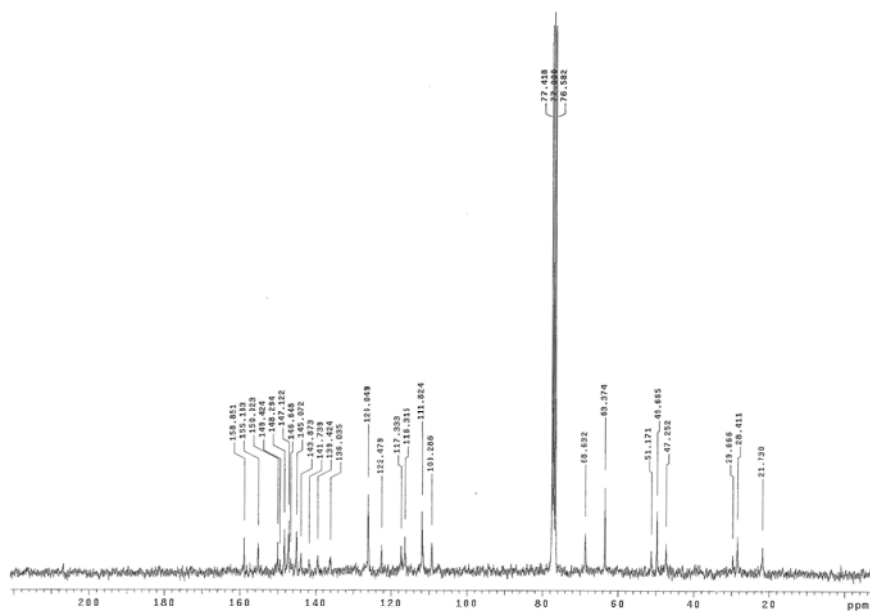


Fig. S28 ¹³C NMR spectrum of G3-PFPh-TB in chloroform-*d*.

13C NMR spectrum of compound 1. The x-axis represents chemical shift in ppm, ranging from 220 to 0. The spectrum shows several peaks in the aromatic region (112-155 ppm), a carbonyl peak at 195.477 ppm, a solvent peak at 69.257 ppm, and aliphatic peaks at 21.234 and 21.238 ppm. A cluster of peaks is visible between 38 and 42 ppm.

Chemical Shift (ppm)
155.477
150.262
147.748
146.385
145.178
115.035
112.742
69.257
41.284
40.262
39.755
39.248
38.841
38.647
21.238
21.234

Fig. S30 ^{13}C NMR spectrum of **G4-PFPh-TB** in $\text{DMSO-}d_6$.

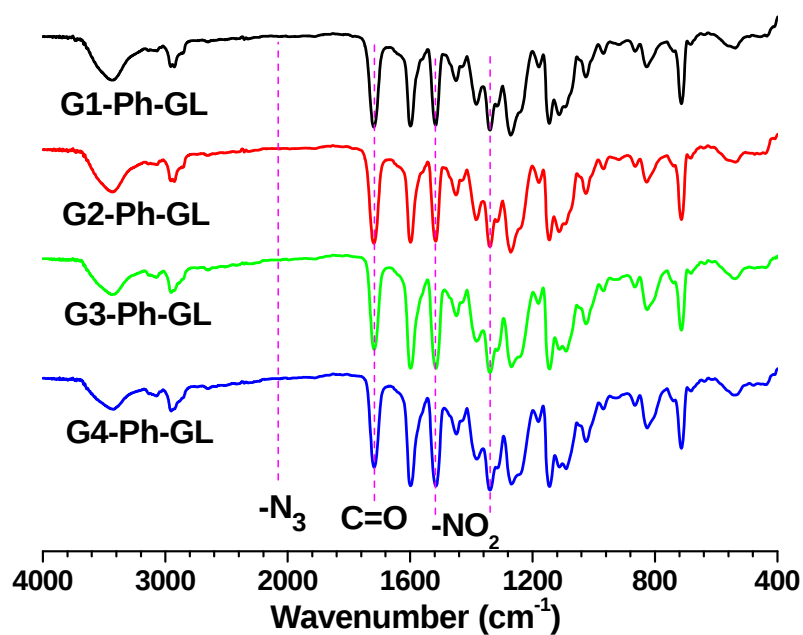


Fig. S31 The FT-IR spectra of dendrimers **G1-Ph-TB-G4-Ph-TB**.

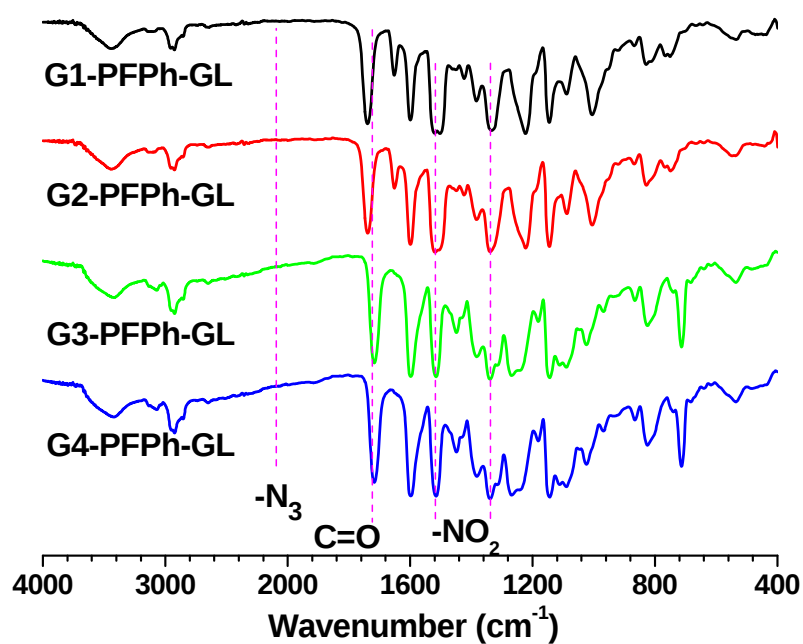


Fig. S32 The FT-IR spectra of dendrimers **G1-PFPh-TB-G4-PFPh-TB**.

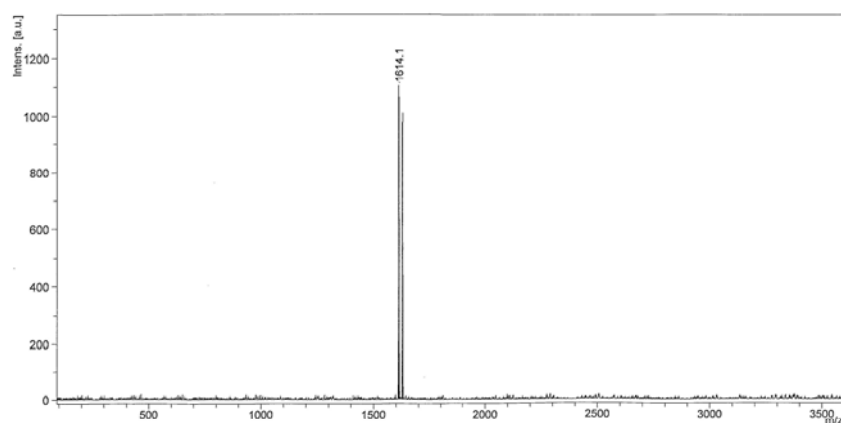


Fig. S33 The MALDI-TOF Mass spectrum of **G1-6Cl-TB**.

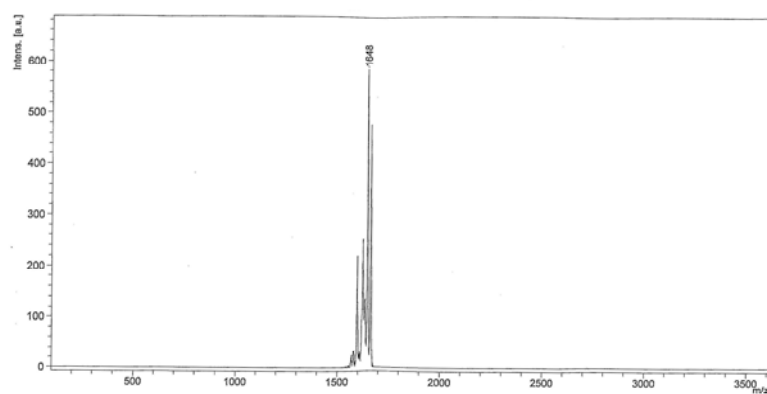


Fig. S34 The MALDI-TOF Mass spectrum of **G1-6N₃-TB**.

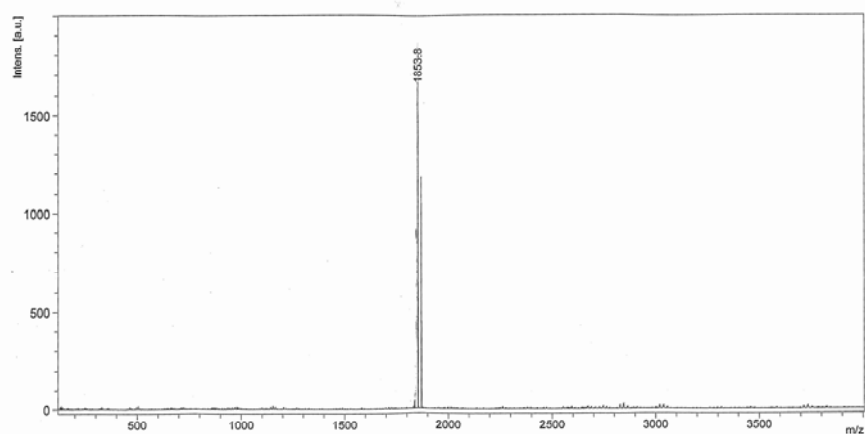


Fig. S35 The MALDI-TOF Mass spectrum of **G1-PFPh**.

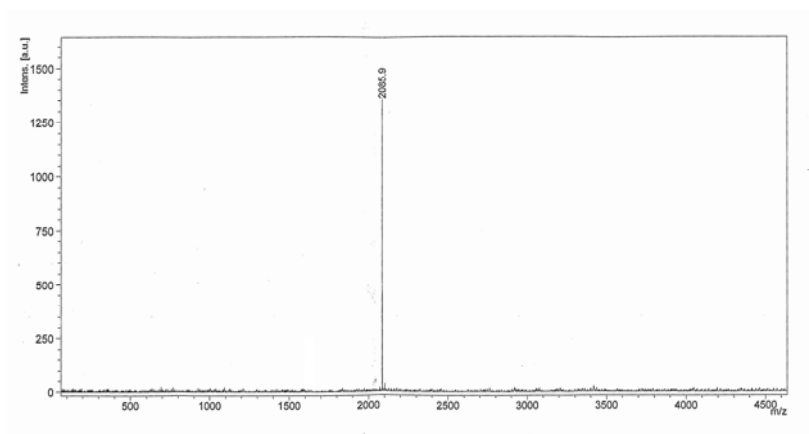


Fig. S36 The MALDI-TOF Mass spectrum of **G1≡-PFPh**.

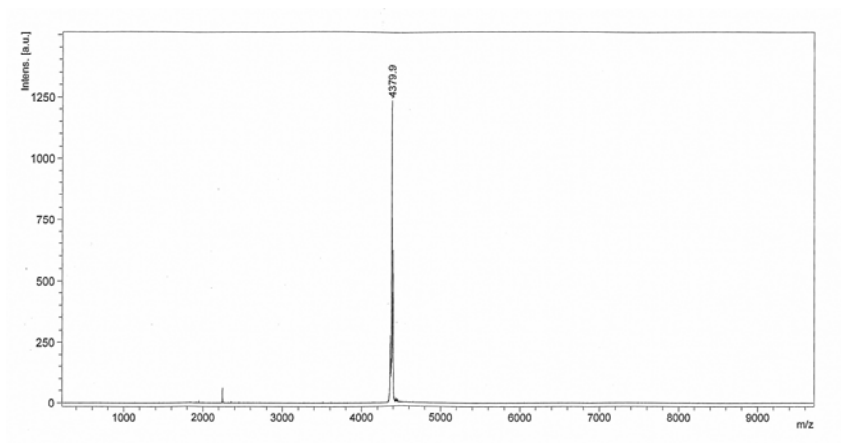


Fig. S37 The MALDI-TOF Mass spectrum of **G2-PFPh**.

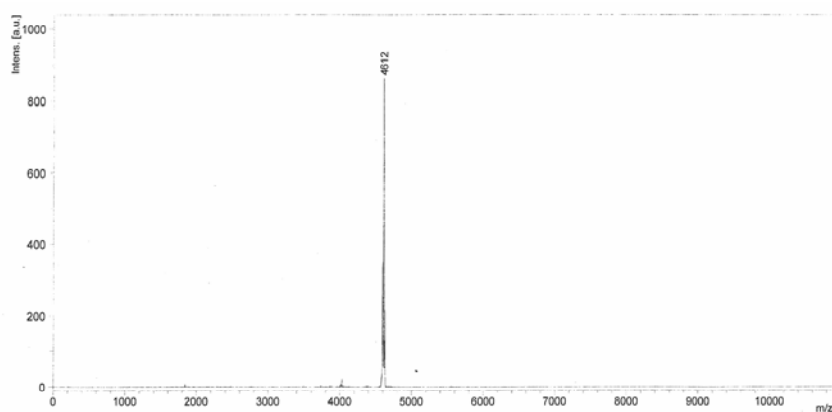


Fig. S38 The MALDI-TOF Mass spectrum of **G2≡-PFPh**.

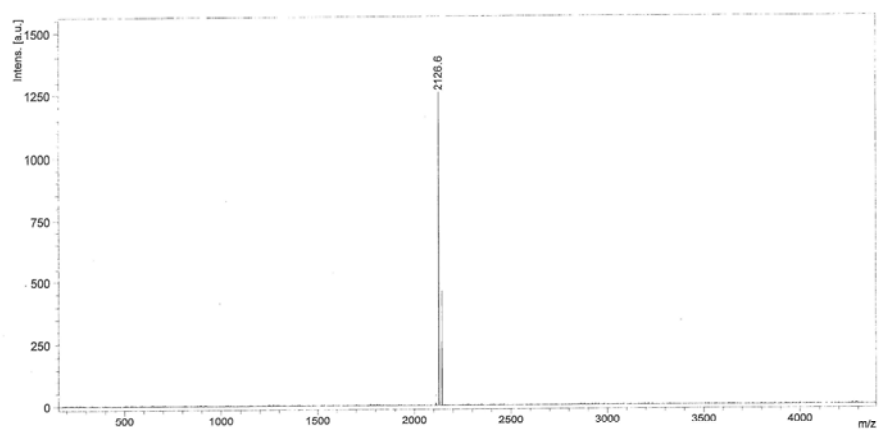


Fig. S39 The MALDI-TOF Mass spectrum of **G1-Ph-TB**.

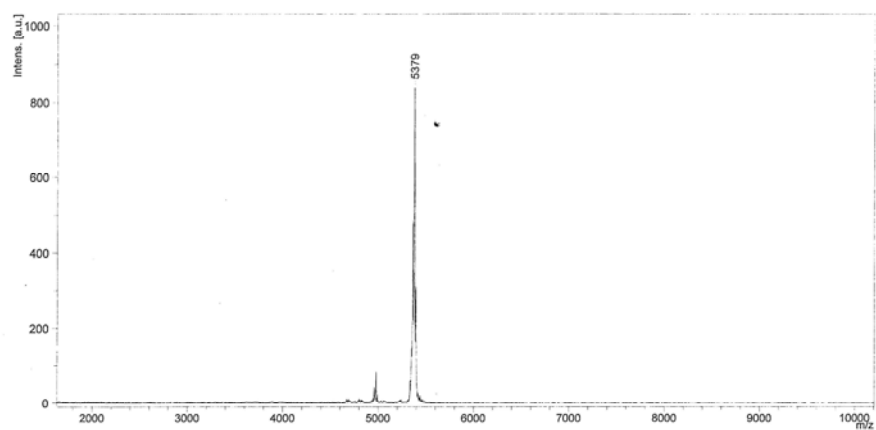


Fig. S40 The MALDI-TOF Mass spectrum of **G2-Ph-TB**.

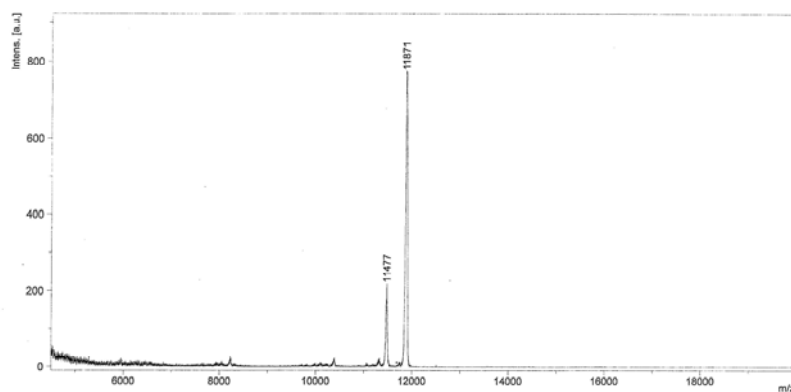


Fig. S41 The MALDI-TOF Mass spectrum of **G3-Ph-TB**.

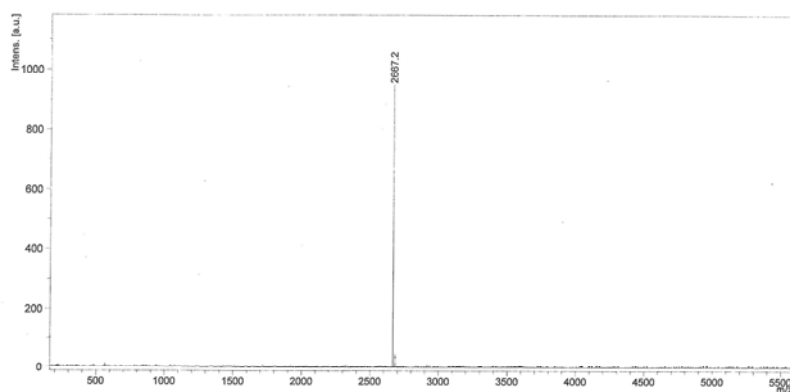


Fig. S42 The MALDI-TOF Mass spectrum of **G1-PFPh-TB**.

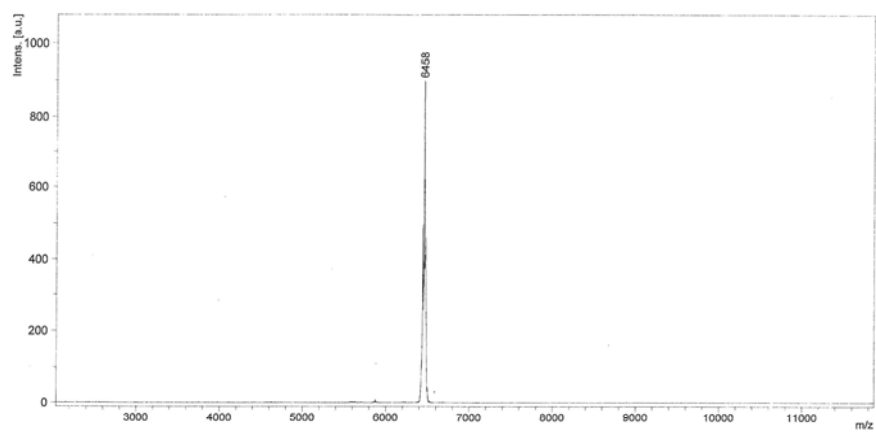


Fig. S43 The MALDI-TOF Mass spectrum of **G2-PFPh-TB**.

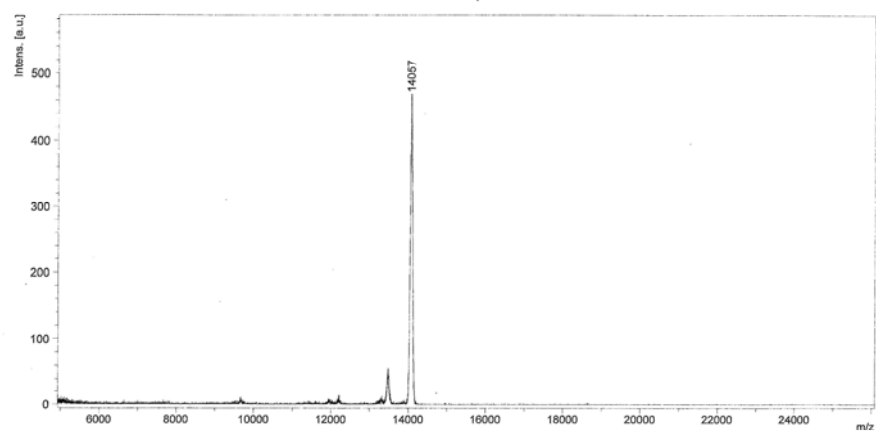


Fig. S44 The MALDI-TOF Mass spectrum of **G3-PFPh-TB**.

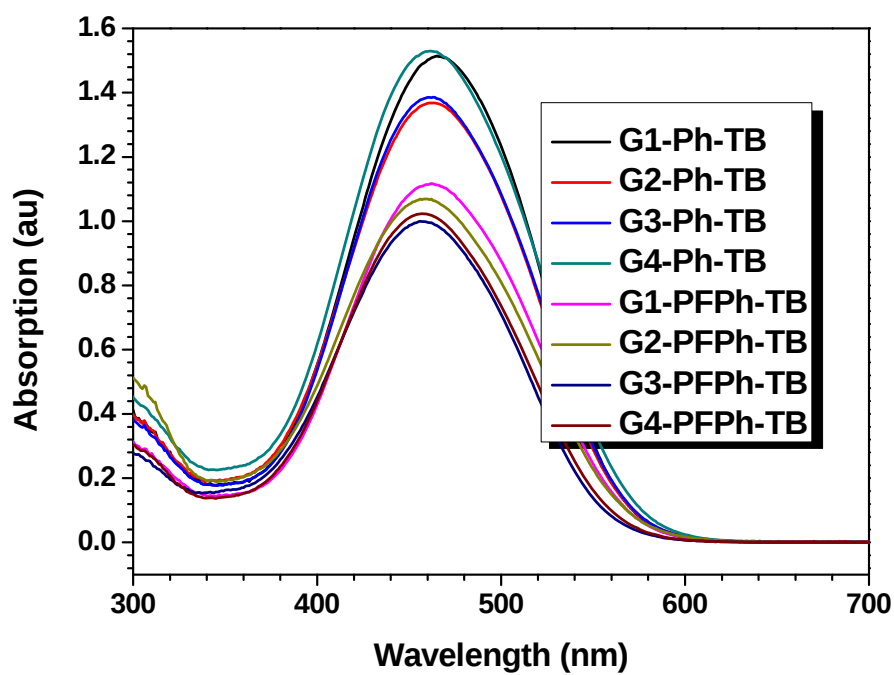


Fig. S45 UV-Vis spectra of THF solutions of dendrimers (0.02 mg/mL).

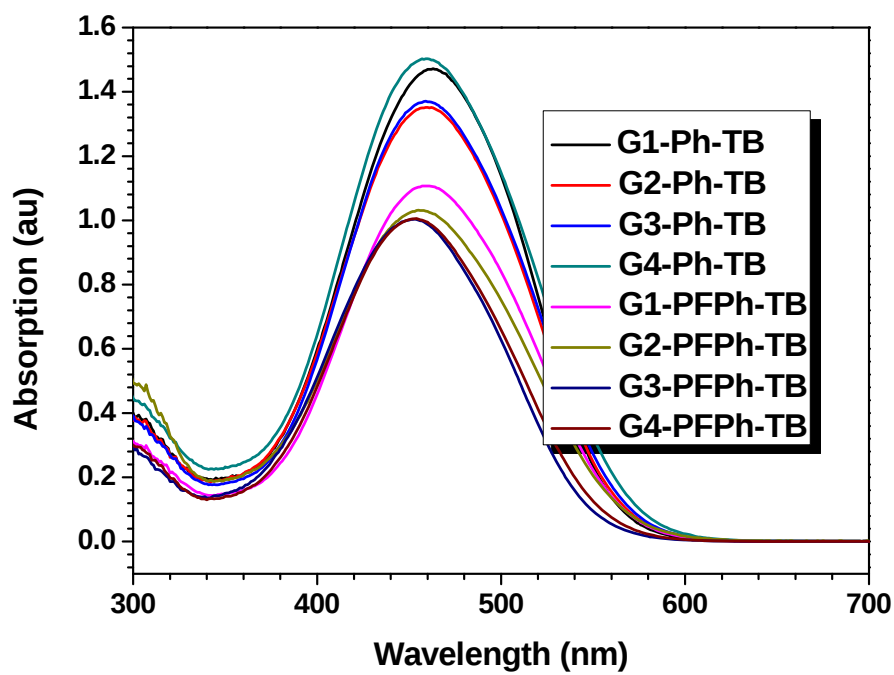


Fig. S46 UV-Vis spectra of 1,4-dioxane solutions of dendrimers (0.02 mg/mL).

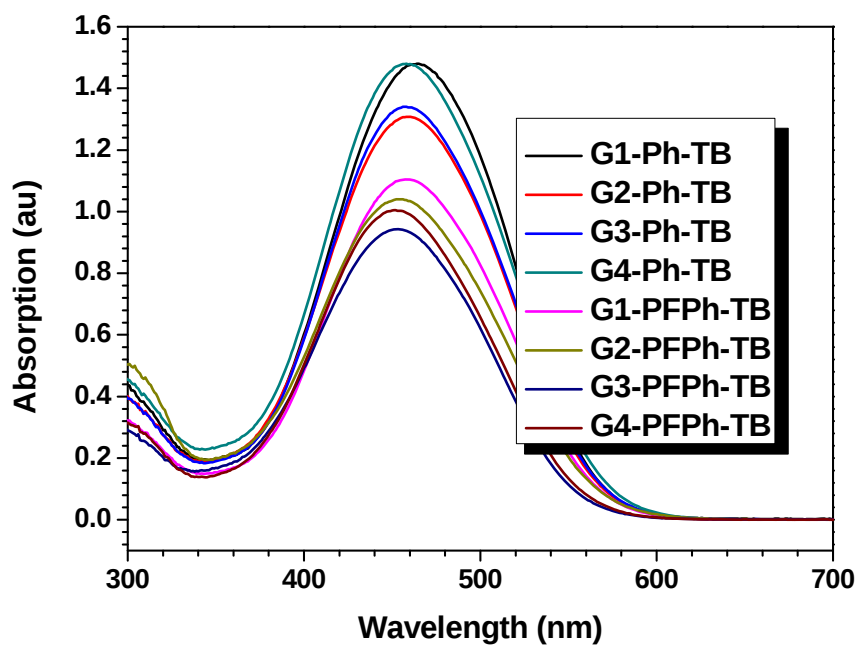


Fig. S47 UV-Vis spectra of chloroform solutions of dendrimers (0.02 mg/mL).

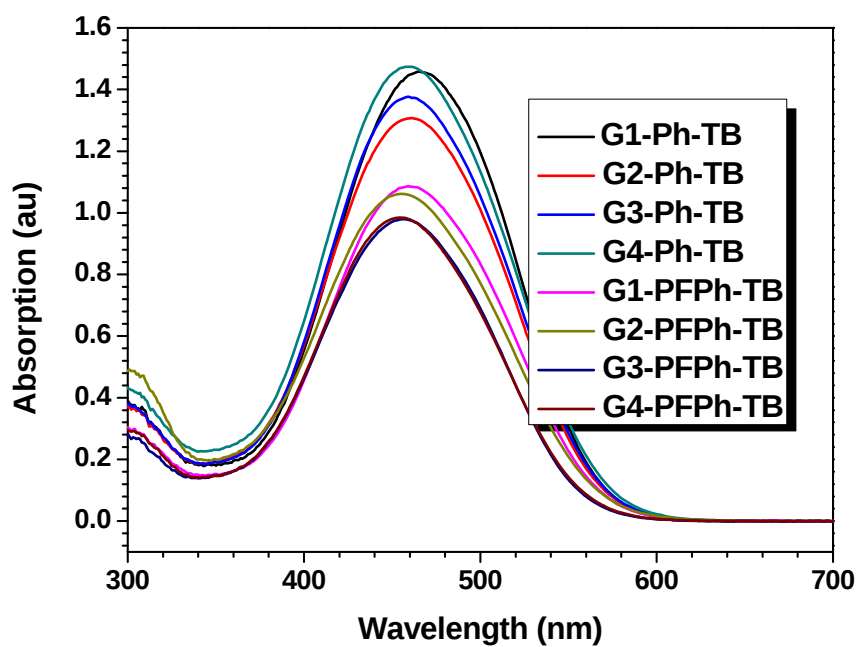


Fig. S48 UV-Vis spectra of dichloromethane solutions of dendrimers (0.02 mg/mL).

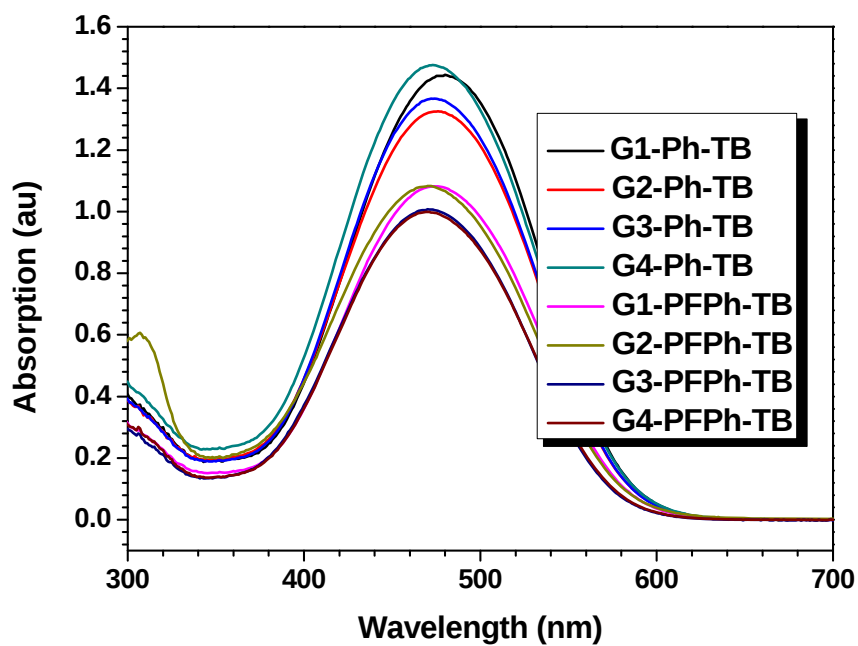


Fig. S49 UV-Vis spectra of DMF solutions of dendrimers (0.02 mg/mL).

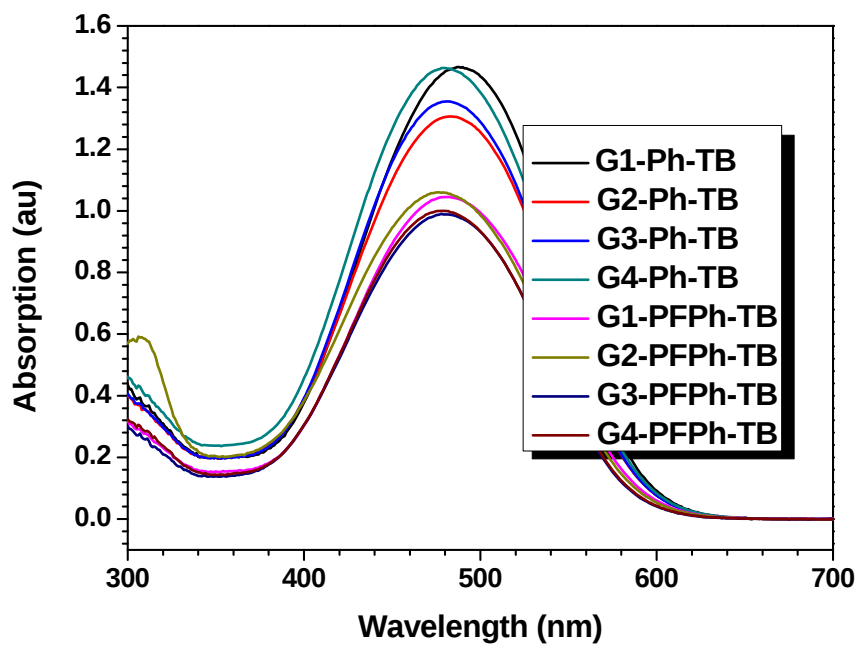


Fig. S50 UV-Vis spectra of DMSO solutions of dendrimers (0.02 mg/mL).

Table S1. The maximum absorption of dendrimers (λ_{max} , nm 0.02 mg/mL).

	THF	1,4-dioxane	chloroform	dichloromethane	DMF	DMSO	film
G1-Ph-TB	465	463	464	466	480	488	478
G2-Ph-TB	462	460	459	461	476	484	475
G3-Ph-TB	463	459	458	459	474	481	470
G4-Ph-TB	461	457	458	458	473	479	470
G1-PFPh-TB	462	458	459	458	474	481	464
G2-PFPh-TB	459	455	456	455	470	477	462
G3-PFPh-TB	456	453	452	455	470	478	461
G4-PFPh-TB	457	454	452	454	470	479	460
G1	462	460	461	465	476	491	479
G2	462	457	456	460	474	485	482
G3	459	454	455	453	472	478	480
G4	459	456	456	456	469	477	470
G5	458	455	456	456	470	478	470

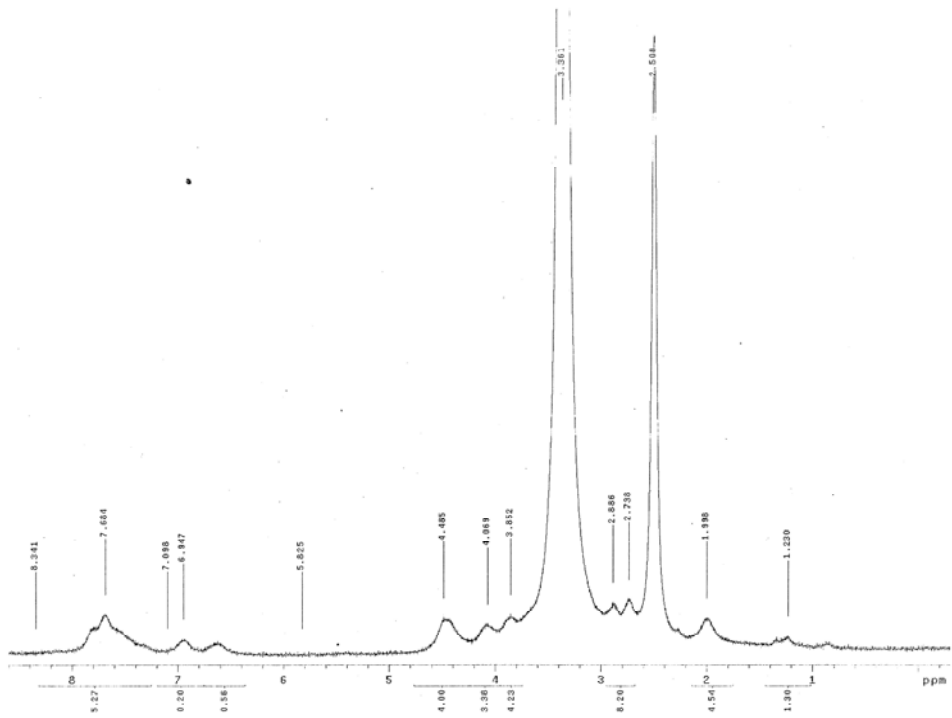


Fig. S51 ^1H NMR spectrum of **G4-PFPh-TB** (1.5 mg/mL) in $\text{DMSO-}d_6$.

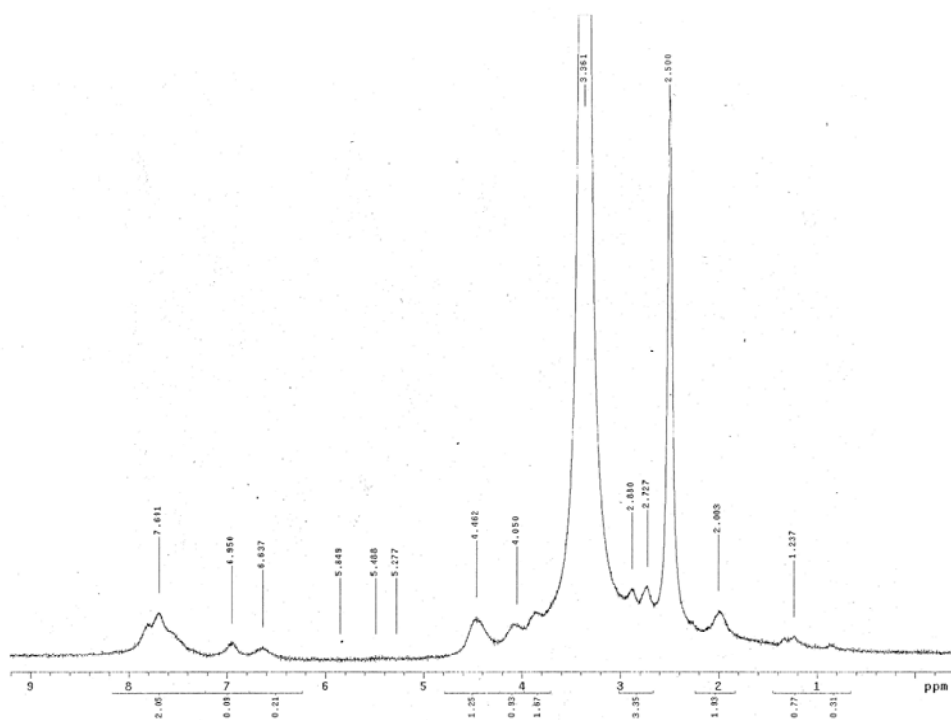


Fig. S52 ¹H NMR spectrum of **G4-PFPh-TB** (3.0 mg/mL) in DMSO-*d*₆.

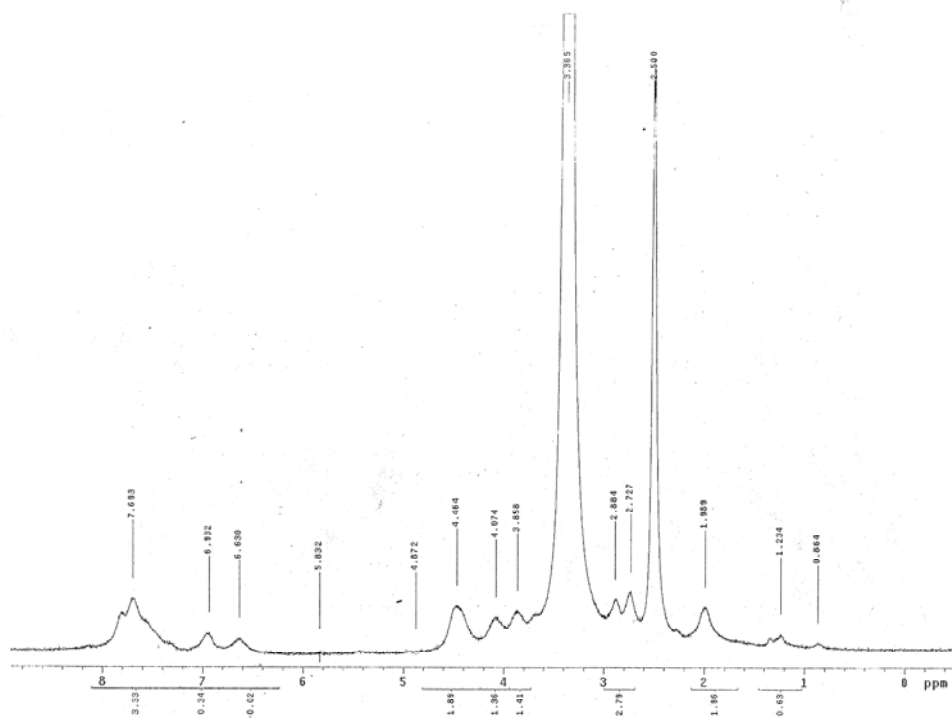


Fig. S53 ¹H NMR spectrum of **G4-PFPh-TB** (5.0 mg/mL) in DMSO-*d*₆.

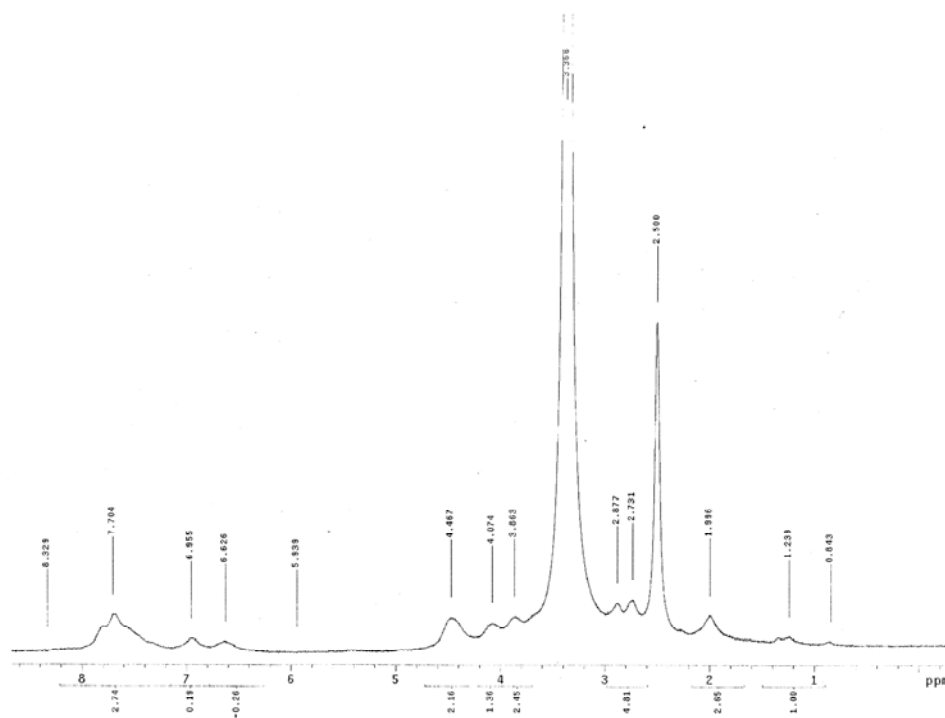


Fig. S54 ¹H NMR spectrum of **G4-PFPh-TB** (7.5 mg/mL) in DMSO-*d*₆.

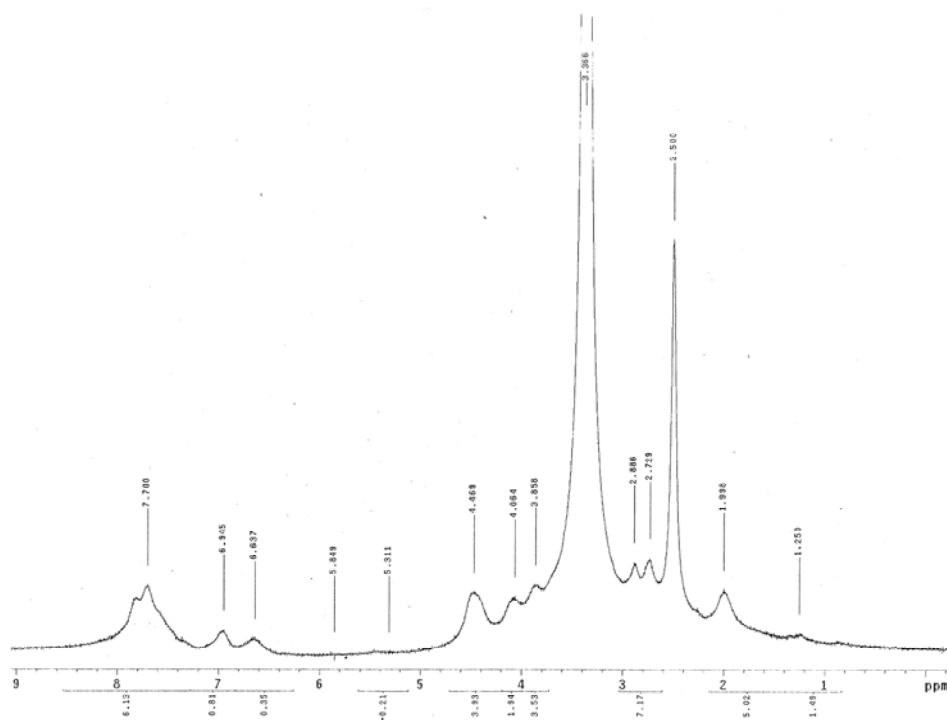


Fig. S55 ¹H NMR spectrum of **G4-PFPh-TB** (10.0 mg/mL) in DMSO-*d*₆.

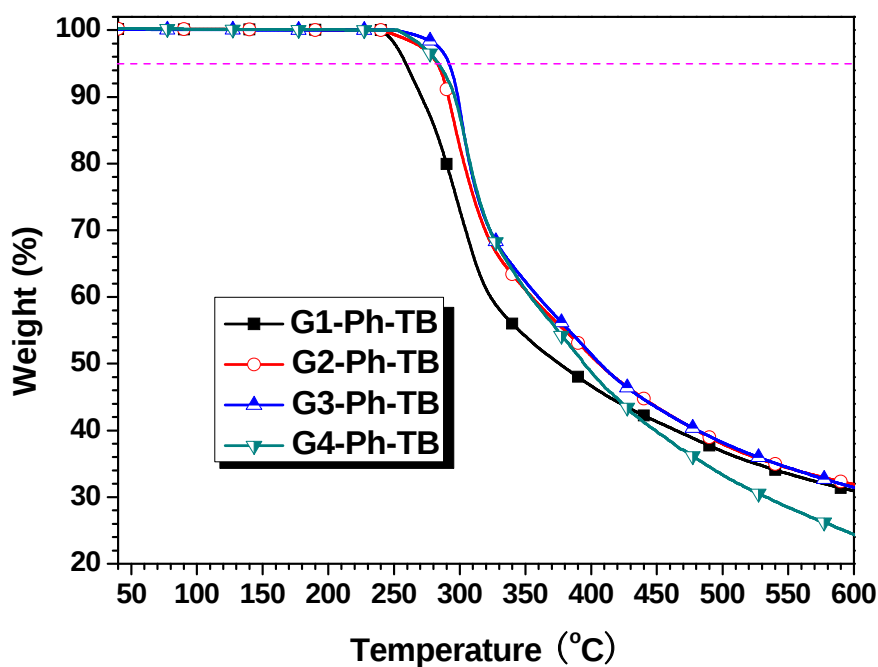


Fig. S56. TGA thermograms of dendrimers **G1-Ph-TB-G4-Ph-TB**, measured in nitrogen at a heating rate of 10 °C/min

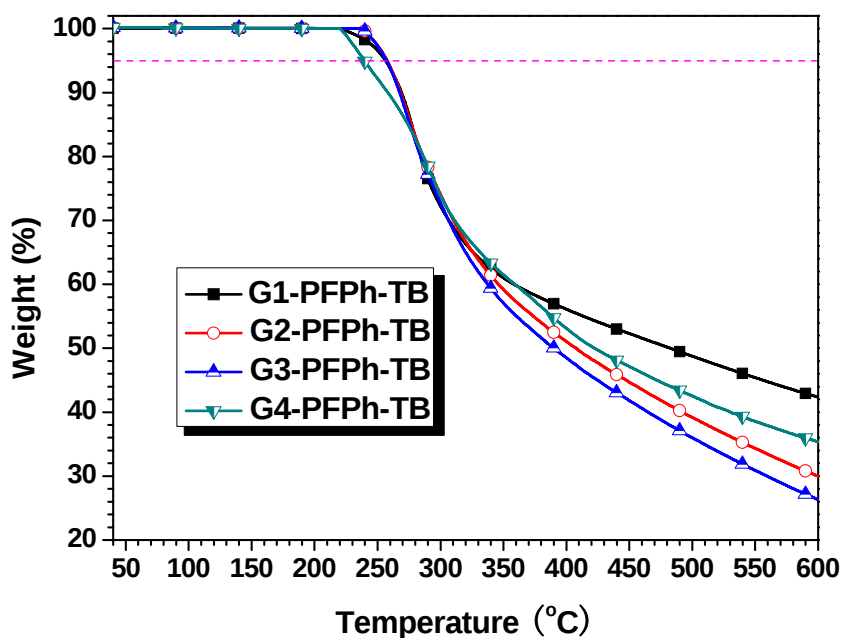


Fig. S57 TGA thermograms of dendrimers **G1-PFPh-TB-G4-PFPh-TB**, measured in nitrogen at a heating rate of 10 °C/min

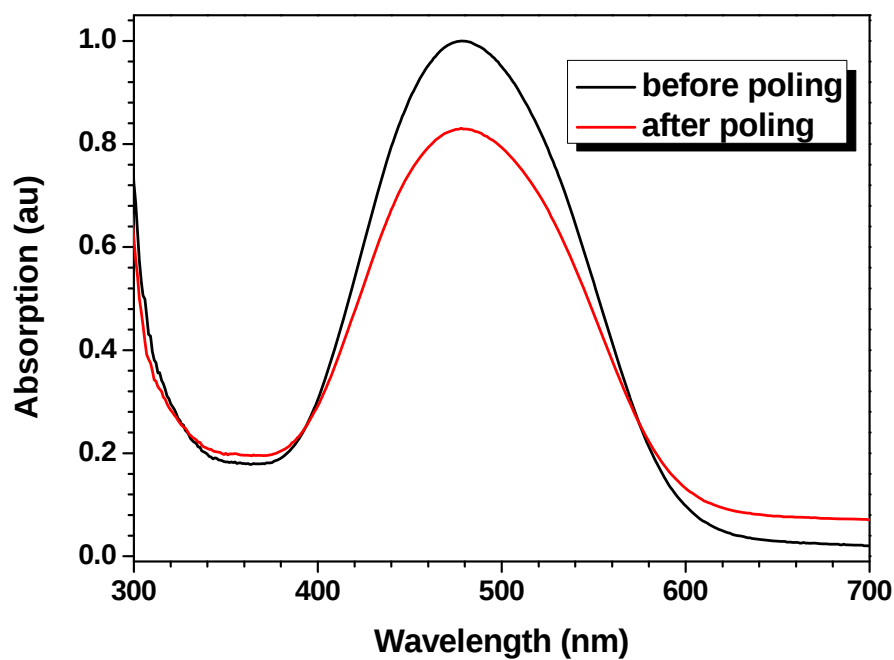


Fig. S58 Absorption spectra of the film of **G1-Ph-TB** before and after poling.

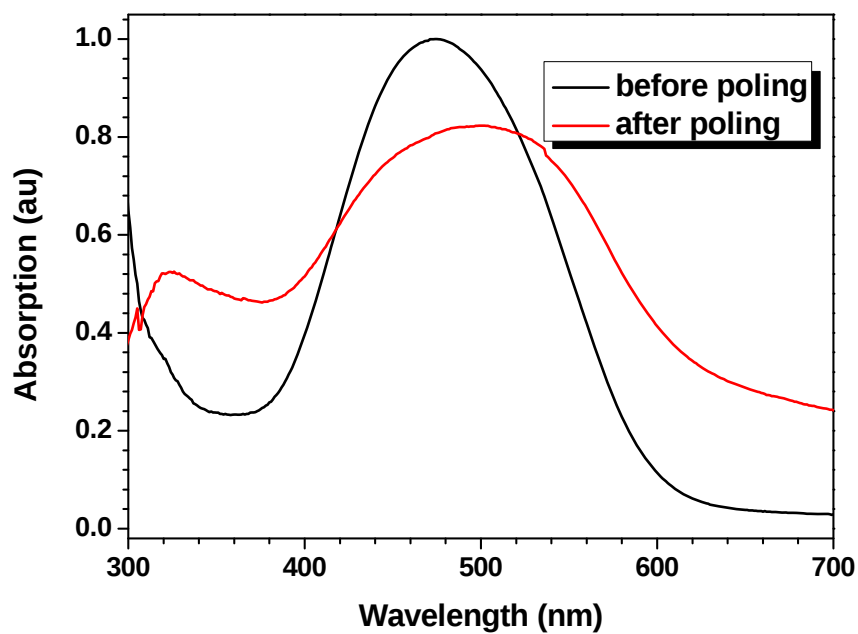


Fig. S59 Absorption spectra of the film of **G2-Ph-TB** before and after poling.

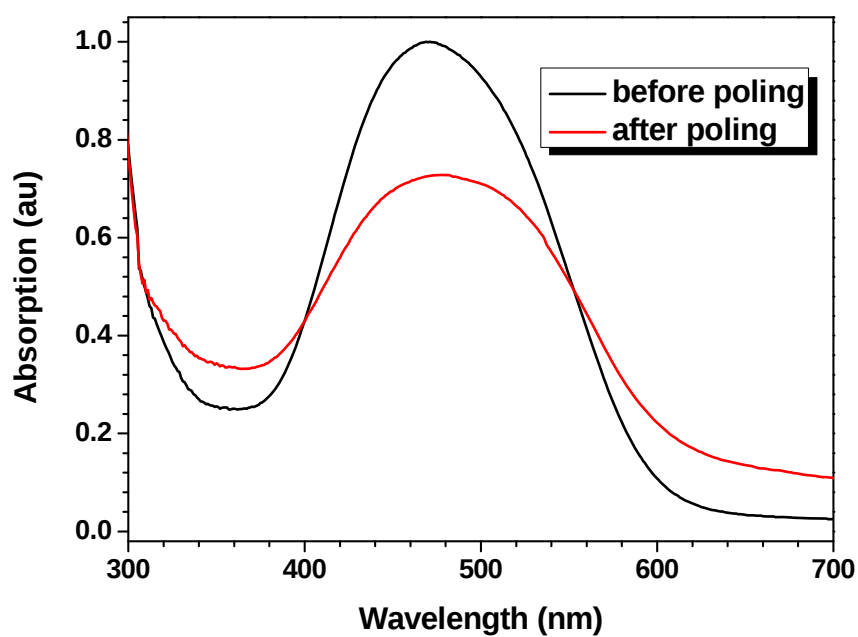


Fig. S60 Absorption spectra of the film of **G3-Ph-TB** before and after poling.

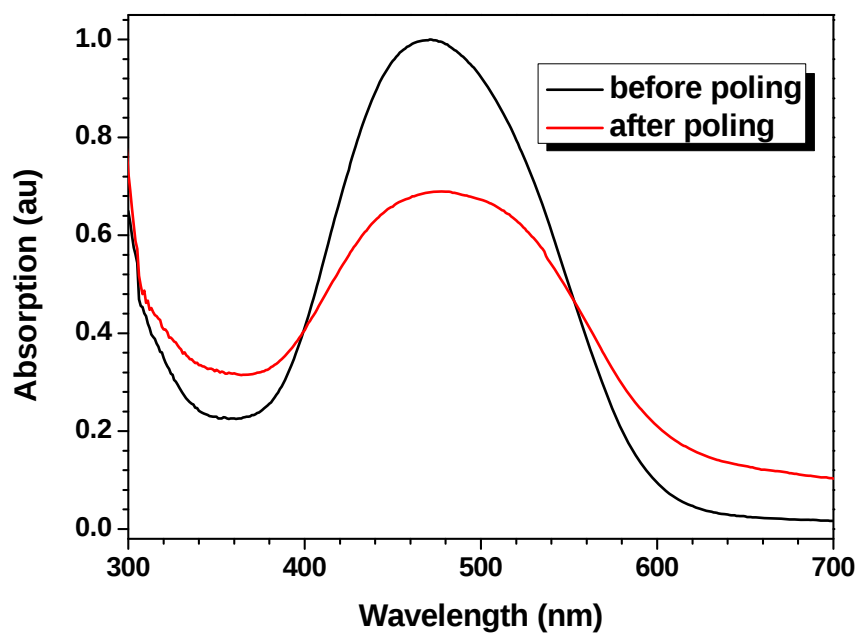


Fig. S61 Absorption spectra of the film of **G4-Ph-TB** before and after poling.

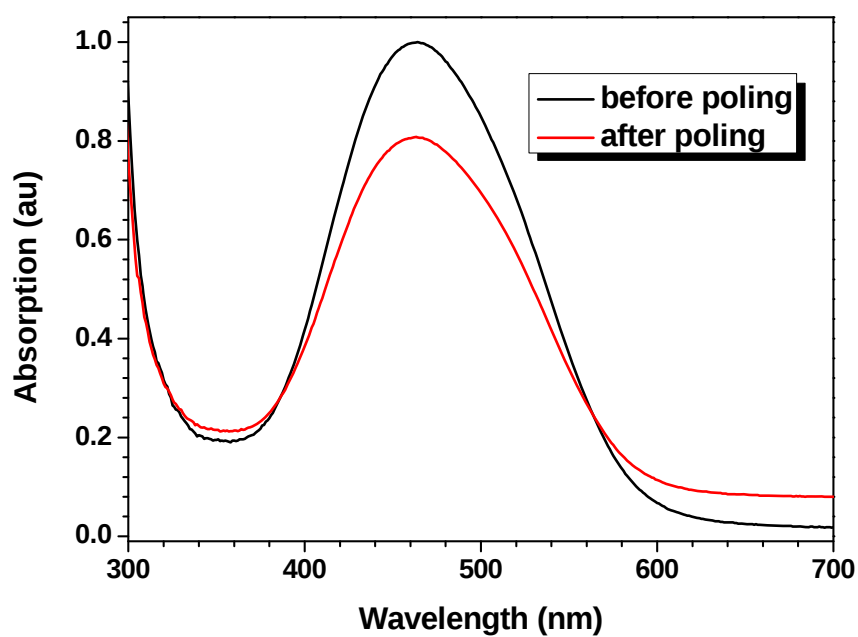


Fig. S62 Absorption spectra of the film of **G1-PFPh-TB** before and after poling.

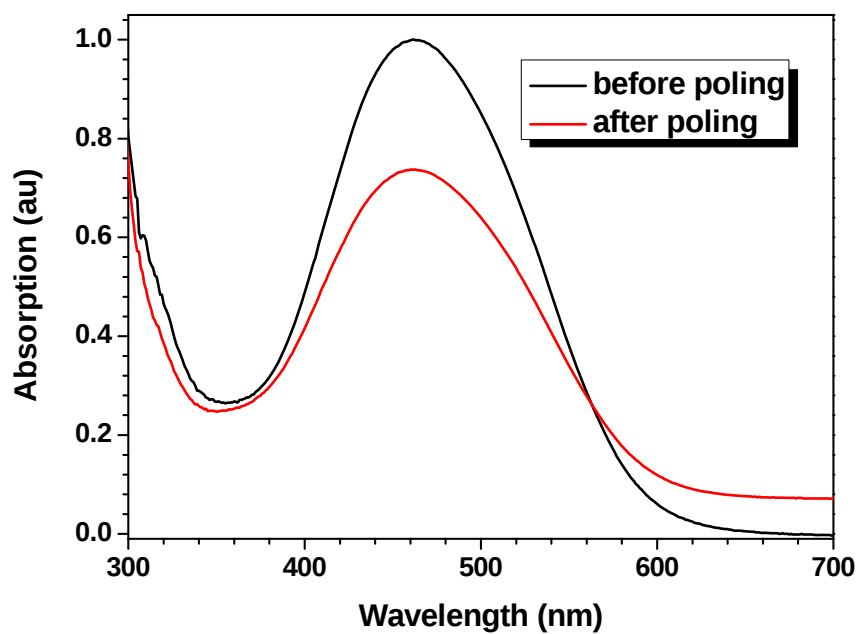


Fig. S63 Absorption spectra of the film of **G2-PFPh-TB** before and after poling.

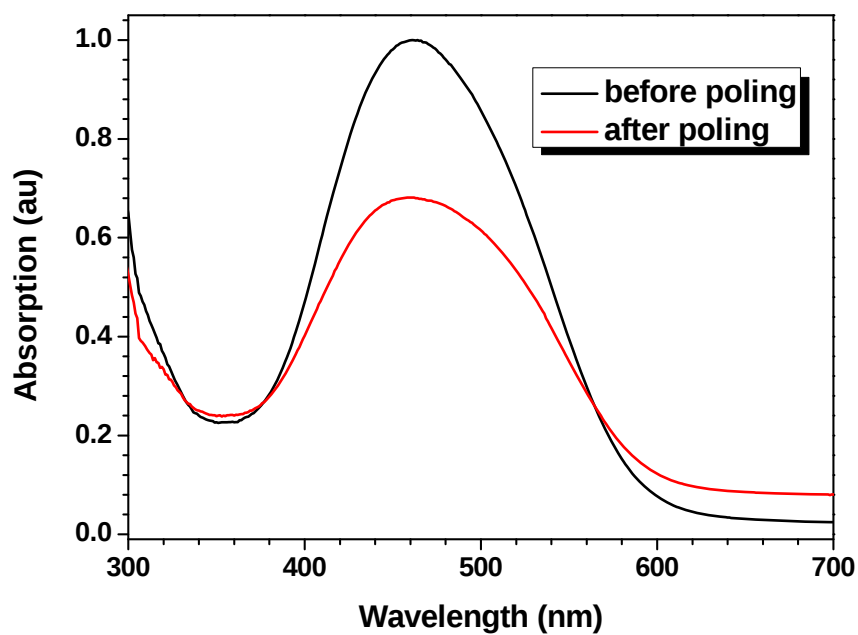


Fig. S64 Absorption spectra of the film of **G3-PFPh-TB** before and after poling.

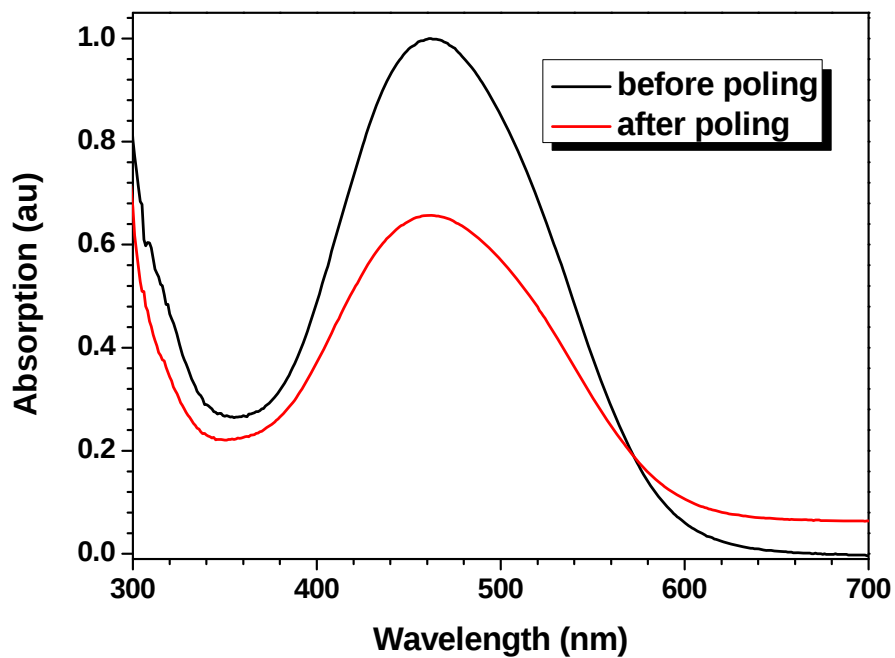


Fig. S65 Absorption spectra of the film of **G4-PFPh-TB** before and after poling.