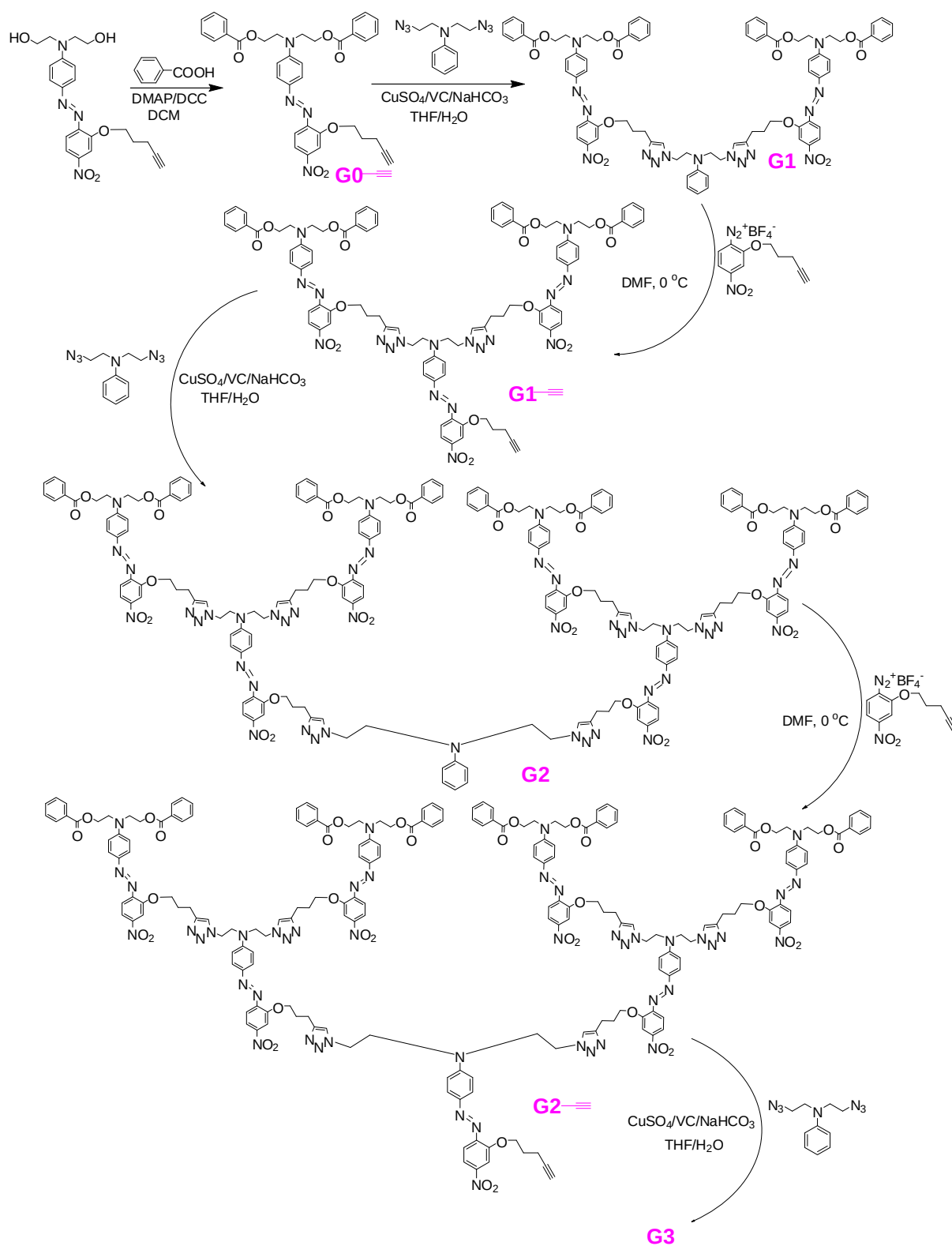


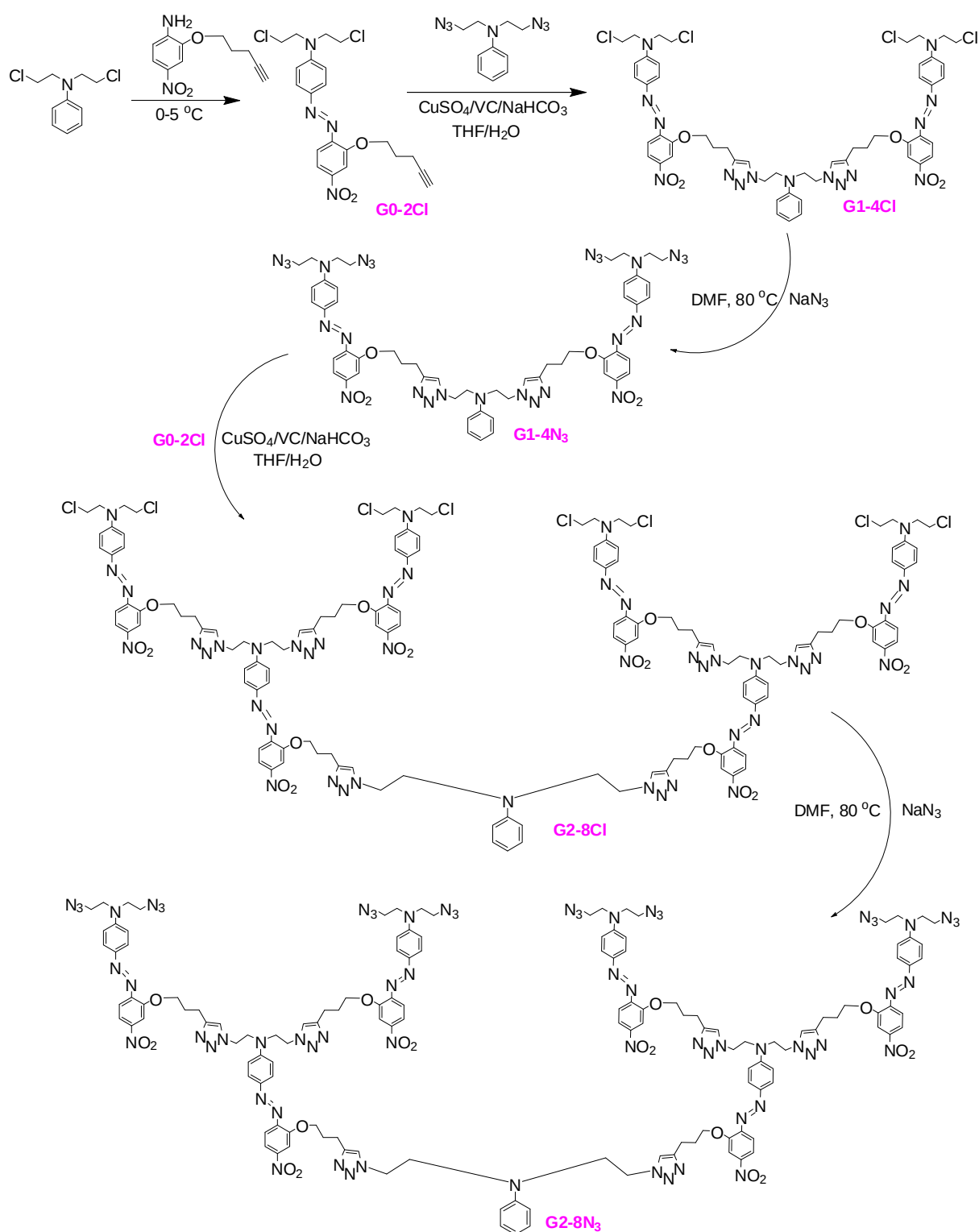
Electronic Supplementary Information:

Using isolation chromophore to further improve the comprehensive performance of nonlinear optical (NLO) dendrimers

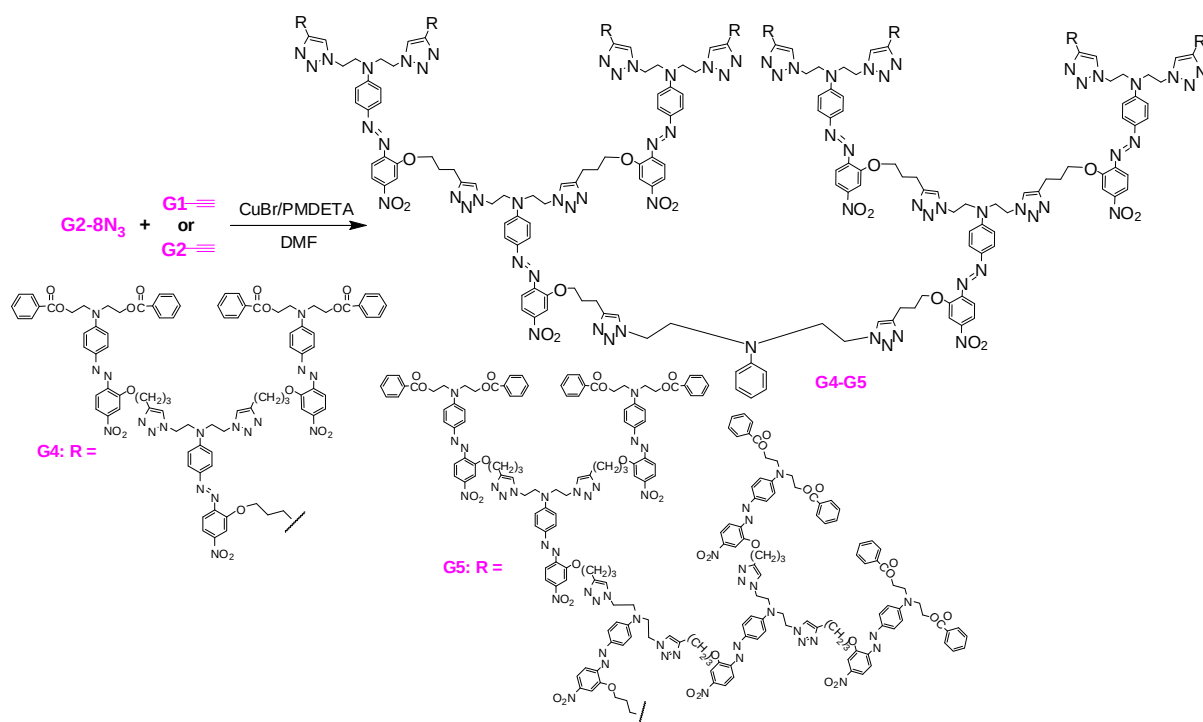
Wenbo Wu,^a Qi Huang,^a Guohua Xu,^b Can Wang,^a Cheng Ye,^c Jingui Qin,^a and Zhen Li^{*a}



Scheme S1. The Synthetic route to the end-capped dendrons (**G1≡** and **G2≡**) of dendrimers.



Scheme S2. The synthesis of the core (G2-8N₃) of dendrimers.



Scheme S3. The synthesis of high generation dendrimers **G4** and **G5**.

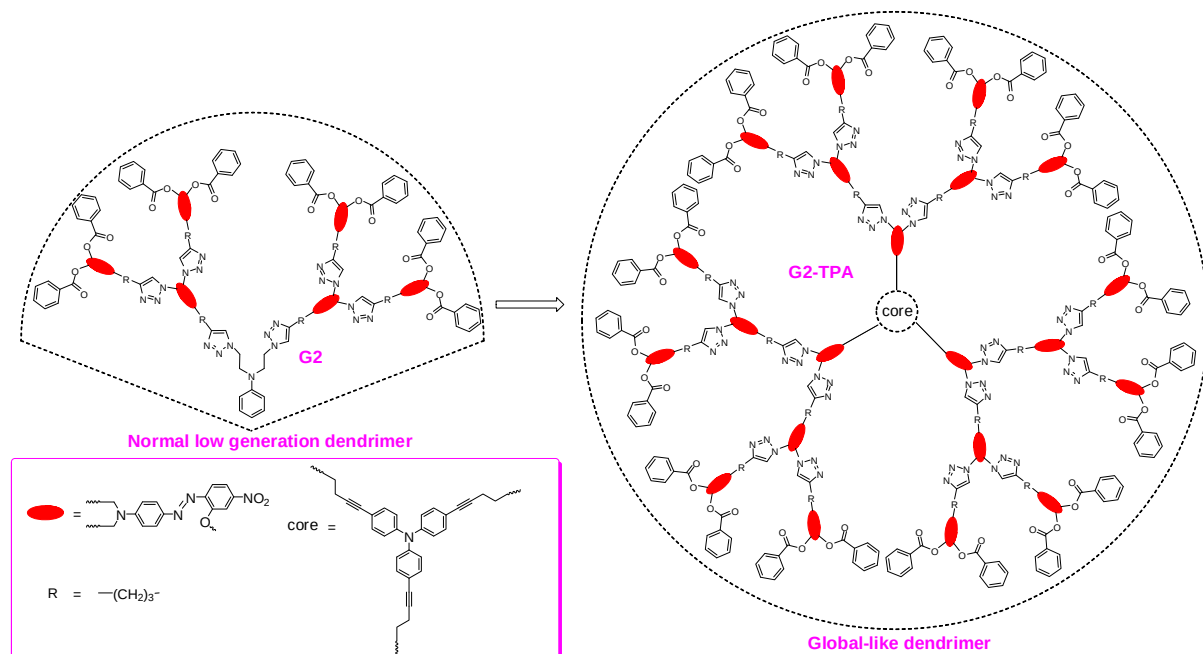
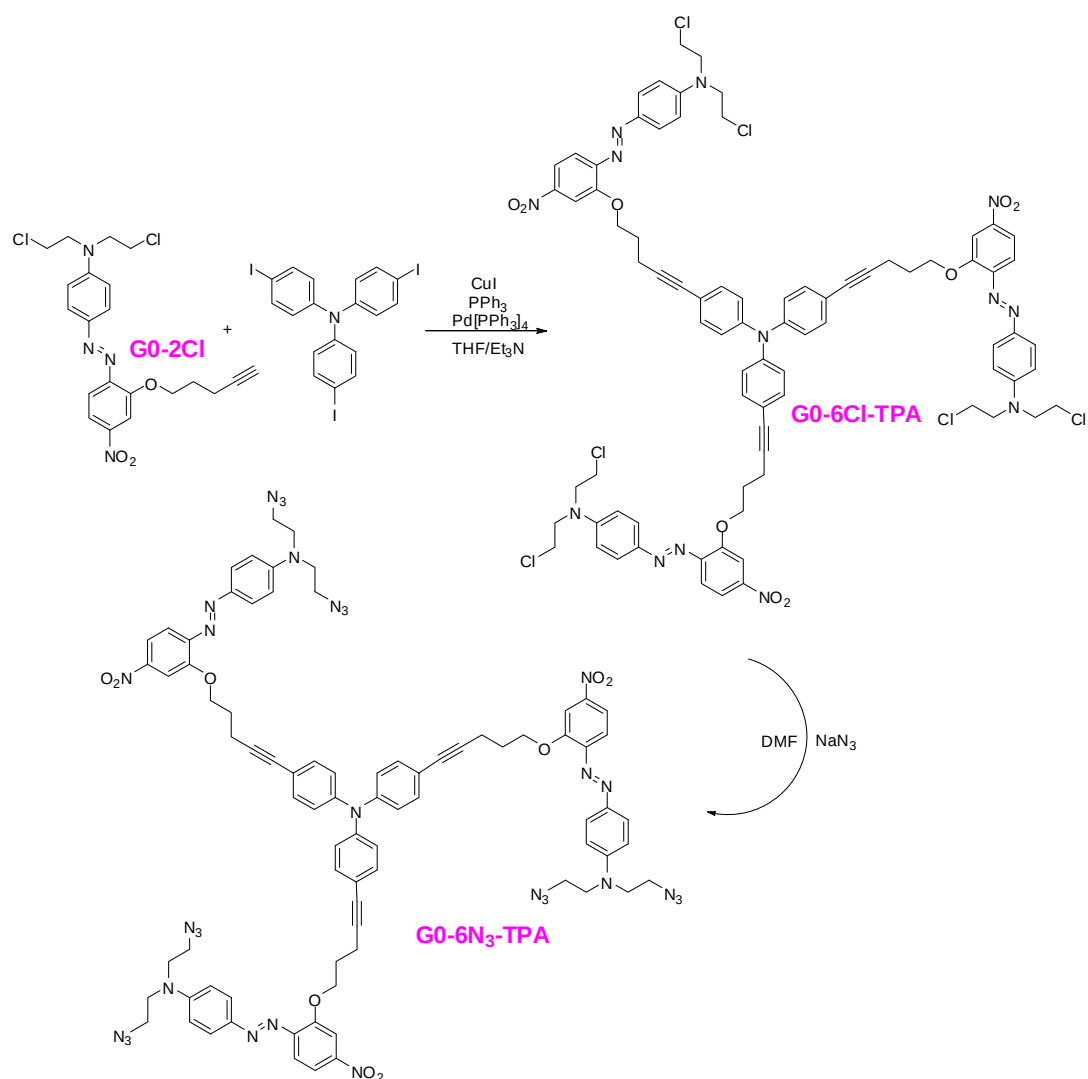
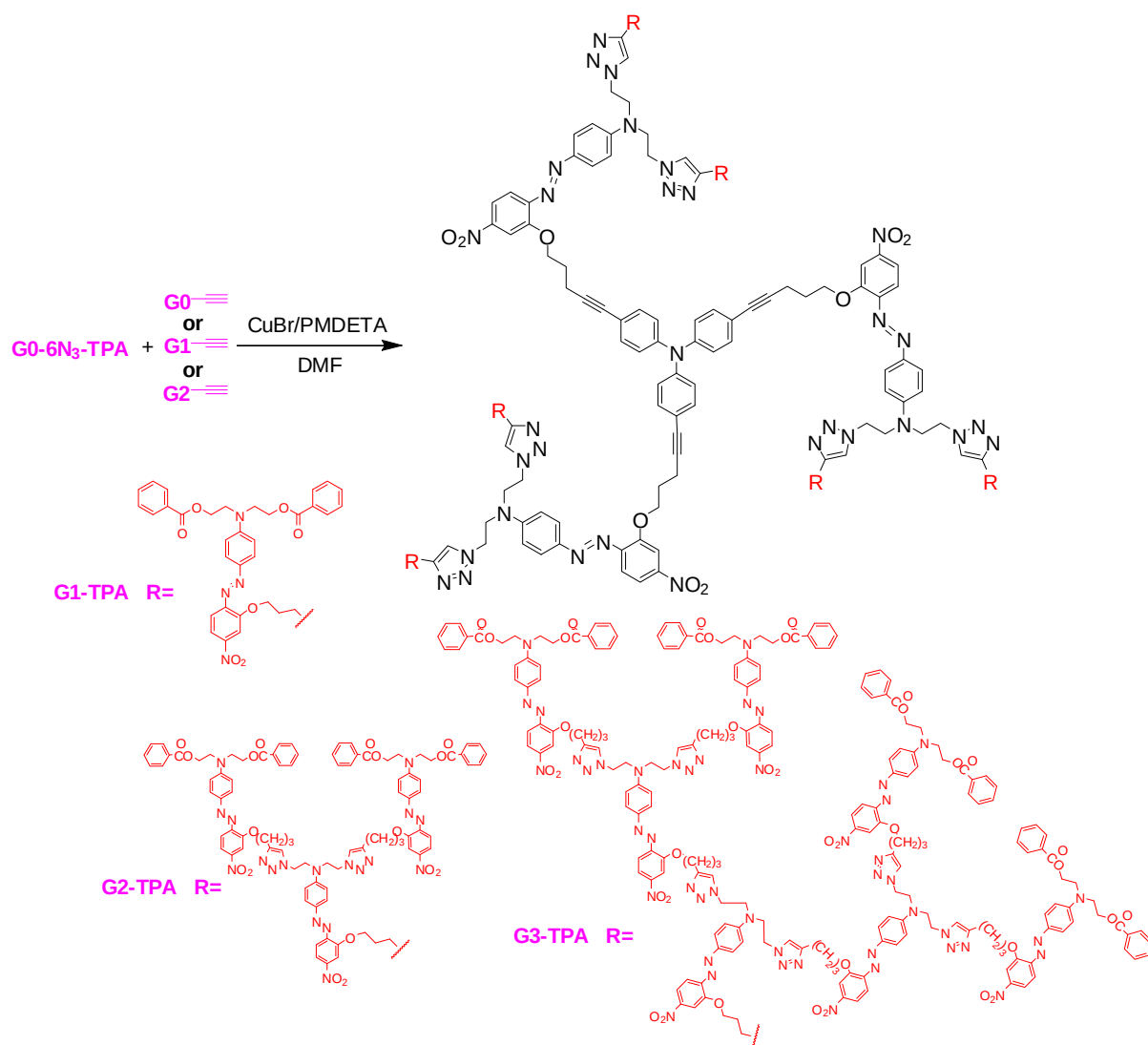


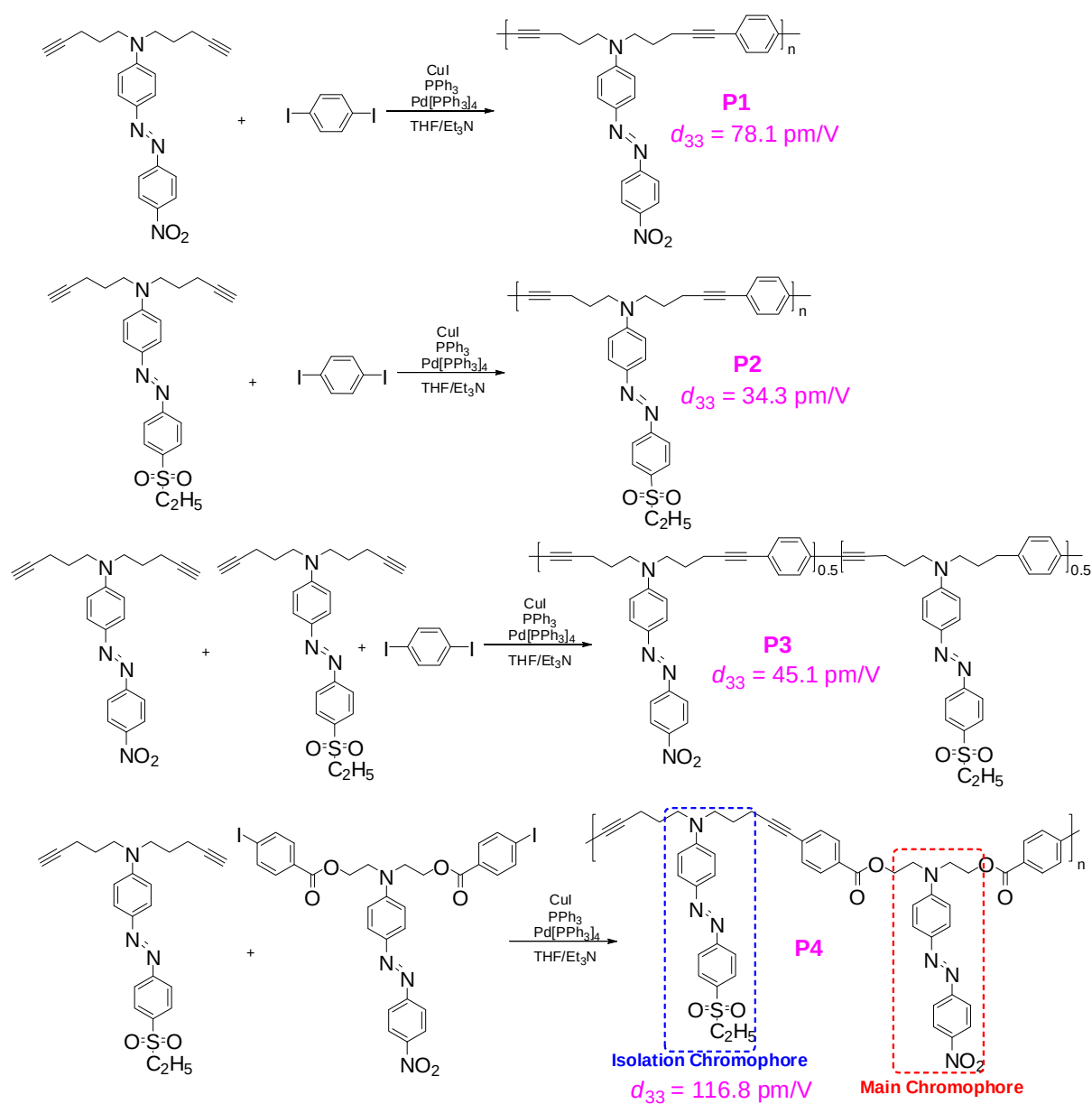
Chart S1. The sketch map differences of dendrimers and global-like dendrimers (**G2** and **G2-TPA** as an example).



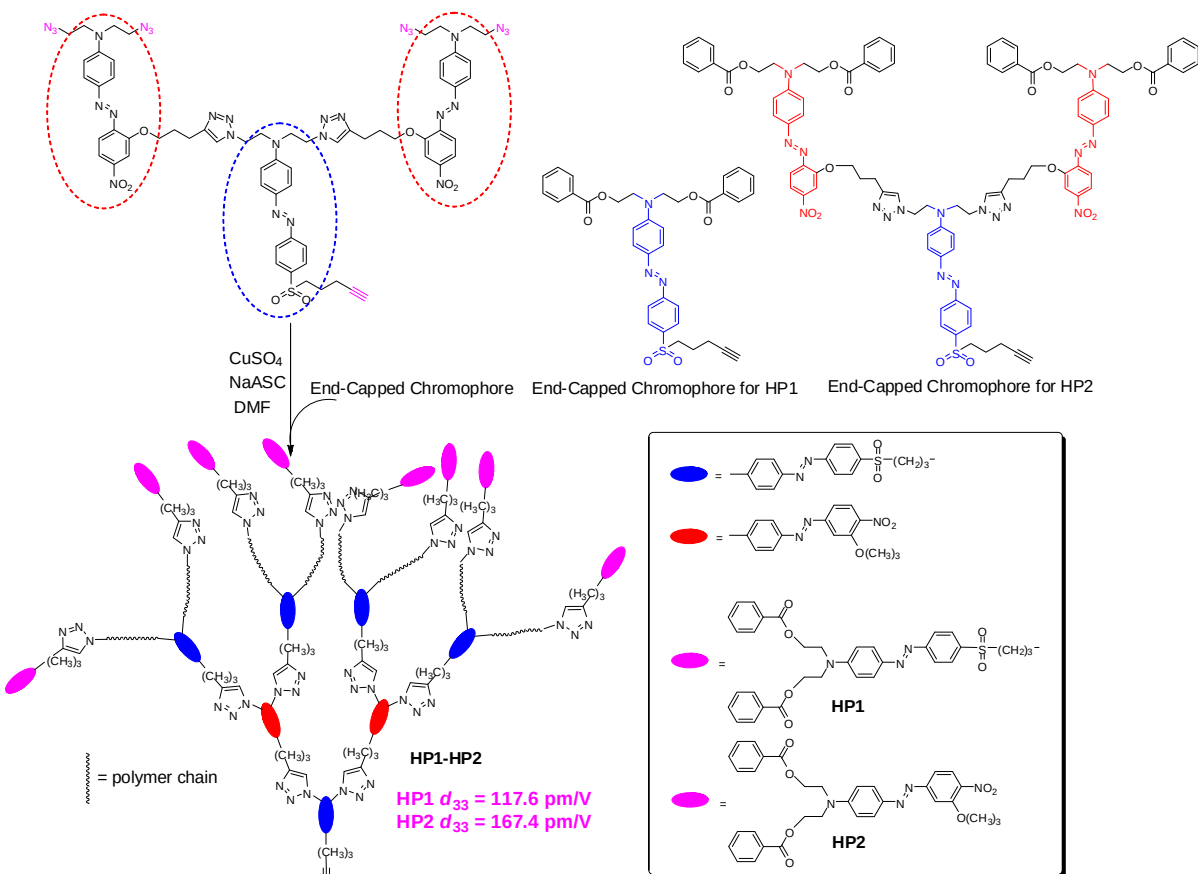
Scheme S4. The synthetic route to the core (**G0-6N₃-TPA**) of dendrimers.



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



Scheme S6. The synthetic route to **P1-P4** and their d_{33} values.



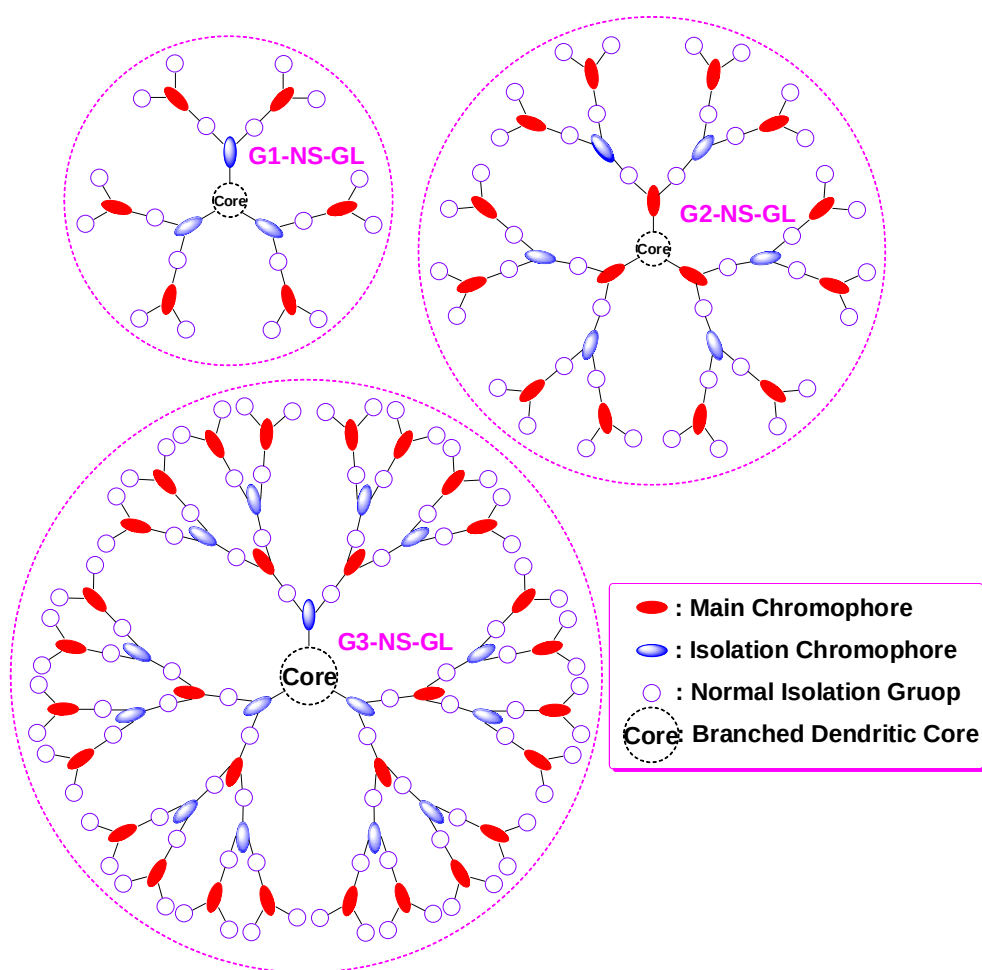


Chart S2. The sketch map of chemical structures of NLO dendrimers **G1-NS-TB** to **G3-NS-TB**.

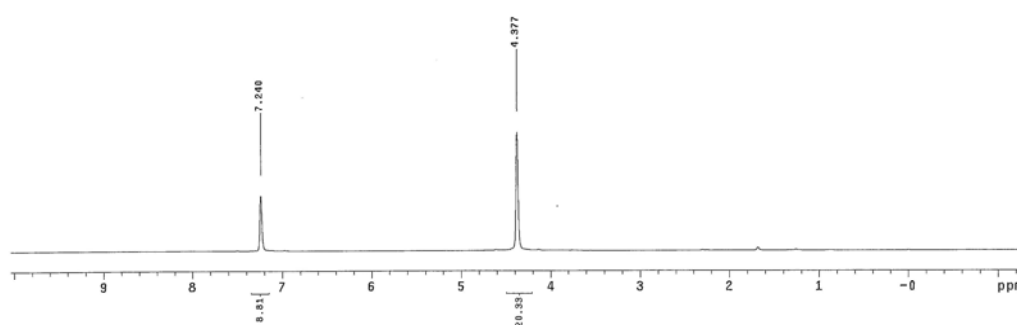


Fig. S1. ¹H NMR spectrum of **S2** in chloroform-*d*.

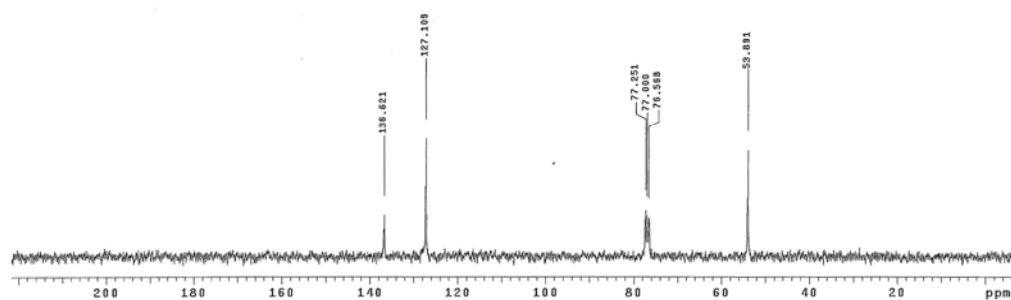


Fig. S2. ^{13}C NMR spectrum of S2 in chloroform-*d*.

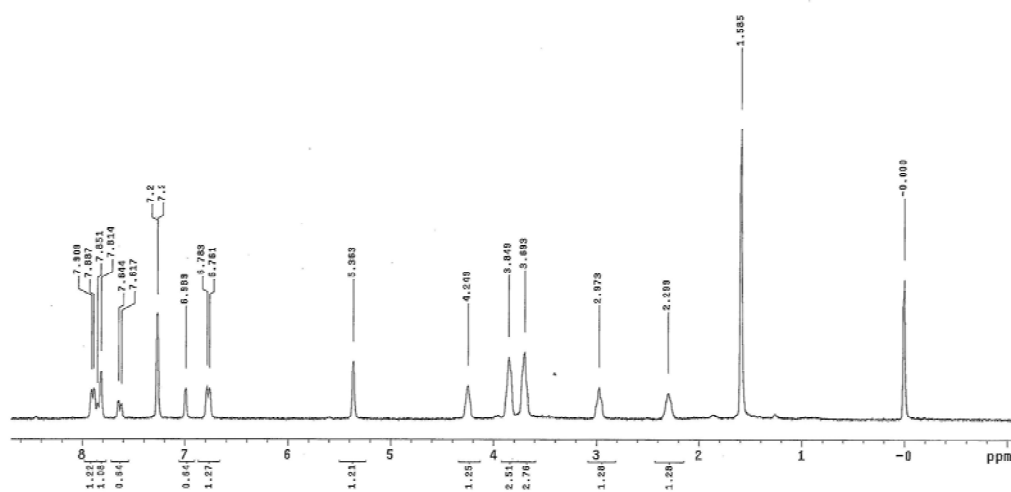


Fig. S3. ^1H NMR spectrum of G0-6Cl-N-TB in chloroform-*d*.

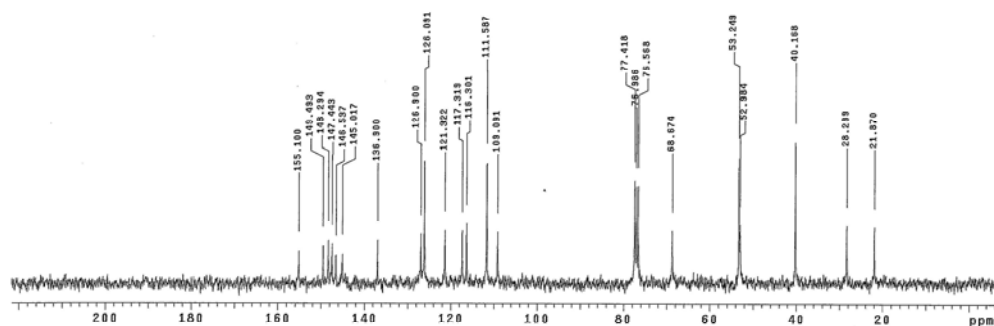


Fig. S4. ^{13}C NMR spectrum of G0-6Cl-N-TB in chloroform-*d*.

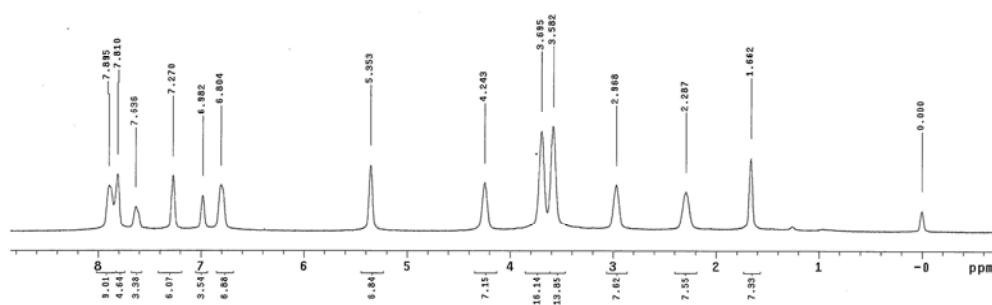


Fig. S5. ¹H NMR spectrum of G0-6N₃-N-TB in chloroform-*d*.

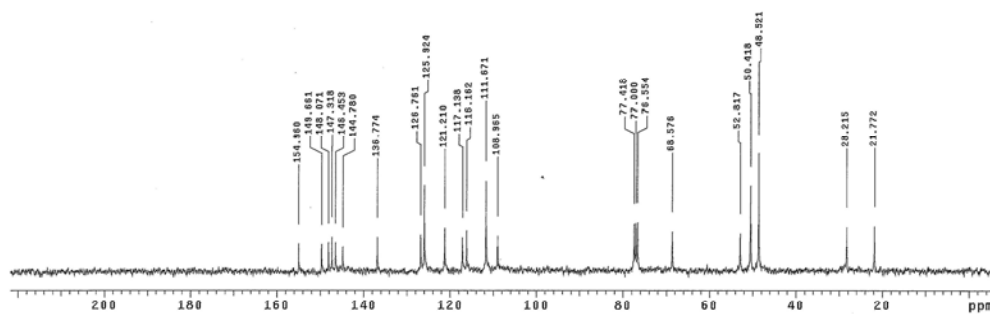


Fig. S6. ¹³C NMR spectrum of G0-6N₃-N-TB in chloroform-*d*.

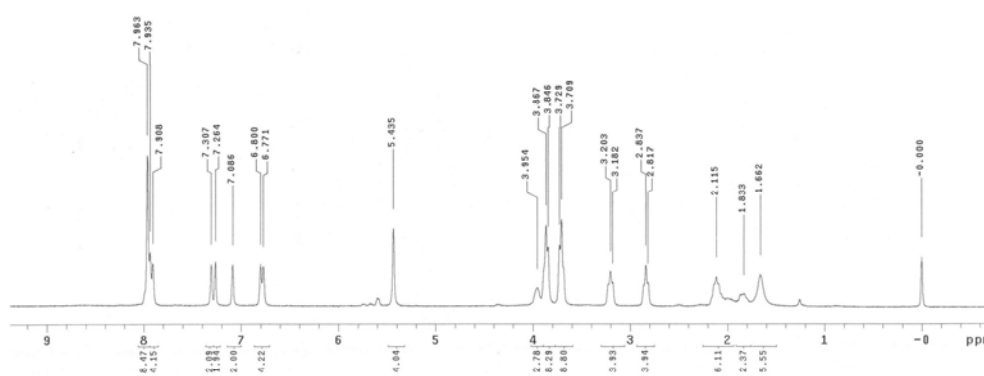


Fig. S7. ¹H NMR spectrum of G0-6Cl-S-TB in chloroform-*d*.

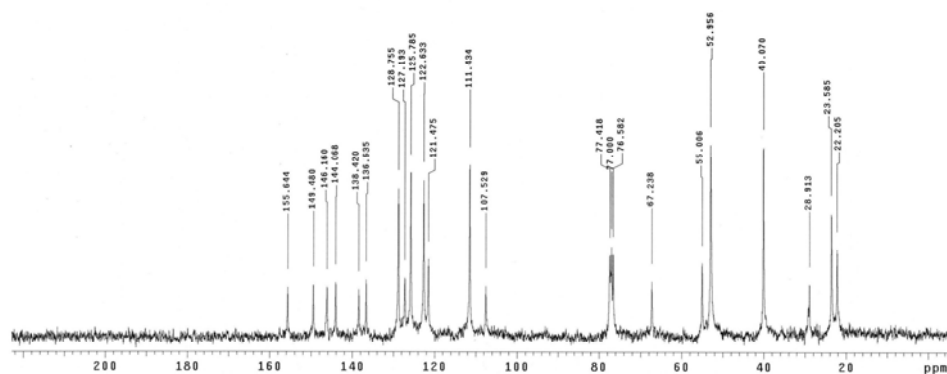


Fig. S8. ^{13}C NMR spectrum of **G0-6Cl-S-TB** in chloroform-*d*.

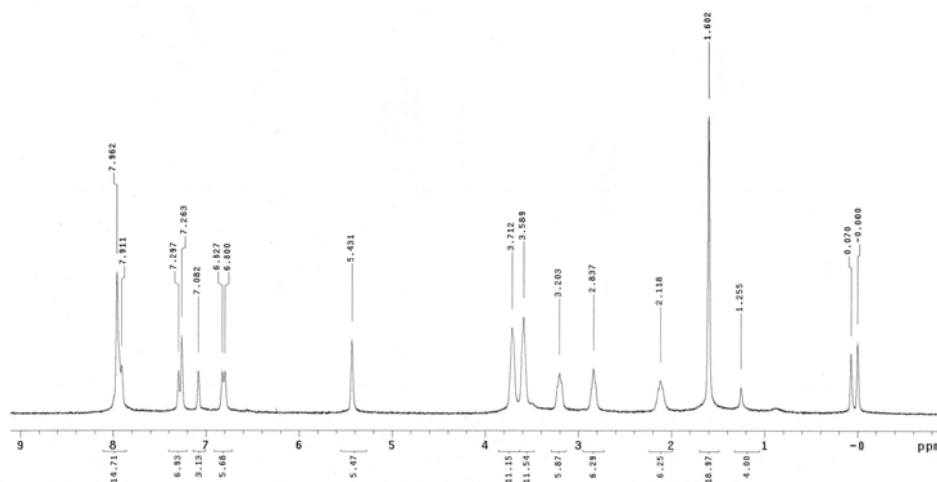


Fig. S9. ^1H NMR spectrum of **G0-6N₃-S-TB** in chloroform-*d*.

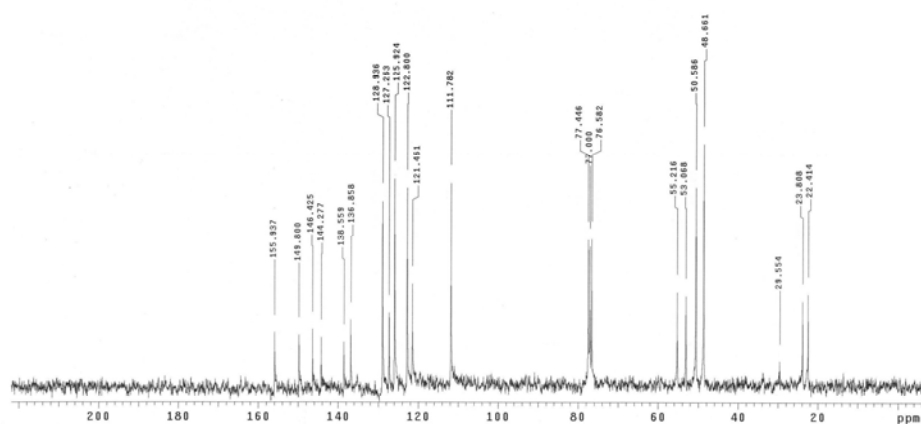


Fig. S10. ^{13}C NMR spectrum of **G0-6N₃-S-TB** in chloroform-*d*.

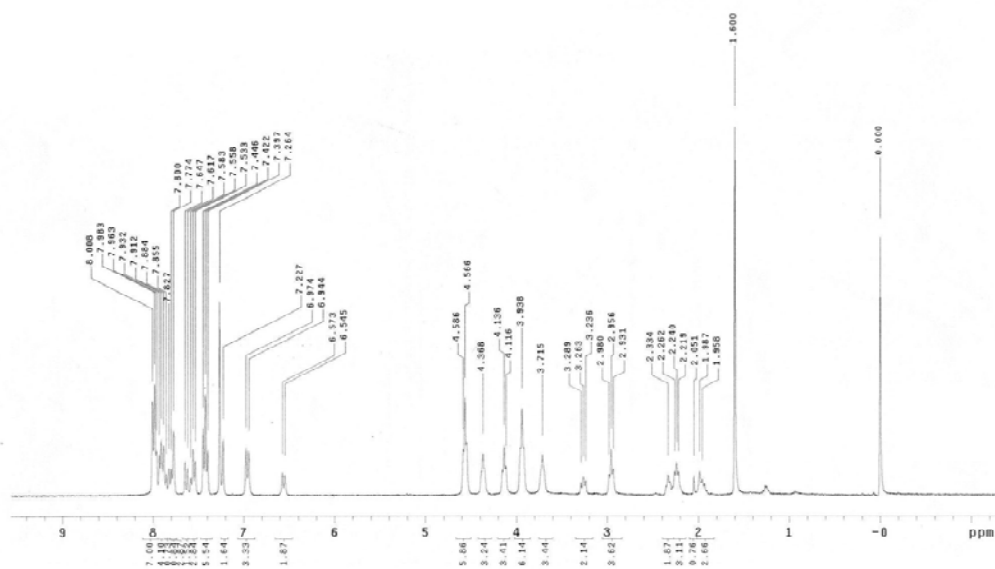


Fig. S11. ^1H NMR spectrum of **G1**≡**NS** in chloroform-*d*.

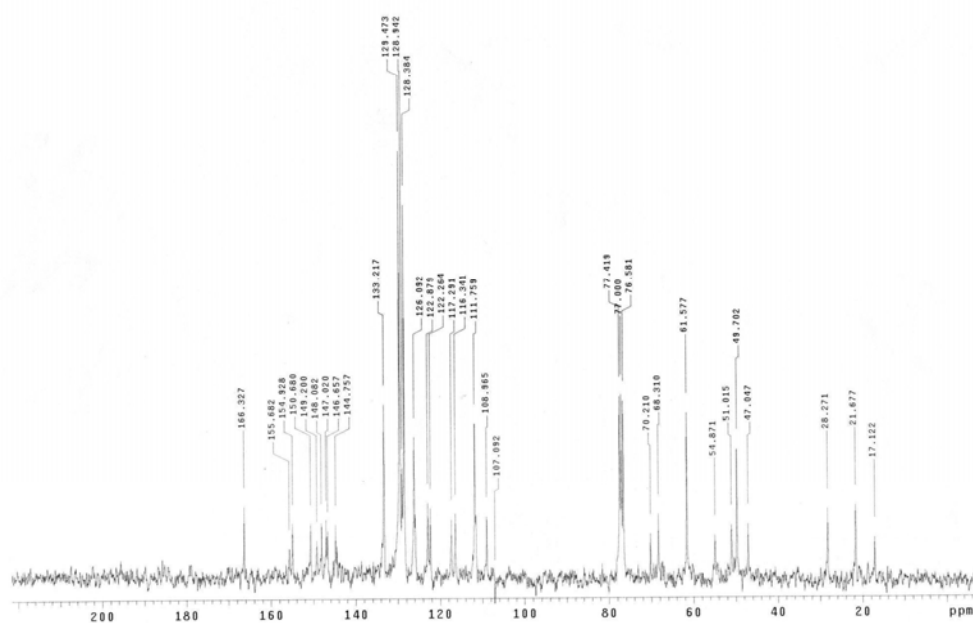


Fig. S12. ^{13}C NMR spectrum of **G1**≡**NS** in chloroform-*d*.

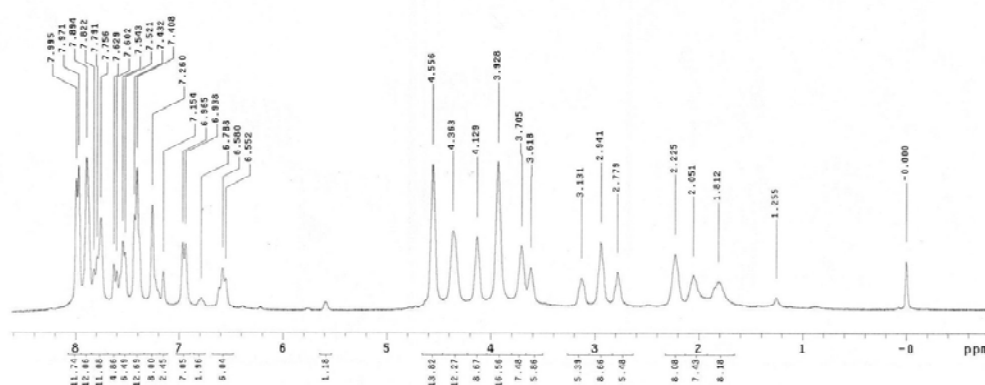


Fig. S13. ^1H NMR spectrum of G2-NS in chloroform-*d*.

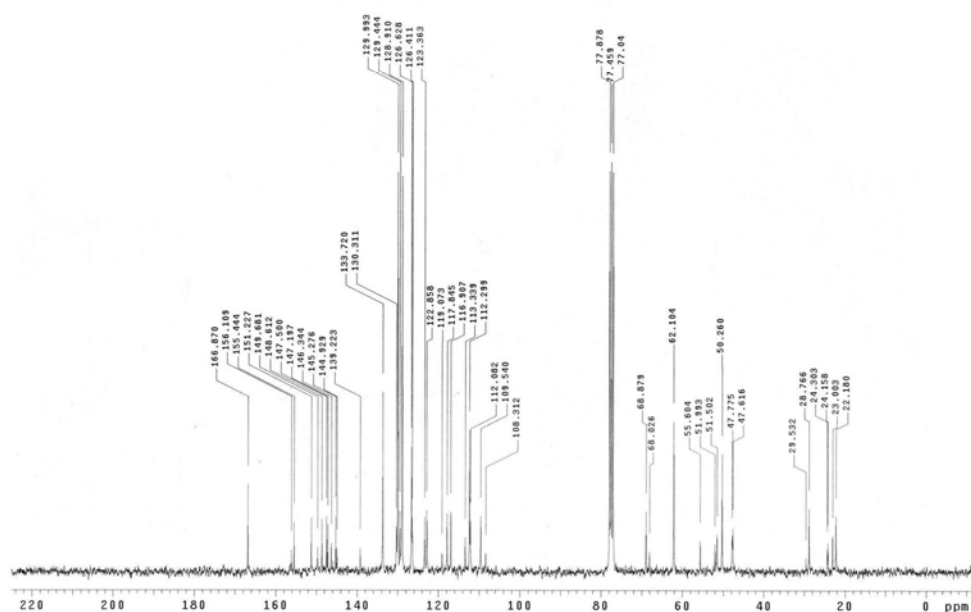


Fig. S14. ^{13}C NMR spectrum of G2-NS in chloroform-*d*.

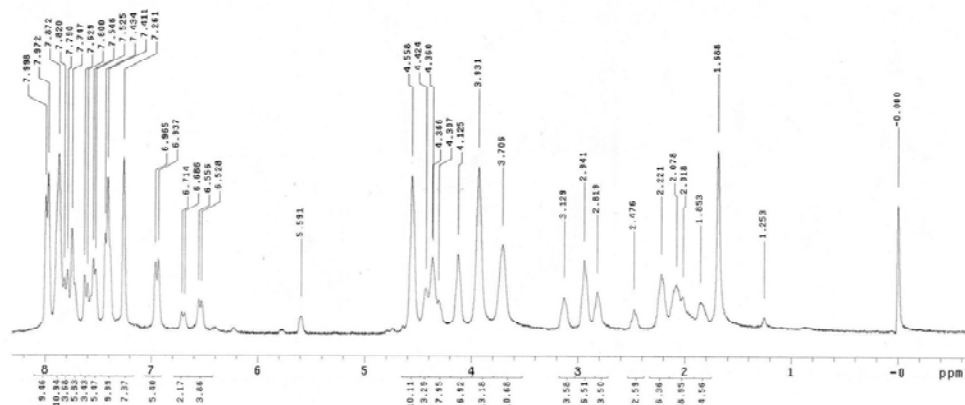


Fig. S15. ^1H NMR spectrum of **G2≡-NS** in chloroform-*d*.

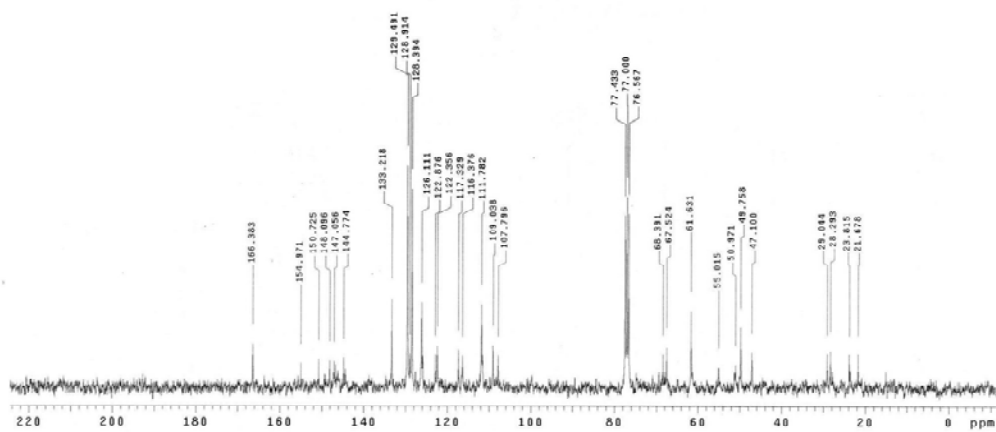


Fig. S16. ^{13}C NMR spectrum of **G2≡-NS** in chloroform-*d*.

Chemical shifts (ppm) labeled on the right side of the spectrum:

- 166.46
- 162.36
- 155.12
- 150.90
- 147.08
- 144.97
- 138.91
- 133.30
- 129.56
- 128.20
- 122.41
- 118.50
- 111.97
- 108.32
- 107.52
- 100.11
- 77.82
- 77.10
- 76.84
- 75.72
- 67.62
- 46.91
- 41.77
- 39.89
- 44.55
- 29.15
- 28.16
- 23.62
- 21.83
- 0.95

-S16-

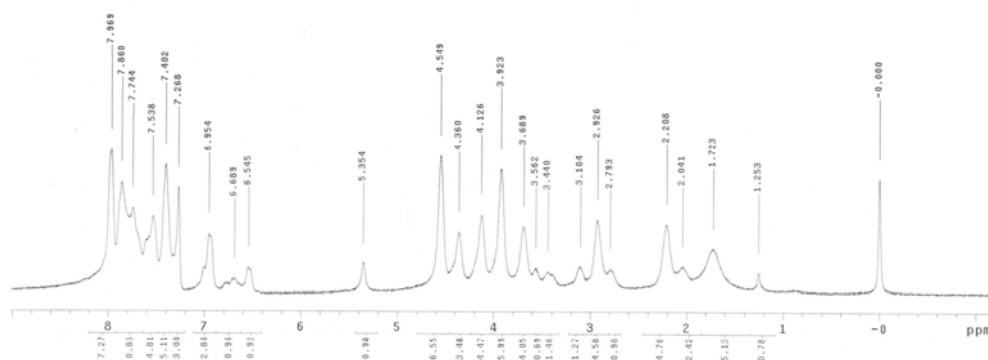


Fig. S19. ¹H NMR spectrum of G2-NS-TB in chloroform-*d*.

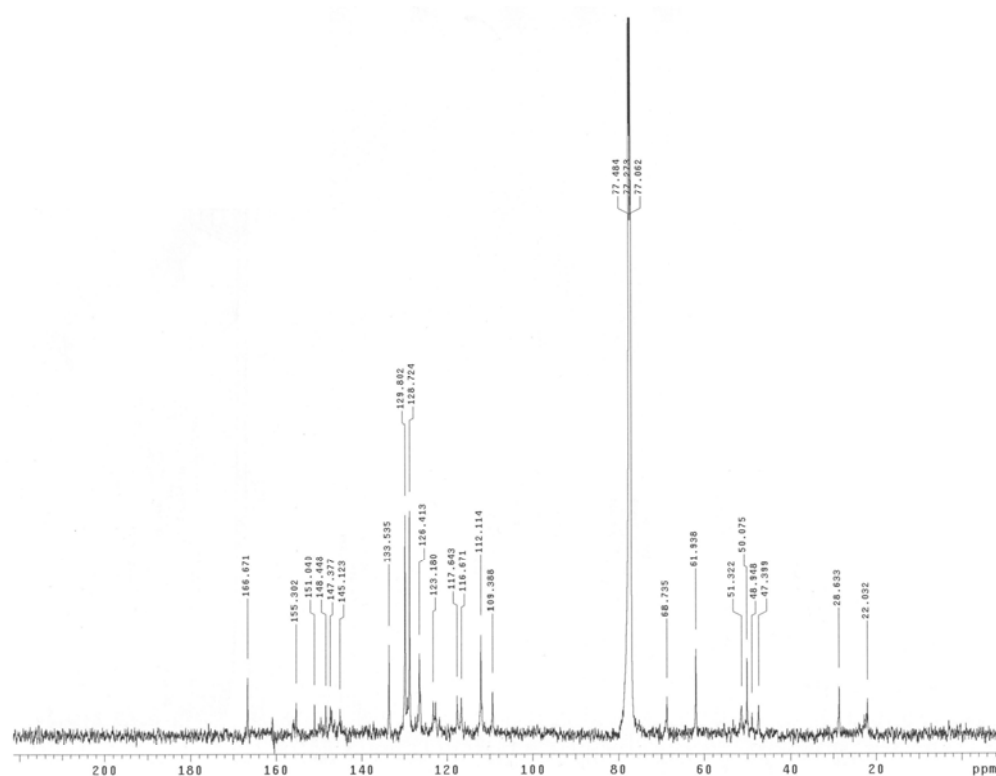


Fig. S20. ¹³C NMR spectrum of G2-NS-TB in chloroform-*d*.

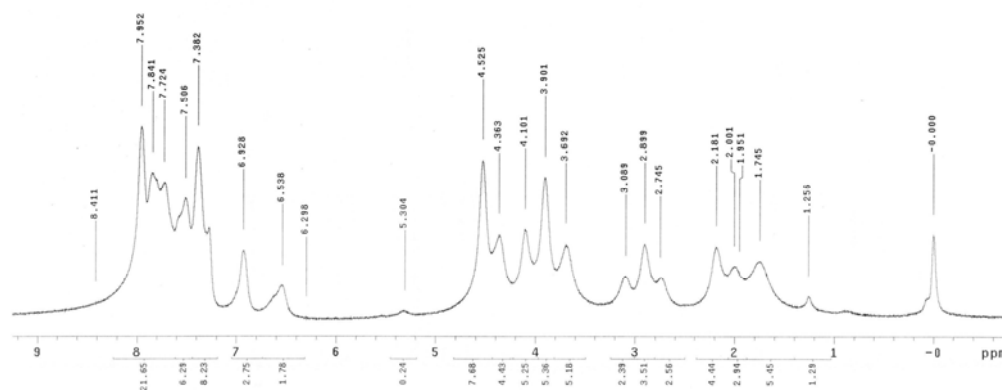


Fig. S21. ¹H NMR spectrum of **G3-NS-TB** in chloroform-*d*.

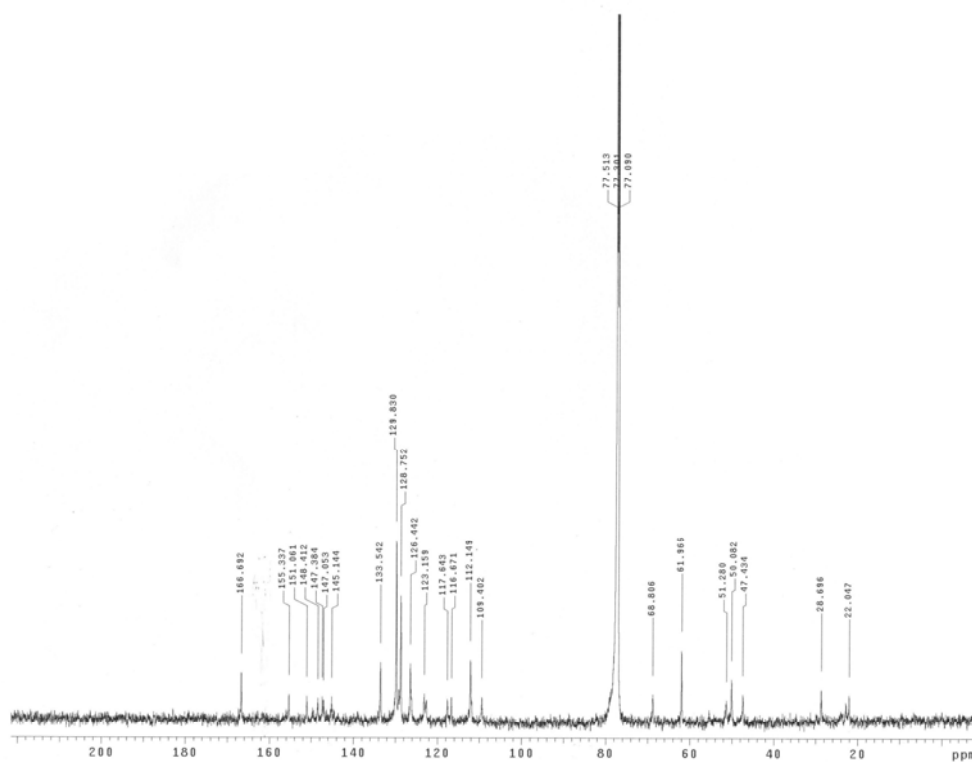


Fig. S22. ¹³C NMR spectrum of **G3-NS-TB** in chloroform-*d*.

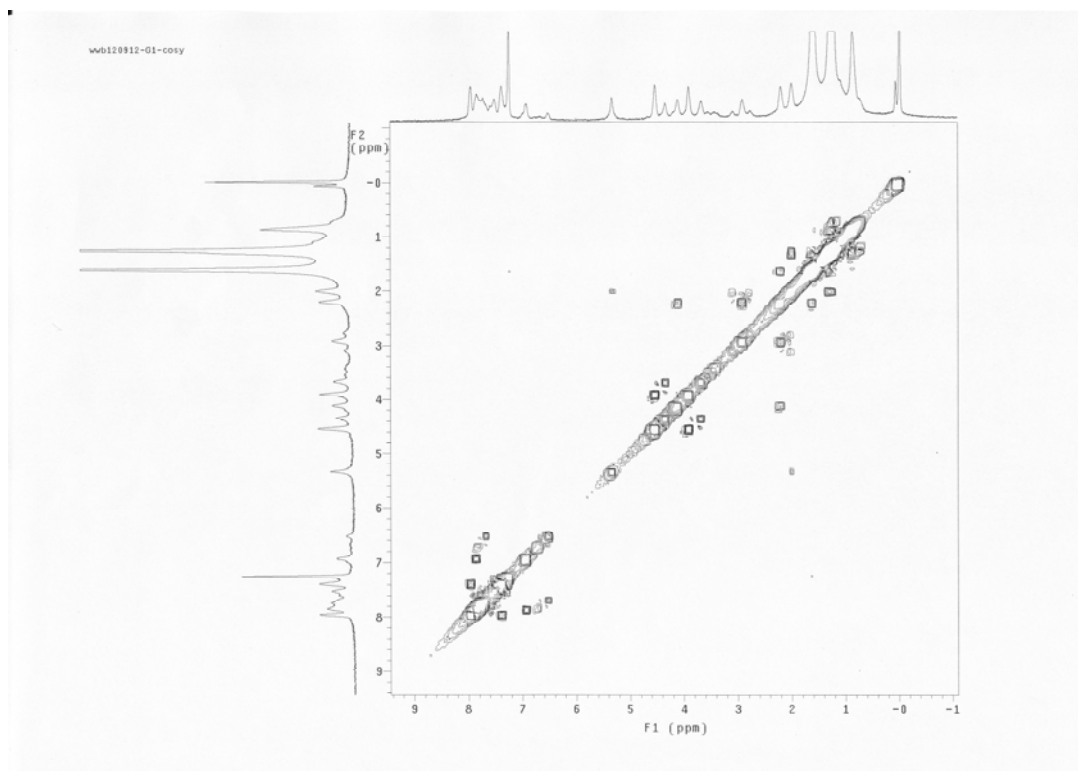


Fig. S23. H,H-cosy NMR spectrum of **G1-NS-TB** in chloroform-*d*.

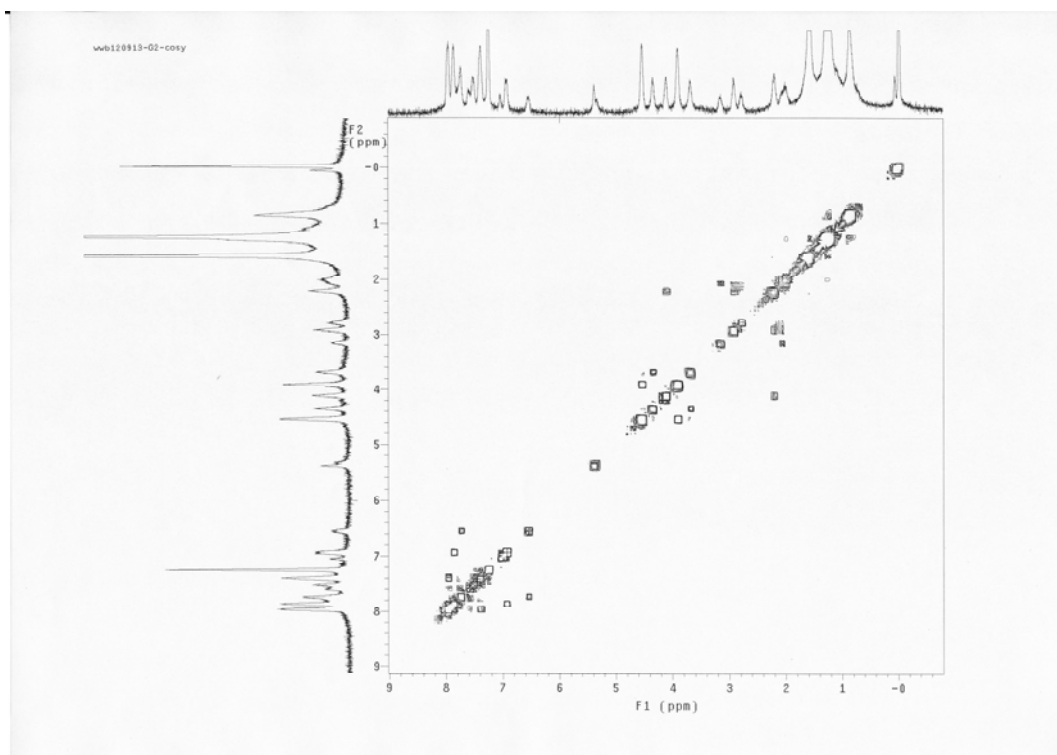


Fig. S24. H,H-cosy NMR spectrum of **G2-NS-TB** in chloroform-*d*.

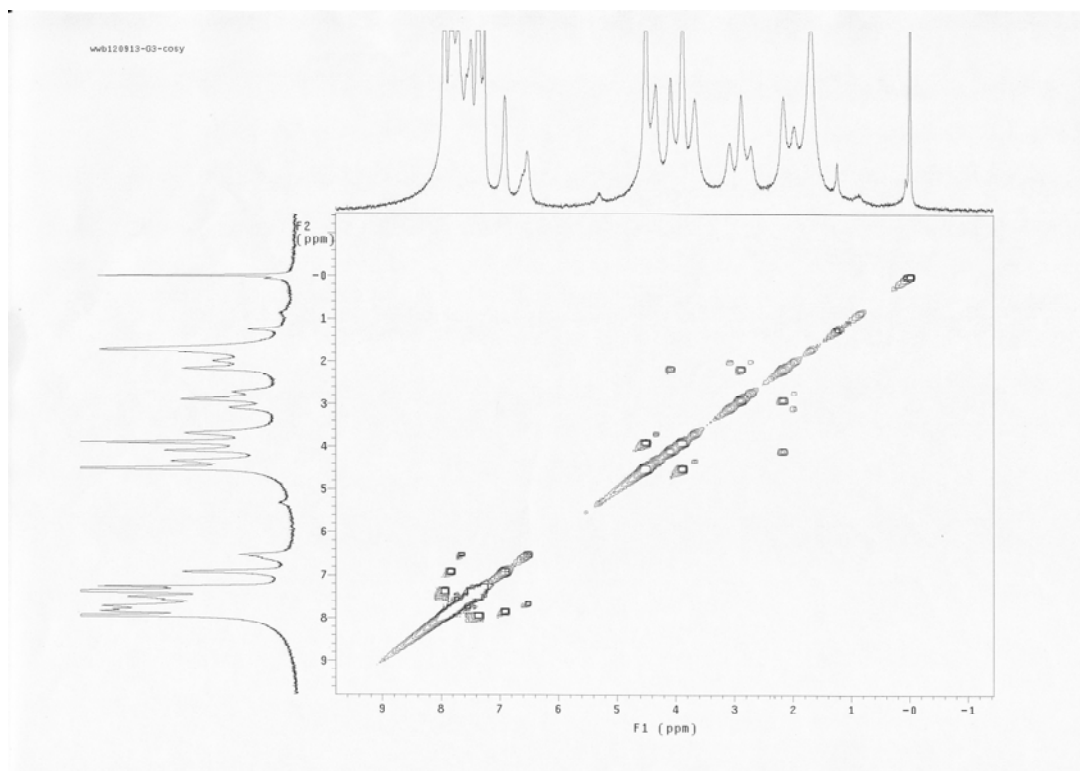


Fig. S25. H,H-cosy NMR spectrum of **G3-NS-TB** in chloroform-*d*.

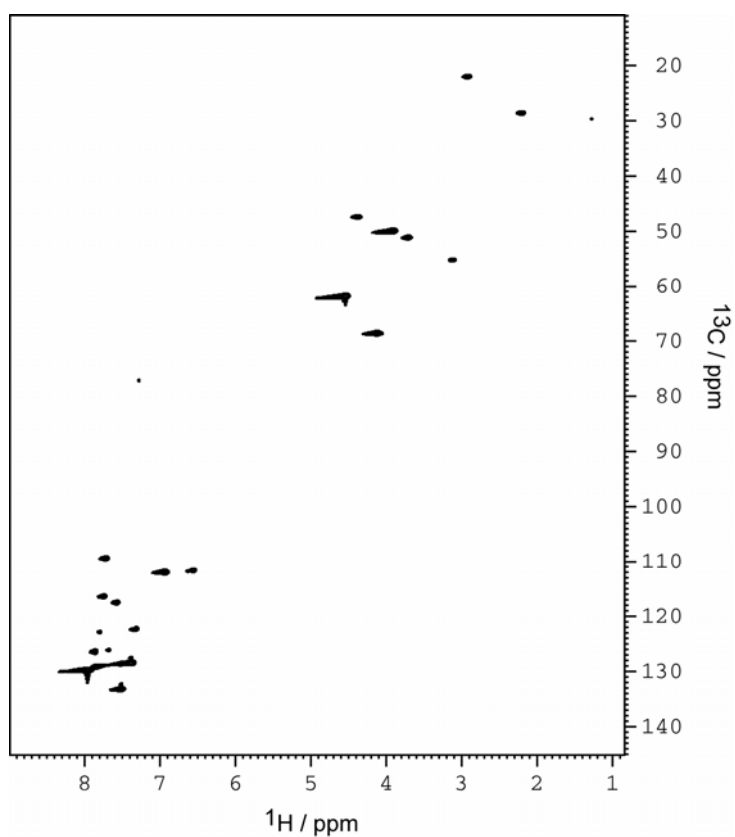


Fig. S26. C,H-cosy NMR spectrum of **G3-NS-TB** in chloroform-*d*.

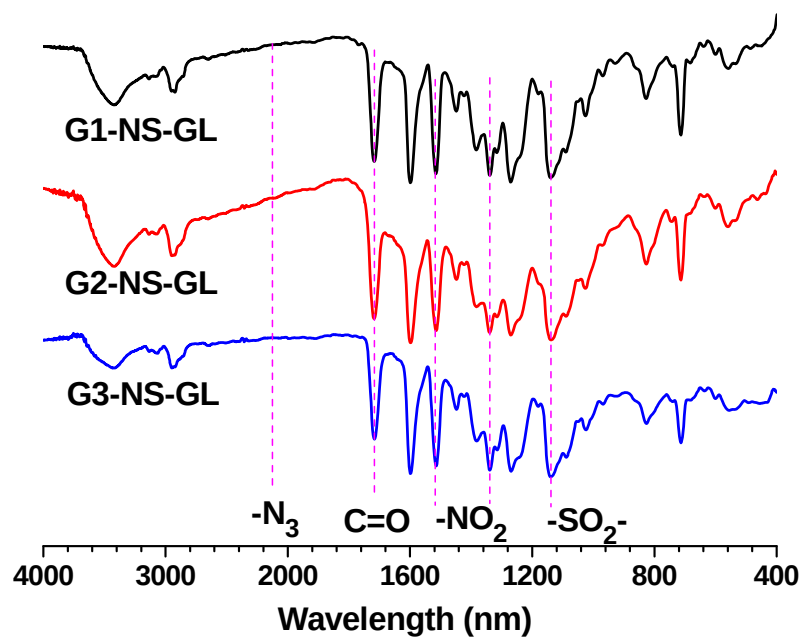


Fig. S27. The FT-IR spectra of dendrimers **G1-NS-TB** to **G3-NS-TB**.

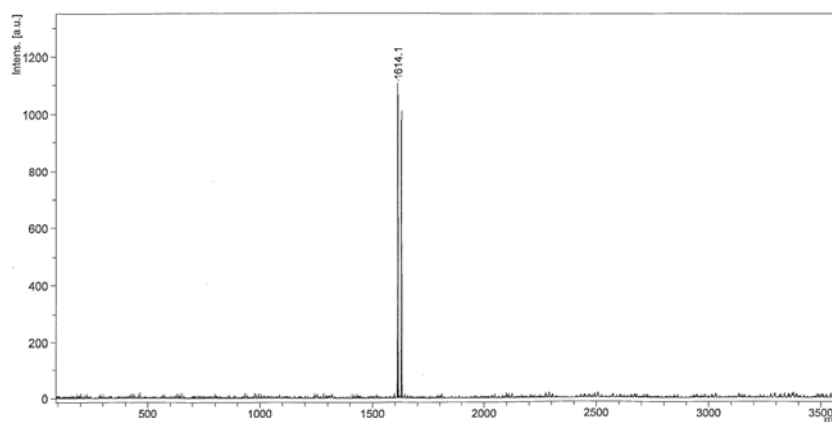


Fig. S28. The MALDI-TOF Mass spectrum of **G1-6Cl-N-TB**.

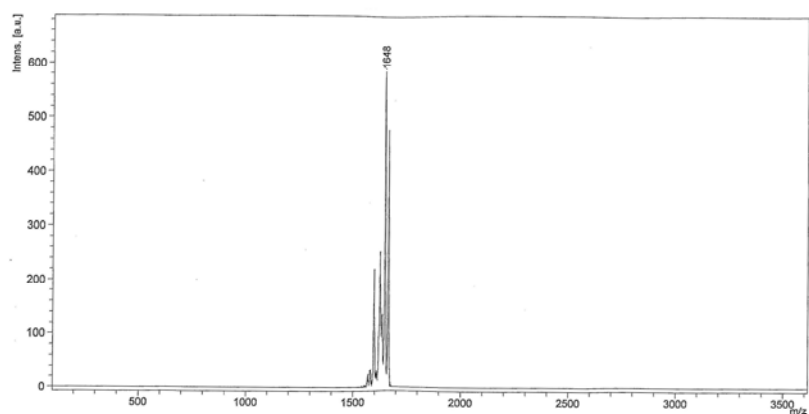


Fig. S29. The MALDI-TOF Mass spectrum of **G1-6N₃-N-TB**.

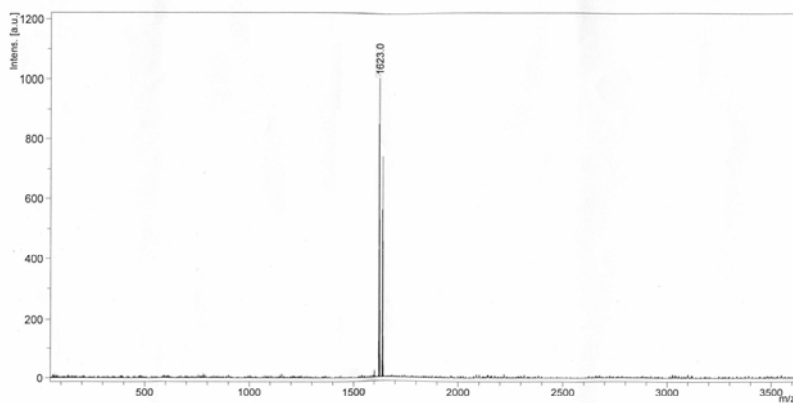


Fig. S30. The MALDI-TOF Mass spectrum of **G1-6Cl-S-TB**.

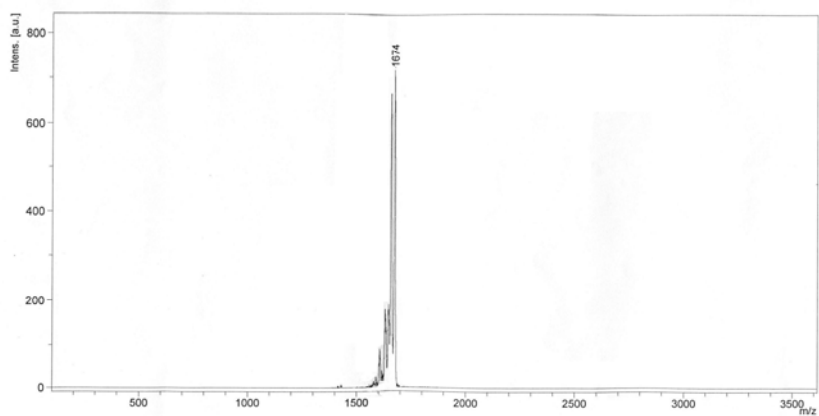


Fig. S31. The MALDI-TOF Mass spectrum of **G1-6N₃-S-TB**.

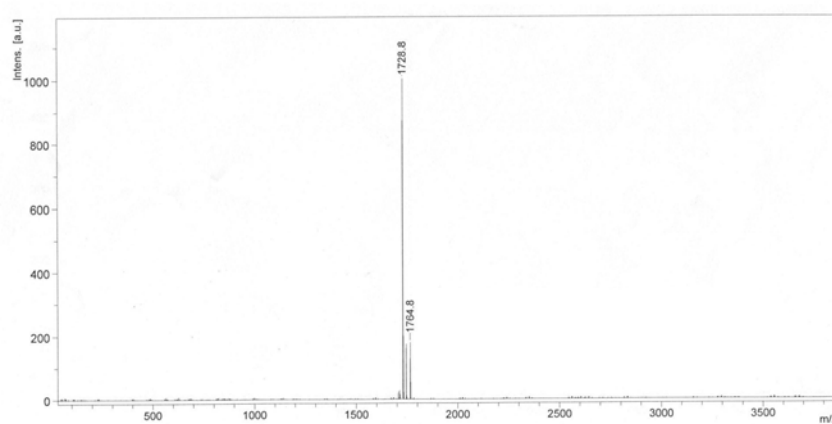


Fig. S32. The MALDI-TOF Mass spectrum of **G1≡-NS**.

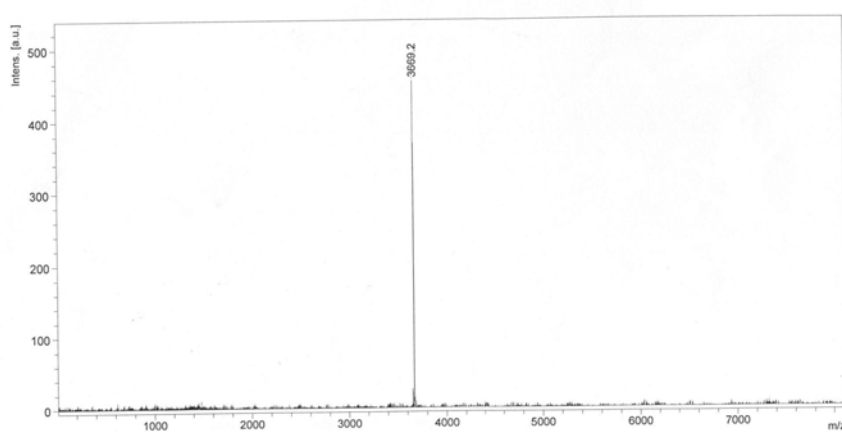


Fig. S33. The MALDI-TOF Mass spectrum of **G2-NS**.

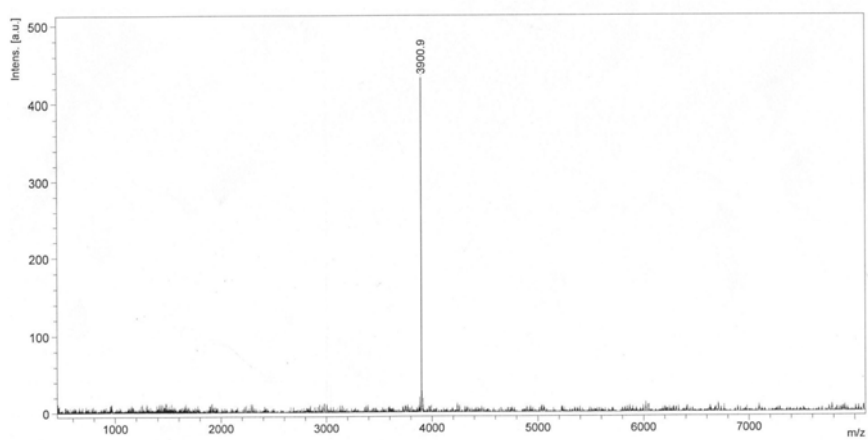


Fig. S34. The MALDI-TOF Mass spectrum of **G2≡-NS**.

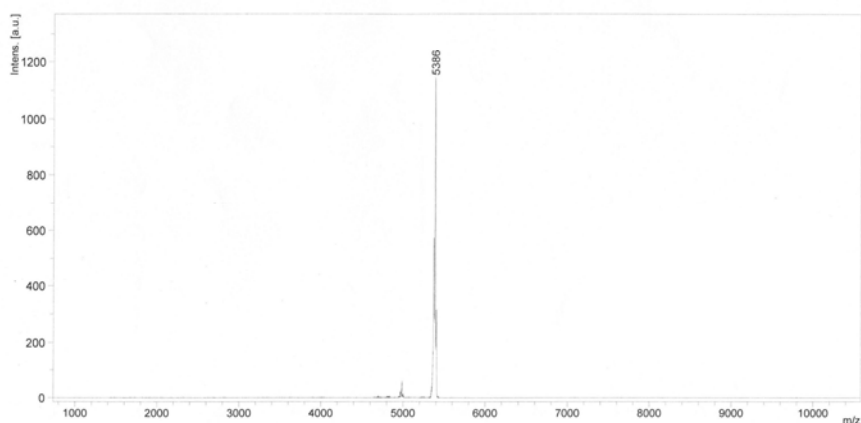


Fig. S35. The MALDI-TOF Mass spectrum of **G1-NS-TB**.

Table S1. Characterization data of dendrimers.

No.	M_w^a	M_w/M_n^a	m/z^b	$m/z(\text{cal})$
G1-6Cl-N-TB	1460	1.03	1614.1	1614.2
G1-6N₃-N-TB	1500	1.04	1648	1654 ^c
G1-6Cl-S-TB	1450	1.03	1623.0	1623.4 ^c
G1-6N₃-S-TB	1540	1.03	1674	1673 ^c
G1-≡-NS	1944	1.04	1728.8	1728.6 ^c
G2-NS	4012	1.04	3669.2	3667.9 ^c
G2-≡-NS	4328	1.04	3900.9	3899.1 ^c
G1-NS-TB	4380	1.03	5386	5387 ^c
G2-NS-TB	7540	1.06	^d	11872
G3-NS-TB	12300	1.07	^d	24897

^a Determined by GPC in THF on the basis of a polystyrene calibration. ^b Measured by MALDI-TOF mass spectroscopy. ^c Calculated for $[M+Na]^+$ ^d Not obtained.

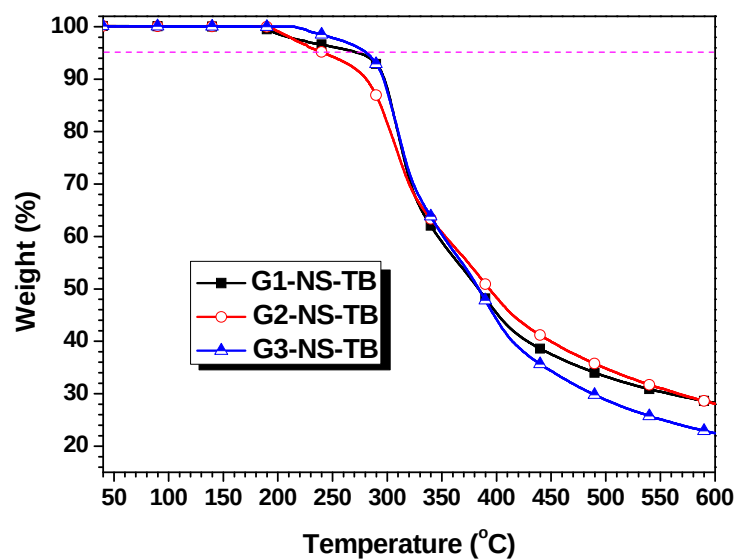


Fig. S36. TGA thermograms of dendrimers **G1-NS-TB** to **G3-NS-TB**, measured in nitrogen at a heating rate of 10 °C/min.

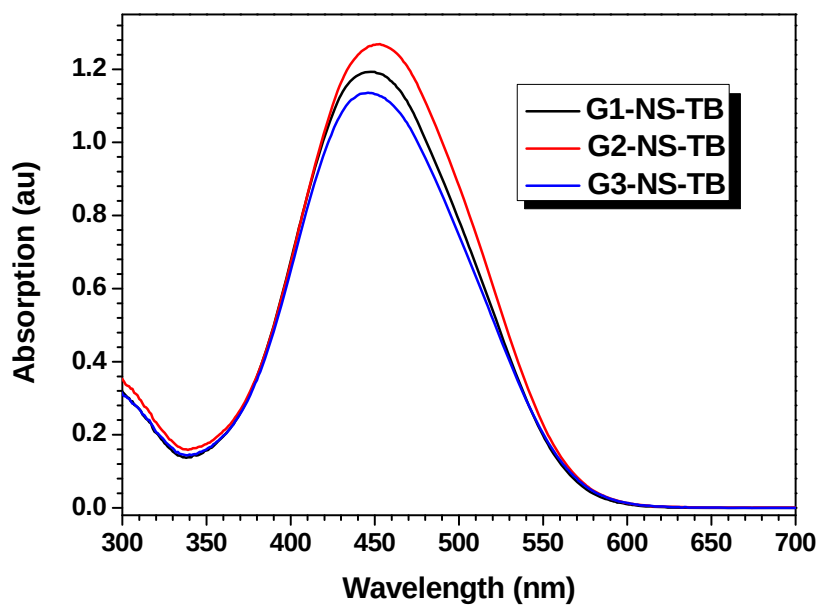


Fig. S37. UV-Vis spectra of THF solutions of dendrimers (0.02 mg/mL).

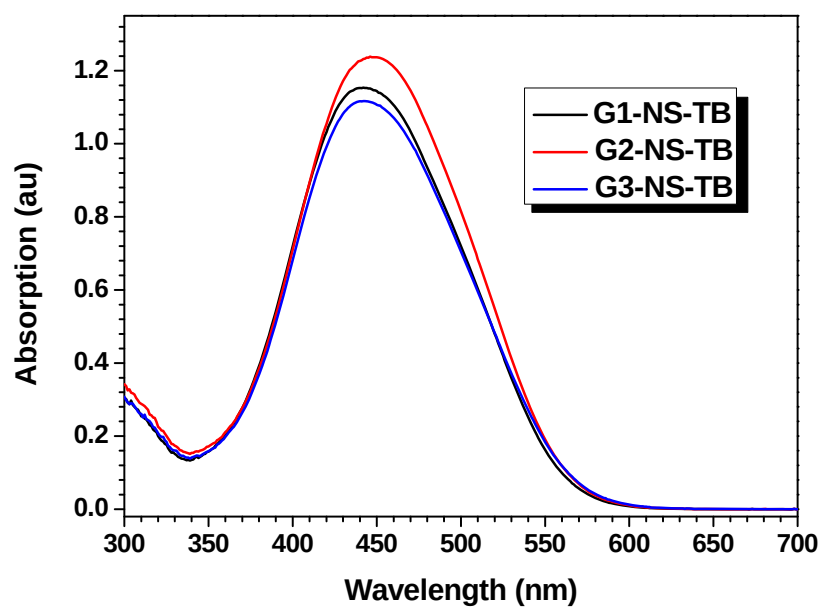


Fig. S38. UV-Vis spectra of 1,4-dioxane solutions of dendrimers (0.02 mg/mL).

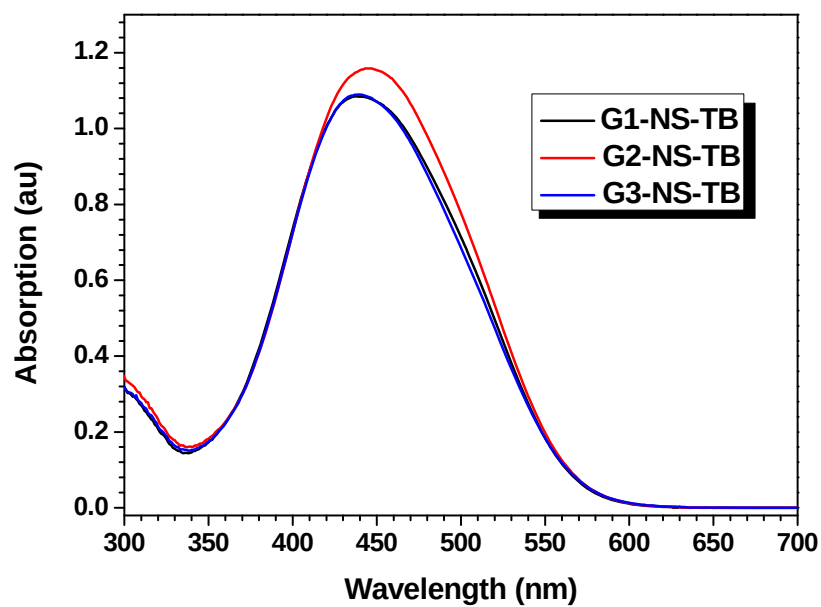


Fig. S39. UV-Vis spectra of chloroform solutions of dendrimers (0.02 mg/mL).

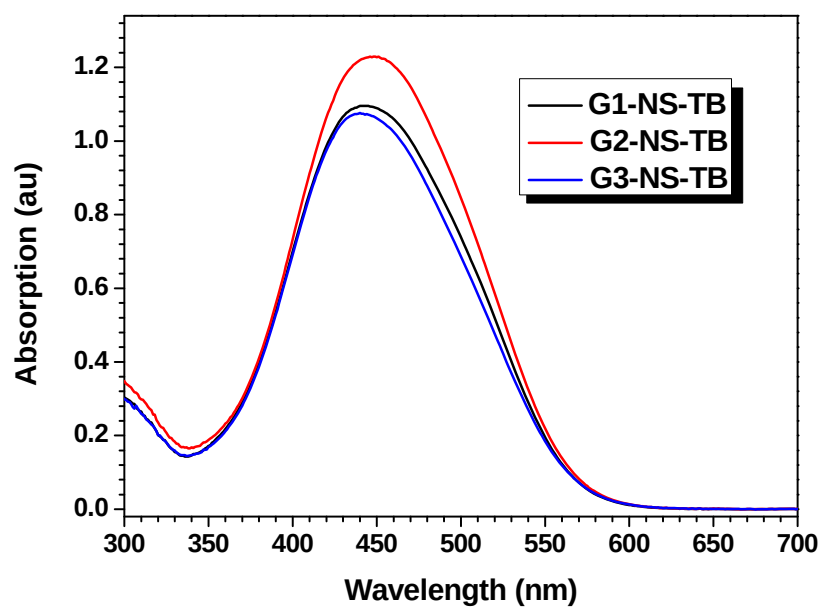


Fig. S40. UV-Vis spectra of dichloromethane solutions of dendrimers (0.02 mg/mL).

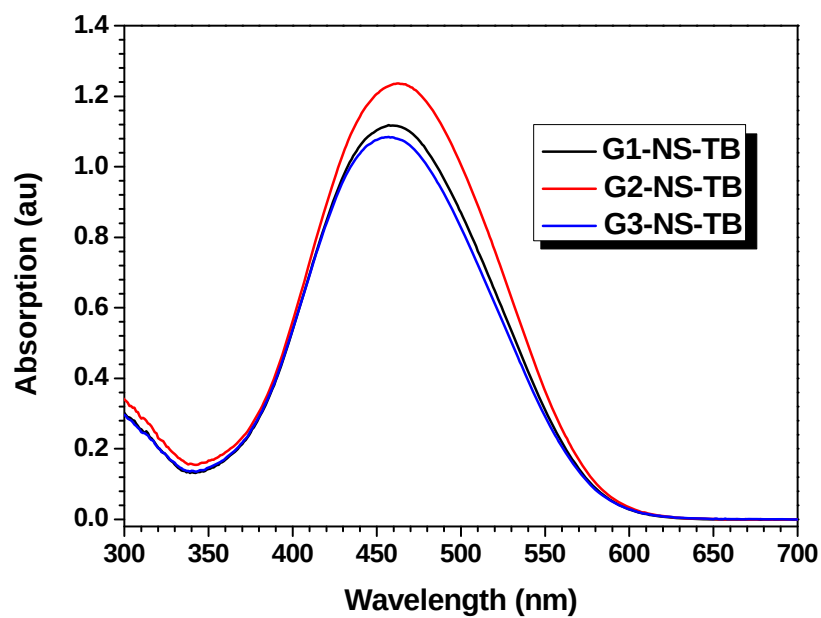


Fig. S41. UV-Vis spectra of DMF solutions of dendrimers (0.02 mg/mL).

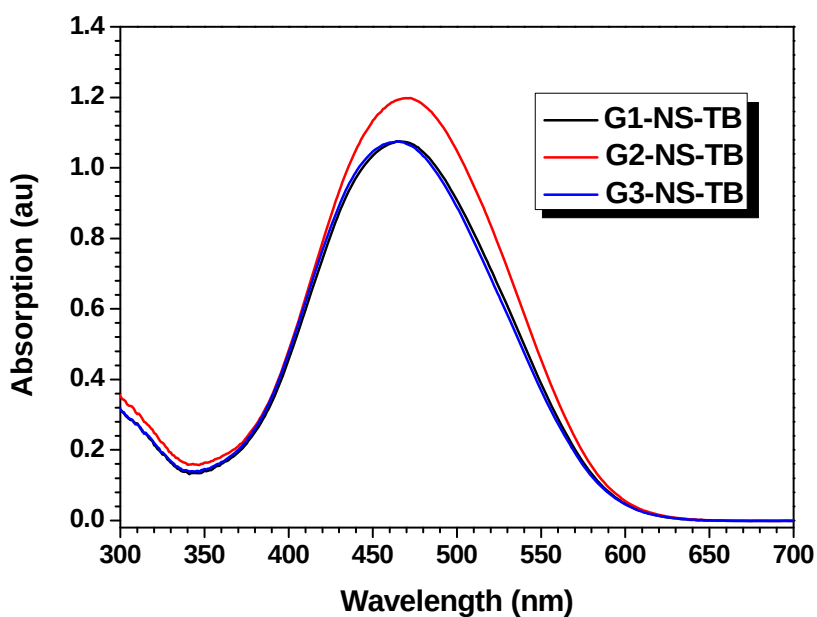


Fig. S42. UV-Vis spectra of DMSO solutions of dendrimers (0.02 mg/mL).

Table S2. The maximum absorption of dendrimers (λ_{max} , nm, 0.02 mg/mL).							
	THF	1,4-dioxane	chloroform	dichloromethane	DMF	DMSO	film
G1-NS-TB	446	442	438	441	457	466	450
G2-NS-TB	453	446	444	446	463	472	453
G3-NS-TB	446	443	440	440	457	464	446
G1-TPA	461	456	457	458	473	483	470
G2-TPA	458	456	455	458	472	482	470
G3-TPA	458	457	457	457	470	476	470
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

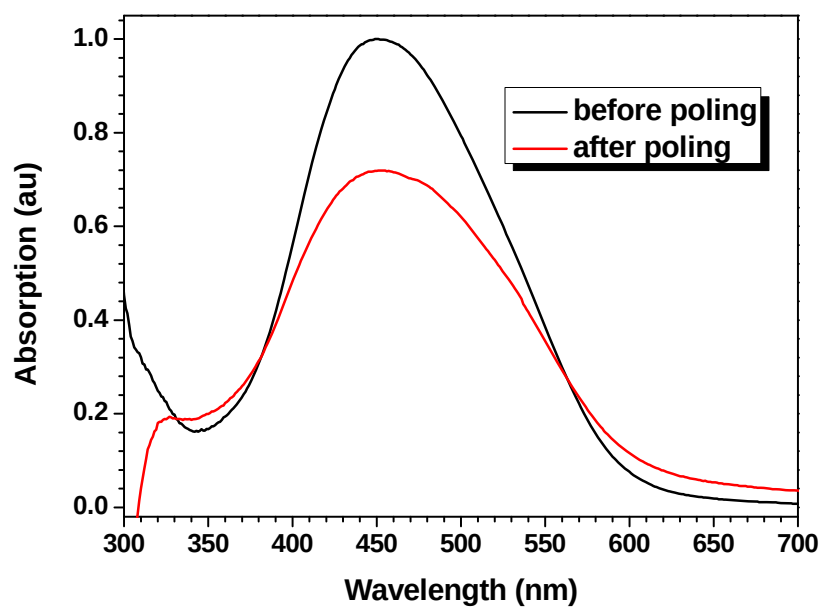


Fig. S43. Absorption spectra of the film of **G1-NS-TB** before and after poling.

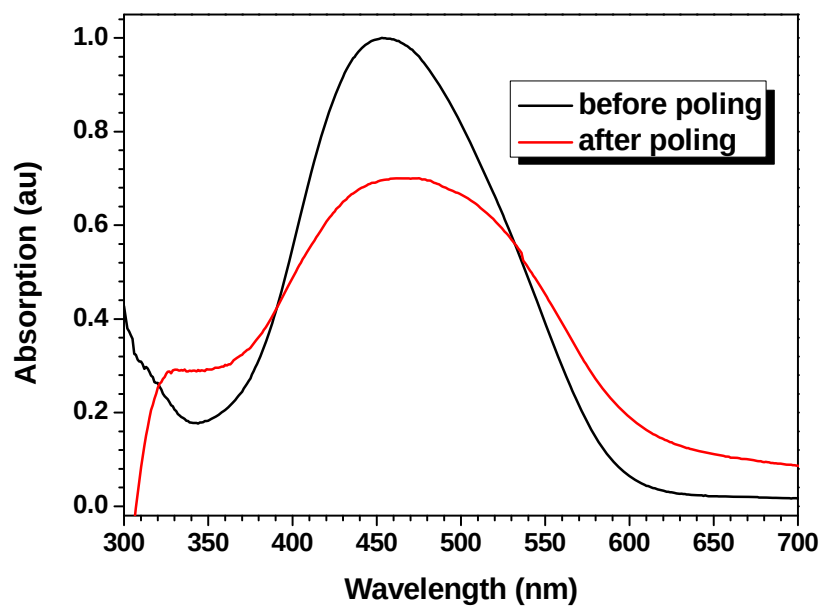


Fig. S44. Absorption spectra of the film of **G2-NS-TB** before and after poling.

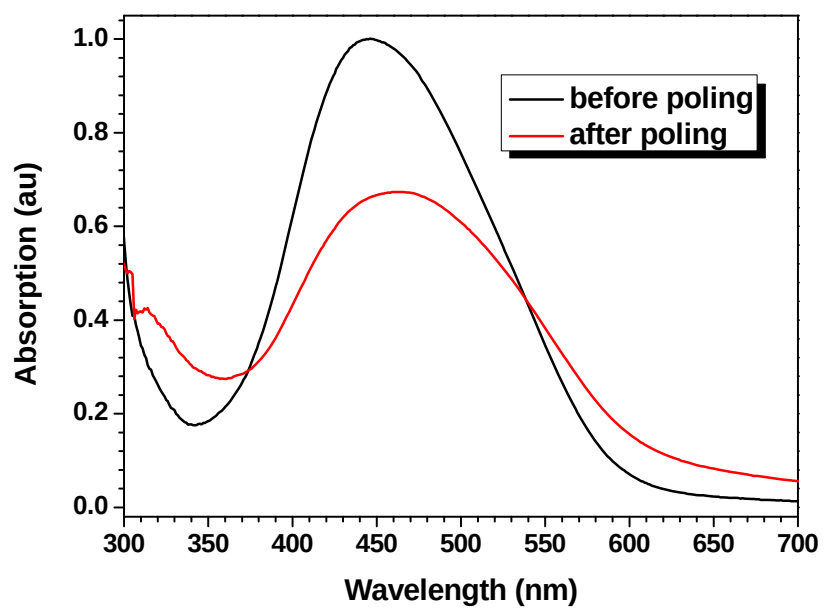


Fig. S45. Absorption spectra of the film of **G3-NS-TB** before and after poling.