Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Salen-Based Enantiomeric Polymers for Enantioseletive Recognition

Manas Kumar Bera, ChanchalChakraborty and Sudip Malik*

Polymer Science Unit, Indian Association for the Cultivation of Science, 2A & 2B Raja S. C. Mullick Road, Jadavpur, Kolkata – 700032, India.

Email: psusm2@iacs.res.in

Table of contents **Page**

NMR Study:

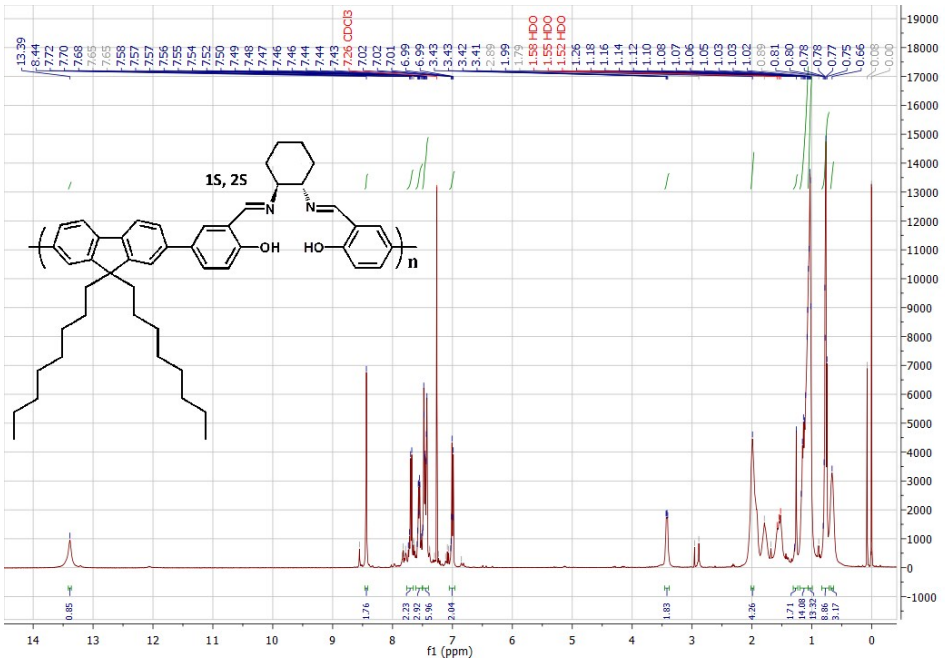

Fig. S1 ^{1}H-NMR of P2 polymer.

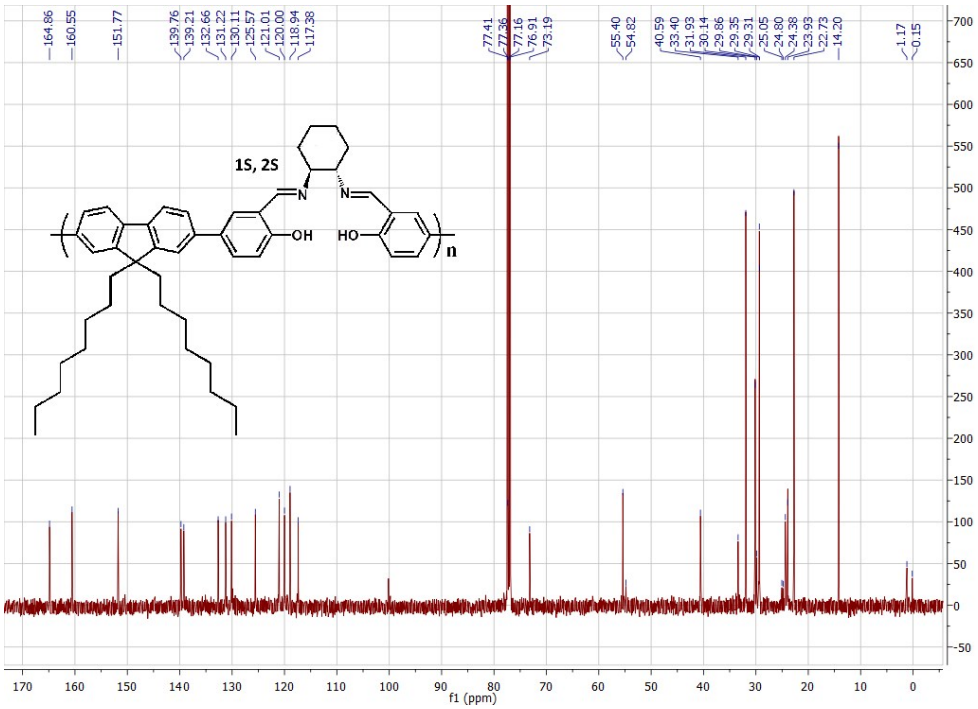

Fig. S2 ^{13}C-NMR of P2 polymer.

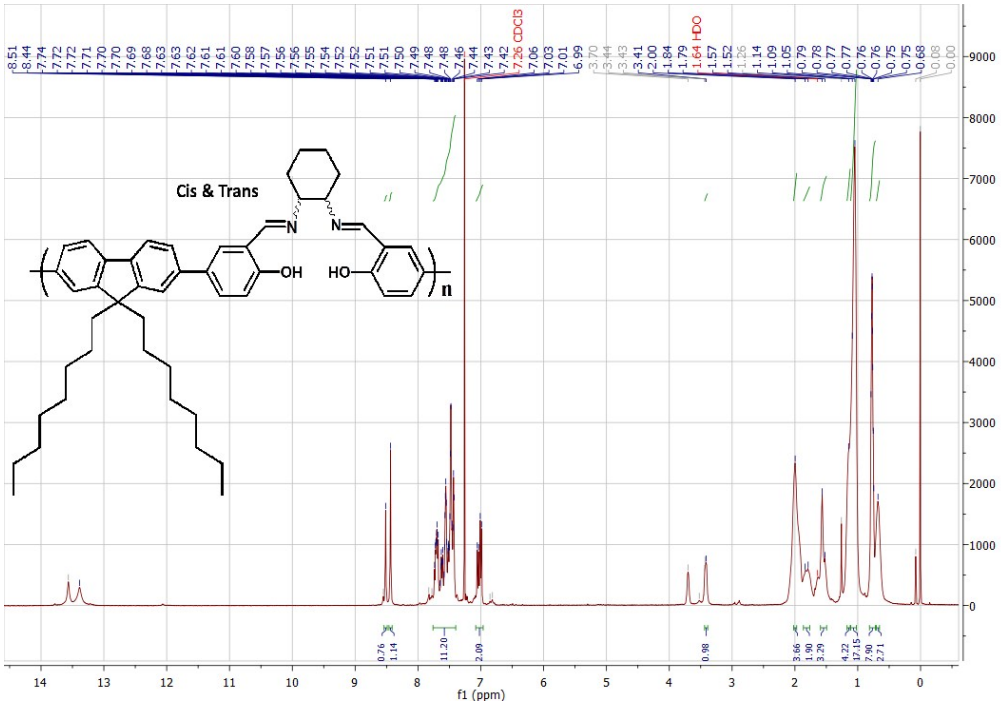

Fig. S3 ^{1}H-NMR of P3 polymer.

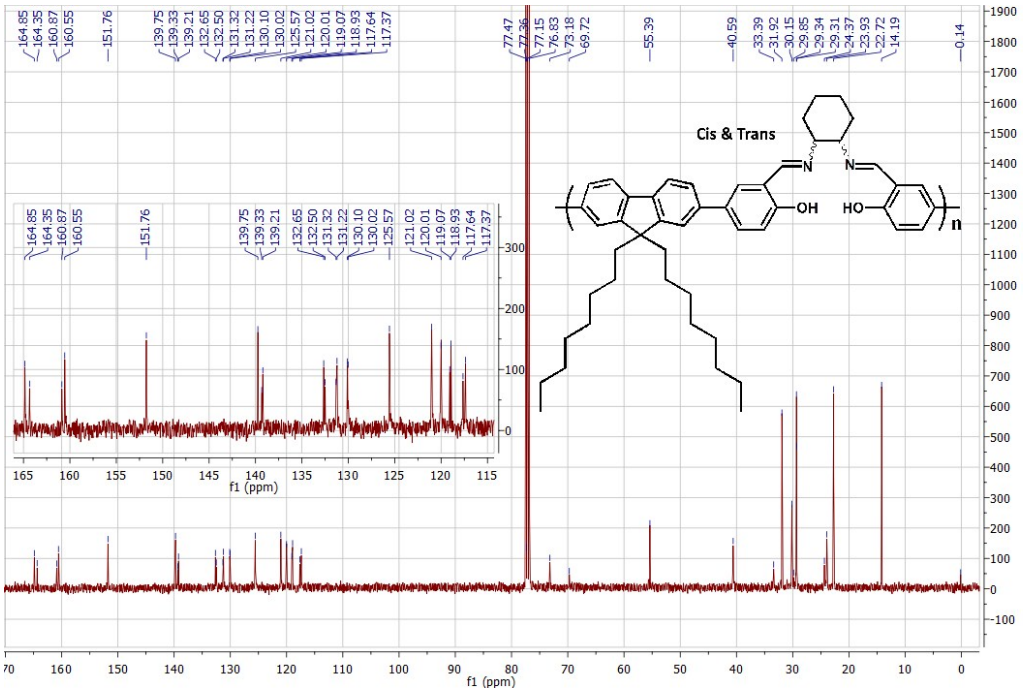

Fig. S4 ^{13}C-NMR of P3 polymer.

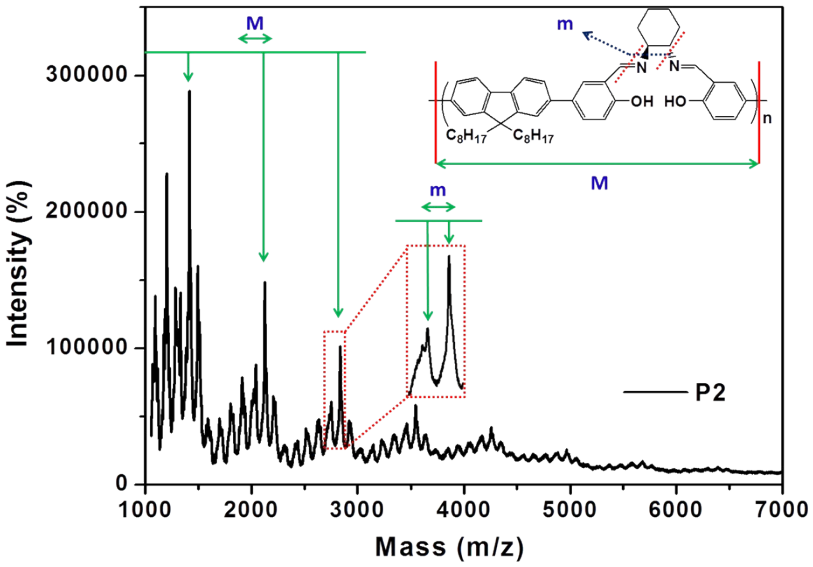

Fig. S5 MALDI-TOF spectrum of P2 in ditranol matrix bearing repetitive monomeric units (with their corresponding mass fragments M and m) up to a degree of polymerization (DP) of 9 (M_W ~ 6400).

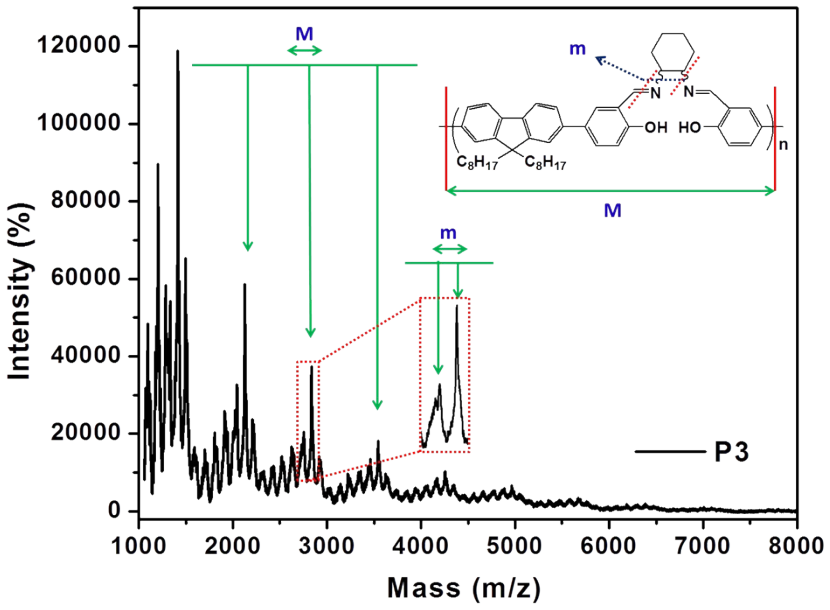

Fig. S6 MALDI-TOF spectrum of P3 in ditranol matrix bearing repetitive monomeric units (with their corresponding mass fragments M and m) up to a degree of polymerization (DP) of 9 (M_W ~ 6400).

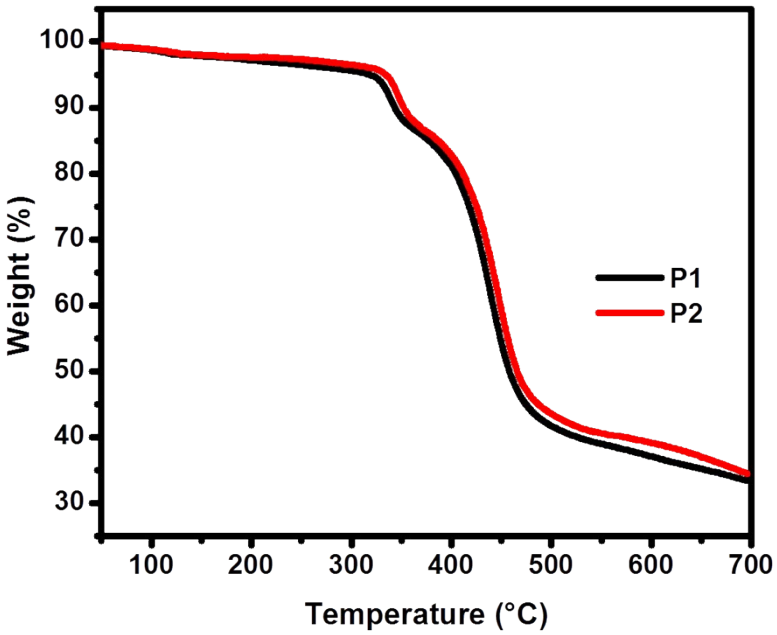

Fig. S7 TGA thermograms of P1and P2.

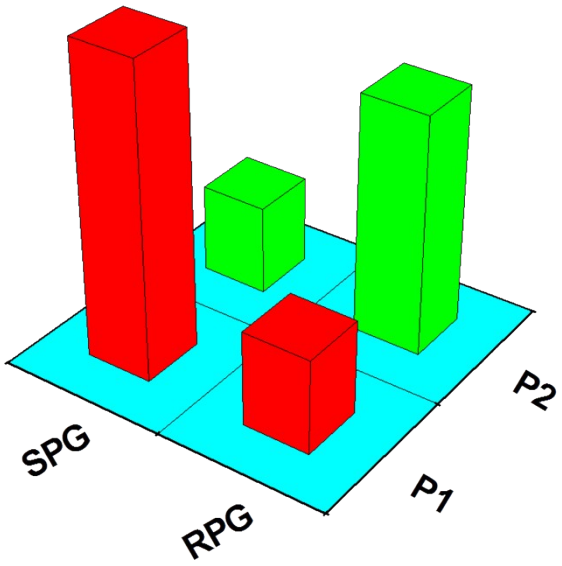

Fig. S8 Bar plot showing the fluorescence change of P1 and P2 in presence of 600 equiv. of (*R*)- and (*S*)-phenylglycinol.

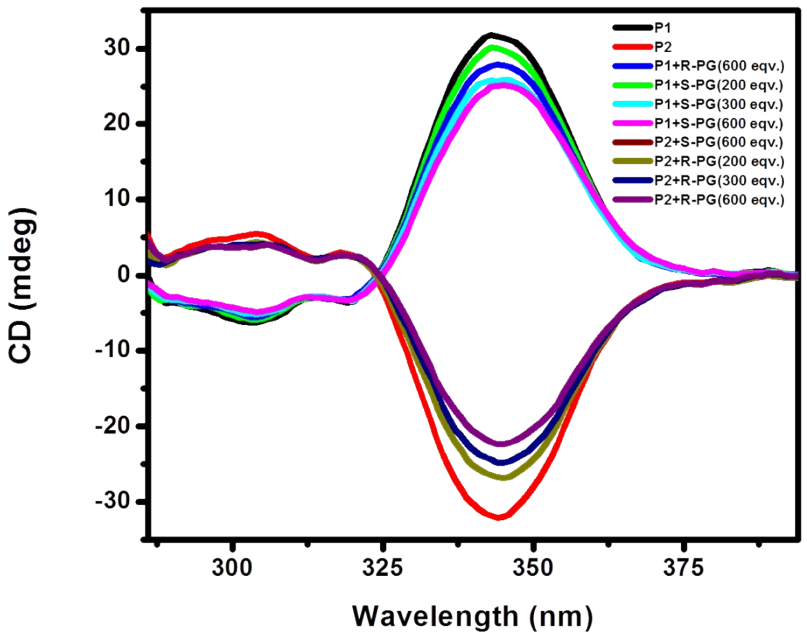

Fig. S9 CD titration spectra of P1 (10 μM in THF) and P2 (10 μM in THF) with different molar ratio of (*S*)- and (*R*)-phenylglycinol in THF.

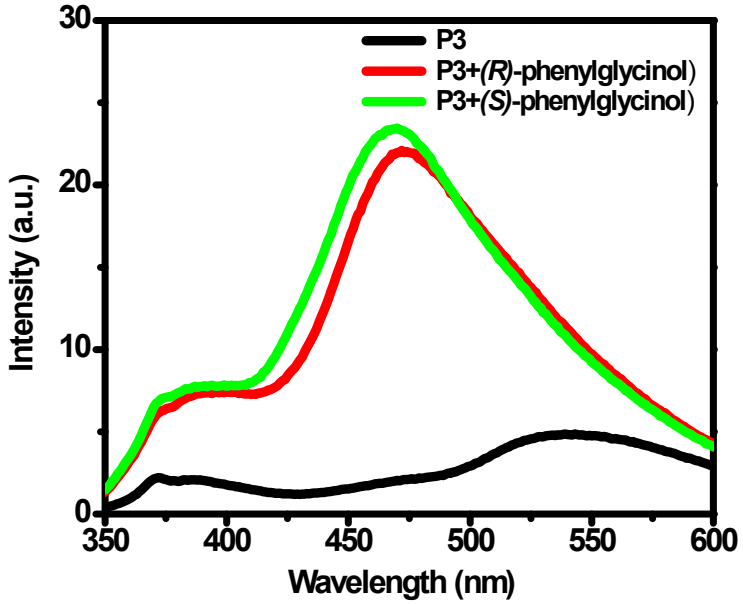

Fig. S10 Fluorescence spectra of P3 (10 μM in THF) with and without 600 equiv. (*R*)- and (*S*)-phenylglycinol in THF. Excitation at 333 nm (slit 5/5).

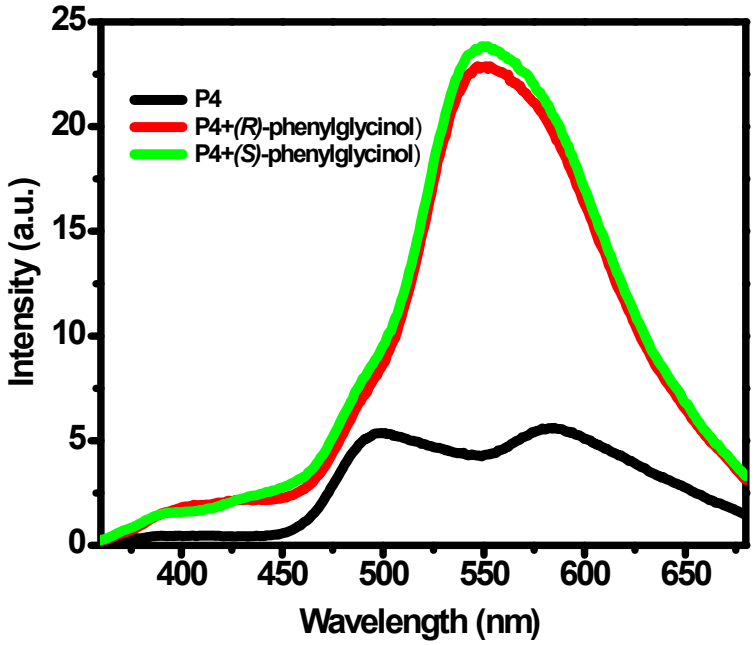

Fig. S11 Fluorescence spectra of P4 (10 μM in THF) with and without 600 equiv. (*R*)- and (*S*)-phenylglycinol in THF. Excitation at 340 nm (slit 5/5).

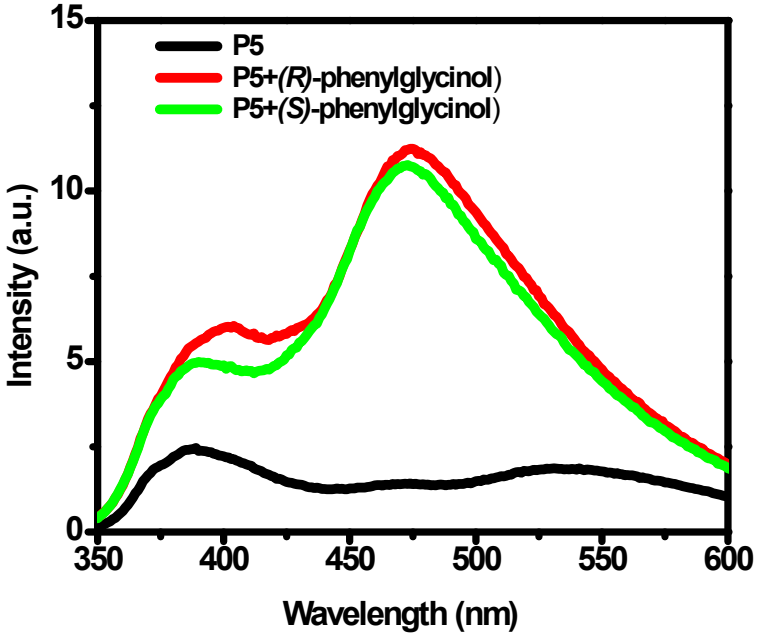

Fig. S12 Fluorescence spectra of P5 (10 μM in THF) with and without 600 equiv. (*R*)- and (*S*)-phenylglycinol in THF. Excitation at 334 nm (slit 5/5).

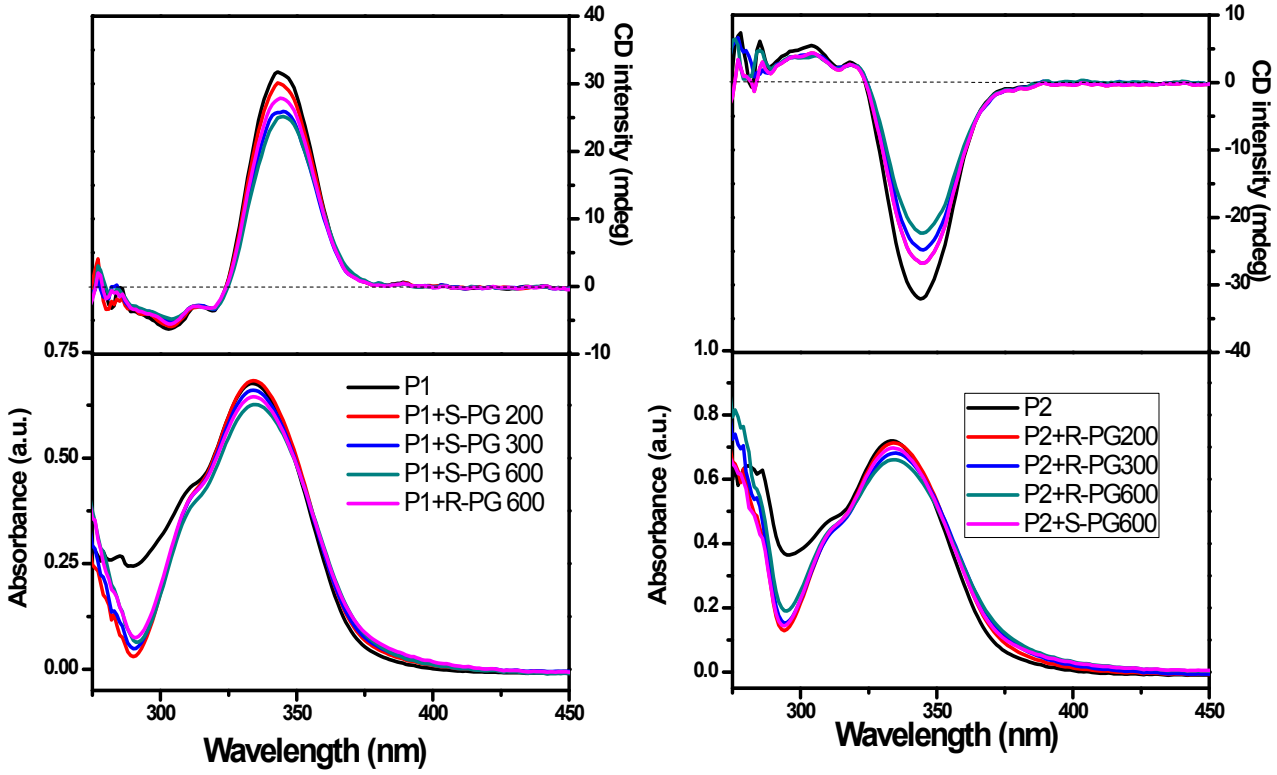

Fig. S13 UV and CD titration spectra of P1 (10 μM in THF) and P2 (10 μM in THF) with different molar ratio of (*S*)- and (*R*)-phenylglycinol in THF.

Kuhn's factor (g):

CD effect is converted into the molar ellipticity using the relation (1).[S1]

$$\Delta\epsilon = \frac{CD(mdeg)}{(32980 \times c \times l)} \quad \text{.....(1)}$$

Where "c" is the concentration of the solution and "l" is the path length of the cuvette.

The anisotropy value or g-value was calculated using the below given relation (2).

$$g = \frac{\Delta\epsilon}{\epsilon} = \frac{CD(mdeg)}{32980 \times A} \quad \text{.....(2)}$$

	***R*-PG (equiv.)**	***S*-PG (equiv.)**	**Calculated g**
Polymer P1	0	0	1.30×10^{-3}
	0	200	1.28×10^{-3}
	0	300	1.17×10^{-3}
	0	600	1.11×10^{-3}
	600	0	1.26×10^{-3}
Polymer P2	0	0	1.29×10^{-3}
	200	0	1.09×10^{-3}
	300	0	1.05×10^{-3}
	600	0	0.95×10^{-3}
	0	600	1.19×10^{-3}

Table ST1. Anisotropy values (g) of the polymers.

NMR Titration Procedure: First polymer was solubilized in $CDCl_3$ (10 mM with respect to monomeric unit) and analyte in $CDCl_3$ was added in different equivalent. Then, solution was shaken for 5 min followed by data acquisition. The OH proton gradually becomes broden upon analyte addition.

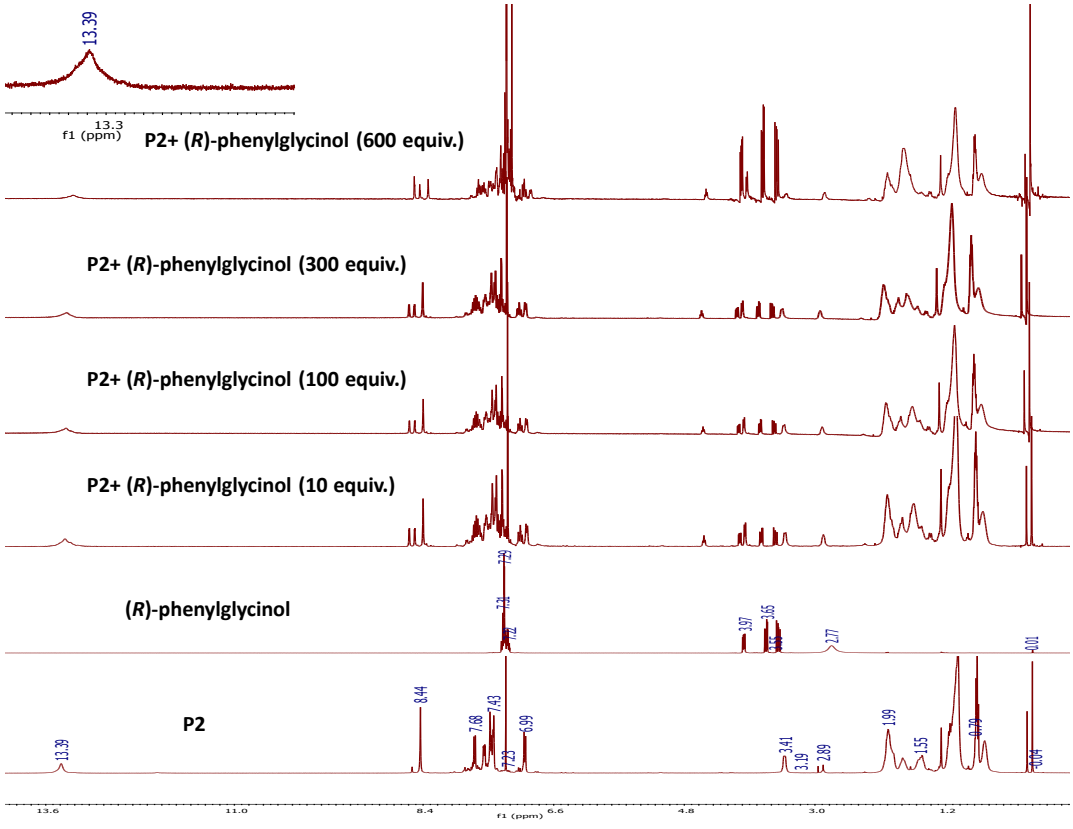

Fig. S14 NMR titration spectra of P2 with (*R*)-phenylglycinol in $CDCl_3$.

Binding constant:

Polymer	Binding constant with *R*-PG (M^{-1})	Binding constant with *S*-PG (M^{-1})
P1	3.7×10^2	10.9×10^3
P2	8.8×10^3	2.8×10^2

Table ST2. Binding constant values of the polymers towards analytes.

Reference:

S1. C. Kulkarni, R. Manirathinam and S. J. George, *Chem. – Eur. J.*, 2013, **19**, 11270.