Electronic Supplementary Information (ESI)

A Facile Method for Colorimetric Determination of the Enantiomeric Purity of Amino Acids Using Poly(phenylacetylene) Possessing (*S*)-Mandelamide Receptors

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1. CD and UV-vis absorption spectra and photograph of the poly-1 solution in the presence of various amino acid guests

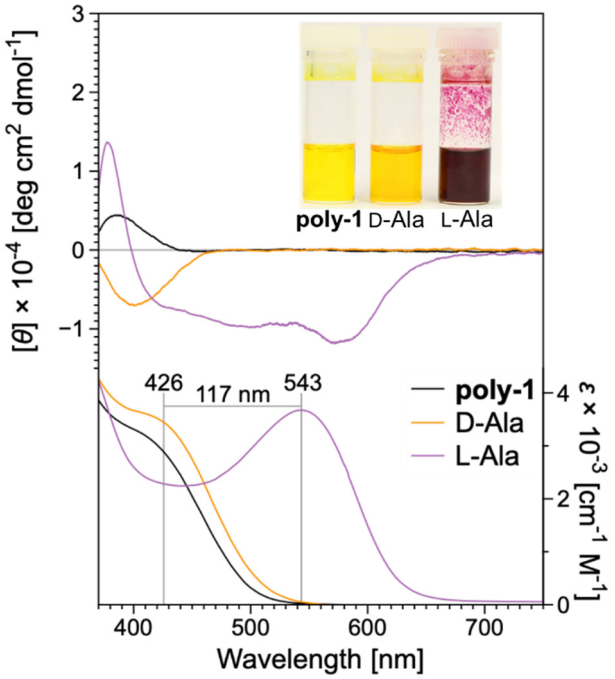

Figure S1. CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of D- and L-Ala in THF at 20 °C. Inset shows the photograph of the THF solutions of **poly-1** in the presence of D- and L-Ala at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Ala]/[monomeric units in **poly-1**] = 20). Peak deconvolution was applied to the absorption spectrum obtained by the D-Ala addition to determine the λ_{max} value. Gel-like precipitates partially formed with the addition of L-Ala.

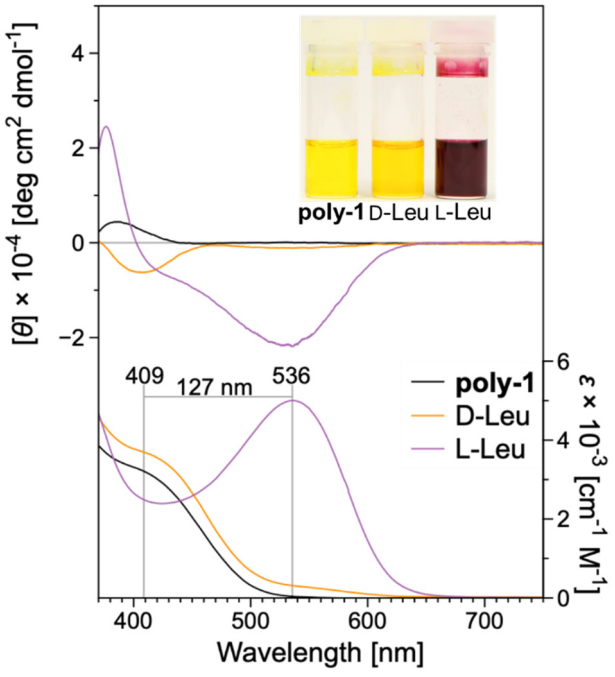

Figure S2. CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of D- and L-Leu in THF at 20 °C. Inset shows the photograph of the THF solutions of **poly-1** in the presence of D- and L-Leu at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Leu]/[monomeric units in **poly-1**] = 20). Peak deconvolution was applied to the absorption spectrum obtained by the D-Leu addition to determine the λ_{max} value.

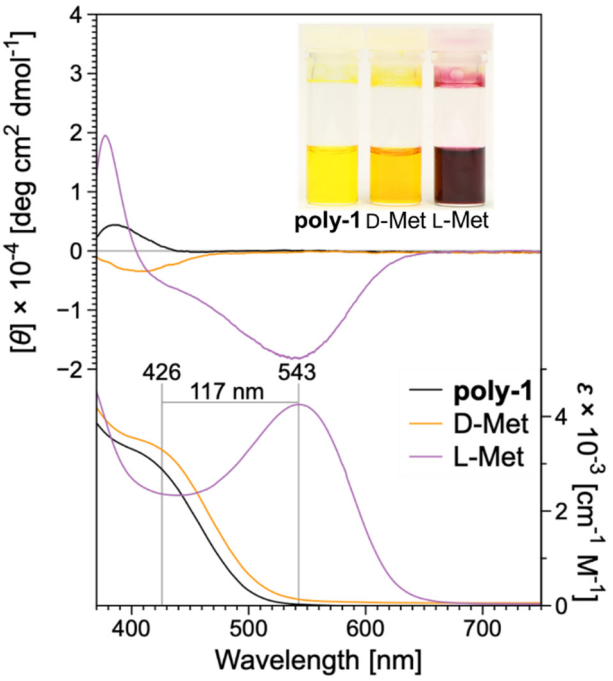

Figure S3. CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of D- and L-Met in THF at 20 °C. Inset shows the photograph of the THF solutions of **poly-1** in the presence of D- and L-Met at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Met]/[monomeric units in **poly-1**] = 50). Peak deconvolution was applied to the absorption spectrum obtained by the D-Met addition to determine the λ_{max} value.

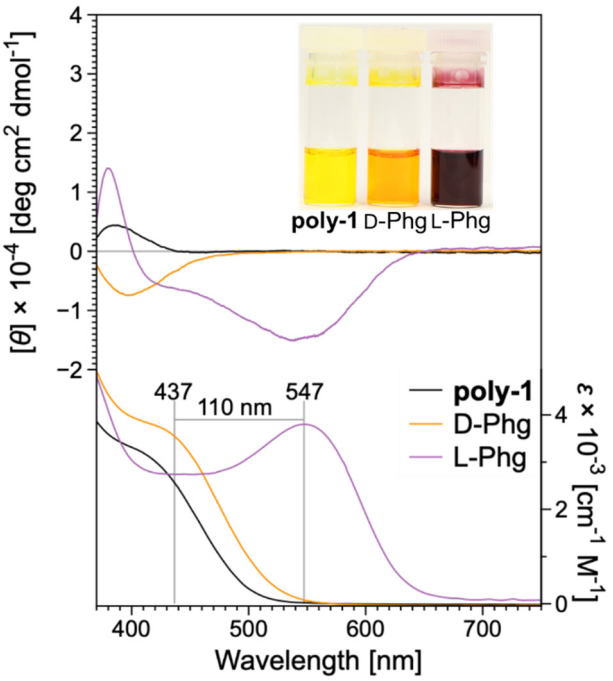

Figure S4. CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of D- and L-Phg in THF at 20 °C. Inset shows the photograph of the THF solutions of **poly-1** in the presence of D- and L-Phg at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Phg]/[monomeric units in **poly-1**] = 100). Peak deconvolution was applied to the absorption spectrum obtained by the D-Phg addition to determine the λ_{max} value.

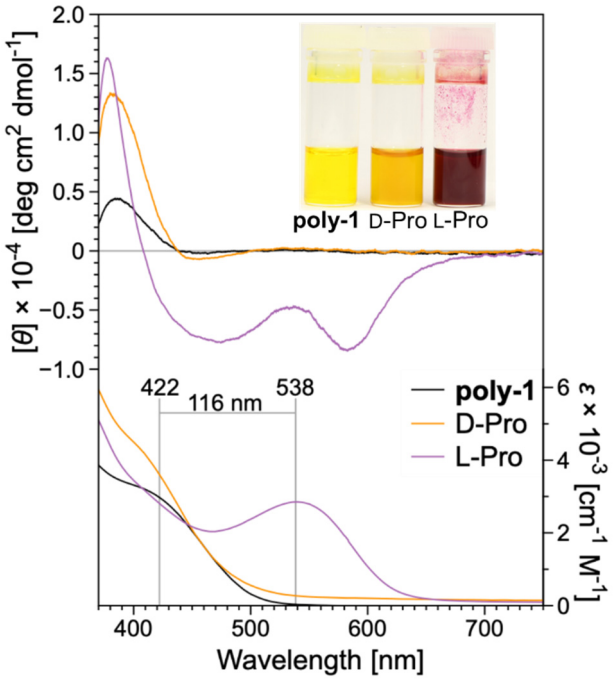

Figure S5. CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of D- and L-Pro in THF at 20 °C. Inset shows the photograph of the THF solutions of **poly-1** in the presence of D- and L-Pro at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Pro]/[monomeric units in **poly-1**] = 10). Peak deconvolution was applied to the absorption spectrum obtained by the D-Pro addition to determine the λ_{max} value. Gel-like precipitates partially formed with the addition of L-Pro.

2. Colorimetric response and changes in CD and absorption spectra for titration experiment

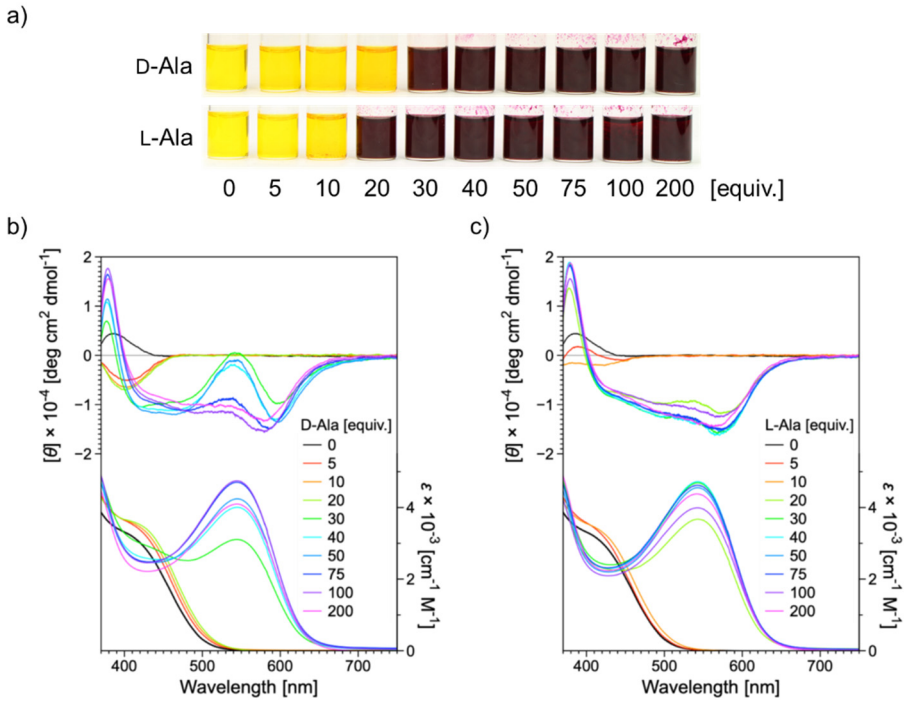

Figure S6. (a) Visible color change of **poly-1** upon the addition of D- and L-Ala guests in THF at 20 °C. Changes in the CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of (b) D-Ala and (c) L-Ala guests in THF at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Ala]/[monomeric units in **poly-1**] = 0–200). Gel-like precipitates partially formed with the addition of more than 40 equiv. of D-Ala and more than 20 equiv. of L-Ala.

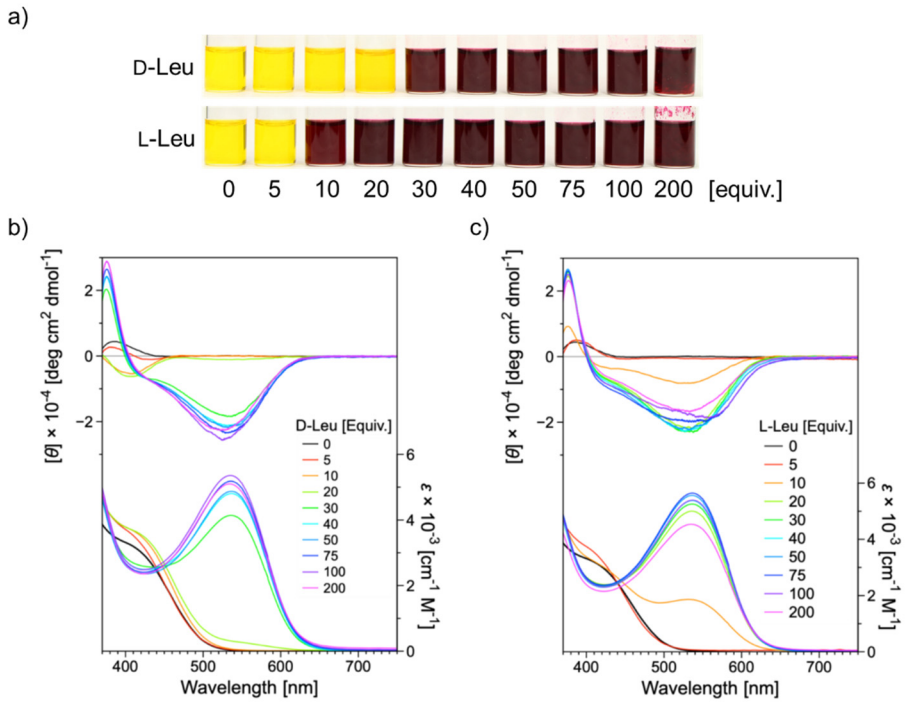

Figure S7. (a) Visible color change of **poly-1** upon the addition of D- and L-Leu guests in THF at 20 °C. Changes in the CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of (b) D-Leu and (c) L-Leu guests in THF at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Leu]/[monomeric units in **poly-1**] = 0–200). Gel-like precipitates partially formed with the addition of 200 equiv. of L-Leu.

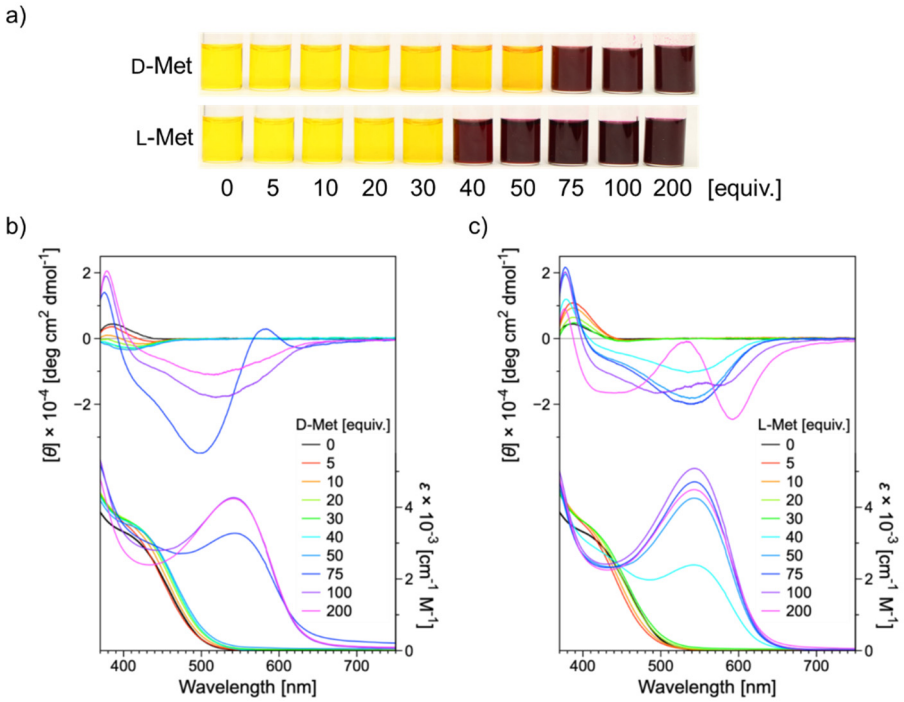

Figure S8. (a) Visible color change of **poly-1** upon the addition of D- and L-Met guests in THF at 20 °C. Changes in the CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of (b) D-Met and (c) L-Met guests in THF at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Met]/[monomeric units in **poly-1**] = 0–200).

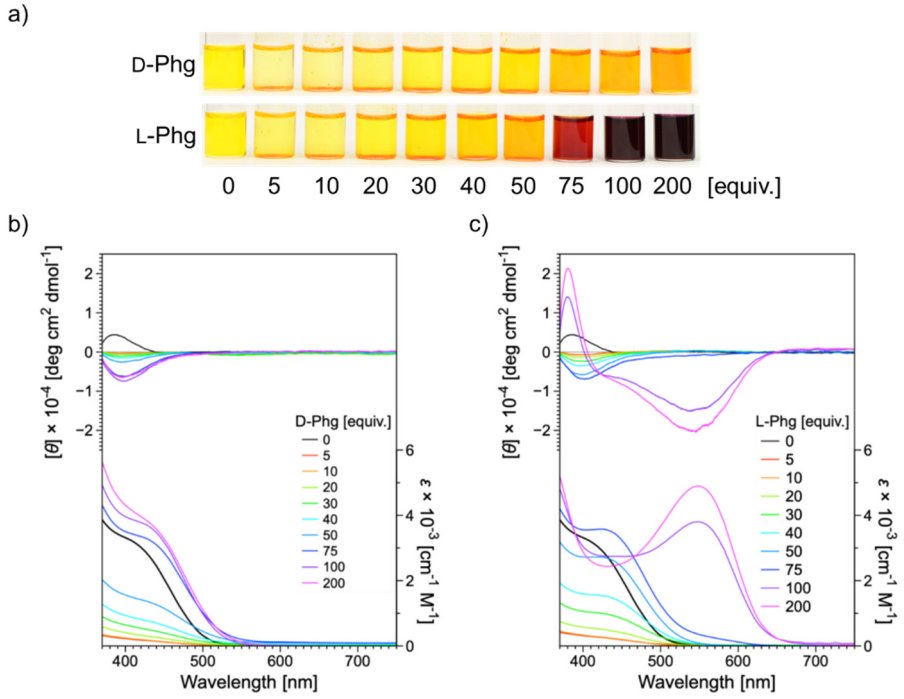

Figure S9. (a) Visible color change of **poly-1** upon the addition of D- and L-Phg guests in THF at 20 °C. Changes in the CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of (b) D-Phg and (c) L-Phg guests in THF at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Phg]/[monomeric units in **poly-1**] = 0–200). Precipitates partially formed with the addition of 5–75 equiv. of D-Phg and 5–50 equiv. of L-Phg. Due to the precipitate formation, the decrease in the apparent polymer concentration was observed in both photographs and absorption spectra.

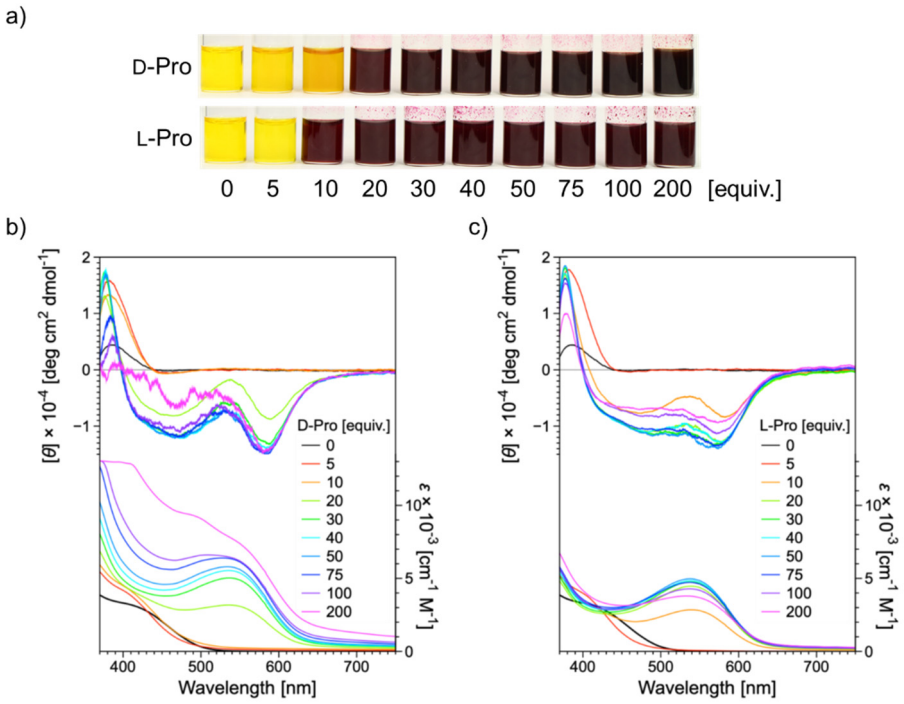

Figure S10. (a) Visible color change of **poly-1** upon the addition of D- and L-Pro guests in THF at 20 °C. Changes in the CD (upper) and UV-vis absorption (lower) spectra of **poly-1** in the presence of (b) D-Pro and (c) L-Pro guests in THF at 20 °C. The polymer concentration was 1.00 g L^{-1} ([Pro]/[monomeric units in **poly-1**] = 0–200). Gel-like precipitates partially formed with the addition of more than 20 equiv. of D-Pro and more than 10 equiv. of L-Pro.

3. CD and UV-vis absorption spectra and photograph of poly-1 in the presence of guest with a varying composition of D- and L-enantiomers

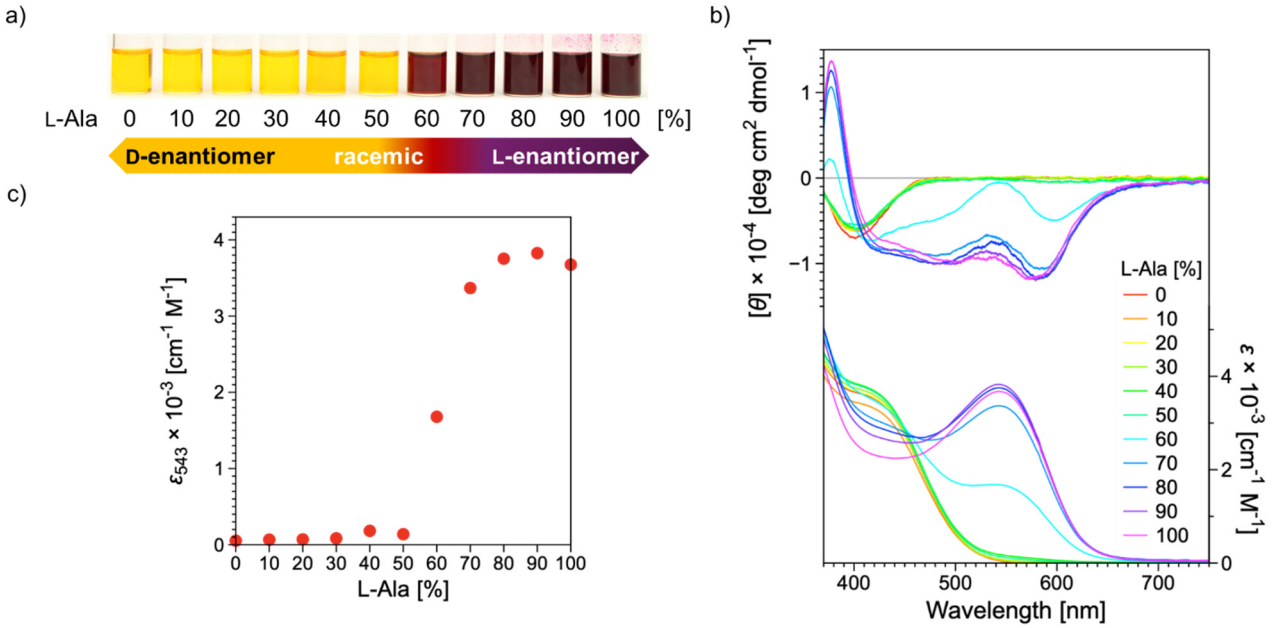

Figure S11. (a) Photograph and (b) CD (upper) and UV-vis absorption (lower) spectra of the THF solution of **poly-1** in the presence of Ala guests with a varying composition of D- and L-enantiomers. (c) The relationship between the resulting ε value at 543 nm and the composition of L-Ala (mol%) in the added guest. The polymer concentration was 1.00 g L^{-1} ([Ala]/[monomeric units in **poly-1**] = 20). The experiments were conducted at 20 °C.

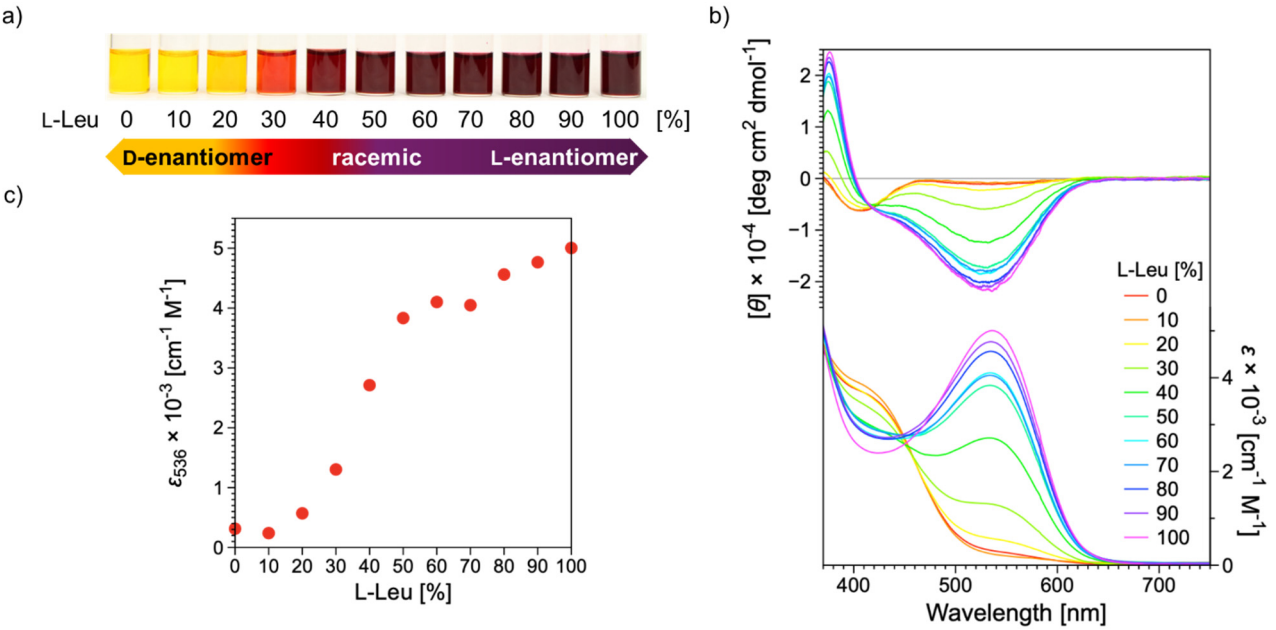

Figure S12. (a) Photograph and (b) CD (upper) and UV-vis absorption (lower) spectra of the THF solution of **poly-1** in the presence of Leu guests with a varying composition of D- and L-enantiomers. (c) The relationship between the resulting ε value at 536 nm and the composition of L-Leu (mol%) in the added guest. The polymer concentration was 1.00 g L^{-1} ([Leu]/[monomeric units in **poly-1**] = 20). The experiments were conducted at 20 °C.

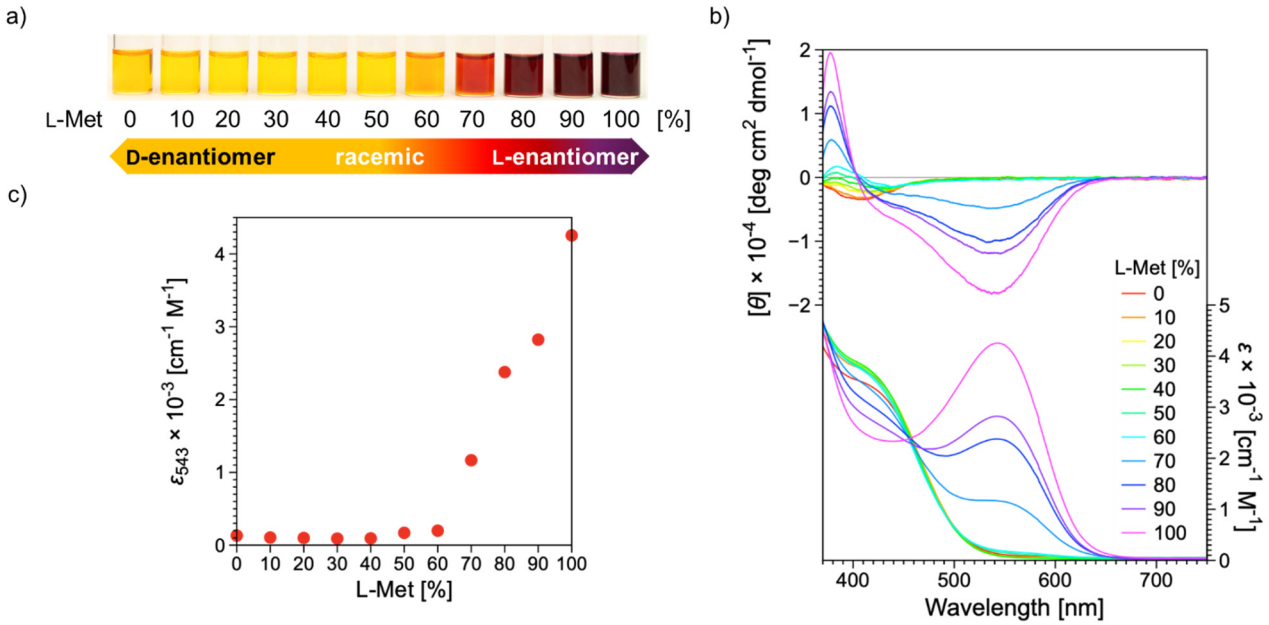

Figure S13. (a) Photograph and (b) CD (upper) and UV-vis absorption (lower) spectra of the THF solution of **poly-1** in the presence of Met guests with a varying composition of D- and L-enantiomers. (c) The relationship between the resulting ε value at 543 nm and the composition of L-Met (mol%) in the added guest. The polymer concentration was 1.00 g L^{-1} ([Met]/[monomeric units in **poly-1**] = 50). The experiments were conducted at 20 °C.

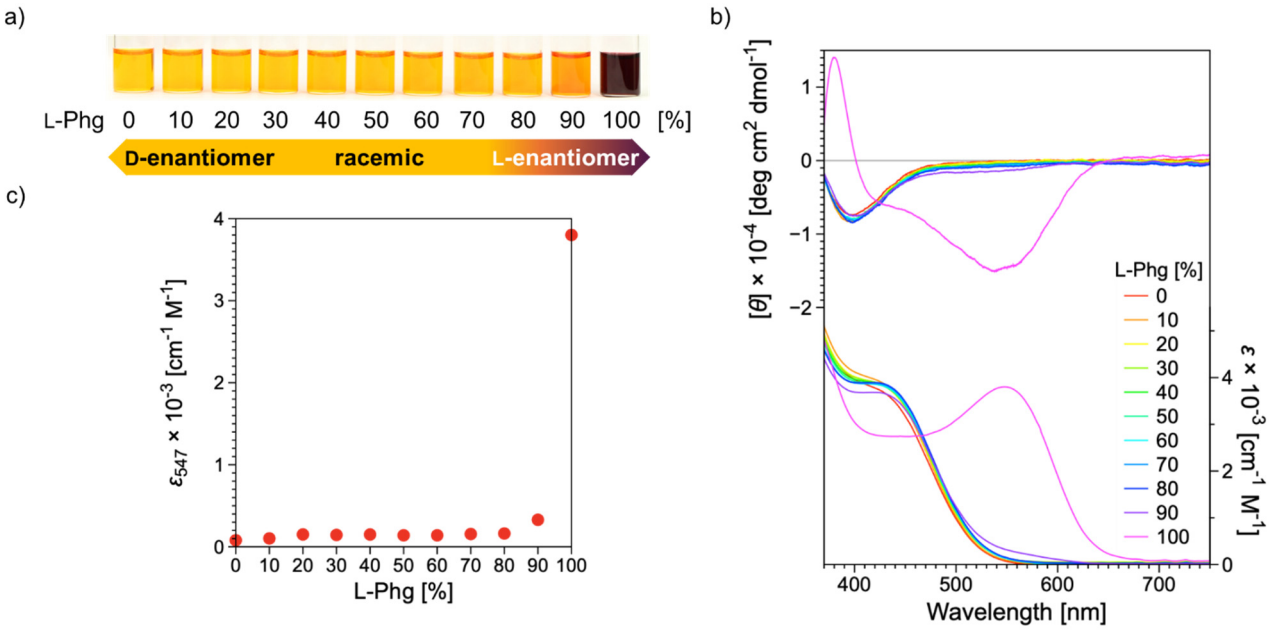

Figure S14. (a) Photograph and (b) CD (upper) and UV-vis absorption (lower) spectra of the THF solution of **poly-1** in the presence of Phg guests with a varying composition of D- and L-enantiomers. (c) The relationship between the resulting ε value at 547 nm and the composition of L-Phg (mol%) in the added guest. The polymer concentration was 1.00 g L^{-1} ([Phg]/[monomeric units in **poly-1**] = 100). The experiments were conducted at 20 °C.

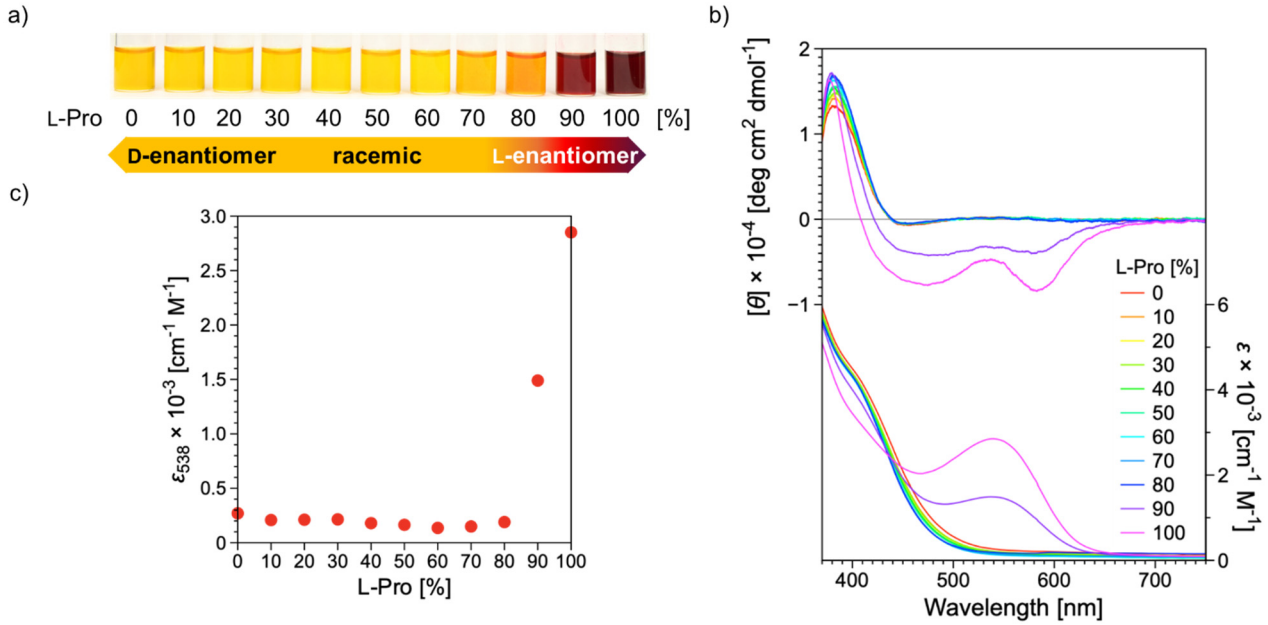

Figure S15. (a) Photograph and (b) CD (upper) and UV-vis absorption (lower) spectra of the THF solution of **poly-1** in the presence of Pro guests with a varying composition of D- and L-enantiomers. (c) The relationship between the resulting ε value at 538 nm and the composition of L-Pro (mol%) in the added guest. The polymer concentration was 1.00 g L^{-1} ([Pro]/[monomeric units in **poly-1**] = 10). The experiments were conducted at 20 °C.

4. NMR spectra

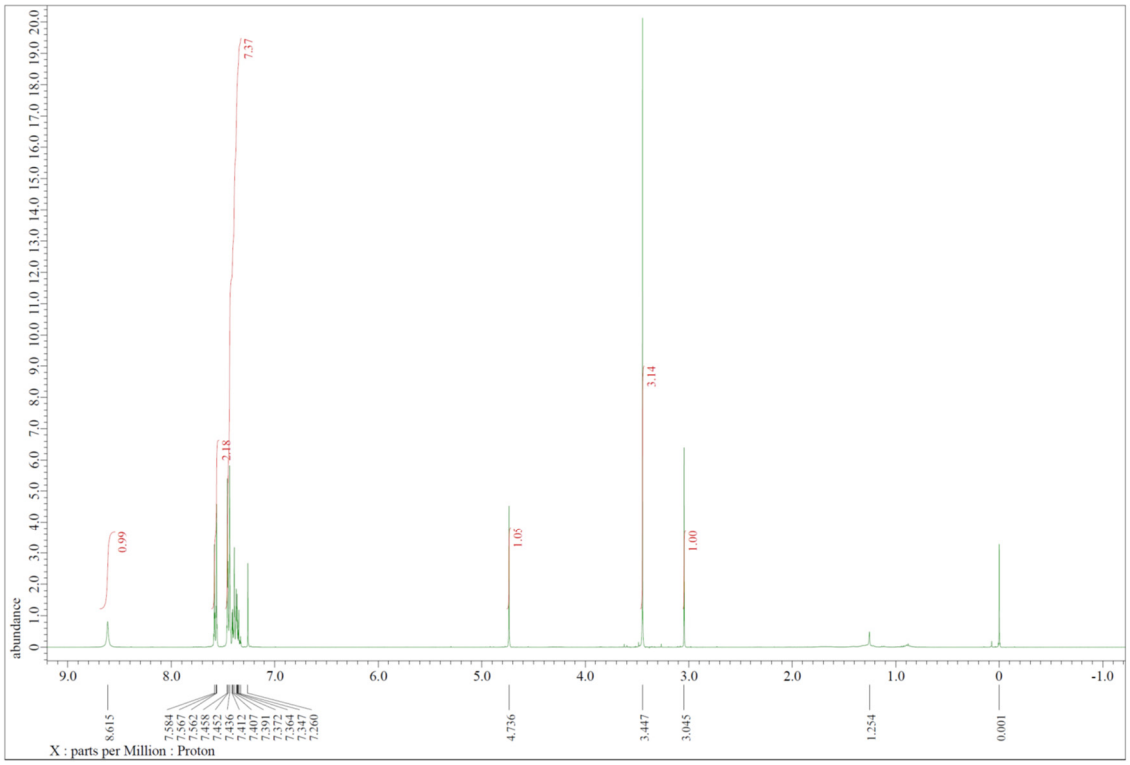

Figure S16. ^{1}H NMR spectrum of **1** in $CDCl_3$ at room temperature (400 MHz).

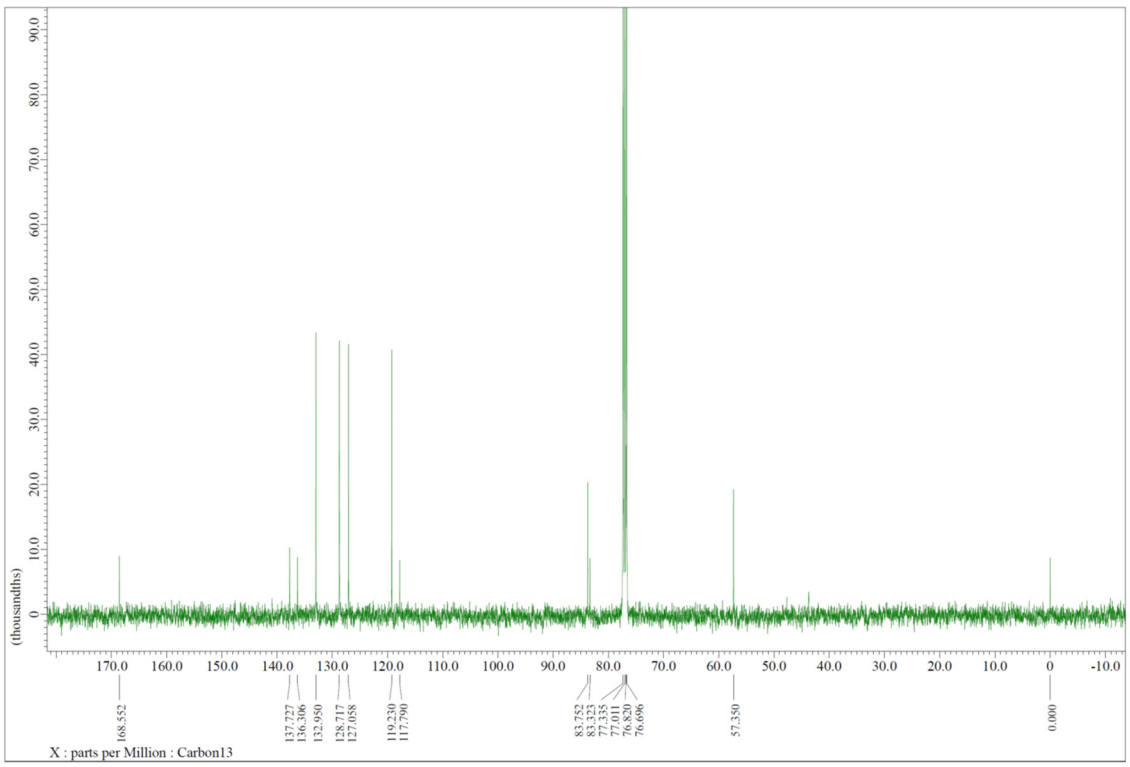

Figure S17. ^{13}C NMR spectrum of **1** in $CDCl_3$ at room temperature (101 MHz).

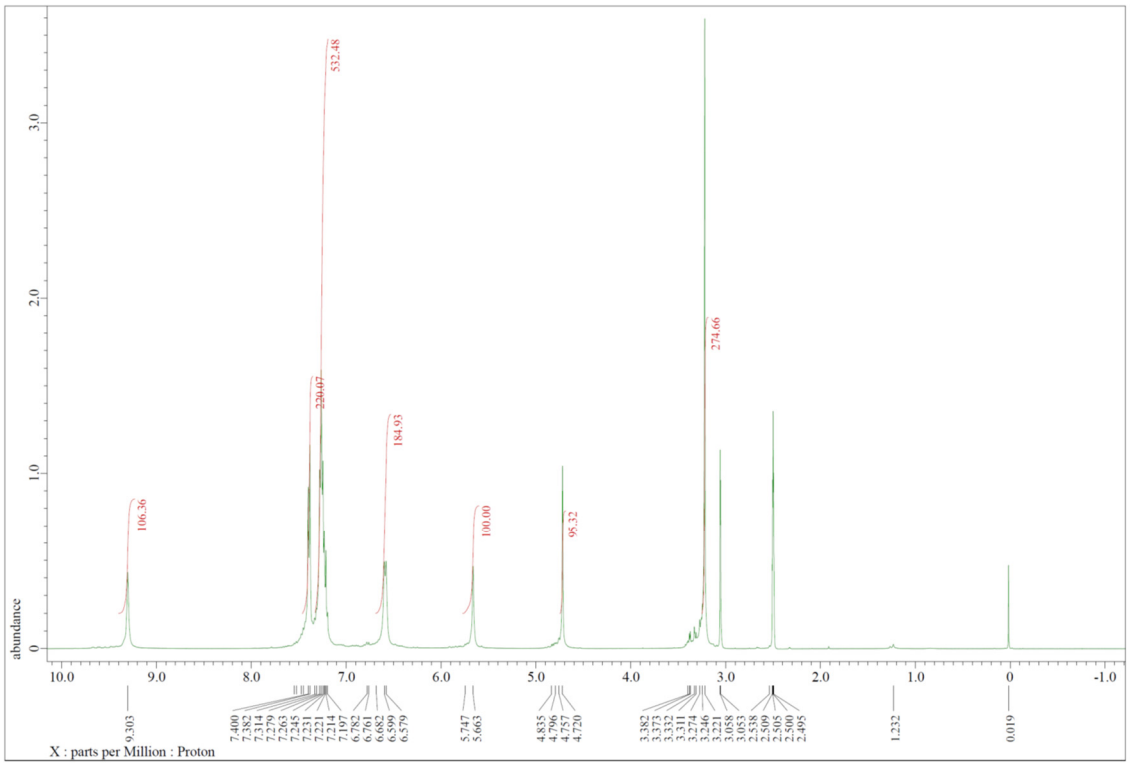

Figure S18. ^{1}H NMR spectrum of **poly-1** in DMSO-d_6 at 80 °C (400 MHz).

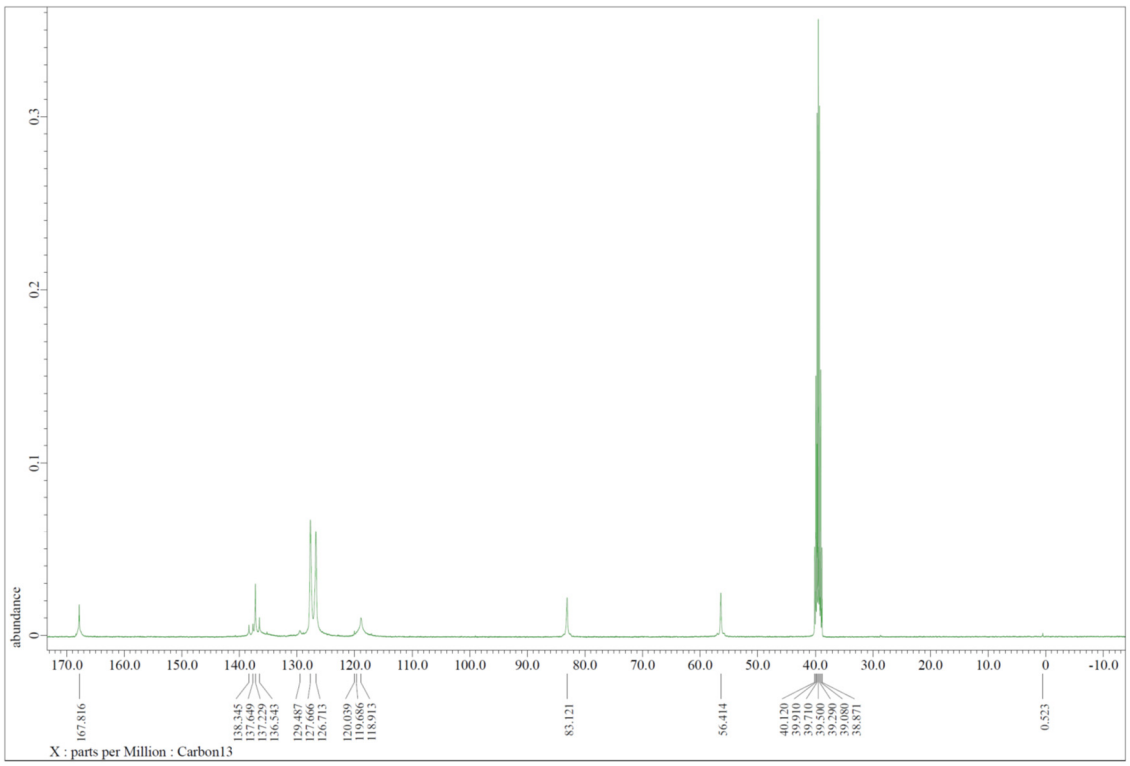

Figure S19. ^{13}C NMR spectrum of **poly-1** in DMSO-d_6 at 80 °C (101 MHz).