(Supporting Information)

Macromolecular Chirality Induction on Optically Inactive Poly(4-carboxyphenyl isocyanide) with Chiral Amines: A Dynamic Conformational Transition of Poly(phenyl isocyanide) Derivatives

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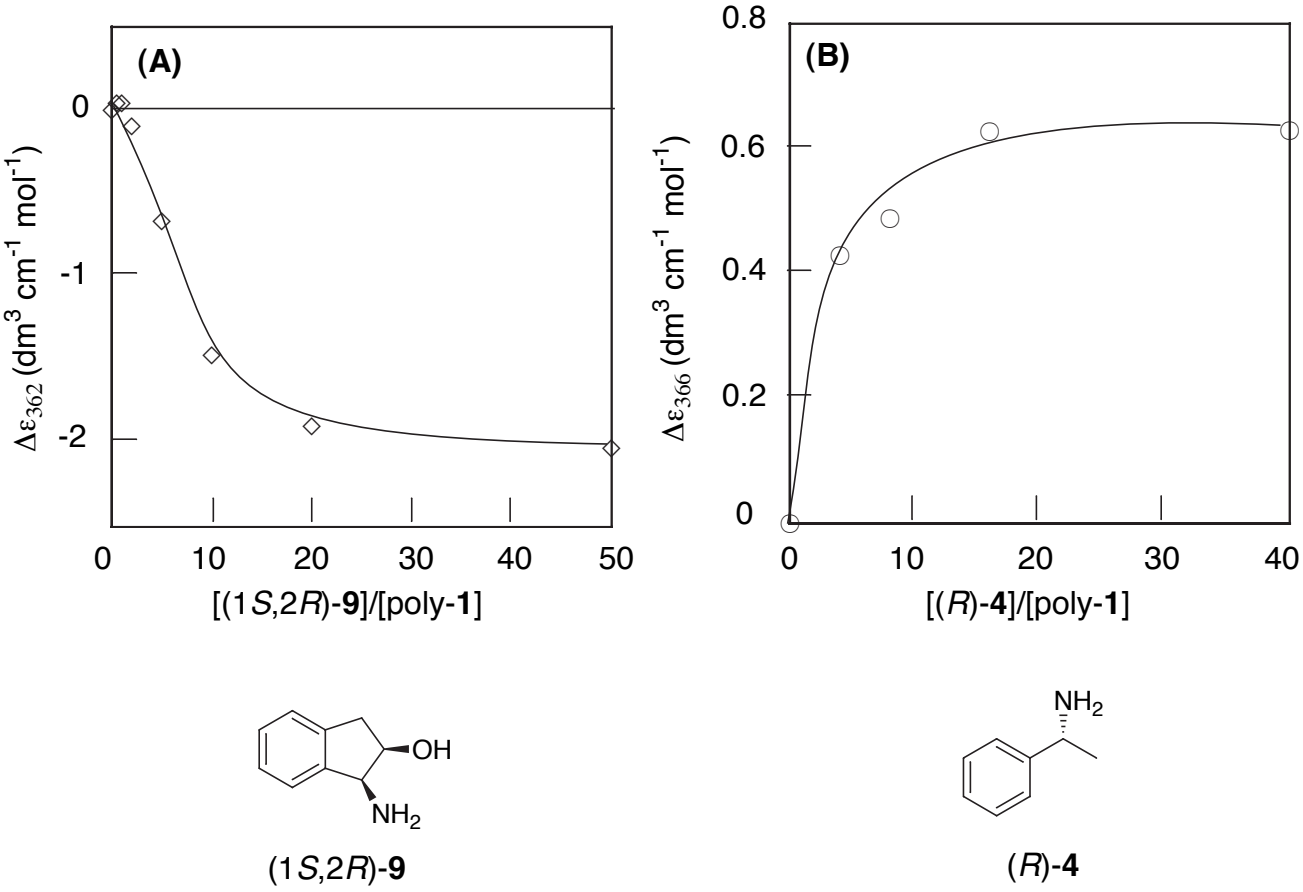


Figure S-1. CD titrations in the complexation of poly-**1** (1 mg/mL) with (1*S*,2*R*)-**9** (A) and (*R*)-**4** (B) in DMSO at ambient temperature (ca. 20 - 25 °C).

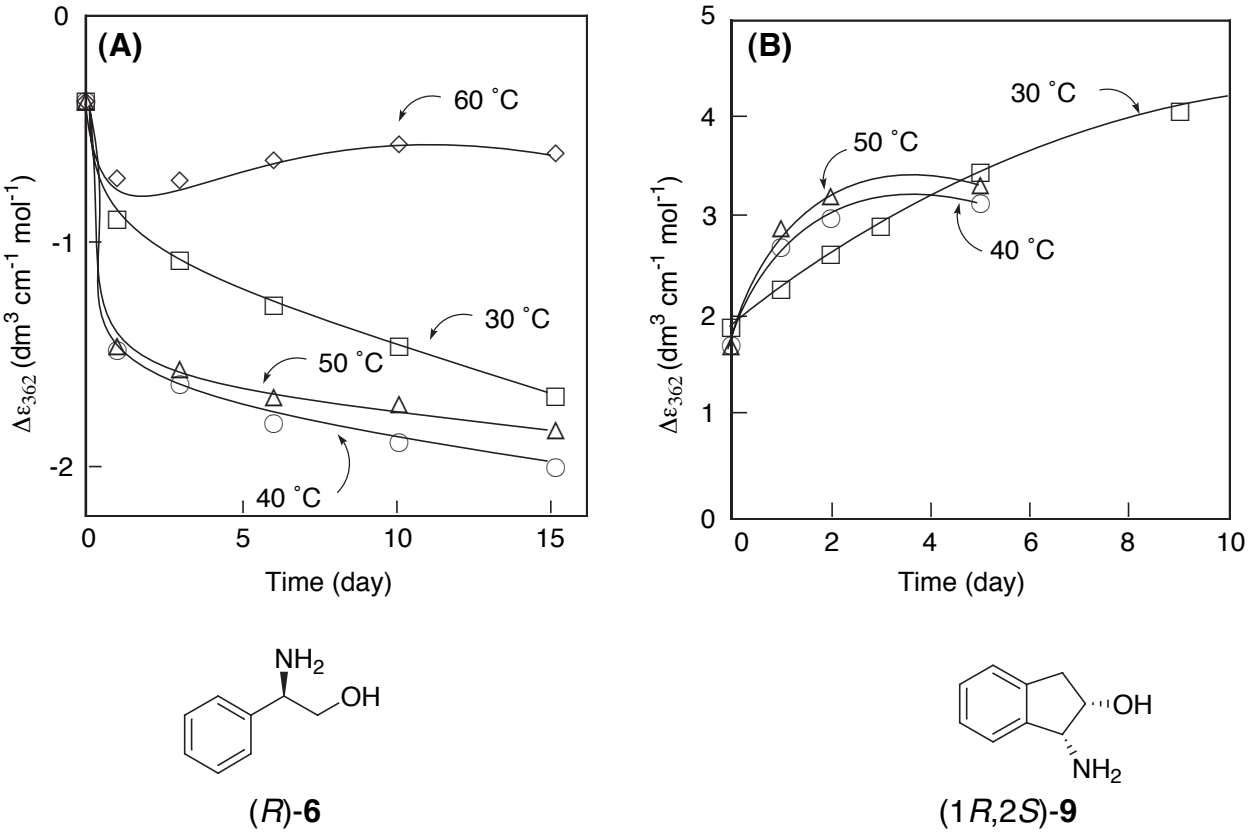


Figure S-2. Changes in the CD intensity of the complexes of poly-**1** with (*R*)-**6** (A) and (1*R*,2*S*)-**9** (B) at various temperatures in DMSO with a poly-**1** concentration of 1.0 mg/mL; molar ratio of amines to monomeric unit of poly-**1** is 20 (**6**) and 50 (**9**), respectively.

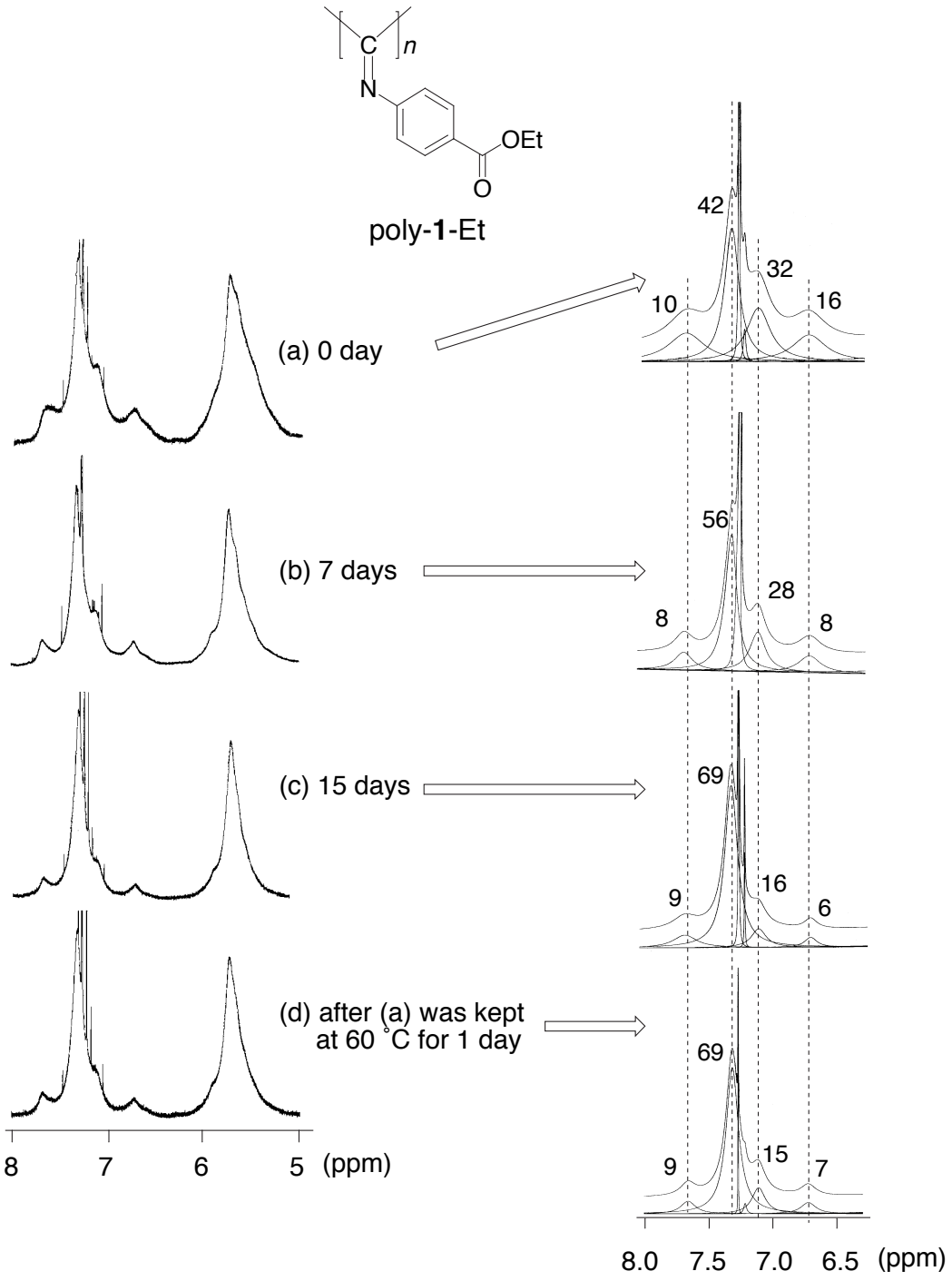


Figure S-3. Time-dependent ^{1}H NMR changes of poly-**1**-Et (10 mg/mL) in $CDCl_3$ at 30 °C (left). Curve fitting results are also shown (right).

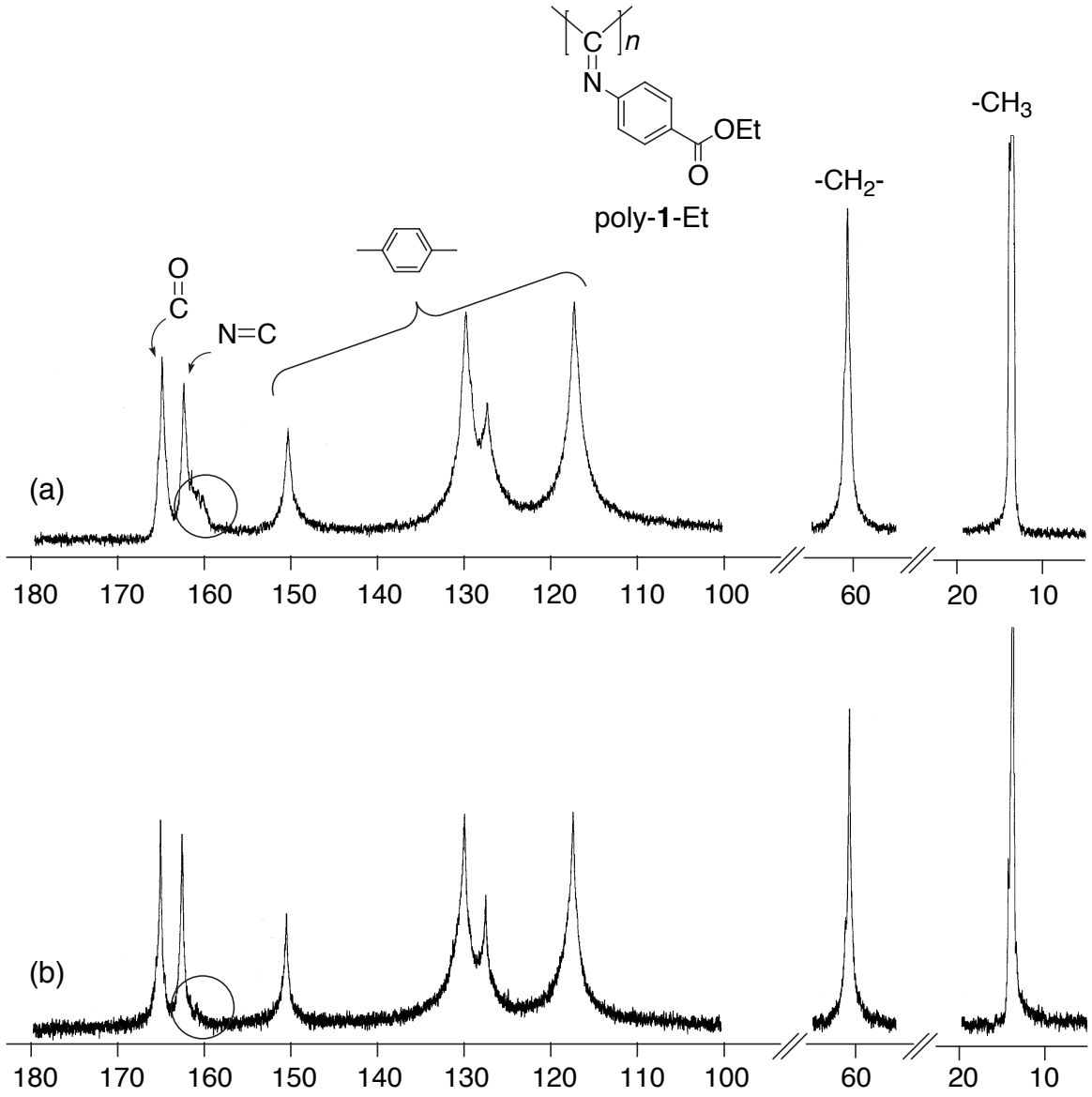


Figure S-4. Time dependent ^{13}C NMR spectral changes of poly-**1**-Et in $CDCl_3$ at 30 °C after 0 (a) and 28 days (b).

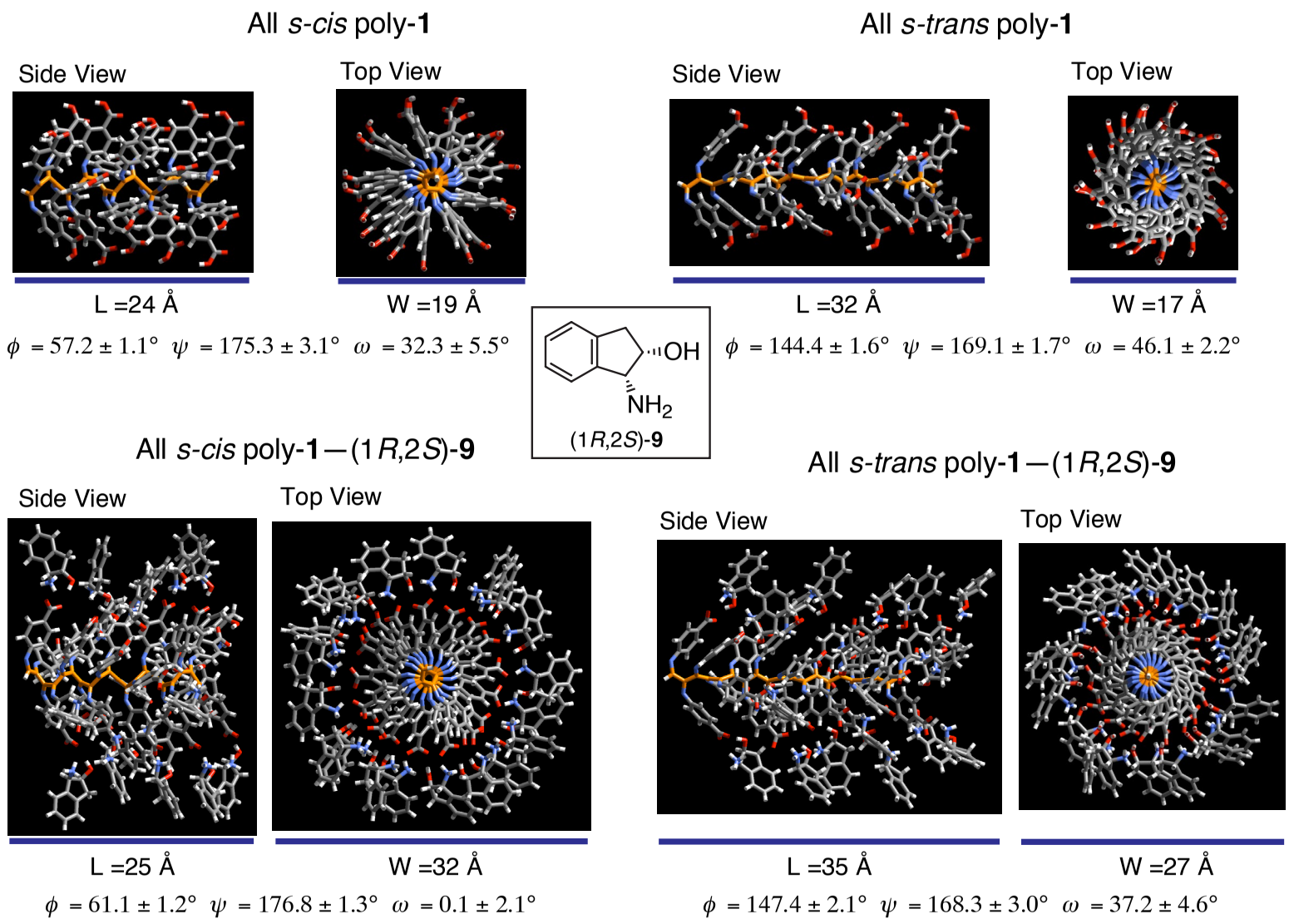
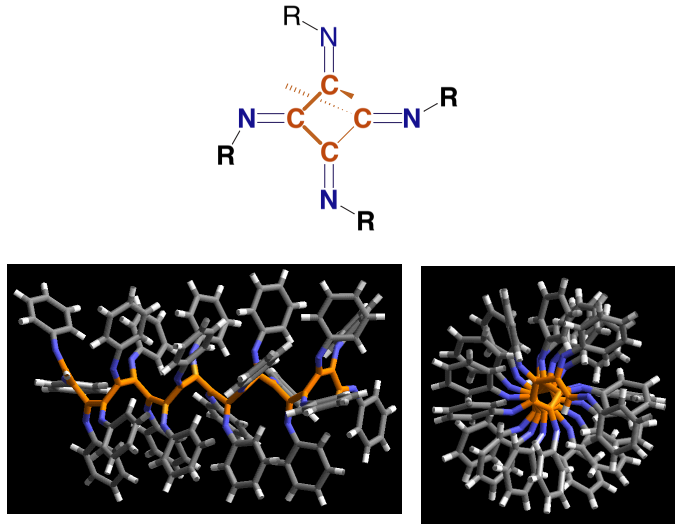
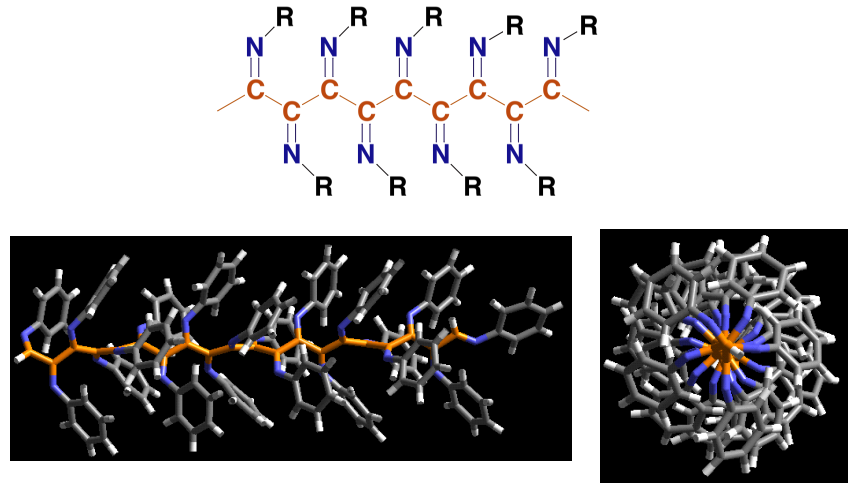


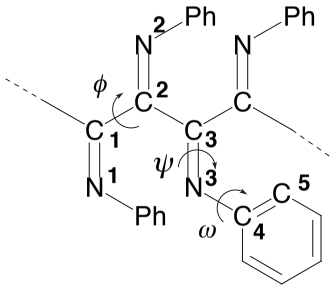
Figure S-5. Optimized all *s-cis* (left) and *s-trans* (right) helical structures of poly-**1** and the poly-**1**—(1*R*,2*S*)-**9** complexes (20 mer). The average dihedral angles, the length, and the width are also shown.

All s-*cis* (4_1 helix) PPI



All s-*trans* PPI





ϕ (N_1-C_1-C_2-N_2) = 59.9 ± 1.8°
ψ (C_2-C_3-N_3-C_4) = 178.0 ± 1.4°
ω (C_3-N_3-C_4-C_5) = –0.2 ± 3.1°

ϕ (N_1-C_1-C_2-N_2) = 146.4 ± 3.9°
ψ (C_2-C_3-N_3-C_4) = 166.4 ± 1.2°
ω (C_3-N_3-C_4-C_5) = 37.2 ± 3.0°

Figure S-6. Optimized all *s-cis* (left) and *s-trans* (right) helical structures of PPI (20 mer). The average dihedral angles are also shown.