

# Hydrodynamic Characteristics and Conformational Parameters of Ferrocene-Terpyridine Based Polymers

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**Table S1.** The experimentally determined solvent parameters<sup>1</sup> used in hydrodynamic study.

|         | $\rho_0$ ,<br>g/cm <sup>3</sup> | $\eta_0$ ,<br>cP |
|---------|---------------------------------|------------------|
|         | 20 °C                           |                  |
| THF     | 0.8878                          | 0.50             |
| THF-d8  | 0.9903                          | 0.54             |
| Toluene | 0.8669                          | 0.589            |
| DMF     | 0.9490                          | 0.82             |

<sup>1</sup> – solvent density  $\rho_0$  and dynamic viscosity  $\eta_0$ .

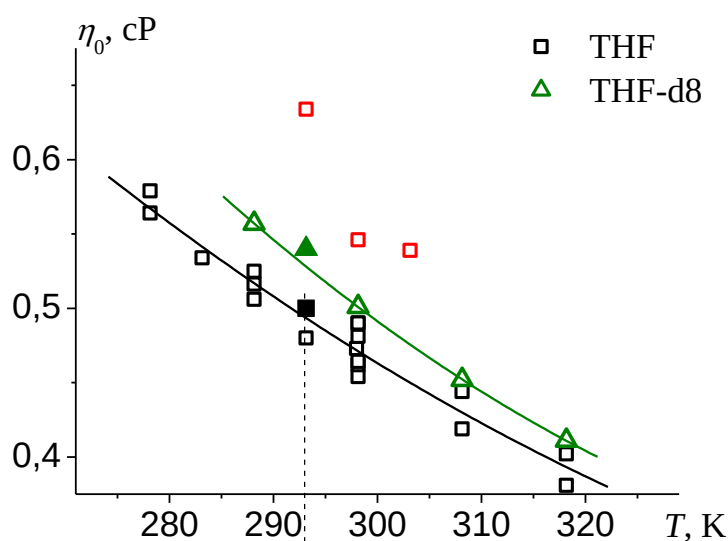
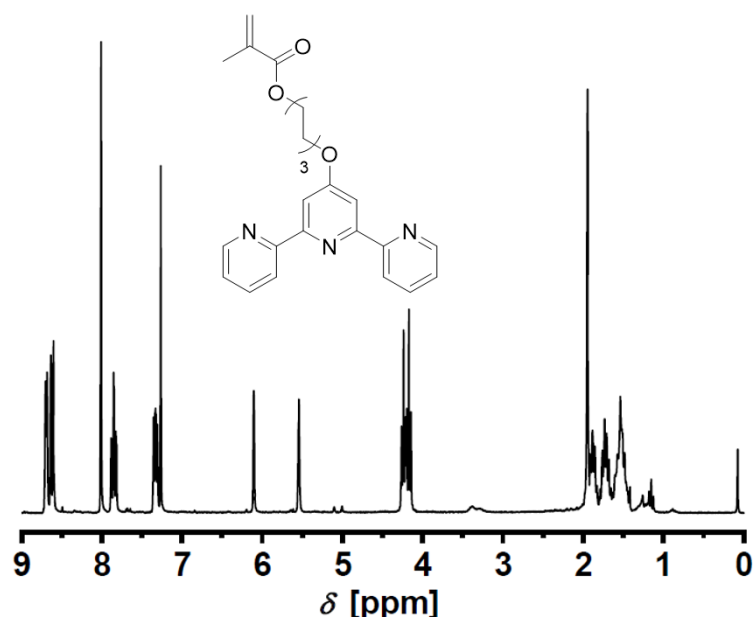


**Figure S1.** The dynamic viscosity data on THF (squares) and THF-d8 (triangles) known from the literature (open symbols) [1-8] and determined experimentally (filled symbols) in this study. The data points in red were not included in extrapolation of data (solid lines).

**Table S2.** Experimental details for the polymer synthesis.

| Polymer                | Synthesis details                                                                                                                             |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <i>poly</i> (Fc)       | Fc monomer: 0.750 g (2.192 mmol)                                                                                                              |
|                        | CPDB: 0.846 mg ( $9.13 \times 10^{-3}$ mmol); monomer-to-CPDB ratio: 240; 0.607 mL of a stock solution (6.66 mg CPDB in 2 mL toluene)         |
|                        | AIBN: 0.375 mg ( $2.28 \times 10^{-3}$ mmol); CPDB-to-AIBN ratio: 4; 0.347 mL of a stock solution (2.16 mg AIBN in 2 mL toluene)              |
|                        | Toluene: 1.786 mL                                                                                                                             |
| <i>poly</i> (tpy)      | Tpy monomer: 0.415 g (0.994 mmol)                                                                                                             |
|                        | CPDB: 2.02 mg ( $3.82 \times 10^{-3}$ mmol); monomer-to-CPDB ratio: 260; 0.447 mL of a stock solution (5.68 mg CPDB in 3 mL toluene)          |
|                        | AIBN: 0.157 mg ( $9.55 \times 10^{-4}$ mmol); CPDB-to-AIBN ratio: 4; 0.175 mL of a stock solution (2.69 mg AIBN in 3 mL toluene)              |
|                        | Toluene: 0.620 mL                                                                                                                             |
| (Fc)- <i>co</i> -(tpy) | Fc monomer: 0.246 g (0.719 mmol)                                                                                                              |
|                        | Tpy monomer: 0.300 g (0.719 mmol)                                                                                                             |
|                        | CPDB: 1.325 mg ( $5.99 \times 10^{-3}$ mmol); monomer-to-CPDB ratio: 240; 0.543 mL of a stock solution (4.88 mg CPDB in 2 mL toluene)         |
|                        | AIBN: 0.246 mg ( $1.49 \times 10^{-3}$ mmol); CPDB-to-AIBN ratio: 4; 0.168 mL of a stock solution (2.93 mg AIBN in 2 mL toluene)              |
| (Fc)- <i>bl</i> -(tpy) | Fc monomer: 0.233 g (0.652 mmol)                                                                                                              |
|                        | Tpy monomer: 0.300 g (0.719 mmol)                                                                                                             |
|                        | <i>poly</i> (tpy): 67.88 mg ( $2.72 \times 10^{-3}$ mmol); monomer-to- <i>poly</i> (tpy) ratio: 240                                           |
|                        | AIBN: 0.111 mg ( $6.78 \times 10^{-4}$ mmol); <i>poly</i> (tpy)-to-AIBN ratio: 4; 0.151 mL of a stock solution (2.22 mg AIBN in 3 mL toluene) |
|                        | Toluene: 0.664 mL                                                                                                                             |

**Figure S2.** <sup>1</sup>H-NMR spectra of the tpy monomer (1, 300 MHz, 25 °C, CDCl<sub>3</sub>).

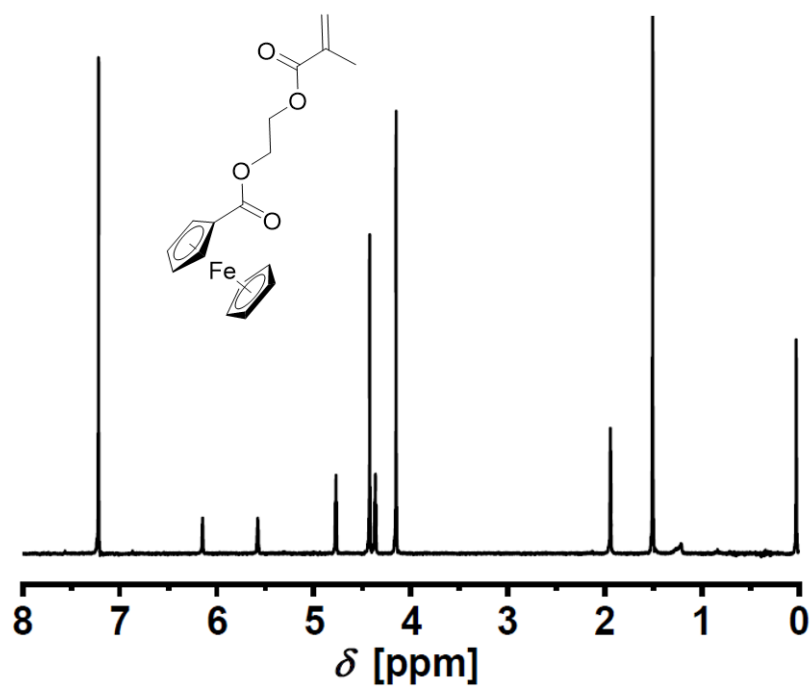


Figure S3.  $^1\text{H}$ -NMR spectra of the Fc monomer (2, 300 MHz, 25  $^\circ\text{C}$ ,  $\text{CDCl}_3$ ).

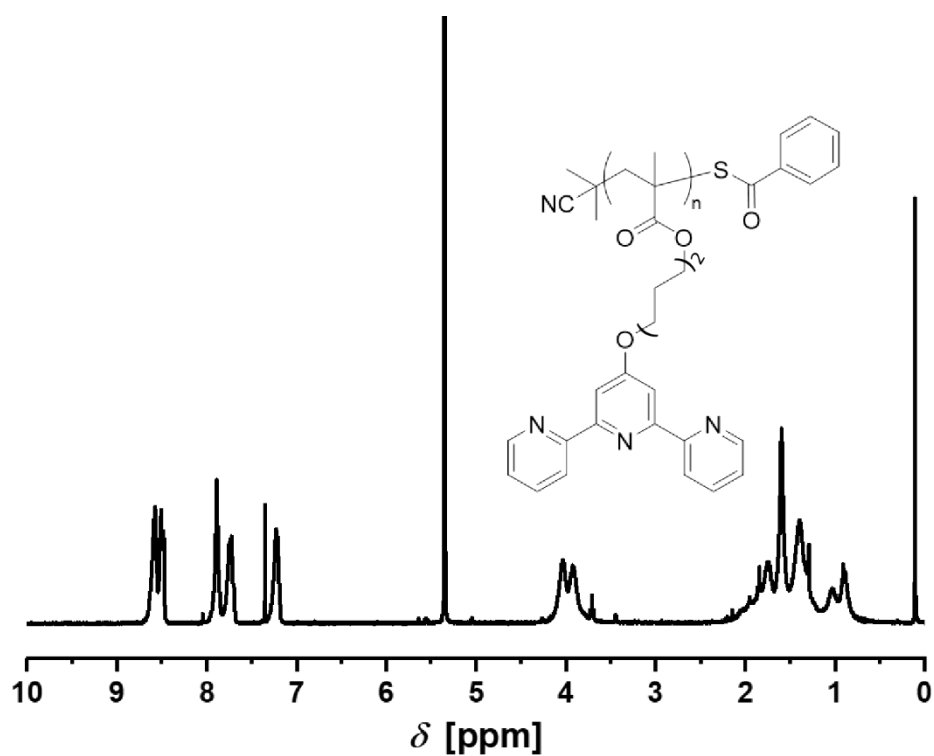


Figure S4.  $^1\text{H}$ -NMR spectra of  $\text{poly}(\text{tpy})$  (300 MHz, 25  $^\circ\text{C}$ ,  $\text{CD}_2\text{Cl}_2$ ).

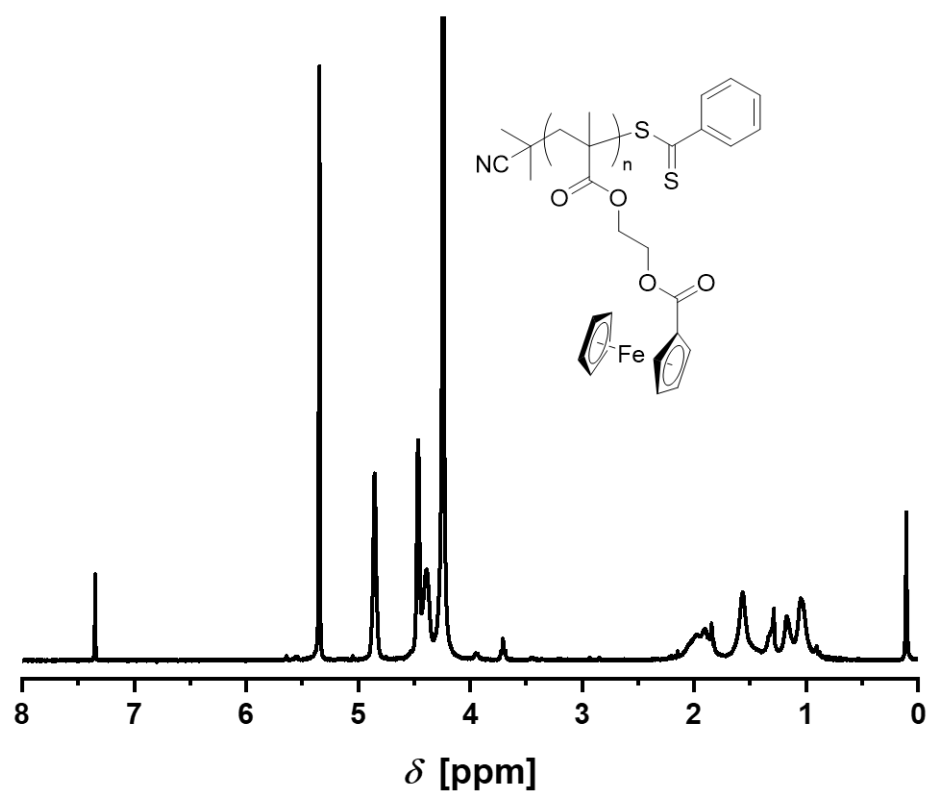


**Figure S5.**  $^1\text{H}$ -NMR spectra of  $\text{poly}(\text{Fc})$  (300 MHz, 25  $^\circ\text{C}$ ,  $\text{CD}_2\text{Cl}_2$ ).

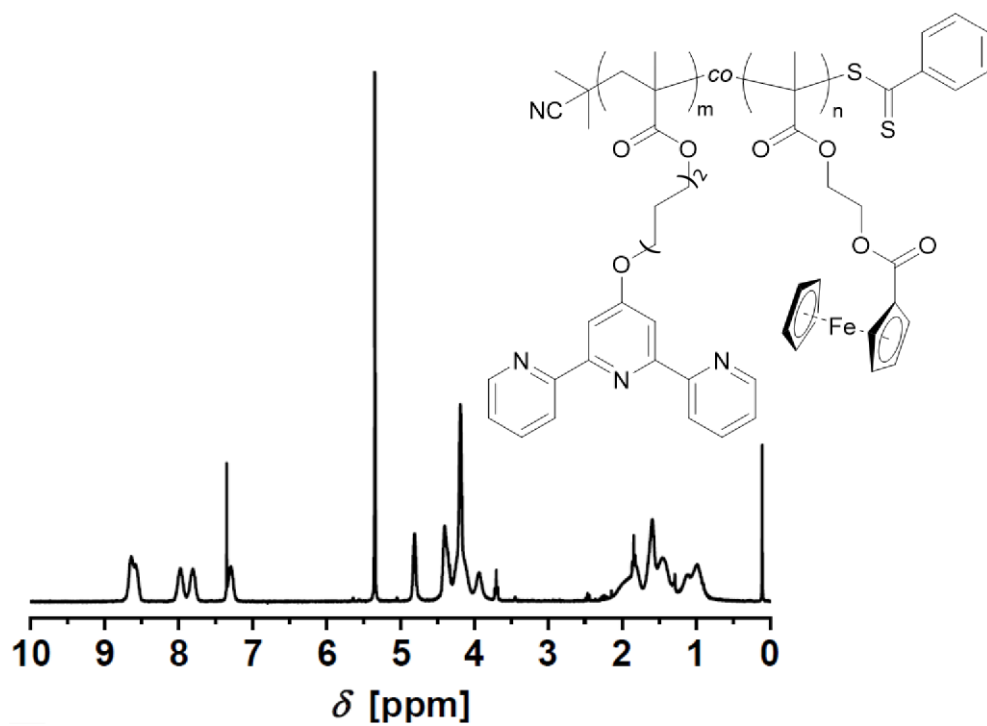


**Figure S6.**  $^1\text{H}$ -NMR spectra of  $(\text{Fc})\text{-co-}(\text{tpy})$  (300 MHz, 25  $^\circ\text{C}$ ,  $\text{CD}_2\text{Cl}_2$ ).

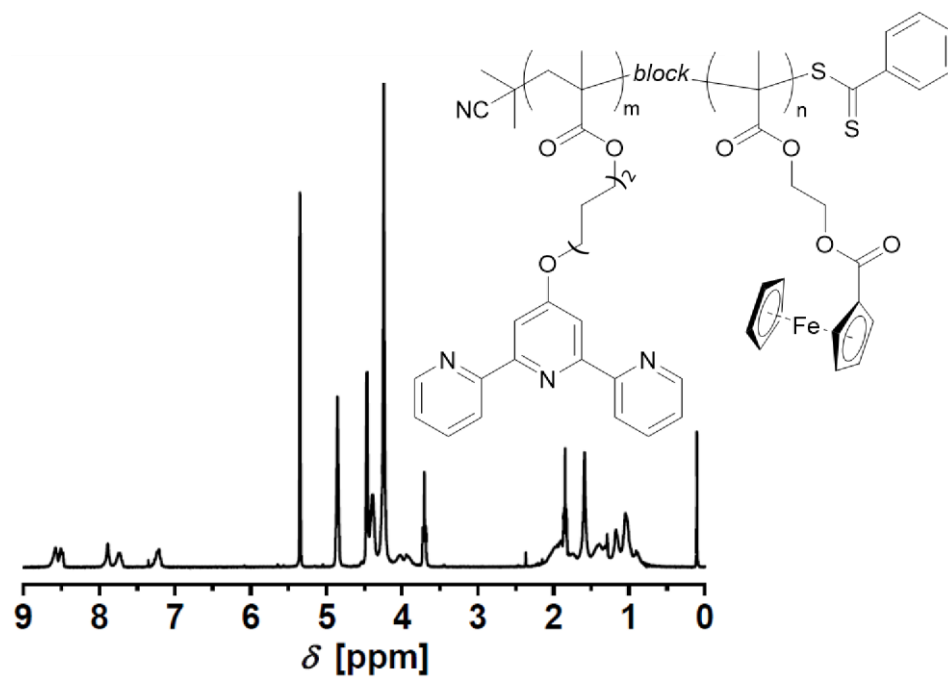


**Figure S7.**  $^1\text{H}$ -NMR spectra of (Fc)-bl-(tpy) (300 MHz, 25 °C,  $\text{CD}_2\text{Cl}_2$ ).

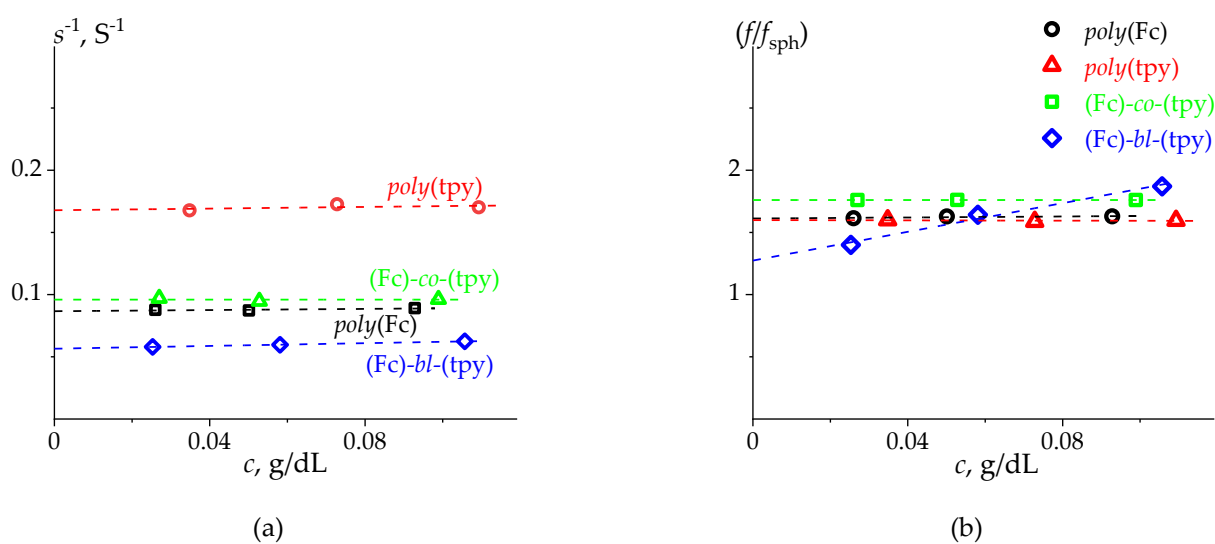


**Figure S8.** The concentration dependences of reciprocal sedimentation coefficients  $s^{-1}$  (a) and frictional ratios  $(f/f_{\text{sph}})$  values (b) resolved with Sedfit for all of the studied systems in THF solutions. All data were obtained at 20 °C.

**Table S3.** The initial DLS data: inverse relaxation times  $1/\tau$  vs. scattered vector squared  $q^2$  acquired for the studied systems at 20 °C.

| Sample            | Solvent | $c$ , g/dL | $1/\tau$ vs. $q^2$ |
|-------------------|---------|------------|--------------------|
| <i>poly</i> (Fc)  | THF     | 0.61       |                    |
|                   | Toluene | 0.71       |                    |
|                   | DMF     | 0.13       |                    |
| <i>poly</i> (tpy) | THF     | 0.28       |                    |
|                   | Toluene | 0.16       |                    |

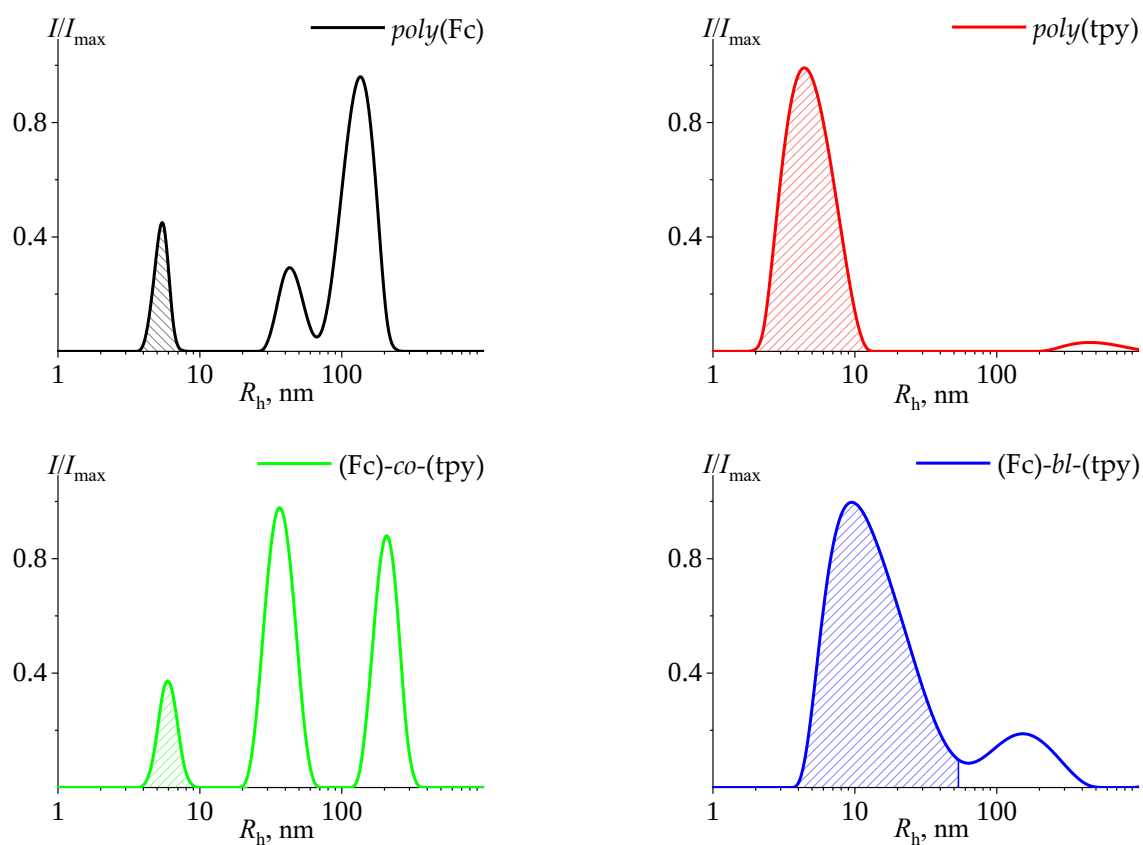
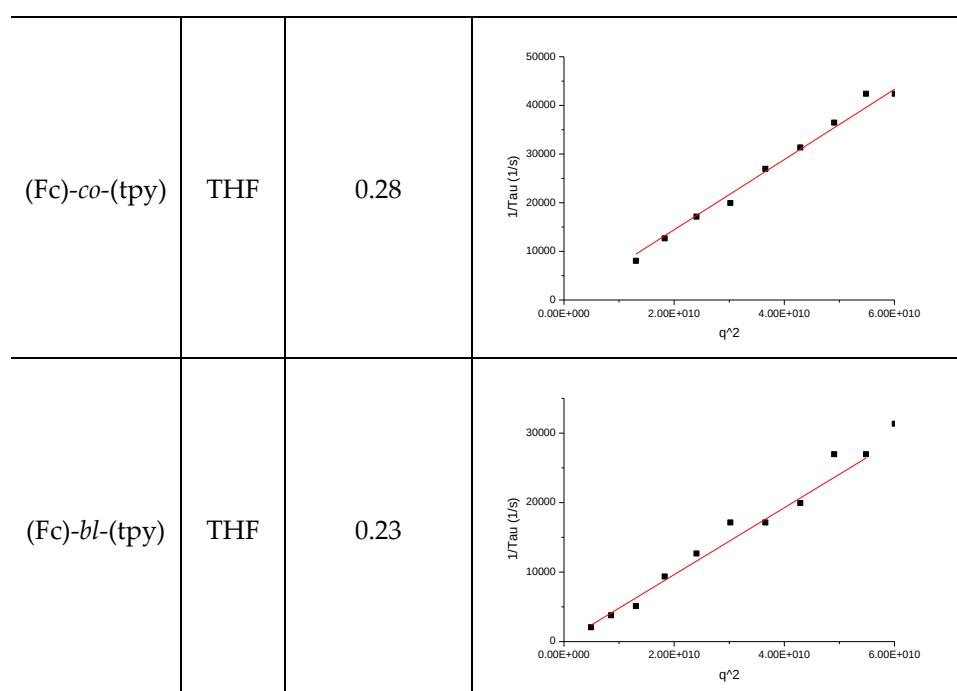


**Figure S9.** The normalized scattered light intensity distributions  $I/I_{max}$  over hydrodynamic radii  $R_h$  for the studied polymers and copolymers in THF solutions. All data were obtained at 20 °C. The diffusion coefficients at infinite dilution limit  $D_0$  are presented in Table 3.

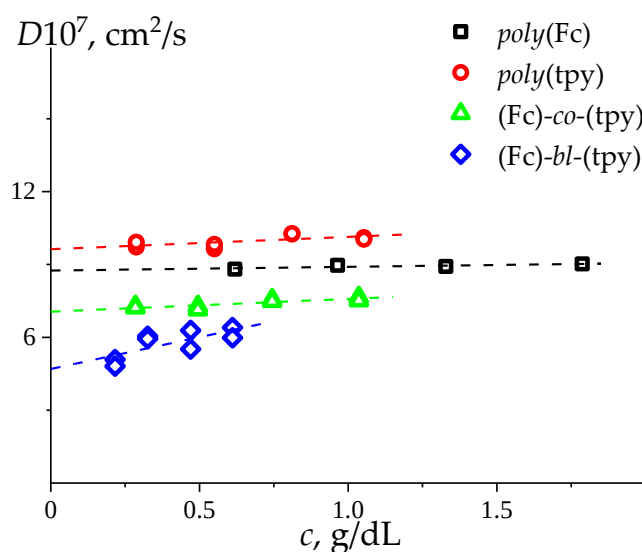


**Figure S10.** The concentration dependences of diffusion coefficients obtained for THF solutions of studied polymers and copolymers. All data were obtained at 20 °C.

## References

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