

A Candidate for Multitopic Probes for Ligand Discovery in Dynamic Combinatorial Chemistry

Keiko Yoneyama, Rina Suzuki, Yusuke Kuramochi, and Akiharu Satake

GPC charts

Column: TOSOH TSKgel
(G2000H_{HR}+ G2500H_{HR} × 2)
Eluent: pyridine
Flow rate: 1.0 mL/min
Detection: 565 nm
Injection: 10 µL

Size exclusion

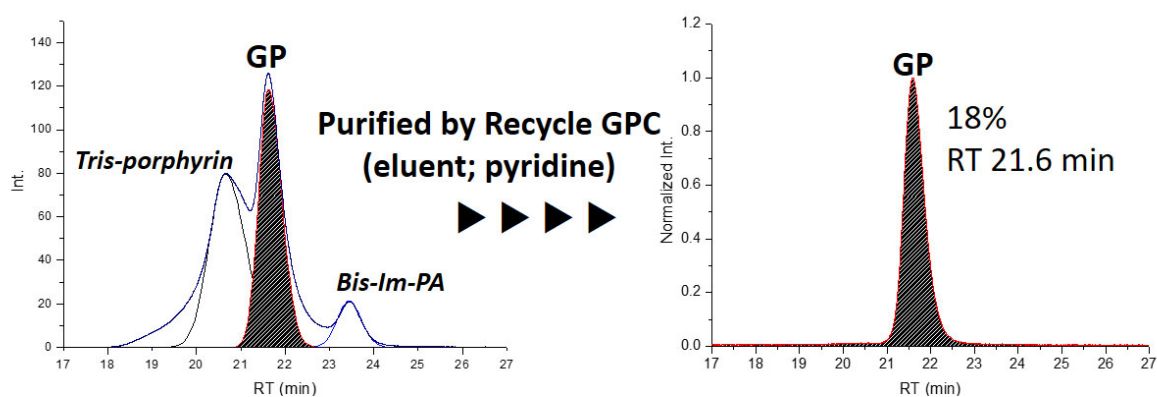


Figure S1. Analytical gel permeation chromatography (GPC) charts of **GP1Fb**. (left: a crude sample, right: purified)

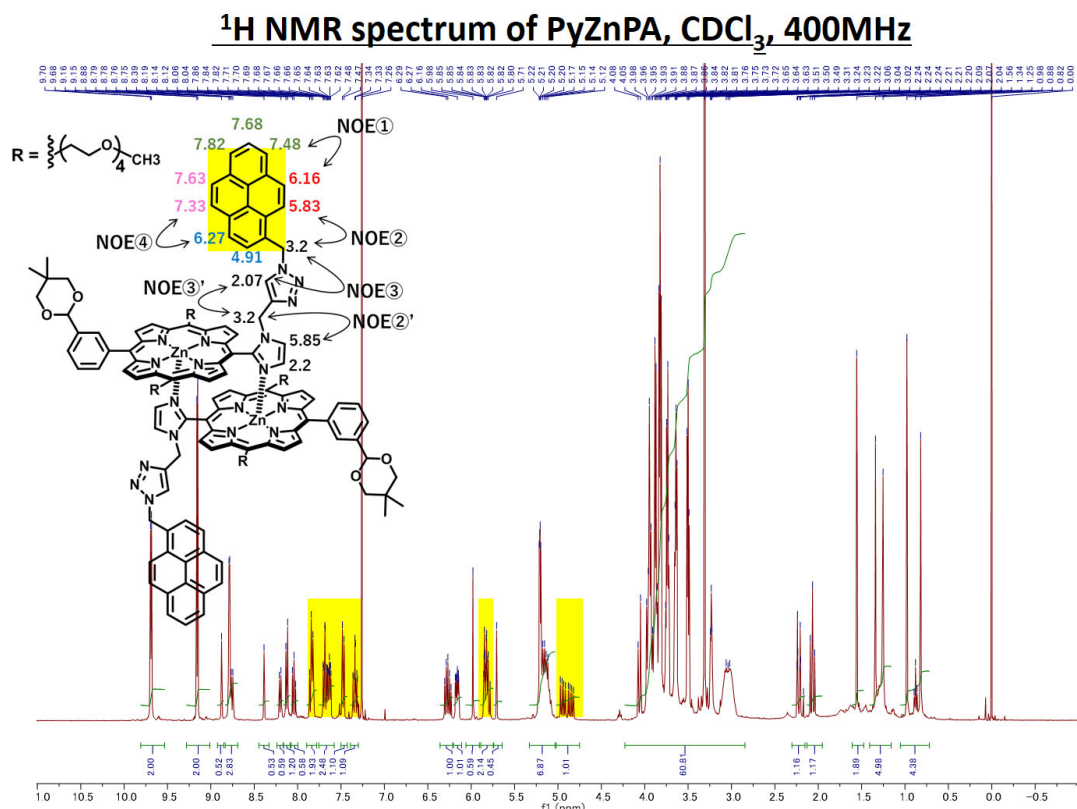


Figure S2. ^1H NMR spectrum (400 MHz, CDCl_3) of **PY-5Zn**

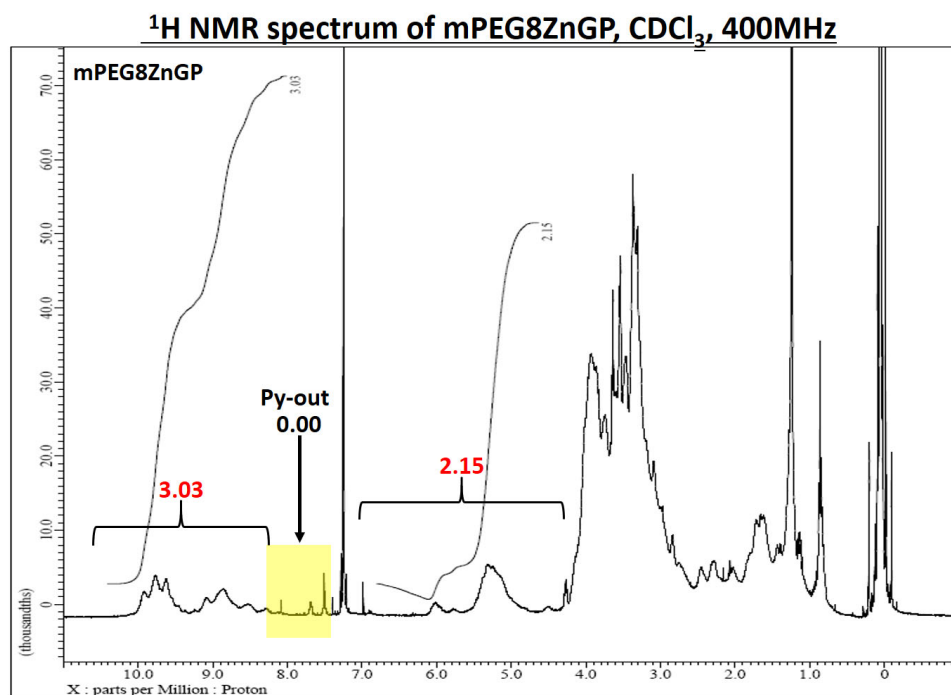


Figure S3. ^1H NMR spectrum (400 MHz, CDCl_3) of **PEG8-GP1**

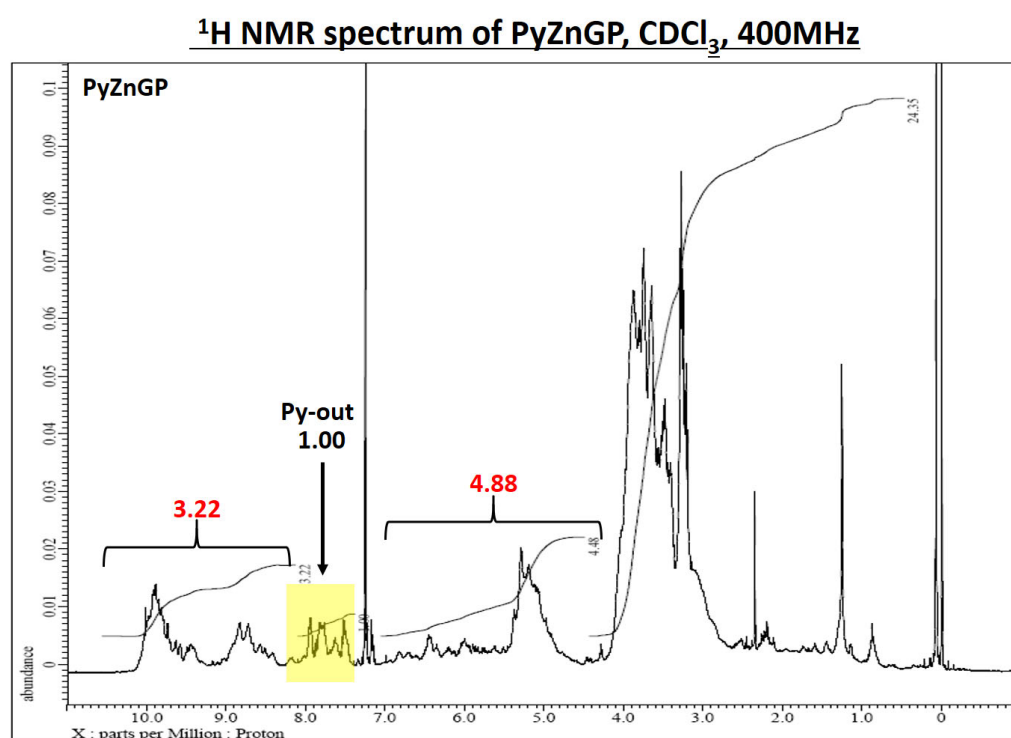


Figure S4. ^1H NMR spectrum (400 MHz, CDCl_3) of **PY-GP1**

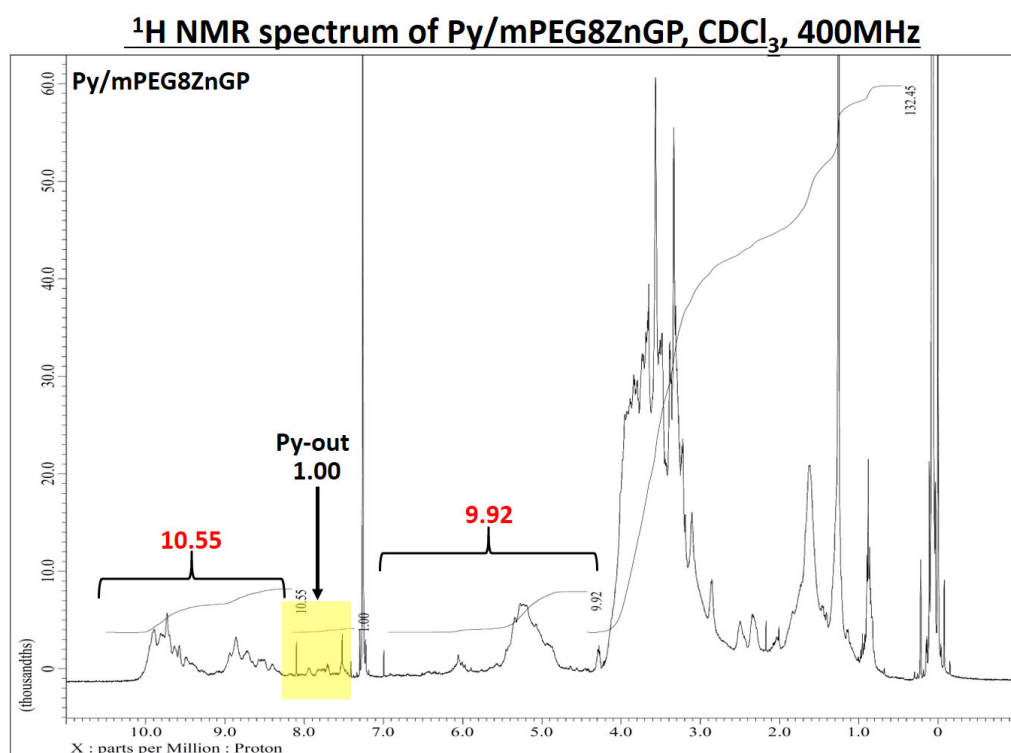


Figure S5. ^1H NMR spectrum (400 MHz, CDCl_3) of a reconstituted sample of **PEG8-GP 1** and **PY-GP 1** (1:1)

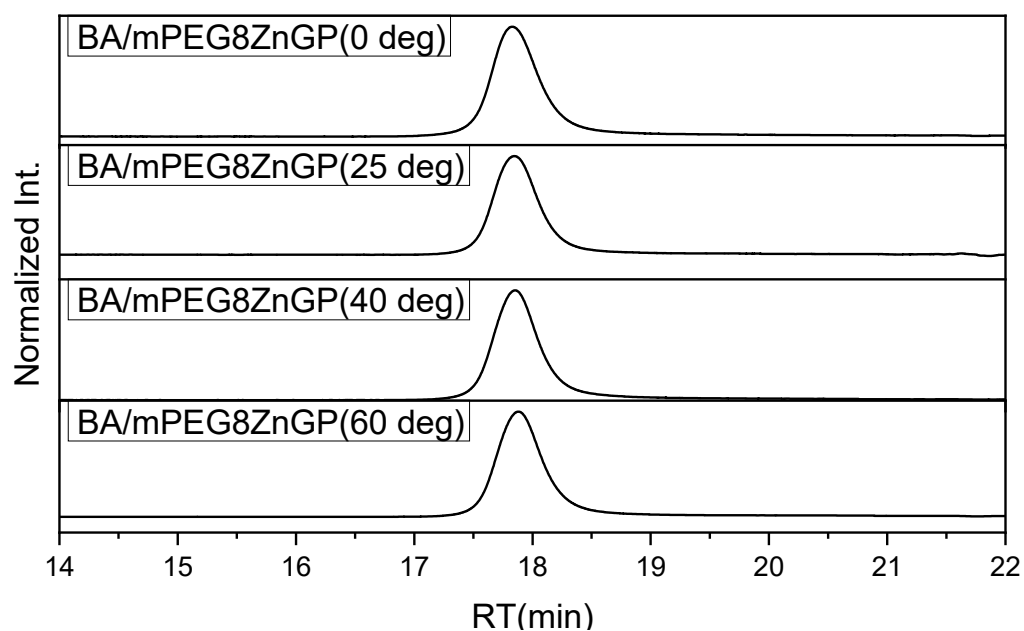


Figure S6. GPC charts of reconstituted samples of 1:1 mixture of **BA-GP1** and **PEG8-GP1**. The reconstituted temperatures are (a) 0 °C, (b) 25 °C, (c) 40 °C, and (d) 60 °C. (from top to bottom) Little change was observed among them. (column; TOSOH TSKgel G4000H_{HR}×2 (exclusion limit; 400,000 Da), eluent; CHCl₃:THF=95:5, flow rate; 1.0 mL/min, detection; 565 nm).

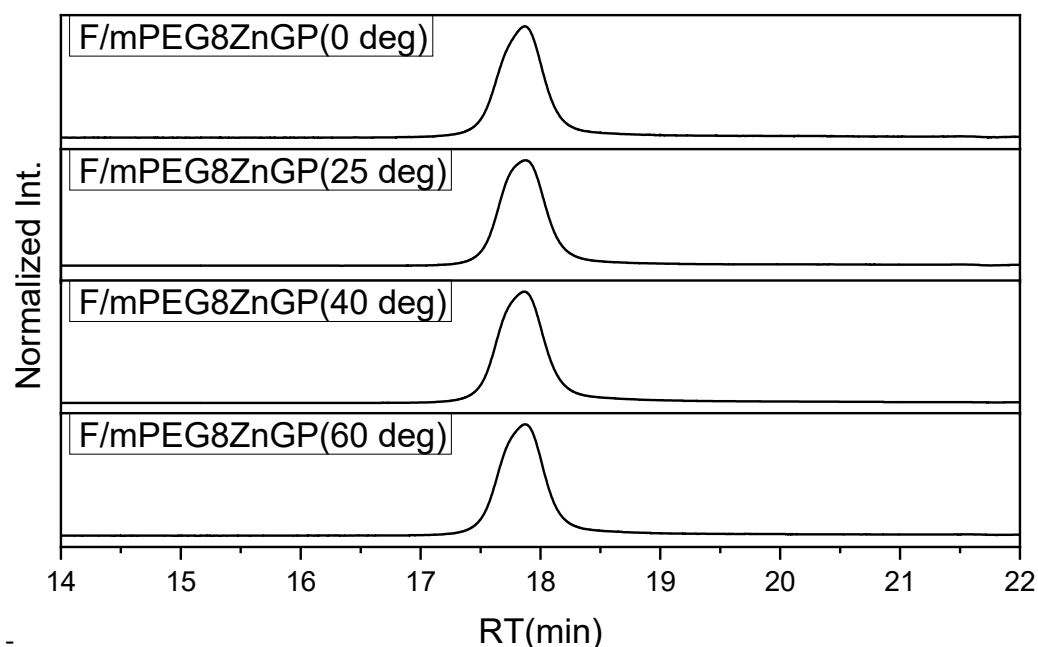


Figure S7. GPC charts of reconstituted samples of 1:1 mixture of **F9-GP1** and **PEG8-GP1**. The reconstituted temperatures are (a) 0 °C, (b) 25 °C, (c) 40 °C, and (d) 60 °C. (from top to bottom) Little change was observed among them. (column; TOSOH TSKgel G4000H_{HR}×2 (exclusion limit; 400,000 Da), eluent; CHCl₃:THF=95:5, flow rate; 1.0 mL/min, detection; 565 nm).

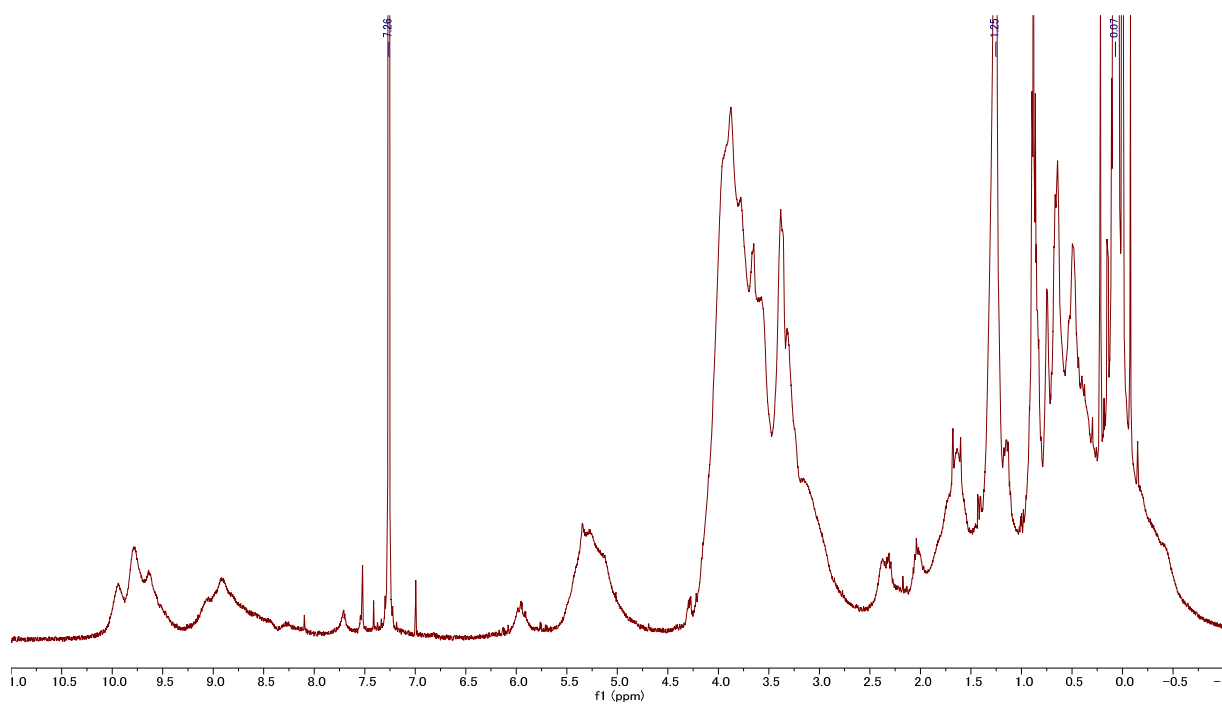


Figure S8. ^1H NMR spectrum (400 MHz, CDCl_3) of a reorganized sample of **BA-GP1**.

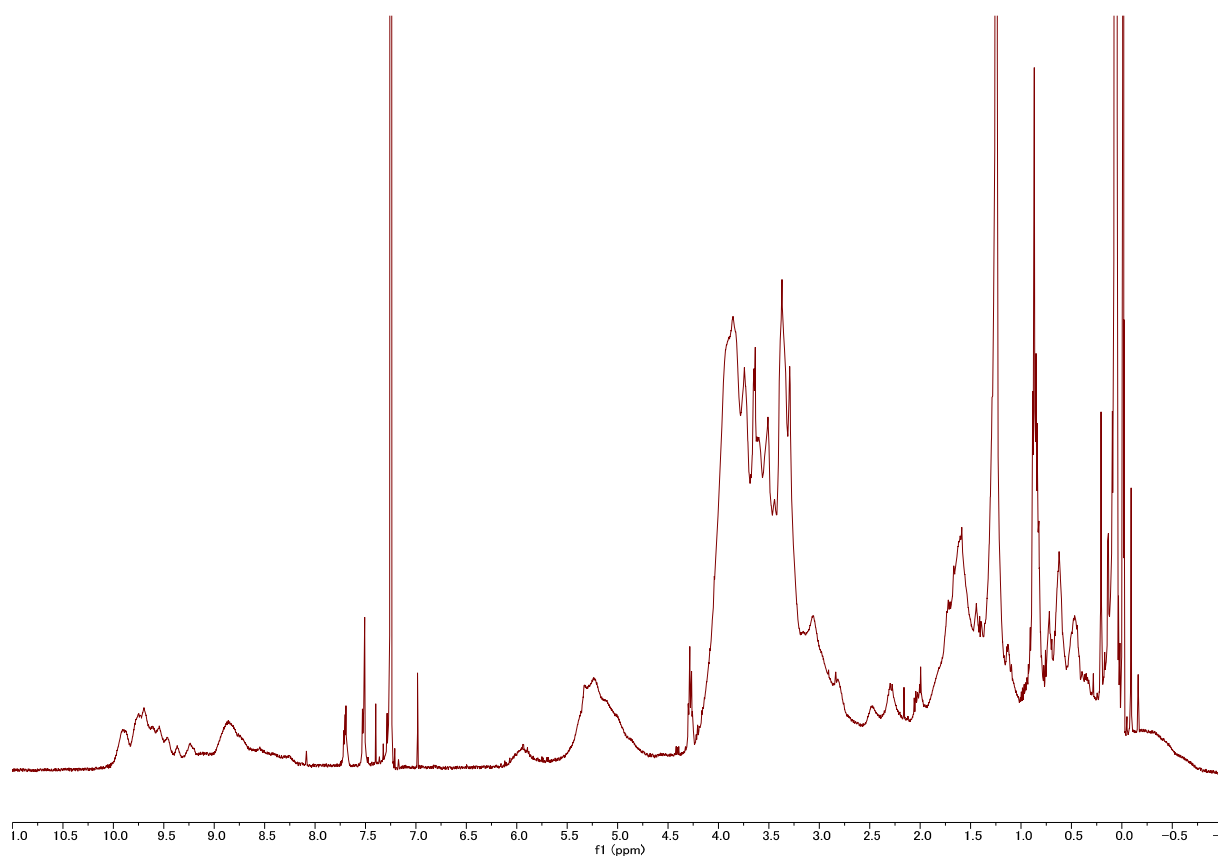


Figure S9. ^1H NMR spectrum (400 MHz, CDCl_3) of a reconstituted sample of **PEG8-GP1** and **BA-GP1** (1:1)

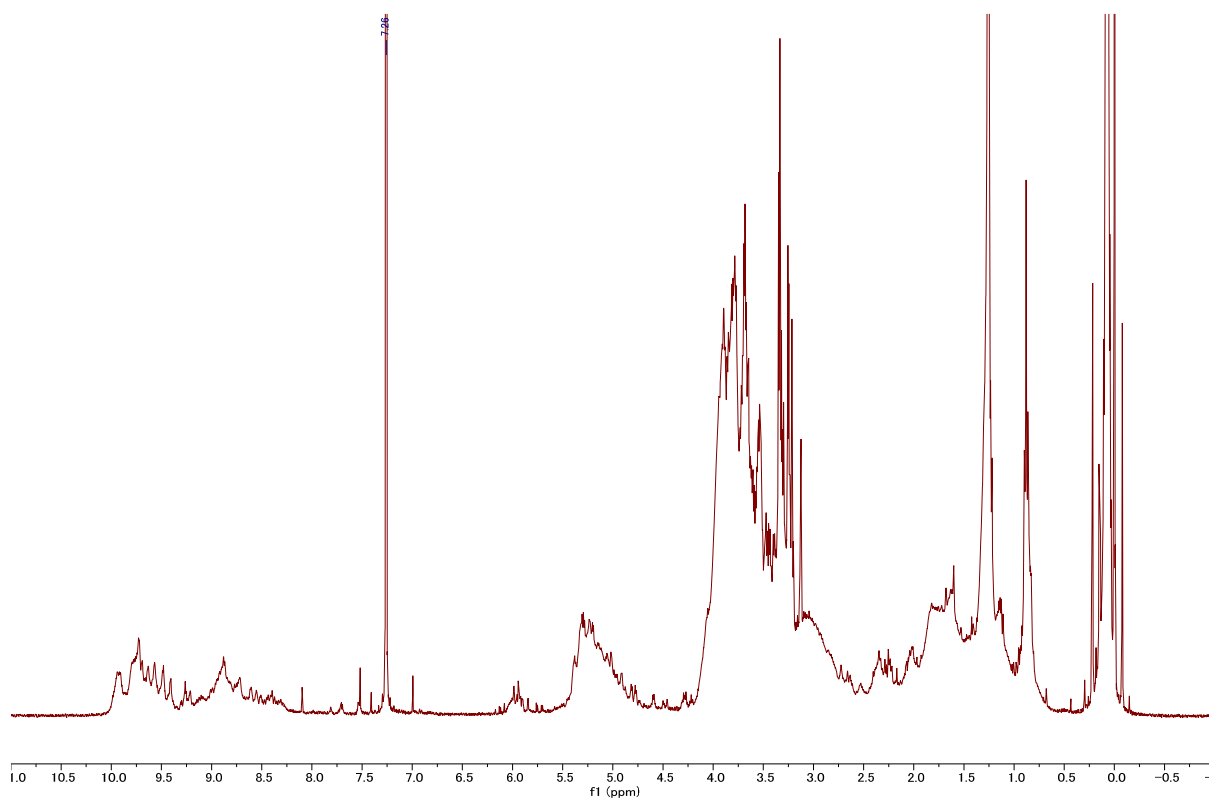


Figure S10. ^1H NMR spectrum (400 MHz, CDCl_3) of a reorganized sample of **F9-GP1**.

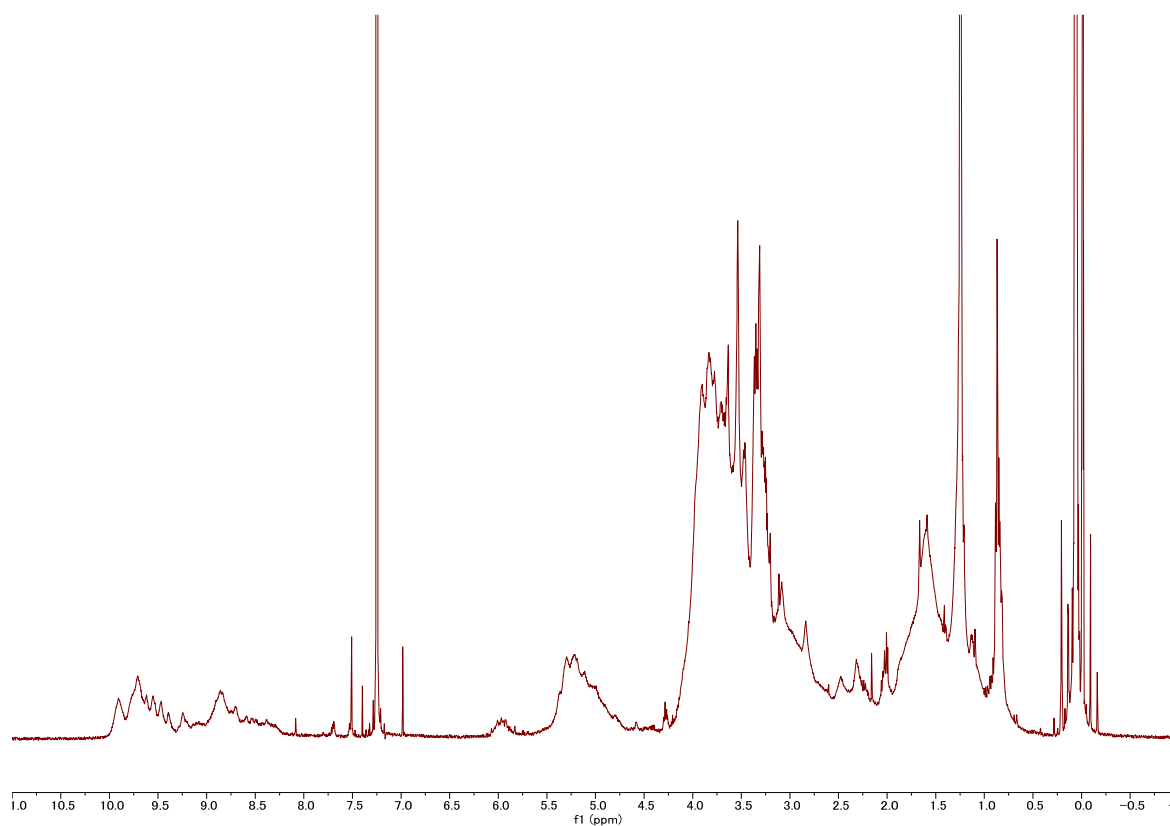


Figure S11. ^1H NMR spectrum (400 MHz, CDCl_3) of a reconstituted sample of **PEG8-GP1** and **F9-GP1** (1:1).