Electronic Supplementary Information

Synthesis and Optoelectronic Properties of Air-stable π-Conjugated Polymers Containing Both Thiophene-2,5-diyl and Fused Titanacycle Units

Alvin Tanudjaja, Makoto Higuchi, Tomohiro Imai, Yoshimasa Matsumura, Ryoyu Hifumi, Shinsuke Inagi, and Ikuyoshi Tomita*

Department of Chemical Science and Engineering, School of Materials and Chemical

Technology, Tokyo Institute of Technology, Nagatsuta-cho 4259-G1-9, Midori-ku, Yokohama

226-8502, Japan

E-mail: tomita@cap.mac.titech.ac.jp

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1. NMR Spectra

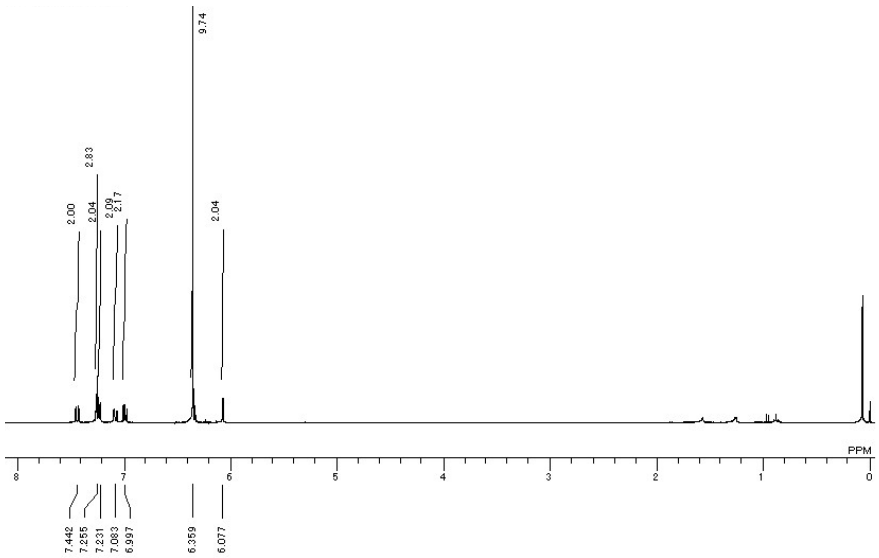

Figure S1. ^{1}H NMR spectrum of **4**.

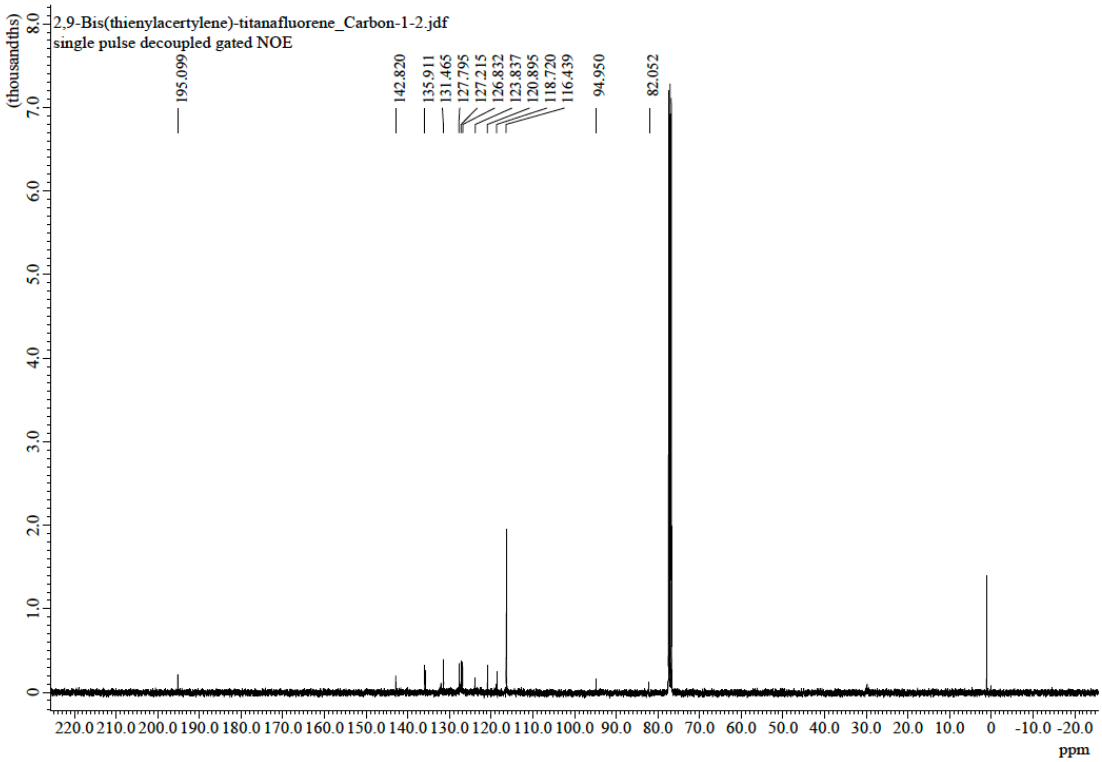

Figure S2. ^{13}C{^{1}H}NMR spectrum of **4**.

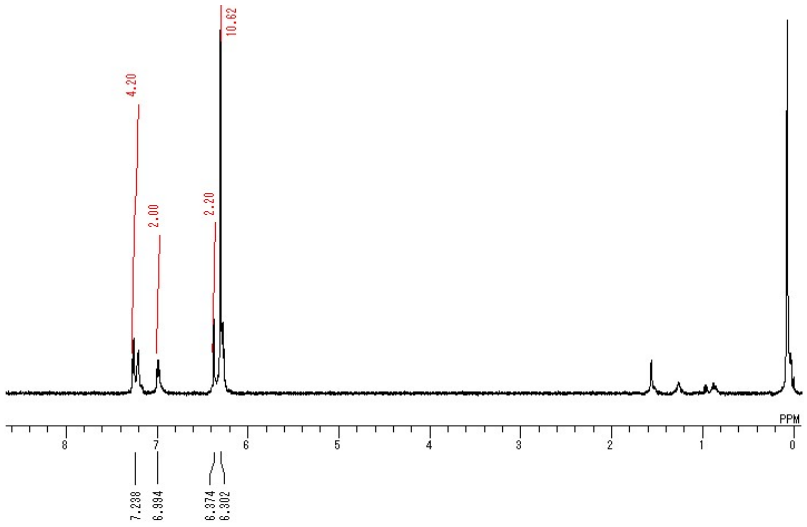

Figure S3. ^{1}H NMR spectrum of **5**.

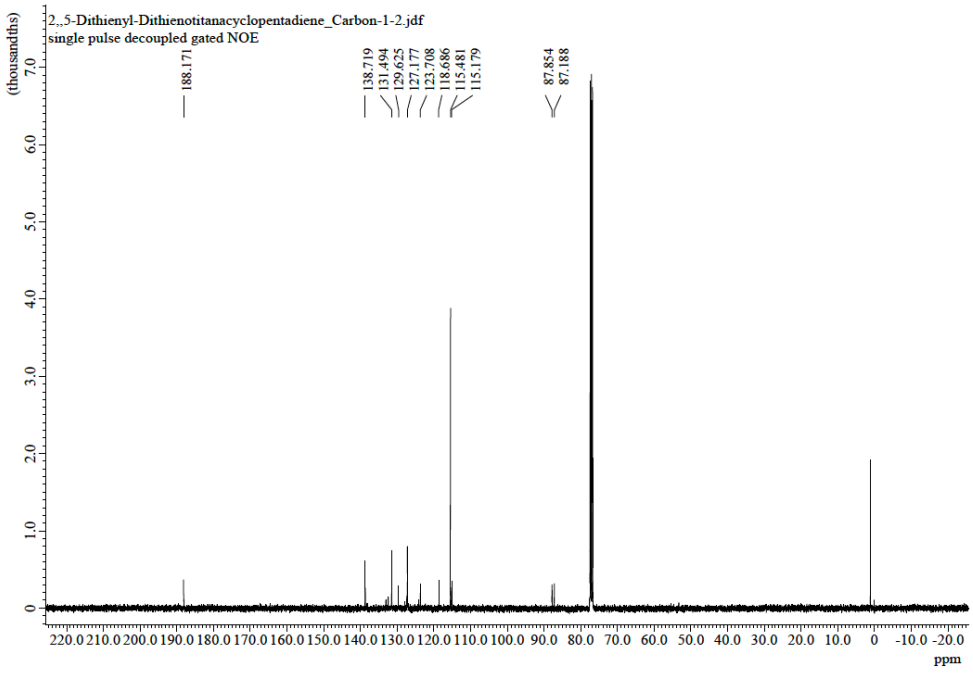

Figure S4. ^{13}C{^{1}H} NMR spectrum of **5**.

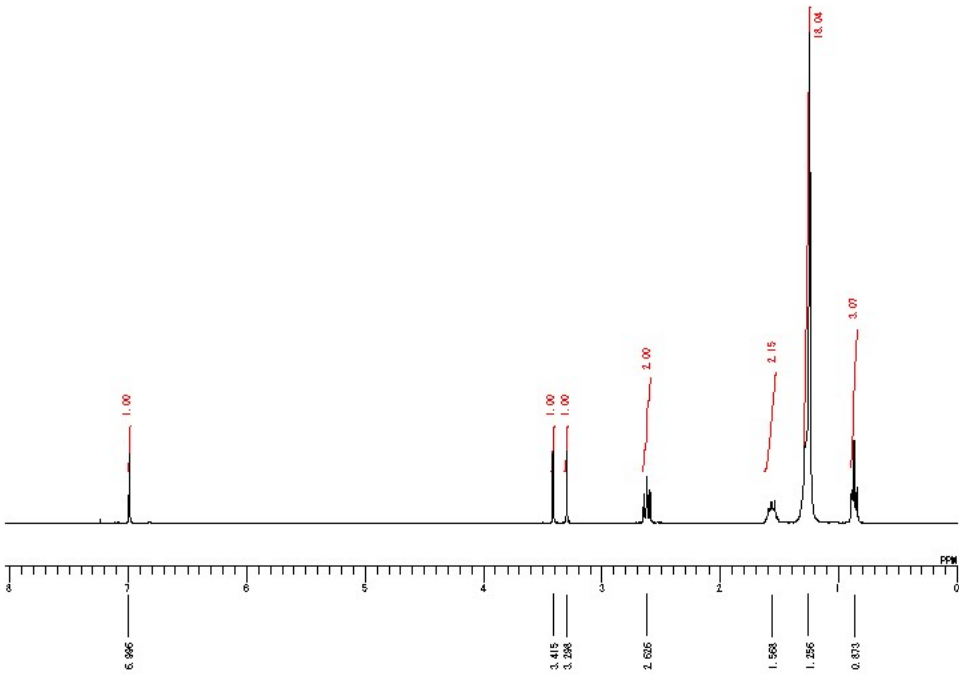

Figure S5. ^{1}H NMR spectrum of **6**.

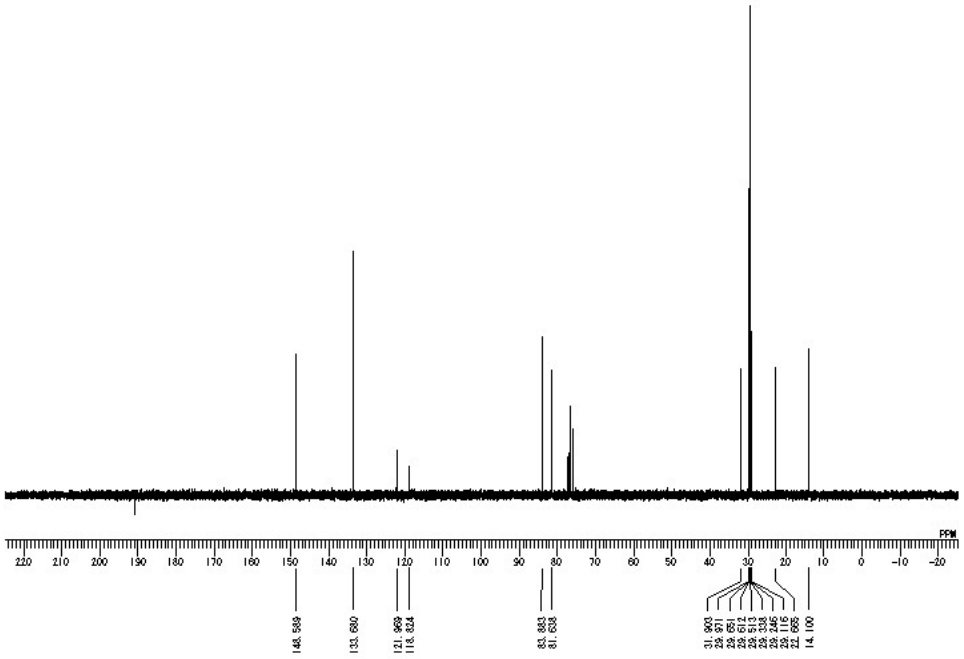

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **6**.

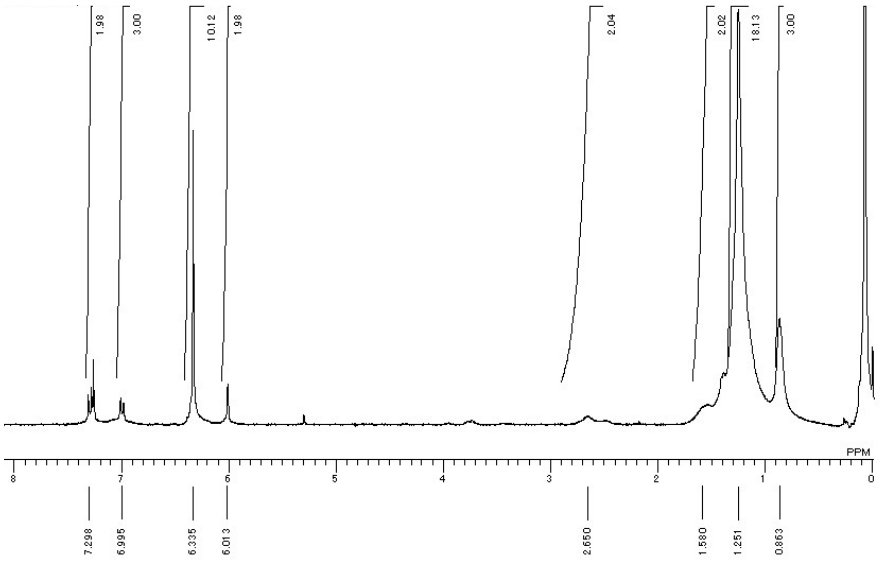

Figure S7. ^{1}H NMR spectrum of **7**.

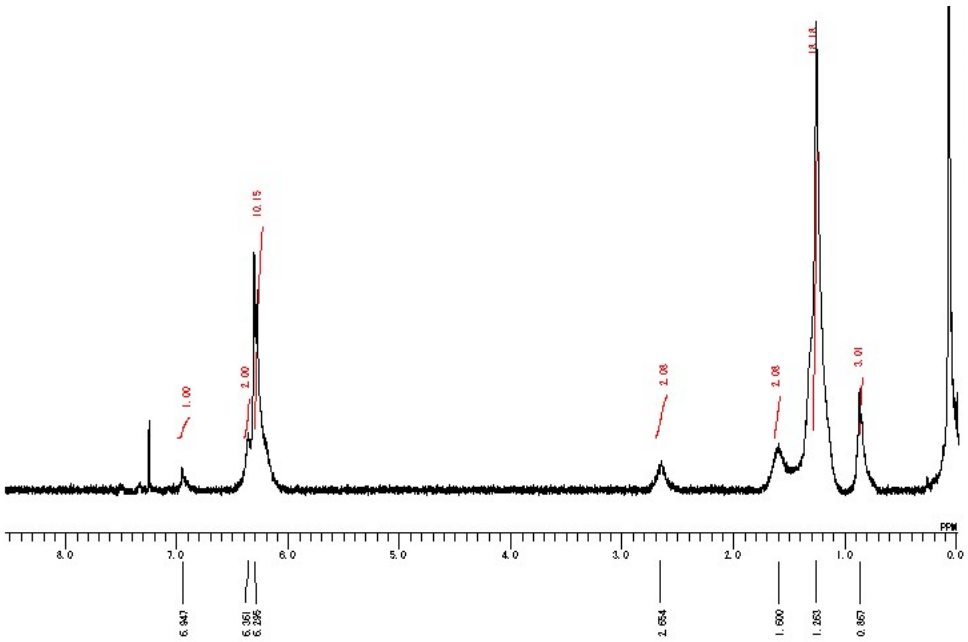

Figure S8. ^{1}H NMR spectrum of **8**.

2. IR Spectra

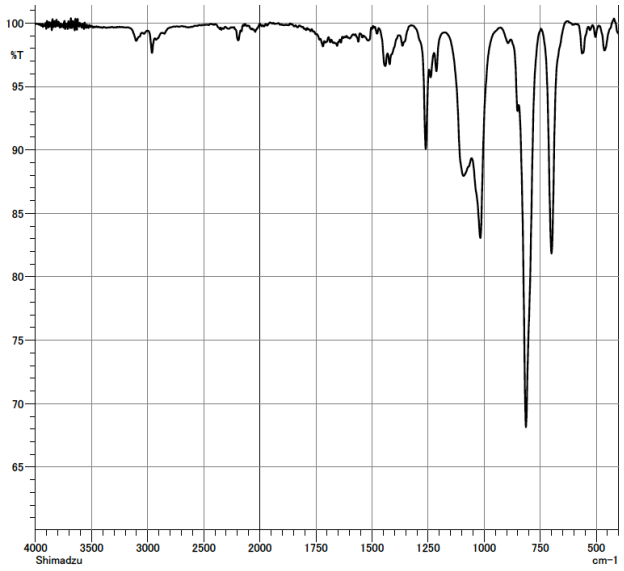

Figure S9. IR Spectrum of **4**.

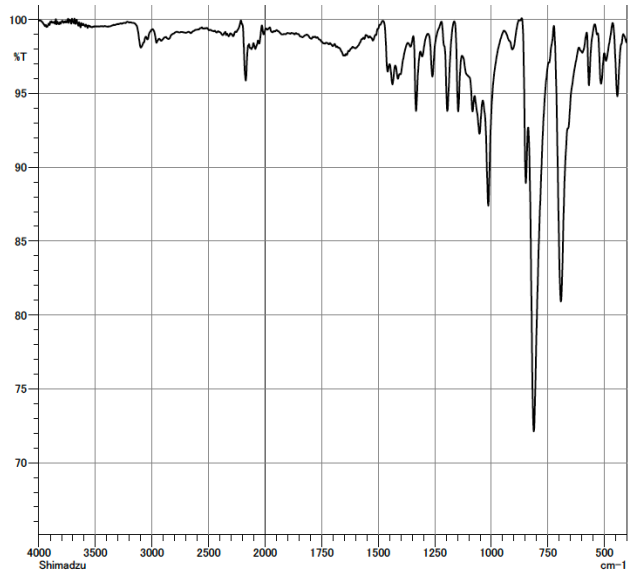

Figure S10. IR Spectrum of **5**.

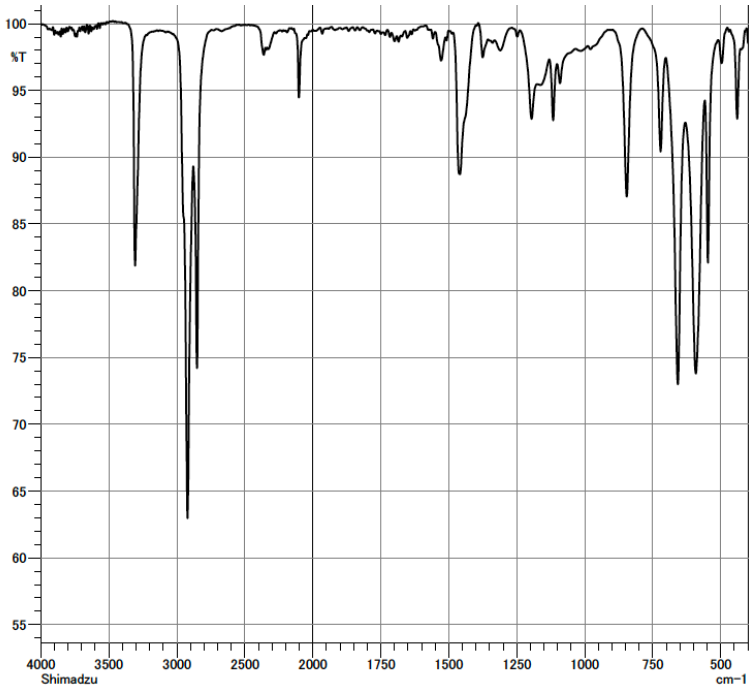

Figure S11. IR Spectrum of **6**.

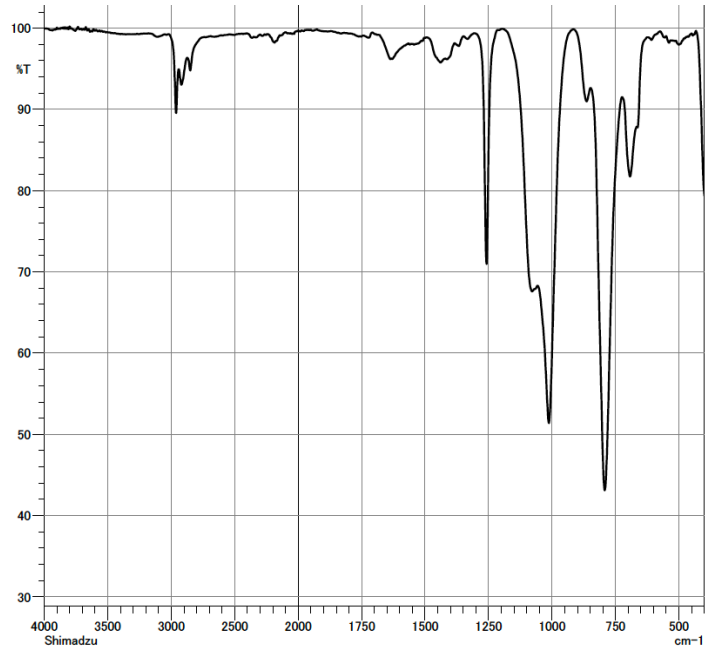

Figure S12. IR Spectrum of **7**.

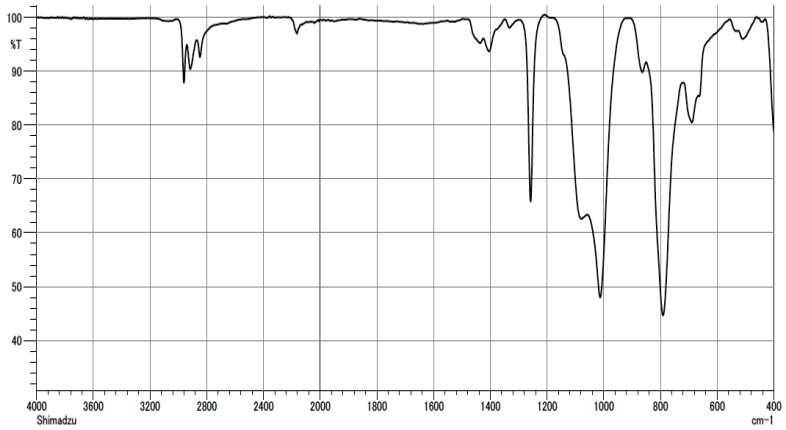

Figure S13. IR Spectrum of **8**.

3. Size Exclusion Chromatographic (SEC) Profiles

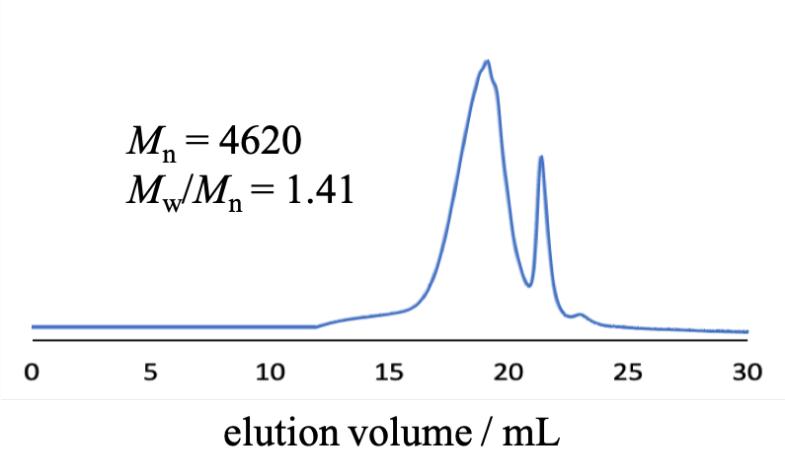

Figure S14. SEC profile of **7** after precipitation into ethanol/ethyl acetate (v/v = 9/1).

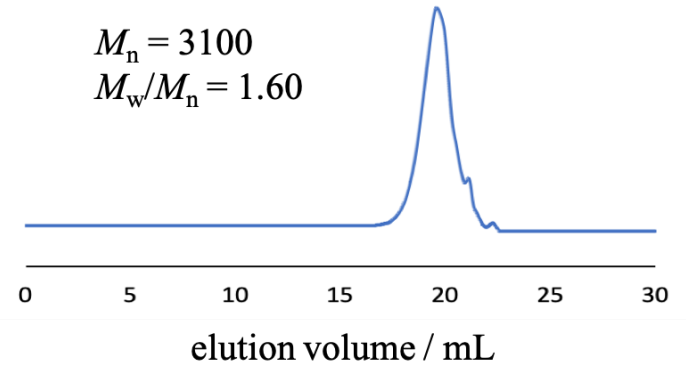

Figure S15. SEC profile of **8** after precipitation into ethanol/ethyl acetate (v/v = 9/1).

4. DFT and TD-DFT Optimized Molecular Diagrams

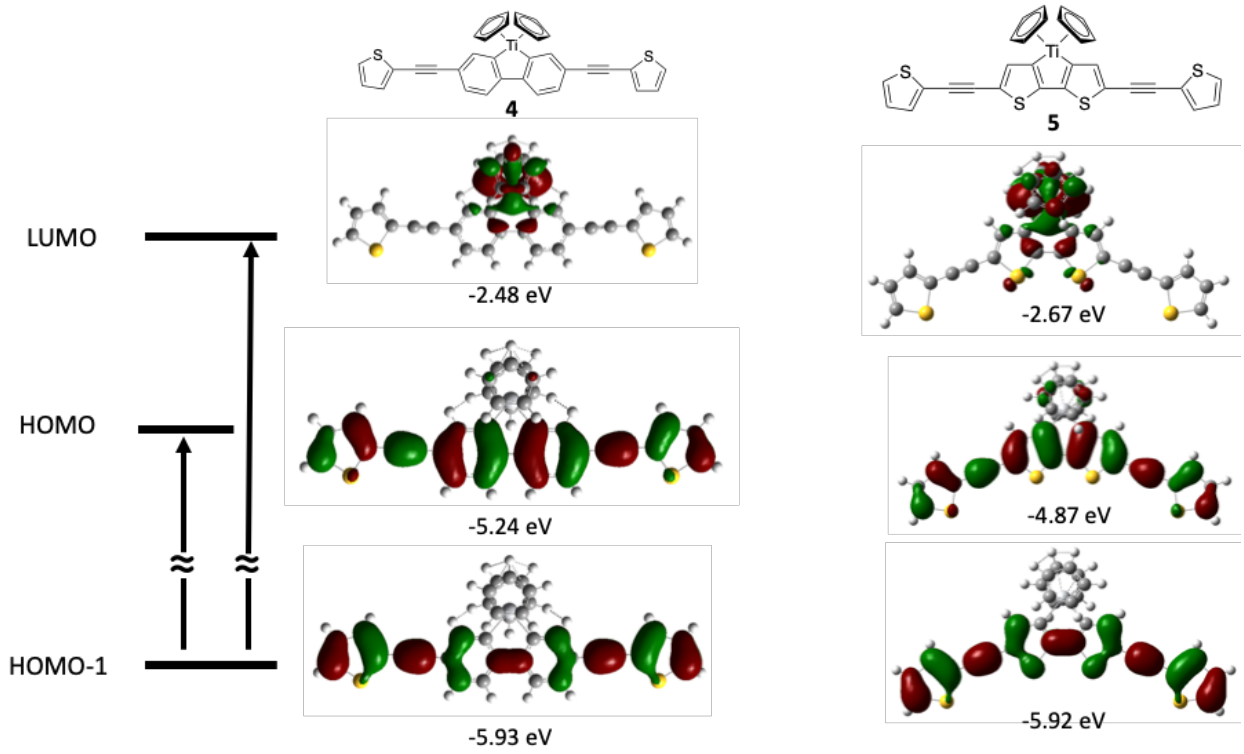

Figure S16. Energy profiles and molecular orbital diagrams of HOMO-1**,** HOMO, and LUMO of **4** and **5**.

Table S1. HOMO to LUMO and HOMO-1 to LUMO transitions by TD-DFT calculations.

Assignment	**4**		**5**	
	HOMO-1 to LUMO	HOMO to LUMO	HOMO-1 to LUMO	HOMO to LUMO
λ_{max} (nm) [a)]	446.06	570.99	766.85	939.12
f [b)]	0.0499	0.0219	0.0058	0.0085
Excitation energy (eV)	2.7795	2.714	1.6168	1.3202

a) Calculated absorption maximum in the UV-vis spectrum. b) Oscillator strength.