

Supplementary Information

Diketopyrrolopyrrole-based semiconducting polymer bearing thermocleavable side chains

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Supplementary Information

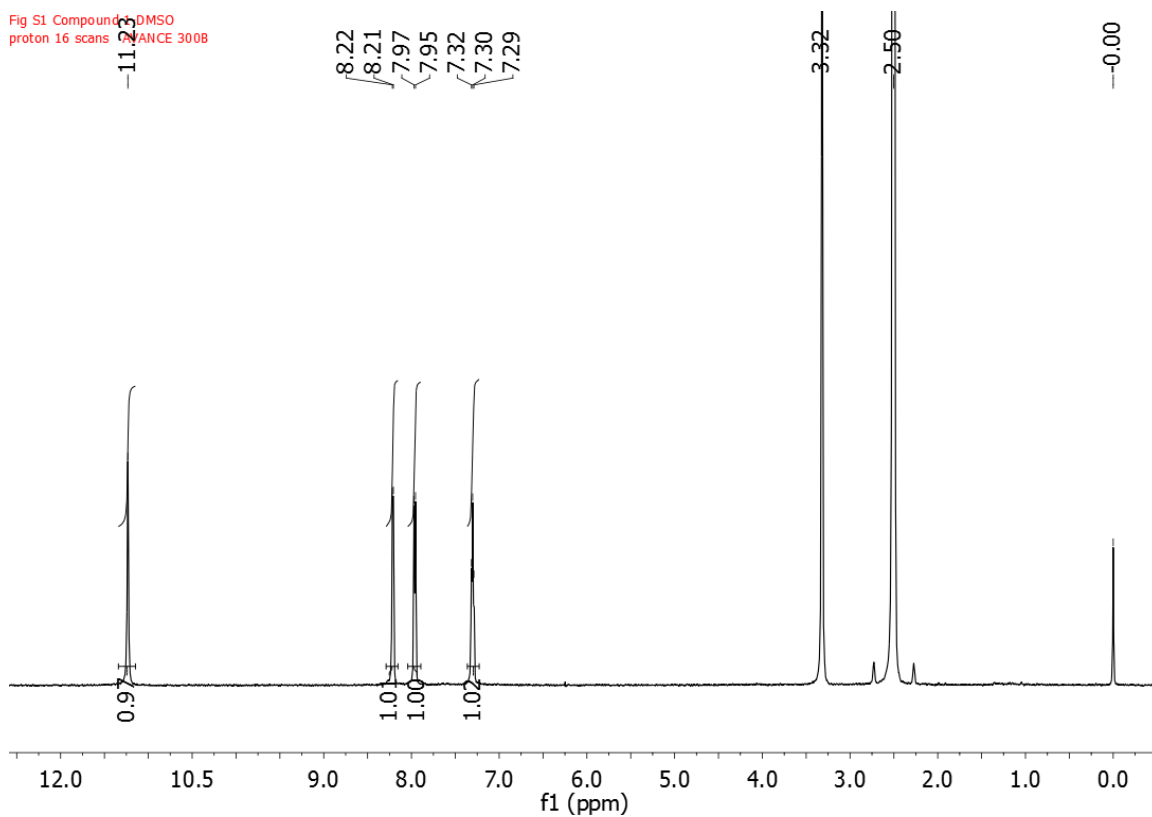


Figure S1. 300 MHz ^1H NMR spectrum of 2,5-dihydro-3,6-di-2-thienyl-pyrrolo[3,4-*c*]pyrrole-1,4-dione (1) in DMSO-*d*₆.

Supplementary Information

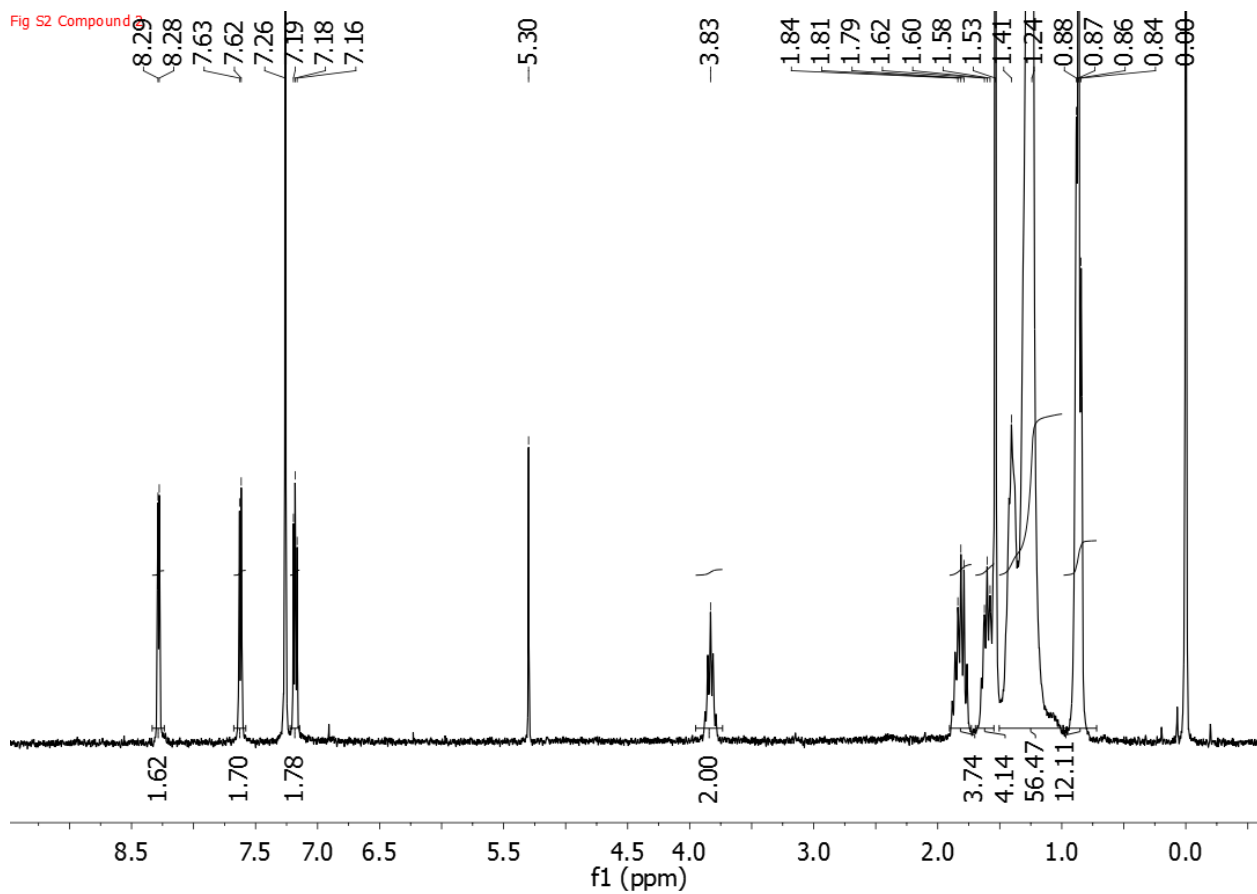


Fig. S2. 300 MHz ^1H NMR spectrum of 2,5-bis(2-octyldodecanoyl)-3,6-di(thiophen-2-yl)pyrrolo[3,4-*c*]pyrrole-1,4(2*H*,5*H*)-dione (**2**) in CDCl_3 .

Supplementary Information

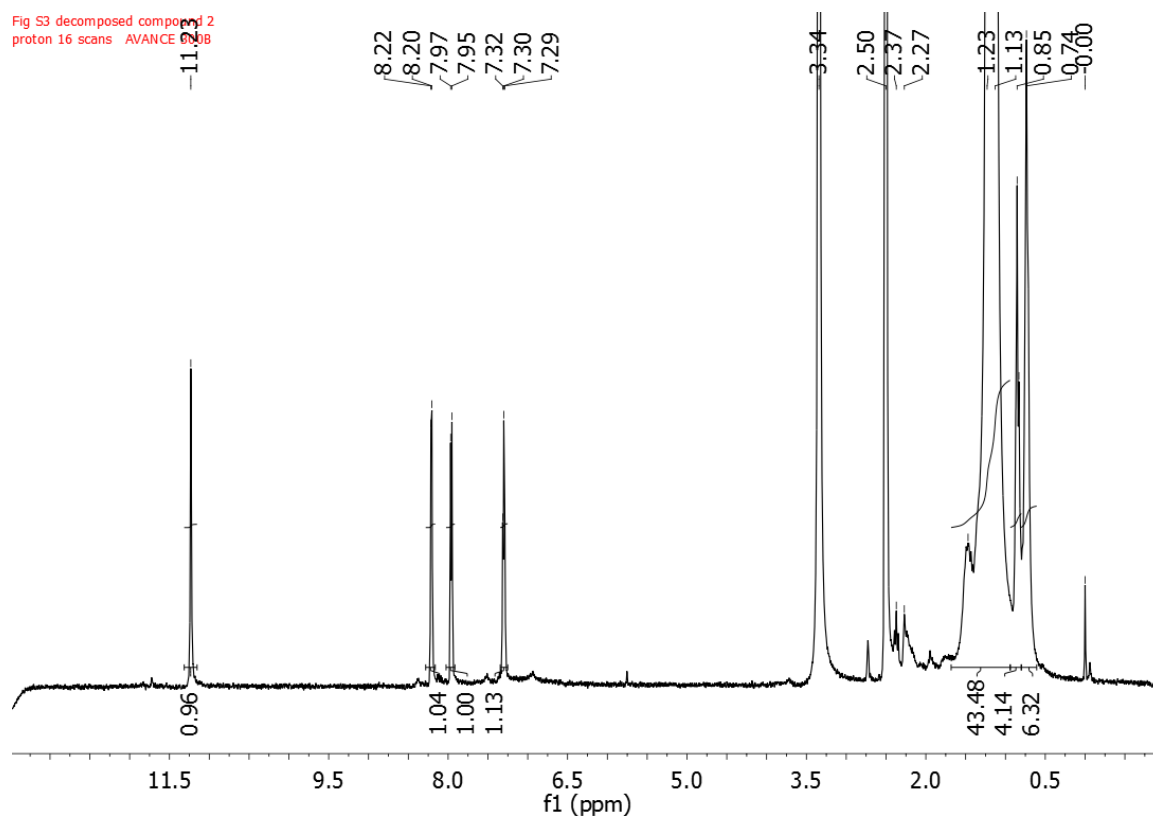


Fig. 3. 300 MHz ^1H NMR of the mixture of the decomposed compound **2** at 250 °C for 20 min measured in DMSO- d_6 . It can be clearly seen that the aromatic peaks of compound **2** disappeared completely and the aromatic peaks corresponding to those of compound **1** appeared.

Supplementary Information

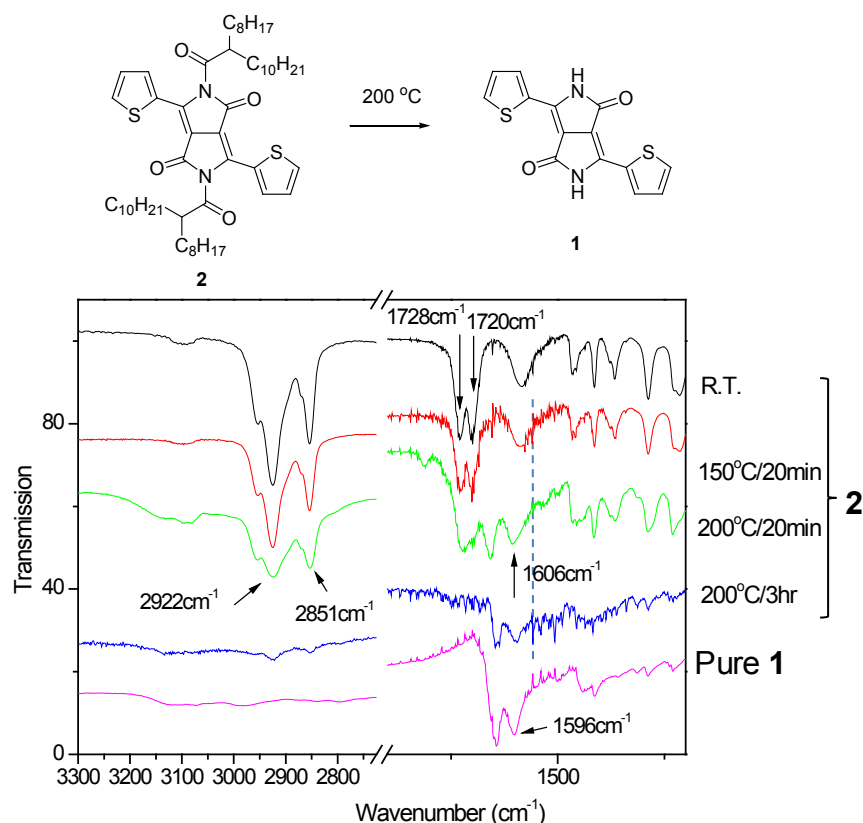


Fig. S4 Top: The proposed thermal decomposition reaction of compound **2** to form compound **1**. Bottom: FT-IR spectra of pure compound **1** on a KBr substrate and compound **2** films on Si wafer substrates annealed at different temperatures in nitrogen. The intense peaks at 2922 cm⁻¹ and 2851 cm⁻¹ of the non-annealed **2** originate from the stretching vibrations of the side chain C-H bonds, which decreased significantly after heating at 200 °C for 3 hr. The peaks at 1728 and 1720 cm⁻¹ are from the stretching vibrations of the C=O groups on the 2-octyldodecanoyl substituents of compound **2**, which disappeared after heating at 200 °C for 3 hr. The new peak appeared at 1596 cm⁻¹ in the thin film annealed at 200 °C for 3 hr is due to the bending of the N-H groups of the recovered compound **1**. The spectrum of the sample annealed at 200 °C for 3 hr resembles the one of the pure compound **1**, indicating that compound **2** was thermally decomposed to form compound **1**.

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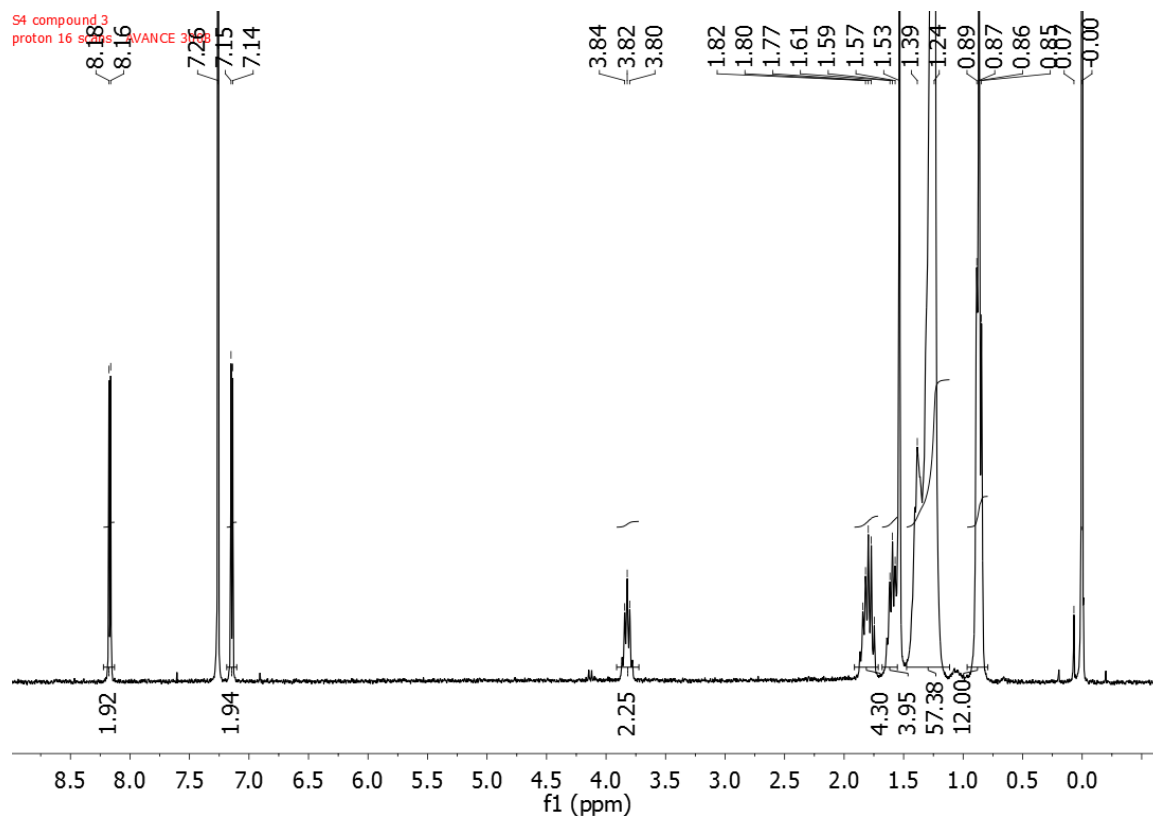


Fig. S5. 300 MHz ^1H NMR spectrum of 3,6-bis(5-bromothiophen-2-yl)-2,5-bis(2-octyldodecanoyl)pyrrolo[3,4-c]pyrrole-1,4(2*H*,5*H*)-dione (**3**) in CDCl_3 .

Supplementary Information

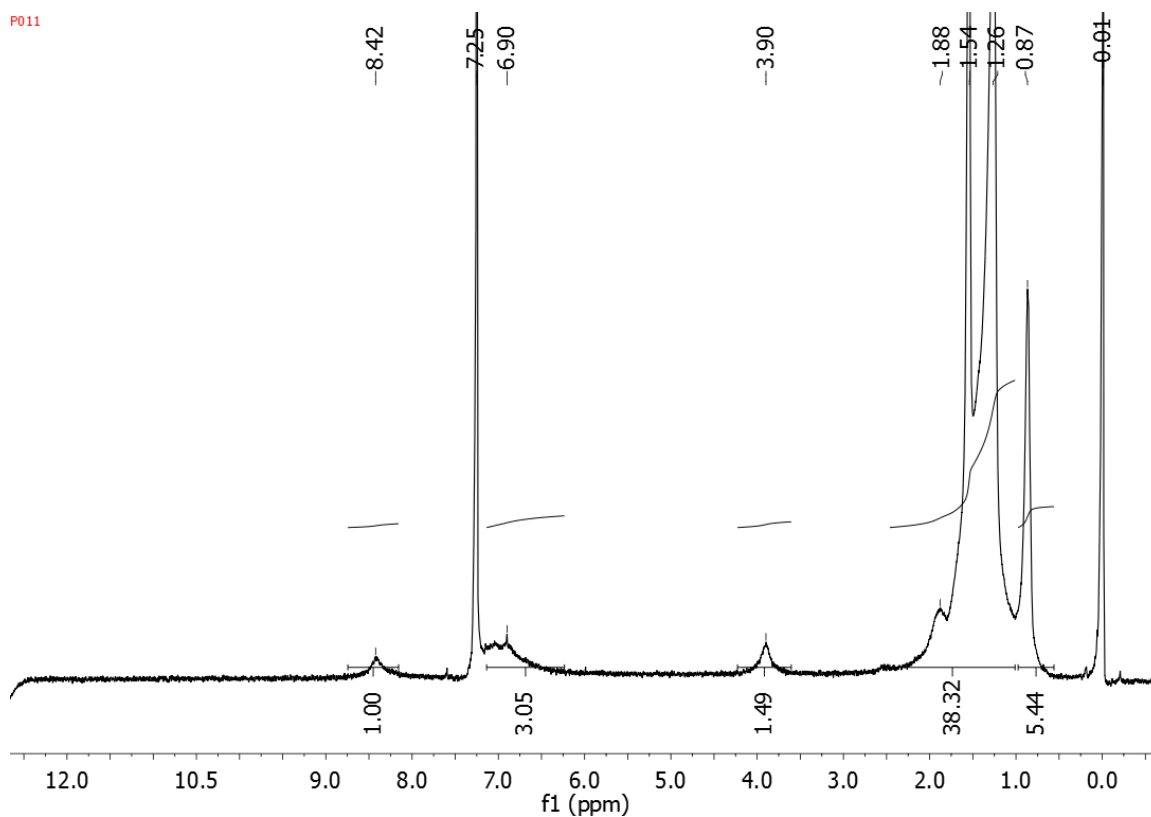


Fig. S6. 300 MHz ^1H NMR spectrum of **PDQT-tc** in CDCl_3 .

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SAMPLE INFORMATION

Sample Name:	P011	Acquired By:	PHOT
Sample Type:	Broad Unknown	Sample Set Name:	june 11
Vial:	2	Acq. Method Set:	Zhao April15
Injection #:	1	Processing Method:	ClBenzAug25_2011
Injection Volume:	50.00 ul	Channel Name:	410
Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	
Date Acquired:	6/11/2012 10:50:11 AM EDT		
Date Processed:	6/11/2012 12:11:05 PM EDT		

GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		24344	95014	75323	431356	1514513		3.902967		

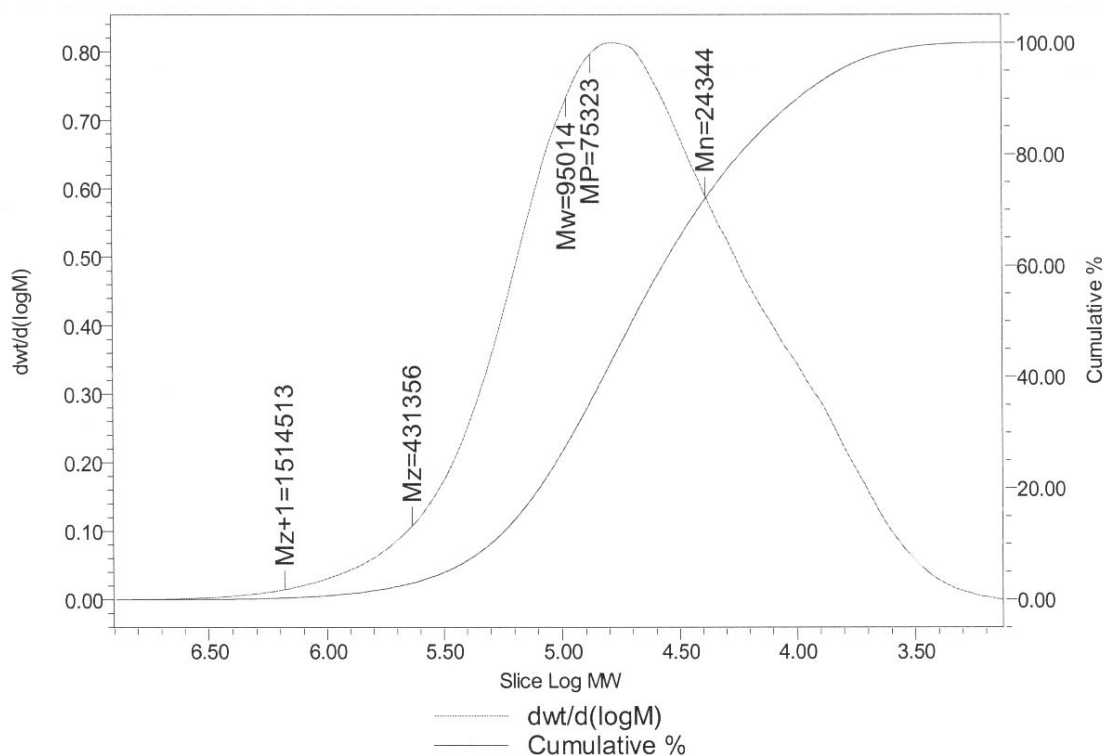


Fig. S7. GPC profile of **PDQT-tc** using chlorobenzene as an eluent and polystyrene as standards at column temperature of 40 °C.

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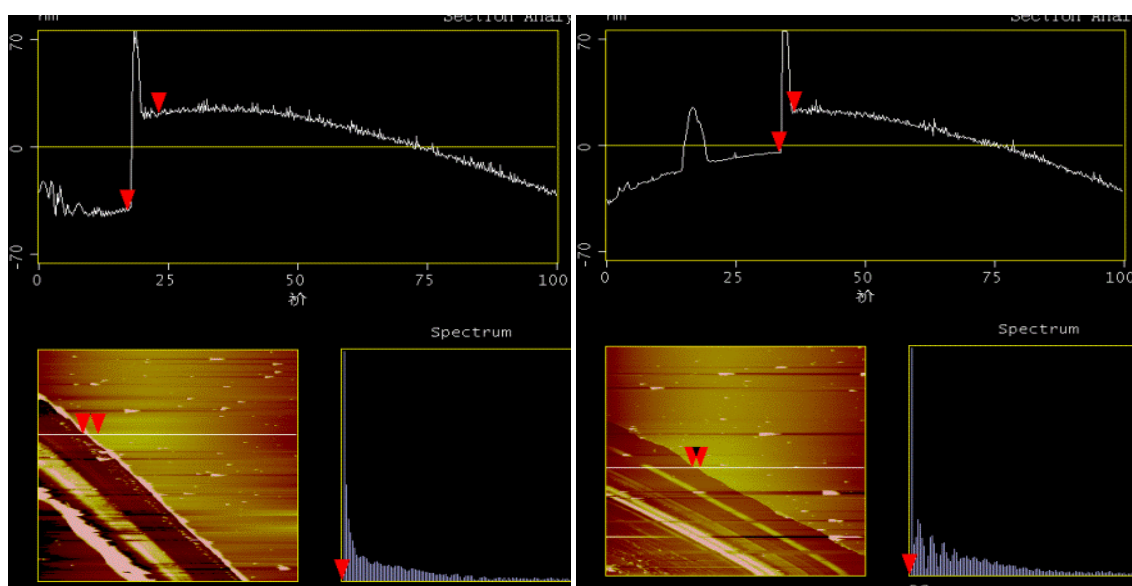


Fig. S8 Film thickness analysis of **PDQT-tc** thin films using AFM: left) before (63 nm) and right) after (26 nm) thermal annealing at 200 °C for 3 hr.