Supporting Information

Sulfur-Containing Polymers from Terpolymerization of Active Methylene Compounds, Carbon Disulfide, and Dihalohydrocarbons: Synthesis and Properties

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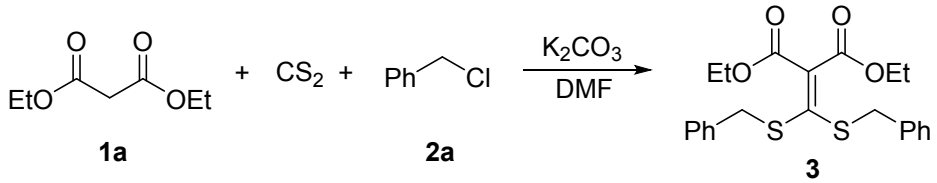
1. General information

All of the reagents and solvents were used without further purification. All the reactions were carried out in air. ^{1}H NMR and ^{13}C NMR spectra were recorded at 25 ºC on a Varian 500 MHz and 125 MHz, respectively. Their peak frequencies were referenced versus an internal standard (TMS) shifts at 0 ppm for ^{1}H NMR and against the solvent, $CDCl_3$ at 77.4 ppm for ^{13}C NMR, respectively. Molecular weights and molecular weight distributions of the resultant copolymers were determined with a PL-GPC220 chromatograph equipped with an HP 1100 pump from Agilent Technologies. The GPC columns were eluted with THF with 1.0 mL/min at 40 °C. The sample concentration was 0.4 wt %, and the injection volume was 100 μL. Calibration was performed using monodisperse polystyrene standards covering the molecular-weight range from 580 to 460 000 Da. Infrared spectra were recorded by using a Bruker Vector 22 FT-IR spectrophotometer. Thermogravimetric analysis (TGA) was carried out on a Perkin-Elmer Pyris I instrument under a N_2 atmosphere at a heating rate of 10 °C/min from room temperature to 400 °C. Samples for thermal analyses were all purified. The refractive index of the copolymer film was measured on an AUEL-III autolaser ellipsometer equipped with a He–Ne laser (I = 632.8 nm).

2. Synthetic procedures of compounds 3

Model compound **3** wAS synthesized by following previously reported procedures.[1-2]



1a **2a** **3**

To a solution of diethyl malonate **1a** (10 mmol) in DMF (50 mL), K_2CO_3 (22 mmol) was added. After stirring at room temperature for 30 min, the reaction mixture was cooled to 0 ºC, then CS_2 (12 mmol) was added. After stirring at 0 ºC for 1.0 h, (chloromethyl)benzene (22 mmol) was added. Then the resulting mixture was stirred overnight at room temperature. The resulting mixture was poured into ice-water and extracted with CH_2Cl_2 (3 × 30 mL). The combined organic extracts were washed with H_2O (3 × 30 mL), dried (Mg_2CO_3), filtered, and concentrated in vacuo to give a yellow oil. Purification was carried out by flash chromatography (silica gel, acetone-EtOAc, 1:4) to afford the product **3** as a yellowish oil; yield: 85%.

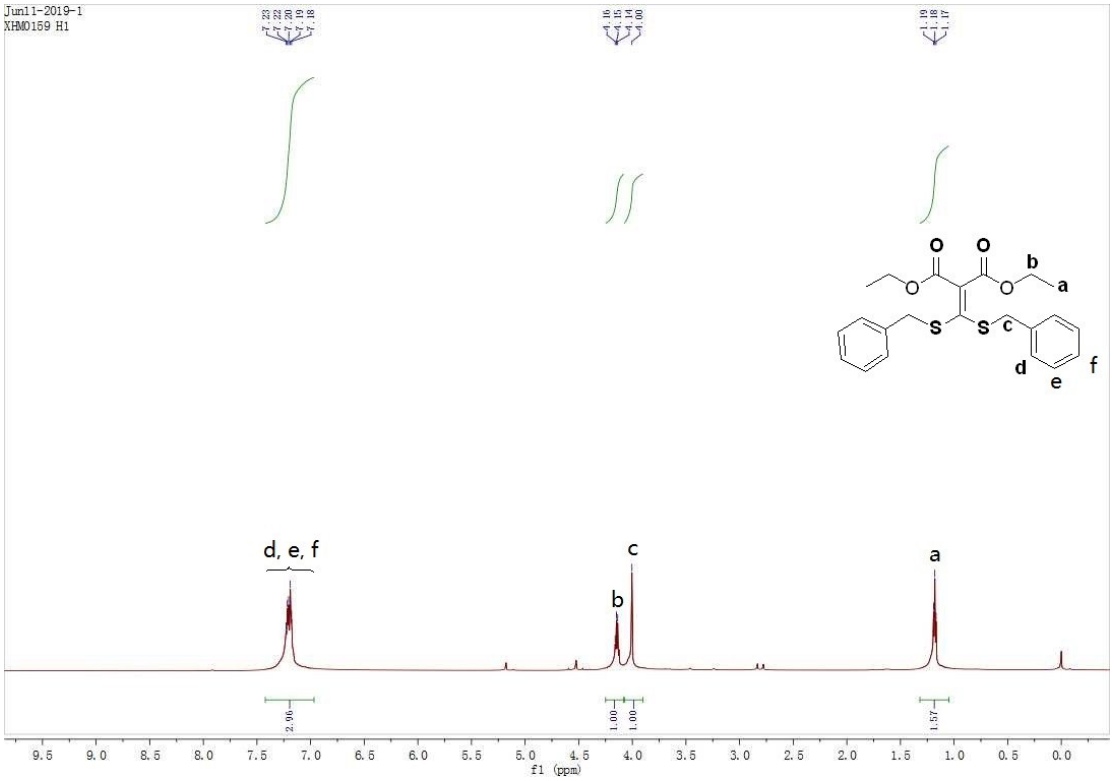
References:

(1) Dong, Y.; Wang, M.; Liu, J.; Ma, W.; Liu, Q. *Chem. Commun.* **2011**, *47*, 7380–7382.

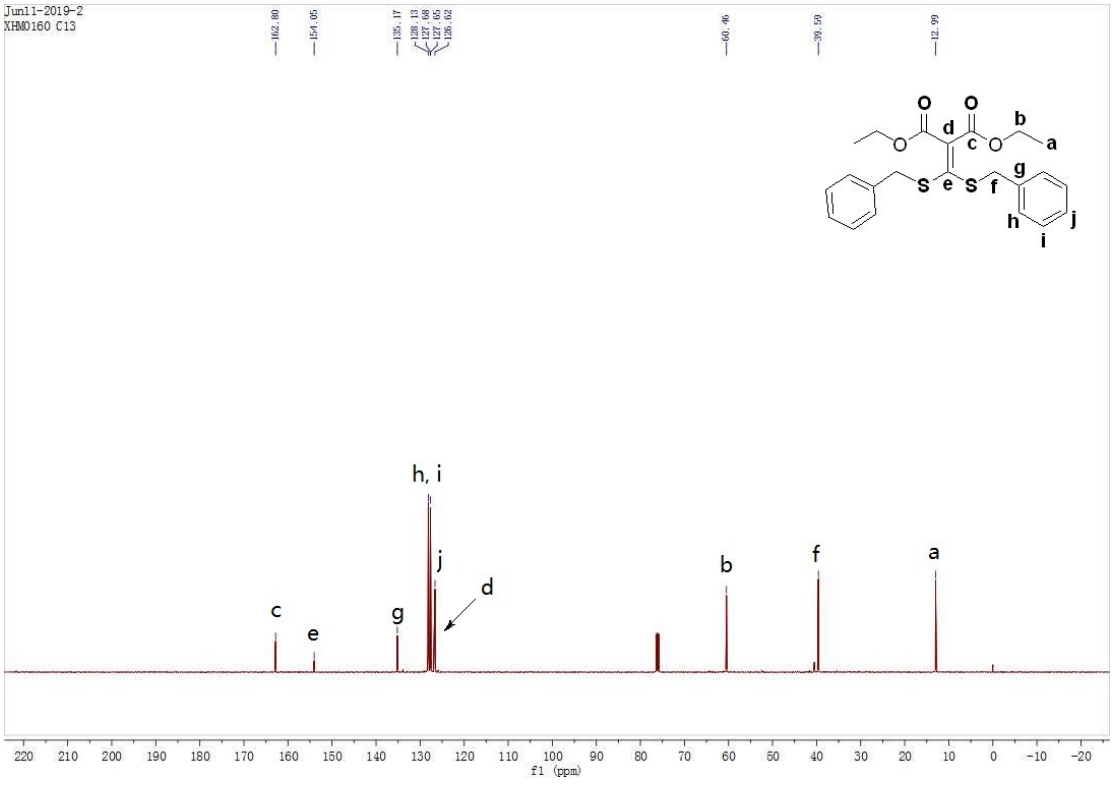
(2) Wang, M.; Ai, L.; Zhang, J. Y.; Liu, Q.; Gao, L. X. *Chin. J. Chem.* **2002**, *20*, 1591–1597.

3. Copies of ^{1}H NMR and ^{13}C NMR spectra of compounds 3 and PKDTA I–V

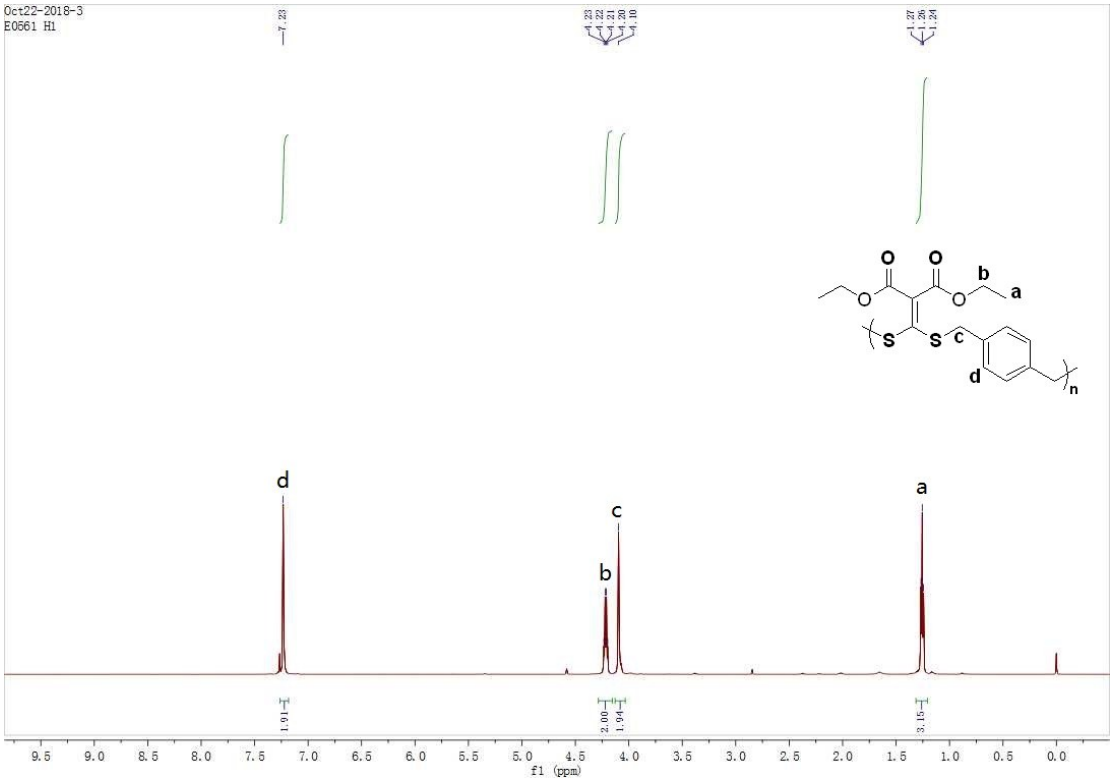
^{1}HNMR (600 MHz, $CDCl_3$) for 3



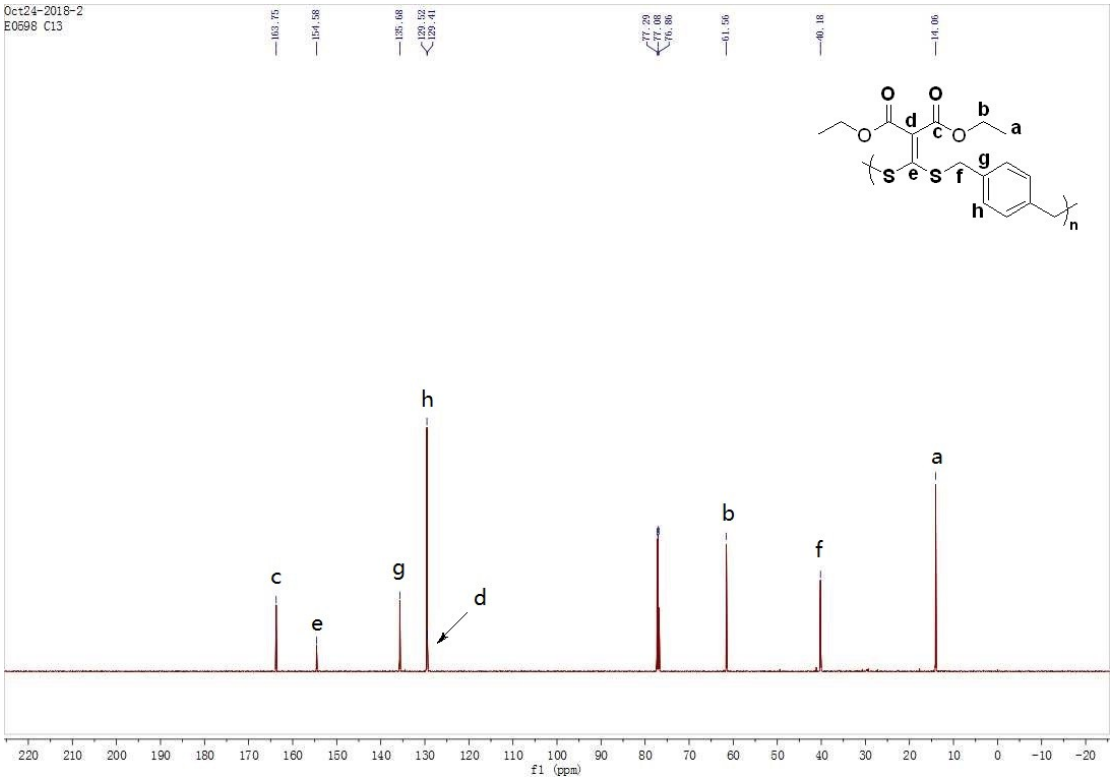
^{13}C NMR (151 MHz, $CDCl_3$) for 3



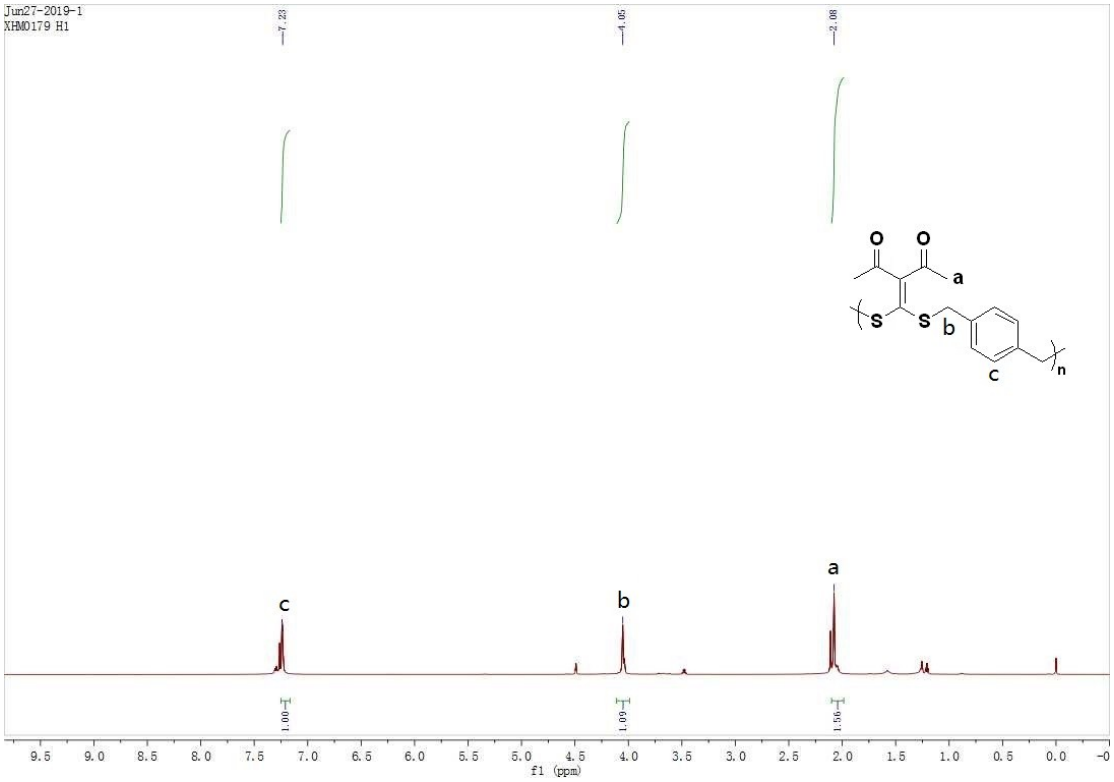
^{1}HNMR (600 MHz, $CDCl_3$) for PKDTA I



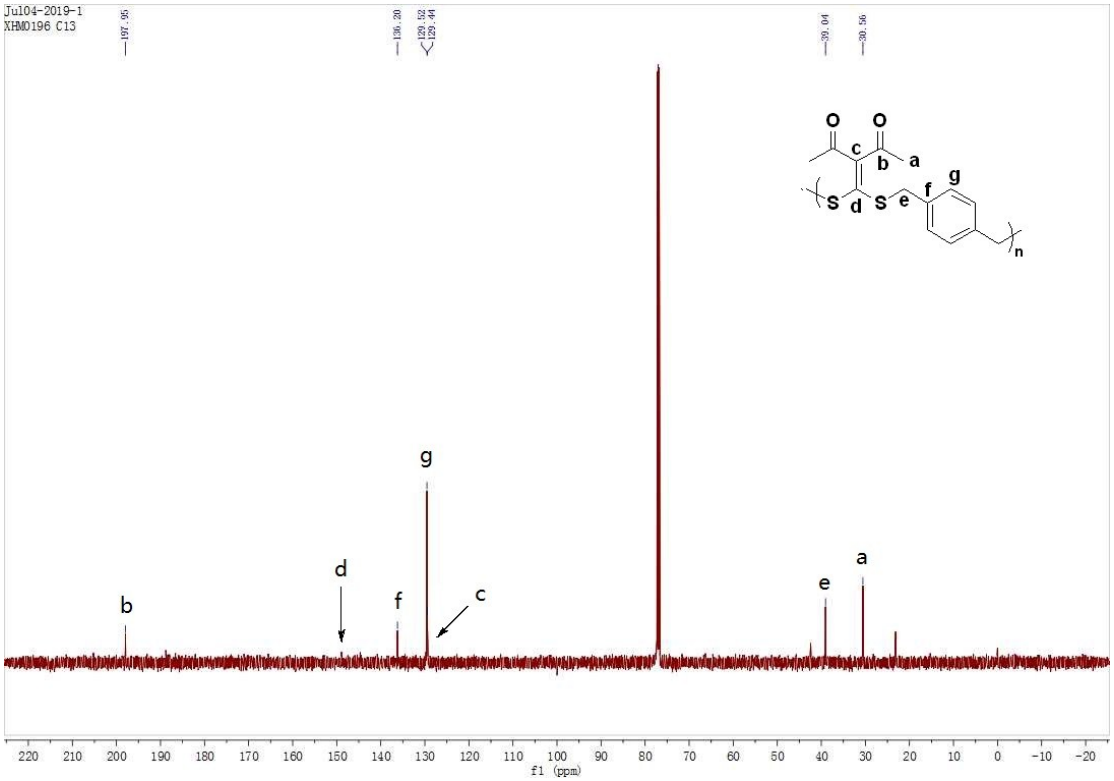
^{13}C NMR (151 MHz, $CDCl_3$) for PKDTA I



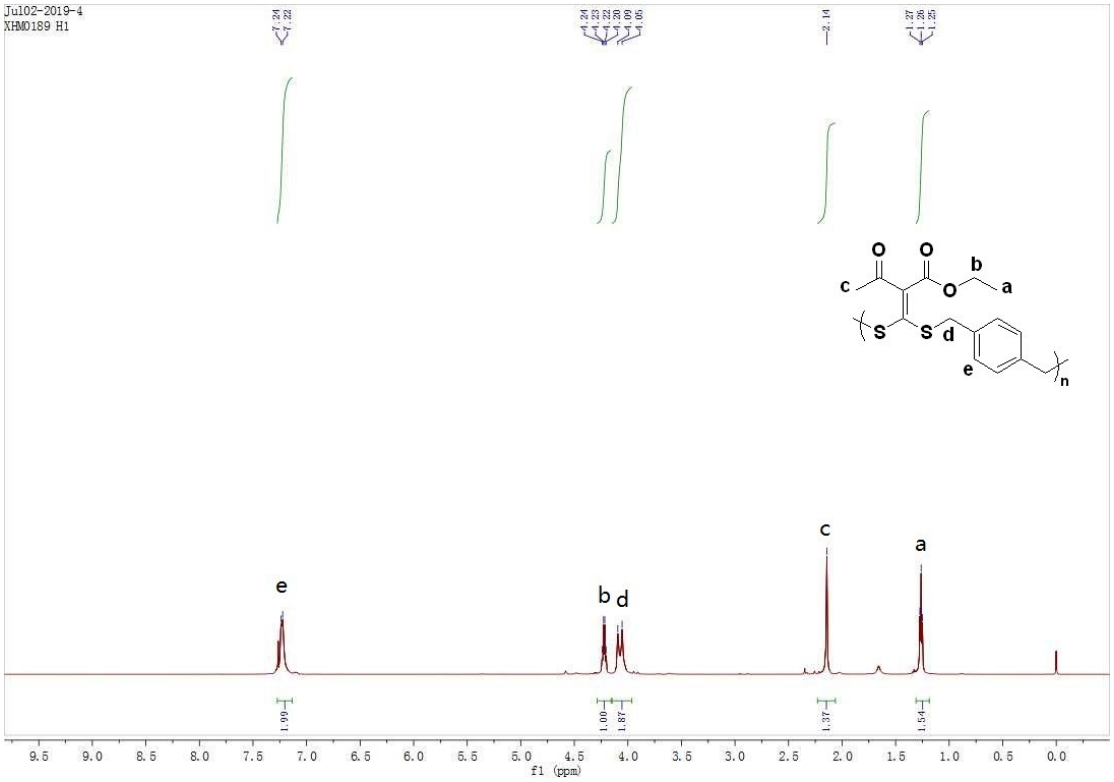
^{1}HNMR (600 MHz, $CDCl_3$) for PKDTA II



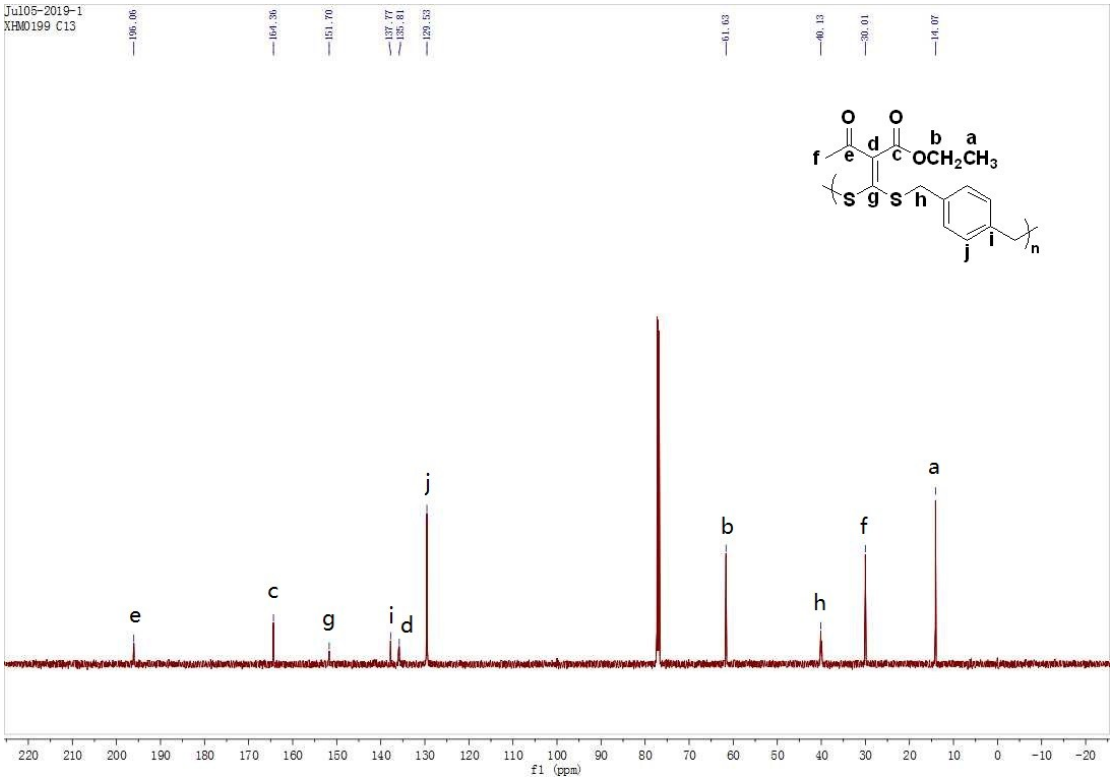
^{13}C NMR (151 MHz, $CDCl_3$) for PKDTA II



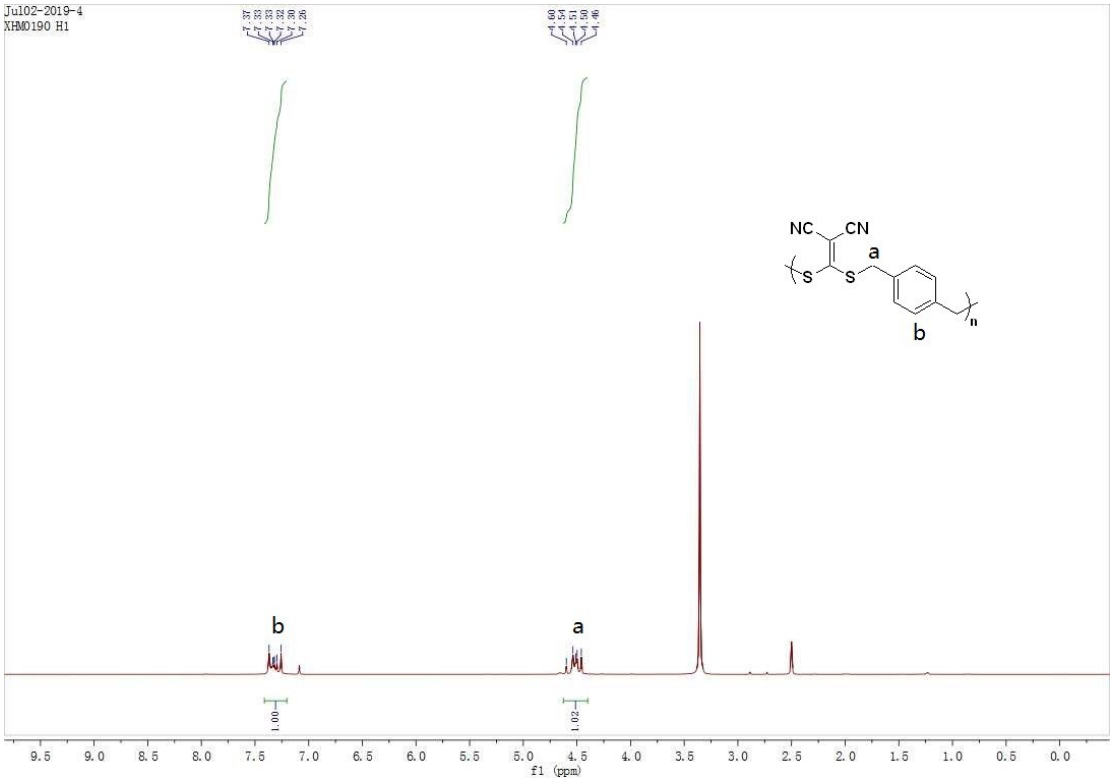
^{1}HNMR (600 MHz, $CDCl_3$) for PKDTA III



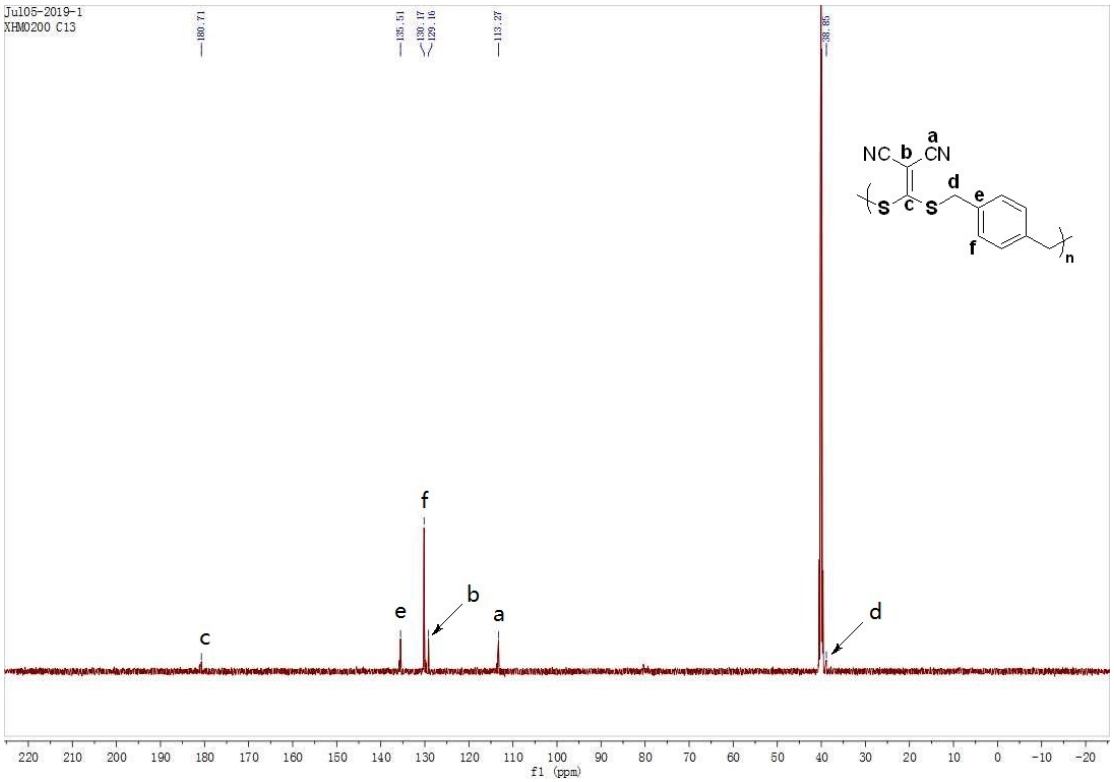
^{13}C NMR (151 MHz, $CDCl_3$) for PKDTA III



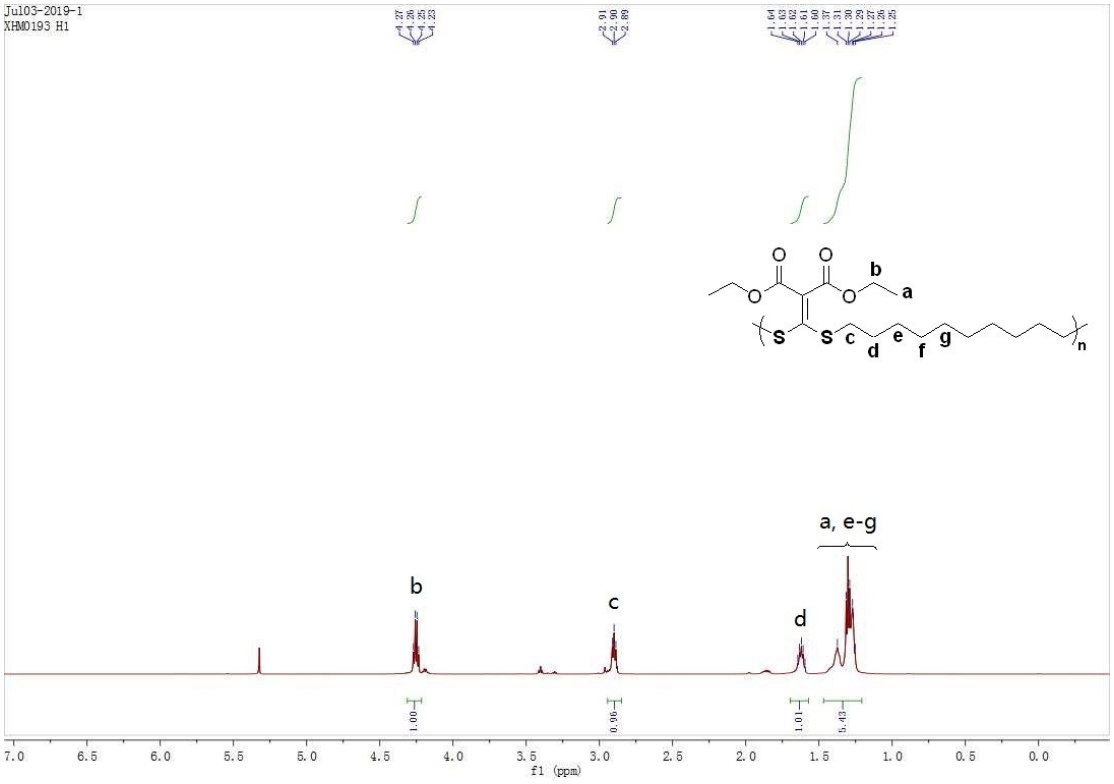
^{1}HNMR (600 MHz, DMSO-d_6) for PKDTA IV



^{13}C NMR (151 MHz, DMSO-d_6) for PKDTA IV



^{1}HNMR (600 MHz, DMSO-d_6) for PKDTA V



^{13}C NMR (151 MHz, CDCl $_3$) for PKDTA V