Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Synthesis of Differentiated Sulfur-Containing Polymers by Regiodivergent Polymerization of Morita−Baylis−Hillman Acetates and Thiols

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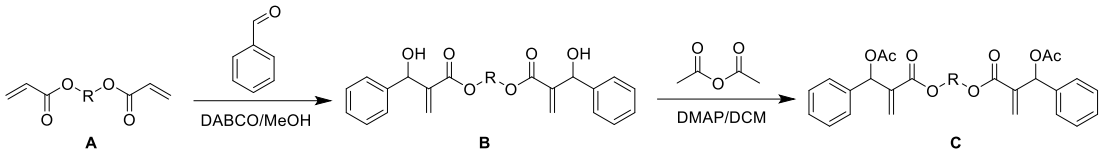
General Information

Materials. The organic solvents such as dimethyl sulfoxide (DMSO), *N*, *N*-dimethylformamide (DMF), toluene, dichloromethane (DCM)， *N*-methylpyrrolidone (NMP), and tetrahydrofuran (THF) were of analytical purity grade and used as received. 1,2-ethanedithiol (EDT), 1,4-butanedithiol, 1,6-hexanedithiol, 3,6-dioxa-1,8-octanedithiol (EGDT) and 4,4'-thiobisbenzenethiol were purchased from Macklin or Bidepharm and purified by flash column chromatography before polymerization. The reagents such as triethylamine (Et_3N), *N*, *N*-dimethylethanolamine (DABCO), 4-dimethylaminopyridine (DMAP) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) were purchased from Sigma-Aldrich and used directly without further purification. Other reagents were purchased from either Macklin, Sigma-Aldrich, or Bidepharm and used without further purification. Other commercially available reagents were used without further purification. Thin layer chromatography (TLC) was performed using Huanghai TLC silica gel plates (SHGF254) and visualized using UV light.

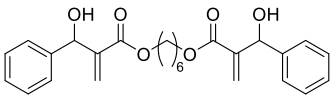
Characterization. ^1H (400 MHz) and ^{13}C (100 MHz) nuclear magnetic resonance (NMR) spectroscopy were recorded in $CDCl_3$, unless otherwise noted, on either an AVANCE III HD 400 or an ASCEND TM 500 spectrometer using residual chloroform (δ = 7.26 for ^1H and δ = 77.16 for ^{13}C) as internal standard. SEC system HLC-8320SEC with LC-20AD pump at 40 °C and a flow rate of 0.6 mL/min. HPLC grade tetrahydrofuran (THF) was used as the eluent. Polystyrene standards (Shodex, SM-105) were used to determine the molecular weight and molecular weight distribution of polymers. The polymers were dissolved in the THF solution and filtered through a 0.45 μm PTFE filter before being injected into the SEC system. Thermogravimetric analysis (TGA) of the polymer samples was performed under a nitrogen atmosphere using a TG 209 F1 (NETZSCH) at a heating rate of 10 ℃/min. Differential scanning calorimetry (DSC) analyses were conducted under a nitrogen atmosphere on DSC 250 (NETZSCH). The DSC curves were recorded as second heating curves from -60 to 120 °C at a heating rate of 10 °C/min and a cooling rate of 10 °C/min. Fourier transform infrared (FTIR) spectra were performed by Thermo Fisher Scientific NICOLET iS10. Polymer thin films were fabricated on silicon wafers (1.0 × 1.0 cm) from their chloroform solutions (0.02 M) via a spin-coating process (900 rpm; 30 seconds). The *n* values were recorded on a Woollam ellipsometer (model Alpha-SE) with wavelength ranging from 380 to 900 nm at a 70° incident angle.

Scheme S1. General procedure for the synthesis of monomers **1a-1c**.



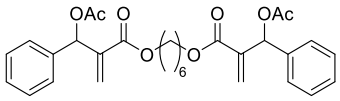
Procedure 1. Following a slightly modified procedure from the literature,[1] in a 100 mL flask, DABCO (1.0 equiv) was dissolved in MeOH (1.0 equiv). To this solution was added diacrylate **A** (1.0 equiv) and benzaldehyde (2.5 equiv). After stirring at room temperature for 48 h, the reaction mixture was diluted with ethyl acetate (50 mL), washed with 1 M hydrochloric acid (3 x 30 mL) and brine (30 mL), dried over Na_2SO_4, and concentrated *in vacuo*. The crude product was purified by flash column chromatography with petroleum ether/ethyl acetate to afford **B** as a colorless oil.

Procedure 2. Following a slightly modified procedure from the literature,[2] in a 100 mL flask, **B** (1.0 equiv) and acetic anhydride (2.5 equiv) were dissolved in DCM (10 mL). then DMAP (0.5 equiv) was slowly added to the mixture at 0 °C. After stirring at room temperature for 48 h, the reaction mixture was treated with water (10 mL) and extracted with DCM (3 x 10 mL). The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The crude product was purified by flash column chromatography with petroleum ether/ethyl acetate to afford **C** as a colorless oil.



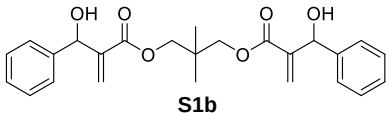
S1a

Following the procedure 1, the reaction of hexamethylene diacrylate (22.6 g, 100 mmol) and benzaldehyde (26.5 g, 250 mmol) afforded **S1a** as a colorless oil (25.5 g, 58% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): 7.40–7.26 (m, 10H), 6.34 (s, 2H), 5.84 (s, 2H), 5.56 (d, *J* = 5.7 Hz, 2H), 4.09 (td, *J* = 6.5, 1.9 Hz, 4H), 3.01 (dd, *J* = 5.5, 3.4 Hz, 2H), 1.57 (t, *J* = 5.7 Hz, 4H), 1.25 (p, *J* = 3.8 Hz, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.3, 142.2, 141.4, 128.4, 127.8, 126.6, 125.9, 73.3, 64.8, 28.3, 25.5; **IR (KBr, thin film)**: 3467, 3030, 2938, 2860, 1716, 1628, 1492, 1454, 1271, 1152, 1401, 958, 765, 700 cm^{-1}; **HRMS (m/z)** $[M-H]^-$ calc'd for $C_{26}H_{29}O_6$, 437.1970, found 437.1972.



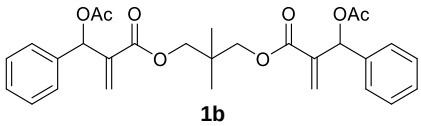
1a

Following the procedure 2, the reaction of **S1a** (7.0 g, 16 mmol) and acetic anhydride (4.0 g, 40 mmol) afforded **1a** as a colorless oil (5.8 g, 70% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.40–7.26 (m, 10H), 6.68 (s, 2H), 6.41 (s, 2H), 5.89–5.82 (m, 2H), 4.14–4.00 (m, 4H), 2.10 (s, 6H), 1.62–1.44 (m, 4H), 1.19 (p, *J* = 3.7 Hz, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.4, 165.0, 139.8, 137.9, 128.5, 128.4, 127.8, 125.7, 73.2, 64.9, 28.3, 25.4, 21.1; **IR (KBr, thin film)**: 3034, 2938, 2860, 1743, 1634, 1495, 1455, 1371, 1230, 1077, 1025, 960, 815, 699 cm^{-1}; **HRMS (m/z)** $[M+Na]^+$ calc'd for $C_{30}H_{34}O_8Na$, 545.2146, found, 545.2151.



S1b

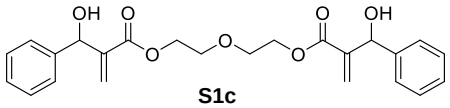
Following the procedure 1, the reaction of neopentyl glycol diacrylate (1.2 g, 5.3 mmol) and benzaldehyde (1.4 g, 13.4 mmol) afforded **S1b** as a colorless oil (1.9 g, 85% yield). **^{1}H NMR (**400 MHz, $CDCl_3$): δ 7.37–7.26 (m, 10H), 6.34 (s, 2H), 5.86 (s, 2H), 5.52 (d, *J* = 4.1 Hz, 2H), 3.84–3.75 (m, 4H), 3.03 (s, 2H), 0.79 (t, *J* = 2.9 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.0, 141.9, 141.3, 128.5, 127.9, 126.6, 126.4, 73.1, 69.3, 69.3, 34.9, 21.6; **IR (KBr, thin film)**: 3447, 2966, 2871, 1717, 1628, 1491, 1456, 1375, 1265, 1151, 989, 765, 700 cm^{-1}; **HRMS (m/z)** $[M-H]^-$ calc'd for $C_{25}H_{27}O_6$, 423.1813, found 423.1815.



1b

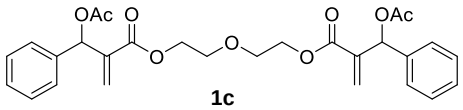
Following the procedure 2, the reaction of **S1b** (1.3 g, 3.3 mmol) and acetic anhydride (0.8 g, 8.2 mmol) afforded **1b** as a colorless oil (1.1 g, 67% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.37–7.27 (m, 10H), 6.65 (s, 2H), 6.41 (s, 2H), 5.87 (s, 2H), 3.86–3.68 (m, 4H), 2.09 (s, 6H), 0.79–0.74 (m, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.4, 164.7, 139.3, 137.7, 128.6, 128.5, 127.7, 127.6, 126.5, 73.1, 69.5, 34.8, 21.5, 21.1; **IR (KBr, thin film)**: 3034,

2966, 2868, 1743, 1635, 1456, 1372, 1024, 988, 760, 699 cm^{-1}; **HRMS (m/z)** $[M+Na]^+$ calc'd for $C_{29}H_{32}O_8Na$, 531.1989, found 531.1992.



S1c

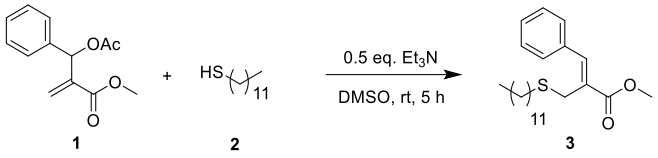
Following the procedure 1, the reaction of diethylene glycol diacrylate (6.1 g, 28.5 mmol) and benzaldehyde (7.6 g, 71.2 mmol) afforded **S1c** as a colorless oil (10.7 g, 87% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38–7.26 (m, 10H), 6.36 (s, 2H), 5.82 (s, 2H), 5.55 (s, 2H), 4.27–4.14 (m, 4H), 3.65–3.55 (m, 4H), 3.25 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.1, 142.07, 142.0, 141.3, 128.4, 127.8, 126.6, 126.6, 73.1, 73.0, 68.8, 63.7.; **IR (KBr, thin film)**: 3481, 3032, 2953, 2893, 1716, 1635, 1491, 1455, 1396, 1271, 1080, 1044, 960, 839, 765, 700 cm^{-1}; **HRMS (m/z)** $[M-H]^-$ calc'd for $C_{24}H_{25}O_7$, 425.16058, found 425.16080.



1c

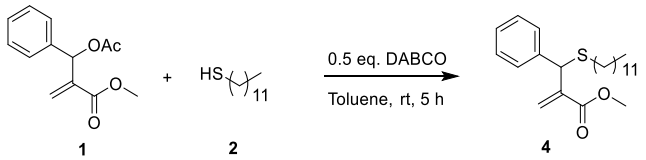
Following the procedure 2, the reaction of **S1c** (8.7 g, 20.4 mmol) and acetic anhydride (5.2 g, 50.9 mmol) afforded **1c** as a colorless oil (6.0 g, 57% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.39–7.26 (m, 10H), 6.68 (s, 2H), 6.42 (s, 2H), 5.86 (s, 2H), 4.26–4.14 (m, 4H), 3.56 (t, *J* = 4.8 Hz, 4H), 2.09 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.4, 164.8, 139.5, 137.8, 128.4, 128.4, 127.7, 126.2, 73.1, 68.8, 64.0, 21.1; **IR (KBr, thin film)**: 3033, 2953, 2877, 1717, 1635, 1507, 1456, 1372, 1132, 1026, 995, 960, 762, 699 cm^{-1}; **HRMS (m/z)** $[M+Na]^+$ calc'd for $C_{28}H_{30}O_9Na$, 533.1782, found 533.1786.

Scheme S2. General procedure of α-regioselective model reaction.



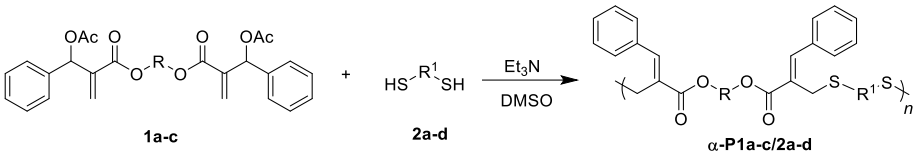
A 3 mL vial equipped with a stir bar was charged with compound **1** (46.9 mg, 0.2 mmol), followed by the Et_3N (10.1 mg, 0.1 mmol) and DMSO (1.0 mL). To the solution, thiol **2** (40.5 mg, 0.2 mmol) was added. The vial was sealed, and the reaction mixture was stirred at room temperature for 5 h. The conversion and yield were calculated using ^{1}H NMR spectroscopy. The crude product was directly purified by flash column chromatography to afford **3** (61.4 mg, 82%) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.74 (s, 1H), 7.57–7.29 (m, 5H), 3.85 (s, 3H), 3.64 (s, 2H), 2.59–2.45 (m, 2H), 1.25 (s, 20H), 0.88 (t, *J* = 6.7 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 167.9, 140.3, 135.1, 129.8, 129.6, 128.8, 128.6, 128.4, 128.2, 52.2, 32.9, 31.9, 29.7, 29.7, 29.6, 29.6, 29.4, 29.3, 28.9, 28.6, 22.7, 14.1; **IR (KBr, thin film)**: 3059, 2925, 2853, 1717, 1457, 1264, 1217, 1202, 1080, 782, 756, 698 cm^{-1}; **LRMS (m/z)** $[M+H]^+$ calc'd for $C_{23}H_{37}O_2S$, 377.25, found 377.1.

Scheme S3. General procedure of γ-regioselective model reaction.

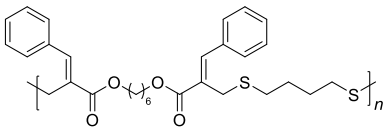


A 3 mL vial equipped with a stir bar was charged with compound **1** (46.9 mg, 0.2 mmol), followed by the DABCO (11.2 mg, 0.1 mmol) and toluene (1.0 mL). After the mixture was stirred at room temperature for 10 min, thiol **2** (40.5 mg, 0.2 mmol) was added to the solution. The vial was sealed, and the reaction mixture was stirred at room temperature for 5 h. The conversion and yield were calculated using ^{1}H NMR spectroscopy. The crude product was directly purified by flash column chromatography to afford **4** (57.5 mg, 76%) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.42–7.19 (m, 5H), 6.44 (s, 1H), 6.05 (s, 1H), 5.05 (s, 1H), 3.71 (s, 3H), 2.40 (t, *J* = 7.4 Hz, 2H), 1.24 (s, 20H), 0.88 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.6, 140.6, 140.0, 129.6, 128.6, 128.4, 128.3, 127.3, 126.9, 52.1, 49.1, 32.6, 31.9, 29.7, 29.6, 29.5, 29.4, 29.2, 29.1, 28.9, 22.7, 14.1; **IR (KBr, thin film)**: 3027, 2922, 2853, 1730, 1493, 1436, 1249, 1202, 1074, 949, 755, 701 cm^{-1}. **LRMS (m/z)** $[M+H]^+$ calc'd for $C_{23}H_{37}O_2S$, 377.25, found 377.1.

Scheme S4. General procedure of α-regioselective polymerization.



A 3 mL vial equipped with a stir bar was charged with monomer MBH acetate **1** (0.2 mmol), followed by the Et_3N (0.1 mmol) and DMSO (1.0 mL). To the solution, monomer dithiol **2** (0.2 mmol) was added. The vial was sealed, and the reaction mixture was stirred at room temperature for 12 h. After the reaction, the reaction mixture was diluted with a minimum amount of DCM and precipitated in hexane. The resulting polymer was re-dissolved with a minimum amount of DCM for further precipitation. The obtained polymer was dried in vacuo overnight and then characterized using SEC, FT-IR, ^{1}H NMR, and ^{13}C NMR.



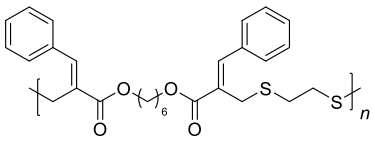
α-P1a/2a

α-P1a/2a: 88% yield, >99:1 *rr*, M_n = 18900, $Đ$ = 1.68**.**

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.71 (s, 1.73H), 7.51–7.19 (m, 10H), 6.72 (s, 0.27H), 4.30–4.02 (m, 4H), 3.67–3.40 (m, 4H), 2.44 (dt, *J* = 11.9, 6.4 Hz, 4H), 1.85–1.12 (m, 12H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.4, 140.1, 135.1, 129.9, 129.5, 128.9, 128.6, 65.1, 32.3, 28.7, 28.6, 28.5, 25.8.

IR (KBr, thin film): 3055, 2931, 2853, 1708, 1634, 1447, 1265, 1215, 1201, 1081, 782, 757, 699 cm^{-1}.



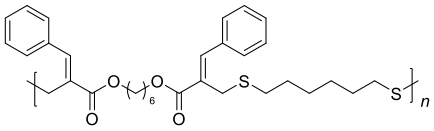
α-P1a/2b

α-P1a/2b: 89% yield, >99:1 *rr*, M_n = 22500, $Đ$ = 1.52.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.71 (s, 1.77H), 7.53–7.26 (m, 10H), 6.72 (s, 0.23H), 4.29–4.03 (m, 4H), 3.70–3.45 (m, 4H), 2.63 (s, 4H), 1.81–1.64 (m, 4H), 1.48 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.3, 140.5, 134.9, 129.5, 129.5, 128.9, 128.7, 65.2, 40.9, 32.7, 28.6, 25.7.

IR (KBr, thin film): 3056, 2935, 2857, 1709, 1627, 1492, 1447, 1264, 1170, 1081, 782, 758, 699 cm^{-1}.



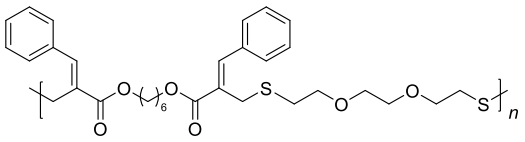
α-P1a/2c

α-P1a/2c: 84% yield, >99:1 *rr*, M_n = 17700, *Đ* = 1.84.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.71 (s, 1.72H), 7.53–7.27 (m, 10H), 6.73(s, 0.28H), 4.31–4.06 (m, 4H), 3.62 (s, 4H), 2.47 (t, *J* = 7.3 Hz, 4H), 1.83–1.67 (m, 4H), 1.53–1.16 (m, 12H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.5, 140.0, 135.1, 130.0, 129.5, 128.8, 128.6, 65.1, 32.8, 29.5, 28.6, 28.5, 28.4, 25.8.

IR (KBr, thin film): 3026, 2922, 2852, 1715, 1653, 1507, 1457, 1362, 1158, 1070, 977, 752, 696 cm^{-1}.



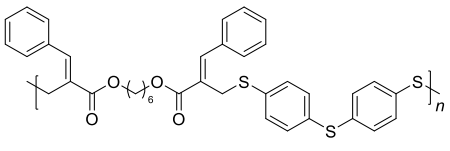
α-P1a/2d

α-P1a/2d: 89% yield, >99:1 *rr*, M_n = 16400, *Đ* = 1.73.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.72 (s, 1.77H), 7.53–7.27 (m, 10H), 6.76 (s, 0.23H), 4.28–4.06 (m, 4H), 3.66 (s, 4H), 3.58–3.42 (m, 8H), 2.71 (t, *J* = 6.9 Hz, 4H), 1.82–1.67 (m, 4H), 1.49 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.3, 140.4, 135.0, 129.7, 129.6, 128.9, 128.7, 70.7, 70.2, 65.1, 32.2, 29.1, 28.6, 25.7.

IR (KBr, thin film): 3025, 2925, 2855, 1715, 1653, 1507, 1457, 1418, 1260, 1167, 1081, 755, 696 cm^{-1}.



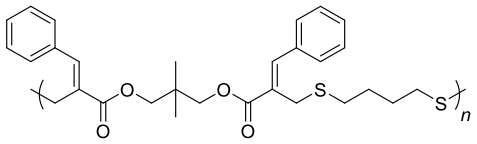
α-P1a/2e

α-P1a/2e: 92% yield, >99:1 *rr*, M_n = 45600, *Đ* = 2.14.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.75 (s, 1.92H), 7.41–7.28 (m, 10H), 7.25–7.07 (m, 10H), 6.53 (s, 0.08H), 4.23 (t, *J* = 6.6 Hz, 4H), 4.02 (s, 4H), 1.80–1.66 (m, 4H), 1.47 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.1, 141.5, 135.3, 134.7, 133.9, 131.3, 131.2, 129.4, 129.0, 128.6, 128.2, 126.7, 65.2, 40.9, 32.2, 28.6, 25.7.

IR (KBr, thin film): 3026, 2933, 2856, 1716, 1558, 1456, 1244, 1130, 1074, 952, 750, 701 cm^{-1}.



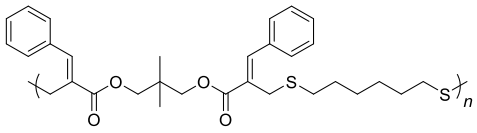
α-P1b/2a

α-P1b/2a: 78% yield, >99:1 *rr*, M_n = 10100, *Đ* = 1.47.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.74 (s, 1.70H), 7.52–7.26 (m, 10H), 6.73 (s, 0.30H), 4.20–3.78 (m, 4H), 3.64–3.41 (m, 4H), 2.54–2.32 (m, 4H), 1.35 (d, *J* = 73.8 Hz, 4H), 1.14–0.79 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.2, 140.6, 134.9, 129.5, 128.9, 128.6, 128.2, 70.0, 35.3, 32.2, 28.6, 28.6, 22.1.

IR (KBr, thin film): 3025, 2931, 1715, 1627, 1491, 1447, 1267, 1201, 1080, 982, 756, 698 cm^{-1}.



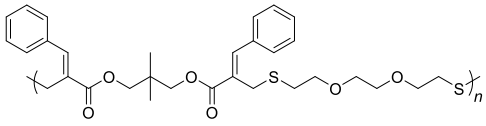
α-P1b/2c

α-P1b /2c: 74% yield, >99:1 *rr*, M_n = 21100, *Đ* = 1.89.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.75 (d, *J* = 17.1 Hz, 1.67H), 7.56–7.32 (m, 10H), 6.76 (s, 0.33H), 4.23–3.78 (m, 4H), 3.69–3.46 (m, 4H), 2.48 (q, *J* = 7.2 Hz, 4H), 1.51–1.38 (m, 4H), 1.32–1.18 (m, 4H), 1.15 (s, 4H), 0.89 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): 167.3, 140.5, 135.0, 129.5, 128.9, 128.6, 128.3, 70.0, 35.3, 32.7, 29.5, 28.7, 28.5, 22.1.

IR (KBr, thin film): 3025, 2922, 2852, 1715, 1635, 1558, 1507, 1457, 1362, 1158, 977, 752, 696 cm^{-1}.



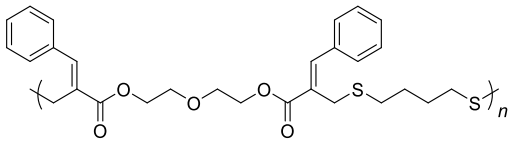
α-P1b/2d

α-P1b/2d: 80% yield, >99:1 *rr*, M_n = 13200, *Đ* = 1.50.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.72 (d, *J* = 18.0 Hz, 1.77H), 7.53–7.27 (m, 10H), 6.77 (s, 0.23H), 4.18–3.78 (m, 4H), 3.67 (s, 4H), 3.59–3.43 (m, 8H), 2.69 (t, *J* = 6.9 Hz, 4H), 1.11 (s, 4H), 0.85 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.1, 140.9, 134.8, 129.6, 129.0, 128.7, 128.3, 70.6, 70.1, 70.0, 35.3, 32.2, 29.2, 22.1.

IR (KBr, thin film): 3034, 2923, 2851, 1715, 1635, 1507, 1457, 1266, 1201, 1083, 982, 756, 699 cm^{-1}.



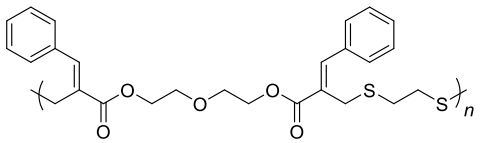
α-P1c/2a

α-P1c/2a: 72% yield, >99:1 *rr*, M_n = 21300, *Đ* = 1.44.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): 7.73 (d, *J* = 7.9 Hz, 1.74H), 7.48–7.28 (m, 10H), 6.72 (s, 0.26H), 4.35 (dt, *J* = 48.2, 4.8 Hz, 4H), 3.88–3.78 (m, 4H), 3.59 (s, 4H), 2.46 (d, *J* = 33.9 Hz, 4H), 1.51 (d, *J* = 48.6 Hz, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): 167.3, 140.6, 134.9, 129.5, 128.9, 128.6, 128.6, 69.2, 64.2, 32.3, 28.7, 28.5.

IR (KBr, thin film): 3024, 2944, 2859, 1715, 1635, 1507, 1456, 1201, 1137, 1080, 935, 757, 698 cm^{-1}.



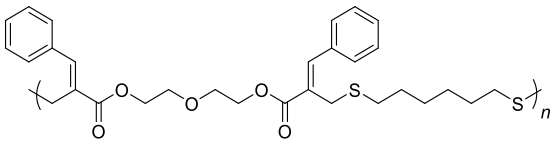
α-P1c/2b

α-P1c/2b: 83% yield, >99:1 *rr*, M_n = 8300, *Đ* = 1.74.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.77 (d, *J* = 8.7 Hz, 1.79H), 7.53–7.31 (m, 10H), 6.74 (s, 0.21H), 4.36 (dt, *J* = 49.2, 4.4 Hz, 4H), 3.90–3.76 (m, 4H), 3.58 (s, 4H), 2.64 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.1, 141.0, 134.7, 129.5, 129.2, 129.0, 128.7, 69.1, 64.2, 32.7, 28.5.

IR (KBr, thin film): 3024, 2948, 1715, 1635, 1507, 1456, 1202, 1135, 1080, 936, 758, 699 cm^{-1}.



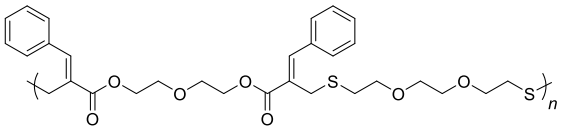
α-P1c/2c

α-P1c/2c: 83% yield, >99:1 *rr*, M_n = 19100, *Đ* = 1.90.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.73 (d, *J* = 7.9 Hz, 1.75H), 7.51–7.28 (m, 10H), 6.73 (s, 0.25H), 4.35 (dt, *J* = 52.8, 4.7 Hz, 4H), 3.84 (dd, J = 5.7, 3.8 Hz, 4H), 3.61 (s, 4H), 2.53–2.40 (m, 4H), 1.50–1.37 (m, 4H), 1.24–1.16 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.3, 140.5, 135.0, 129.6, 129.5, 128.9, 128.6, 69.2, 64.2, 32.8, 29.5, 28.5.

IR (KBr, thin film): 3024, 2928, 2855, 1715, 1684, 1507, 1456, 1201, 1137, 1081, 934, 757, 698 cm^{-1}.



α-P1c/2d

α-P1c/2d: 81% yield, >99:1 *rr*, M_n = 12500, *Đ* = 1.46.

^{1}H NMR (400 MHz, $CDCl_3$, *E*/*Z*): δ 7.76 (d, *J* = 8.1 Hz, 1.74H), 7.52–7.31 (m, 10H), 6.79(s, 0.26H), 4.37 (dt, *J* = 49.7, 4.6 Hz, 4H), 3.84 (d, *J* = 4.6 Hz, 4H), 3.66 (d, *J* = 6.0 Hz, 4H), 3.58–3.48 (m, 8H), 2.74 (q, *J* = 7.0, 6.5 Hz, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, *E* isomer): δ 167.2, 140.9, 134.8, 129.6, 129.3, 129.0, 128.7, 70.6, 70.2, 69.2, 64.2, 32.2, 29.1.

IR (KBr, thin film): 3056, 3024, 2928, 2864, 1715, 1507, 1456, 1201, 1171, 1133, 935, 757, 698 cm^{-1}.

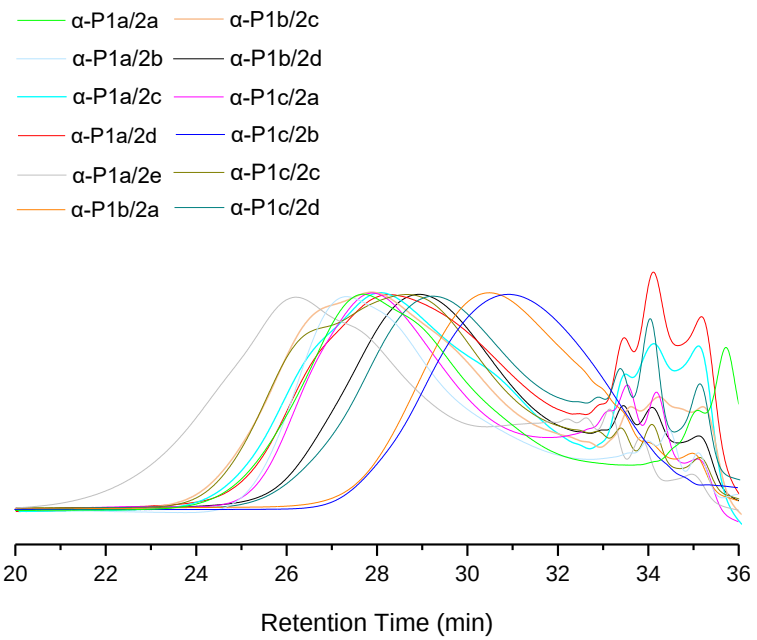


Figure S1. SEC traces of all resulting α-polymers.

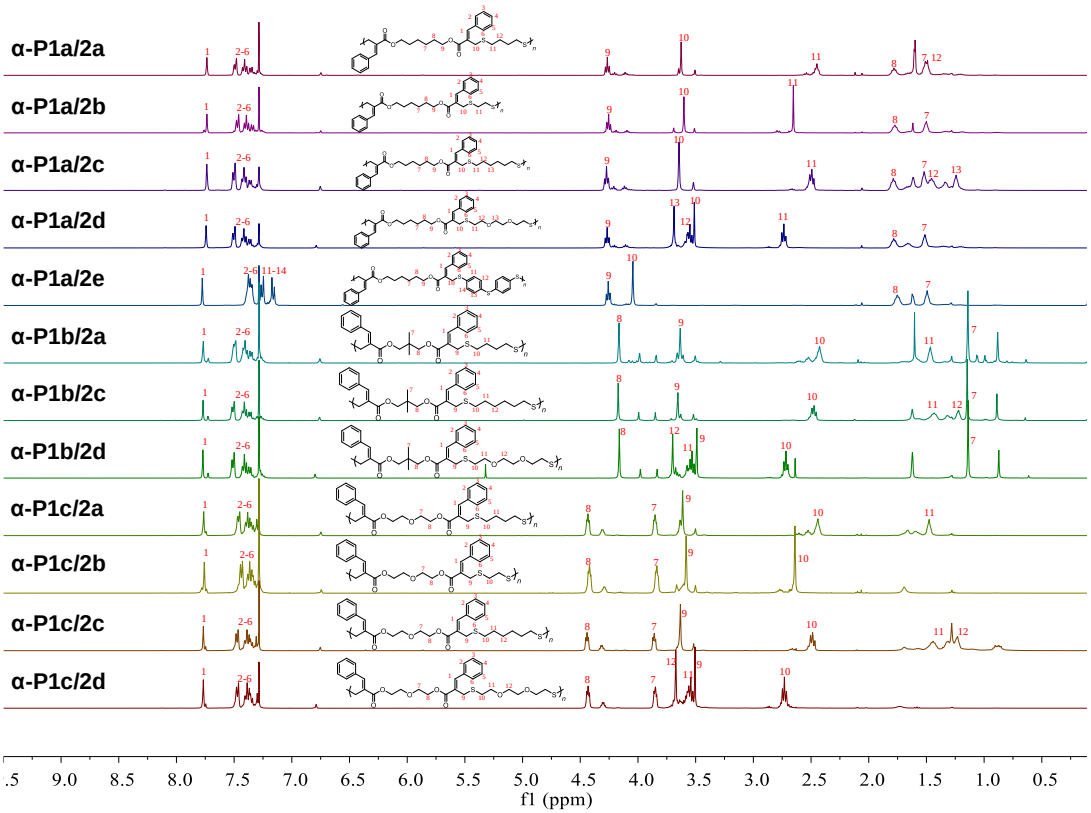
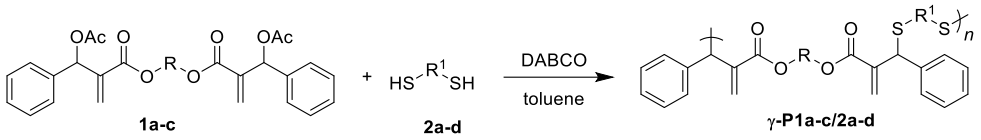
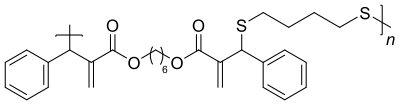


Figure S2. ^{1}H NMR spectral of all resulting α-polymers.

Scheme S5. General procedure of γ-regioselective polymerization.



A 3 mL vial equipped with a stir bar was charged with monomer MBH acetate **1** (0.2 mmol), followed by the DABCO (0.1 mmol) and toluene (1.0 mL). After the mixture was stirred at room temperature for 10 min, monomer dithiol **2** (0.2 mmol) was added to the solution. The reaction mixture continued stirring at room temperature for 12 h. After the reaction, the reaction mixture was diluted with a minimum amount of DCM and precipitated in hexane. The resulting polymer was re-dissolved with a minimum amount of DCM for further precipitation. The obtained polymer was dried in vacuo overnight and then characterized using SEC, FT-IR, ^{1}H NMR, and ^{13}C NMR.



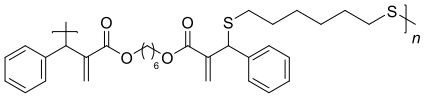
γ-P1a/2a

γ-P1a/2a: 70% yield, 2:98 *rr*, M_n = 14100, $Đ$ = 1.58.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35–7.17 (m, 10H), 6.43 (s, 2H), 6.02 (s, 2H), 5.00 (s, 2H), 4.14–3.97 (m, 4H), 2.35 (s, 4H), 1.62–1.48 (m, 8H), 1.21 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0, 140.5, 139.9, 128.4, 128.3, 127.3, 126.9, 65.0, 49.2, 45.4, 31.9, 28.1, 25.5.

IR (KBr, thin film): 3026, 2933, 2856, 1716, 1684, 1489, 1456, 1313, 1244, 1130, 952, 701, 651 cm^{-1}.



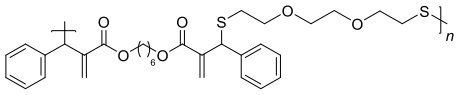
γ-P1a/2c

γ-P1a/2c: 65% yield, 3:97 *rr*, M_n = 11900, $Đ$ = 1.46.

^{1}H NMR (400 MHz, $CDCl_3$): 7.41–7.17 (m, 10H), 6.36 (s, 2H), 5.96 (s, 2H), 4.94 (s, 2H), 4.08–3.91 (m, 4H), 2.31 (dq, *J* = 12.9, 6.4, 5.6 Hz, 4H), 1.46 (dq, *J* = 18.4, 7.3, 6.7 Hz, 8H), 1.19 (dd, *J* = 19.2, 11.5 Hz, 8H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 140.6, 140.0, 128.4, 128.3, 127.3, 126.8, 64.9, 49.3, 45.4, 32.4, 28.9, 28.4, 25.5.

IR (KBr, thin film): 3027, 2924, 2852, 1717, 1630, 1558, 1456, 1243, 1128, 950, 751, 701 cm^{-1}.



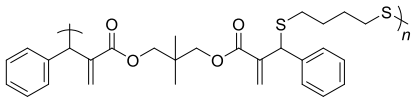
γ-P1a/2d

γ-P1a/2d: 76% yield, 6:94 *rr*, M_n = 16900, *Đ* = 1.68.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51–7.27 (m, 10H), 6.44 (s, 2H), 6.05 (s, 2H), 5.10 (s, 2H), 4.16–3.96 (m, 4H), 3.59–3.48 (m, 8H), 2.60 (t, *J* = 6.8 Hz, 4H), 1.60–1.46 (m, 4H), 1.21 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 167.3, 140.4, 135.0, 129.7, 129.6, 128.9, 128.7, 70.7, 70.2, 65.1, 32.2, 29.1, 28.6, 25.7.

IR (KBr, thin film): 3027, 2934, 2860, 1715, 1627, 1489, 1453, 1291, 1201, 953, 755, 702 cm^{-1}.



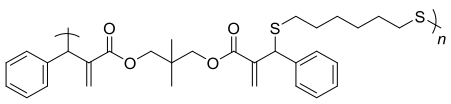
γ-P1b/2a

γ-P1b/2a: 68% yield, 5:95 *rr*, M_n = 6800, *Đ* = 1.67.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30–7.15 (m, 10H), 6.42 (s, 2H), 6.02 (s, 2H), 4.96 (s, 2H), 3.91–3.67 (m, 4H), 2.35 (s, 4H), 1.64–1.44 (m, 4H), 0.84–0.69 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 140.2, 139.7, 128.5, 128.2, 127.4,127.4, 69.7, 49.3, 45.4, 31.9, 28.1, 21.6.

IR (KBr, thin film): 3026, 2933, 2856, 1716, 1635, 1540, 1456, 1200, 1130, 952, 750, 701 cm^{-1}.



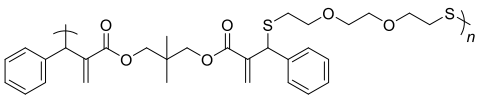
γ-P1b/2c

γ-P1b/2c: 70% yield, 4:96 *rr*, M_n = 14500, *Đ* = 1.53.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35–7.15 (m, 10H), 6.43 (s, 2H), 6.04 (s, 2H), 4.97 (s, 2H), 3.91–3.69 (m, 4H), 2.45–2.27 (m, 4H), 1.53–1.40 (m, 4H), 1.27 (t, *J* = 5.1 Hz, 4H), 0.84–0.76 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 140.2, 139.8, 128.5, 128.2, 127.4, 127.4, 69.7, 49.3, 45.5, 32.4, 28.9，28.4, 21.6.

IR (KBr, thin film): 3027, 2924, 2852, 1717, 1629, 1558, 1456, 1410, 1312, 1128, 990, 751, 701 cm^{-1}.



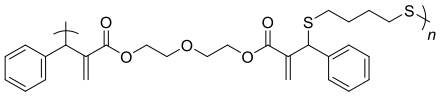
γ-P1b/2d

γ-P1b/2d: 73% yield, 2:98 *rr*, M_n = 13000, *Đ* = 1.56.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37–7.15 (m, 10H), 6.43 (s, 2H), 6.05 (s, 2H), 5.06 (s, 2H), 3.61–3.43 (m, 8H), 2.60 (t, *J* = 6.7 Hz, 4H), 0.80 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.6, 140.1, 139.6, 128.5, 128.3, 127.5, 127.4, 70.4, 70.2, 69.7, 49.5, 34.9, 31.7, 21.6.

IR (KBr, thin film): 3027, 2834, 2860, 1715, 1627, 1489, 1453, 1291, 1130, 953, 755, 702 cm^{-1}.



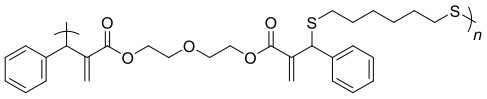
γ-P1c/2a

γ-P1b/2c: 71% yield, 7:93 *rr*, M_n = 10600, *Đ* = 1.52.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49–7.16 (m, 10H), 6.44 (s, 2H), 6.03 (s, 2H), 5.00 (s, 2H), 4.30–4.10 (m, 4H), 3.56 (t, *J* = 4.7 Hz, 4H), 2.34 (s, 4H), 1.63–1.52 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.9, 140.3, 139.8, 128.5, 128.3, 127.4, 127.3, 68.9, 64.0, 49.2, 31.9, 28.0.

IR (KBr, thin film): 3027, 2946, 2852, 1716, 1558, 1507, 1456, 1312, 1246, 1200, 1030, 954, 755, 702 cm^{-1}.



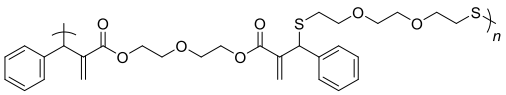
γ-P1c/2c

γ-P1c/2c: 71% yield, 7:93 *rr*, M_n = 16300, *Đ* = 1.52.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49–7.20 (m, 10H), 6.44 (s, 2H), 6.04 (s, 2H), 5.01 (s, 2H), 4.20 (tq, *J* = 12.4, 8.1, 6.7 Hz, 4H), 3.56 (t, *J* = 4.7 Hz, 4H), 2.36 (t, *J* = 6.2 Hz, 4H), 1.56–1.37 (m, 4H), 1.27 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.9, 140.4, 134.0, 128.4, 128.3, 127.3, 127.2, 68.9, 64.0, 49.2, 32.4, 28.9, 28.3.

IR (KBr, thin film): 3027, 2927, 2855, 1716, 1507, 1489, 1312, 1124, 1030, 953, 755, 702 cm^{-1}.



γ-P1c/2d

γ-P1c/2d: 70% yield, 1:99 *rr*, M_n = 10100, *Đ* = 1.67.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39–7.16 (m, 10H), 6.45 (s, 2H), 6.06 (s, 2H), 5.10 (s, 2H), 4.27–4.10 (m, 4H), 3.57 (tt, *J* = 9.0, 4.1 Hz, 8H), 3.51 (s, 4H), 2.59 (t, *J* = 6.8 Hz, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 140.3, 139.8, 128.5, 128.4, 127.4, 127.4, 70.4, 70.2, 68.9, 64.0, 49.4, 31.7.

IR (KBr, thin film): 3055, 2919, 2864, 1716, 1646, 1507, 1455, 1290, 1248, 1122, 1031, 957, 736, 702 cm^{-1}.

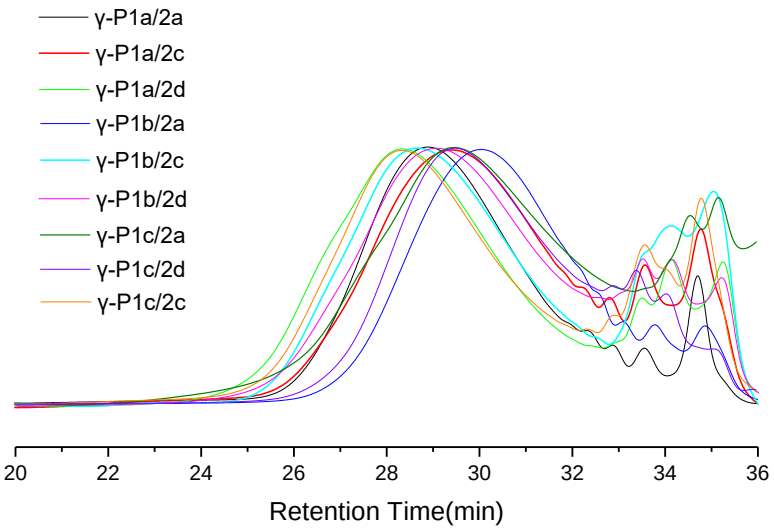


Figure S3. SEC traces of all resulting γ-polymers.

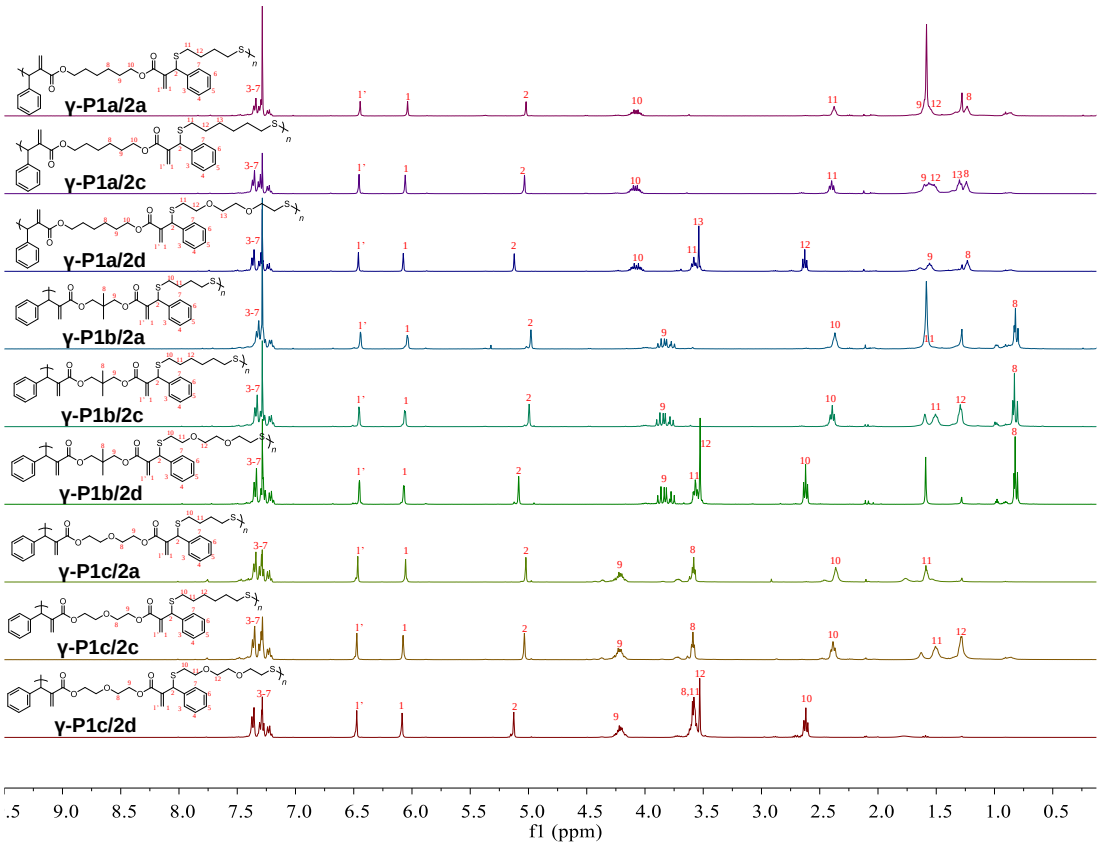


Figure S4. ^{1}H NMR spectral of all resulting γ-polymers.

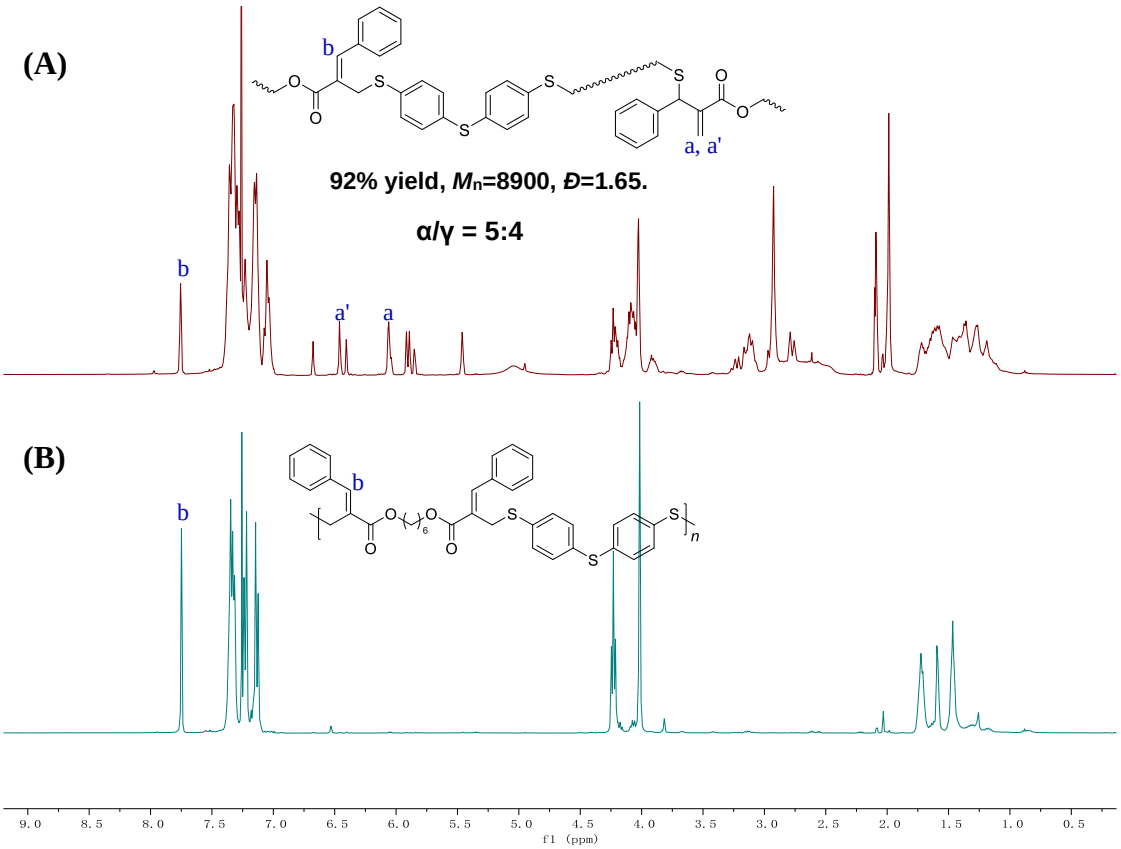
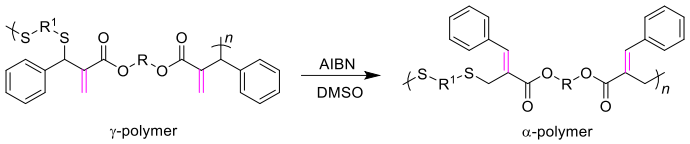


Figure S5. ^{1}H NMR spectral for the γ-regioselective polymerization of aryl thiol and MBH acetate. (A) the polymer formed from the γ-regioselective polymerization. (B) **α-P1a/2e** was used for comparison.

Scheme S6. General procedure of the transformation of γ-polymers to α-polymers.



A 10 mL Schlenk vial equipped with a stir bar was charged with γ-polymers (0.2 mmol), followed by the AIBN (0.01 mmol) and DMSO (2.0 mL). The vial was sealed, and the solution was deoxygenated via three freeze-pump-thaw cycles and then backfilled with nitrogen. After stirring at 70 °C for 15 h, the vial was cooled in an ice bath and exposed to air to stop the reaction. Next, the reaction mixture was diluted with a minimum amount of DCM and precipitated in hexane, yielding the polymer that was then characterized using SEC and ^{1}H-NMR.

NMR analysis of the conversion of γ-P1a/2a.

Determination of the conversion for the polymer backbone modification of **γ-P1a/2a** was made based on the assumption that the integral of the peak at δ = 6.02 ppm (Peak a, Figure S6) corresponds to the vinyl group of the polymer **γ-P1a/2a**, and the integral of the peak at δ = 7.71 ppm (Peak b, Figure S6) corresponds to internal alkene of **α-P1a/2a**. When the integral of Peak a is normalized to 1, the monomer conversion α is calculated based on the following equation:

$$\lambda = \frac{b}{a+b} \times 100\%$$

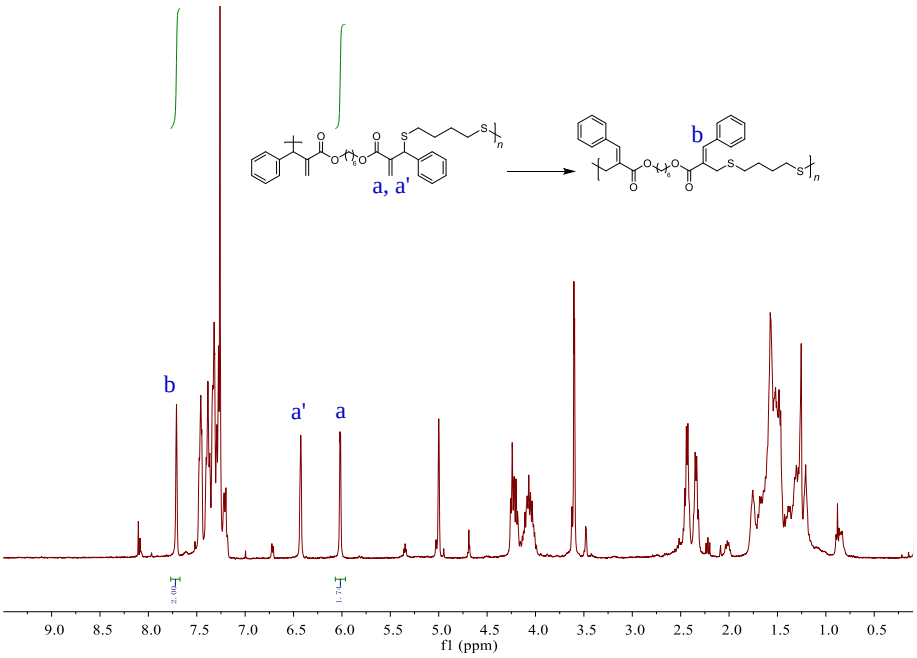


Figure S6. NMR determination of conversion for the transformation of **γ-P1a/2a** to **α-P1a/2a**.

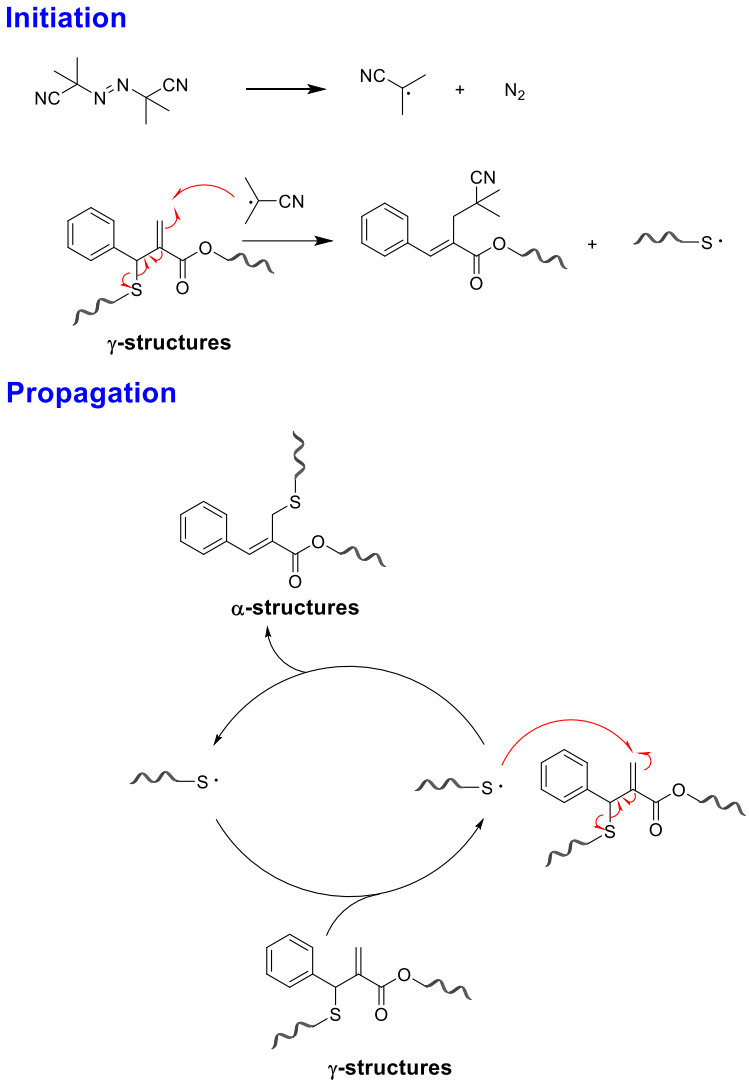
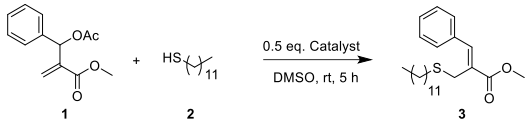


Figure S7. Reaction mechanism for the transformation of γ-polymers to α-polymers**.**

Optimization of Model Reaction

Table S1. Effect of different catalysts on the α-regioselective model reaction.



Entry[a]	Catalysts	Conversion(%)[b]	Yield (%)[b]	*rr*[c]
1	Et_3N	>99	88	>99:1
2	K_2CO_3	>99	74	>99:1
3	1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU)	>99	61	>99:1
4	Diazabicyclononene (DBN)	>99	62	>99:1
5	KO^tBu	>99	76	>99:1
6	1,1,3,3-Tetramethylguanidine (TMG)	>99	76	89:11

[a] Experimental conditions: [**M**] = 0.2 M, reacted at room temperature for 5 h, unless otherwise noted. [b] Conversion and yield were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an external standard. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, calculated by ^{1}H NMR spectroscopy.

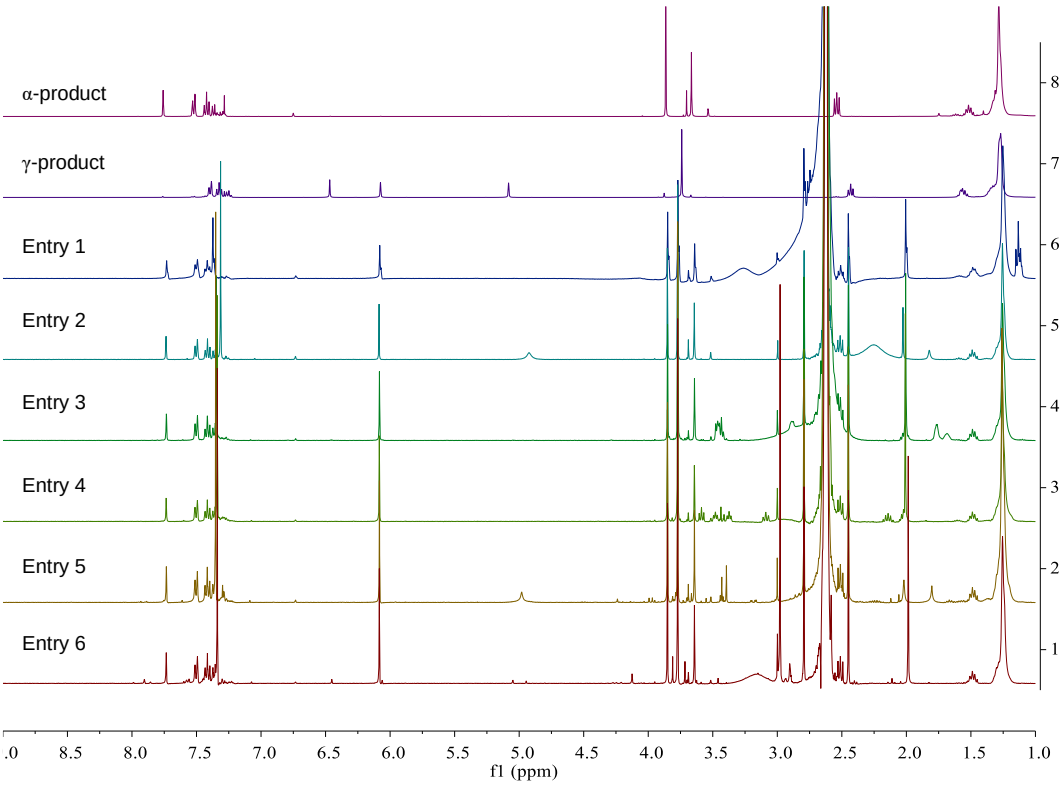
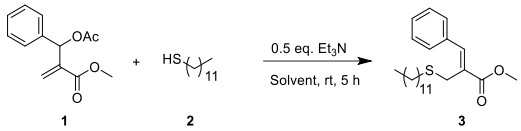


Figure S8. ^{1}H NMR traces for the α-regioselective model reaction catalyzed by different catalysts.

Table S2. Effect of different solvents on the α-regioselective model reaction.



Entry[a]	Solvents	Conversion(%)[b]	Yield (%)[b]	*rr*[c]
1	DMF	99	75	>99:1
2	NMP	99	74	>99:1
3	Toluene	5	4	>99:1
4	THF	14	9	>99:1
5	DCM	20	13	>99:1
6	DMSO	>99	88	>99:1

[a] Experimental conditions: [**M**] = 0.2 M, reacted at room temperature for 5 h, unless otherwise noted. [b] Conversion and yield were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an external standard. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, calculated by ^{1}H NMR spectroscopy.

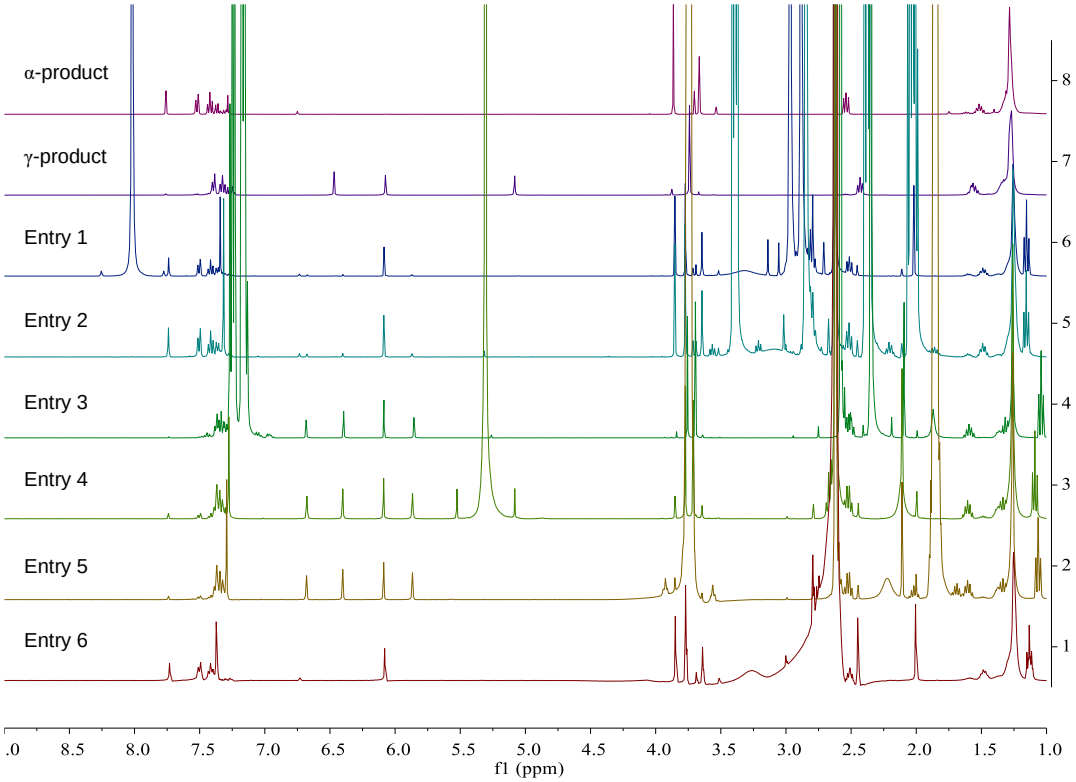
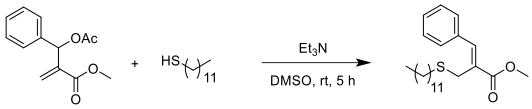


Figure S9. ^{1}H NMR traces for the α-regioselective model reaction in different solvents.

Table S3. Effect of different amounts of Et_3N on the α-regioselective model reaction.



Entry[a]	Equiv. of Et_3N	Conversion(%)[b]	Yield (%)[b]	*rr*[c]
1	0	86	65	>99:1
2	0.2	>99	80	>99:1
3	0.5	>99	88	>99:1
4	1.0	>99	83	>99:1

[a] Experimental conditions: [**M**] = 0.2 M, reacted at room temperature for 5 h, unless otherwise noted. [b] Conversion and yield were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an external standard. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, calculated by ^{1}H NMR spectroscopy.

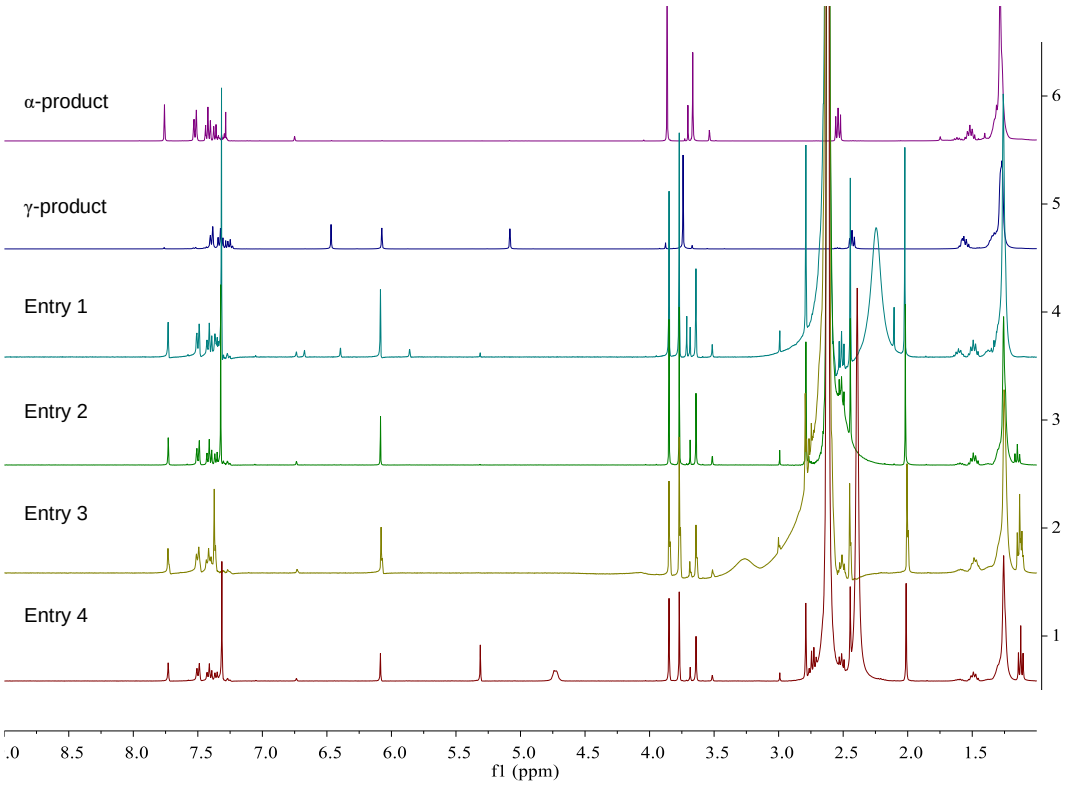
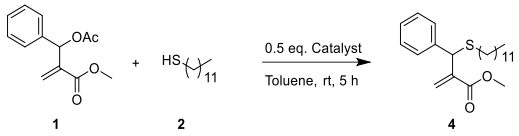


Figure S10. ^{1}H NMR traces for the α-regioselective model reaction in different amounts of Et_3N.

Table S4. Effect of different catalysts on the γ-regioselective model reaction.



Entry[a]	Catalysts	Conversion(%)[b]	Yield (%)[b]	*rr*[c]
1	DABCO	>99	96	1:>99
2	DMAP	88	73	3:97
3	Triphenylphosphine	33	13	1:>99
4	Dimethylphenylphosphine	94	44	1:>99
5	Diphenylpropylphosphine	>99	38	1:>99

[a] Experimental conditions: [**M**] = 0.2 M, reacted at room temperature for 5 h, unless otherwise noted. [b] Conversion and yield were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an external standard. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, calculated by ^{1}H NMR spectroscopy.

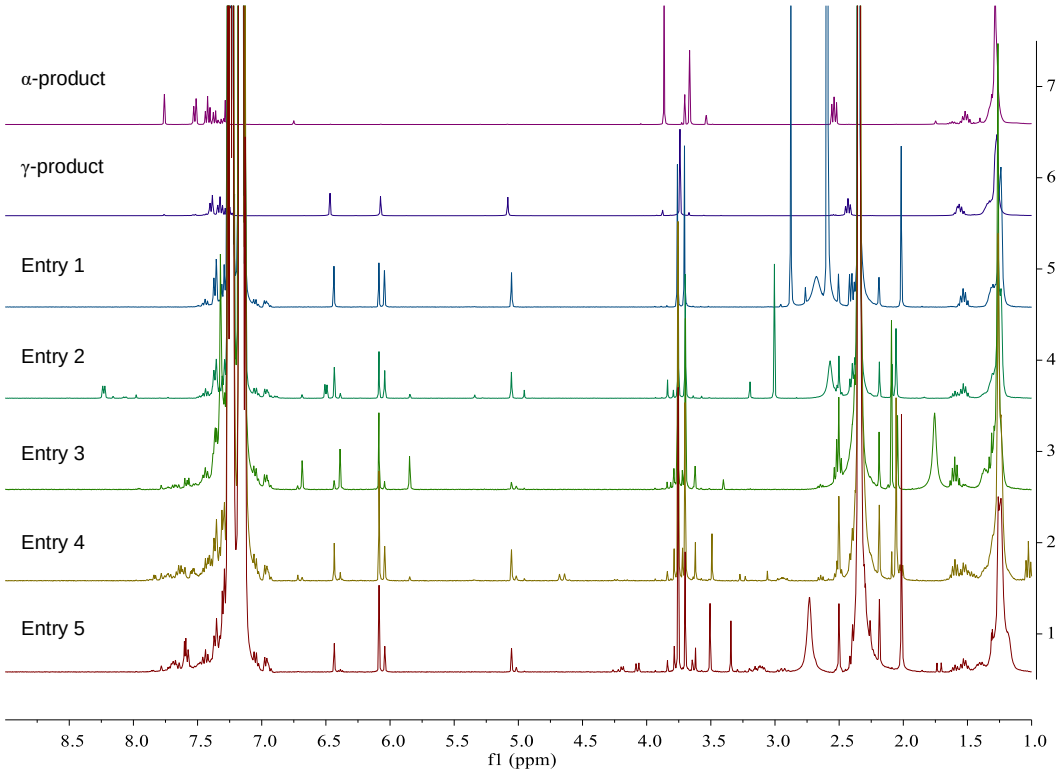
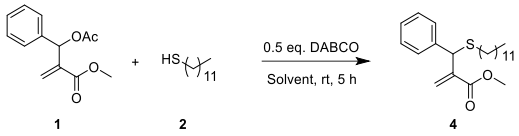


Figure S11. ^{1}H NMR traces for the γ-regioselective model reaction catalyzed by different catalysts.

Table S5. Effect of different solvents on the γ-regioselective model reaction.



1 2 4

Entry[a]	Solvents	Conversion(%)[b]	Yield (%)[b]	*rr*[c]
1	DMSO	>99	65	14:86
2	DMF	>99	84	10:90
3	NMP	>99	82	10:90
4	THF	>99	94	1:>99
5	DCM	98	96	1:>99
6	Toluene	>99	96	1:>99

[a] Experimental conditions: [**M**] = 0.2 M, reacted at room temperature for 5 h, unless otherwise noted. [b] Conversion and yield were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an external standard. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, calculated by ^{1}H NMR spectroscopy.

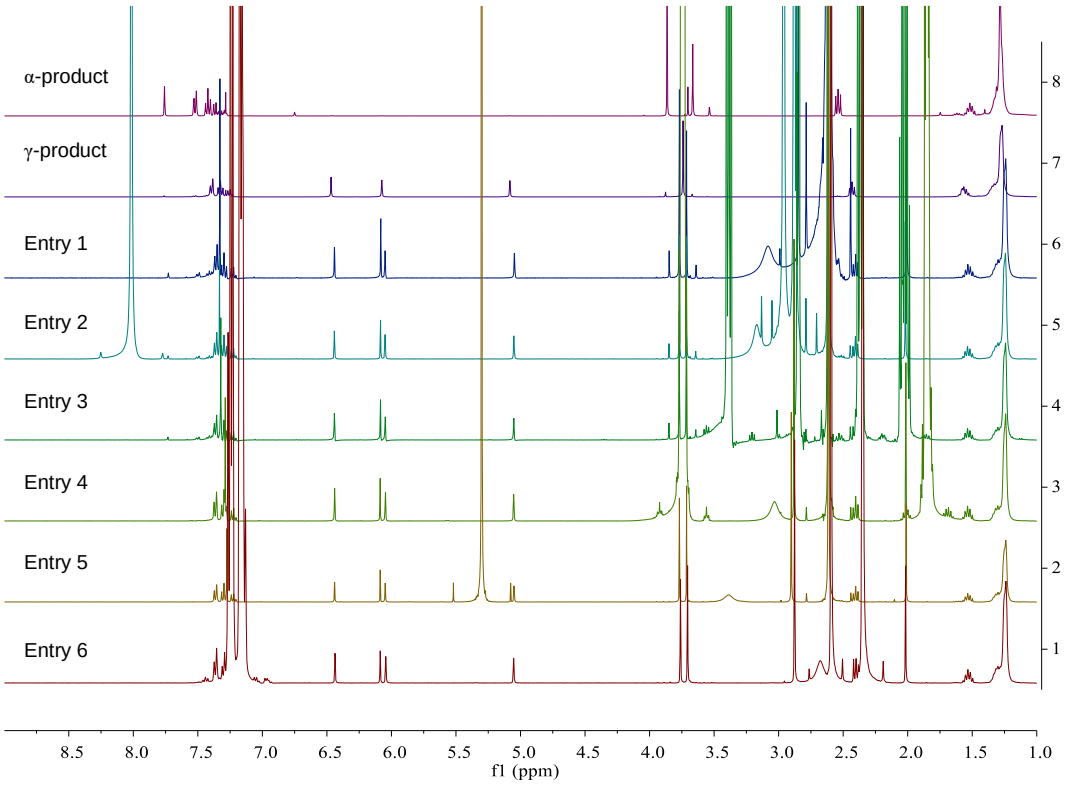
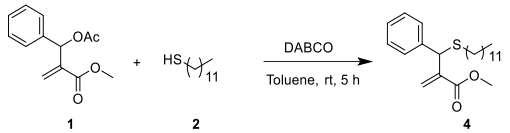


Figure S12. ^{1}H NMR traces for the γ-regioselective model reaction in different solvents.

Table S6. Effect of different amounts of DABCO on the γ-regioselective model reaction.



Entry[a]	Equiv. of DABCO	Conversion(%)[b]	Yield (%)[b]	*rr*[c]
1	0.2	55	53	1:>99
2	0.5	>99	96	1:>99
3	1.0	>99	100	1:>99

[a] Experimental conditions: [**M**] = 0.2 M, reacted at room temperature for 5 h, unless otherwise noted. [b] Conversion and yield were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an external standard. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, calculated by ^{1}H NMR spectroscopy.

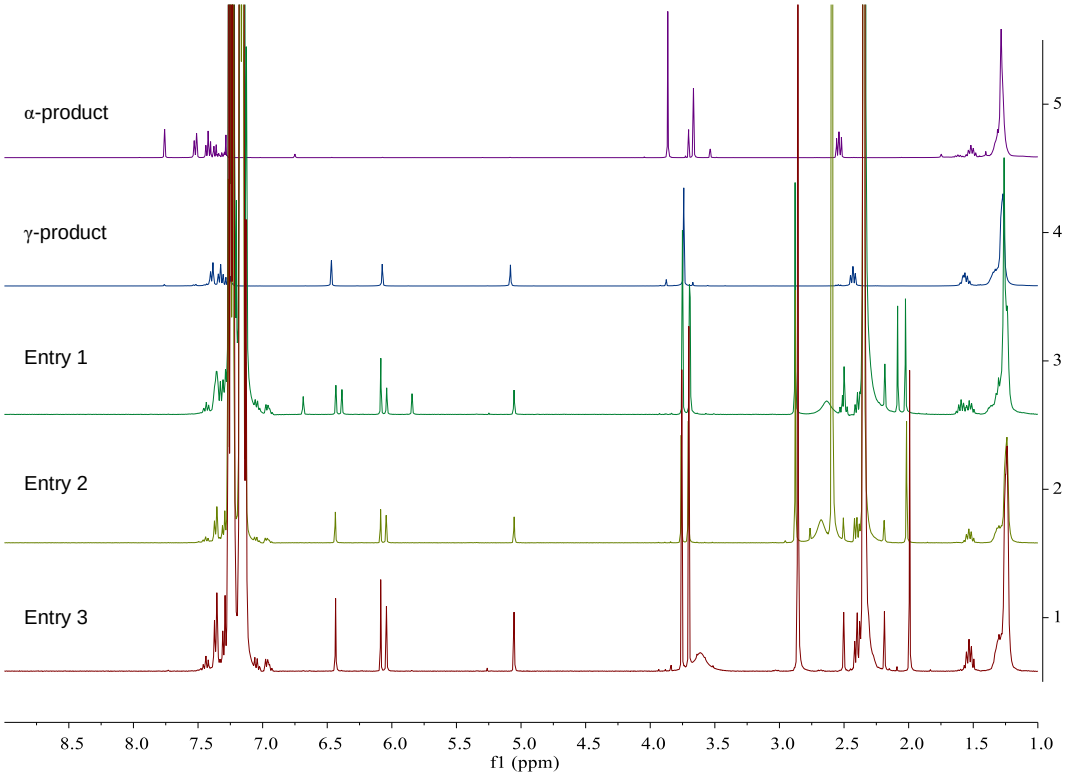
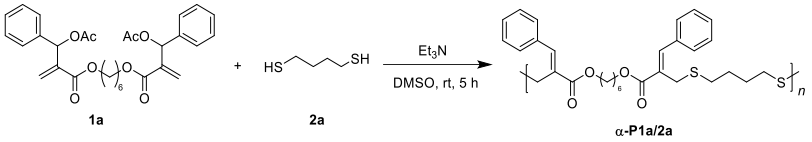


Figure S13. ^{1}H NMR traces for the γ-regioselective model reaction in different amounts of DABCO.

Optimization of Polymerization

Table S7. Effect of different amounts of Et_3N on the α-regioselective polymerization.



Entry[a]	Equiv. of Et_3N	Yield (%)	$M_{n\ (SEC)}$[b]	$Đ$[b]	rr[c]
1	0	37	1100	1.49	>99:1
2	0.2	57	6400	1.75	>99:1
3	0.5	82	8800	1.98	>99:1
4	1.0	81	7700	1.92	>99:1

[a] Experimental conditions: [**M**] = 0.2 M, room temperature for 5 h, unless otherwise noted. [b] $M_{n\ (SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [c] The regioselectivity ratio (rr) is the equivalent ratio of α-structures to γ-structures, which was determined by ^{1}H NMR spectroscopy.

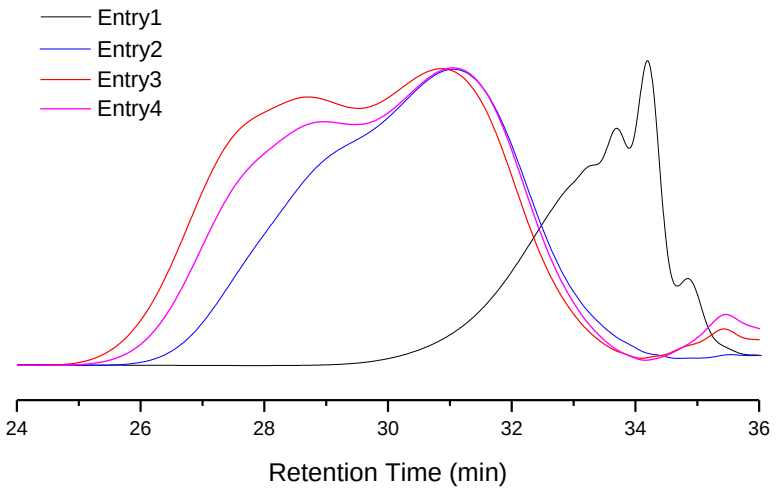
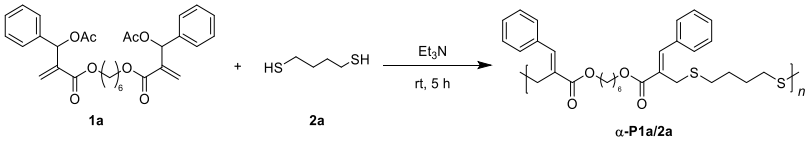


Figure S14. SEC traces for the α-regioselective polymerization in different amounts of Et_3N.

Table S8. Effect of different solvents on the α-regioselective polymerization.



Entry[a]	Solvent	Yield (%)	$M_{n\ (SEC)}$[b]	$Đ$[b]	rr[c]
1	DMF	56	1700	1.90	>99:1
2	NMP	47	1600	1.84	>99:1
3	DMSO	82	8800	1.98	>99:1
4[d]	DCM	--	--	--	--
5[d]	THF	--	--	--	--
6[d]	Toluene	--	--	--	--
7[e]	DMF	63	4000	1.57	>99:1
8[e]	NMP	62	3700	1.49	>99:1
9[f]	DMF	74	5700	1.95	>99:1
10[f]	NMP	79	6100	2.15	>99:1

[a] Experimental conditions: [**M**] = 0.2 M, 0.5 equiv. Et_3N, room temperature for 5 h, unless otherwise noted. [b] $M_{n\ (SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [c] The regioselectivity ratio (rr) is the equivalent ratio of α-structures to γ-structures, which was determined by ^1H NMR spectroscopy. [d] No polymers precipitated in hexane. [e] 12h. [f] 1.0 equiv. Et_3N, 12h.

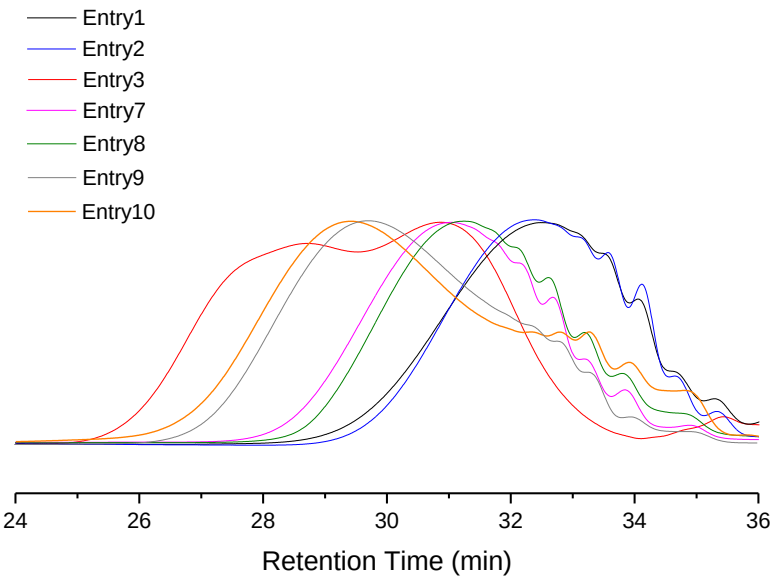
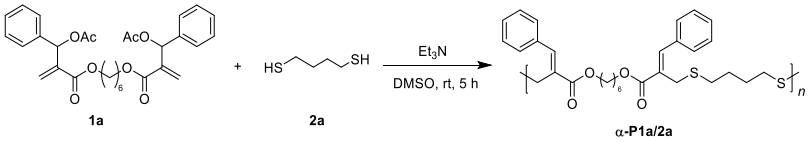


Figure S15. SEC traces for the α-regioselective polymerization in different solvents.

Table S9. Effect of different monomer concentrations on the α-regioselective polymerization.



Entry[a]	Concentration of monomer	Yield (%)	$M_{n\,(SEC)}$[b]	$Đ$[b]	*rr*[c]
1	0.1 mol/L	25	1400	1.29	>99:1
2	0.2 mol/L	82	8800	1.98	>99:1
3	0.4 mol/L	79	6000	1.86	>99:1
4[d]	0.4 mol/L	83	10100	2.25	>99:1

[a] Experimental conditions: room temperature under air for 5 h, unless otherwise noted. [b] $M_{n\,(SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, which was determined by ^{1}H NMR spectroscopy. [d] 10 h.

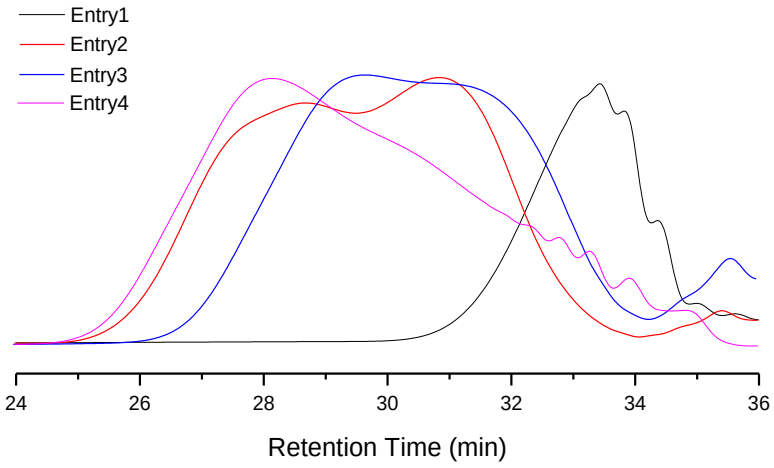
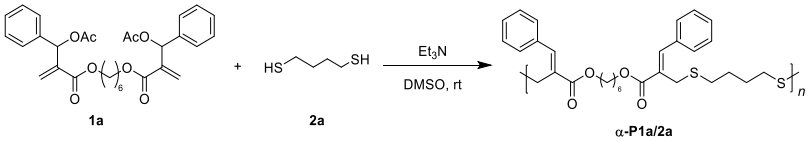


Figure S16. SEC traces for the α-regioselective polymerization at different monomer concentrations.

Table S10. Reaction time effect on the α-regioselective polymerization.



Entry[a]	Time	Yield (%)	$M_{n\,(SEC)}$[b]	$Đ$[b]	*rr*[c]
1	5 h	82	8800	1.98	>99:1
2	12 h	88	18900	1.68	>99:1
3	16 h	87	21100	1.92	>99:1

[a] Experimental conditions: [**M**] = 0.2 M, 0.5 equiv. Et_3N, room temperature for a given time, unless otherwise noted. [b] $M_{n\,(SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, which was determined by ^{1}H NMR spectroscopy.

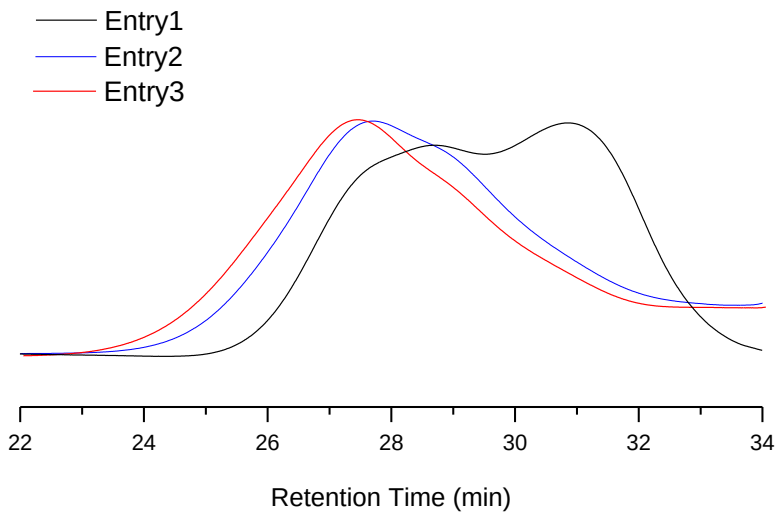
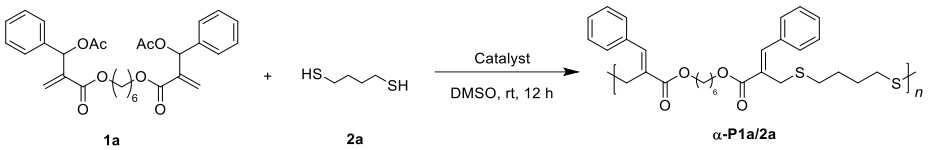


Figure S17. SEC traces for the α-regioselective polymerization at different reaction time.

Table S11. Screen of different catalysts for the regioselective polymerization.



1a **2a** **α-P1a/2a**

Entry[a]	Catalyst	Yield (%)	$M_{n\,(SEC)}$[b]	$Đ$[b]	*rr*[c]
1	Et_3N	88	18900	1.68	>99:1
2	DBU	85	2800	2.01	>99:1
3	DMAP	76	8100	2.74	50:50
4	DABCO	69	5100	1.94	41:59

[a] Experimental conditions: [**M**] = 0.2 M, 0.5 equiv. catalyst, room temperature for 12 h, unless otherwise noted. [b] $M_{n\,(SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [c] The regioselectivity ratio (*rr*) is the equivalent ratio of α-structures to γ-structures, which was determined by ^{1}H NMR spectroscopy.

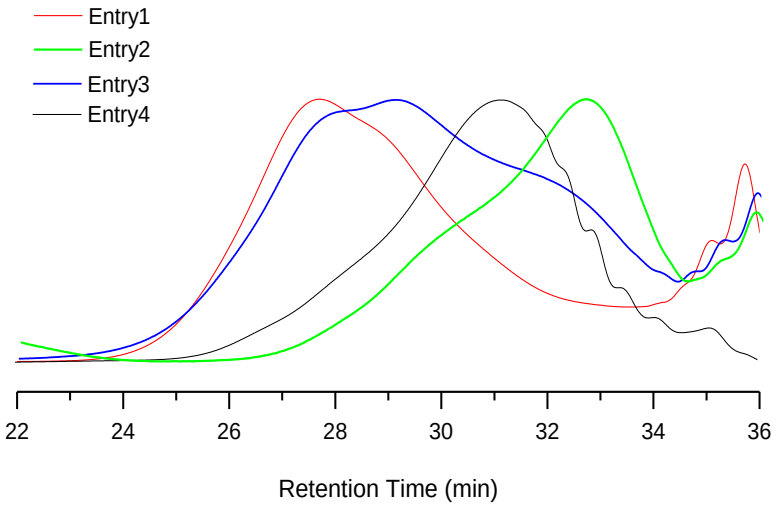
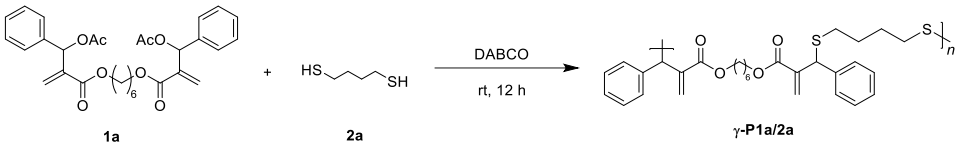


Figure S18. SEC traces for the regioselective polymerization catalyzed by different catalysts.

Table S12. Effect of different solvents on the γ-regioselective polymerization.



Entry[a]	Solvent[a]	Yield (%)	$M_{n\ (SEC)}$[b]	$Đ$[b]	rr[c]
1	DMSO	69	5100	1.94	41:59
2	DMF	65	3300	1.65	52:48
3	NMP	75	3700	1.93	39:61
4	THF	73	6800	1.49	3:97
5	Toluene	70	14100	1.58	2:98
6[d]	Toluene	74	15100	1.68	2:98

[a] Experimental conditions: [**M**] = 0.2 M, 0.5 equiv. DABCO, room temperature under air for 12 h, unless otherwise noted. [b] $M_{n\ (SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [c] The regioselectivity ratio (rr) is the equivalent ratio of α-structures to γ-structures, which was determined by ^{1}H NMR spectroscopy. [d] Reaction time was 16 h.

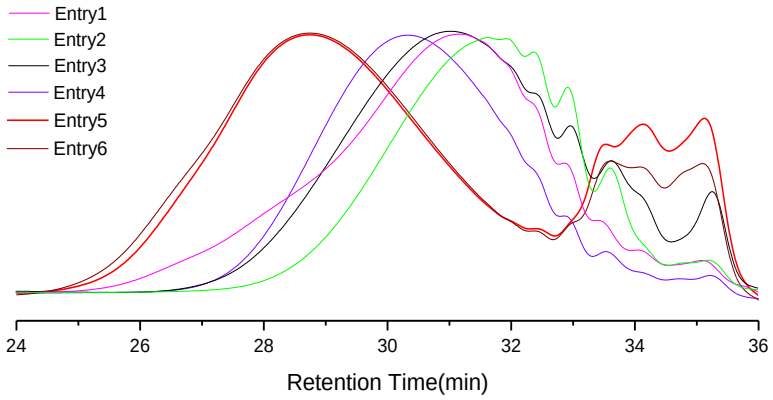
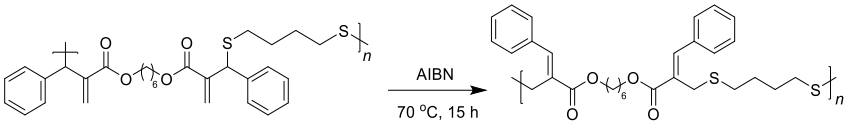


Figure S19. SEC traces for the γ-regioselective polymerization in different solvents.

Optimization of Transformation of γ-Polymers to α-Polymers

Table S13. Screen of different solvents for the polymer transformation.



γ-**P1a/2a** α-**P1a/2a**

Entry[a]	Solvent	Conversion (%)[b]	$M_{n\ (SEC)}$[c]	$Đ$[c]
1	NMP	90	3500	1.54
2	THF	65	15200	2.72
3	DMF	87	5300	1.54
4	DMSO	94	8600	1.71

[a] Experimental conditions: M_n = 14100, $Đ$ = 1.58, [**M**] = 0.1 M, 0.05 equiv. AIBN, 70 °C under nitrogen for 15 h, unless otherwise noted. [b] The conversion was determined based on alkenes of polymers by ^{1}H NMR spectroscopy. [c] $M_{n\ (SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards.

Note: Monomer conversion is the criterion for optimization.

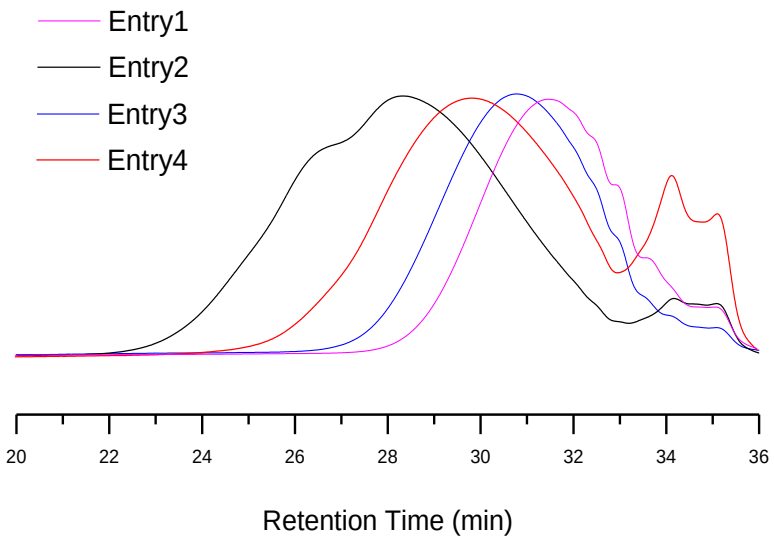
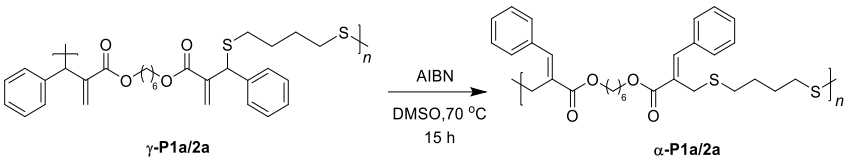


Figure S20. SEC traces for the polymer transformation in different solvents.

Table S14. Effect of different concentrations on the polymer transformation.



γ-P1a/2a α-P1a/2a

Entry[a]	Concentration[b]	Conversion (%)[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	0.05 mol/L	77	5300	1.60
2	0.1 mol/L	94	8600	1.71
3	0.2 mol/L	96	9700	1.76

[a] Experimental conditions: M_n = 14100, $Đ$ = 1.58, 0.05 equiv. AIBN, 70 ℃ under nitrogen for 15 h, unless otherwise noted. [b] Calculated according to the molecular weight of the repeat unit. [c] The conversion was determined based on alkenes of polymers by ^{1}H NMR spectroscopy. [d] $M_{n\ (SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards.

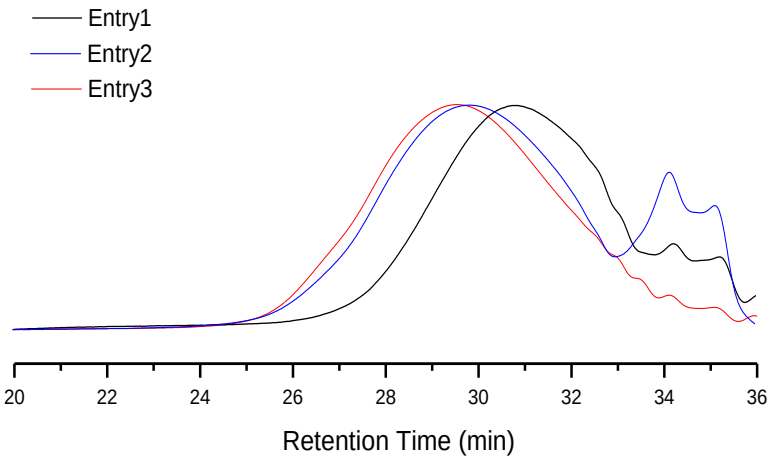
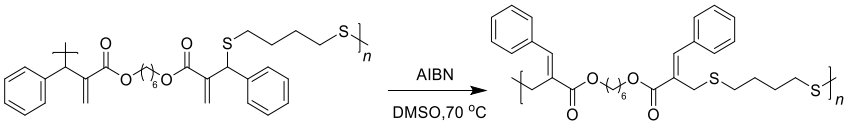


Figure S21. SEC traces for the polymer transformation at different concentrations.

Table S15. Polymer transformation at different reaction time.



γ-P1a/2a α-P1a/2a

Entry	Time (h)	Conversion (%)[b]	$M_{n\,(SEC)}$[c]	$Đ$[c]
1	5	69	6300	1.81
2	10	94	7500	1.64
3	15	96	9700	1.76
4[d]	15	92	8900	1.55
5[d]	25	93	8500	1.51

[a] Experimental conditions: M_n = 14100, $Đ$ = 1.58, [**M**] = 0.2 M, 0.05 equiv. AIBN, 70 ℃ under nitrogen, unless otherwise noted. [b] The conversion was determined based on alkenes of polymers by ^{1}H NMR spectroscopy. [c] $M_{n\,(SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [d] M_n = 16100, $Đ$ = 1.66.

Note: After nearly complete conversion, the polymer's molecular weight was almost unchanged when increasing the reaction time (entry 4 & entry 5), which was probably because this transformation involves fragmentation and recombination of the polymer chains.

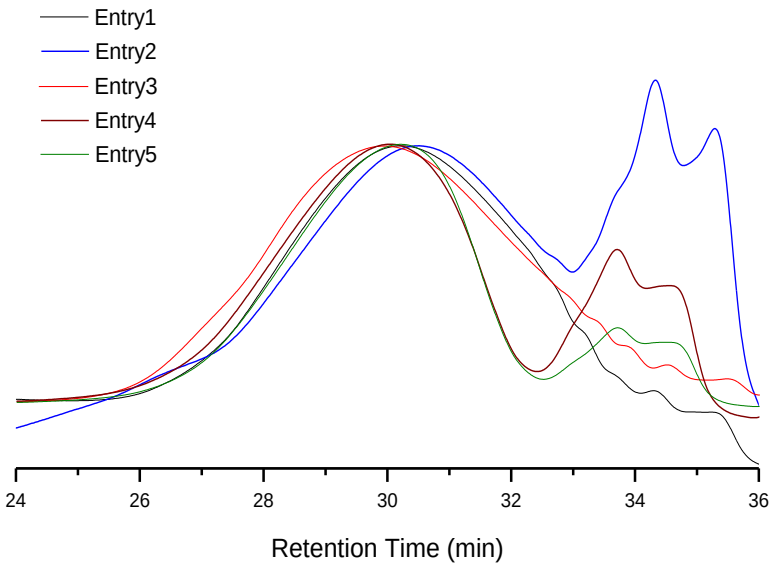
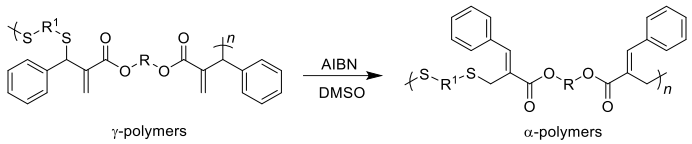


Figure S22. SEC traces for the polymer transformation at different reaction time.

Table S16. Transformation of different γ-polymers.



Entry	γ-Polymers	α-Polymers	Conversion (%)[b]	$M_{n\,(SEC)}$[c]	$Đ$[c]
1	γ-P1a/2a	α-P1a/2a	96	9700	1.76
2[d]	γ-P1a/2a	α-P1a/2a	92	8900	1.55
3	γ-P1a/2d	α-P1a/2d	>99	8900	1.85
4[d]	γ-P1a/2d	α-P1a/2d	>99	7800	1.55
5	γ-P1c/2c	α-P1c/2c	>99	8400	1.67
6[d]	γ-P1c/2c	α-P1c/2c	>99	8400	1.63

[a] Experimental conditions: [**M**] = 0.2 M, 15 h, 0.05 equiv. AIBN, 70 ℃ under nitrogen for 15 h, unless otherwise noted. [b] Conversion was determined based on alkenes of polymers by ^{1}H NMR spectroscopy. [c] $M_{n\,(SEC)}$ and $Đ$ were determined by SEC analysis calibrated to polystyrene standards. [d] Repeating experiment.

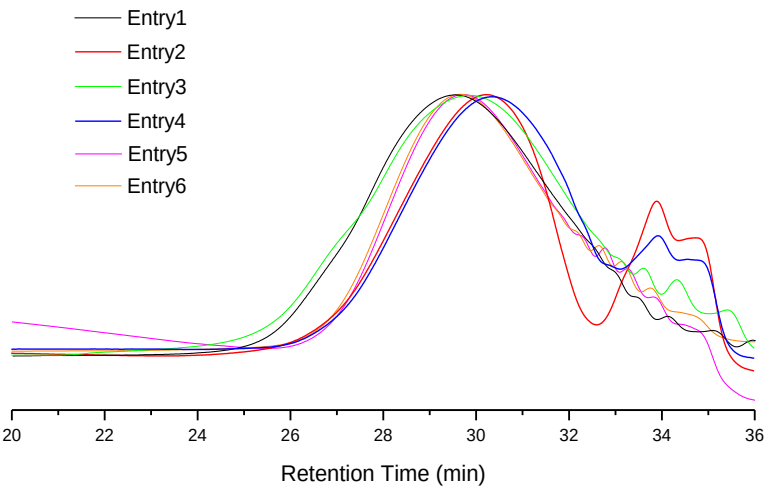


Figure S23. SEC traces for different polymer transformations.

DFT calculations

All geometry optimizations and frequency calculations were carried out employing the M06-2X/6-31+G(d,p) method and the SMD solvation model in toulene. All computed frequencies are real except the transition state structures, which have one imaginary frequency. Single-point energies were calculated using the M06-2X/def2-TZVP and the SMD solvation model in toulene. Gibbs free energies (298.15 K and 1.0 atm) were computed as the sum of the single-point energies and the Gibbs free energy corrections using unscaled normal mode frequencies. All quantum chemical calculations were carried out with the Gaussian computer program.[3]

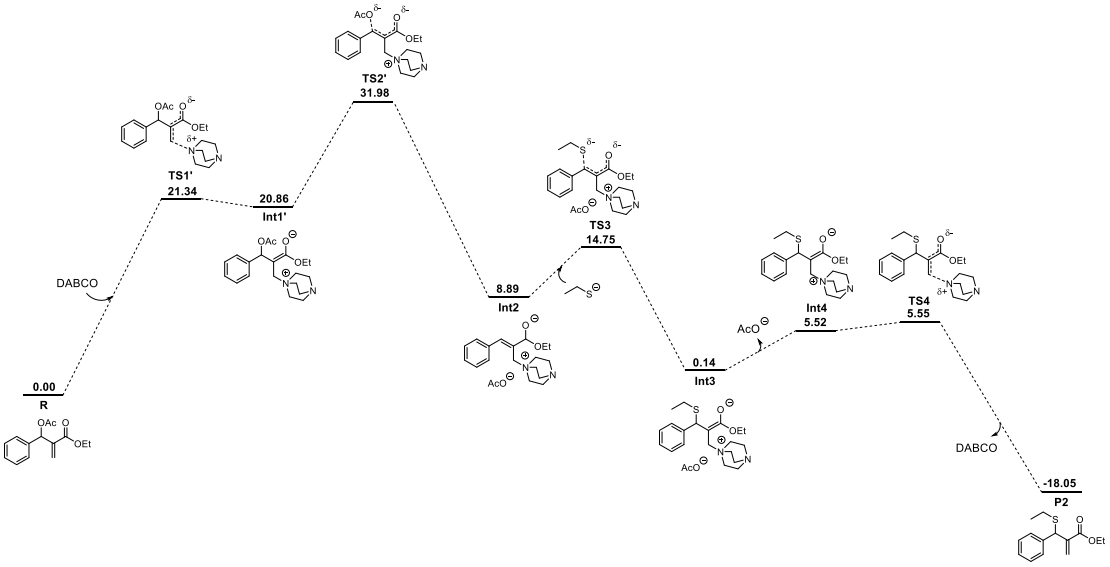


Figure S24. DFT calculation details of pathway B.

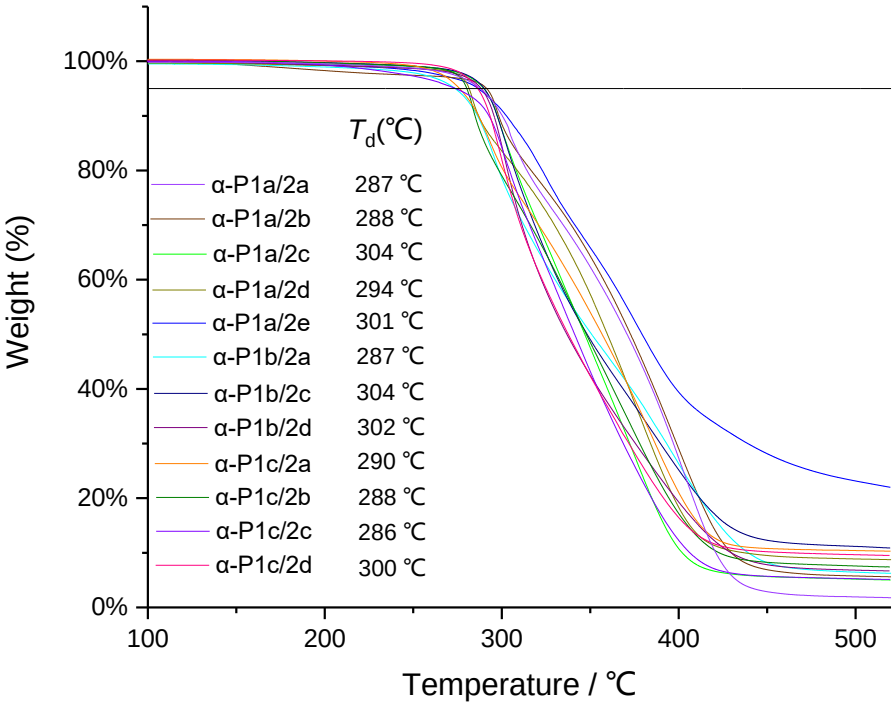


Figure S25. TGA thermograms of different α-polymers recorded under nitrogen at a heating rate of 10 °C /min.

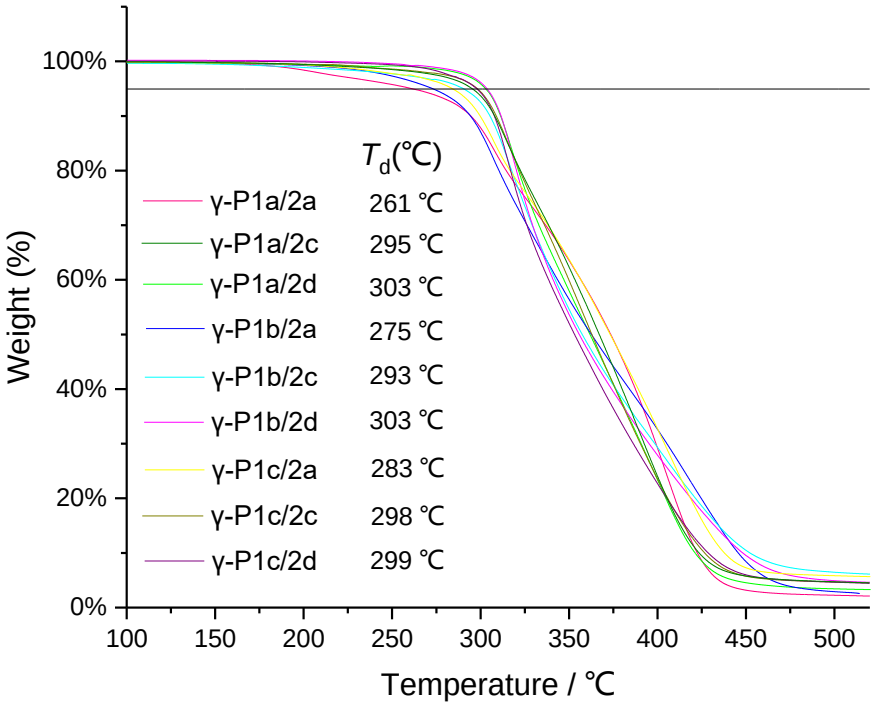


Figure S26. TGA thermograms of different γ-polymers recorded under nitrogen at a heating rate of 10 °C /min.

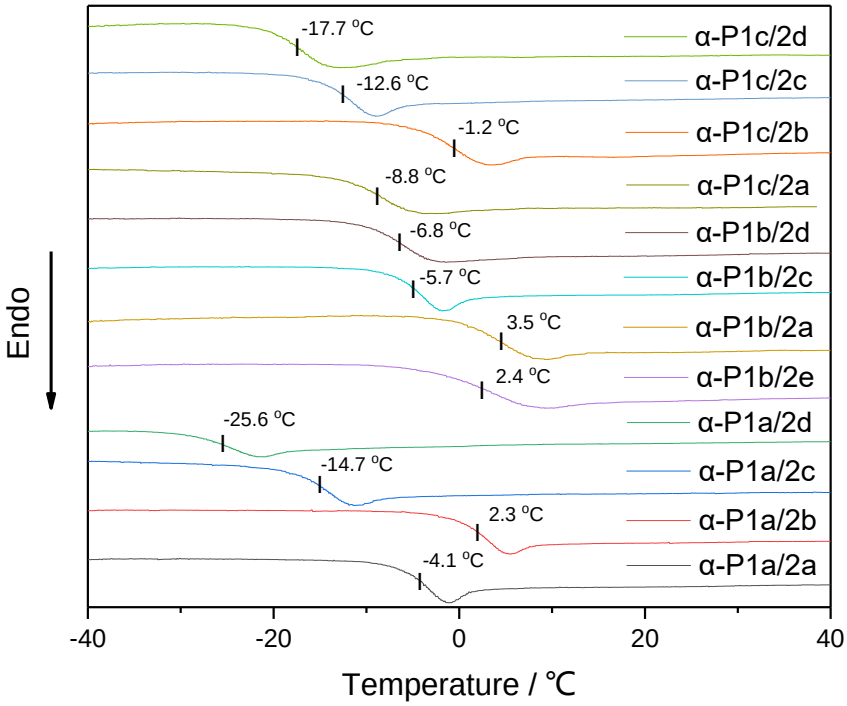


Figure S27. DSC thermograms of different α-polymers recorded under nitrogen during the second heating cycle at a heating rate of 10 °C /min.

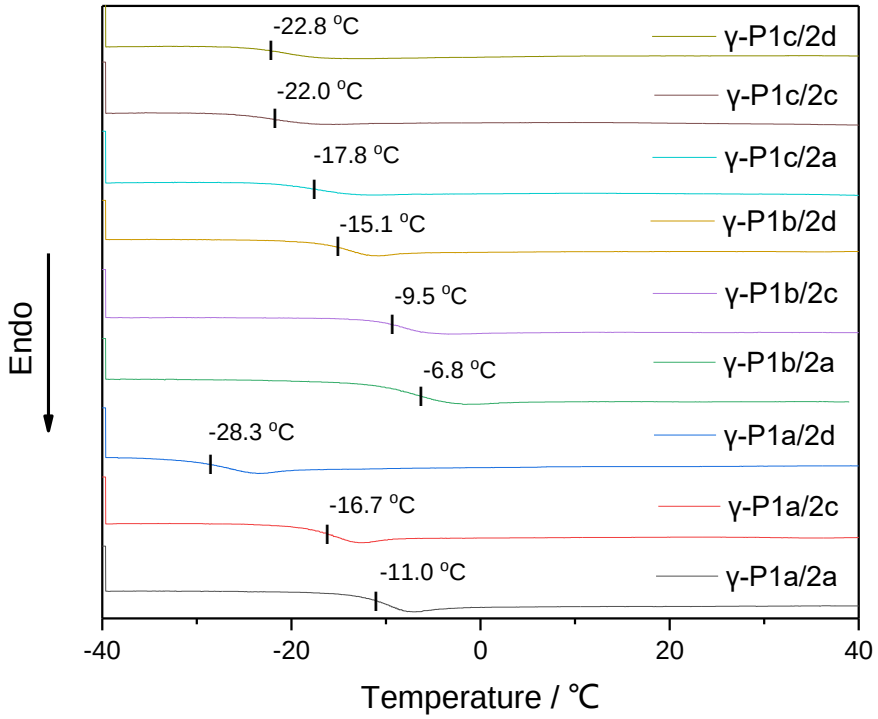


Figure S28. DSC thermograms of different γ-polymers recorded under nitrogen during the second heating cycle at a heating rate of 10 °C /min.

Reference

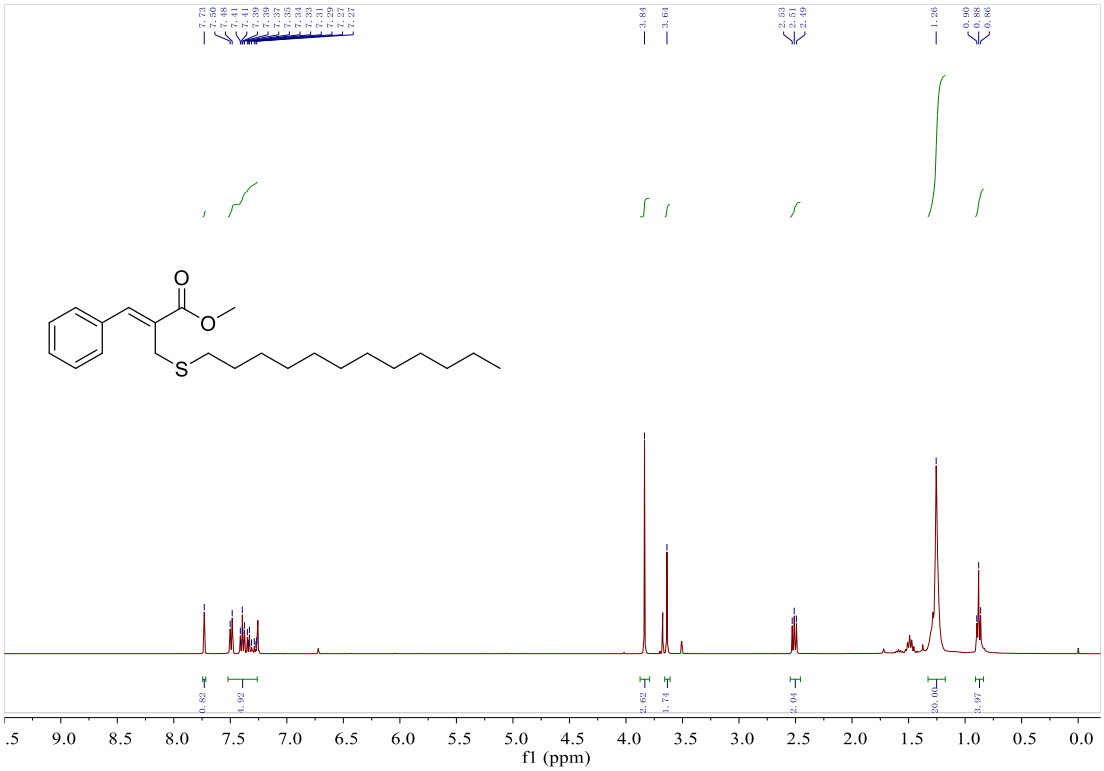
(1) Y.-H. Hu, C.-X. Liu, J.-C. Wang, X.-H. Ren, X. Kan and Y.-B. Dong, TiO2@UiO-68-CIL: A Metal–Organic-Framework-Based Bifunctional Composite Catalyst for a One-Pot Sequential Asymmetric Morita–Baylis–Hillman Reaction, *Inorg. Chem.* 2019, **58**, 4722-4730.

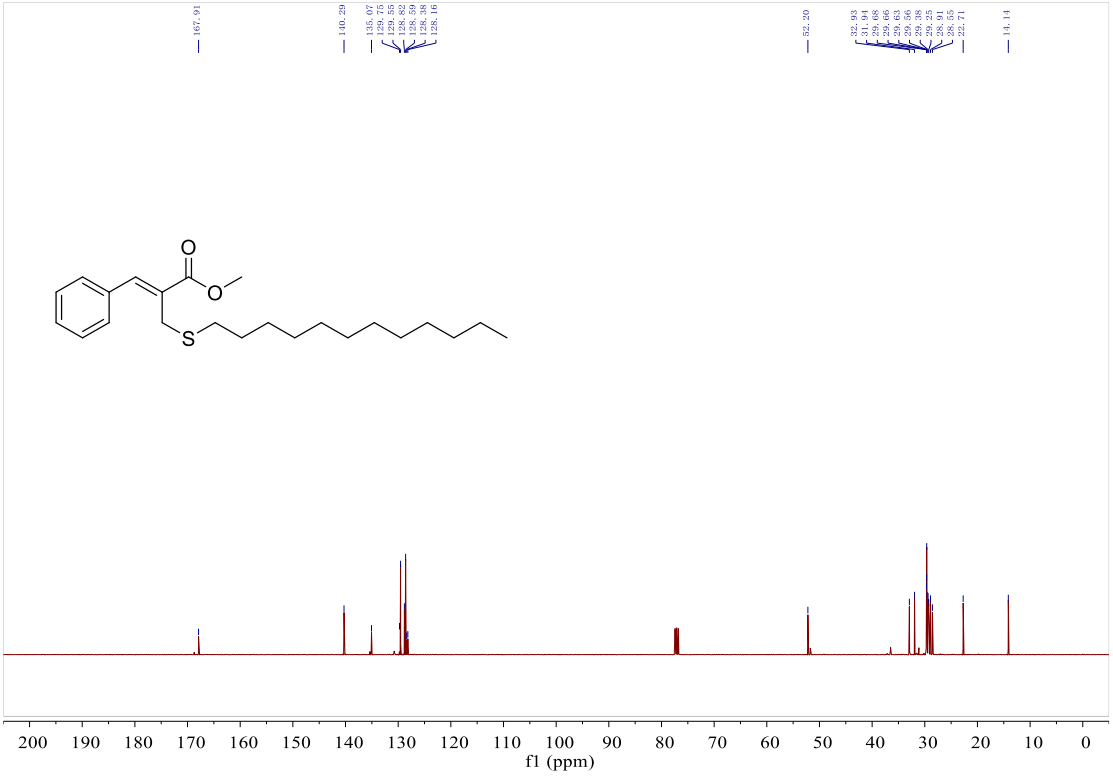
(2) W. X. Wang, Q. Z. Zhang, T. Q. Zhang, Z. S. Li, W. Zhang and W. Yu, *N*-Bromosuccinimide-Mediated Radical Cyclization of 3-Arylallyl Azides: Synthesis of 3-Substituted Quinolines, *Adv. Synth. Catal*. 2015, **357**, 221-226.

(3) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

NMR spectra

NMR of **3**





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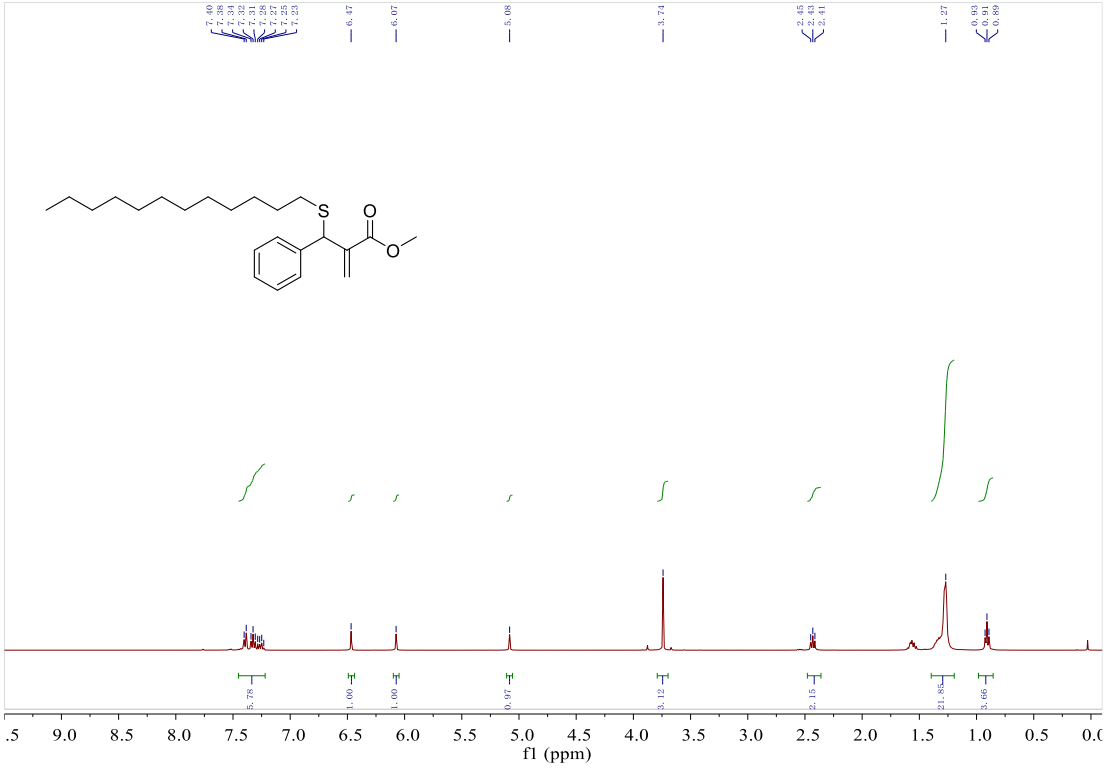
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2.45
2.43
2.41
1.27
0.93
0.91
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O
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1.00
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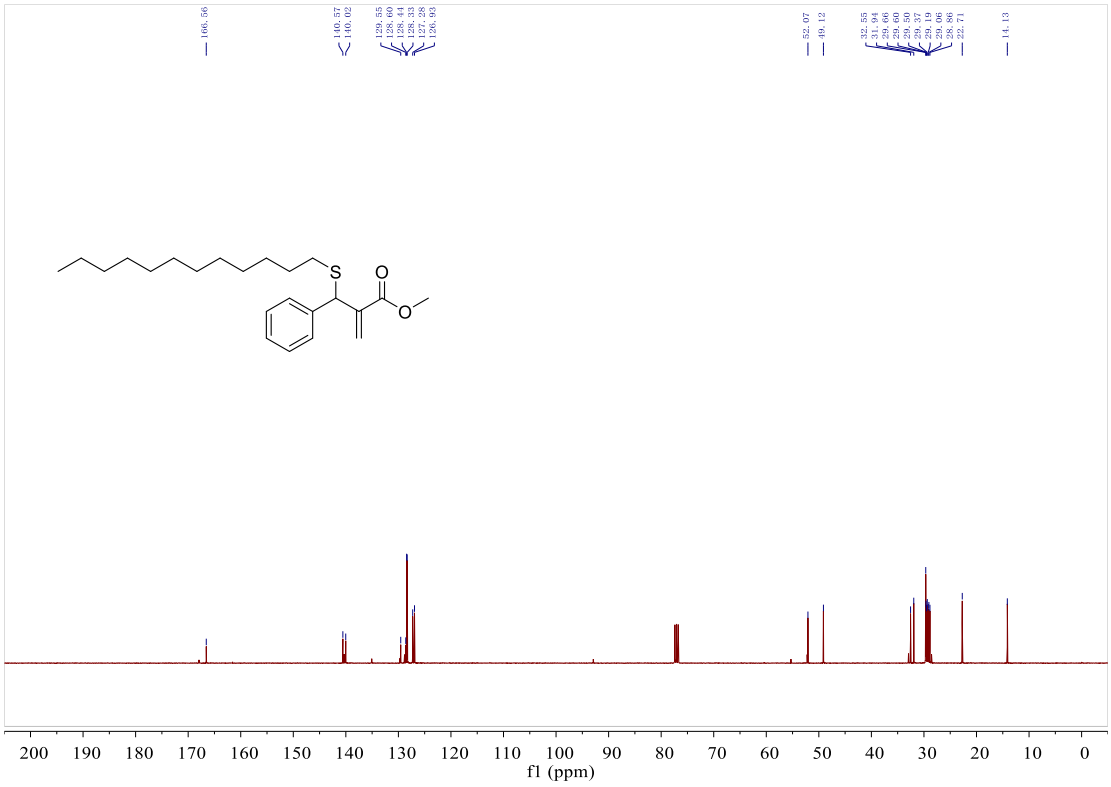
3.66
f1 (ppm)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31.94
29.66
29.60
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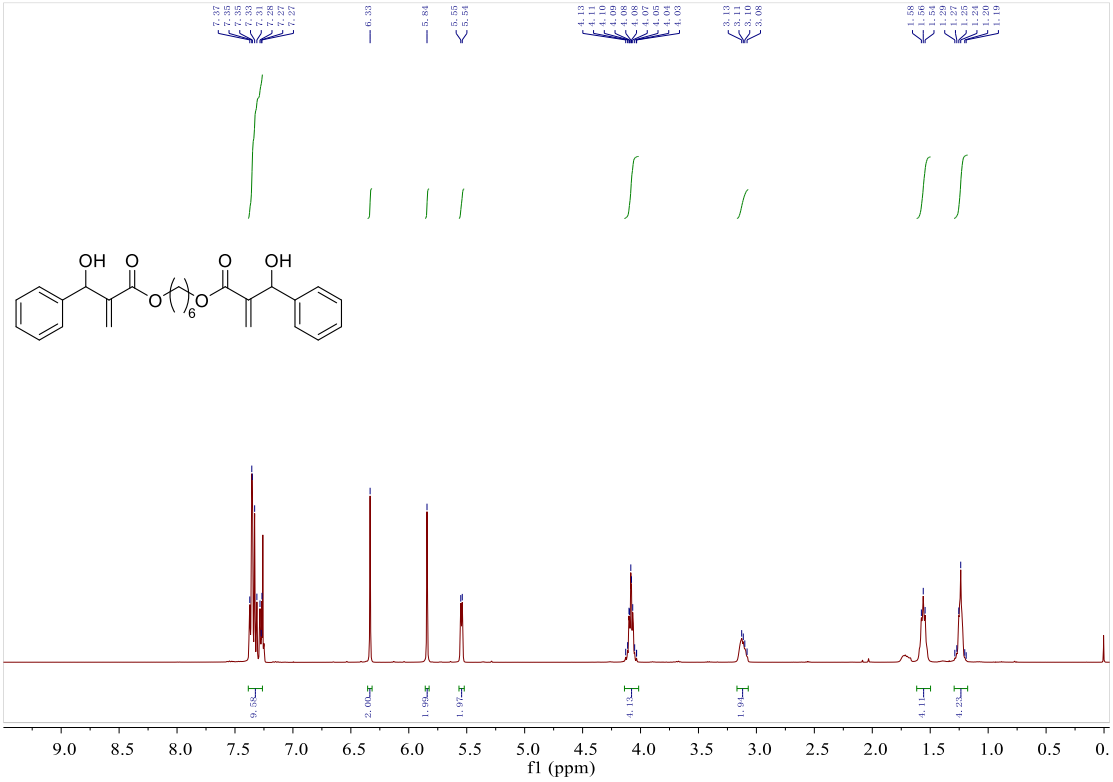
14.13
S
O
O
f1 (ppm)

NMR of **S1a**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4.08
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4.04
4.03
3.13
3.11
3.10
3.08
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1.27
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OH
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7.0
6.5
6.0
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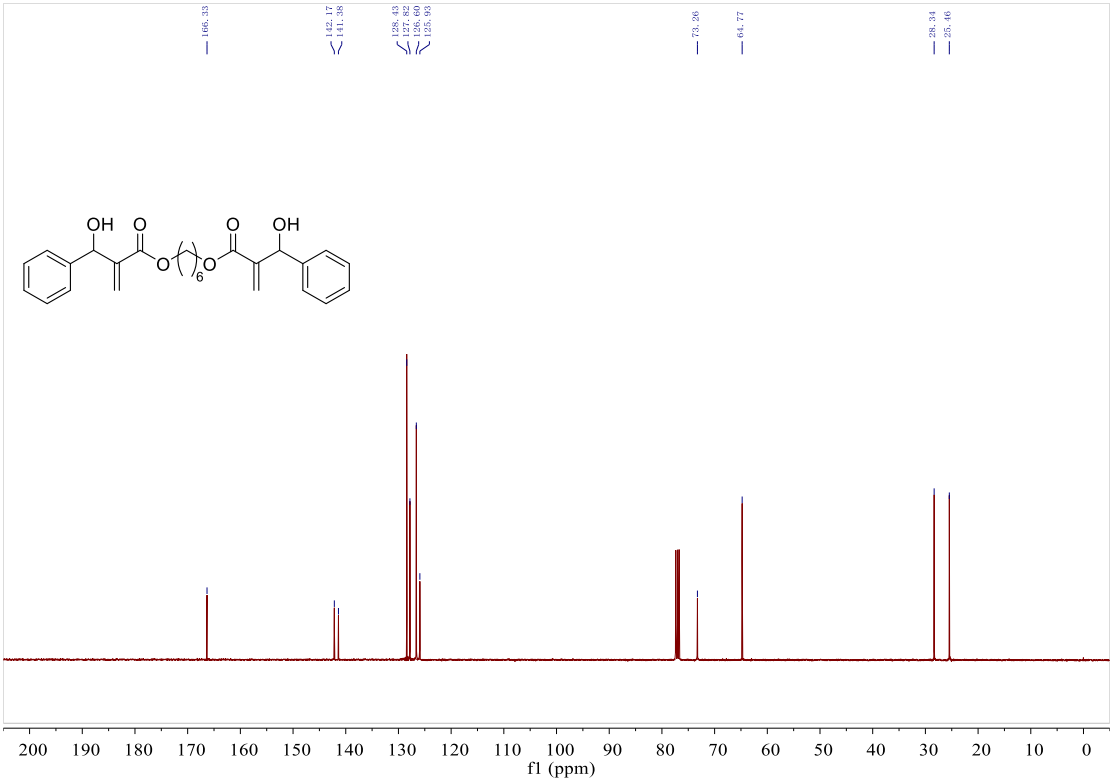
f1 (ppm)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O
O
OH
6
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180
170
160
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20
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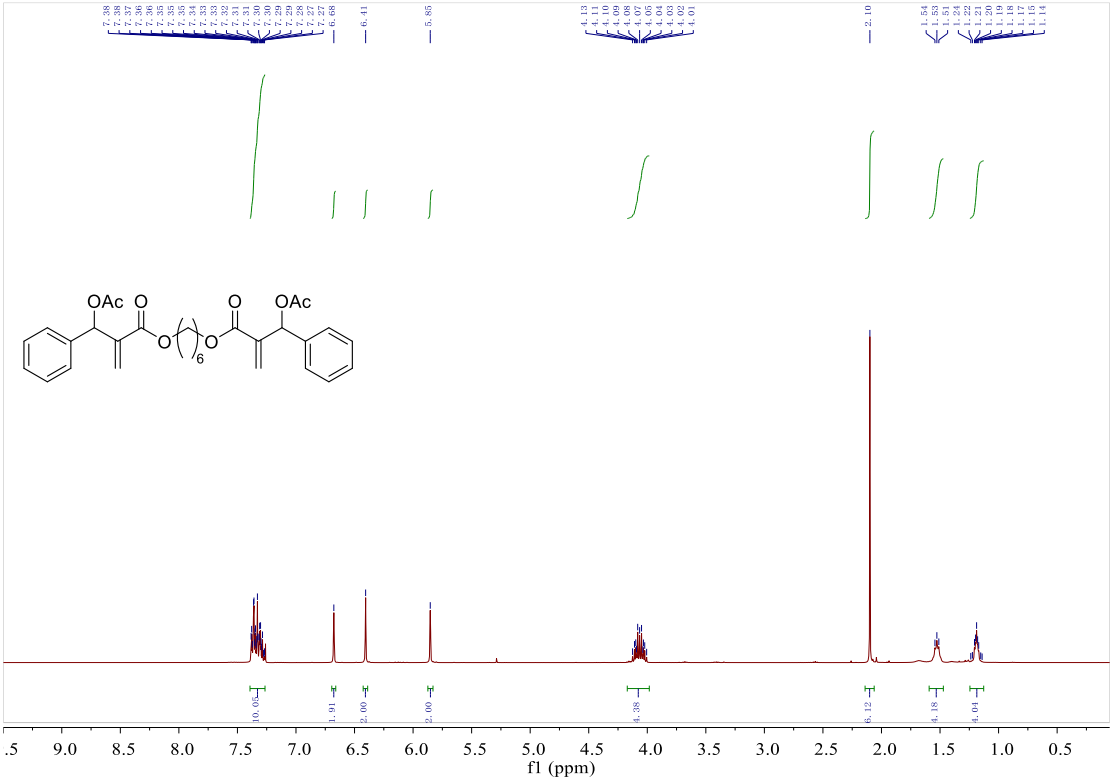
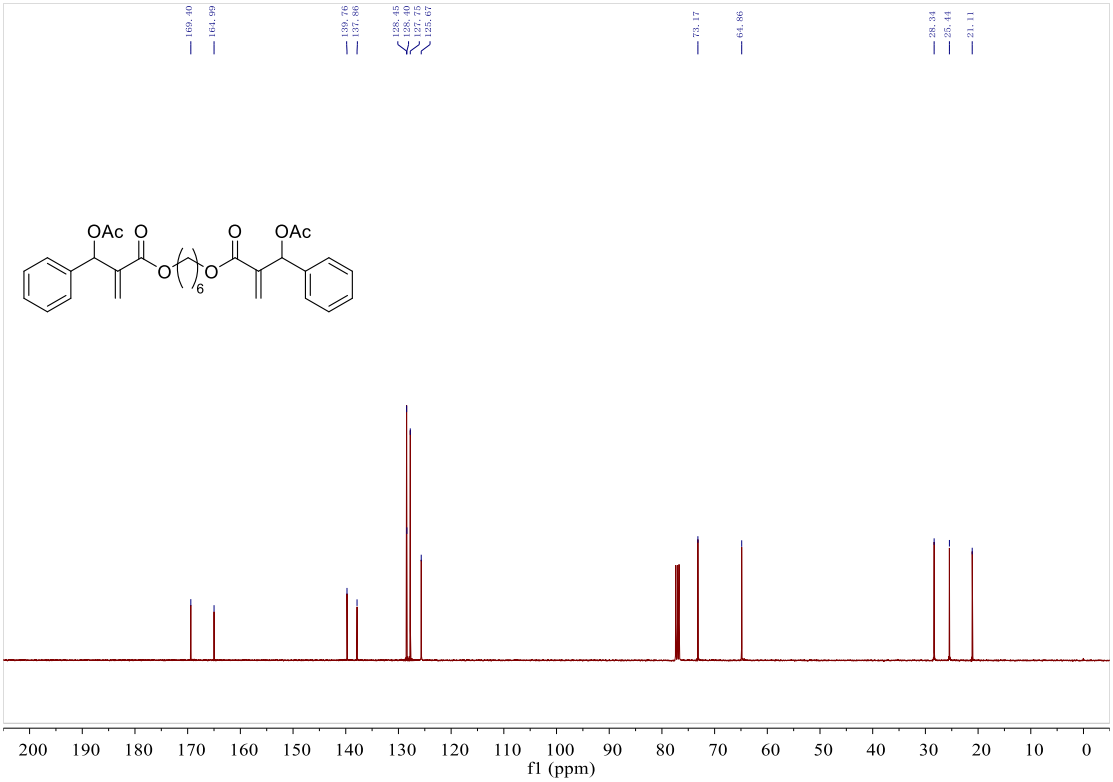
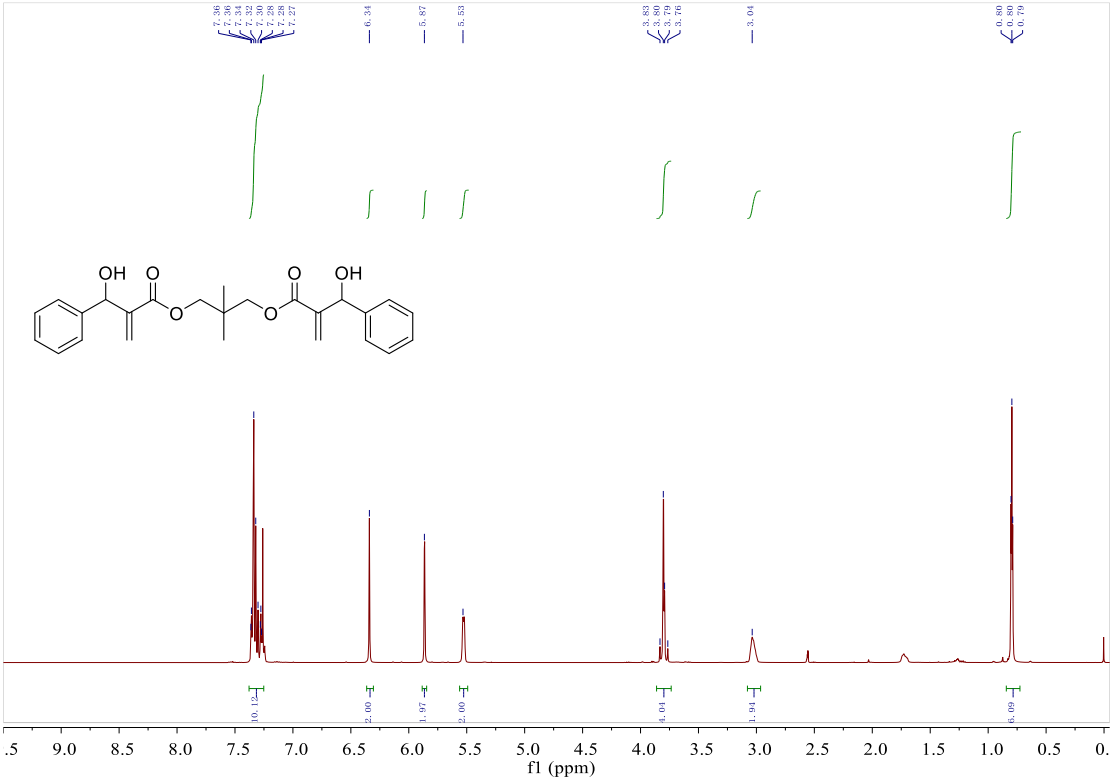
f1 (ppm)

NMR of **1a**





NMR of **S1b**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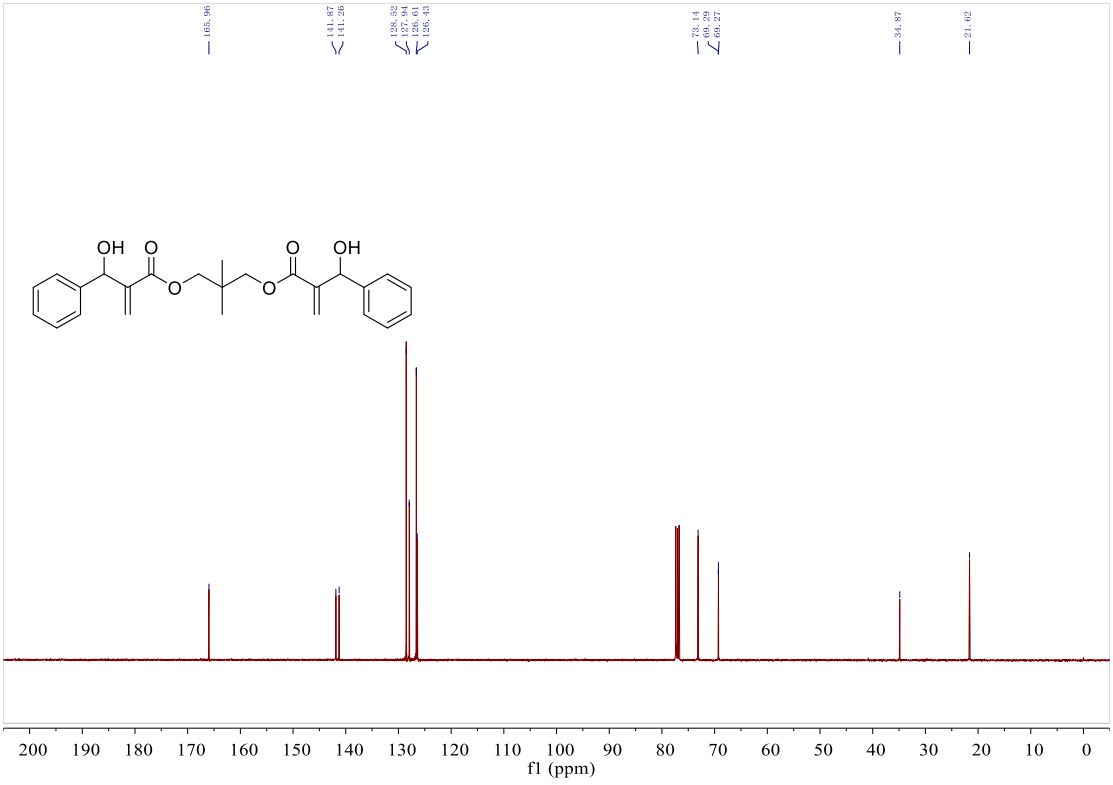
f1 (ppm)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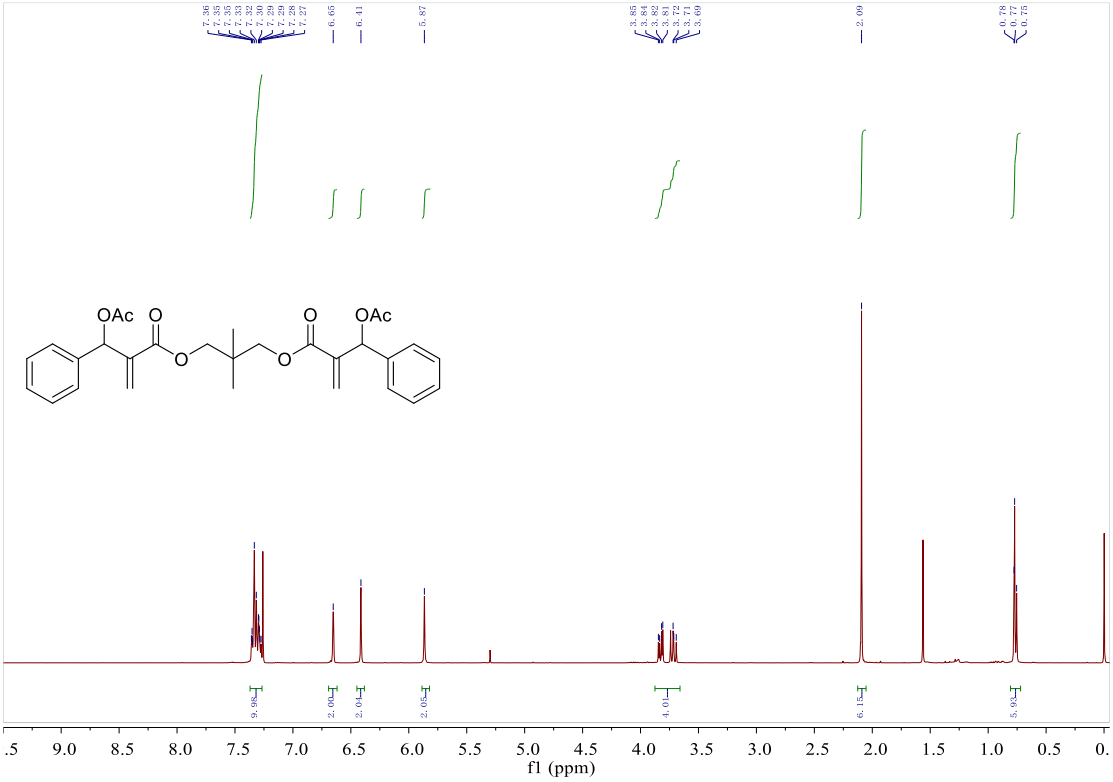
O
OH
f1 (ppm)

NMR of **1b**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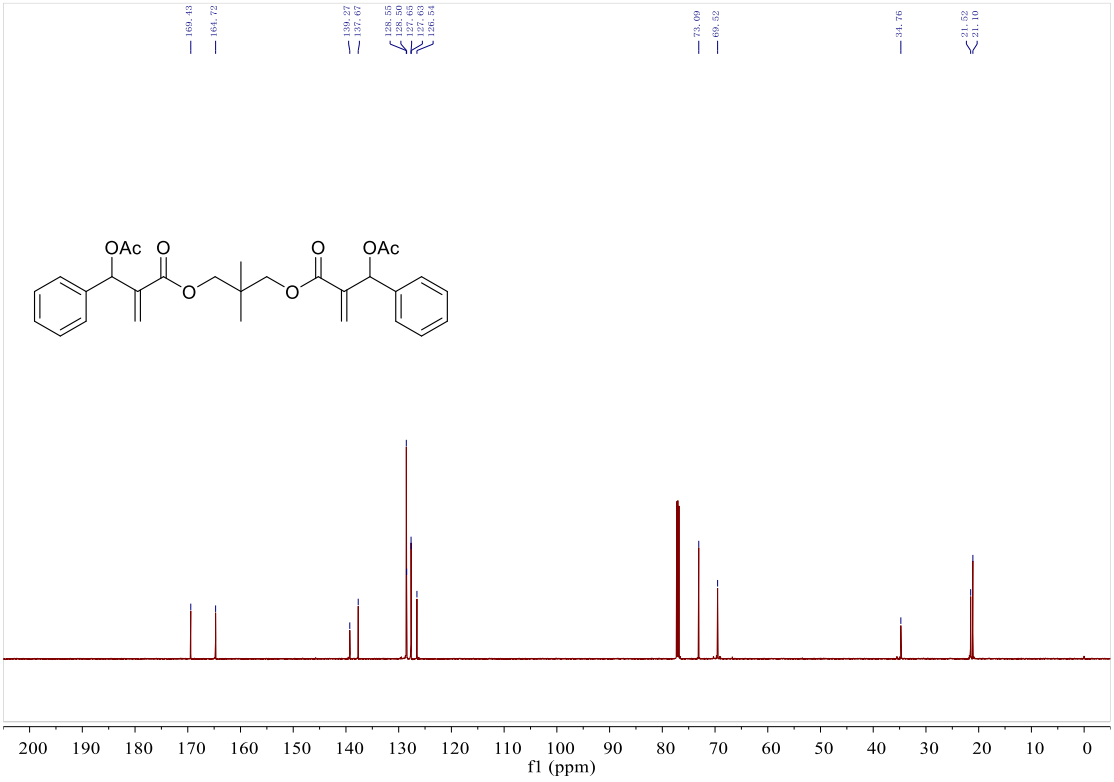
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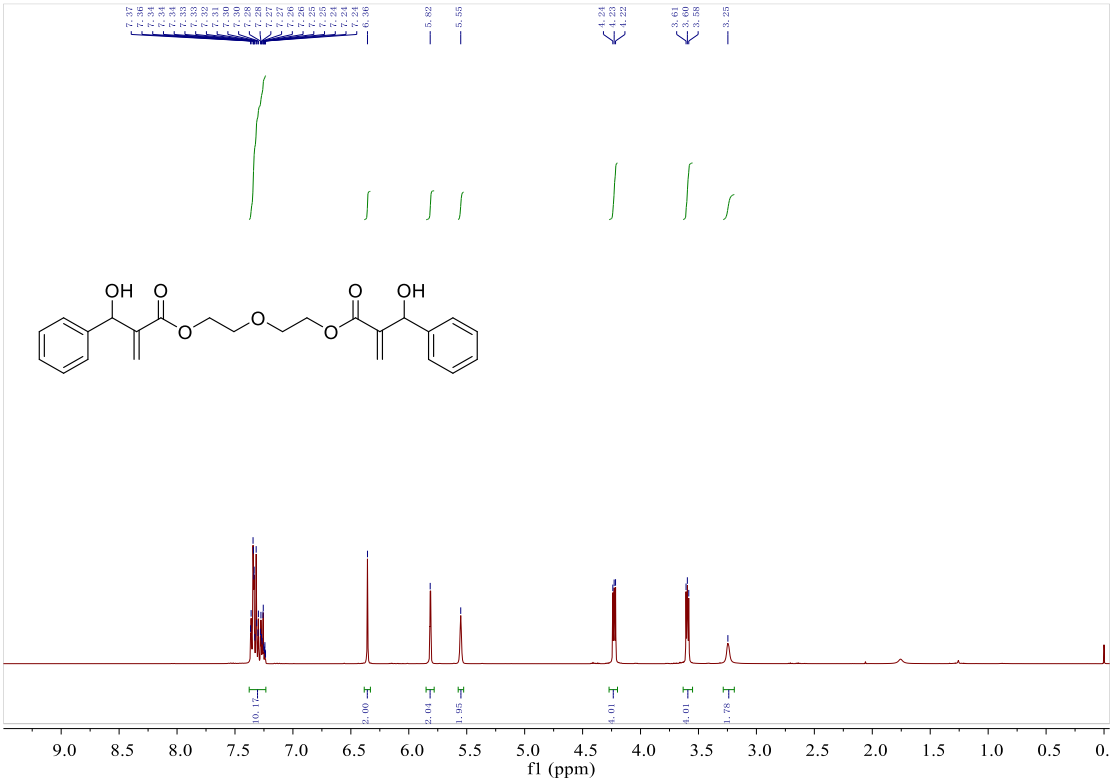
OAc
O
O
O
O
OAc
f1 (ppm)

NMR of **S1c**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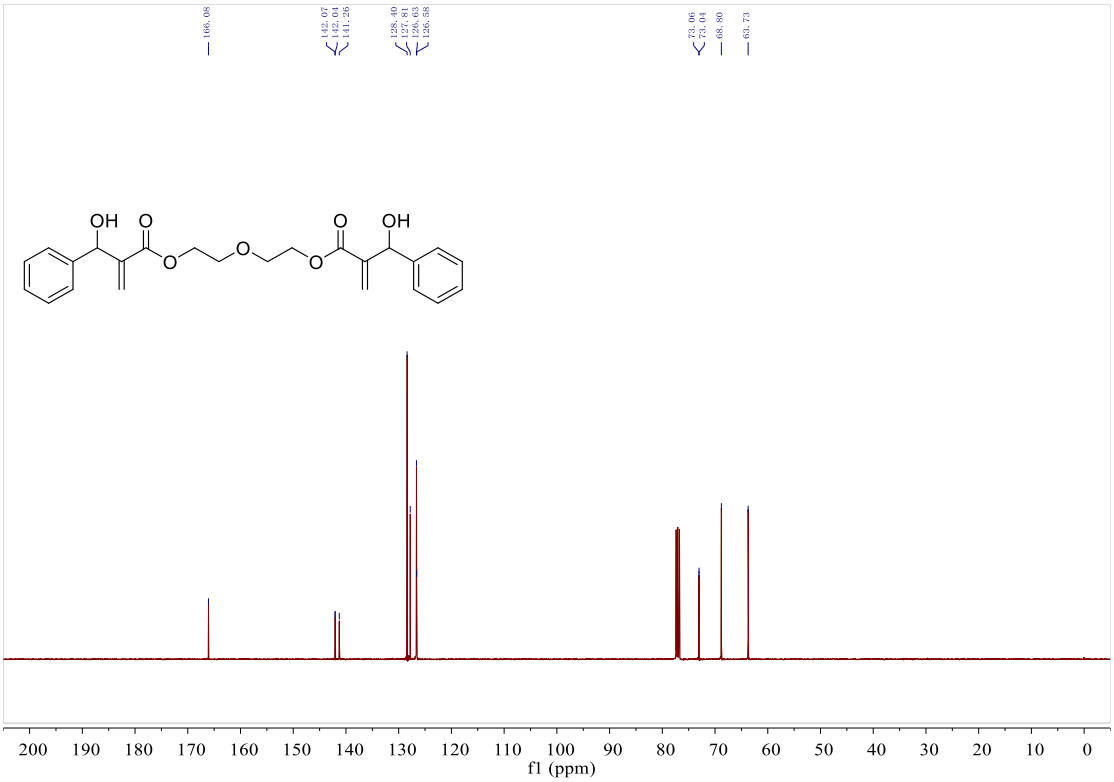
1.0
0.5
f1 (ppm)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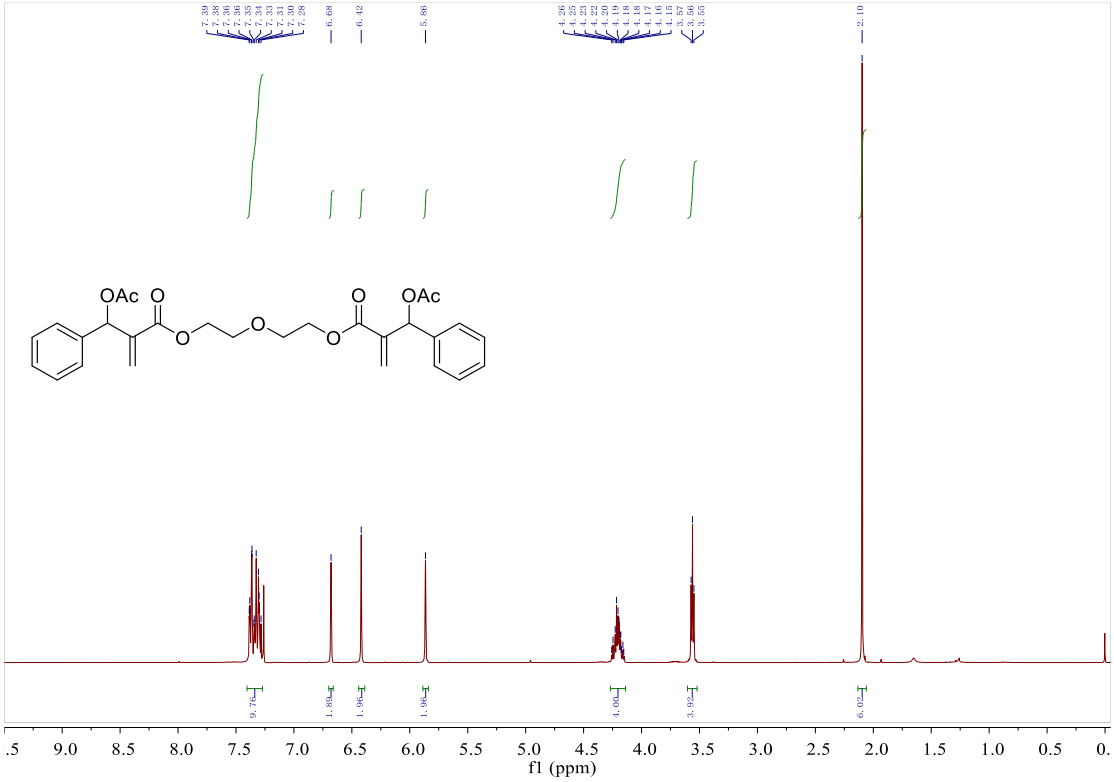
f1 (ppm)

NMR of **1c**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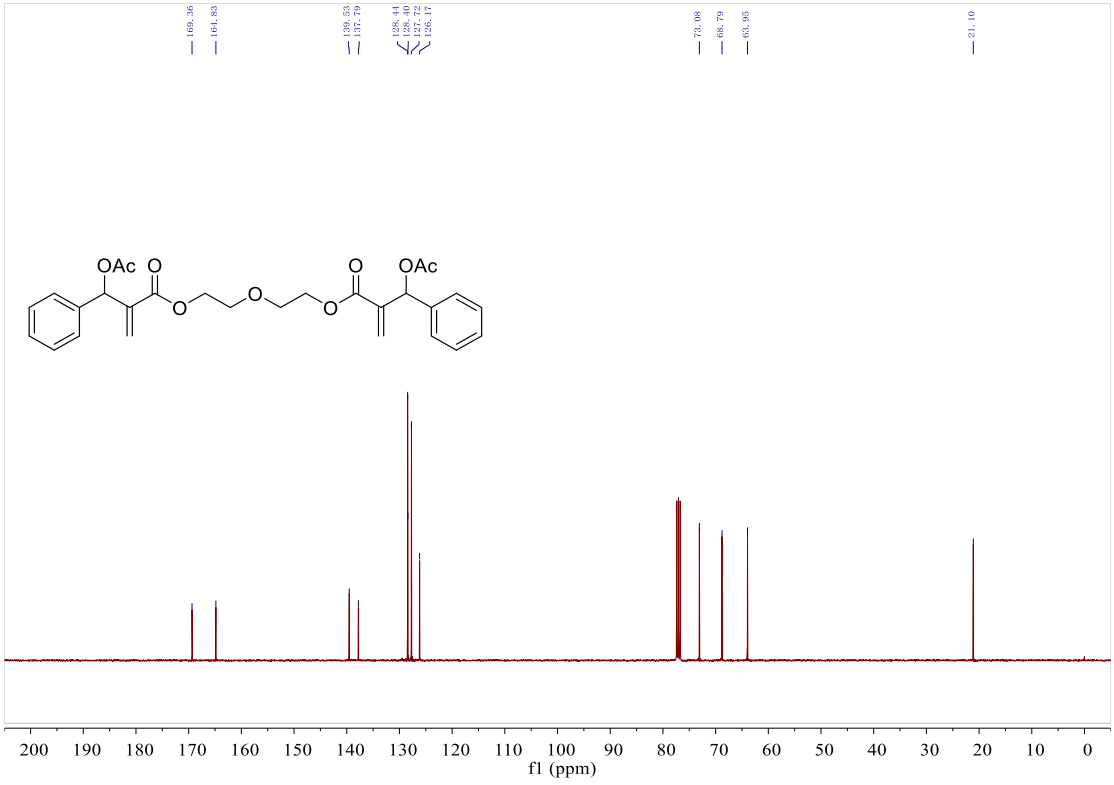
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OAc
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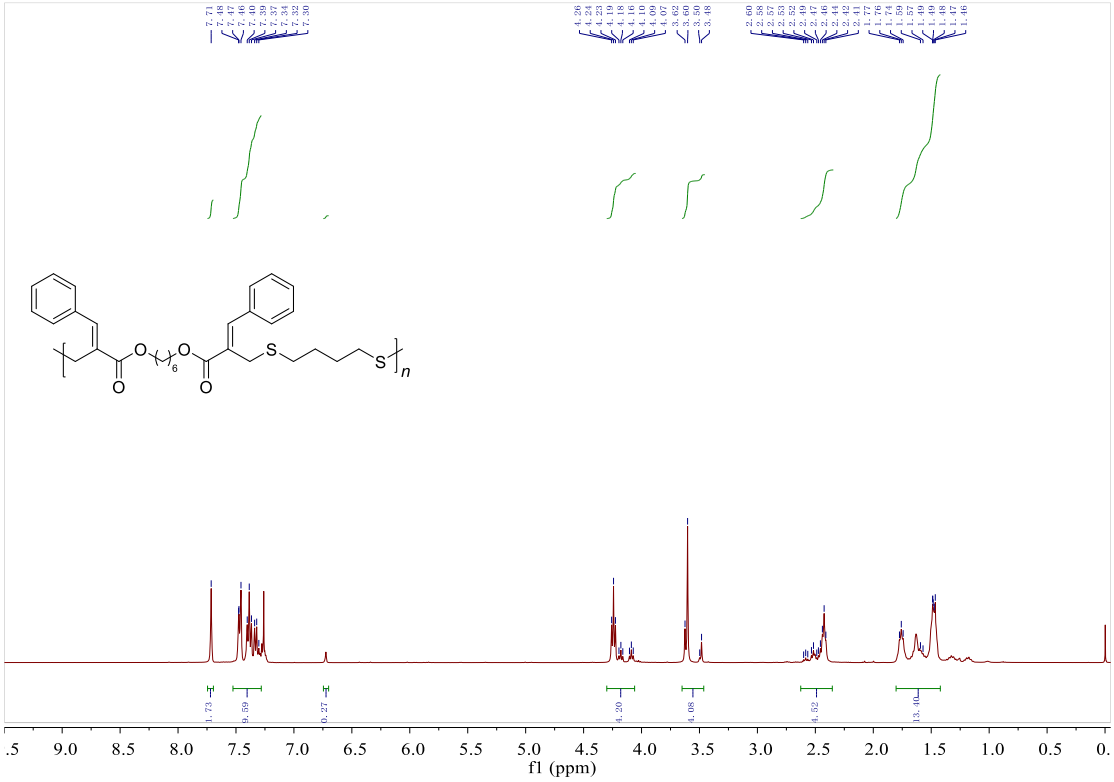
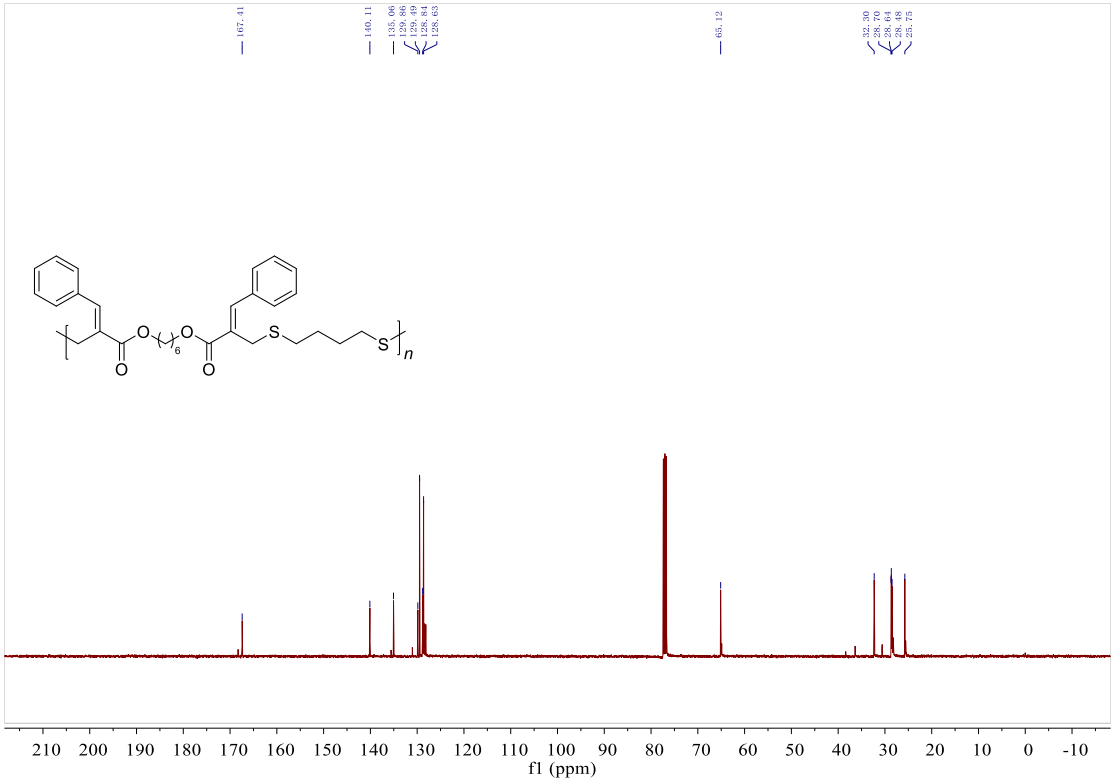
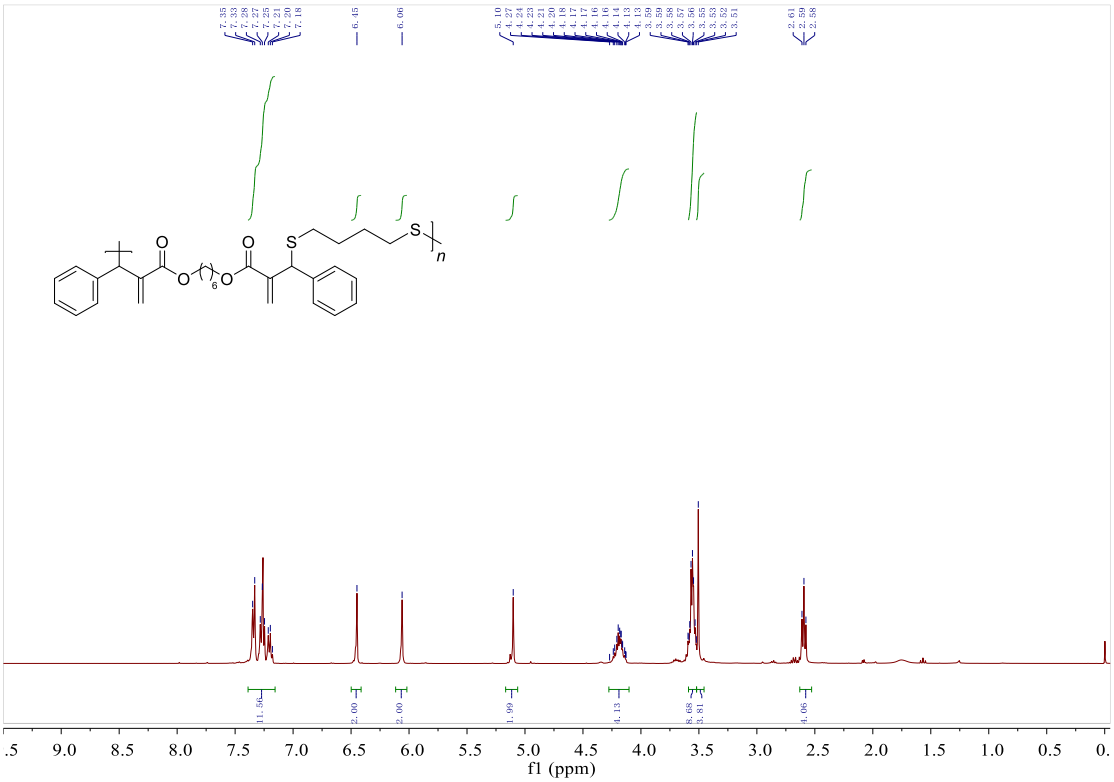
O
O
O
O
OAc
f1 (ppm)

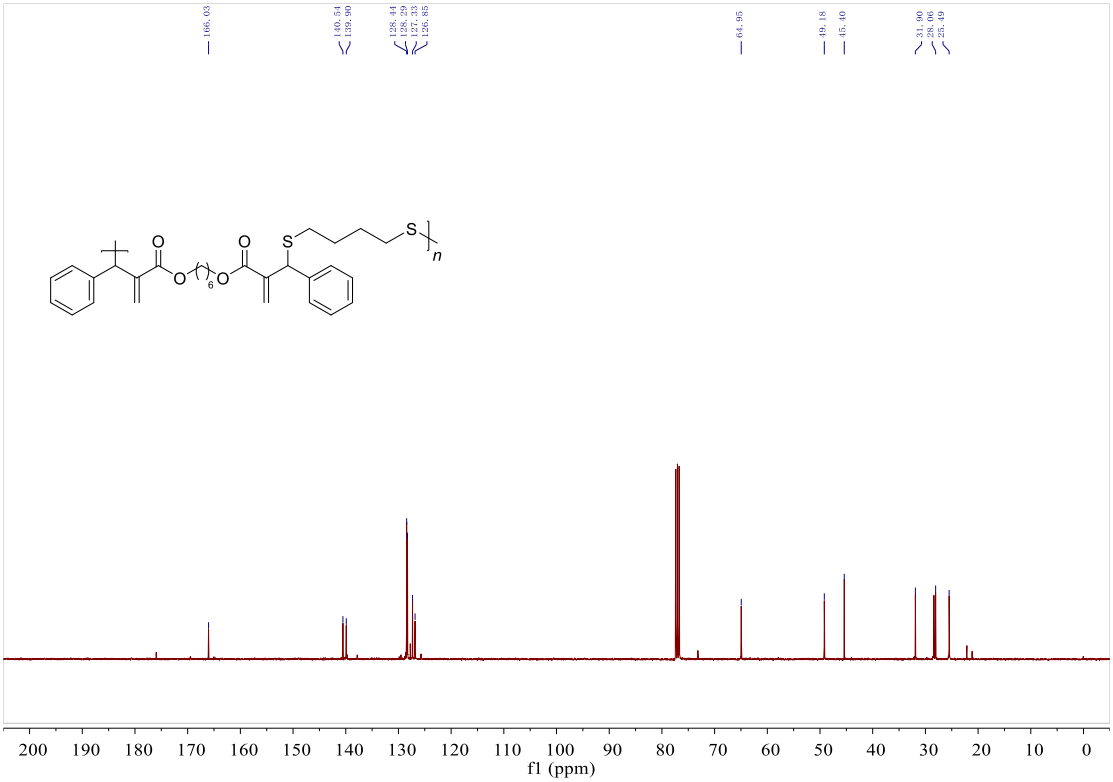
NMR of **α-P1a/2a**



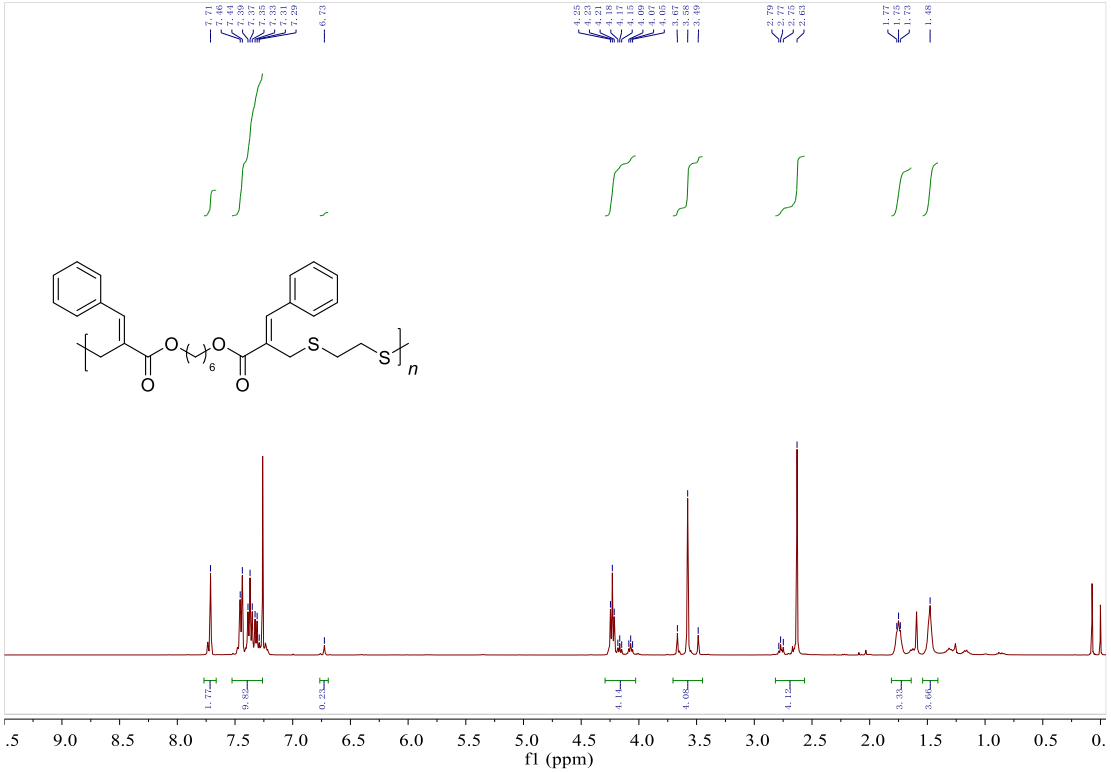


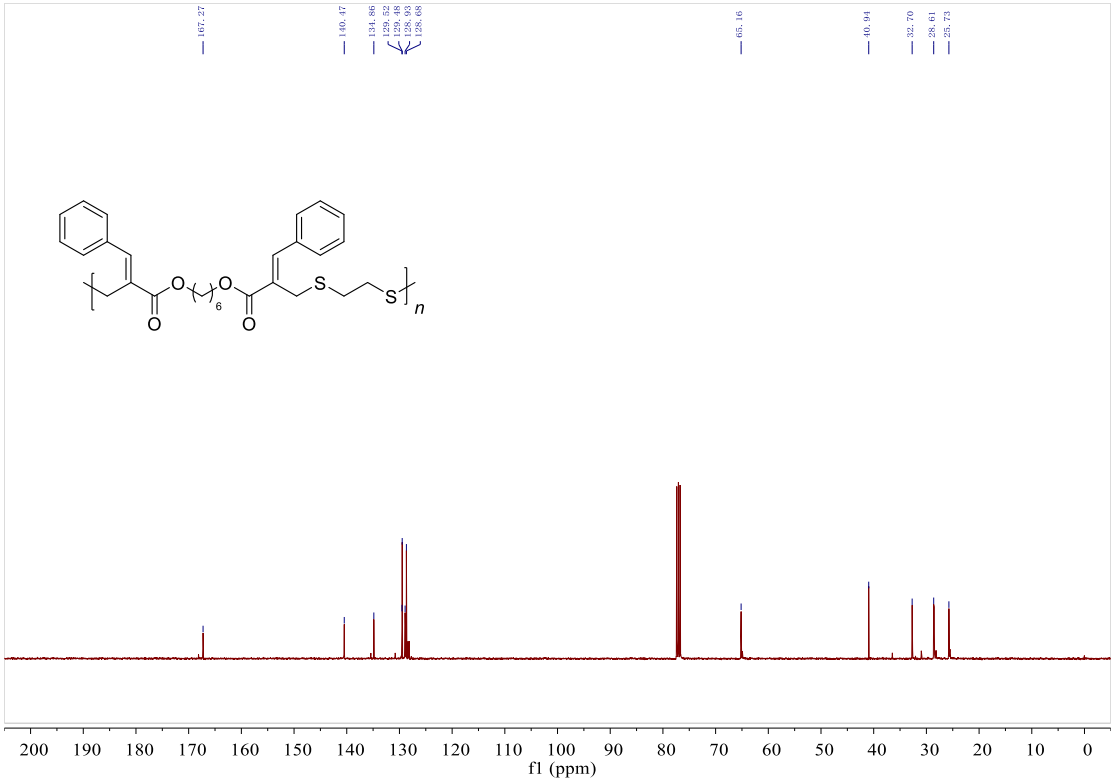
NMR of **γ-P1a/2a**



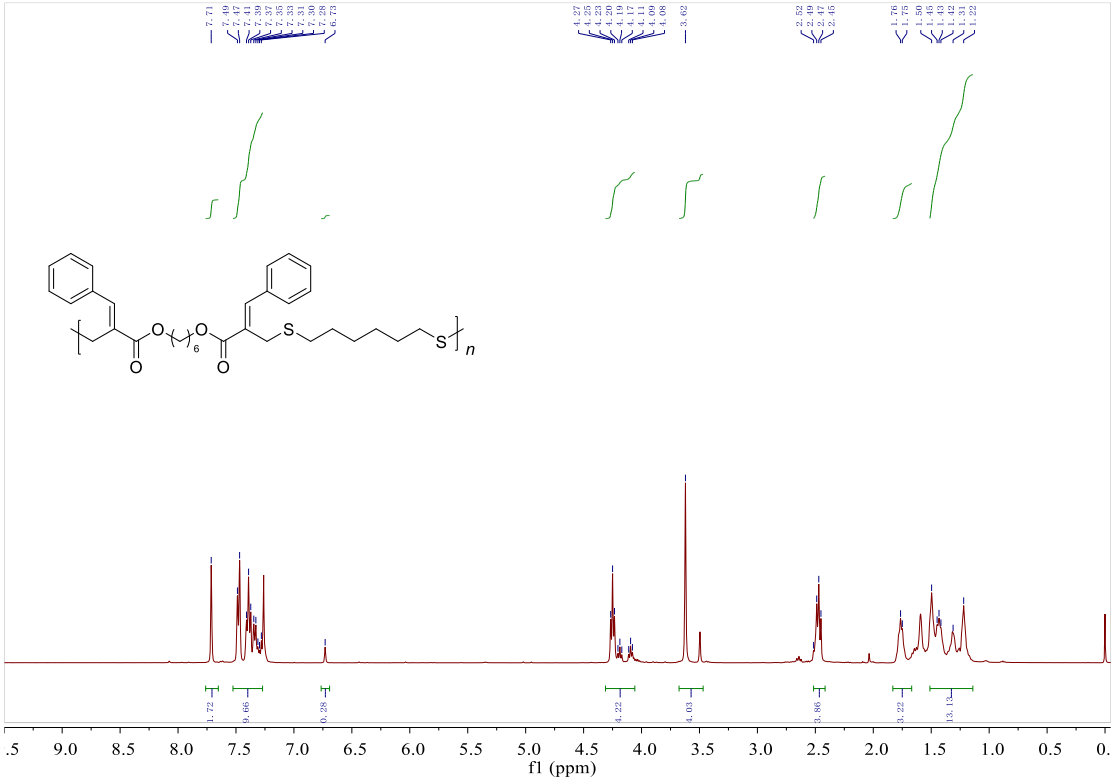


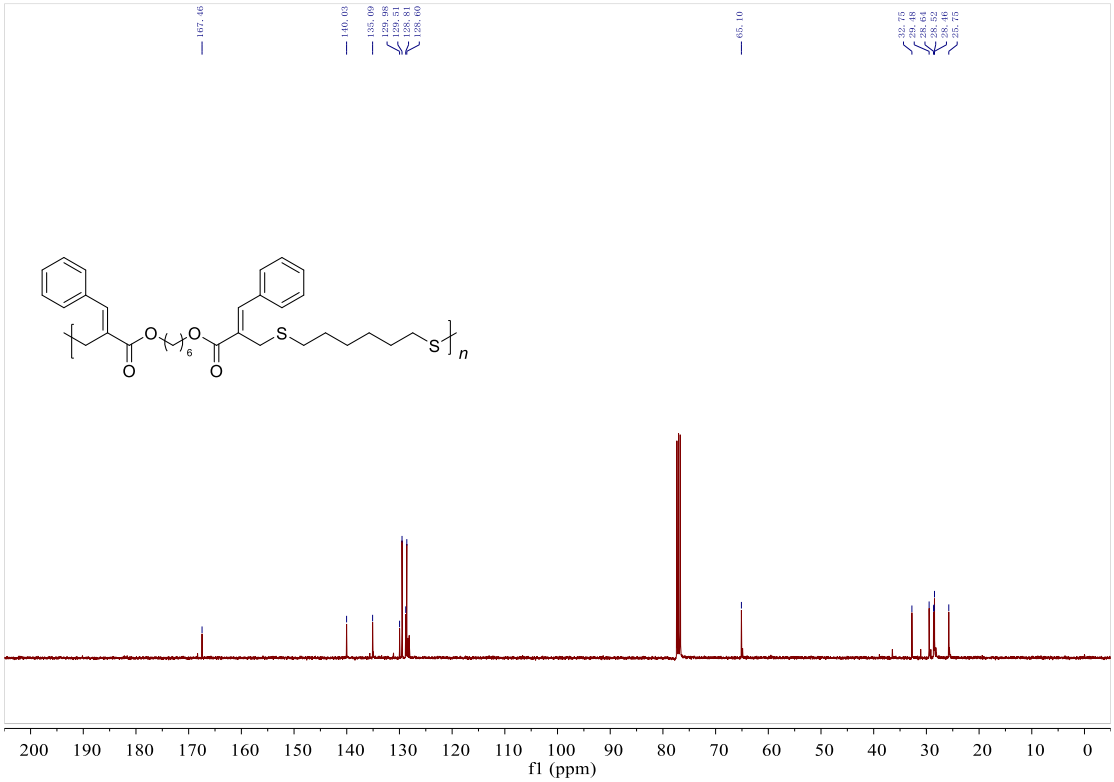
NMR of **α-P1a/2b**



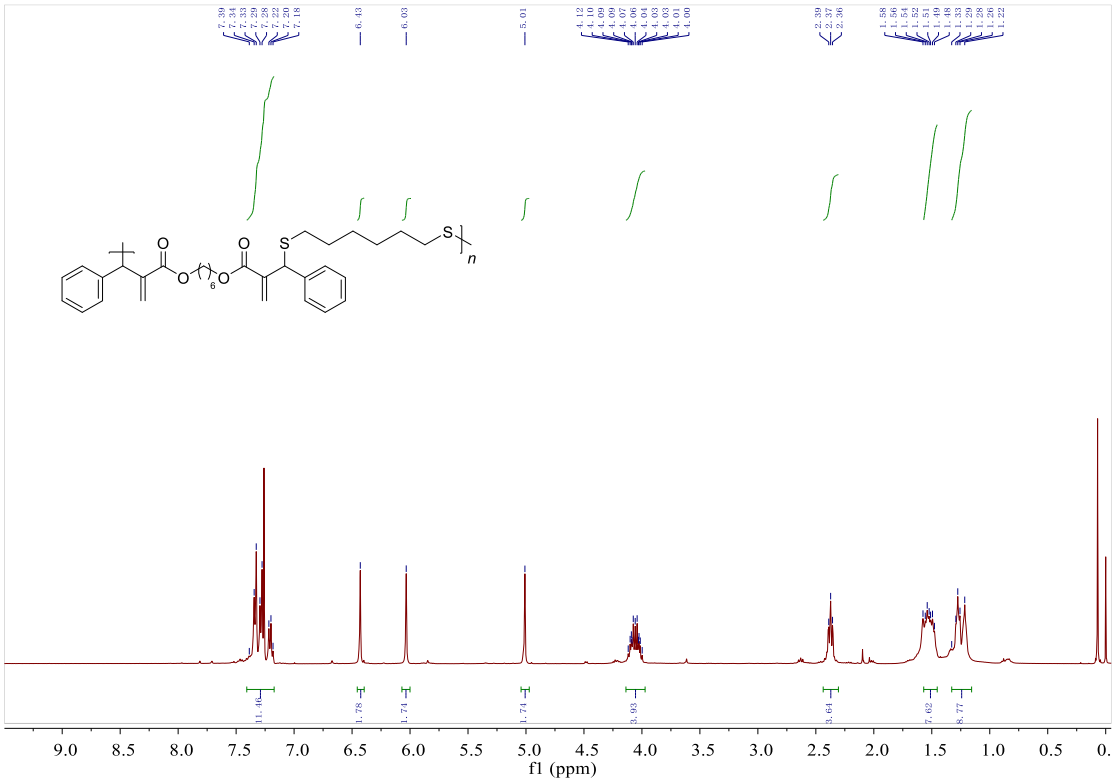


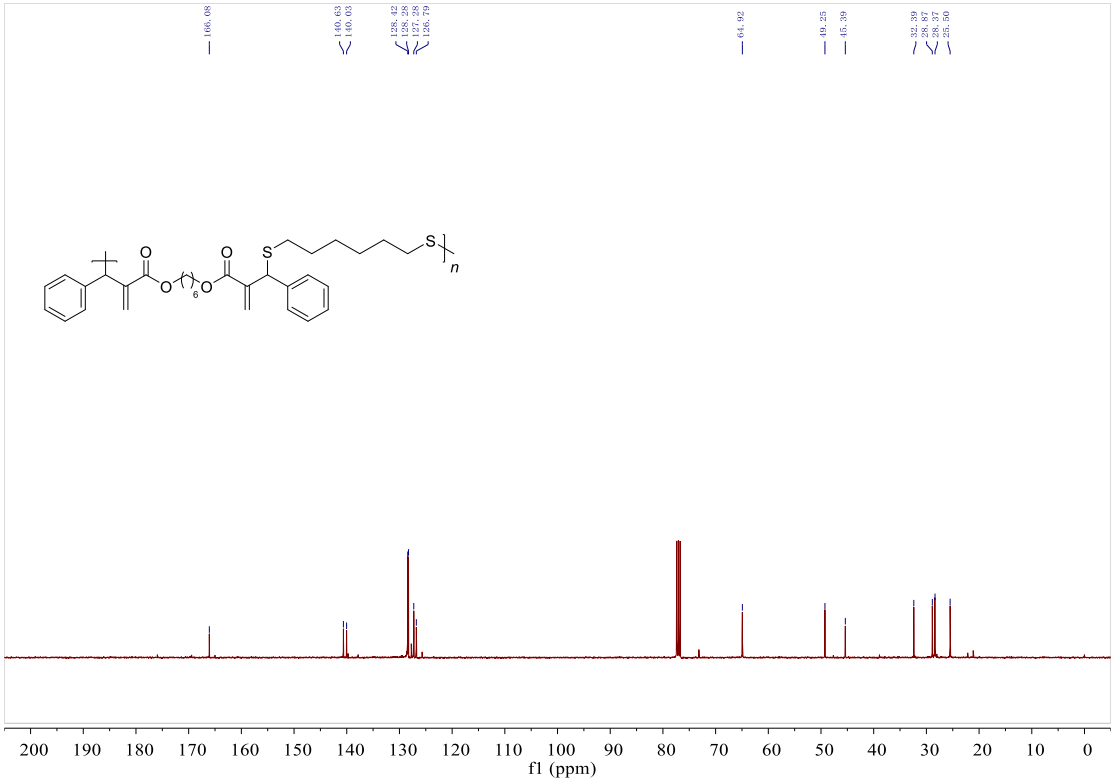
NMR of **α-P1a/2c**



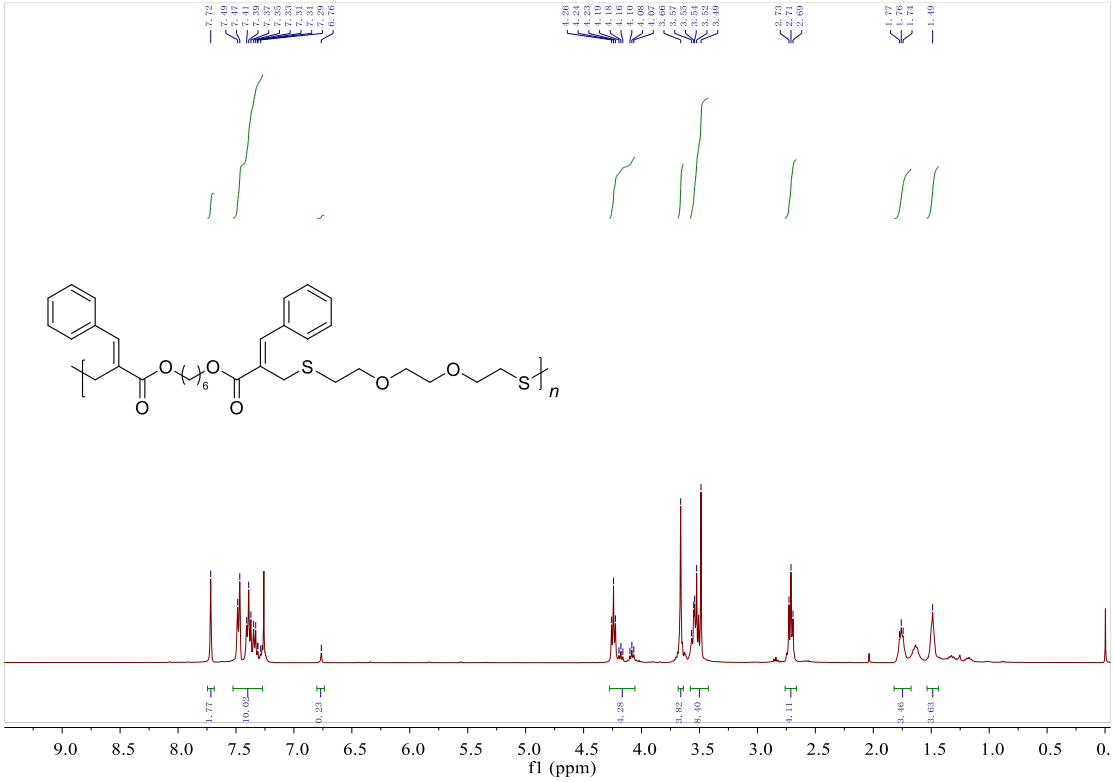


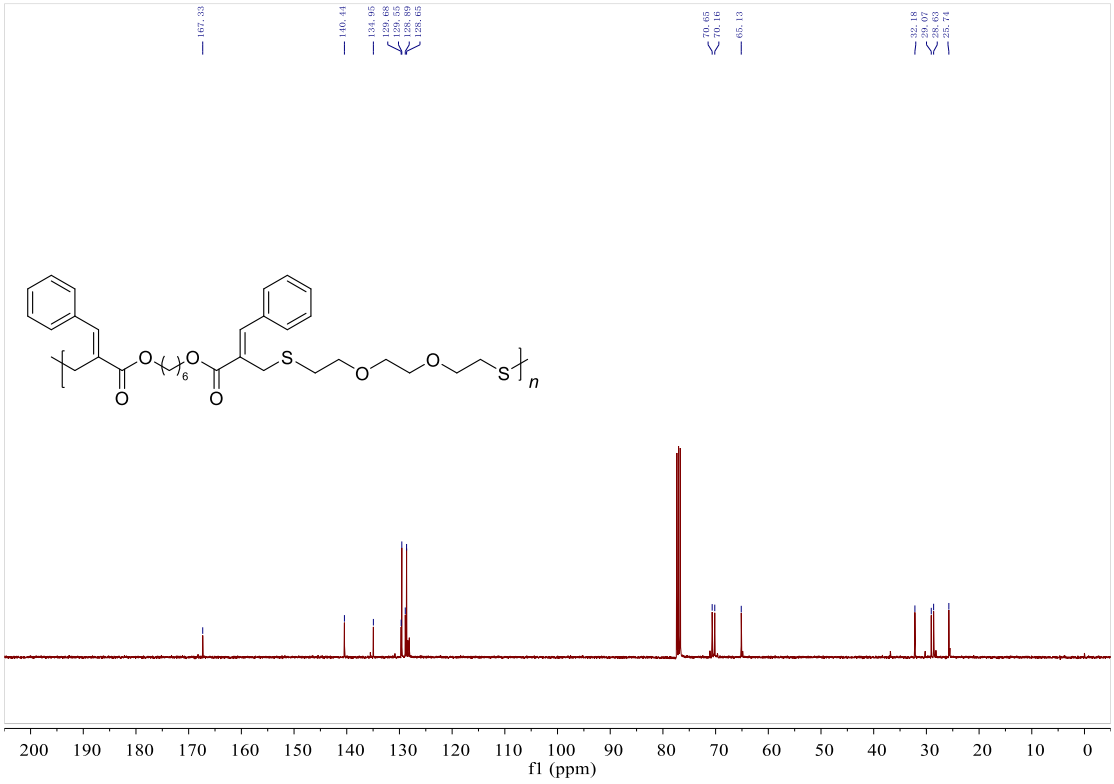
NMR of **γ-P1a/2c**



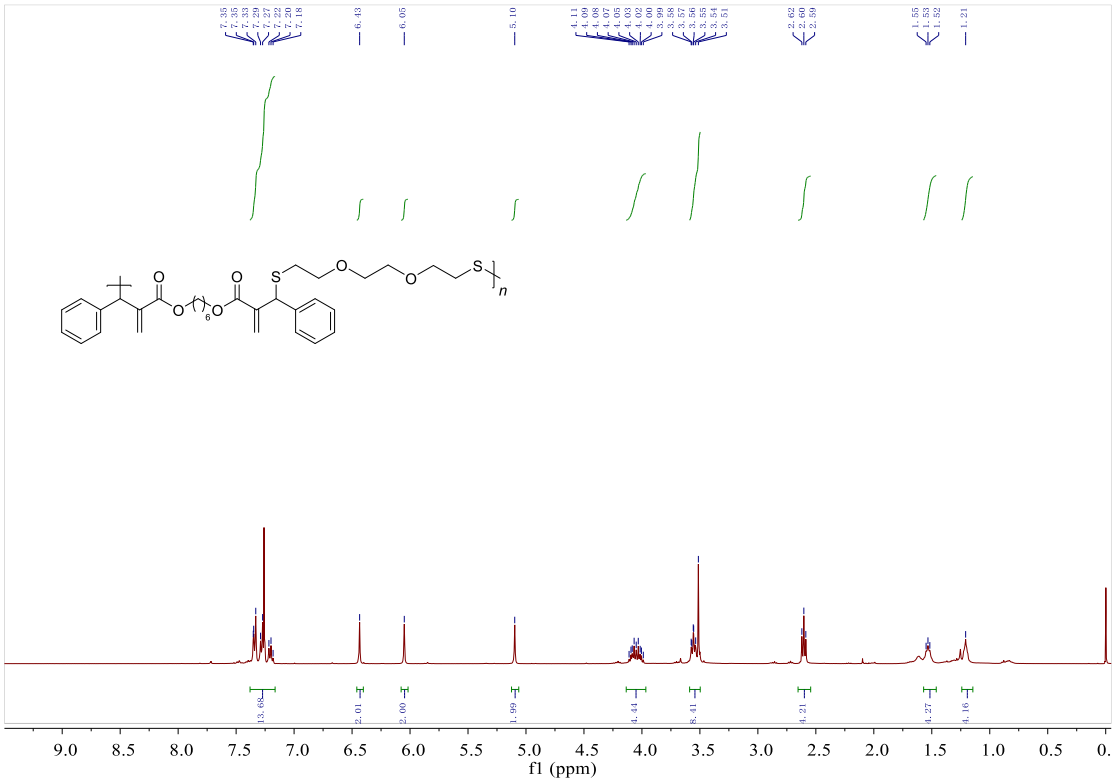


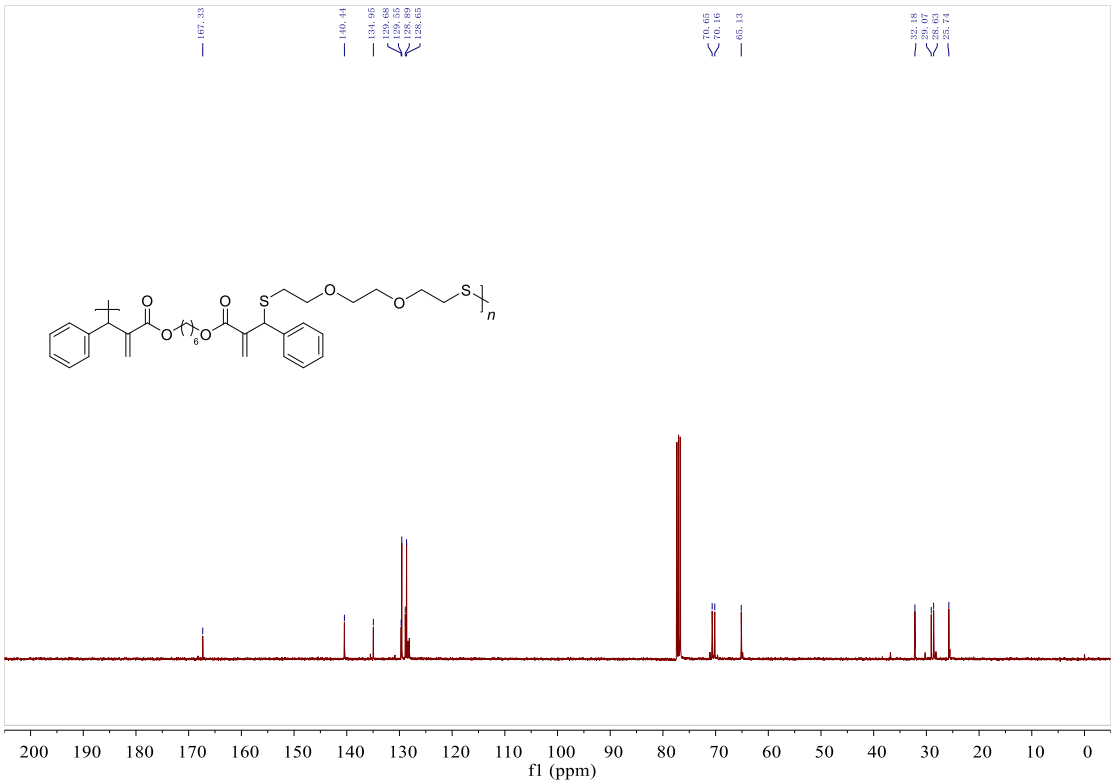
NMR of **α-P1a/2d**



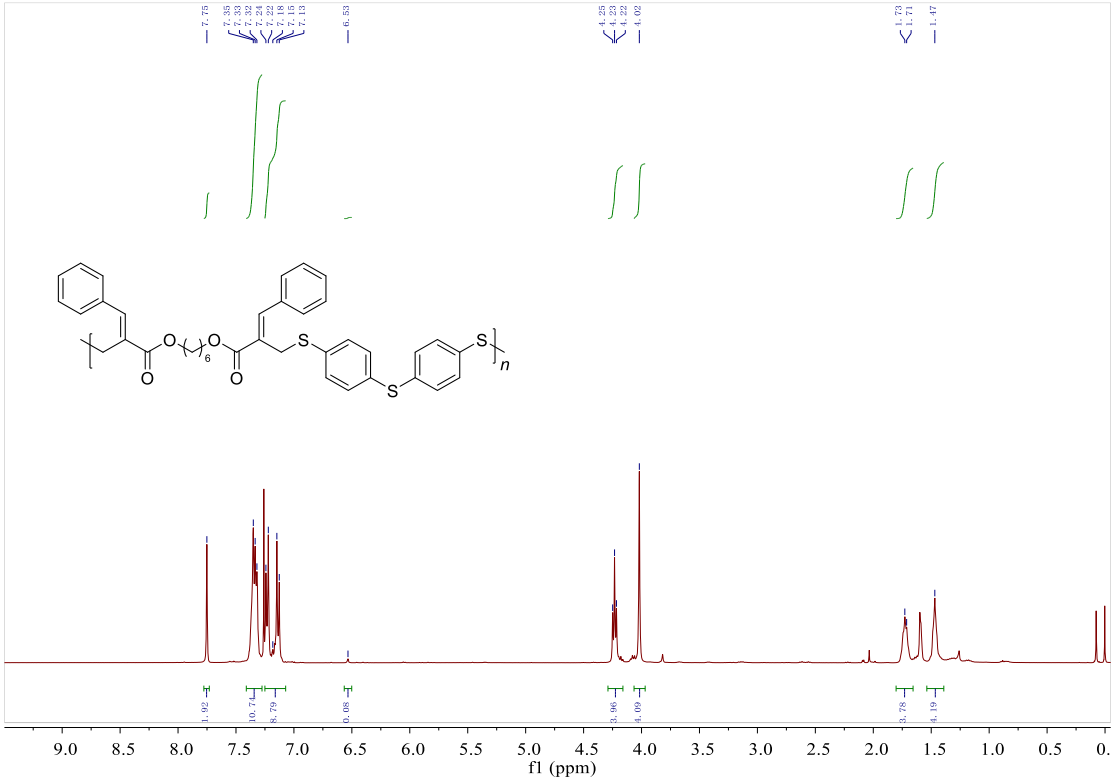


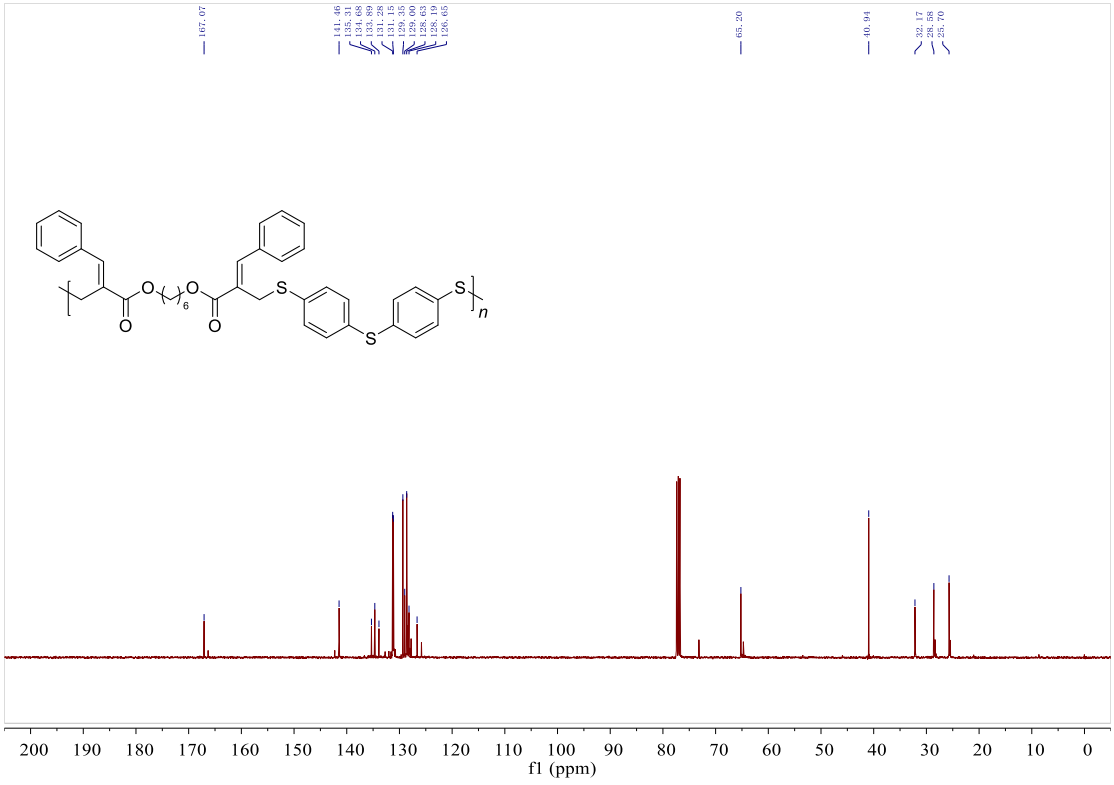
NMR of **γ-P1a/2d**



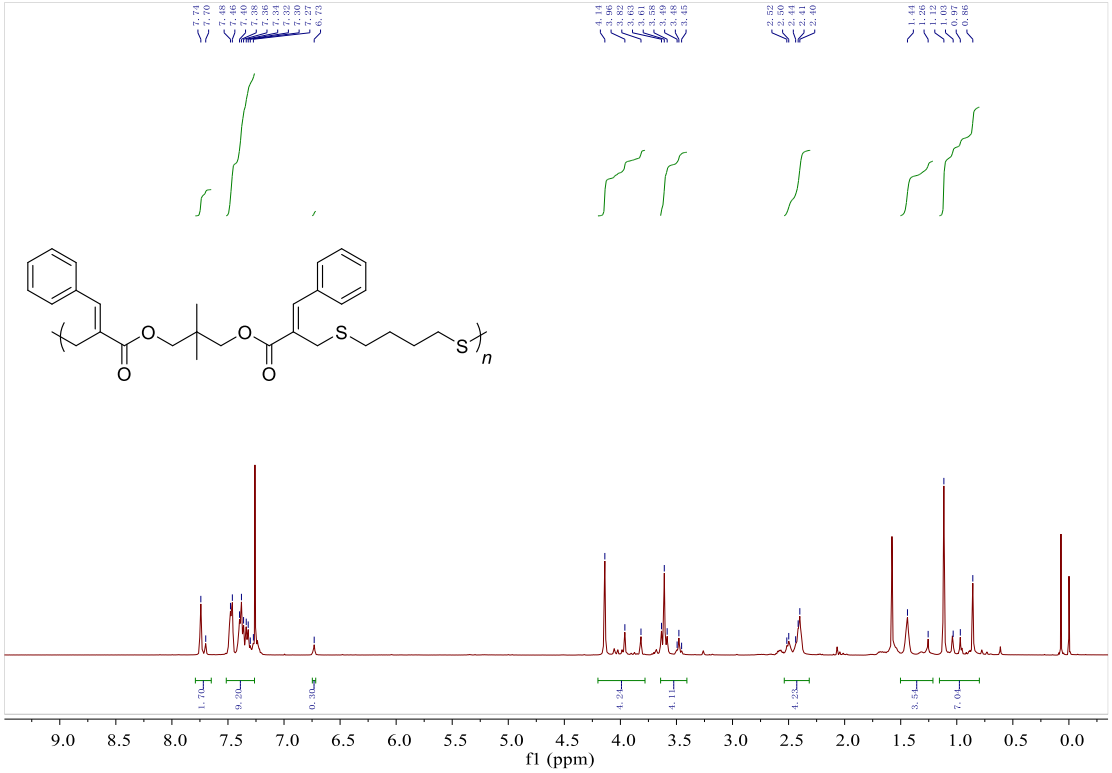


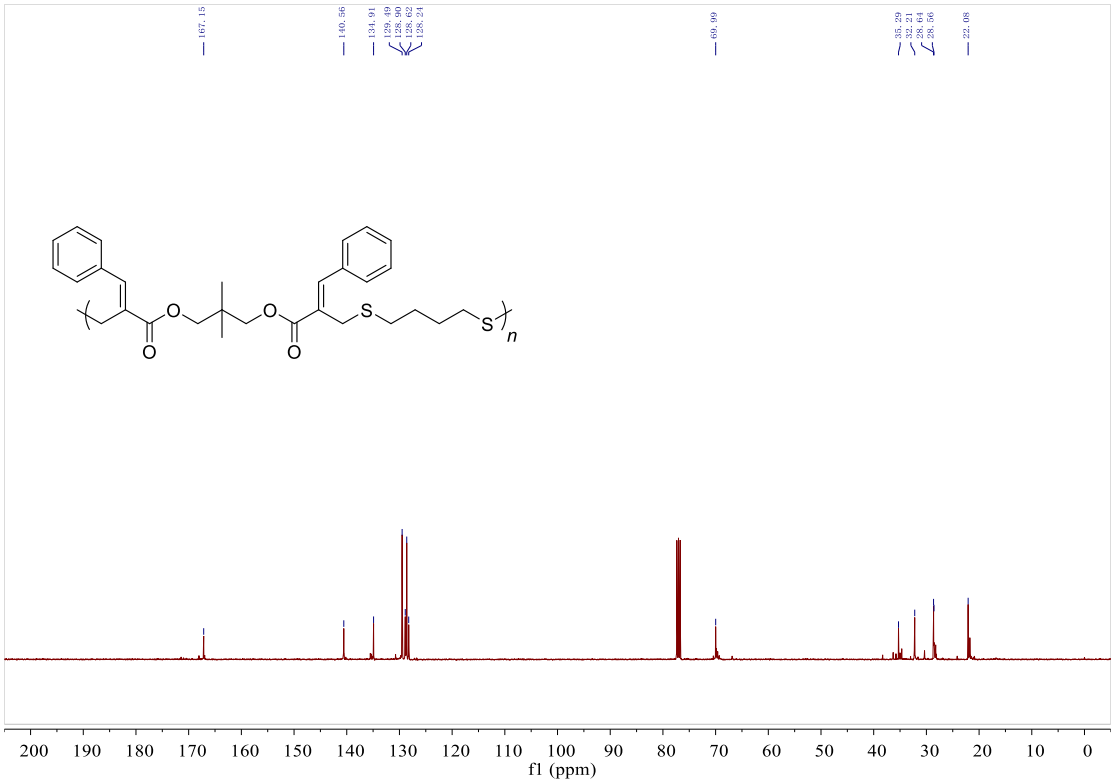
NMR of **α-P1a/2e**



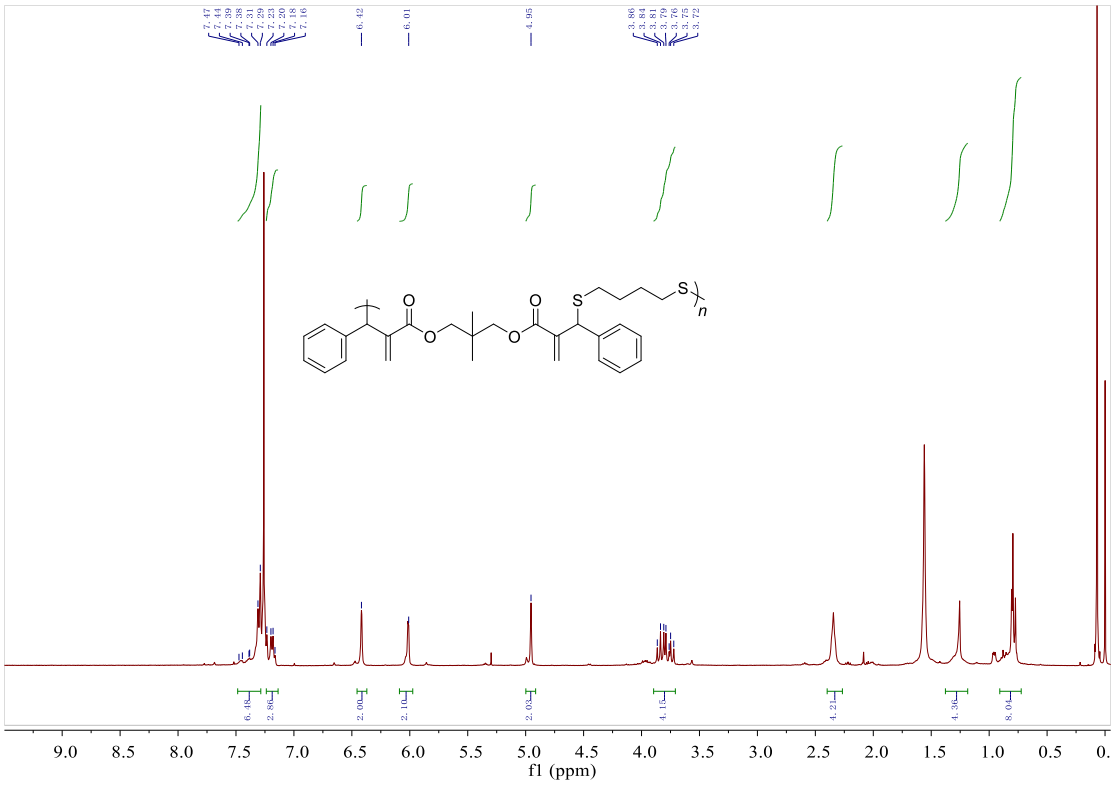


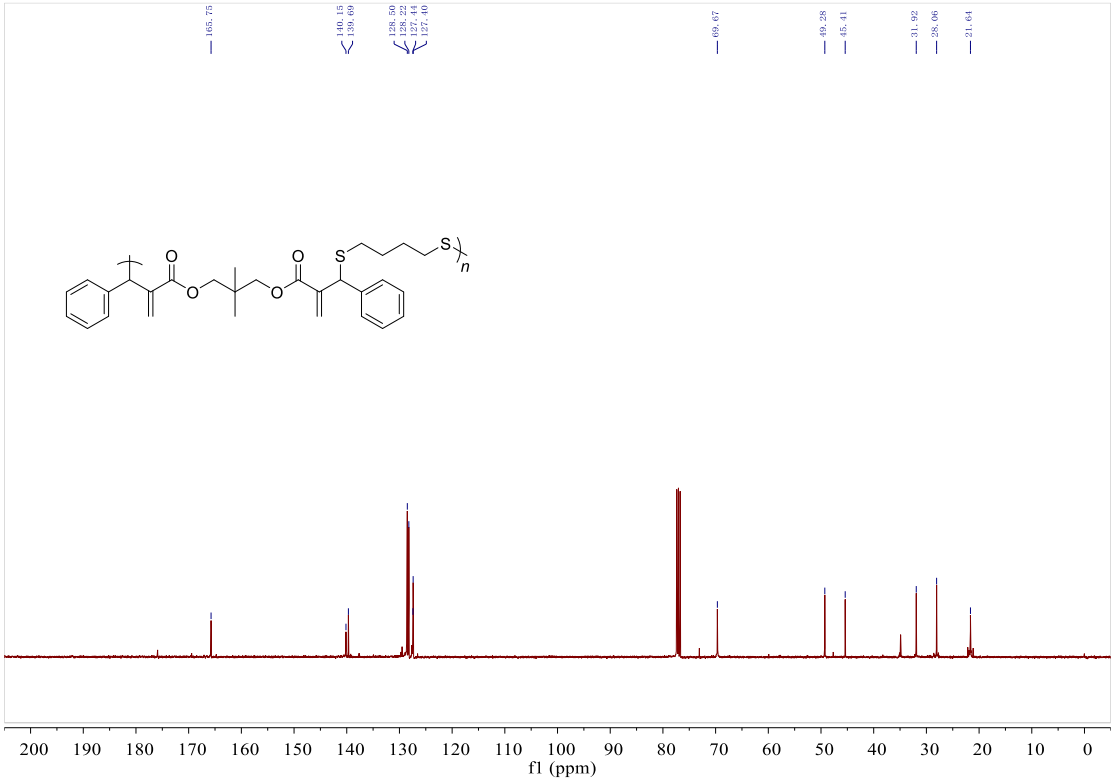
NMR of **α-P1b/2a**



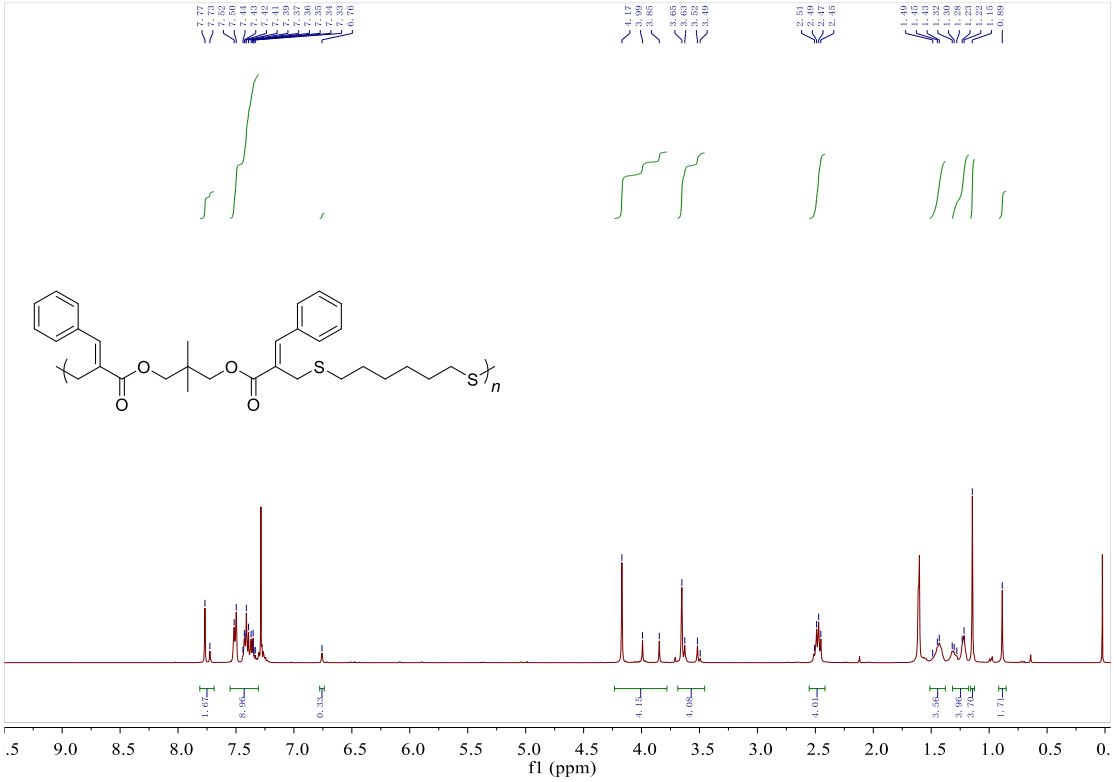


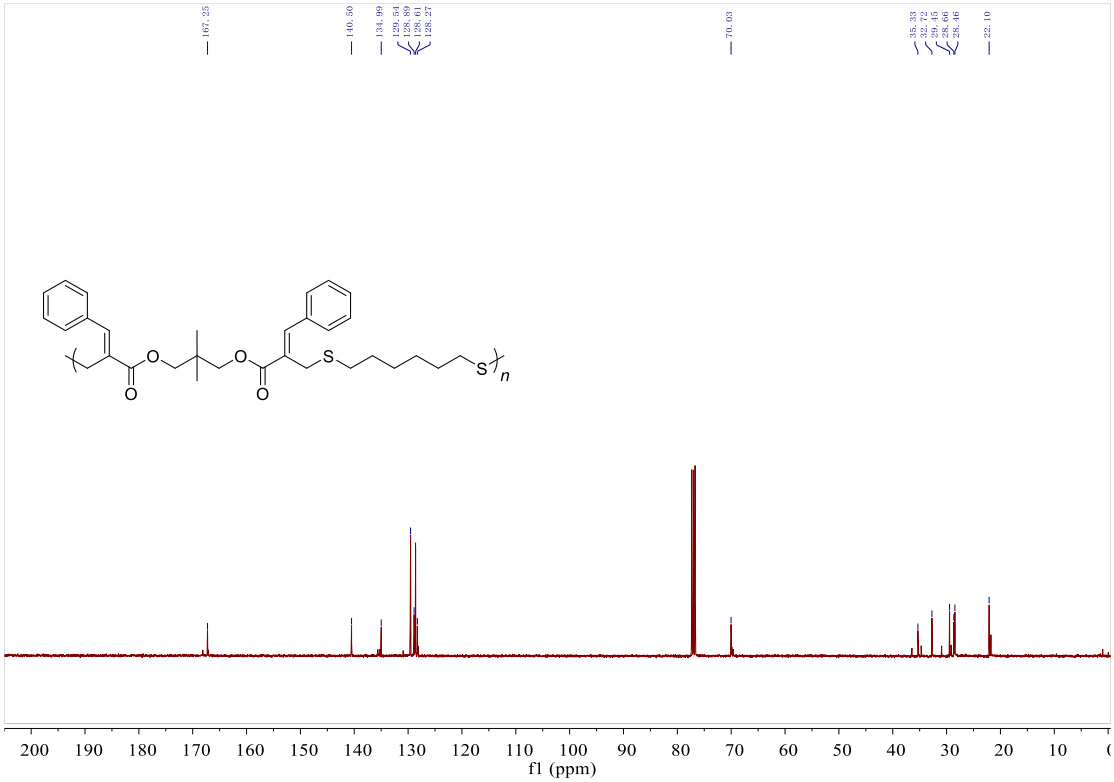
NMR of **γ-P1b/2a**



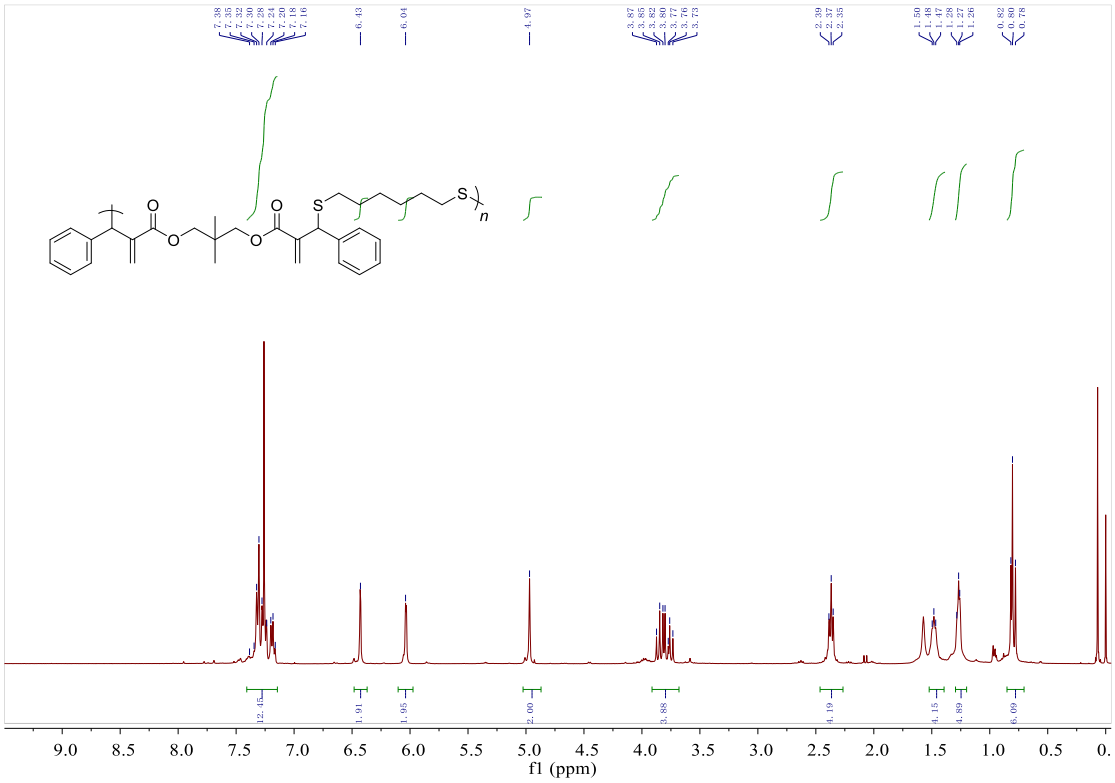


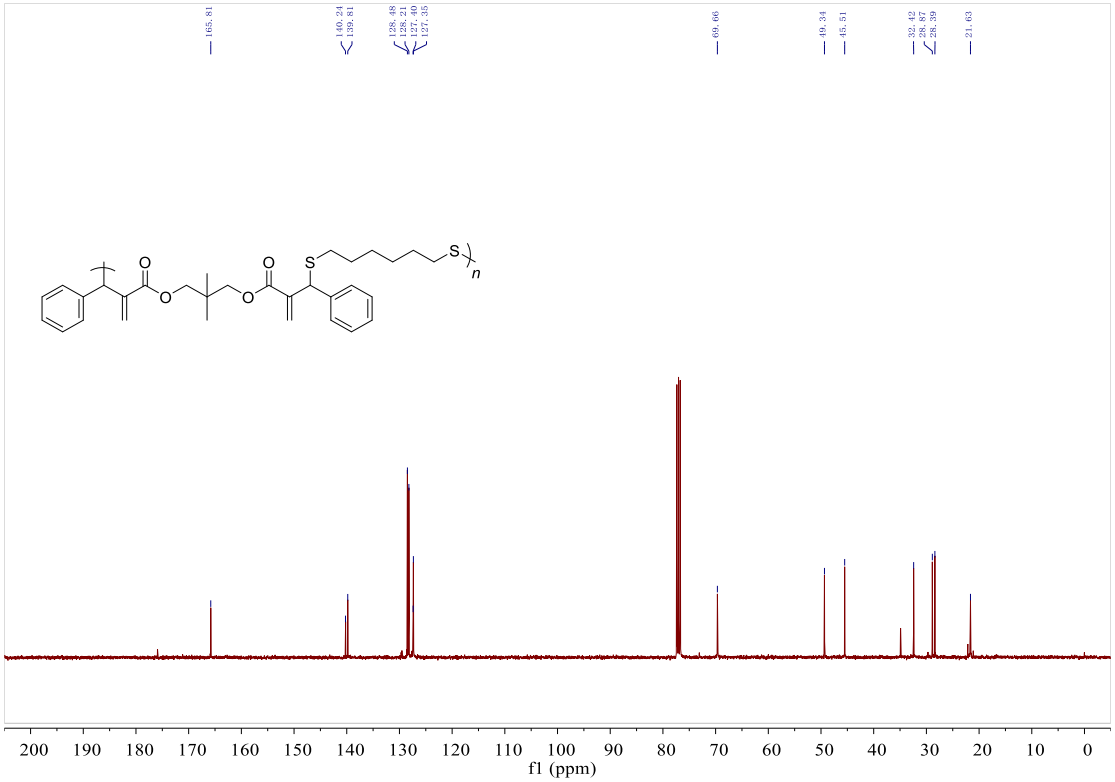
NMR of **α-P1b/2c**



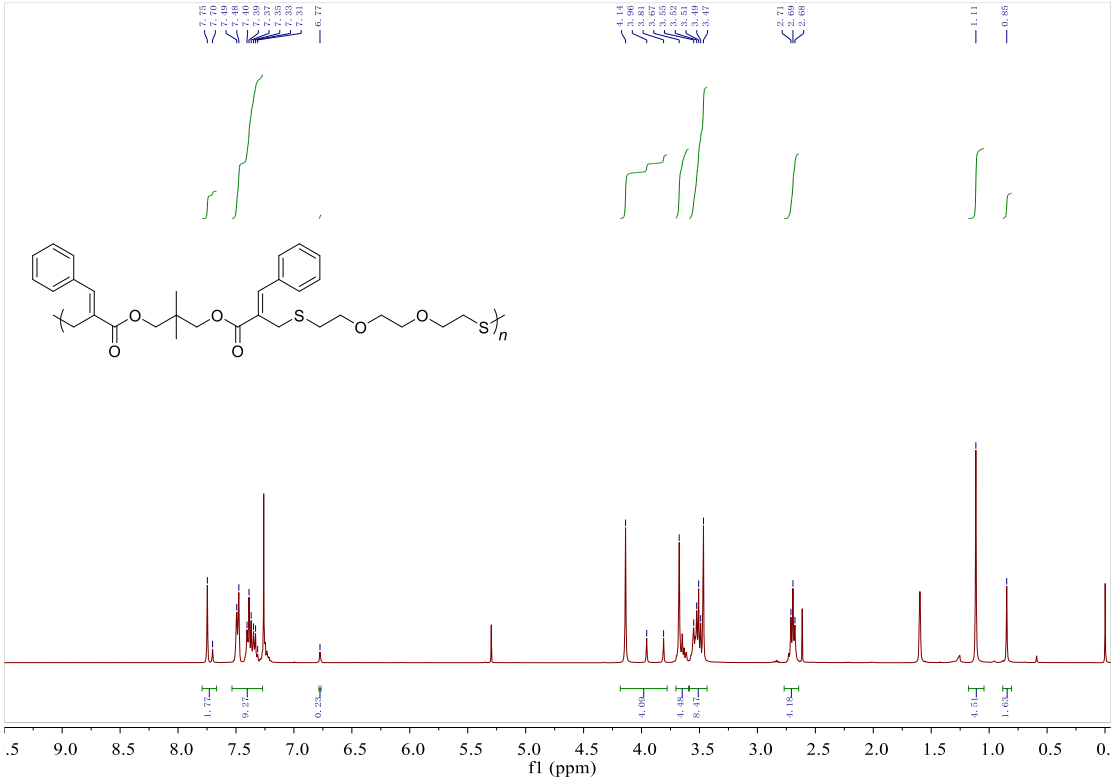


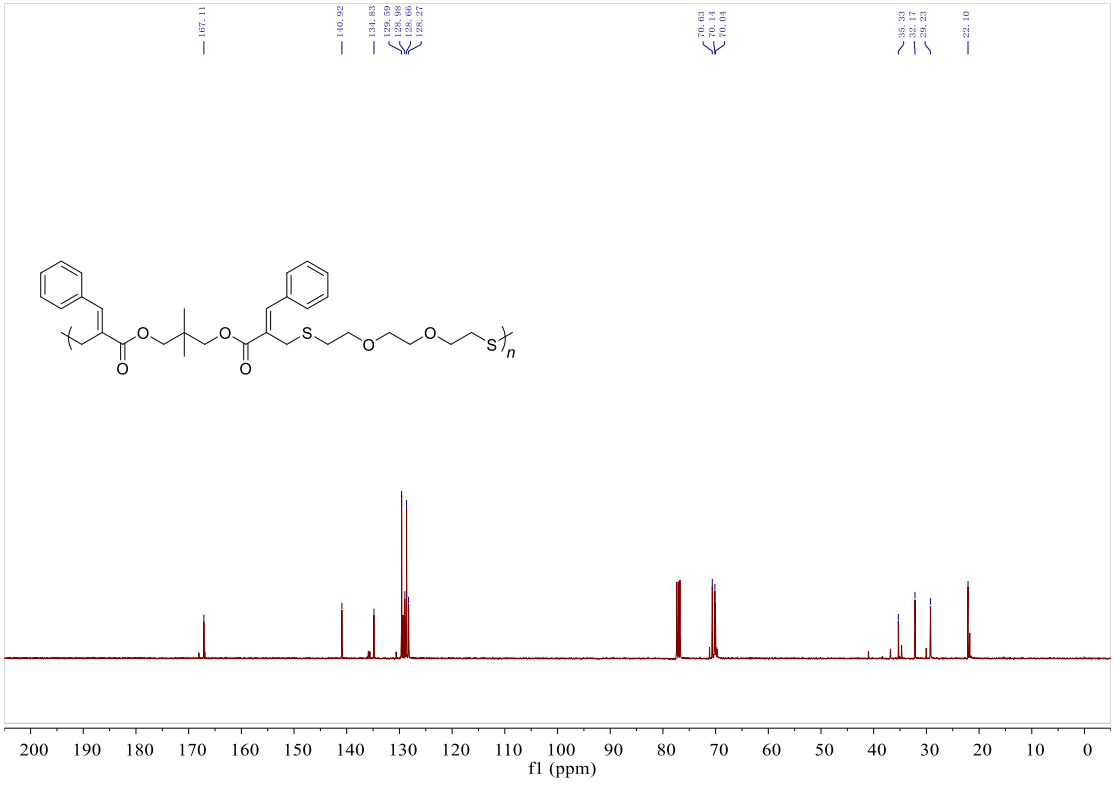
NMR of **γ-P1b/2c**



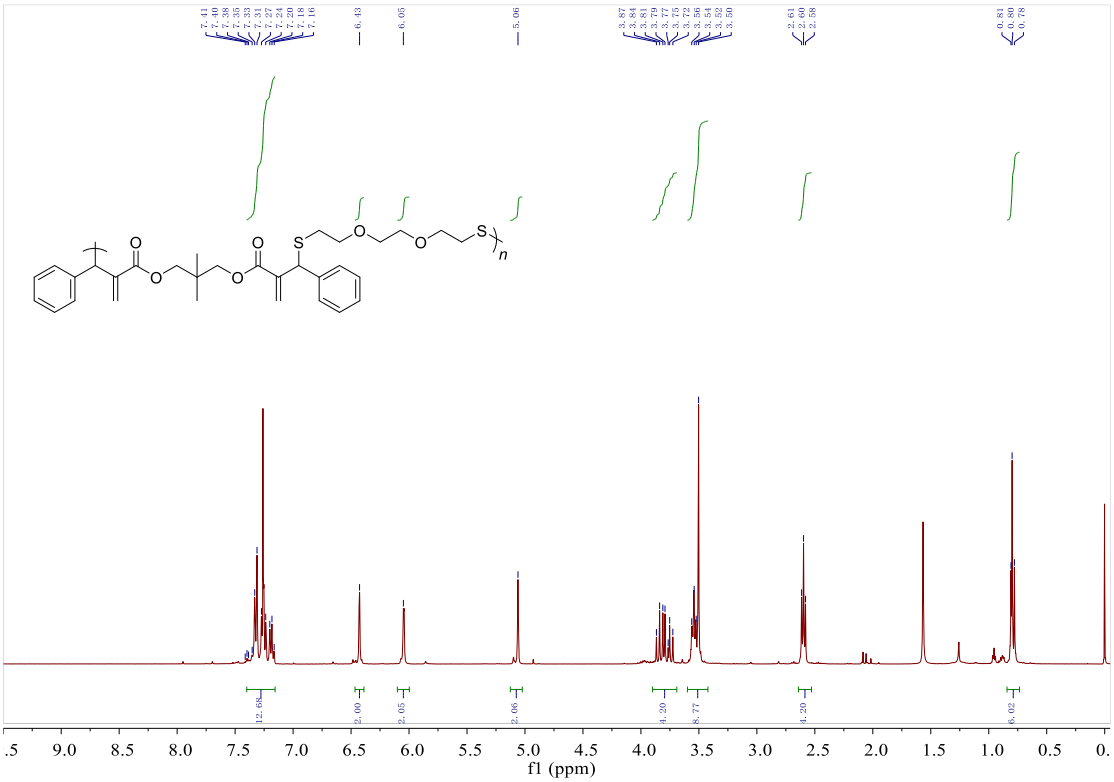


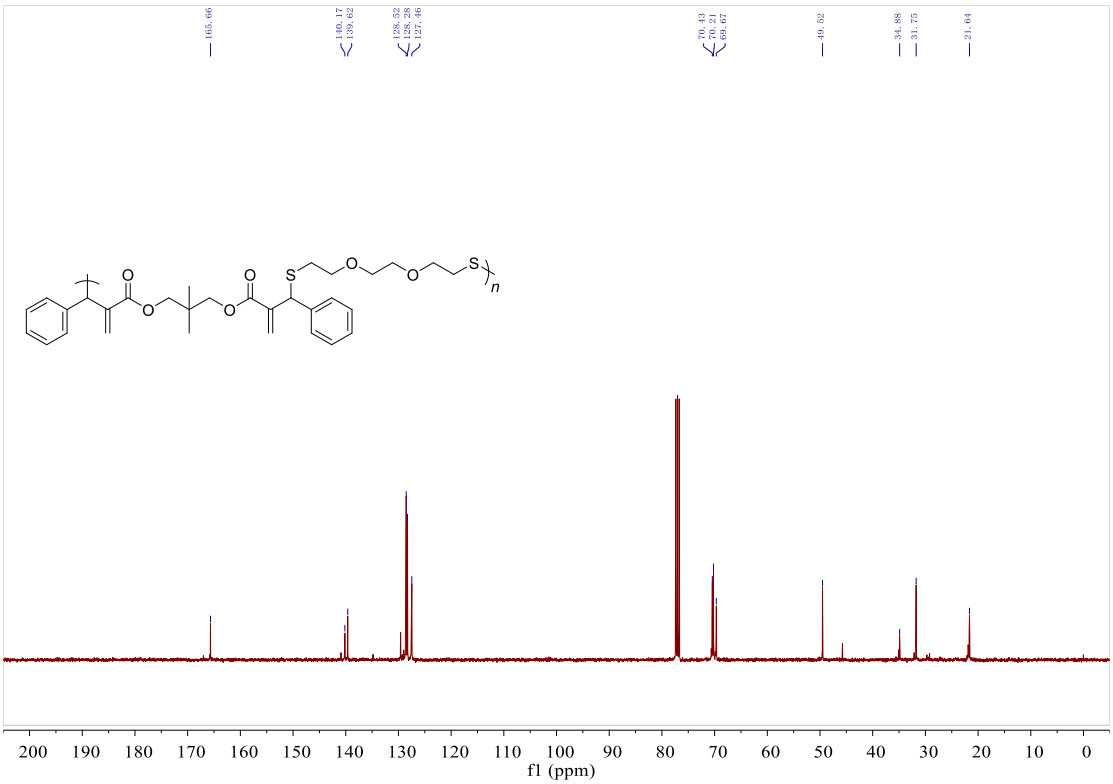
NMR of **α-P1b/2d**



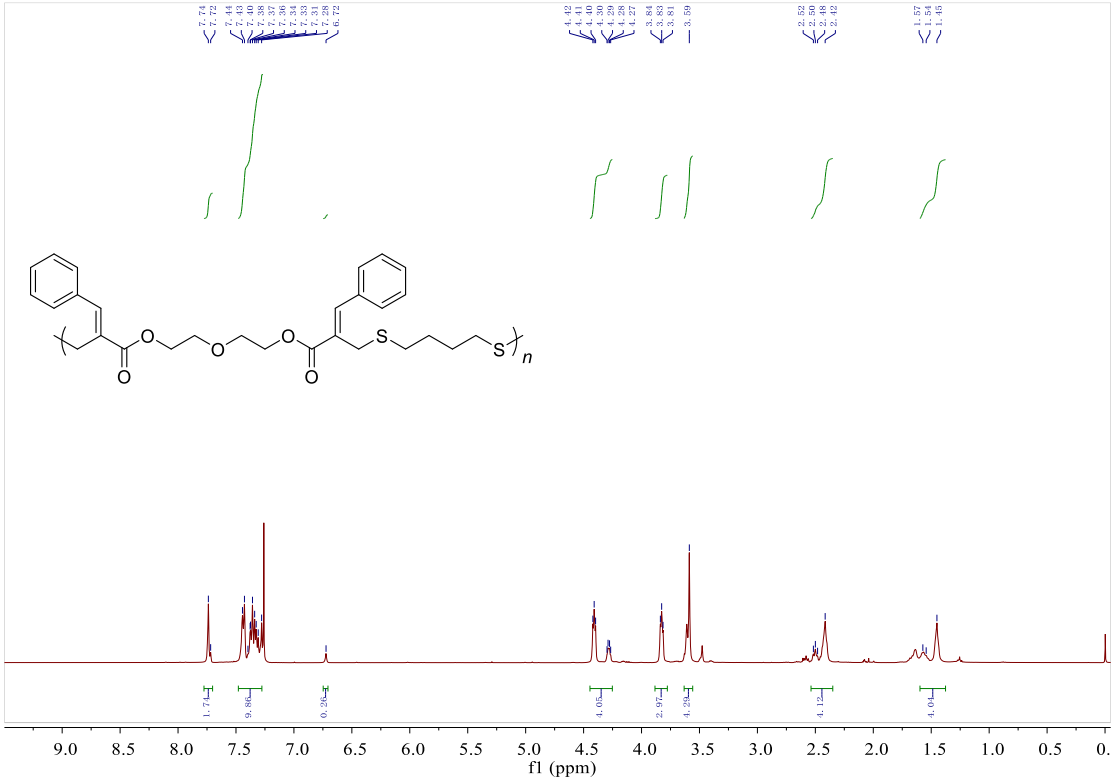


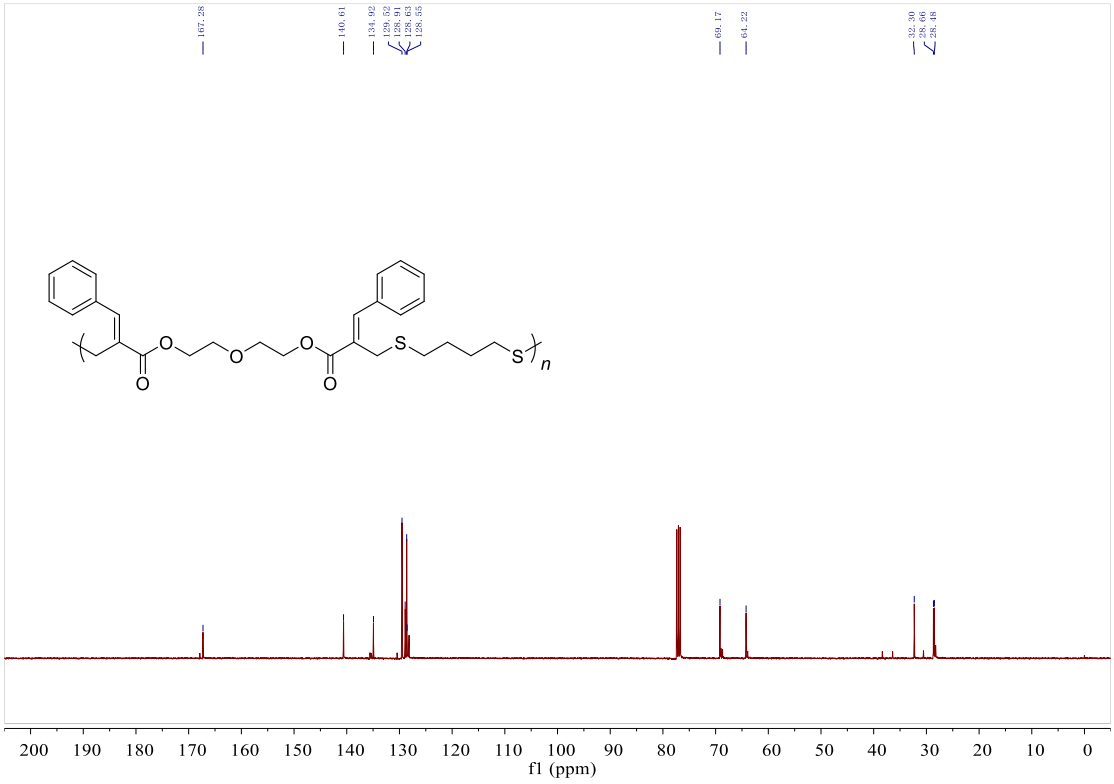
NMR of **γ-P1b/2d**



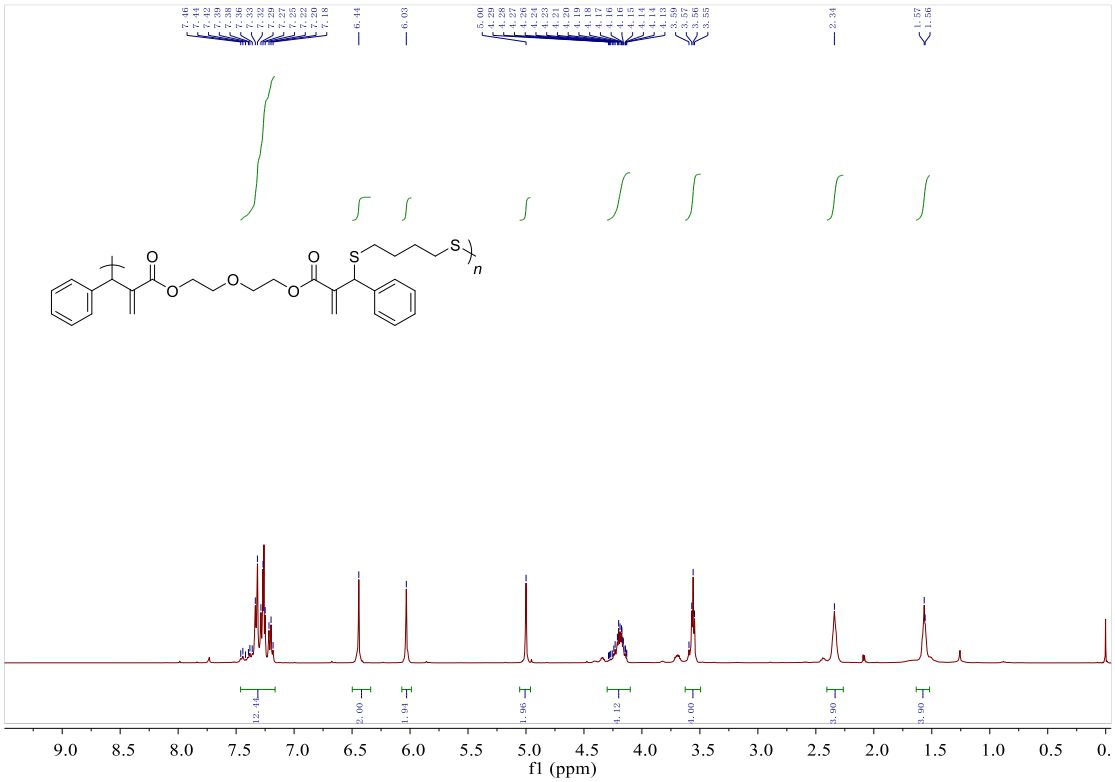


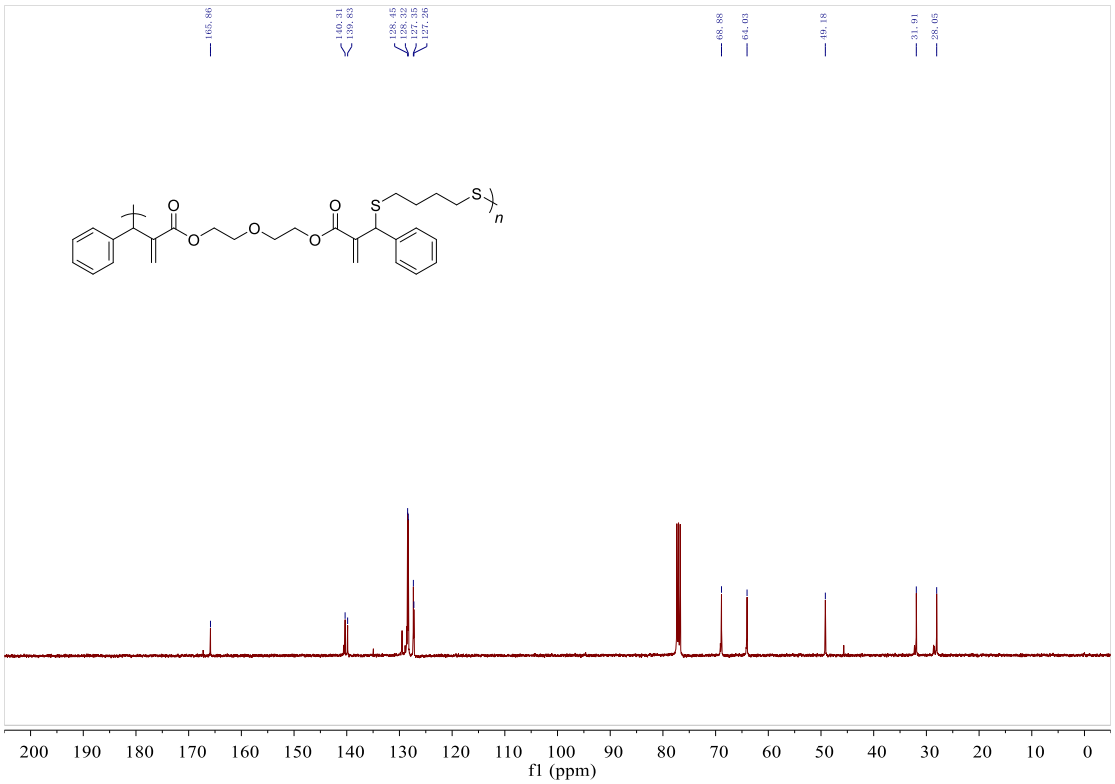
NMR of **α-P1c/2a**



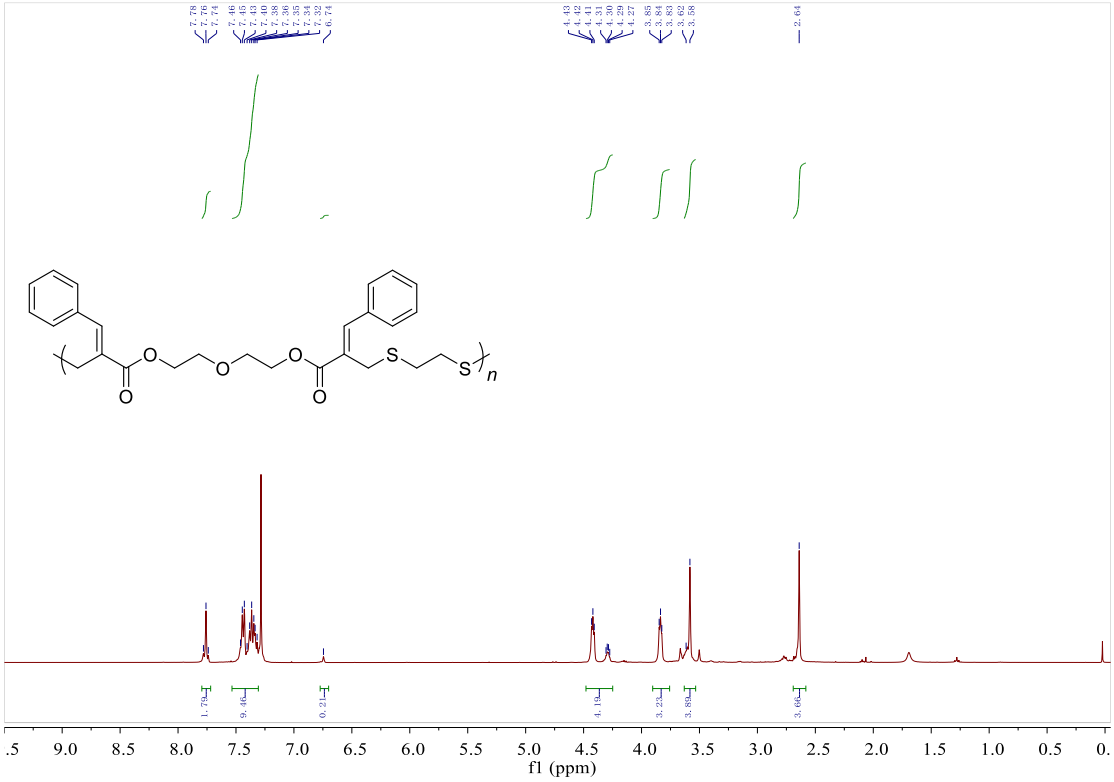


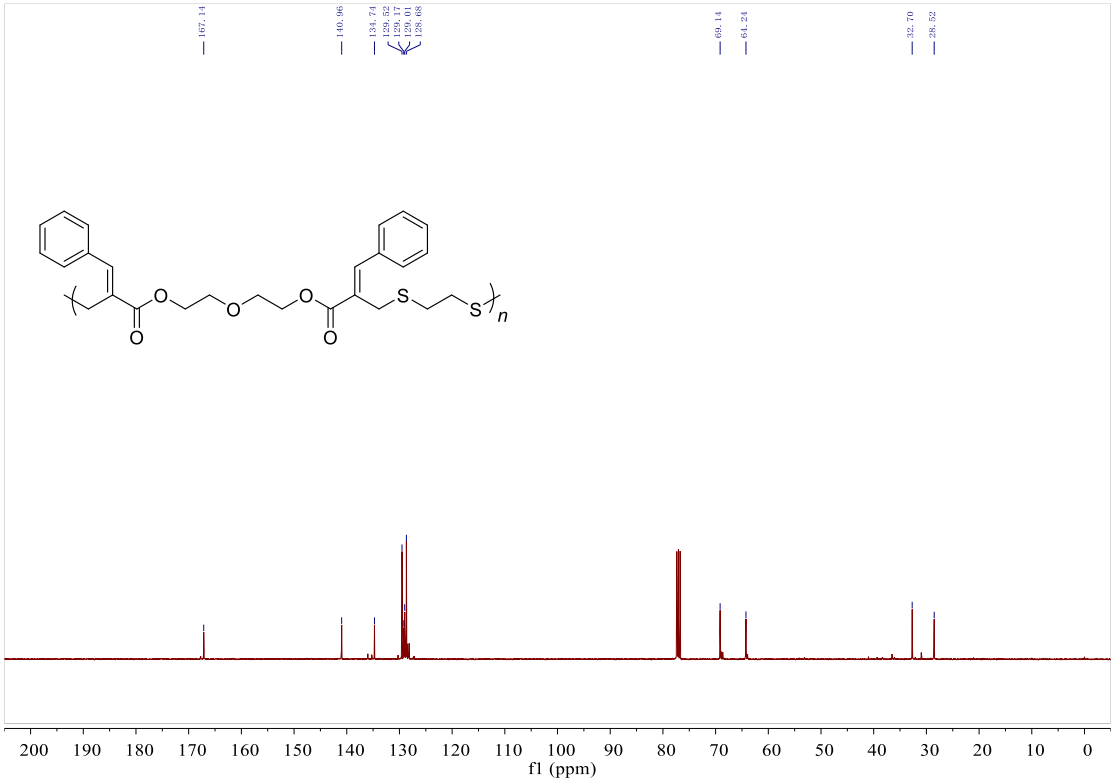
NMR of **γ-P1c/2a**



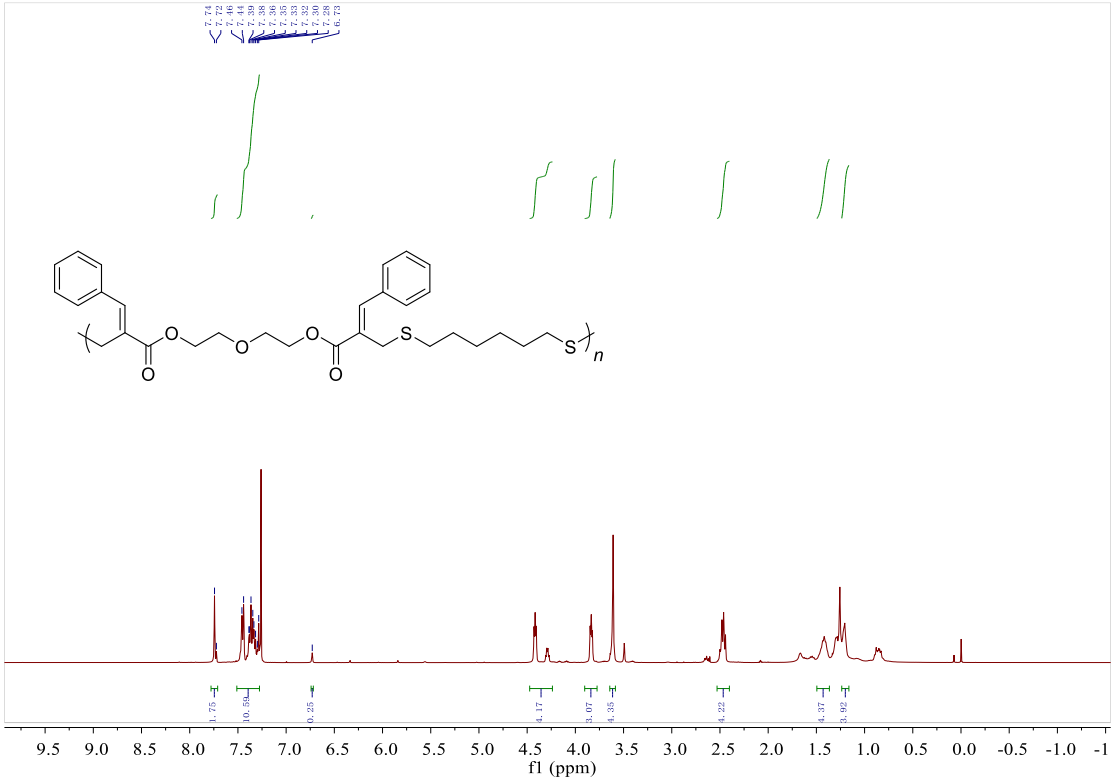


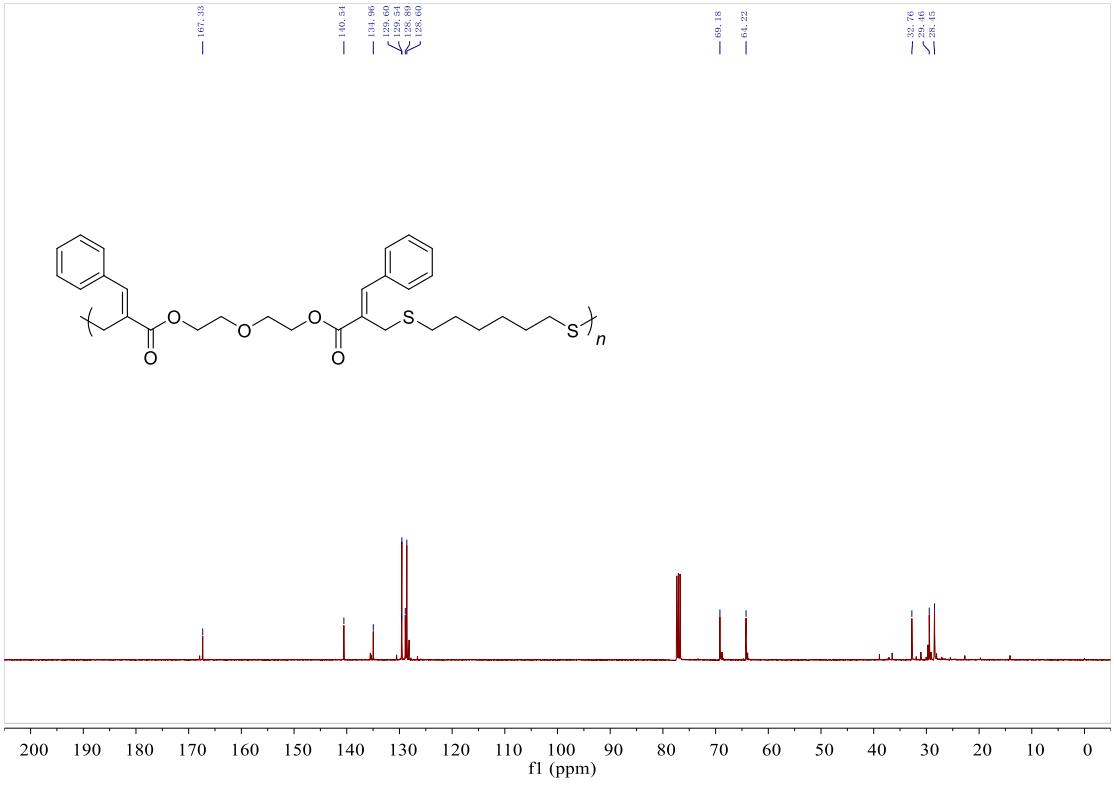
NMR of **α-P1c/2b**



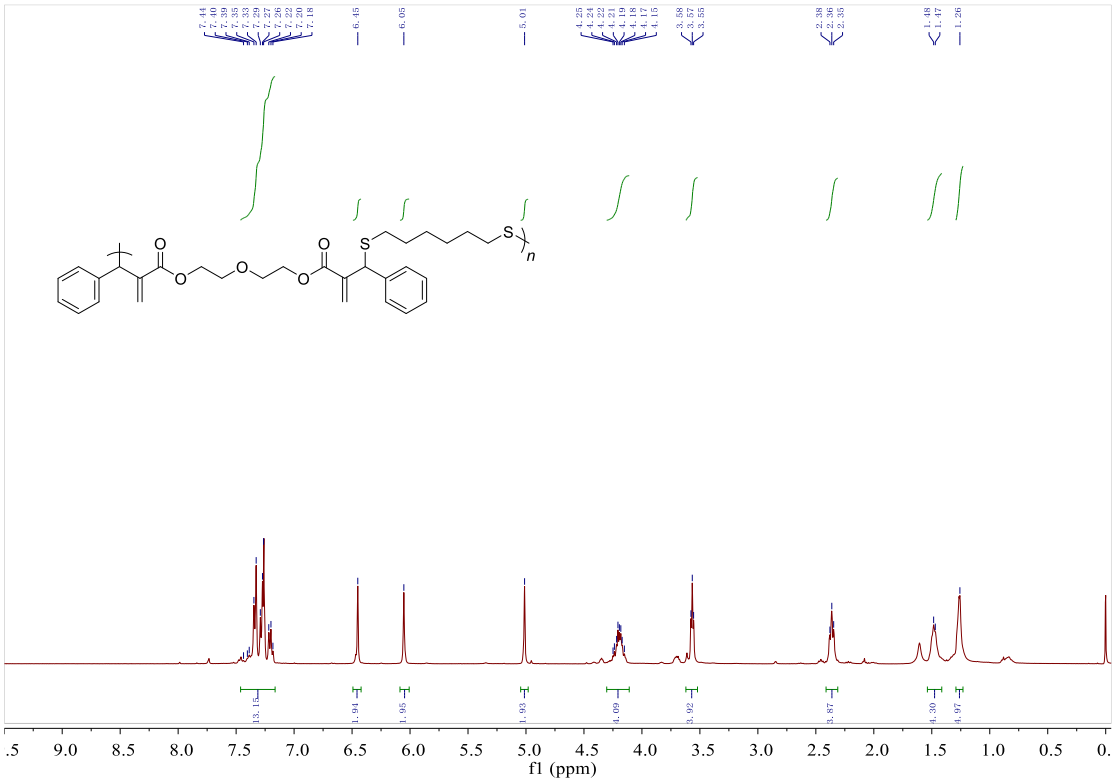


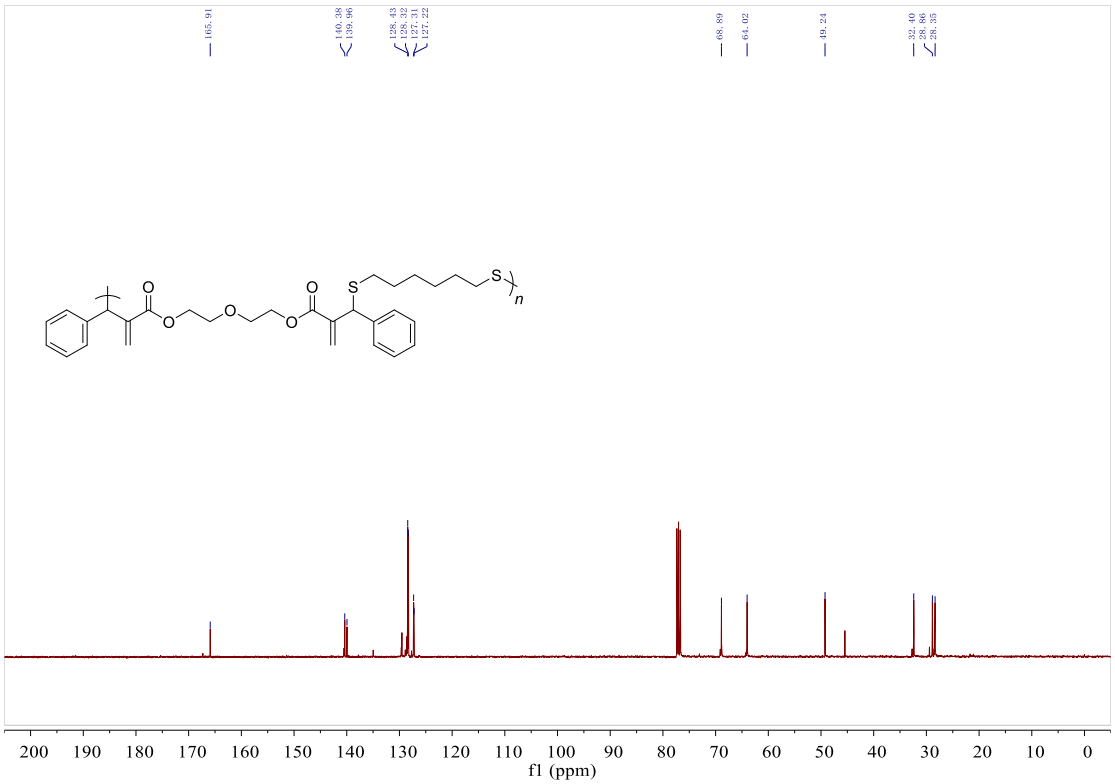
NMR of **α-P1c/2c**



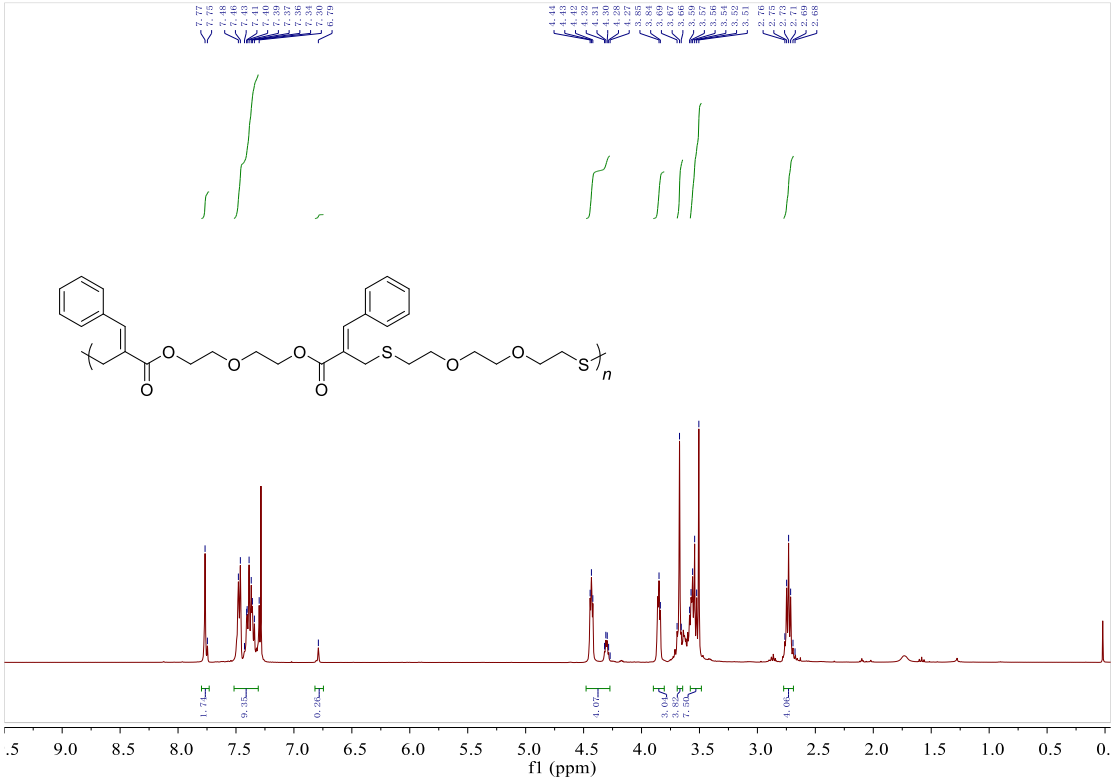


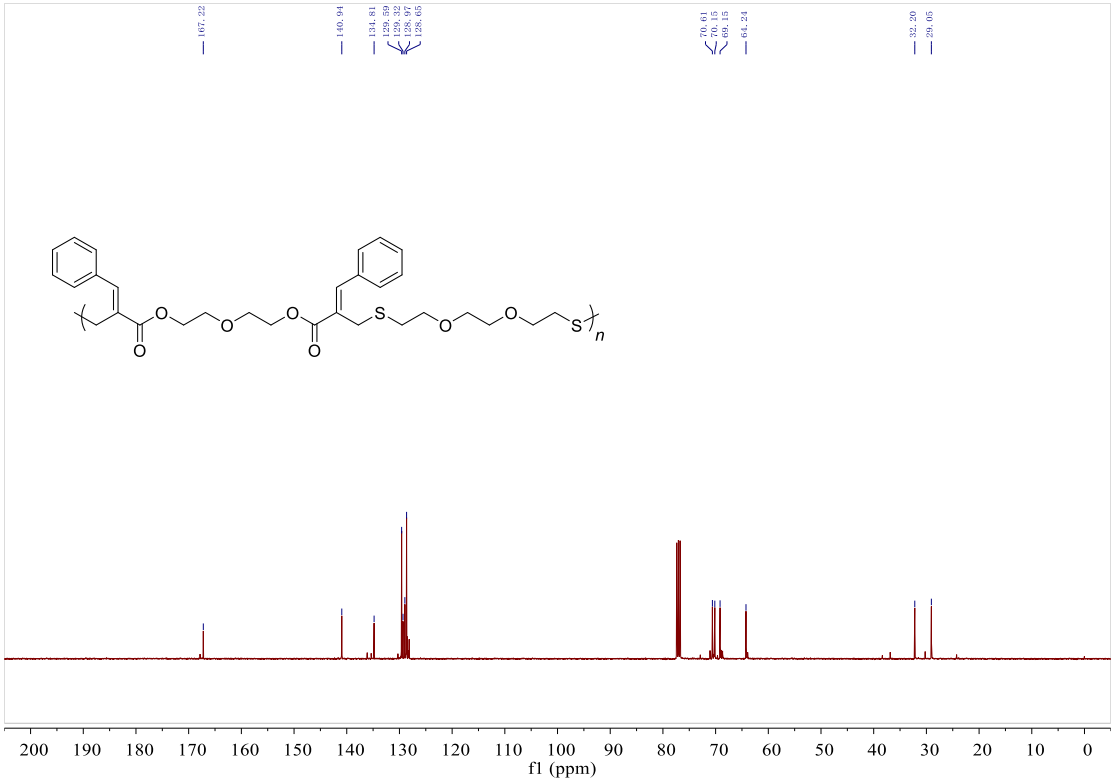
NMR of **γ-P1c/2c**



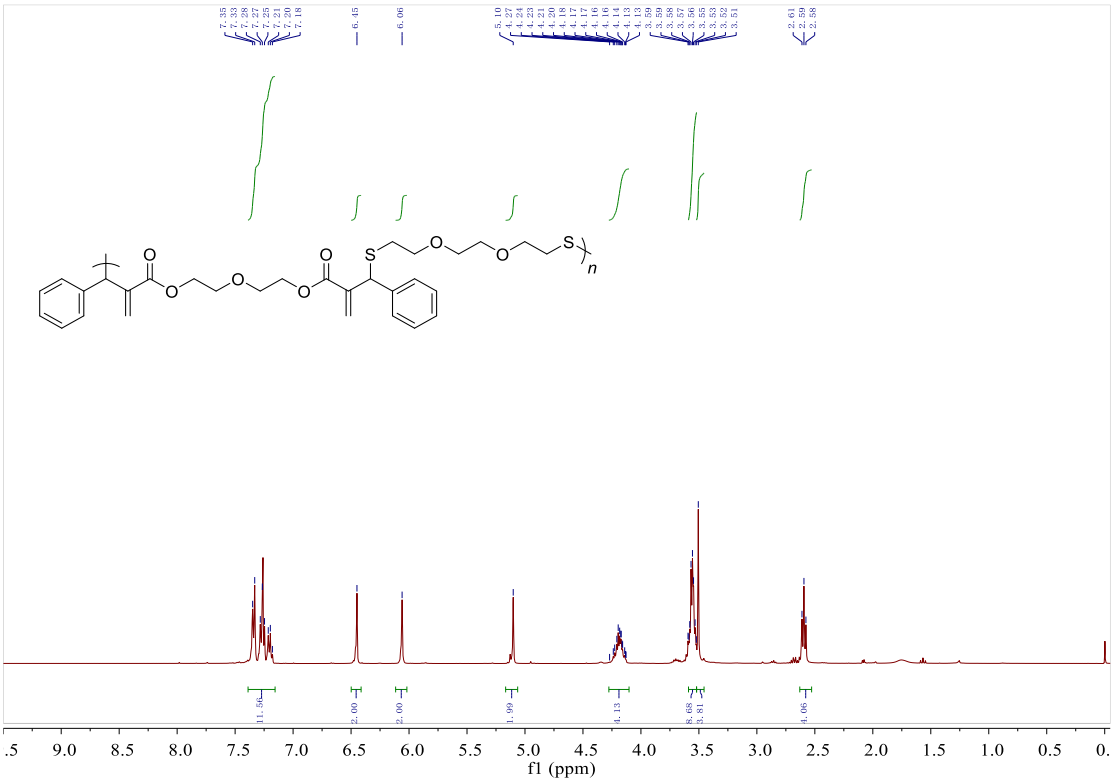


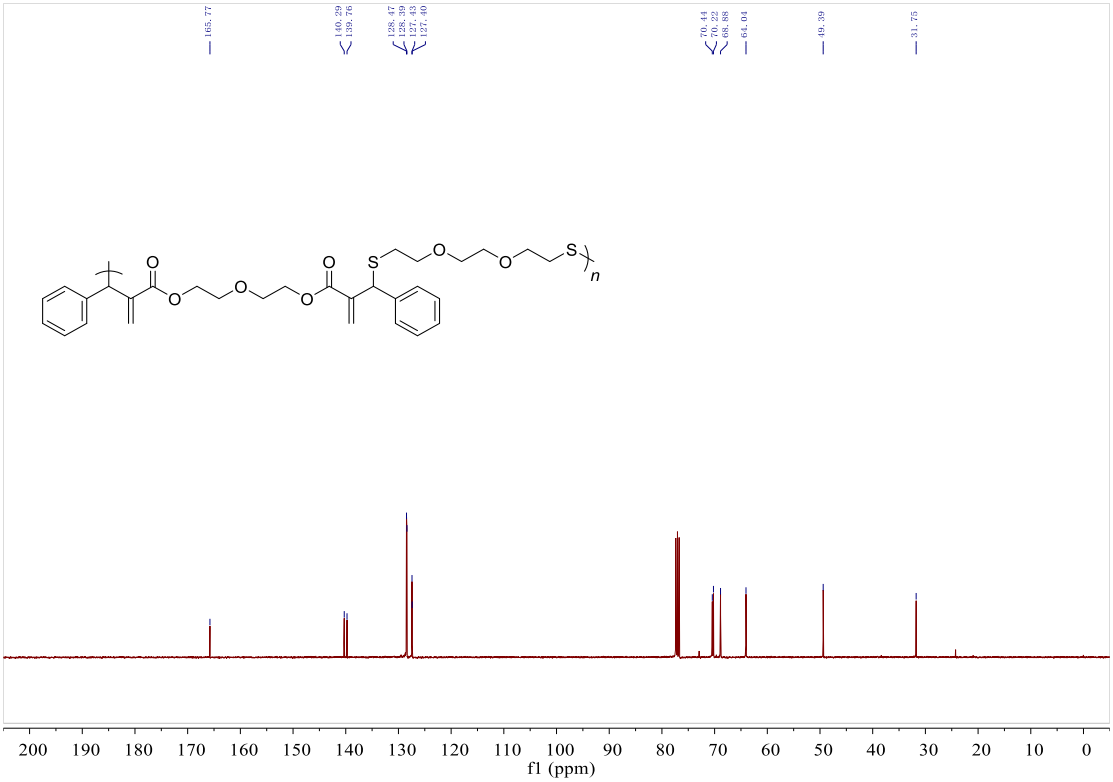
NMR of **α-P1c/2d**



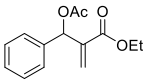


NMR of **γ-P1c/2d**





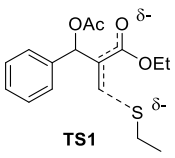
Cartesian coordinates of all optimized structures



R

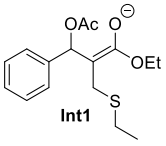
C	0.741663	-0.78303	0.018004
C	-0.3546	0.21635	0.319115
H	-0.20147	0.569852	1.343915
C	2.104394	-0.28293	0.383725
O	2.282723	0.671734	1.110868
O	3.093788	-0.99842	-0.15377
C	4.432272	-0.57689	0.176761
H	4.554774	0.463611	-0.13734
H	4.554259	-0.62338	1.263061
C	5.385933	-1.50204	-0.54204
H	5.242354	-2.53739	-0.22099
H	5.239918	-1.44629	-1.62407
H	6.415724	-1.21088	-0.31715
C	-1.75591	-0.33353	0.172118
C	-2.45925	-0.19605	-1.02536
C	-2.34451	-1.00891	1.244468
C	-3.74154	-0.73234	-1.14798
H	-2.0035	0.332998	-1.85721
C	-3.62293	-1.5481	1.119451
H	-1.79894	-1.11261	2.180227
C	-4.32443	-1.4095	-0.0787
H	-4.28382	-0.61887	-2.08177
H	-4.07448	-2.06846	1.958775
H	-5.32342	-1.82361	-0.17542
O	-0.1231	1.294932	-0.59985
C	-0.51569	2.560408	-0.31749
O	-0.38055	3.396028	-1.17629
C	-1.07446	2.85132	1.050775
H	-1.40456	3.888658	1.063824
H	-1.91635	2.194573	1.287534
H	-0.29991	2.710471	1.811235
C	0.550599	-1.99605	-0.49961
H	-0.44675	-2.35895	-0.73009
H	1.390906	-2.65299	-0.69754

C	0.455994	0.643262	7.71E-05
C	1.609173	-0.35706	-6.6E-05
H	2.58852	0.145684	0.000214
H	1.552888	-1.00318	0.882941
H	1.553116	-1.00265	-0.88347
H	0.55963	1.294992	-0.87828
H	0.559369	1.2944	0.878901
S	-1.19957	-0.14574	-0.00042



TS1

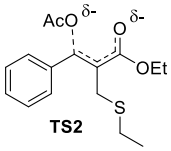
C	-0.27846	-0.25742	-0.48995
C	1.056876	-0.32742	0.203026
H	0.877494	-0.4871	1.269472
C	-1.18566	-1.31425	-0.07964
O	-0.93868	-2.14865	0.787705
O	-2.36848	-1.32249	-0.74169
C	-3.32817	-2.28339	-0.30243
H	-2.93469	-3.29225	-0.46936
H	-3.49293	-2.16342	0.774102
C	-4.59721	-2.0419	-1.09069
H	-4.98387	-1.03558	-0.90388
H	-4.41122	-2.14651	-2.16368
H	-5.36197	-2.76804	-0.79849
C	1.935558	0.897732	0.048155
C	3.168382	0.845659	-0.6035
C	1.499678	2.111979	0.592284
C	3.959864	1.99225	-0.70638
H	3.506156	-0.09126	-1.03451
C	2.287992	3.253714	0.485064
H	0.519203	2.167566	1.060529
C	3.524375	3.197581	-0.1622
H	4.917139	1.938299	-1.21731
H	1.928873	4.191433	0.899365
H	4.137796	4.090066	-0.24785
O	1.762481	-1.48221	-0.31847
C	2.291006	-2.43255	0.464323
O	2.871382	-3.35556	-0.06691
C	2.150715	-2.319	1.961884
H	2.678832	-3.16025	2.408581
H	2.580052	-1.38252	2.330607
H	1.092907	-2.35287	2.237736
C	-0.66929	0.751292	-1.33138
H	0.058079	1.459144	-1.71079
H	-1.58055	0.643015	-1.90679
S	-1.90322	2.715075	-0.25865
C	-3.45511	1.760263	-0.07714
H	-3.52627	1.034142	-0.89724
H	-4.3092	2.440701	-0.18336
C	-3.56153	1.023561	1.255146
H	-3.55001	1.735696	2.087651
H	-4.48884	0.435249	1.319668
H	-2.71271	0.345252	1.393415



Int1

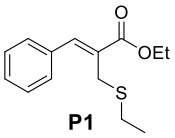
C	-0.2368	-0.63409	-0.22837
C	1.134873	-0.77298	0.328948
H	1.063822	-1.21641	1.326257
C	-1.3042	-1.1062	0.536873
O	-1.27665	-1.66721	1.656281
O	-2.54834	-0.90417	-0.06474
C	-3.67608	-1.31195	0.689553
H	-3.65297	-2.39753	0.847271

H	-3.65661	-0.84091	1.679516
C	-4.91097	-0.90064	-0.0882
H	-4.94833	0.186713	-0.20991
H	-4.91089	-1.35662	-1.08326
H	-5.81619	-1.21946	0.438852
C	1.886787	0.542602	0.432375
C	2.839168	0.94512	-0.50483
C	1.546375	1.420281	1.467704
C	3.42497	2.209712	-0.42067
H	3.116094	0.267265	-1.30529
C	2.134849	2.677192	1.557846
H	0.791571	1.116055	2.190195
C	3.075919	3.080797	0.607751
H	4.154678	2.513282	-1.1664
H	1.853594	3.348419	2.36479
H	3.529078	4.066135	0.670053
O	1.997857	-1.62957	-0.50908
C	1.902406	-2.96047	-0.48534
O	2.49796	-3.6048	-1.32769
C	1.117566	-3.61107	0.624002
H	1.091253	-4.68388	0.436004
H	1.617298	-3.42603	1.581528
H	0.106984	-3.2049	0.710963
C	-0.41738	0.049466	-1.53516
H	0.454147	-0.10782	-2.18232
H	-1.2927	-0.3311	-2.06773
S	-0.59508	1.919525	-1.58149
C	-2.23212	2.137793	-0.80585
H	-2.865	1.305785	-1.12823
H	-2.64429	3.059622	-1.23069
C	-2.199	2.229407	0.715311
H	-1.58629	3.077742	1.038494
H	-3.21337	2.365699	1.113044
H	-1.77615	1.321853	1.152673



TS2

C	-1.08483	0.482117	-0.80477
C	-0.50887	-0.61281	0.035596
C	0.847411	-0.69835	0.34686
H	1.075442	-1.43404	1.113452
C	-1.33124	-1.70894	0.479121
O	-0.97895	-2.67955	1.14666
O	-2.63756	-1.58526	0.086372
C	-3.52143	-2.60911	0.530354
H	-3.17692	-3.57907	0.155258
H	-3.50473	-2.65557	1.625028
C	-4.90313	-2.26903	0.01262
H	-5.22834	-1.29618	0.393072
H	-4.90824	-2.23067	-1.08075
H	-5.62277	-3.0278	0.336023
C	1.703999	0.529104	0.389749
C	2.240046	1.13174	-0.75282
C	1.949661	1.115345	1.637135
C	2.985091	2.305481	-0.64877
H	2.088026	0.654848	-1.71549
C	2.698133	2.285609	1.74238
H	1.534659	0.652904	2.529957
C	3.216522	2.888517	0.596842
H	3.396099	2.75936	-1.54644
H	2.874528	2.726417	2.719616
H	3.801796	3.800449	0.674162
O	1.705051	-1.62864	-1.05024
C	2.784919	-2.31971	-0.8959
O	3.373229	-2.88046	-1.8265
C	3.33973	-2.45611	0.519589
H	4.292513	-2.98543	0.485755
H	3.483802	-1.47452	0.98276
H	2.637616	-3.02256	1.140764
S	-1.78739	1.854478	0.213904
C	-2.35884	2.946378	-1.12865
H	-1.50228	3.205385	-1.76106
H	-3.08158	2.401435	-1.74638
C	-2.99424	4.208041	-0.55811
H	-2.27826	4.763806	0.055262
H	-3.33178	4.86542	-1.36616
H	-3.85981	3.96448	0.065934
H	-0.31915	0.924342	-1.44821
H	-1.89433	0.110848	-1.43881



P1

C	-1.02225	0.949964	-0.55908
C	-0.561	-0.11328	0.394601
C	0.641994	-0.17054	0.991231
H	0.768036	-0.94234	1.749916
C	-1.55591	-1.15569	0.811876
O	-1.41508	-1.91589	1.746173
O	-2.62752	-1.17671	0.009853
C	-3.65695	-2.12141	0.352134
H	-3.23762	-3.13074	0.298106
H	-3.96907	-1.93652	1.384131
C	-4.79215	-1.92528	-0.62596
H	-5.19279	-0.91024	-0.555
H	-4.45805	-2.1011	-1.65229
H	-5.59716	-2.63003	-0.39953
C	1.803765	0.711598	0.763704
C	2.282593	1.007314	-0.51962
C	2.485056	1.229432	1.873906
C	3.395534	1.828516	-0.6874
H	1.798817	0.567322	-1.38715
C	3.589154	2.060082	1.705287
H	2.134015	0.986345	2.873462
C	4.045889	2.364295	0.423084
H	3.760283	2.042624	-1.68756
H	4.096695	2.464743	2.575637
H	4.911839	3.005664	0.290361
S	-2.11965	2.116134	0.339481
C	-3.14784	2.68114	-1.05641
H	-2.49593	3.100148	-1.82938

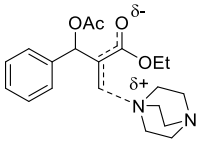
H	-3.66849	1.81335	-1.47483
C	-4.14488	3.725929	-0.57443
H	-3.63241	4.59915	-0.16034
H	-4.76852	4.06079	-1.40863
H	-4.80278	3.316134	0.197858
H	-0.18437	1.506134	-0.97732
H	-1.60419	0.510681	-1.37317

AcO$^{\ominus}$

O	-0.74833	-1.13006	0.002688
C	-0.19899	-0.00037	-0.01132
O	-0.7538	1.126606	0.005019
C	1.347962	0.002915	-0.00635
H	1.743169	0.902424	-0.48689
H	1.691018	9.41E-05	1.035535
H	1.746389	-0.89218	-0.49247

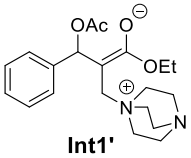
DABCO

C	3.038561	0.170855	0.029147
C	4.26868	-0.62391	0.55858
H	3.337479	0.931419	-0.70042
H	2.509033	0.67959	0.841809
H	5.20845	-0.20917	0.178087
H	4.316552	-0.60519	1.652926
C	2.76508	-1.35767	-1.78697
H	2.062032	-2.06136	-2.24597
H	2.976049	-0.57241	-2.52079
C	4.068731	-2.07516	-1.32853
H	4.079387	-3.12532	-1.63982
H	4.959115	-1.59539	-1.74928
C	2.973535	-2.62509	0.722017
H	2.90426	-3.65913	0.36728
H	3.099281	-2.65456	1.809723
C	1.717904	-1.79872	0.315065
H	0.958219	-2.42941	-0.1593
H	1.255553	-1.31905	1.184703
N	4.180042	-2.02753	0.135323
N	2.097452	-0.74229	-0.6321



TS1'

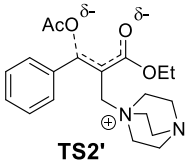
C	-2.85239	0.251998	-0.16885
C	-4.01772	-0.63742	-0.6886
H	-3.19894	1.013538	0.537629
H	-2.31903	0.763583	-0.97593
H	-4.98544	-0.23223	-0.37814
H	-4.01219	-0.6938	-1.78145
C	-2.51115	-1.18421	1.732877
H	-1.78147	-1.85712	2.19559
H	-2.7249	-0.37276	2.437104
C	-3.8025	-1.93946	1.299487
H	-3.80649	-2.95973	1.694084
H	-4.69774	-1.43174	1.671542
C	-2.65301	-2.59016	-0.68897
H	-2.52871	-3.58011	-0.23921
H	-2.76107	-2.724	-1.76942
C	-1.43544	-1.67868	-0.35993
H	-0.63149	-2.23005	0.138623
H	-1.01642	-1.20353	-1.25162
N	-3.889	-2.00075	-0.16316
N	-1.88142	-0.60145	0.537814
C	-0.37142	0.543647	1.127355
H	0.028005	-0.24511	1.763846
H	-1.07942	1.209677	1.615454
C	0.445666	1.060821	0.135501
C	1.807799	0.497437	-0.16009
H	2.15762	0.958067	-1.08655
C	0.171371	2.347569	-0.47509
O	0.914878	2.941639	-1.2468
O	-1.02705	2.880694	-0.1099
C	-1.31598	4.184275	-0.62654
H	-0.55171	4.88634	-0.27756
H	-1.26975	4.15749	-1.71979
C	-2.69346	4.570068	-0.13408
H	-3.44968	3.869684	-0.50137
H	-2.72736	4.578885	0.959221
H	-2.94963	5.570577	-0.4944
C	1.875333	-1.00955	-0.29552
C	2.106953	-1.83306	0.809381
C	1.686913	-1.5938	-1.55169
C	2.107684	-3.2214	0.66537
H	2.297106	-1.38361	1.780308
C	1.689817	-2.97877	-1.6978
H	1.527116	-0.95382	-2.41757
C	1.890781	-3.798	-0.58539
H	2.288462	-3.85219	1.53098
H	1.544645	-3.42017	-2.67961
H	1.8976	-4.87799	-0.69799
O	2.683586	0.914788	0.926807
C	4.014995	1.019594	0.759307
O	4.704803	1.205005	1.735739
C	4.576356	0.937312	-0.63867
H	5.65959	1.02503	-0.57151
H	4.315297	-0.01052	-1.11838
H	4.183313	1.753095	-1.25368



Int1'

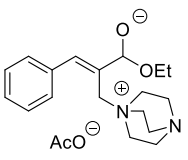
C	2.444265	1.878991	-0.01464
C	3.829847	1.765052	0.664238
H	2.416479	2.63062	-0.80769
H	1.636403	2.094073	0.685667
H	4.436192	2.644012	0.430001
H	3.724152	1.71016	1.751415
C	3.085737	0.332728	-1.7824

H	2.907937	-0.68506	-2.14077
H	2.838079	1.034287	-2.58243
C	4.526116	0.529758	-1.24806
H	5.168613	-0.28472	-1.59261
H	4.949448	1.469725	-1.6128
C	3.808381	-0.61076	0.711832
H	4.256591	-1.50451	0.268076
H	3.933347	-0.67612	1.795815
C	2.304598	-0.51821	0.35683
H	1.916263	-1.44606	-0.07086
H	1.678555	-0.24471	1.207097
N	4.533152	0.561024	0.214931
N	2.121135	0.566536	-0.66137
C	0.652799	0.5843	-1.24145
H	0.600776	-0.37004	-1.77778
H	0.712581	1.400918	-1.96813
C	-0.4461	0.746661	-0.28026
C	-1.38393	-0.38815	-0.04329
H	-2.10836	-0.04943	0.700236
C	-1.02094	2.026972	-0.05782
O	-2.08451	2.281138	0.517339
O	-0.25449	3.068187	-0.55192
C	-0.8149	4.372602	-0.41517
H	-1.76629	4.420164	-0.9557
H	-1.02616	4.573953	0.640032
C	0.188617	5.357307	-0.97744
H	1.128803	5.319447	-0.41793
H	0.40037	5.139245	-2.0288
H	-0.20704	6.375199	-0.91133
C	-0.75205	-1.68588	0.422512
C	-0.45846	-2.72763	-0.46135
C	-0.41387	-1.83124	1.773003
C	0.199936	-3.87474	-0.01125
H	-0.74775	-2.64016	-1.50486
C	0.238331	-2.97487	2.224663
H	-0.65188	-1.02711	2.466905
C	0.558675	-3.99917	1.329314
H	0.42418	-4.67448	-0.71136
H	0.492733	-3.07266	3.276263
H	1.065304	-4.89307	1.680764
O	-2.10443	-0.66381	-1.29746
C	-3.32697	-1.21443	-1.30822
O	-3.79613	-1.57078	-2.36768
C	-4.07703	-1.33392	-0.00391
H	-5.03312	-1.81378	-0.20724
H	-3.51719	-1.92846	0.723924
H	-4.24983	-0.34194	0.424858



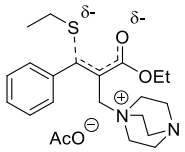
TS2'

C	-2.84432	0.086145	-0.34319
C	-3.89887	-0.93434	-0.83851
H	-3.2598	0.849248	0.31906
H	-2.32573	0.5821	-1.16441
H	-4.90543	-0.54939	-0.65668
H	-3.79217	-1.10587	-1.91293
C	-2.45732	-1.19619	1.698787
H	-1.70931	-1.82528	2.188419
H	-2.68225	-0.34725	2.347639
C	-3.72564	-1.98439	1.289935
H	-3.75193	-2.94492	1.810169
H	-4.6285	-1.42945	1.559109
C	-2.46856	-2.8141	-0.55428
H	-2.30501	-3.71266	0.046734
H	-2.52874	-3.11756	-1.60223
C	-1.30533	-1.81057	-0.36134
H	-0.45789	-2.24456	0.174522
H	-0.94131	-1.38941	-1.30055
N	-3.74346	-2.21758	-0.15338
N	-1.80762	-0.65091	0.457223
C	-0.65456	0.277138	0.874461
H	-0.01862	-0.35095	1.500272
H	-1.12544	1.035414	1.504322
C	0.110524	0.901264	-0.24249
C	1.358035	0.468423	-0.62406
H	1.823806	1.035899	-1.4253
C	-0.26942	2.231054	-0.73377
O	0.285209	2.846014	-1.62568
O	-1.35034	2.742395	-0.088
C	-1.7443	4.066911	-0.47689
H	-0.89638	4.742871	-0.33478
H	-1.9985	4.065256	-1.54159
C	-2.92405	4.459793	0.383578
H	-3.76764	3.779903	0.229459
H	-2.65247	4.448325	1.442933
H	-3.24955	5.471018	0.123792
C	1.859242	-0.92292	-0.44748
C	2.214827	-1.47284	0.789406
C	1.935068	-1.72412	-1.59372
C	2.598127	-2.81053	0.877237
H	2.235294	-0.82958	1.66361
C	2.312945	-3.06272	-1.50319
H	1.689102	-1.29437	-2.56269
C	2.637407	-3.61298	-0.26355
H	2.889095	-3.22002	1.840152
H	2.365684	-3.66997	-2.40221
H	2.943148	-4.65232	-0.19028
O	2.595582	1.371384	0.818926
C	3.87479	1.260438	0.814969
O	4.579773	1.158178	1.828579
C	4.544448	1.239276	-0.55996
H	5.62404	1.365354	-0.46373
H	4.350531	0.273395	-1.04274
H	4.13257	2.024507	-1.2012



Int2

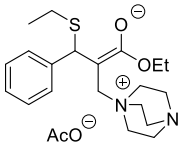
C	2.197445	-2.06017	0.738906
C	2.20049	-3.52227	1.255853
H	3.021168	-1.8531	0.053464
H	2.219906	-1.33196	1.55424
H	2.920078	-4.12295	0.692353
H	2.495268	-3.54175	2.308415
C	0.771225	-2.9308	-1.0479
H	-0.09387	-2.66102	-1.65913
H	1.690622	-2.90531	-1.64051
C	0.566805	-4.27206	-0.31166
H	-0.47927	-4.57103	-0.40669
H	1.207529	-5.04339	-0.74827
C	-0.1196	-3.26112	1.726664
H	-1.08829	-3.76589	1.707903
H	0.165623	-3.08877	2.768922
C	-0.23743	-1.92753	0.952539
H	-1.14202	-1.90194	0.341094
H	-0.17887	-1.05672	1.607841
N	0.882539	-4.13329	1.112659
N	0.91869	-1.83334	-0.01476
C	0.894506	-0.50512	-0.7494
H	-0.09606	-0.46301	-1.20199
H	1.629042	-0.60386	-1.55033
C	1.236824	0.68345	0.112213
C	0.394923	1.480134	0.809062
C	2.679374	1.091303	0.201197
O	3.125303	1.912529	0.974233
O	3.452878	0.450885	-0.69023
C	4.851734	0.799722	-0.68346
H	4.942586	1.871026	-0.88323
H	5.25412	0.605366	0.315347
C	5.52986	-0.03553	-1.7442
H	5.430589	-1.10325	-1.52803
H	5.101697	0.163895	-2.7301
H	6.595097	0.20892	-1.77499
C	-1.06035	1.491057	1.007799
C	-2.00458	0.854878	0.185113
C	-1.52204	2.217346	2.120546
C	-3.3601	0.924026	0.491199
H	-1.72424	0.299019	-0.70234
C	-2.87679	2.275852	2.429089
H	-0.8026	2.7347	2.750446
C	-3.80162	1.624499	1.613833
H	-4.07052	0.421631	-0.15914
H	-3.20975	2.833803	3.298743
H	-4.86113	1.669358	1.847642
O	-1.8778	-1.39008	-2.00613
C	-2.6726	-2.31723	-1.67177
O	-2.40601	-3.24959	-0.87126
C	-4.06487	-2.31645	-2.30428
H	-4.82409	-2.50221	-1.53937
H	-4.26956	-1.37639	-2.82031
H	-4.12504	-3.13714	-3.02706
H	0.904493	2.266363	1.365861



TS3

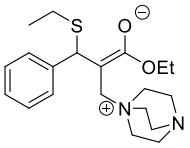
C	2.826078	0.78294	0.777293
C	4.008769	-0.02646	1.3717
H	3.150682	1.564932	0.088403
H	2.200608	1.234593	1.550989
H	4.953018	0.296121	0.922576
H	4.073575	0.145286	2.450012
C	2.798568	-0.85391	-1.03411
H	2.110149	-1.46878	-1.62072
H	3.232627	-0.06192	-1.65169
C	3.867089	-1.70729	-0.31289
H	3.644092	-2.76298	-0.48008
H	4.865209	-1.47563	-0.69736
C	2.557149	-1.89519	1.662495
H	2.461096	-2.97125	1.502125
H	2.539361	-1.68684	2.736665
C	1.387473	-1.18458	0.942646
H	0.817129	-1.87941	0.323954
H	0.726857	-0.65027	1.628145
N	3.850883	-1.45726	1.130729
N	1.95219	-0.15405	0.000453
C	0.818278	0.573594	-0.73071
H	0.253829	-0.232	-1.1984
H	1.315191	1.144667	-1.51707
C	-0.00205	1.476491	0.140011
C	-1.19867	1.178926	0.739328
C	0.424723	2.878849	0.298693
O	-0.04632	3.690195	1.075188
O	1.447758	3.222152	-0.53065
C	1.882405	4.584437	-0.44965
H	1.036471	5.240013	-0.67748
H	2.203816	4.79819	0.575367
C	3.010726	4.760006	-1.44186
H	3.852868	4.104102	-1.20004
H	2.673028	4.533364	-2.45689
H	3.365417	5.794597	-1.41909
C	-1.85961	-0.12294	0.945369
C	-1.86976	-1.18201	0.026442
C	-2.51759	-0.30181	2.172571
C	-2.47228	-2.39349	0.351846
H	-1.43212	-1.08208	-0.95882
C	-3.12557	-1.51285	2.49578
H	-2.5556	0.527079	2.875665
C	-3.09626	-2.57044	1.588116
H	-2.4535	-3.1992	-0.37705
H	-3.62621	-1.62609	3.453276
H	-3.56749	-3.51782	1.833591
O	0.215086	-2.46345	-1.95101
C	0.577865	-3.59457	-1.52811
O	1.533042	-3.81354	-0.73519
C	-0.20104	-4.81989	-2.01955
H	-0.54252	-5.40667	-1.16103
H	-1.05388	-4.53251	-2.63789

H	0.469088	-5.46089	-2.60239
H	-1.59926	1.975382	1.356627
S	-3.37049	2.06171	-0.84074
C	-4.7235	0.938446	-0.33483
H	-5.06939	1.202488	0.673393
H	-4.33989	-0.0894	-0.27593
C	-5.91633	0.963941	-1.28826
H	-5.60333	0.67868	-2.29813
H	-6.7039	0.269957	-0.96162
H	-6.34596	1.969839	-1.34631



Int3

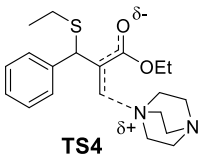
C	-1.87567	-1.27219	-0.95871
C	-1.55907	-2.57362	-1.73789
H	-2.74496	-1.3664	-0.30631
H	-2.03473	-0.40654	-1.60613
H	-2.23969	-3.37511	-1.43303
H	-1.69167	-2.41304	-2.81223
C	-0.42398	-2.11489	0.804493
H	0.391749	-1.80544	1.46557
H	-1.33766	-2.2947	1.379321
C	-0.02388	-3.32567	-0.07255
H	1.028298	-3.55835	0.106431
H	-0.63862	-4.19807	0.17162
C	0.730184	-1.93297	-1.84481
H	1.755798	-2.28115	-1.70089
H	0.580985	-1.6833	-2.90039
C	0.494185	-0.69864	-0.94484
H	1.326959	-0.54635	-0.25773
H	0.295815	0.212655	-1.51176
N	-0.18841	-3.02276	-1.49876
N	-0.71066	-0.94092	-0.08693
C	-1.01024	0.305128	0.826994
H	-0.07479	0.400353	1.390794
H	-1.78922	-0.08929	1.488136
C	-1.41461	1.559146	0.158696
C	-0.49923	2.755112	0.140058
C	-2.77717	1.862222	-0.05162
O	-3.27257	2.929605	-0.4459
O	-3.63792	0.799362	0.227215
C	-5.02125	1.06786	0.053896
H	-5.33158	1.874185	0.728681
H	-5.20955	1.411948	-0.96946
C	-5.77393	-0.21422	0.349093
H	-5.48473	-1.00669	-0.34891
H	-5.56811	-0.55942	1.367119
H	-6.85198	-0.05056	0.251929
C	0.868742	2.542972	-0.48065
C	1.949805	1.999785	0.220429
C	1.038468	2.846871	-1.83756
C	3.154697	1.732405	-0.42931
H	1.845042	1.737575	1.270191
C	2.244096	2.58849	-2.48791
H	0.202252	3.270816	-2.39064
C	3.308433	2.022116	-1.78459
H	3.969921	1.278131	0.128374
H	2.351915	2.827129	-3.5427
H	4.247303	1.808431	-2.28758
O	2.082734	-0.56358	2.0892
C	3.004832	-1.22841	1.546451
O	2.864086	-2.10411	0.651939
C	4.435952	-0.96923	2.041272
H	5.154746	-1.08017	1.224669
H	4.524573	0.019926	2.497984
H	4.680898	-1.71887	2.802848
H	-1.0143	3.531776	-0.43151
S	-0.37704	3.435274	1.872163
C	0.671307	4.906598	1.620852
H	0.261949	5.48516	0.784683
H	1.684072	4.591176	1.349045
C	0.70112	5.751828	2.888866
H	1.095556	5.177169	3.733085
H	1.341886	6.628844	2.748553
H	-0.3022	6.099103	3.153707



Int4

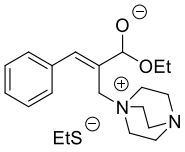
C	2.807909	0.356906	0.110387
C	3.961332	-0.57377	0.555361
H	3.133805	1.145849	-0.57246
H	2.286706	0.82597	0.945535
H	4.92611	-0.10944	0.333633
H	3.917103	-0.75643	1.632837
C	2.411761	-0.95444	-1.90143
H	1.695455	-1.65074	-2.34693
H	2.527847	-0.09693	-2.5692
C	3.764145	-1.63131	-1.56723
H	3.847077	-2.58515	-2.09481
H	4.600957	-1.00037	-1.87981
C	2.675412	-2.55815	0.333787
H	2.54626	-3.46222	-0.26847
H	2.815177	-2.86569	1.37355
C	1.433986	-1.64034	0.213583
H	0.588931	-2.14526	-0.25926
H	1.10062	-1.23859	1.171452
N	3.881658	-1.86703	-0.12791
N	1.79423	-0.45842	-0.63252
C	0.521621	0.431903	-0.99264
H	-0.05	-0.24294	-1.64022
H	0.98529	1.215702	-1.60082
C	-0.27336	0.949651	0.12252
C	-1.65816	0.418193	0.391783
H	-2.00312	0.891656	1.315836
C	-0.01754	2.241748	0.649971
O	-0.69976	2.869594	1.465639

O	1.150606	2.815686	0.16347
C	1.415429	4.144511	0.603387
H	0.607391	4.807467	0.274596
H	1.438867	4.174199	1.697724
C	2.744889	4.561734	0.009581
H	3.551978	3.912729	0.364767
H	2.714875	4.513229	-1.08338
H	2.981189	5.589534	0.301148
C	-1.74566	-1.08761	0.566402
C	-2.00827	-1.97129	-0.48529
C	-1.48777	-1.62609	1.833622
C	-1.96947	-3.35312	-0.28843
H	-2.24702	-1.56716	-1.46603
C	-1.44669	-3.00338	2.03606
H	-1.29307	-0.94828	2.662635
C	-1.67754	-3.87607	0.97015
H	-2.17566	-4.02062	-1.12066
H	-1.24161	-3.39817	3.027347
H	-1.65079	-4.95042	1.126442
C	-4.42126	0.446196	-0.33983
C	-5.54472	1.060442	-1.16604
H	-6.51511	0.691464	-0.81895
H	-5.54318	2.151089	-1.08218
H	-5.44401	0.799949	-2.22459
H	-4.45299	-0.64657	-0.40307
H	-4.52392	0.726474	0.714274
S	-2.80337	1.048663	-0.93207



TS4

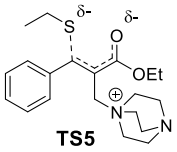
C	2.869047	0.314718	0.088056
C	4.06291	-0.55491	0.567901
H	3.172092	1.073533	-0.64017
H	2.359435	0.824968	0.90983
H	5.010818	-0.14164	0.211111
H	4.104078	-0.5951	1.660467
C	2.465927	-1.15526	-1.78377
H	1.724646	-1.84266	-2.20385
H	2.640911	-0.35158	-2.50668
C	3.781257	-1.88785	-1.39
H	3.779699	-2.91344	-1.76991
H	4.653386	-1.37548	-1.80726
C	2.72299	-2.51972	0.653056
H	2.591358	-3.51831	0.225411
H	2.875902	-2.63349	1.730136
C	1.480391	-1.6314	0.361939
H	0.668364	-2.20059	-0.0988
H	1.088504	-1.14597	1.259715
N	3.92956	-1.92646	0.067785
N	1.875143	-0.55802	-0.5713
C	0.412912	0.511362	-1.08664
H	-0.03733	-0.25446	-1.71934
H	1.059001	1.201641	-1.62753
C	-0.3765	1.033795	-0.05543
C	-1.72424	0.459566	0.324387
H	-1.99089	0.872281	1.302008
C	-0.04938	2.294056	0.565601
O	-0.68796	2.852884	1.451329
O	1.095212	2.868495	0.073993
C	1.456655	4.123715	0.651671
H	0.651247	4.846482	0.485383
H	1.575455	4.004468	1.733992
C	2.746466	4.569169	-0.00299
H	3.54817	3.84715	0.180891
H	2.616431	4.677008	-1.08387
H	3.057444	5.535806	0.404177
C	-1.78357	-1.05276	0.417214
C	-1.95992	-1.87781	-0.69921
C	-1.61764	-1.6564	1.668797
C	-1.92509	-3.26661	-0.5742
H	-2.14026	-1.42408	-1.67043
C	-1.5829	-3.04365	1.799727
H	-1.49879	-1.02575	2.547632
C	-1.72692	-3.85603	0.674793
H	-2.06286	-3.88955	-1.45375
H	-1.45047	-3.49048	2.781049
H	-1.70503	-4.93724	0.773708
C	-4.51873	0.507838	-0.12555
C	-5.72272	1.09593	-0.85075
H	-6.65042	0.705278	-0.42117
H	-5.73984	2.186418	-0.76585
H	-5.70832	0.836605	-1.9141
H	-4.52643	-0.58521	-0.19142
H	-4.5363	0.785166	0.934101
S	-2.97399	1.143761	-0.85792



Int5

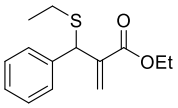
C	2.251349	-0.82538	1.133322
C	2.497959	-2.01445	2.097925
H	3.021438	-0.74245	0.364524
H	2.167232	0.127374	1.66302
H	3.259909	-2.68622	1.692473
H	2.856282	-1.63897	3.059899
C	0.965013	-2.46257	-0.12879
H	0.111346	-2.56772	-0.80288
H	1.893657	-2.53313	-0.70231
C	0.915309	-3.4557	1.050582
H	-0.09136	-3.86971	1.152557
H	1.609051	-4.28118	0.871003
C	0.193251	-1.85821	2.659348
H	-0.68669	-2.43122	2.96132
H	0.52181	-1.26097	3.514988
C	-0.17037	-0.95839	1.457642
H	-1.08227	-1.28301	0.942803
H	-0.255	0.093944	1.735432

N	1.271529	-2.78201	2.303053
N	0.939222	-1.05799	0.435703
C	0.696561	-0.09608	-0.71409
H	-0.31403	-0.32201	-1.06071
H	1.393183	-0.39882	-1.49729
C	0.918091	1.351071	-0.36029
C	0.013513	2.259352	0.071963
H	0.450148	3.240066	0.25957
C	2.298895	1.910665	-0.55149
O	2.677418	2.987164	-0.14057
O	3.095686	1.089488	-1.25386
C	4.432857	1.56558	-1.50845
H	4.364633	2.510582	-2.05454
H	4.920814	1.761666	-0.54885
C	5.147336	0.499421	-2.30528
H	5.207009	-0.43825	-1.7449
H	4.634655	0.310239	-3.25203
H	6.16595	0.830476	-2.52529
C	-1.42458	2.21657	0.363454
C	-2.31441	1.19798	-0.01819
C	-1.935	3.316373	1.078467
C	-3.66034	1.278013	0.324529
H	-2.00609	0.32192	-0.58147
C	-3.27906	3.388775	1.426663
H	-1.26114	4.120255	1.364293
C	-4.14778	2.365015	1.049667
H	-4.32597	0.47601	0.01797
H	-3.64761	4.244267	1.984161
H	-5.19971	2.416828	1.314158
C	-3.99449	-2.09226	-1.75183
C	-4.12653	-1.05739	-2.8648
H	-5.16856	-0.95678	-3.19809
H	-3.77823	-0.07377	-2.52976
H	-3.51643	-1.34536	-3.72721
H	-4.35996	-3.05883	-2.11733
H	-4.64743	-1.81361	-0.91494
S	-2.27573	-2.29729	-1.14462



TS5

C	2.863923	-0.04415	0.185656
C	4.094035	-0.9846	0.136375
H	3.041893	0.92182	-0.2889
H	2.503179	0.130237	1.202385
H	4.856233	-0.5845	-0.53773
H	4.53624	-1.07379	1.131475
C	2.23925	-1.10773	-1.91907
H	1.375345	-1.44035	-2.49904
H	2.645682	-0.2038	-2.38002
C	3.302715	-2.2173	-1.74079
H	2.904152	-3.18729	-2.04959
H	4.176943	-1.99895	-2.35889
C	2.58395	-2.79627	0.453702
H	2.38543	-3.84107	0.202689
H	2.864568	-2.75152	1.509387
C	1.321821	-1.94042	0.188171
H	0.581651	-2.45051	-0.43527
H	0.834381	-1.61276	1.107023
N	3.714542	-2.31461	-0.3409
N	1.735584	-0.70193	-0.56084
C	0.548603	0.24989	-0.74778
H	-0.18512	-0.32925	-1.30886
H	0.92405	1.052158	-1.38611
C	-0.04105	0.790835	0.513387
C	-1.21173	0.325363	1.042722
H	-1.58381	0.862553	1.910696
C	0.446228	2.069702	1.065122
O	0.082736	2.565875	2.112939
O	1.382169	2.657861	0.280727
C	1.811063	3.964483	0.695838
H	0.93555	4.618715	0.739737
H	2.236381	3.897834	1.702076
C	2.824491	4.451184	-0.31511
H	3.699925	3.794774	-0.34426
H	2.383517	4.49643	-1.31472
H	3.161711	5.455323	-0.04299
C	-1.80774	-1.0172	0.814224
C	-2.28141	-1.47539	-0.42103
C	-1.84976	-1.88461	1.914713
C	-2.75137	-2.78044	-0.55595
H	-2.33163	-0.77183	-1.24698
C	-2.31624	-3.19152	1.778256
H	-1.50876	-1.53008	2.884921
C	-2.76181	-3.64695	0.538198
H	-3.13251	-3.11499	-1.51678
H	-2.34156	-3.84737	2.643606
H	-3.13683	-4.66034	0.43038
C	-4.38463	2.107474	-1.12564
C	-5.06316	0.776952	-1.43751
H	-6.11613	0.918659	-1.71652
H	-4.55718	0.269401	-2.26684
H	-5.02721	0.110996	-0.56812
H	-4.93875	2.615874	-0.32779
H	-4.43986	2.757723	-2.00779
S	-2.62614	1.932494	-0.63031



P2

C	0.47071	0.421916	-0.80924
H	0.29611	-0.56691	-1.22394
H	1.413033	0.90972	-1.0329
C	-0.44327	1.013805	-0.03666
C	-1.79495	0.420106	0.298715
H	-2.06992	0.792925	1.290897
C	-0.18206	2.354847	0.580956
O	-0.84627	2.816527	1.484239
O	0.873025	2.982291	0.051869
C	1.207293	4.256092	0.634542
H	0.344762	4.921562	0.535133
H	1.405457	4.111502	1.701046

C	2.417879	4.783268	-0.10006
H	3.264435	4.098777	0.002989
H	2.200575	4.91421	-1.16353
H	2.705371	5.752626	0.316646
C	-1.79906	-1.09704	0.332281
C	-2.10558	-1.88714	-0.77791
C	-1.43712	-1.7268	1.528376
C	-2.04125	-3.27873	-0.69532
H	-2.40332	-1.40941	-1.70708
C	-1.37205	-3.11522	1.613162
H	-1.20096	-1.11901	2.399218
C	-1.6741	-3.89704	0.498119
H	-2.28256	-3.87958	-1.5673
H	-1.09127	-3.58639	2.55044
H	-1.62927	-4.98001	0.562208
C	-4.5454	0.741559	-0.00995
C	-5.73615	1.284669	-0.78833
H	-6.66578	1.028129	-0.27174
H	-5.68702	2.373794	-0.87818
H	-5.77949	0.858012	-1.79489
H	-4.604	-0.34791	0.07816
H	-4.51239	1.170829	0.996434
S	-2.99515	1.173193	-0.86844