Electronic Supplementary Material (ESI) for Polymer Chemistry.

SUPPORTING INFORMATION

For

Mechanical Activation of a Dithioester Derivative-based Retro RAFT-HDA Reaction

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Supporting Information

1. Materials and Characterizations:

Picolychloride hydrochloride (97 %, J&K Chemicals), benzenesulfinic acid salt (97 %, J&K Chemicals), tetrapropylammonium bromide (98 %, J&K Chemicals), 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (98 %, J&K Chemicals), elemental sulfur (powder, Sinopharm Chemical Reagent Co. Ltd.), potassium *tert*-butanolate (97 %, TCI chemicals), *p*-xylylene bromide (97 %, Adamas)， trans,trans-2,4-hexadien-1-ol (98 %, stab. with 0.1% a-tocopherol, Alfa Aesar), 2-bromo-2-methylpropionyl bromide (98 %, J&K Chemicals), hydroquinone (99 %, Xilong Huagong), triethylamine (99.5 %, Sigma-Aldrich), 1-(hydroxymethyl) pyrene (98 %, Adamas) nickelocene (98 %, TCI chemicals), triphenylphosphine (99 %, J&K Chemicals), sodium iodide (99 %, Tianjin Jinke) and trifluoroacetic acid (TFA) (99 %, Sigma-Aldrich) were used as received. Azodiisobutyonitrile (AIBN) was recrystallized from methanol. Tetrahydrofuran (THF), methyl acylate (MA), styrene (St) and chloroform was distilled following the standard procedures. Other solvents and reagents, unless stated specifically, were purchased from Beijing Chemical Reagent Co. and used as received.

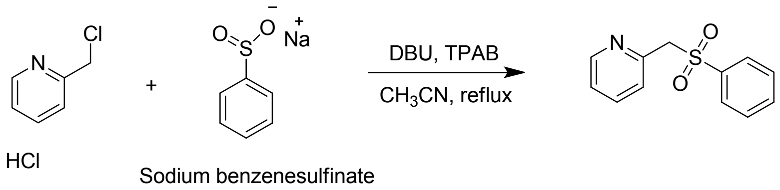
^{1}H and ^{13}C NMR data were collected on Bruker 400 MHz spectrometers operated at room temperature with $CDCl_3$ as the solvent. Chemical shifts (δ) are reported in ppm with $(CH_3)_4Si$ and the residual solvent peak as the reference, respectively. UV-Vis spectra were recorded on the Perkin-Elmer Instruments Lambda spectrometer. High resolution mass spectra (HRMS) were measured by Bruker APEX IV Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. Molecular weight and PDI were measured by a gel permeation chromatograph (GPC) equipped with a Waters 410 refractive-index detector, a Waters 515 HPLC pump, and HT1, 2, 4 columns with THF as an eluent at a flow rate of 1.0 mL/min at 35℃. Monodispersity polystyrene standards were used for calibration.

General Sonication Conditions:

The sonication experiments were performed using a JY96-II Ultrasonic Cell Crusher Instrument (Ningbo Scientz Biotechnology Co. LTD) operating at 20 kHz equipped with 6 mm tip titanium probe. The whole system was immersed in an ice-salt bath and pulsed ultrasound was applied (1.0 s on and 1.0 s off) at 300 W for 3 h for each experiment.

2. Synthesis:

Synthesis of 2-picoly phenyl sulfone



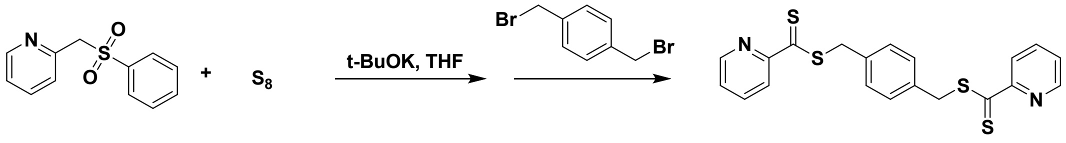
The synthetic procedures were same as the description in the literature.[S1] Picolychloride (2.81 g, 17.1 mmol), sodium benzenefulfinate (4.20 g, 25.6 mmol) and tetrapropylammonium bromide (0.94 g, 3.53 mmol) were dissolved in 40 mL acetonitrile. A solution of DBU (2.60 g, 17.1 mmol) in 10 mL acetonitrile was added into the mixture dropwise. The mixture was refluxed overnight. After that, the solvent was evaporated under vacuum, and the crude product was dissolved in dichloromethane (50 mL) and washed with water (100 mL). The organic phase was dried over anhydrous Na_2SO_4 and collected under vacuum. The targeted compound was obtained as a brown solid. Yield: 86 %.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dd, J = 4.9, 0.8 Hz, 1H), 7.74 (td, J = 7.7, 1.8 Hz, 1H), 7.70 (dd, J = 8.3, 1.1 Hz, 2H), 7.65 – 7.57 (m, 1H), 7.53 – 7.43 (m, 3H), 7.32 – 7.24 (m, 2H), 4.61 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.94, 148.53, 138.22, 137.43, 133.86, 129.03, 128.43, 126.04, 123.59, 64.04.

HR-ESI-MS: $C_{12}H_{12}NO_2S$, Mass Calculated: 234.05833, Mass Measured: 234.05811

Synthesis of dithioester ***1***



1

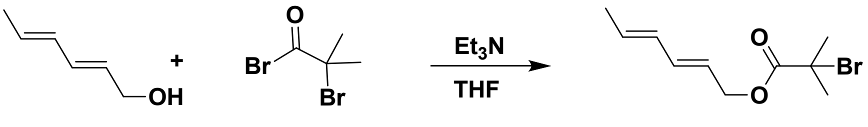
A mixture of 2-picoyl phenyl sulfone (1.60 g, 6.87 mmol) and elemental sulfur (S8, 0.69 g, 21.6 mmol) in THF (20 mL) was cooled in an ice-salt bath. Then, potassium *tert*-butanolate (2.32 g, 20.7 mmol) was added. The mixture turned red and was stirred overnight. A solution of *p*-xylylene bromide (0.79 g, 3.0 mmol) in 10 mL THF was added and the mixture was stirred for another 8 h. The solution was dried and dissolved in 100 mL dichloromethane. The organic phase was washed with water (30 mL) until the aqueous phase was slightly yellowish. The organic phase was dried over anhydrous Na_2SO_4 and evaporated under vacuum. The crude product was purified through a silica column with dichloromethane as the eluent. The product was given as a red solid. Yield: 23 %.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, J = 4.0 Hz, 1H), 8.32 (d, J = 8.0 Hz, 1H), 7.80 (td, J = 7.8, 1.7 Hz, 1H), 7.52 – 7.44 (m, 1H), 7.35 (s, 2H), 4.52 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.29, 147.89, 136.96, 134.50, 129.66, 126.77, 122.22, 41.11.

HR-ESI-MS: $C_{20}H_{17}N_2S_4$, Mass Calculated: 413.02691, Mass Measured: 413.02641

Synthesis of the open-chain diene ***2***



2

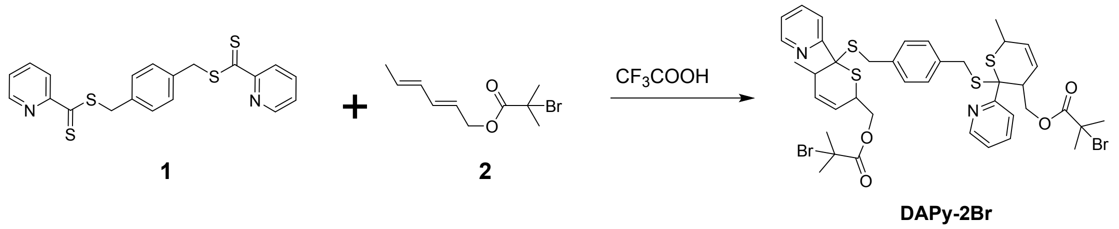
The *trans*, *trans*-hexadien-1-ol (1.00 g, 10.2 mmol) was dissolved in 20 mL anhydrous THF, and triethylamine (TEA) (1.52 g, 15.0 mmol) was added dropwise. The mixture was cooled in an ice salt bath for 20 min. Then α-bromoisobutyryl bromide (2.87 g, 12.5 mmol) was added dropwise. After the solution was stirred at room temperature for 12 h, the resulting salt TEA·HBr was filtrated. The filtrate was collected and evaporated in vacuo. The crude product was purified through a silica column with ethyl acetate/petrolum ether (1/20) as the eluent. The product was given as pale yellow oil. Yield: 90 %.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.30 (dd, *J* = 15.2, 10.5 Hz, 1H), 6.07 (ddd, *J* = 14.7, 10.5, 1.2 Hz, 1H), 5.78 (dd, *J* = 15.0, 6.8 Hz, 1H), 5.70 – 5.59 (m, 1H), 4.67 (d, *J* = 6.6 Hz, 2H), 1.93 (s, 6H), 1.77 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.31, 135.23, 131.50, 130.30, 122.77, 66.32, 55.76, 30.71, 18.06.

HR-ESI-MS: $C_{10}H_{15}BrNaO_2$, Mass Calculated: 269.01476, Mass Measured: 269.01448

Synthesis of ***DAPy-2Br***



A mixture of compound **2** (0.32 g, 1.3 mmol) and compound **1** (0.08 g, 0.2 mmol) in 5 mL $CHCl_3$ was stirred in room temperature for 2 d. Then the solution was evaporated under vacuum and the crude product was purified through a silica column with $CHCl_3$ as the eluent. The product was obtained as a colorless solid. Yield: 35 %.

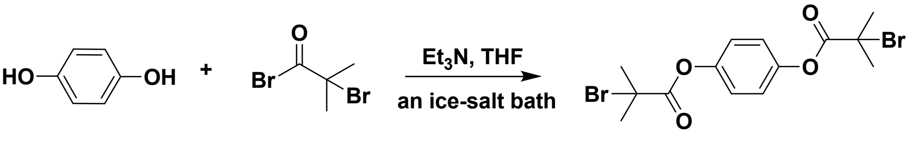
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.5 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.18 (dd, *J* = 7.4, 4.0 Hz, 1H), 6.85 (s, 2H), 5.86 (dt, *J* = 19.5, 6.5 Hz, 2H), 4.10 (dd, *J* = 10.8, 7.4 Hz, 1H), 3.91 (dd, *J* = 10.9, 5.1 Hz, 1H), 3.75 – 3.67 (m, 1H), 3.64 (d, *J* = 12.3 Hz, 1H), 3.19 (d, *J* = 12.2 Hz, 2H), 1.78 (d, *J* = 21.7 Hz, 5H), 1.45 (d, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.23, 147.82, 136.81, 132.21, 129.27, 129.18, 128.91, 125.95, 122.69, 68.15, 55.60, 44.25, 34.61, 34.53, 30.77, 30.61, 30.54, 18.80, 18.25.

HR-ESI-MS: $C_{40}H_{47}Br_2N_2O_4S_4$, Mass Calculated: 905.07799 Mass Measured:

905.07999

*Synthesis of compound **S1***



S1

The compound **S1** was used as a model initiator to obtain the poly(methyl acrylate)s without mechanophore embedded in the polymer chain.

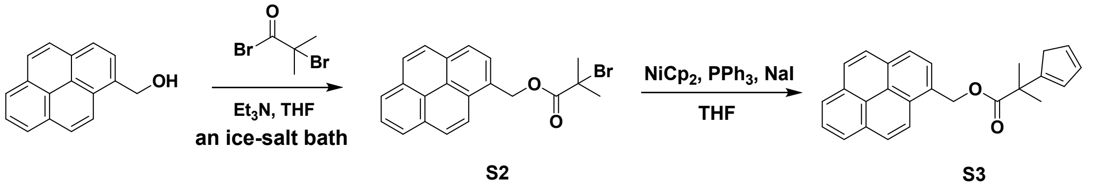
Hydroquinone (2.00 g, 18.2 mmol) was dissolved in THF (50 mL) and triethyl amine (5.20 g, 54.5 mmol) was added. The mixture was put in an ice-salt bath for 20 min. After that, 2-bromo-2-methylpropionyl bromide (10.02 g, 43.6 mmol) was added into the mixture dropwise. The mixture was stirred at ambient temperature overnight and filtrated. The filtrate was concentrated under vacuo. The crude product was purified through a silica column with ethyl acetate/petroleum ether (1/40) as the eluent. Yield: 91 %.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (s, 4H), 2.06 (s, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.02, 148.36, 122.03, 55.17, 30.56.

HR-ESI-MS: $C_{14}H_{17}Br_2O_4$, Mass Calculated: 406.94881 Mass Measured: 406.94908

*Synthesis of the labeled molecule **S3***



S2

S3

1-pyrenemethanol (1.00 g, 4.27 mmol) was dissolved in 20 mL THF, followed by adding triethyl amine (0.66 g, 6.41 mmol) dropwise. The solution was cooled in an ice-salt bath for 20 min. Then the solution of 2-bromo-2-methylpropionyl bromide (1.21 g, 5.26 mmol) in 10 mL THF was added into the mixture dropwise. The mixture was stirred for another 24 h. After that, the mixture was filtrated and the filtrate was concentrated under vacuo. The crude product of **S2** was purified through a silica column with dichloromethane as the eluent. Yield: 84 %.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 9.2 Hz, 1H), 8.18 (dd, *J* = 7.4, 4.6 Hz, 2H), 8.13 (dd, *J* = 8.5, 5.0 Hz, 2H), 8.02 (dt, *J* = 18.7, 7.6 Hz, 4H), 5.88 (s, 2H), 1.92 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 171.50, 131.63, 131.01, 130.50, 129.32, 128.04, 127.97, 127.70, 127.39, 127.16, 125.93, 125.39, 125.34, 124.65, 124.40, 122.67, 66.28, 55.83, 30.71.

HR-ESI-MS: $C_{21}H_{17}BrNaO_2$, Mass Calculated: 403.03041 Mass Measured: 403.03157

Compound **S2** (0.66 g, 1.75 mmol) and triphenylphosphine (0.47 g, 1.75 mmol) were dissolved in 15 mL THF in a Schlenk tube. Sodium iodide (0.79 g, 5.26 mmol) was added into the solution. The tube was sealed and three freeze-pump-thaw cycles were conducted to remove the oxygen. Then, nickelocene (0.20 g, 1.05 mmol) was added into the mixture and another three freeze-pump-thaw cycles were conducted. After being stirred under nitrogen at room temperature for 24 h, the mixture was poured into n-hexane and filtrated. The filtrate was concentrated under vacuo. The crude product was purified through a silica column with ethyl acetate/petroleum ether (1/8) as the eluent. Yield: 77 %.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (m, 9H), 6.58 – 6.29 (m, 2H), 6.28 – 6.07 (m, 1H), 5.80 (d, *J* = 6.1 Hz, 2H), 2.91 (d, *J* = 4.5 Hz, 2H), 1.47 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 176.23, 151.58, 150.13, 133.80, 132.64, 132.14, 131.79, 131.60, 131.57, 131.22, 130.72, 129.41, 129.17, 129.11, 128.01, 127.85, 127.72, 127.69, 127.42, 127.38, 127.35, 126.05, 125.96, 125.45, 125.41, 125.36, 124.84, 124.64, 124.56, 124.53, 123.10, 122.96, 65.23, 44.60, 43.86, 41.16, 41.12, 26.01, 25.23.

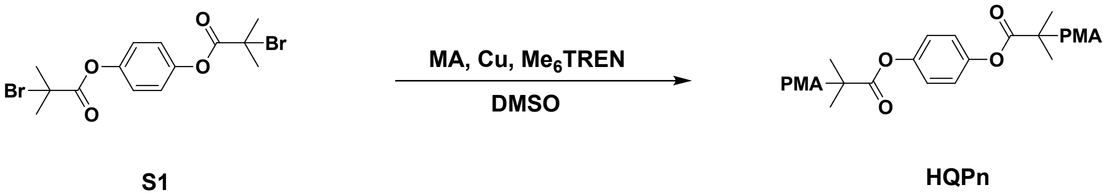
HR-ESI-MS: $C_{26}H_{23}O_2$, Mass Calculated: 367.16926, Mass Measured: 367.16996

Representative Procedures for the synthesis of ***DAPyPn***

The polymerization was conducted using a classical SET-LRP method. A 25 mL

Schlenk flask was charged with 2 mL MA (2.0 mL, 22.1 mmol), 18.23 mg (0.02 mmol) difunctional initiator **DAPy-2Br** and 1 mL DMSO. The solution was stirred for several minutes to ensure the homogeneity. Then two pieces of Cu sheet were cut into small pieces and added into the flask. The flask was sealed and three freeze-pump-thaw cycles were conducted to remove the oxygen. After that, 10 μL Me_6(TREN) was added into the mixture, and the flask was immediately sealed and degassed by another three freeze-pump-thaw cycles. After being stirred in an oil bath for 24 h at 25℃, the flask was opened and 5 mL $CHCl_3$ was added. The solution was filtered through a short column of basic alumina. After the solvent was evaporated in vacuo, the product was precipitated in methanol. The resulting polymer was collected and dried under vacuum at room temperature.

Representative Procedures for the synthesis of ***HQPn***



The polymerization of **HQPn** is similar to the procedures of **DAPyPn**. A 25 mL Schlenk flask was charged with 2 mL MA (2.0 mL, 22.1 mmol), 8.14 mg difunctional initiator **S1** and 1 mL DMSO. The solution was stirred for several minutes to ensure the homogeneity. Then two pieces of Cu sheet were cut into small pieces and added into the flask. The flask was sealed and three freeze-pump-thaw cycles were conducted to remove the oxygen. After that, 20 μL Me_6(TREN) was added into the mixture and the flask was immediately sealed and degassed by another three freeze-pump-thaw cycles. After being stirred in an oil bath for 24 h at 25℃, the flask was opened and 5 mL $CHCl_3$ was added. The solution was filtered through a short column of basic alumina. After the solvent was evaporated in vacuo, the polymer was precipitated in methanol. The resulting polymer was collected and dried under vacuum at room temperature.

Representative Procedures for labelling of DAPyP6-3h by compound S3

DAPyP6 (120.78 mg) was dissolved in 6 mL $CHCl_3$ (20 mg/mL) and the solution was subjected to the pulsed ultrasound in an ice-bath for 3 h. The colorless solution turned into yellow. Then compound **S3** (5.26 mg) was added into the solution. 2 μL CF_3COOH was added into the mixture. After being stirred at room temperature for 2 d, the solution was evaporated under vacuo, and the crude product was precipitated in petroleum ether. The precipitate was collected and characterized by ^1H NMR and GPC.

Representative Procedure for the RAFT polymerization of St

DAPyP6 (109.68 mg) was dissolved in 5 mL $CHCl_3$ (20 mg/mL) and the solution was subjected to the pulsed ultrasound in an ice-bath for 3 h. The colorless solution turned to yellow and was evaporated under vacuo. The product was obtained and named as DAPyP6-3h. After that, DAPyP6-3h was dissolved in St (1.0 mL) in a 25 mL Schlenk tube. 200 μL solution of 1.49 mg AIBN in 7 mL St was injected into the Schlenk tube. The flask was immediately sealed and degassed by another three freeze-pump-thaw cycles. After being stirred in an oil bath for 48 h at 60℃, the mixture was precipitated in methanol. The precipitate was collected and characterized by ^1H NMR and GPC.

Representative Procedures for the radical polymerization of St

The radical polymerization of St was conducted in the same conditions as the above mentioned RAFT polymerization without **DAPyP6-3h** in the system. 1.52 mg AIBN was dissolved in 7 mL St. 200 μL of such solution was injected into the Schlenk tube. Then, 1.0 mL styrene was added. After that, the flask was immediately sealed and degassed by three freeze-pump-thaw cycles. After being stirred in an oil bath for 48 h at 60℃, the mixture was precipitated in methanol. The precipitate was collected and characterized by ^1H NMR and GPC.

3. UV-Vis spectrum of the dithioester 1

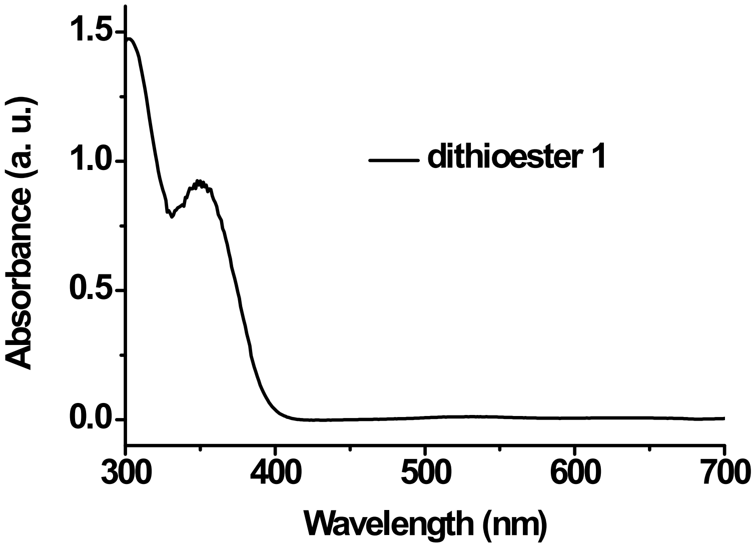
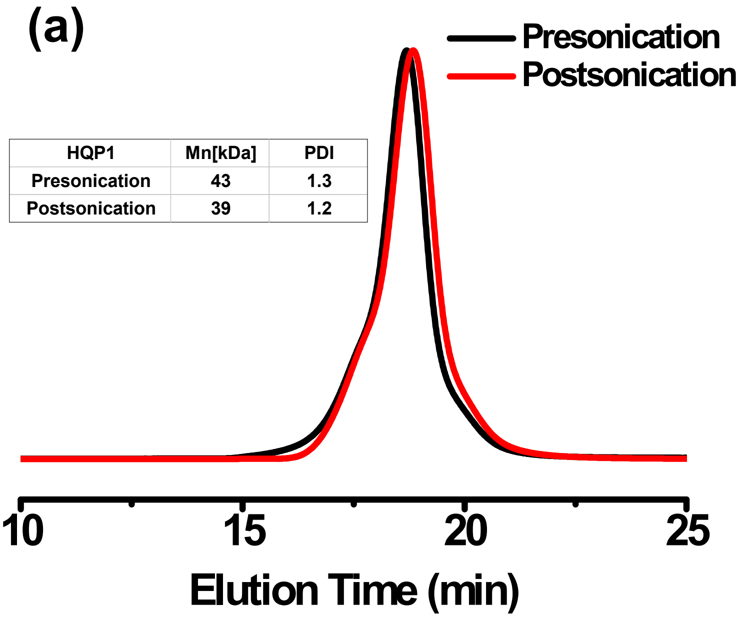
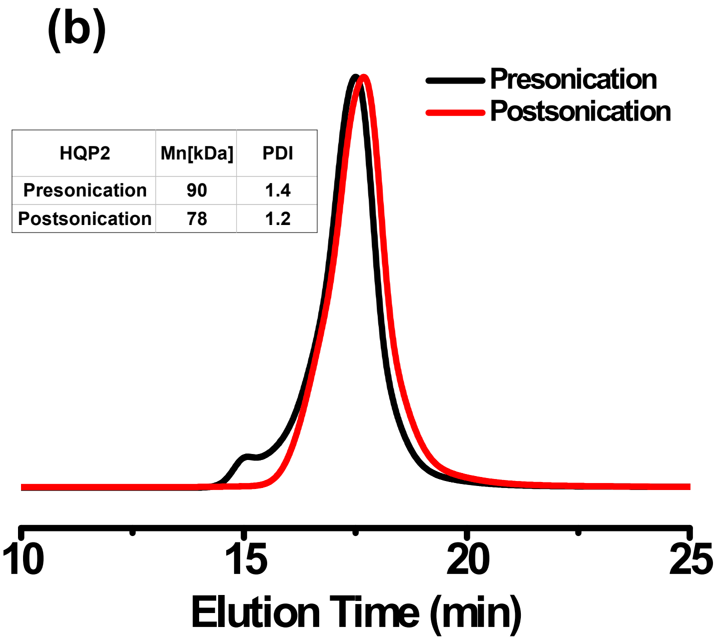


Figure S1. UV-Vis spectrum of dithioester **1**(concentration 1.0×10^{-4} mol/mL)

4. GPC traces of control samples HQPn before and after sonication



HQP1	Mn[kDa]	PDI
Presonication	43	1.3
Postsonication	39	1.2



HQP2	Mn[kDa]	PDI
Presonication	90	1.4
Postsonication	78	1.2

Figure S2. GPC traces of (a) **HQP1** and (b) **HQP2** before and after sonication for 3 h.

5. Photographs of HQP2 (a) before and (b) after sonication for 3 h

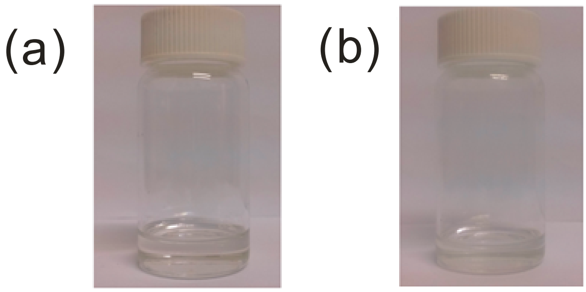


Figure S3. Photographs of **HQP2** (a) before and (b) after sonication for 3 h.

6. ^{1}H NMR spectra of DAPyP6 before and after sonication

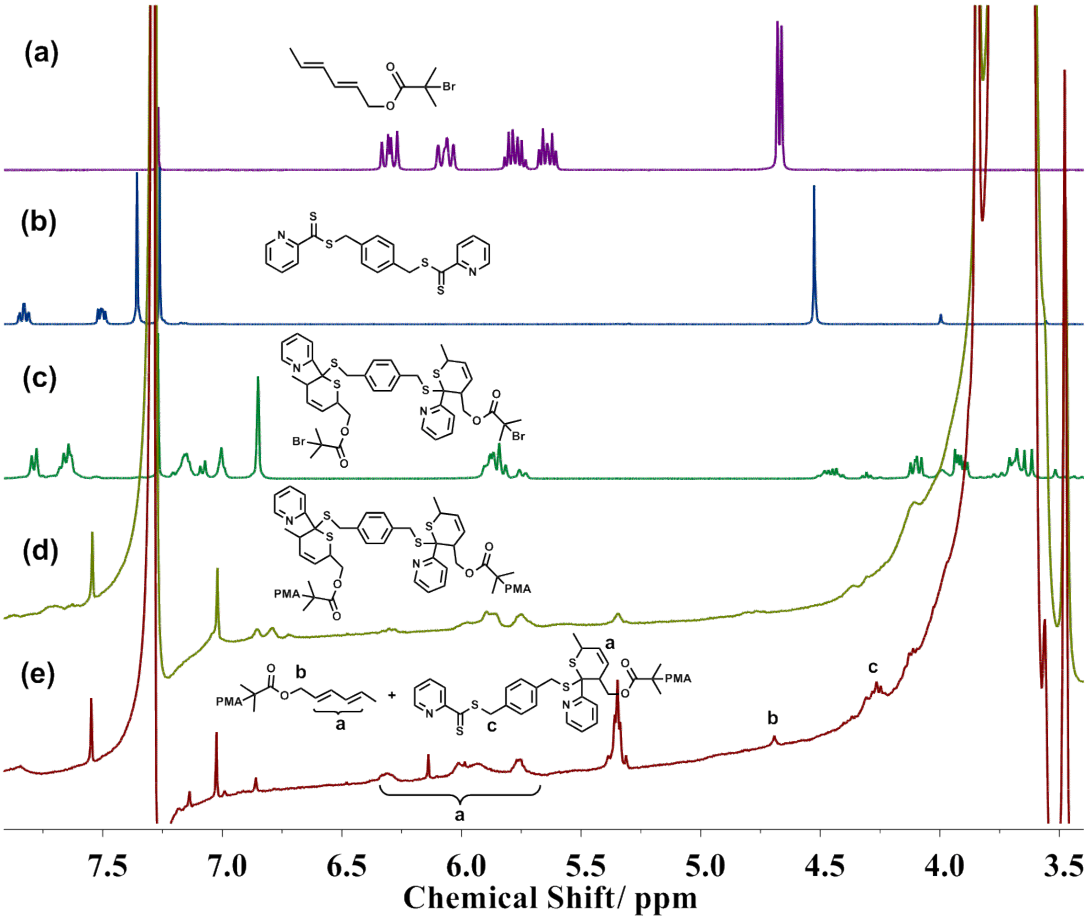


Figure S4. ^{1}H NMR spectra of (a) diene **2**, (b) dithioester **1**, (c) initiator **DAPy-2Br**, (d) and (e) **DAPyP6** before and after sonication.

7. Synthesis of DAPyP6-3h-Py

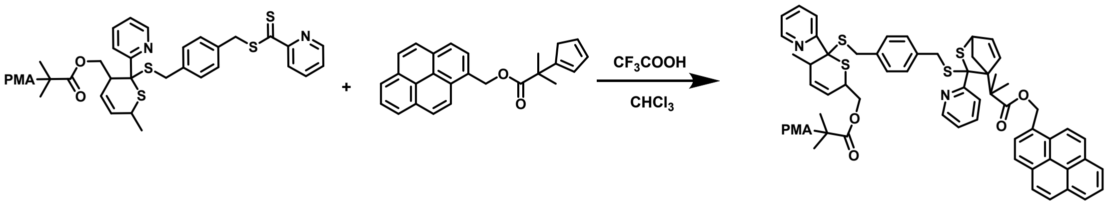


Figure S5. The synthesis of **DAPyP6-3h-Py**.

8. ^{1}H NMR spectra of DAPyP6-3h and DAPyP6-3h-Py

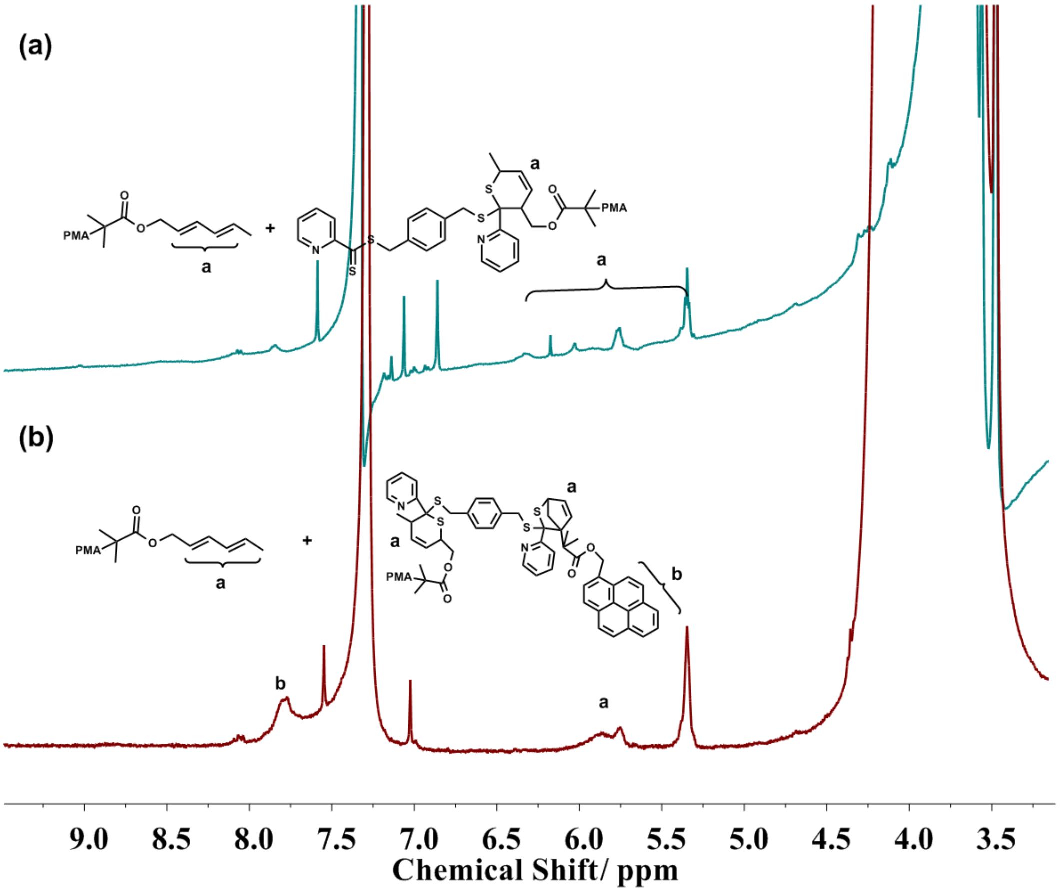


Figure S6. ^{1}H NMR spectra of (a) **DAPy-P6-3h** and (b) **DAPy-P6-3h-Py**

9. Excitation fluorescent spectrum and Emission fluorescent spectrum of DAPyP6-3h-Py

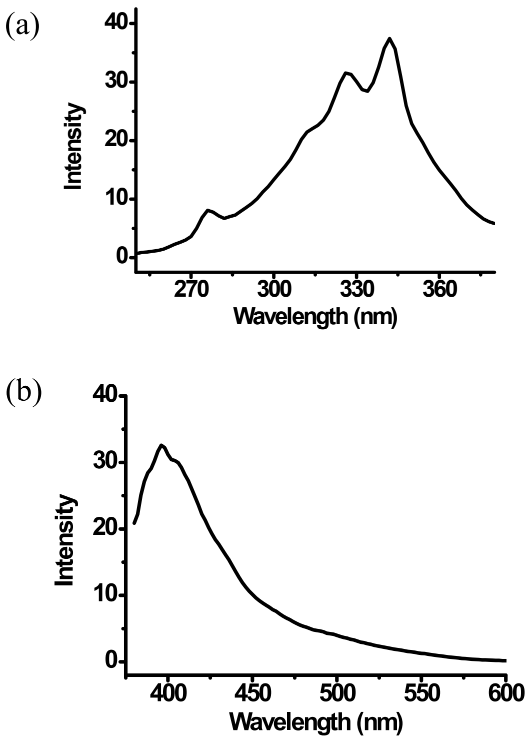


Figure S7. (a) Excitation fluorescent spectrum of **DAPyP6-3h-Py** in THF. The emission was set at 395 nm. (b) Emission fluorescent spectrum of the **DAPyP6-3h-Py** in THF. The excitation wavelength was set at 365 nm.

10. Pictures of DAPyP6-3h, DAPyP6-3h-Py under sunlight and 365 nm UV light.

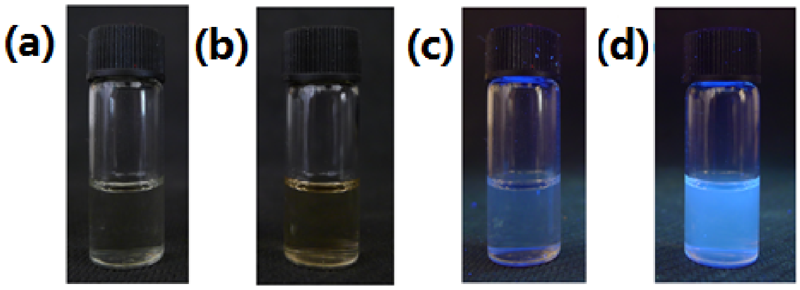


Figure S8. Pictures of (a) **DAPyP6-3h**; (b) **DAPyP6-3h-Py** under sunlight; (c) **DAPyP6-3h** (d) **DAPyP6-3h-Py** under 365 nm UV light. The concentration of the sample is 20 mg/mL.

11. RAFT polymerization of St using released 1 as RAFT agent

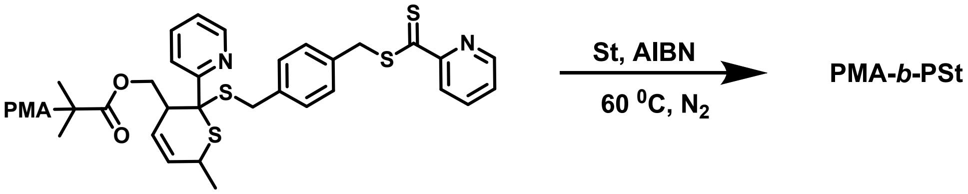


Figure S9. RAFT polymerization of St using released 1 as RAFT agent

12. GPC traces of DAPyP6 after sonication for 3h, DAPyP6-*b*-PSt block polymer and PSt

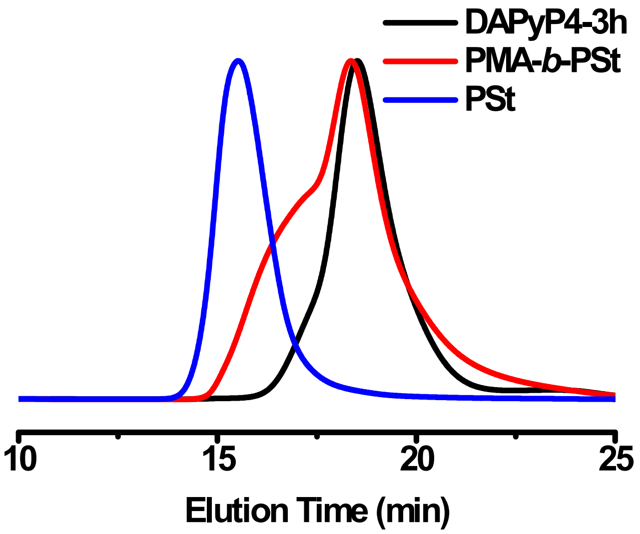


Figure S10. GPC traces of the DAPyP6 after sonication for 3 h (black); the PMA-*b*-PSt block polymer initiated by DAPyP6-3h (red) and Polystyrene synthesized by radical polymerization (blue)

13. ^{1}H NMR spectra of DAPy-P6 after sonication for 3h, PSt obtained from the radical polymerization of St and PMA-*b*-PSt block copolymer

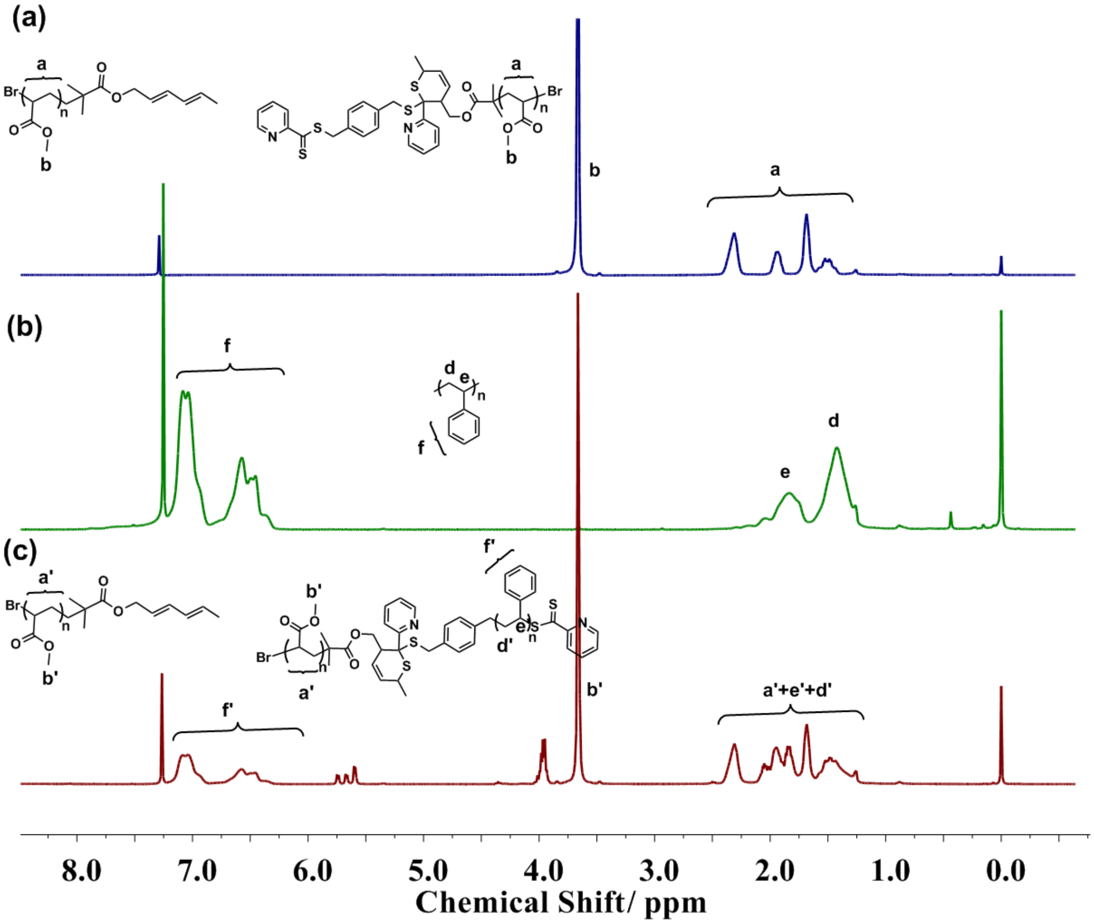


Figure S11. ^{1}H NMR spectra of (a) DAPy-P6 after sonication for 3 h, (b) PSt obtained from the radical polymerization of styrene and (c) PMA-*b*-PSt block copolymer using DAPy-P6-3h as a RAFT agent in the St polymerization.

14. Theoretical Calculation

The activation energy of the chain scission was calculated based on the Extended Bell Theory (EBT).[S2] The EBT calculations were conducted with the Gaussian package using density functional theory, employing the 6-31G* basis set and the B3LYP exchange-correlation energy functional. An analogue of RAFT-HDA adducts with a benzyl ring and a pyridine unit in the structure was employed as a model for simplifying the calculation process. Figure S12 and S13 showed the optimized structures of the model molecule and its transition state. Table S1 demonstrated the ΔR (ΔR refers to the change in the mechanical pulling coordinate) and $\Delta\chi$ ($\Delta\chi$ refers to the change in the compliances of the reactant state and transition state in the pulling along R) for the atom pair in all the possible pulling points for RAFT-HDA mechanophore, which was calculated from the molecules's $(3N\times3N)$ Hessians in the RAFT-HDA adduct and TS configurations. The possible situations were summarized in Figure S14. From Table S1, we can get the values of ΔR and $\Delta\chi$, and applied them in the equation: $E = E_0 - F\Delta R - F^2\Delta\chi/2$ to obtain the change in activation energy in the cycloreversion of DA adduct.

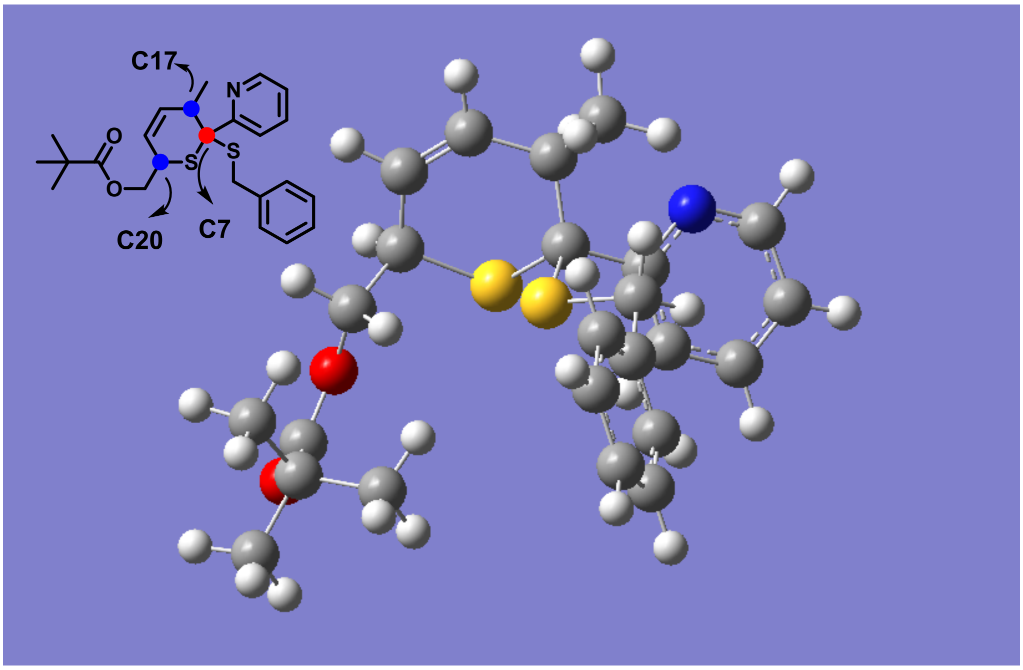


Figure S12. Initial optimized molecular structure of the model molecule.

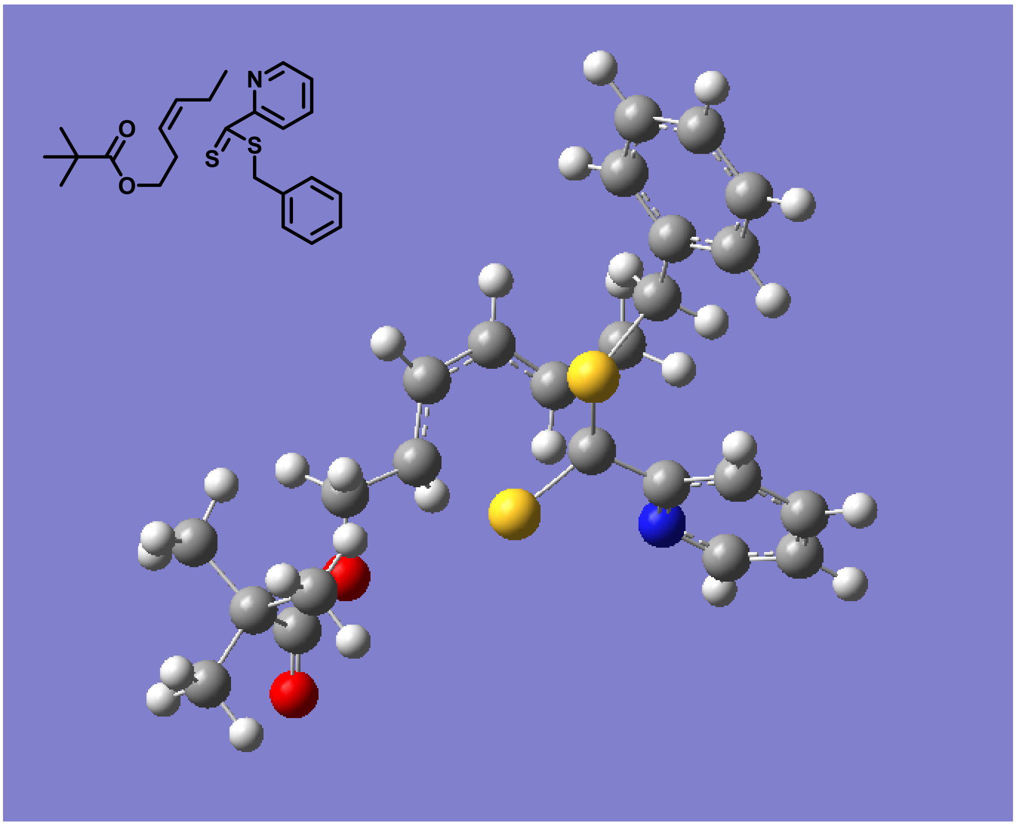


Figure S13. Optimized molecular structure of the transition state.

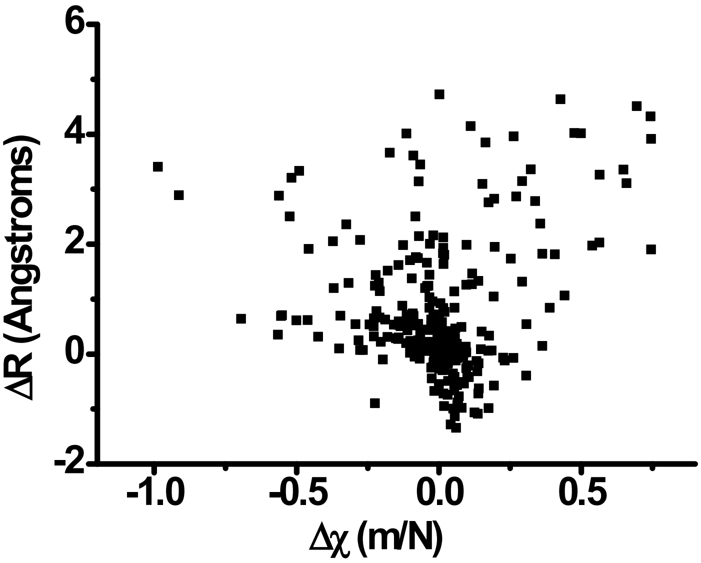


Figure S14. Computed values of ΔR and Δχ for all possible combinations of pulling points for the indicated mechanophore.

Table S1. Compliances and internuclear distances

Atom pairs		ΔR(A)	Δχ(m/N)
12	11	0.000083	0.000001
12	16	-0.00052	0
12	15	-0.00012	-1.2E-05
12	14	0.00013	-7E-06
12	13	-0.00003	0.000003
12	10	-0.00154	-8E-06
12	9	0.010837	0.029491
12	7	-0.04886	-0.08496
12	8	0.271333	-0.14263
12	2	0.235498	-0.10031
12	3	0.072126	-0.26696
12	4	0.317724	-0.22786
12	5	0.611028	-0.50024
12	6	0.689538	-0.55426
12	1	0.543446	-0.29267
12	17	0.032126	0.023328
12	26	0.065008	0.185717
12	18	-0.72153	0.016042
12	19	-0.4167	0.054757
12	20	0.545957	-0.07243
12	21	1.745868	-0.07377
12	22	2.051321	-0.37242
12	23	2.879945	-0.56142
12	27	2.887834	-0.91335
12	24	3.610323	-0.08935
12	28	4.019633	0.475863
12	29	3.449305	-0.06541
12	25	4.01094	-0.11449
11	16	-0.00028	-5E-06
11	15	0.000159	-0.00001
11	14	0.000316	-6E-06
11	13	0.000081	-7E-06
11	10	-0.00079	-7E-06
11	9	0.016732	-9.5E-05
11	7	-0.07619	-0.00334
11	8	-0.01182	-0.0171
11	2	0.197648	-0.02595
11	3	-0.00444	-0.07595

11	4	0.220567	-0.20391
11	5	0.527977	-0.14056
11	6	0.649426	-0.22792
11	1	0.531943	-0.1304
11	17	-0.10291	0.04706
11	26	0.183658	0.063097
11	18	-0.94043	0.064615
11	19	-0.71915	0.138995
11	20	0.131661	0.094643
11	21	1.269577	0.116328
11	22	1.439451	-0.03321
11	23	2.146042	-0.06982
11	27	2.074638	-0.27684
11	24	2.864834	0.271375
11	28	3.262883	0.564361
11	29	2.822574	0.194162
11	25	3.143596	0.292053
16	15	-0.00002	0.000004
16	14	-0.00027	-3E-06
16	13	-0.00061	-5E-06
16	10	0.000312	-0.00013
16	9	0.027402	0.089712
16	7	-0.09077	0.011025
16	8	-0.20826	0.102943
16	2	0.166128	-0.0031
16	3	-0.01837	-0.06866
16	4	0.196529	-0.11458
16	5	0.503294	-0.22897
16	6	0.628585	-0.18823
16	1	0.505252	-0.13507
16	17	-0.22061	-0.0075
16	26	0.307402	-0.18057
16	18	-1.13186	0.055874
16	19	-0.98085	0.080242
16	20	-0.12798	0.131981
16	21	1.043102	0.192762
16	22	1.241548	-0.03683
16	23	1.979097	-0.12543
16	27	1.912208	-0.45759
16	24	2.760132	0.174643
16	28	3.109685	0.659315

16	29	2.78398	0.337715
16	25	3.09427	0.152745
15	14	-0.00019	-3E-06
15	13	-0.0003	0.000001
15	10	0.000106	-5.5E-05
15	9	0.028736	0.096414
15	7	-0.08298	0.030761
15	8	-0.11688	0.230881
15	2	0.18146	-0.00744
15	3	0.021236	-0.1012
15	4	0.248881	-0.28212
15	5	0.556712	-0.10657
15	6	0.661421	-0.20878
15	1	0.514128	-0.11542
15	17	-0.1808	0.031612
15	26	0.279656	-0.14475
15	18	-1.06365	0.125172
15	19	-0.88205	0.065933
15	20	0.057261	0.173911
15	21	1.31568	0.292312
15	22	1.637186	0.016235
15	23	2.504843	-0.08287
15	27	2.502475	-0.52371
15	24	3.359027	0.322946
15	28	3.660153	-0.17208
15	29	3.353281	0.648041
15	25	3.850399	0.163474
14	13	0.000023	-2E-06
14	10	-0.00049	-1.3E-05
14	9	0.023691	0.007137
14	7	-0.06588	-0.00317
14	8	0.105263	-0.05779
14	2	0.211916	-0.079
14	3	0.070762	-0.27694
14	4	0.314579	-0.4239
14	5	0.617854	-0.4612
14	6	0.697443	-0.34598
14	1	0.532691	-0.15849
14	17	-0.07215	0.066974
14	26	0.181431	-0.00909
14	18	-0.89767	-0.22442

14	19	-0.62751	0.139948
14	20	0.406134	0.150345
14	21	1.733175	0.253132
14	22	2.157839	-0.01921
14	23	3.138983	-0.0706
14	27	3.205455	-0.51734
14	24	4.018099	0.498626
14	28	4.321642	0.743647
14	29	3.913033	0.745542
14	25	4.633313	0.427056
13	10	-0.00131	-3E-06
13	9	0.015648	0.012094
13	7	-0.0495	-0.08012
13	8	0.287632	-0.15131
13	2	0.233766	-0.09524
13	3	0.098636	-0.3507
13	4	0.349887	-0.56575
13	5	0.642068	-0.69464
13	6	0.705279	-0.55103
13	1	0.539692	-0.24369
13	17	0.023044	0.020887
13	26	0.08583	0.147483
13	18	-0.74412	0.030491
13	19	-0.41811	0.099747
13	20	0.631788	-0.01852
13	21	1.932367	0.015223
13	22	2.359931	-0.3257
13	23	3.329604	-0.49087
13	27	3.408104	-0.98731
13	24	4.148335	0.111971
13	28	4.509835	0.695021
13	29	3.958349	0.262745
13	25	4.726264	0.002026
10	9	-0.00367	-1.3E-05
10	7	-0.08941	-0.00186
10	8	-0.12815	-0.00351
10	2	0.173491	-0.01146
10	3	-0.08683	-0.06752
10	4	0.120733	-0.08051
10	5	0.430707	-0.11074
10	6	0.593493	-0.14081

10	1	0.525533	-0.0962
10	17	-0.13419	0.026195
10	26	0.188775	0.022801
10	18	-0.94664	0.01796
10	19	-0.77215	0.07045
10	20	-0.11655	0.059284
10	21	0.840491	0.054523
10	22	0.841784	-0.03294
10	23	1.37391	-0.09493
10	27	1.241284	-0.22461
10	24	1.986062	0.096824
10	28	2.371105	0.356401
10	29	2.003339	-0.03105
10	25	2.12109	0.015547
9	7	-0.09263	-0.00135
9	8	-0.10325	-0.00586
9	2	0.043876	-0.00283
9	3	-0.00688	-0.00841
9	4	0.061846	-0.00879
9	5	0.139753	-0.01748
9	6	0.169016	-0.02774
9	1	0.150246	-0.02376
9	17	0.579138	0.011233
9	26	0.835526	0.01521
9	18	-0.0372	0.016054
9	19	-0.05657	0.042517
9	20	0.46528	0.057423
9	21	1.260846	0.096331
9	22	1.140092	0.054151
9	23	1.46414	0.11724
9	27	1.331686	0.138136
9	24	1.823301	0.363152
9	28	1.902177	0.745621
9	29	1.946989	0.195933
9	25	1.814998	0.407114
7	8	-0.15594	-0.00255
7	2	-0.0394	-0.00022
7	3	-0.02386	-0.00028
7	4	-0.02623	-0.00024
7	5	-0.02913	-0.00021
7	6	-0.0373	-0.00012

7	1	-0.02906	-0.00017
7	17	0.92654	0.005448
7	26	0.768295	0.020021
7	18	0.389949	0.007716
7	19	0.175568	0.007875
7	20	0.207323	0.006353
7	21	0.482885	-0.00225
7	22	0.153101	0.02097
7	23	0.258149	0.009756
7	27	0.105444	0.093302
7	24	0.492839	0.07901
7	28	0.544585	0.307293
7	29	0.702106	-0.01339
7	25	0.404335	0.053522
8	2	0.081505	-0.00276
8	3	0.709135	-0.01843
8	4	0.621323	-0.01236
8	5	0.210275	-0.01462
8	6	-0.24934	-0.02681
8	1	-0.44443	-0.02503
8	17	0.463231	0.006163
8	26	0.311429	0.010185
8	18	0.322239	0.003417
8	19	0.176419	0.00803
8	20	0.358678	0.010549
8	21	0.124095	0.013242
8	22	-0.03676	0.058854
8	23	-0.10456	0.047332
8	27	-0.06608	0.225768
8	24	-0.21238	0.100871
8	28	-0.39376	0.306318
8	29	-0.07331	0.060096
8	25	-0.25915	0.096033
2	3	0.001218	0.000006
2	4	0.006626	0.000038
2	5	0.011019	0.00007
2	6	0.004122	0.00004
2	1	0.008934	0.000089
2	17	0.416253	0.026979
2	26	0.116089	0.037362
2	18	0.050722	0.014169

2	19	-0.00062	0.009747
2	20	0.077727	0.016377
2	21	0.393622	-0.00554
2	22	0.077849	0.018324
2	23	0.249671	-0.07283
2	27	0.052377	-0.04284
2	24	0.596323	0.001095
2	28	0.839926	0.3896
2	29	0.737218	-0.09118
2	25	0.512014	-0.02696
3	4	0.001879	0.00002
3	5	0.000982	-6E-06
3	6	-0.00368	0.000016
3	1	0.001372	0.000111
3	17	0.283541	0.057128
3	26	-0.31569	0.13521
3	18	-0.01266	0.036129
3	19	0.223891	0.008239
3	20	0.721617	-0.01884
3	21	1.234959	-0.04142
3	22	1.1995	-0.0483
3	23	1.515883	-0.17942
3	27	1.435096	-0.22184
3	24	1.80554	0.019199
3	28	2.026021	0.564081
3	29	1.764115	-0.08086
3	25	1.834315	0.014405
4	5	-0.0028	-2.1E-05
4	6	-0.00257	0.000018
4	1	0.000445	-5E-06
4	17	0.124226	0.069681
4	26	-0.57367	0.193565
4	18	-0.10286	0.044703
4	19	0.134969	0.008515
4	20	0.54929	-0.00711
4	21	1.03065	-0.03312
4	22	0.958057	-0.02252
4	23	1.298311	-0.21127
4	27	1.198297	-0.36953
4	24	1.660282	-0.04192
4	28	1.970723	0.538256

4	29	1.616185	-0.14156
4	25	1.706257	-0.10183
5	6	0.004595	0.000043
5	1	0.002879	0
5	17	0.030075	0.052961
5	26	-0.53813	0.08813
5	18	-0.14356	0.032292
5	19	-0.0871	0.013511
5	20	-0.01497	0.034368
5	21	0.284671	0.034855
5	22	-0.04979	0.085907
5	23	0.160643	-0.08249
5	27	-0.10086	-0.19674
5	24	0.628057	-0.02709
5	28	1.06431	0.441885
5	29	0.716598	-0.11299
5	25	0.545669	-0.09918
6	1	-0.00604	-4.8E-05
6	17	0.044333	0.029821
6	26	-0.23192	-0.01446
6	18	-0.11873	0.014039
6	19	-0.29058	0.017881
6	20	-0.56729	0.064133
6	21	-0.41975	0.105564
6	22	-0.9871	0.174665
6	23	-0.89104	0.067604
6	27	-1.28062	0.041355
6	24	-0.35402	0.049426
6	28	0.148455	0.363692
6	29	-0.13656	-0.00145
6	25	-0.54817	0.000321
1	17	0.240104	0.021334
1	26	0.174414	0.040651
1	18	-0.01558	0.008153
1	19	-0.29691	0.012735
1	20	-0.66427	0.054351
1	21	-0.51025	0.082059
1	22	-1.08823	0.136753
1	23	-0.99198	0.050562
1	27	-1.34204	0.060478
1	24	-0.4915	0.032263

1	28	-0.07042	0.261599
1	29	-0.23629	-0.02087
1	25	-0.67222	-0.01644
17	26	-0.0388	-0.00033
17	18	-0.12238	-0.0011
17	19	-0.11026	0.000162
17	20	-0.24272	0.006074
17	21	0.135701	-0.00671
17	22	-0.19376	0.014089
17	23	-0.03092	-0.01209
17	27	-0.26854	0.000706
17	24	0.381814	-0.06594
17	28	0.692686	-0.08895
17	29	0.519139	-0.07876
17	25	0.300789	-0.14067
26	18	0.053339	-0.00158
26	19	0.099932	-0.00447
26	20	-0.13142	0.00279
26	21	0.44572	-0.04194
26	22	-0.02216	-0.00409
26	23	0.222384	-0.03888
26	27	-0.15085	-0.01864
26	24	0.876161	-0.12819
26	28	1.293432	-0.31755
26	29	1.143815	-0.20728
26	25	0.780257	-0.21955
18	19	0.058968	0.000272
18	20	-0.07247	0.000825
18	21	0.195571	-0.00748
18	22	0.01274	0.001658
18	23	0.093699	-0.00631
18	27	-0.02097	0.012992
18	24	0.28835	0.002267
18	28	0.331488	0.176391
18	29	0.434867	-0.03192
18	25	0.256928	-0.00563
19	20	-0.08797	-0.00061
19	21	-0.00956	-0.00106
19	22	-0.02285	-0.00153
19	23	-0.02409	-0.00123
19	27	-0.01837	0.000492

19	24	-0.04082	0.01964
19	28	-0.16774	0.139304
19	29	0.057092	-0.01162
19	25	-0.02679	0.013254
20	21	-0.02155	-0.00031
20	22	-0.0059	0.000483
20	23	-0.00459	-0.001
20	27	0.009623	0.002604
20	24	-0.0281	-0.00098
20	28	-0.08846	0.025986
20	29	0.005277	0.008322
20	25	-0.02007	0.013095
21	22	-0.00145	-3.5E-05
21	23	-0.00899	0.001053
21	27	-0.01797	0.00518
21	24	-0.0018	0.002475
21	28	-0.03196	-0.00269
21	29	0.029443	0.006327
21	25	0.001029	0.001911
22	23	0.003297	0.000085
22	27	0.004263	0.000347
22	24	-0.00409	0.00044
22	28	-0.06174	-0.00082
22	29	0.041224	-0.00879
22	25	0.002111	0.000033
23	27	-0.00127	-4E-06
23	24	-0.00028	0.000032
23	28	0.003288	0.000978
23	29	-0.00554	0.001119
23	25	0.00098	0.000201
27	24	0.001626	0.00005
27	28	0.04331	-0.09884
27	29	-0.03737	0.021626
27	25	0.00164	0.000738
24	28	-0.00021	-4E-06
24	29	0.001095	0.000019
24	25	-0.00032	-1E-06
28	29	0.003179	0.000806
28	25	0.000152	0.000014
29	25	-0.001	0.00003

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