

Supporting Information

Bidentate Selenium-Based Chalcogen Bond Catalyzed Cationic Polymerization of *p*-Methoxystyrene

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Materials and Methods

Unless otherwise specified, all polymerization of *p*MOS experiments were conducted in dry nitrogen atmosphere. Diethyl ether (Et₂O) was refluxed with sodium and distilled under nitrogen before use. Chloroform (CHCl₃) and acetonitrile (CH₃CN) were freshly distilled from CaH₂. *p*-Methoxystyrene, *o*-methoxystyrene, 4-dimethylamino-styrene and 4-methoxy- α -methylbenzyl were purchased from Energy Chemical and distilled from CaH₂ before use. 4,4'-dimethoxybenzhydrol was purchased from Energy Chemical and used after sublimation. IBVE-HCL¹, ICCP² and *p*-methylthiostyrene³ were synthesized according to the method of literature. All other chemicals were commercially available and used as received without further purification unless.

Varian INOVA 600 MHz spectrometer and JNMECS 400 MHz spectrometer were used to record ¹H NMR and ¹³C NMR. ¹H NMR chemical shifts are reported in ppm versus residual protons in deuterated solvents as follows: δ 7.26 ppm for chloroform-d. ¹³C NMR chemical shifts are reported in ppm versus residual ¹³C in the solvent: δ 77.0 ppm for chloroform-d. The molecular weights (M_n and M_w) and the molecular mass distributions (\mathcal{D}) of the polymer samples were determined by gel permeation chromatography (GPC) using THF as the eluent (flow rate: 1.0 mL/min at 40 °C), and narrow polystyrene standards as reference samples. The measurements were performed using a Shodex GPC KF-800 system that was equipped with a Shodex RI-201H detector using Shodex-KF-803 and ShodexKF-804 Styragel columns (0.4 - 400 kg/mol). The absolute value of the polymer was detected using a Malvern Viscotek 305 Triple Detector (light scattering, refractive index, and viscometer), and was eluted with tetrahydrofuran at 30 °C at a flow rate of 1.0

mL/min (Shodex-KF-805, 50 - 2000 kg/mol). Differential scanning calorimetry (DSC) measurements: using 2.9 mg material, DSC experiments were performed on a METTLER TOLEDO instrument with a heat (25-300 °C) /cool 300-25 °C/heat (25-300 °C) cycle at a heating rate of 10 °C/min and cooling rate of 10 °C/min under N₂ atmosphere. The T_g values were obtained from a second heating scan. Thermal gravimetric analyzer (TGA): using 8.09 mg of material, TGA experiments were performed on a Linseis PT 1600 instrument, with a heat (40-800 °C) at a rate of 10 °C/min under N₂ atmosphere. Decomposition temperatures ($T_{d, \text{defined}}$ by the temperature of 5 % weight loss). Time of Flight (MALDI-TOF) Mass Spectrometry conditions were as follows. Instrument type: Bruker autoflex speed MALDI-TOF mass spectrometer, adjust to reflection mode, Power 80, P. Ext at 5000.00. The MALDI-TOF mass spectroscopic data were obtained using trans-2-[3-(4-tertbutylphenyl)-2-methyl-2-propenylidene]alonitrile (DCTB) as the matrix (10 mg/mL in THF), sodium trifluoroacetate as the cationization agent (10 mg/mL in THF) and samples were dissolved in THF (10 mg/mL). The solutions of samples, matrix and salt were mixed in a volume ratio of 1:1:1; then the mixed solution (1 μ L) was hand-spotted on a stainless steel MALDI target, which allowed to be dried completely.

Synthesis of catalyst:

1, 4-diiodobutane (9.0 mmol, 2.8 g) was added to phenylselenanylbenzene (6.0 mmol, 1.4 g) solution in 9 ml anhydrous acetonitrile at 23 °C under N₂ atmosphere. Then AgOTf (6.0 mmol, 1.54 g) was added proportionally to the stirring solution under no light conditions. After stirring for 3 days in no-light conditions, the reaction mixture was filtered with diatomite to remove the silver iodide. The residue was cleaned with CH₃CN (5.0 mL), and the filtrate evaporated under reduced pressure at 40 °C. The residue is recrystallized from dichloromethane/ether to obtain pure mono-selenium salt A'. Phenylselenanylbenzene (2.5 mmol, 0.6 g) and mono-selenium salt A' (2 mmol, 1.098 g) were added to 6 ml anhydrous acetonitrile at 23 °C under nitrogen atmosphere. Then, AgOTf (2.0 mmol, 0.514 g) was added proportionally to the stirring solution under no-light conditions. After stirring for 2 days in no-light conditions, the reaction mixture is filtered through diatomite to remove the silver iodide. The residue was cleaned with CH₃CN (5.0 mL), and the filtrate evaporated under reduced pressure at 40 °C. The residue was recrystallized by dichloromethane/ether to obtain pure bis-selenium salt A, which was dried under vacuum at 70 °C for 12 h, and the yield was 0.656 g (40%). ¹H NMR (600 M, Chloroform-d): δ (ppm) 7.73-7.75 (m, 8H, Ar-H), 7.61-7.68 (m, 12H, Ar-H), 4.19 (t, J = 7.6 Hz, 2CH₂, 4H), 2.20-2.25 (m, 2CH₂, 4H). ¹³C NMR (100 M, Chloroform-d): δ (ppm) 133.7, 131.8, 130.8, 125.1, 44.3, 24.3. ¹⁹F NMR (400 M, Chloroform-d): δ (ppm) 78.7. ⁷⁷Se NMR (76 M, Dichloromethane-d₂): δ (ppm) 450.5.

General procedure for polymerization of poly(*p*MOS)

A typical polymerization procedure is illustrated by the synthesis of poly(*p*MOS) ([cat]₀/[I]₀/[M]₀=1:1:25; Table 1, entry 3). 0.01 mmol catalyst, 0.01 mmol 4-methoxy- α -methylbenzyl alcohol (0.1 ml, 0.1 M dichloromethane solution), 0.25 mmol *p*-methoxy-styrene and 0.4 ml dichloromethane were successively added into a 10 ml reaction bottle. The solution was rapidly stirred at 30 °C for 8 hours, then an aliquot was withdrawn to determine monomer conversion by ¹H NMR spectroscopy, and the remaining solution was quenched by NH₃ solution in CH₃OH (0.1 ml). Methanol was added to precipitate the polymer, and the white solid was

obtained by recrystallization and purification of the polymer with dichloride/methanol mixed solution. Finally, poly(*p*MOS) was obtained by vacuum drying.

Table S1 Polymerization of electron-donating styrenic monomers and activation methods of different initiators^a.

Entry	[M] ₀	[I] ₀	[cat]/[I]/[M]	T (°C)	t (h)	Conv. (%) ^b	M _n , obsd (g/mol) ^c	M _n , calcd (g/mol) ^d	D ^d
1	(1)	(1)	1/5/500	30	48	--	--	--	--
2	(2)	(1)	1/5/500	30	72	90	12700	12000	1.55
3	(3)	(1)	1/5/500	30	72	95	13300	14300	1.52
4	(4)	(1)	1/5/500	30	36	98	13800	14400	1.47
5	<i>p</i> MOS	(2)	1/1/25	30	12	99	4300	3500	1.21
6	<i>p</i> MOS	(3)	1/1/25	0	20min	99	8100	3400	1.70
7	<i>p</i> MOS	(4)	1/1/25	0	30min	99	6700	3400	1.79
8	<i>p</i> MOS	(4)	1/1/25	-40	1	99	5520	3400	1.51
9	<i>p</i> MOS	(3)	1/1/25	-78	12	--	--	--	--

^aThe cationic polymerization of *p*MOS was carried out in dry DCM with [*p*MOS]₀ = 0.5 M (N₂ atmosphere). ^bThe conversion of monomer was determined by ¹H NMR. ^cM_n, calcd = M_{monomer} × [M]₀/[I]₀ × Conversion (%) + the molar mass of the initiators. ^dTHF (40 °C, PS calibrated) was used as the eluent of the sample, and the molecular weight was tested by SEC.

Table S2. Polymerization at different temperatures and solvents ^a.

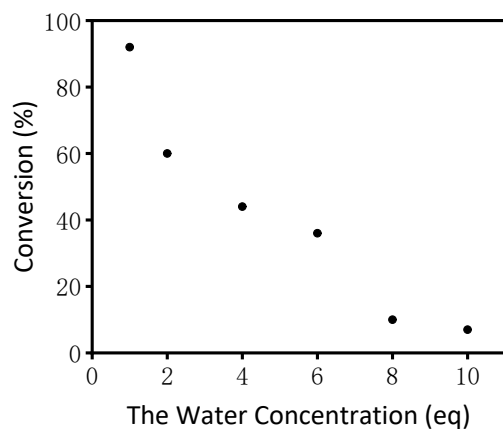
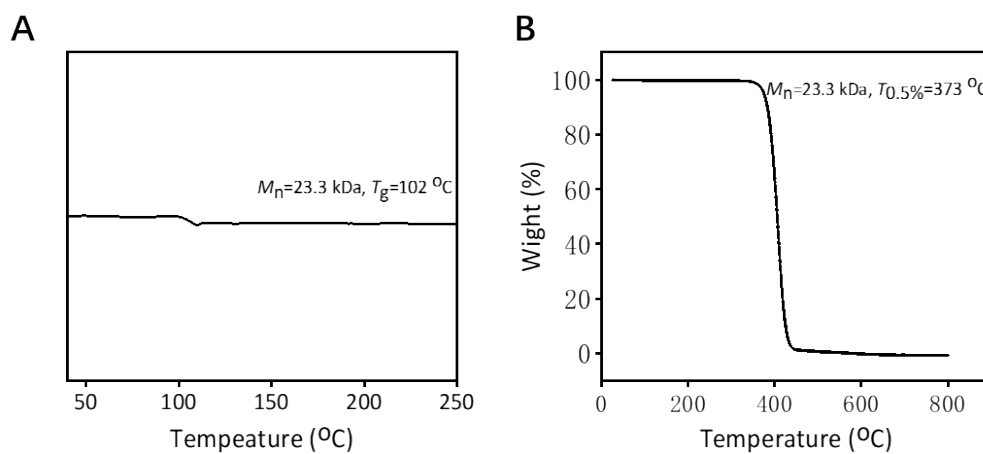
Entry	T (°C)	t (h)	Solv ^b	Conv. (%) ^c	M _n , obsd (g/mol) ^d	M _n , calcd (g/mol) ^e	D ^e
1	50	4	DCM	96	3000	3300	1.28
2	0	24	DCM	85	3100	3000	1.18
3	-40	48	DCM	10	--	--	--
4	30	6	AN	--	--	--	--
5	30	6	THF	--	--	--	--
6	30	8	DCM/AN=9/1	92	2900	3100	1.42
7	30	8	DCM/THF=9/1	84	3900	3000	1.25

^aThe cationic polymerization was carried out with [*p*MOS]₀ = 0.5 M (N₂ atmosphere), and [cat]₀/[initiator]₀/[M]₀ = 1 : 1 : 25. ^bDCM: Dichloromethane, AN: acetonitrile, THF: tetrahydrofuran ^cThe conversion of monomer was determined by ¹H NMR. ^dM_n, calcd = 152.19 + 134.18 × [M]₀ / [I]₀ × Conversion (%). ^eTHF (40 °C, PS calibrated) was used as the eluent of the sample, and the molecular weight was tested by SEC.

Table S3. Effect of water concentration on polymerization^a.

Entry	H ₂ O (eq)	THF (uL) ^b	Conv. (%) ^c	<i>M_n</i> , obsd (g/mol) ^d	<i>M_n</i> , calcd (g/mol) ^e	<i>D</i> ^e
1	0	100	92	2900	3100	1.25
2	1	10	91	3000	3100	1.26
3	2	10	60	2300	2100	1.11
4	4	10	44	1900	1600	1.07
5	6	20	36	--	--	--
6	8	20	10	--	--	--
7	10	40	7	--	--	--

^aThe cationic polymerization was carried out at 30 °C with $[pMOS]_0 = 0.25$ M (N₂ atmosphere), and $[cat]_0/[initiator]_0/[M]_0 = 1 : 1 : 25$. The reaction time was 8 h. ^bAdd 10 uL of 0.01 M, 0.02 M, and 0.04 M water tetrahydrofuran solution to Entry 2-4; 10 uL of 0.02 M and 0.04 M water tetrahydrofuran solution to Entry 5; 20 uL of 0.04 M water tetrahydrofuran solution to Entry 6; and 20 uL of 0.02 M and 0.04 M water tetrahydrofuran solution to Entry 7. ^cThe conversion of monomer was determined by ¹H NMR. ^d M_n , calcd = $152.19 + 134.18 \times [M]_0 / [I]_0 \times \text{Conversion} (\%)$. ^eTHF (40 °C, PS calibrated) was used as the eluent of the sample, and the molecular weight was tested by SEC.

**Fig. S1** Effect of water concentration on catalytic activity**Fig. S2** (A)DSC curves of poly(*p*MOS). (B)TGA (at 10 °C/min heating rate) thermograms of poly(*p*MOS).

The difference between two mechanisms in detail in supporting

Firstly, the mechanism of this work is different to the degenerative chain transfer between C–OR covalent species and C⁺ cations mechanism suggested by Tanaka and You in the publication of *Macromolecules* **2020**, 53, 4303, where TfOH is a catalyst/initiator and alcohol/phenol/ Group 16 Aromatic Nucleophiles act as chain transfer reagents (CTA). In fact, in that publication, TfOH can be considered as an initiator, the proton addition of TfOH to *p*MOS to generate the cation propagation species, and the controllability is modified by the CTAs. While in our system, selenium compound just acts as a catalyst.

There are two possible mechanisms as the following Fig. S3. If the polymerization proceeds with the second mechanism of degenerative chain transfer C–OR covalent species and C⁺ cations as mechanism 2 in the Fig. S3, a chain end of methyl group should appear in the ¹H NMR of the resulting polymer. However, no methyl end group was discovered (Fig. S4, red square). If the polymerization proceeds with the first mechanism of degenerative chain transfer C–OH covalent species and C⁺ cations as mechanism 1 in the Fig. S3, there is no end methyl group theoretically which agree with the ¹H NMR of the resulting polymer (Fig. S4). If methyl group exists, the chemical shift of methyl signals should appear at the same place as that in the polymer obtain using 4-methoxy- α -Methylbenzyl alcohol as an initiator (Fig. S5, red square). But in the Fig. S4, there is no methyl group. Therefore, the mechanism is the dormant-active equilibrium between C–OH covalent species and C⁺ cation–HO-selenium counter species (mechanism 1 in Fig. S3).

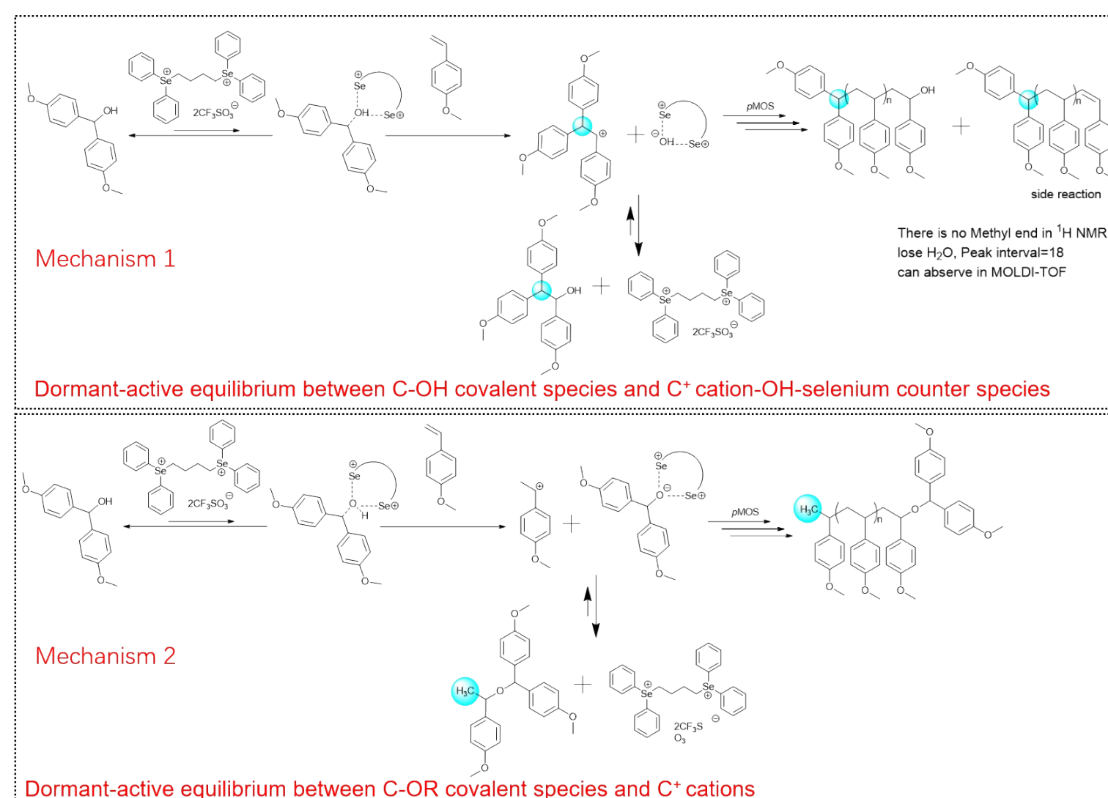


Fig. S3 Mechanism 1: dormant-active equilibrium between C–OH covalent species and C⁺ cation–HO-selenium counter species. Mechanism 2: C–OR covalent species and C⁺ cations.

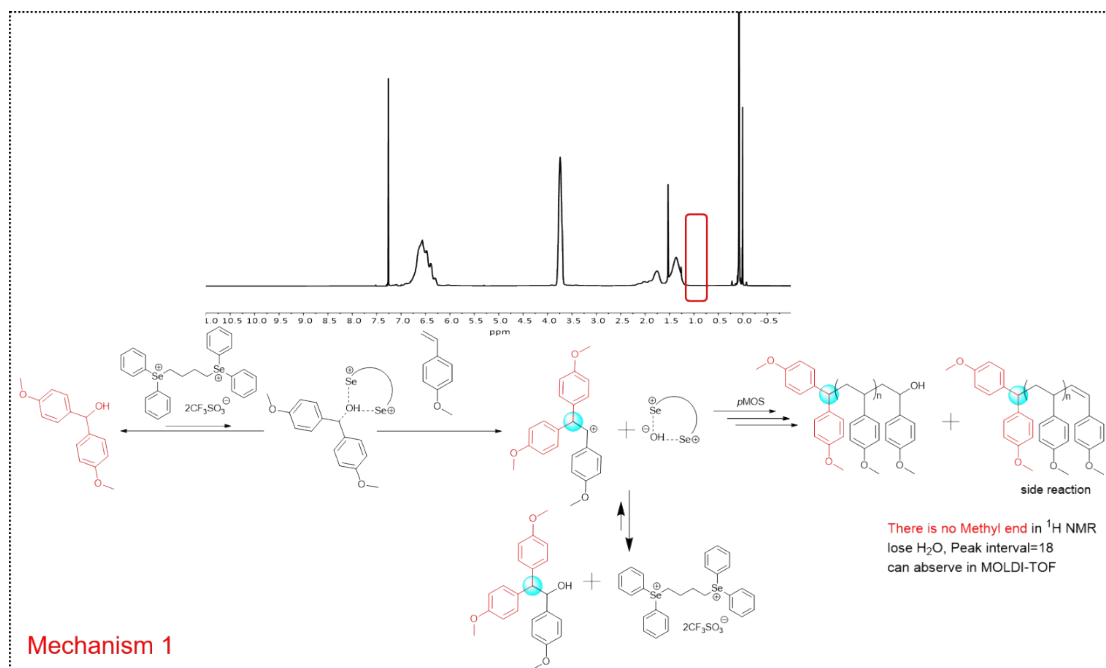


Fig. S4 $^1\text{H NMR}$ spectrum of the resulting polymer using 4,4'-dimethoxybenzhydrol as an initiator (600 MHz, CDCl_3 , 25 °C).

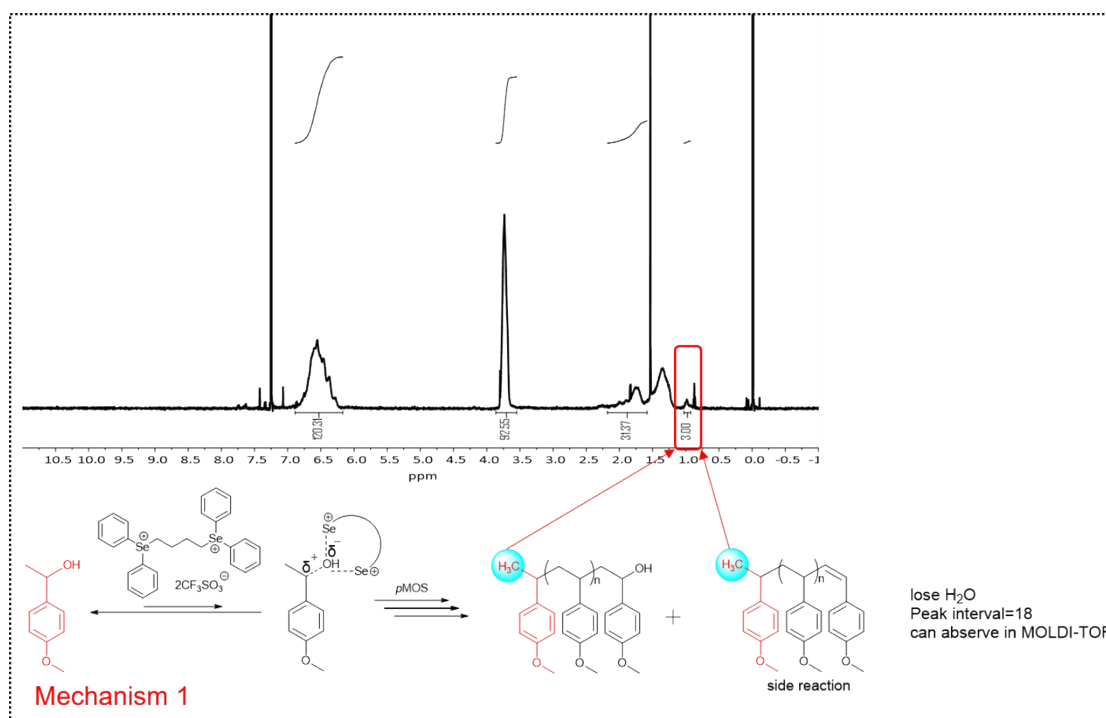


Fig. S5 $^1\text{H NMR}$ spectrum of the resulting polymer using 4-methoxy- α -Methylbenzyl alcohol as an initiator (600 MHz, CDCl_3 , 25 °C).

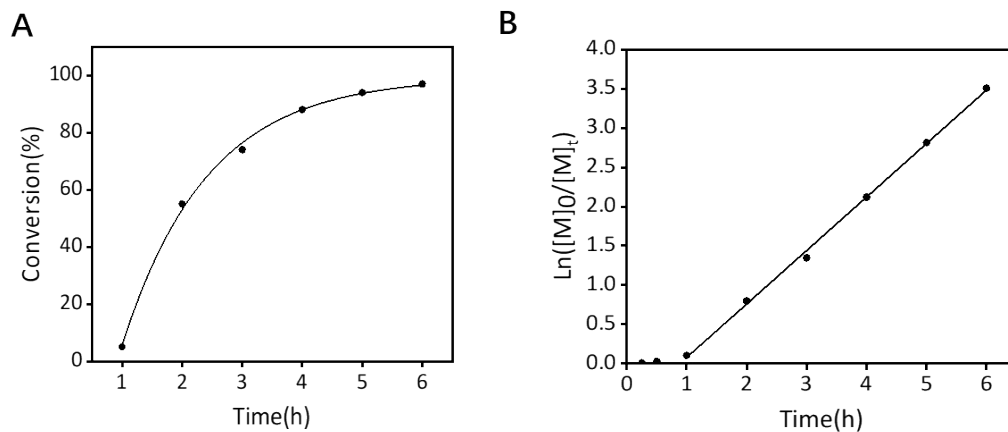


Fig. S6. (A) Time-conversion curves for the entry 3 reaction in Table 1. (B) The curves of $\ln([M]_0/[M]_t)$ versus time.

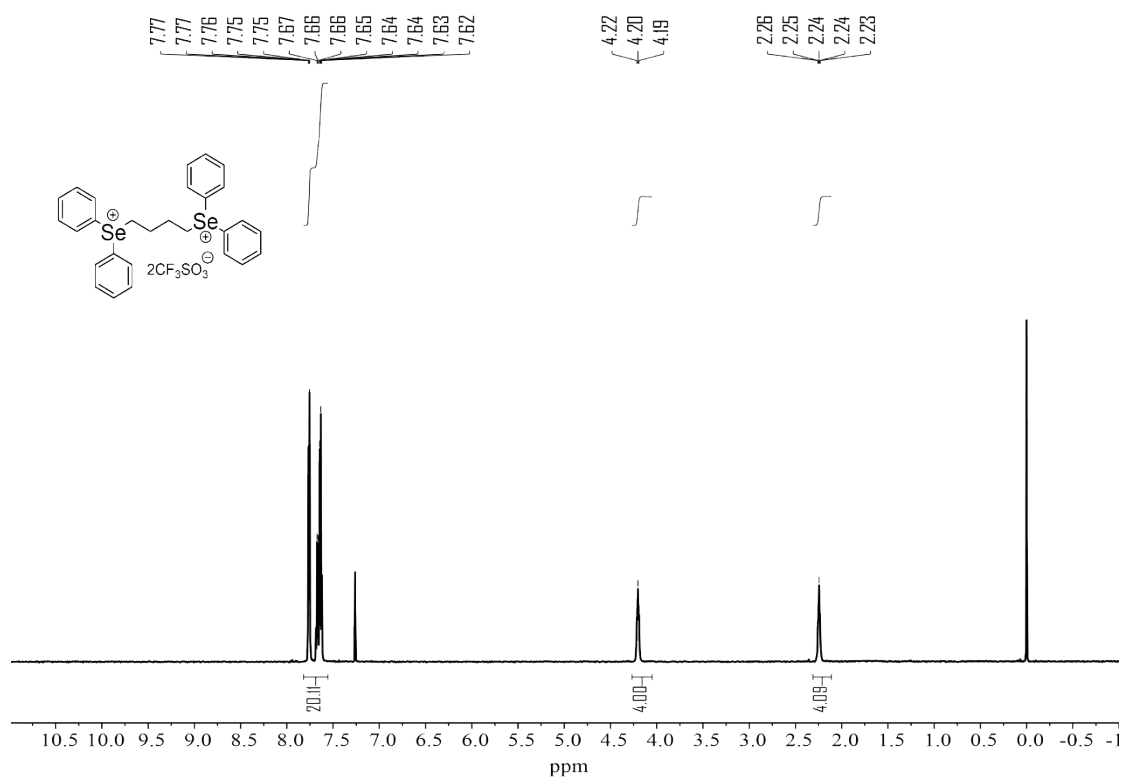


Fig. S7 ^1H NMR of Catalyst (600 M Hz, CDCl_3 , 25 $^\circ\text{C}$).

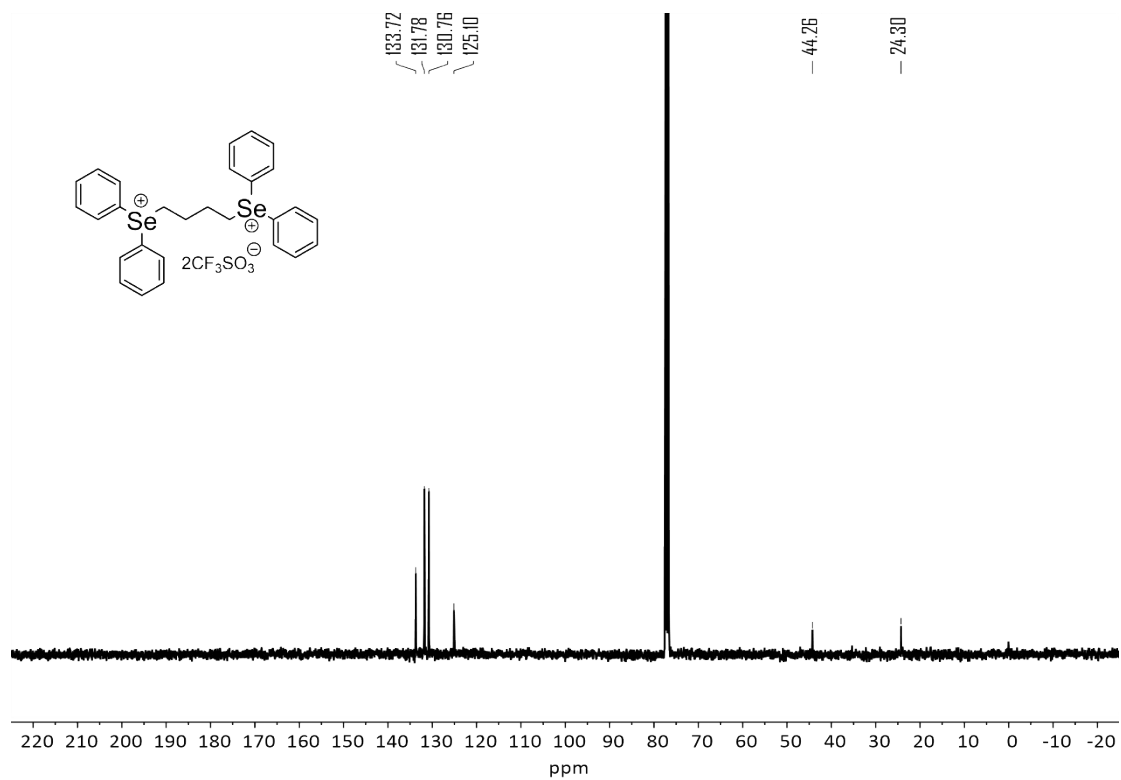


Fig. S8 ^{13}C NMR of Catalyst (100 M Hz, CDCl_3 , 25 °C).

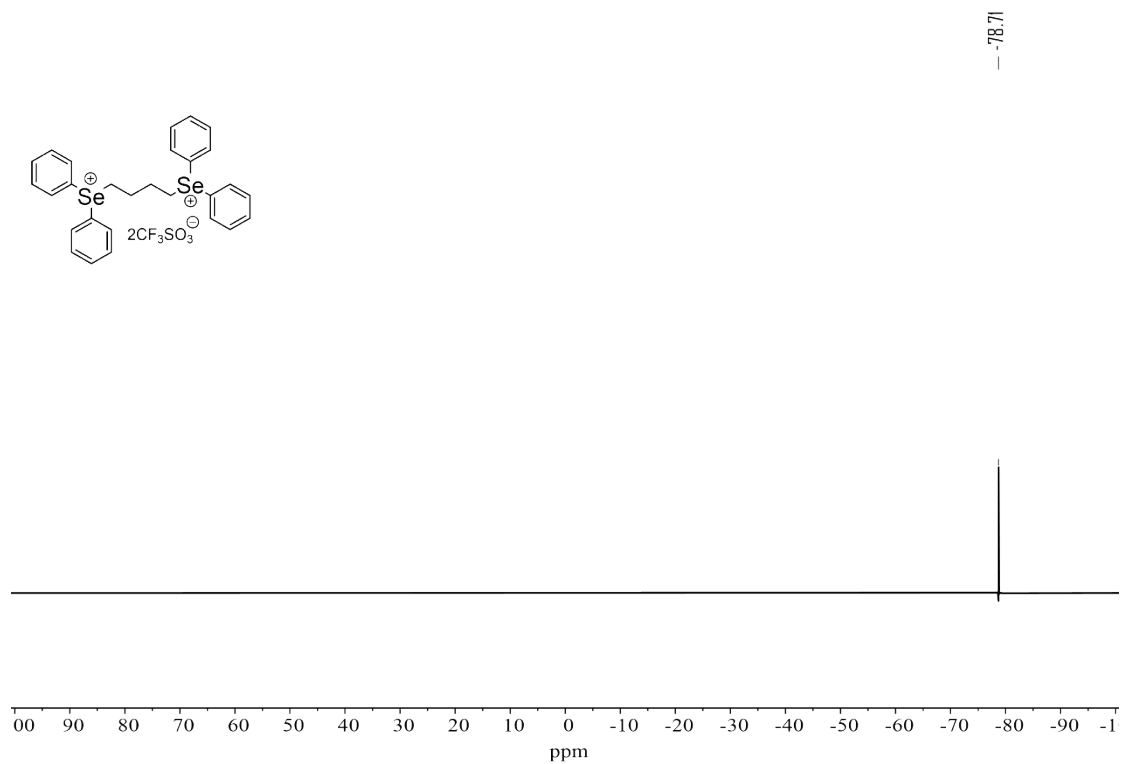


Fig. S9 ^{19}F NMR of Catalyst (400 M Hz, CD_2Cl_2 , 25 °C).

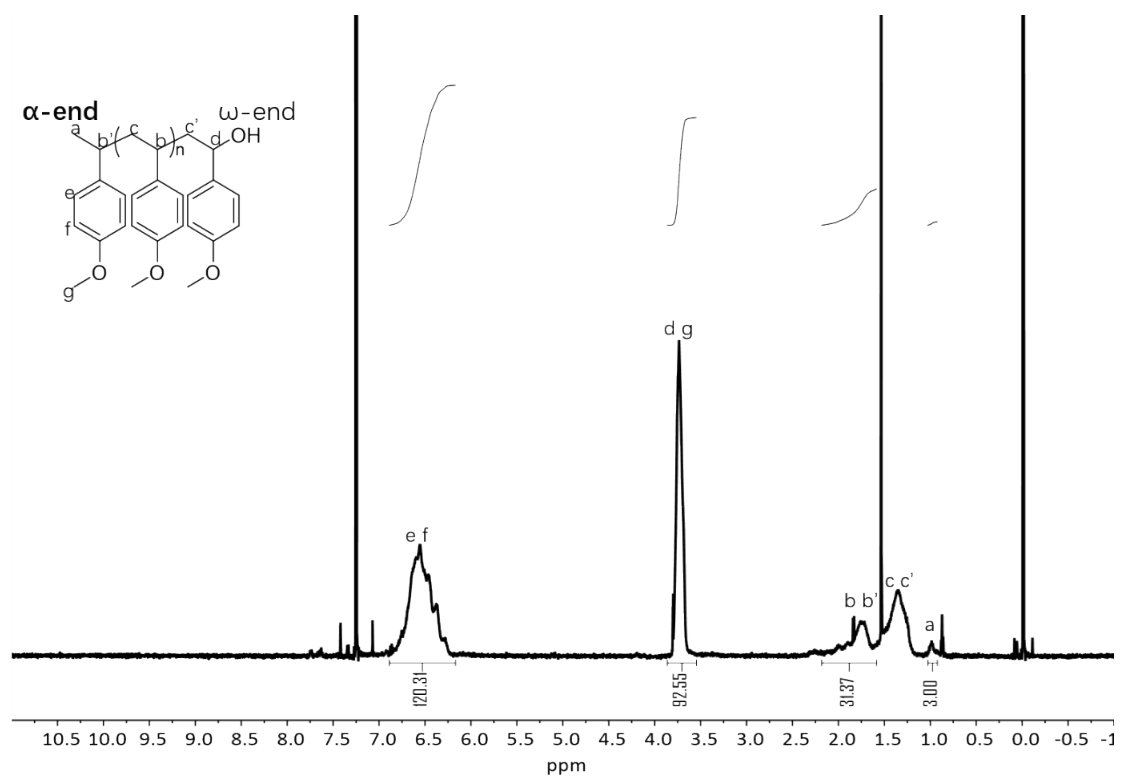


Fig. S10 ¹H NMR of poly(*p*MOS) (600 M Hz, CDCl₃, 25 °C).

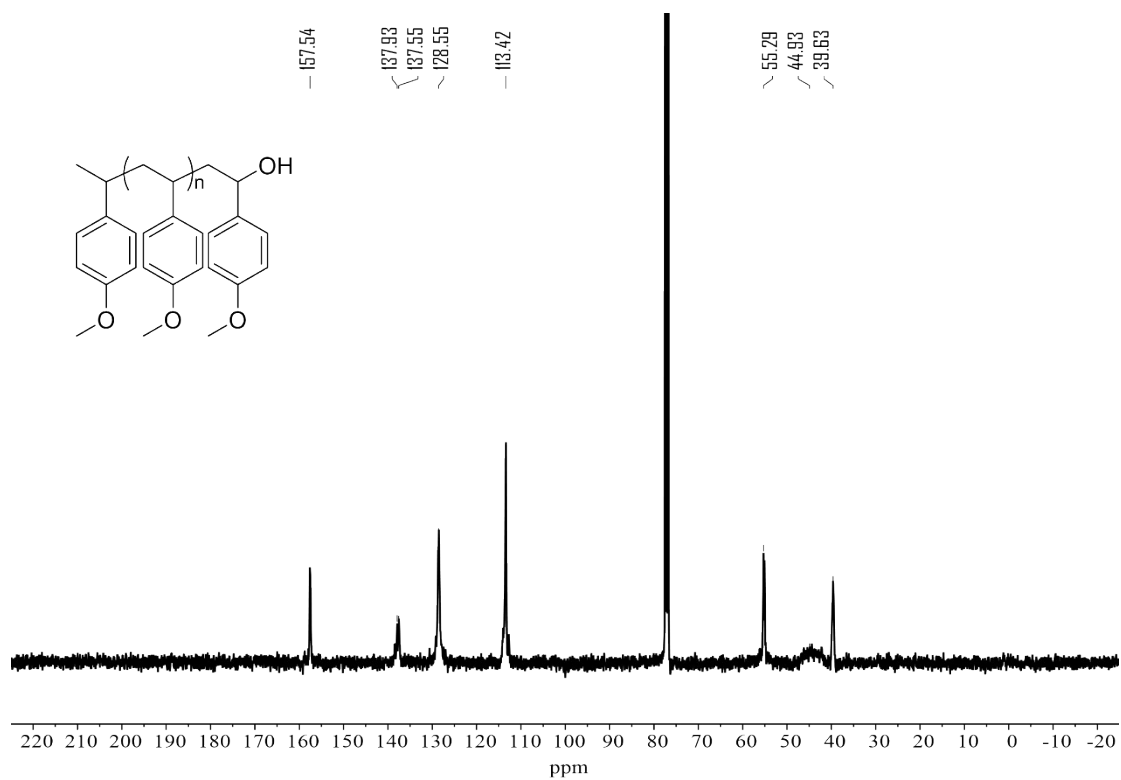


Fig. S11 ¹³C NMR of poly(*p*MOS) (100 M Hz, CDCl₃, 25 °C).

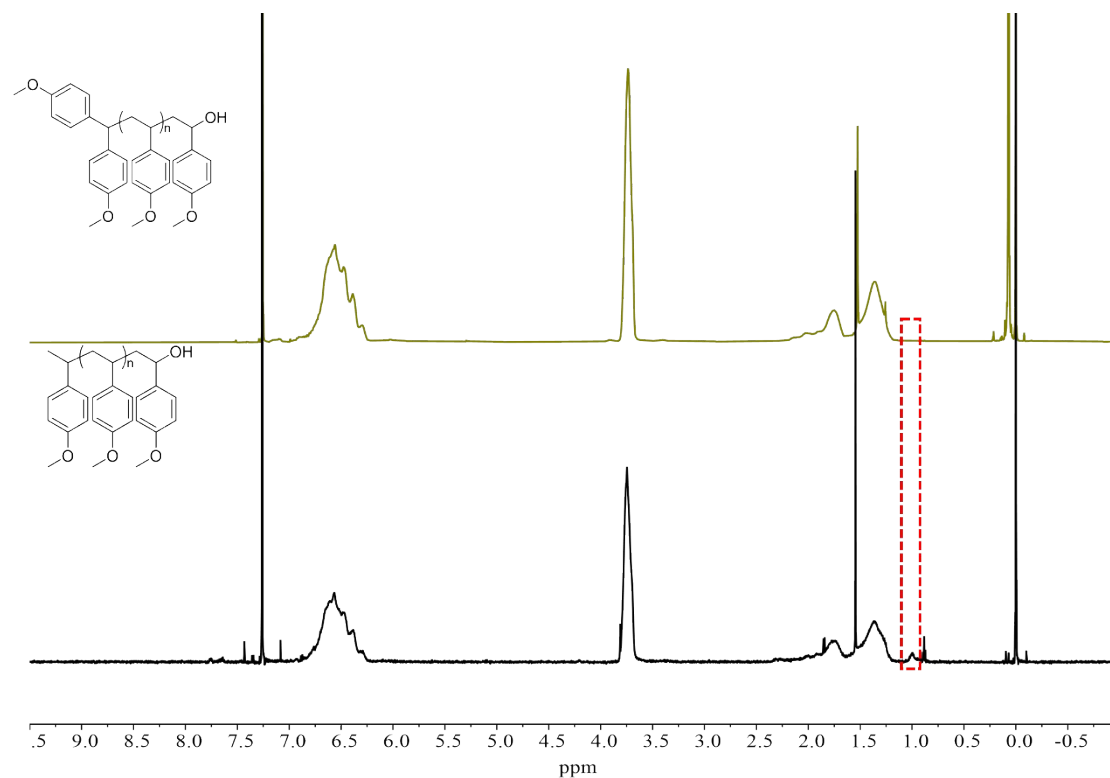


Fig. S12 ^1H NMR of poly(*p*MOS) (400 M Hz, CDCl_3 , 25 $^\circ\text{C}$). The top is triggered by 4,4'-dimethoxybenzhydrol, and the bottom is triggered by 4-methoxy- α -methylbenzyl alcohol, $[\text{cat}]_0/[\text{I}]_0/[\text{M}]_0=1/1/25$.

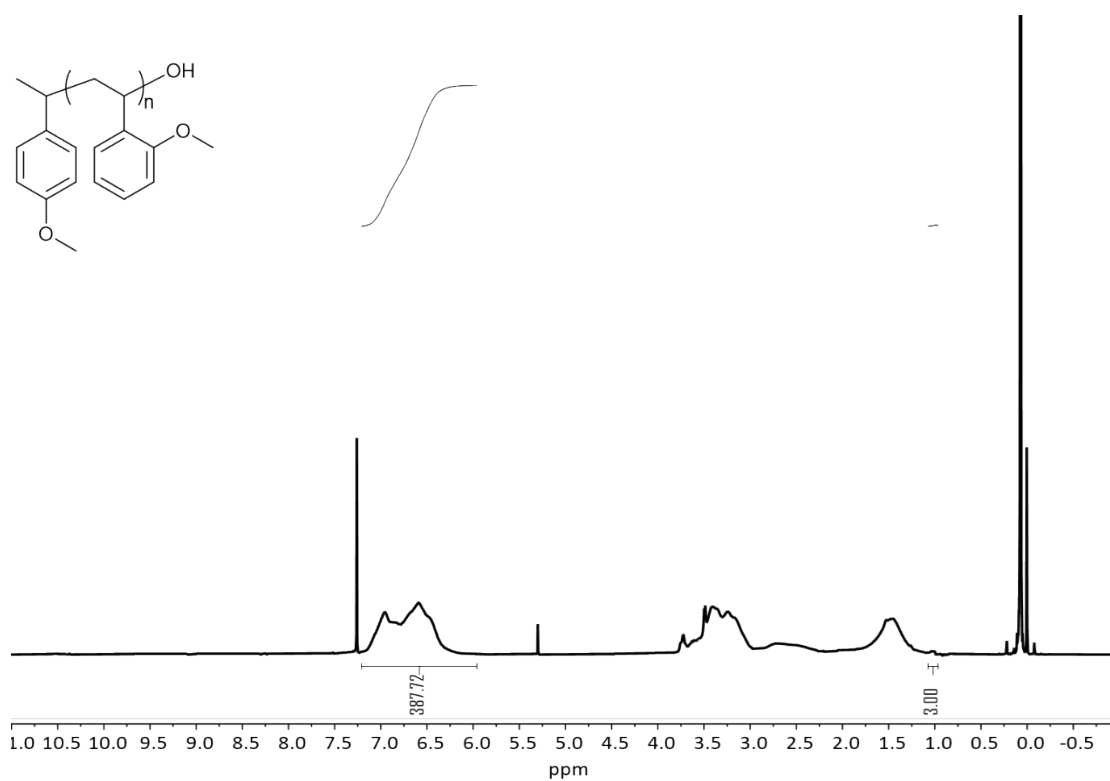


Fig. S13 ^1H NMR of poly(*o*-methoxystyrene) (600 M Hz, CDCl_3 , 25 $^\circ\text{C}$) (Table S1 entry 2).

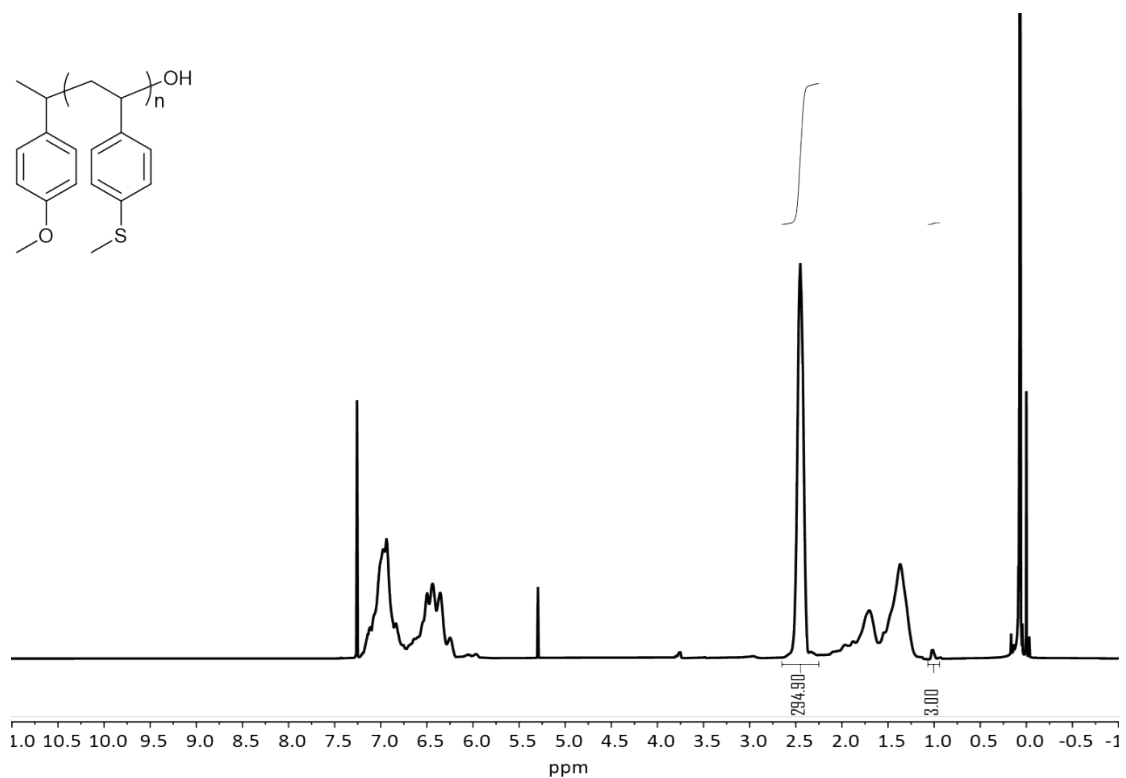


Fig. S14 ¹H NMR of poly(*p*-methylthiostyrene) (600 M Hz, CDCl₃, 25 °C) (Table S1 entry 3).

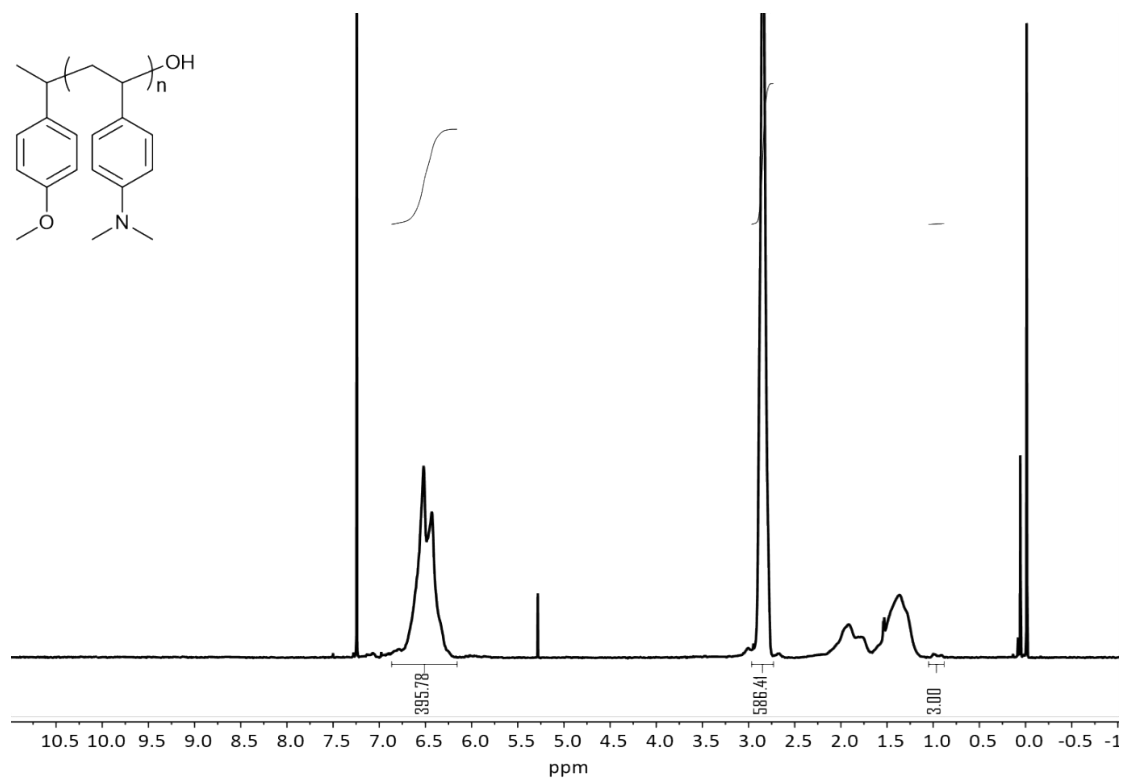


Fig. S15 ¹H NMR of poly(4-dimethylamino-styrene) (600 M Hz, CDCl₃, 25 °C) (Table S1 entry 4).

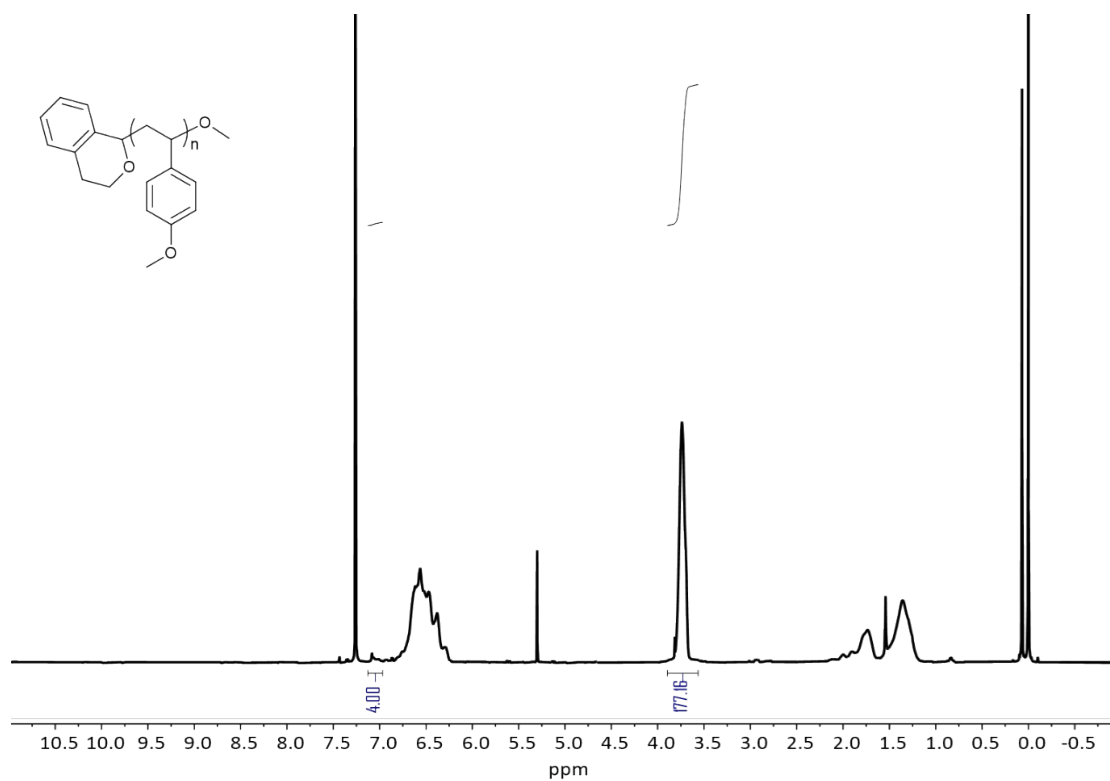


Fig. S16 ^1H NMR of poly(*p*MOS) triggered by ICCI (100 M Hz, CDCl_3 , 25 $^\circ\text{C}$) (Table S1 entry 6).

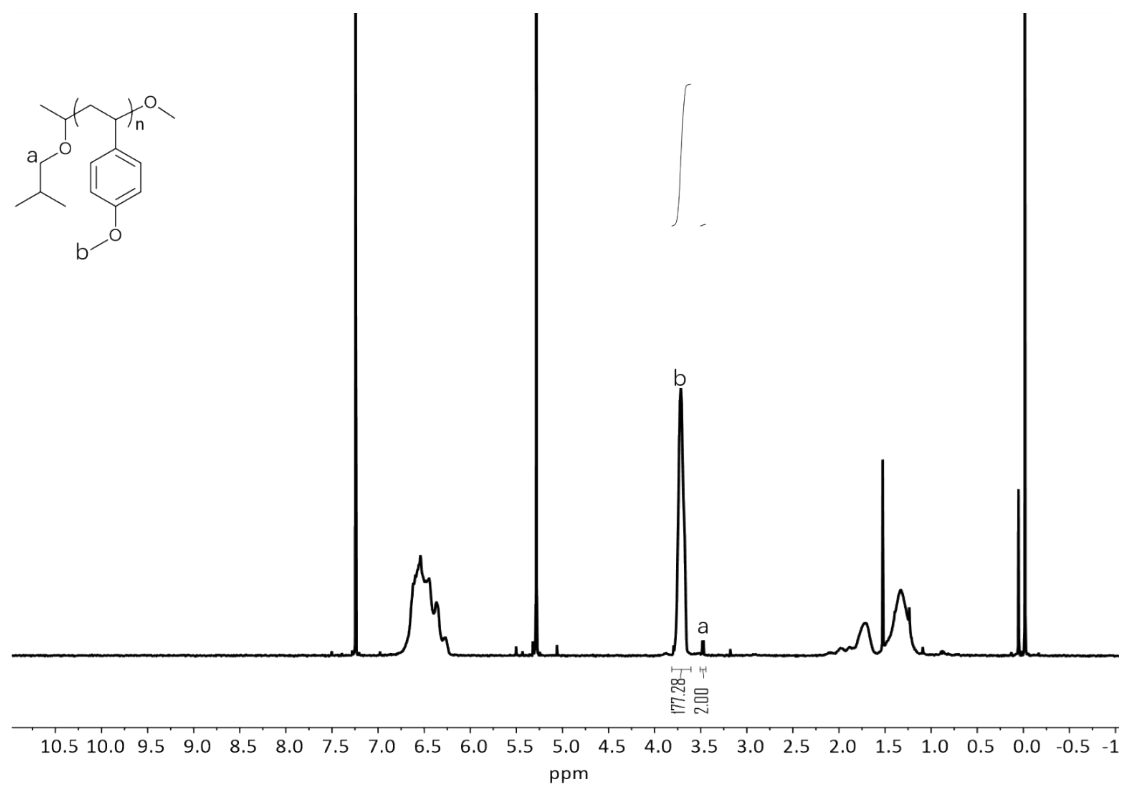


Fig. S17 ^1H NMR of poly(*p*MOS) triggered by IBVE-HCl (100 M Hz, CDCl_3 , 25 $^\circ\text{C}$) (Table S1 entry 7).

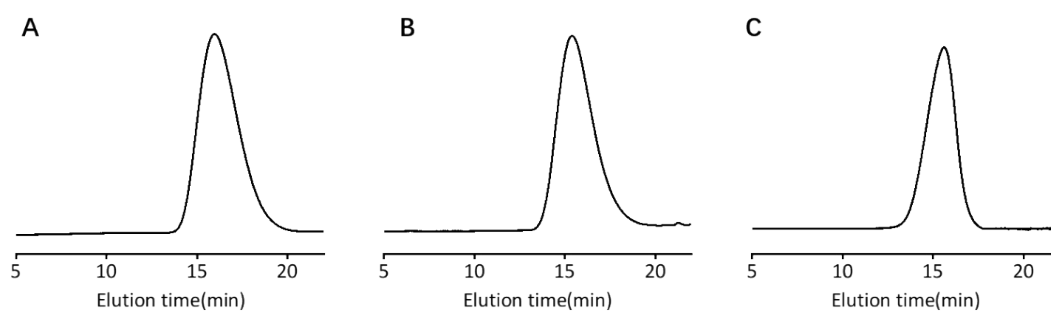


Fig. S18 GPC spectra of synthetic polymers with different monomer. (A) Table S1 entry 2. (B) Table S1 entry 3. (C) Table S1 entry 4.

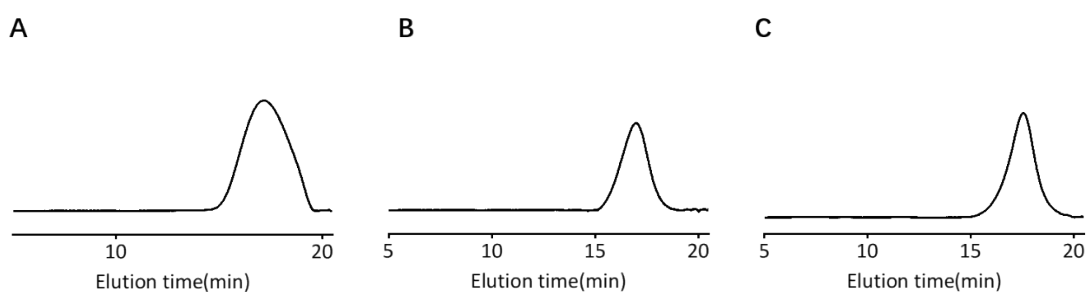


Fig. S19 GPC spectra of synthetic polymers with different initiator. (A) Table S1 entry 6. (B) Table S1 entry 7. (C) Table S1 entry 8.

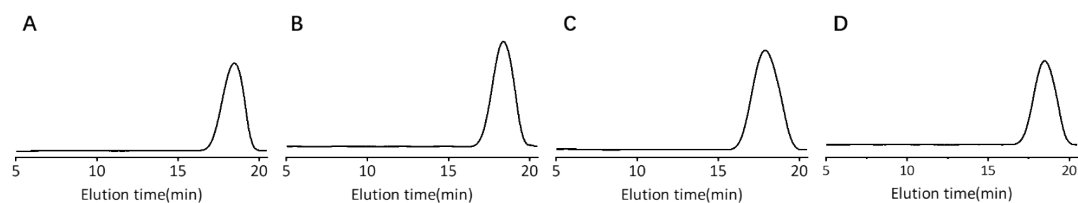


Fig. S20 GPC spectra of synthetic polymers with different temperature and solvent. (A) Table S2 entry 1. (B) Table S2 entry 2. (C) Table S2 entry 6. (D) Table S2 entry 7.

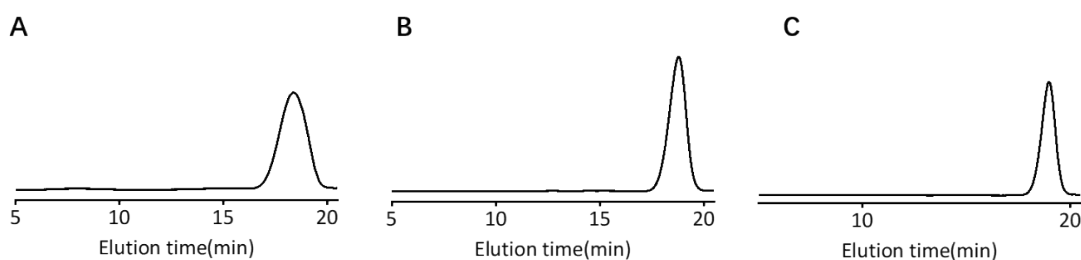


Fig. S21 GPC spectra of synthetic polymers with different water concentration. (A) 1 eq of water (Table S3 entry 2). (B) 2 eq of water (Table S3 entry 3). (C) 4 eq of water (Table S3 entry 4).

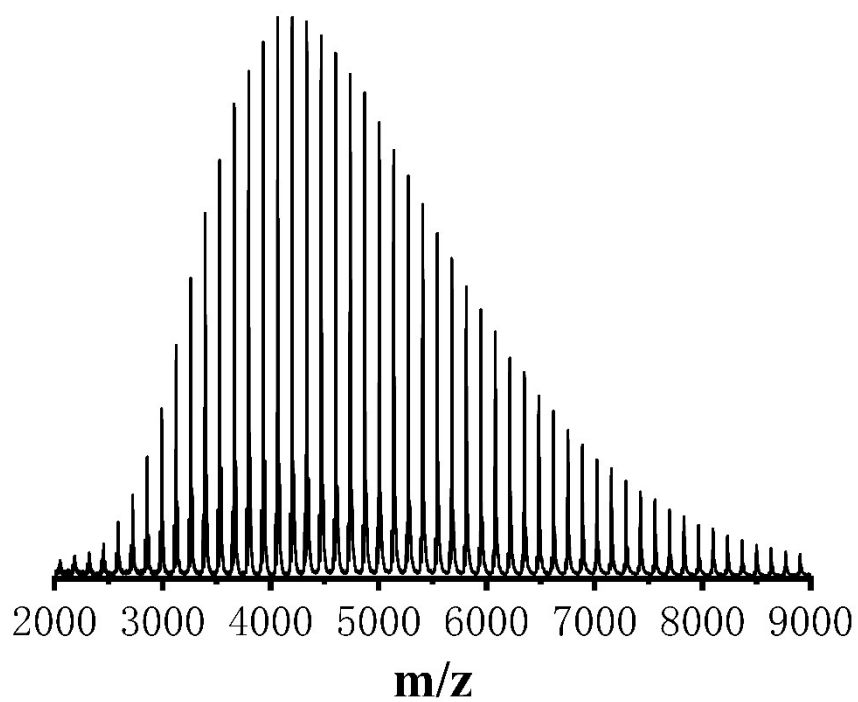


Fig. S22 MALDI-TOF MS of poly (*p*MOS) (Table 1 Entry 2).

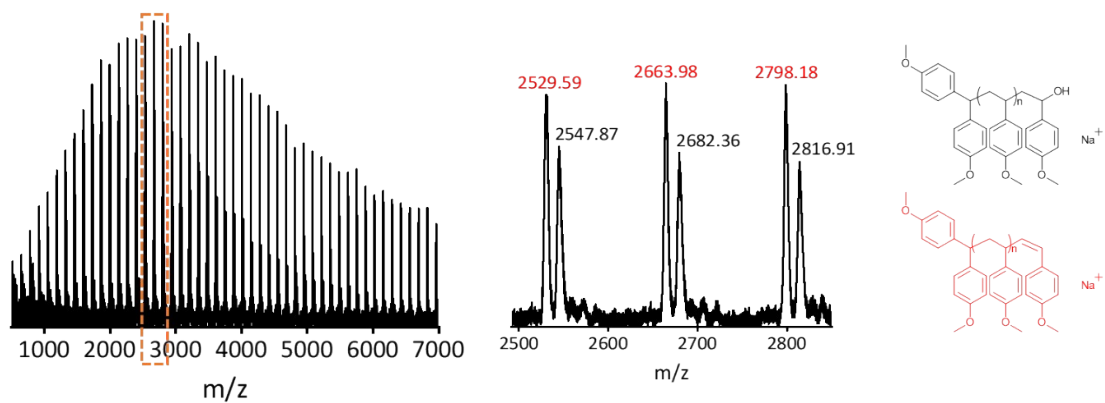


Fig. S23 MALDI-TOF MS of poly (*p*MOS) (Table S1 Entry 1).

Computational studies

All Density Functional Theory (DFT) calculations were carried out using M06-2X hybrid-exchange correlation functional⁴ with Grimme D3⁵ dispersion correction and 6-31G(d,p) basis set by Gaussian 09,⁶ NBO analysis⁷ was carried out to determine the atomic charges. SMD⁸ solvent models were used in all the calculations above. Basis set superposition errors (BSSE) were handled by a counterpoise procedure⁹ in all the binding energy calculations. Multiwfn was carried out to evaluate electrostatic potential,¹⁰ and VMD¹¹ was carried out to draw electrostatic potential maps. All the optimized structures were visualized with CYL view.⁹

Coordinates((M06-2X-D3/6-31G(d,p) (SMD, DCM)).

4-methoxy- α - Methylbenzyl alcohol

C	-0.51540800	1.15604800	0.12014500
C	0.85073300	1.34902500	0.24730300
C	1.73615400	0.28437700	0.05284900
C	1.23382800	-0.97510400	-0.27472900
C	-0.14359200	-1.15032400	-0.40278700
C	-1.03314700	-0.10016200	-0.20669700
H	-1.19513100	1.98782600	0.26429700
H	1.25949400	2.32265500	0.49504900
H	1.89431300	-1.81666200	-0.44012500
H	-0.52436000	-2.13303400	-0.66768700
O	3.05464600	0.57157900	0.19710300
C	3.98174900	-0.48332700	0.00738900
H	3.92019600	-0.88884600	-1.00679700
H	4.96694500	-0.04783900	0.16126400
H	3.82305800	-1.28623500	0.73339500
C	-2.52325500	-0.33584100	-0.29212000
H	-2.70990400	-1.08883500	-1.06938300
C	-3.08112200	-0.84527200	1.03366500
H	-2.90812900	-0.10353600	1.81794500
H	-4.15786700	-1.02505900	0.95394500
H	-2.60172900	-1.78196800	1.32657400
O	-3.14272800	0.89075600	-0.65598200
H	-4.09786900	0.76633200	-0.60754400

Bis-selenonium catalyst

Se	-1.55983700	-0.14358200	0.17780800
C	-1.24680500	-0.51861300	2.08613300
H	-2.11744300	-1.04990400	2.47024400
H	-0.39903000	-1.20800400	2.07432200
C	-0.95577500	0.79597100	2.80626700
H	-1.88110300	1.37329700	2.88867900
H	-0.64816600	0.55331500	3.82976100
C	0.10699600	1.68158000	2.13395200

H	-0.23753700	2.00036600	1.14251500
H	0.20636600	2.59823200	2.72310300
C	1.50577100	1.06897800	2.03809200
H	2.28312000	1.82307700	1.91522500
H	1.74332700	0.43732400	2.89752100
Se	1.71756800	-0.13116600	0.46782100
C	-1.96949100	-1.92531900	-0.43133100
C	-3.27819000	-2.36934600	-0.59069200
C	-0.85999600	-2.73042400	-0.70400200
C	-3.47758200	-3.67719500	-1.03561700
H	-4.12332500	-1.72243400	-0.38777500
C	-1.08109000	-4.03342900	-1.14471100
H	0.14852700	-2.34686700	-0.59411900
C	-2.38619700	-4.50469000	-1.30650400
H	-4.48836800	-4.04629800	-1.17080100
H	-0.23661900	-4.67763100	-1.36384300
H	-2.55257700	-5.51882000	-1.65295000
C	-3.22074700	0.80413100	0.21784800
C	-4.21927500	0.50813000	1.14828300
C	-3.36135600	1.82139400	-0.72902000
C	-5.39470700	1.25561000	1.11846600
H	-4.10672700	-0.28523500	1.87808800
C	-4.54552900	2.55727900	-0.74539800
H	-2.56736000	2.04004800	-1.43613400
C	-5.55571000	2.27518900	0.17579700
H	-6.18409200	1.04195800	1.83081800
H	-4.67511800	3.35021900	-1.47360400
H	-6.47380800	2.85247700	0.16073000
C	3.61918000	-0.47814900	0.47295100
C	4.10543500	-1.08710100	-0.68526000
C	4.44251300	-0.14217700	1.54378400
C	5.46690000	-1.36730400	-0.76574400
H	3.44924000	-1.33012700	-1.51514400
C	5.80464200	-0.43607500	1.44584000
H	4.06128700	0.32057100	2.44571000
C	6.31345400	-1.04209900	0.29742400
H	5.86486100	-1.83698100	-1.65854300
H	6.46326500	-0.18547900	2.27012400
H	7.37266500	-1.26475100	0.22976800
C	1.62729500	1.15693600	-0.94939800
C	2.47679600	2.26314900	-0.92404100
C	0.75806400	0.90920800	-2.01330000
C	2.40739200	3.17896000	-1.97108900
H	3.19432600	2.40375500	-0.12307400

C	0.70508800	1.83441600	-3.05595100
H	0.12796500	0.02802700	-2.03846100
C	1.51950300	2.96801400	-3.03008300
H	3.05494200	4.04895400	-1.96712400
H	0.04303900	1.65837200	-3.89699300
H	1.47600000	3.68180800	-3.84560100

Complex of bis-selenonium catalyst and 4-methoxy- α - Methylbenzyl alcohol

Se	1.16212700	0.41523300	-0.86323000
C	0.80099000	0.63697700	-2.80508000
H	1.76897400	0.77649600	-3.28490400
H	0.41875600	-0.35018600	-3.07047400
C	-0.18854300	1.76314800	-3.09542700
H	0.33543000	2.72203200	-3.08070300
H	-0.55548900	1.62234100	-4.11836900
C	-1.36127600	1.84590500	-2.11127600
H	-0.96813000	2.16872300	-1.13871800
H	-2.04653700	2.63816300	-2.41787300
C	-2.14525600	0.52824900	-1.95967300
H	-3.19407500	0.61249200	-2.24087700
H	-1.68850900	-0.31471800	-2.47375400
Se	-2.12296100	0.04529700	-0.05846700
C	2.85245300	-0.50319200	-1.07498000
C	3.99606600	-0.00957600	-0.45792500
C	2.84572200	-1.69322300	-1.80057600
C	5.18746200	-0.72016800	-0.60717800
H	3.97326400	0.90319900	0.12351000
C	4.04819200	-2.38068200	-1.95280200
H	1.92877400	-2.08994700	-2.21920000
C	5.21468400	-1.89583500	-1.35730200
H	6.08964700	-0.35387900	-0.13029200
H	4.07094700	-3.30075200	-2.52689800
H	6.14575400	-2.43977800	-1.47409100
C	1.76401100	2.18188100	-0.41928400
C	2.56095900	2.93427200	-1.28274200
C	1.37314300	2.66421700	0.83081700
C	2.95411700	4.21084500	-0.88565500
H	2.88602000	2.54082400	-2.23915800
C	1.77659800	3.94222500	1.21784700
H	0.78463600	2.04490300	1.49887700
C	2.56041300	4.71364000	0.35804500
H	3.57187500	4.81233000	-1.54371700
H	1.48538300	4.33171500	2.18743600
H	2.87329400	5.70743200	0.65965300
C	-3.41858400	-1.37579800	0.02873500

C	-3.87599400	-1.69695600	1.30722000
C	-3.80436500	-2.09163100	-1.10200900
C	-4.76360300	-2.76124500	1.45062400
H	-3.56438600	-1.12192400	2.17350000
C	-4.69431300	-3.15583900	-0.93971400
H	-3.45558300	-1.82828000	-2.09359400
C	-5.16799400	-3.49078800	0.32980500
H	-5.13706800	-3.01963100	2.43545300
H	-5.02052100	-3.71783000	-1.80823400
H	-5.85809800	-4.31927600	0.44620000
C	-3.20900600	1.51451500	0.54633100
C	-4.55227400	1.60978500	0.18314100
C	-2.57644300	2.48692800	1.31970000
C	-5.27904000	2.71491000	0.61794500
H	-5.03553000	0.83314600	-0.39979000
C	-3.31663400	3.59105200	1.74421000
H	-1.53136900	2.39040500	1.59341900
C	-4.66235500	3.70223400	1.39356300
H	-6.32728700	2.80752700	0.35514100
H	-2.84558900	4.35687800	2.35066700
H	-5.23723900	4.55819000	1.73013700
C	2.06163700	-3.01414400	0.96613100
C	3.17817600	-2.52889800	1.62649800
C	3.11529800	-1.31130600	2.32118900
C	1.89756200	-0.61743300	2.38770500
C	0.77816300	-1.14449700	1.74330400
C	0.84005100	-2.32355000	0.99466900
H	2.14839900	-3.94657500	0.42077000
H	4.12199500	-3.06011700	1.60296400
H	1.80789500	0.28911600	2.97250500
H	-0.16732700	-0.61630200	1.82391800
O	4.27126100	-0.88732800	2.87310100
C	4.26128500	0.31231000	3.64434500
H	3.96332600	1.17382800	3.03316800
H	3.59024200	0.22409200	4.50549900
H	5.28318500	0.45081800	3.99390500
C	-0.38146900	-2.79418800	0.24522200
C	-0.44507700	-4.28247300	-0.05279700
H	-1.40184300	-4.53522800	-0.52218000
H	0.36214000	-4.59493600	-0.72097500
H	-0.36855800	-4.85997600	0.87128000
O	-0.48087300	-2.03595200	-1.02744800
H	-0.94438700	-2.61748200	-1.64707800
H	-1.26571400	-2.51962400	0.82959700

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