Supporting Information

Controlling thiyl radical polymerization via *in situ* desulfurization

Huajuan Hu,[a,b] Ping Yi,[a,b] Jiayang He,[b] Derong Cao,*[,a] and Hanchu Huang*[,b]

[a]*State Key Laboratory of Luminescent Materials and Devices, School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China*

[b]*School of Materials Science and Engineering, Key Laboratory for Polymeric Composite and Functional Materials of Ministry of Education, Sun Yat-sen University, Guangzhou 510006, China*

*__Corresponding Email addresses__: huanghch9@mail.sysu.edu.cn; drcao@scut.edu.cn

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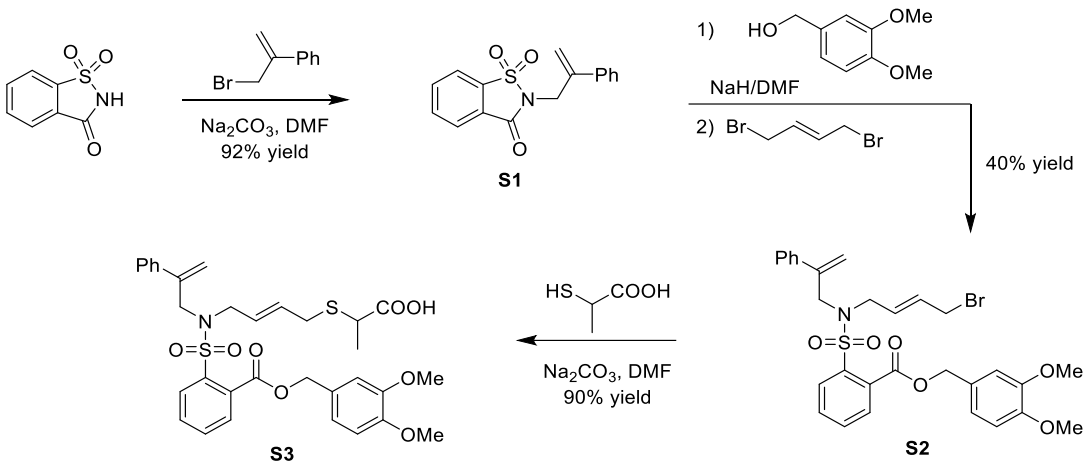
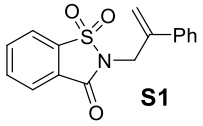
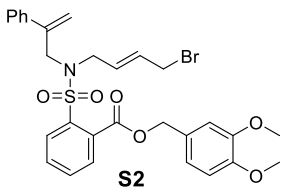
Scheme S1. Synthesis of trigger-testing compounds.





S1

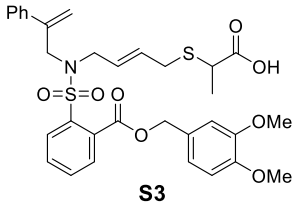
In a 250 mL flask, saccharin (10.99 g, 60 mmol) and (3-bromoprop-1-en-2-yl)benzene (17.74 g, 90 mmol) were dissolved in DMF (60 mL), then Na_2CO_3 (6.36 g, 60 mmol) was added to the mixture, which was heated at 80 °C for 12 hours. The reaction mixture was then poured into water (250 mL) with vigorous stirring. The heterogeneous mixture was filtered to give a crude product, which was then purified by washing with petroleum ether to afford **S1** as a white solid (16.52 g, 92% yield, CAS: 1465901-24-9). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 7.6 Hz, 1H), 7.89 (d, *J* = 7.0 Hz, 1H), 7.87–7.76 (m, 2H), 7.52 (d, *J* = 7.4 Hz, 2H), 7.39–7.27 (m, 3H), 5.47 (s, 1H), 4.83 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.9, 141.4, 138.1, 138.0, 134.9, 134.4, 128.6, 128.3, 127.2, 126.5, 125.4, 121.1, 116.5, 42.8.



S2

In a 250 mL flask, veratryl alcohol (5.55 g, 33 mmol) was dissolved in DMF (30 mL), the mixture was cooled at 0 °C, then NaH (1.58 g，39.6 mmol) was dissolved in DMF (3 mL) and slowly added, the reaction was stirred for 30 min. Compound **S1** (9.88 g，33 mmol) was then added to the mixture and stirred for 20 min at room temperature. The mixture was added dropwise to a DMF (10 mL) solution of *trans*-1,4-dibromo-2-butene (10.59 g，49.5 mmol) and stirred for 40 min at room temperature. The reaction was poured into water (250 mL) and extracted with ethyl acetate (3×100 mL). The organic layer was washed with brine (3×100 mL), dried over Na_2SO_4, and concentrated *in vacuo*. The crude product was purified by flash column chromatography to afford **S2** as a yellowish oil (7.93 g, 40% yield, CAS: 2969136-30-7). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.59–7.53 (t, *J* = 7.5 Hz, 1H), 7.50–7.44 (m, 2H), 7.37–7.32 (m, 2H), 7.30–7.25 (m, 3H), 7.04–

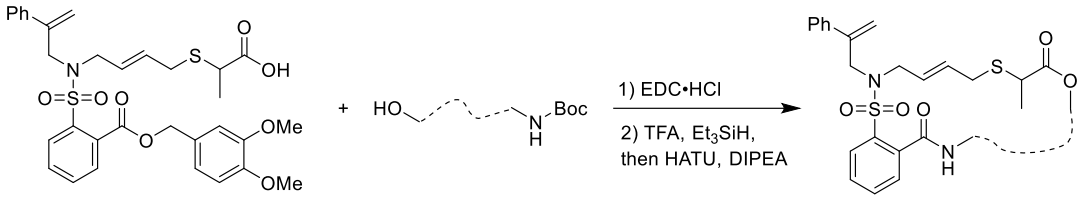
6.96 (m, 2H), 6.82 (d, *J* = 8.1 Hz, 1H), 5.77–5.67 (m, 1H), 5.53 – 5.40 (m, 2H), 5.32 (s, 2H), 5.24 (s, 1H), 4.33 (s, 2H), 3.89–3.77 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 149.4, 149.2, 142.6, 138.6, 138.0, 133.2, 132.4, 130.8, 130.5, 129.5, 129.0, 128.6, 128.5, 128.2, 127.7, 126.6, 121.7, 116.5, 112.3, 111.0, 68.5, 56.1, 56.0, 50.5, 47.5, 31.5.



S3

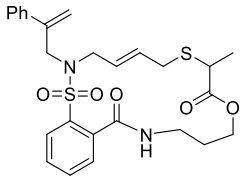
In a 250 mL flask, the reaction mixture of **S2** (6.61 g, 11 mmol), 2-mercaptopropionic acid (1.2 mL, 13.2 mmol), and K_2CO_3 (1.82 g, 13.2 mmol) in DMF (50 mL) was stirred at room temperature for 24 h. After the reaction, the mixture was poured into water (200 mL) and extracted with ethyl acetate (3×100 mL). The organic layer was washed with brine (3×100 mL), dried over Na_2SO_4, and concentrated *in vacuo* to afford the **S3** as a yellowish oil (6.19 g, 90% yield, CAS: 2969136-36-3). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.51–7.44 (m, 2H), 7.37–7.31 (m, 2H), 7.29–7.25 (m, 3H), 7.04–6.95 (m, 2H), 6.81 (d, *J* = 8.2 Hz, 1H), 5.56–5.47 (m, 1H), 5.43 (s, 1H), 5.39–5.28 (m, 3H), 5.23 (s, 1H), 4.39–4.26 (m, 2H), 3.90–3.80 (m, 8H), 3.28–3.18 (m, 2H), 3.12–3..03 (m, 1H), 1.37 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 178.1, 168.2, 149.4, 149.1, 142.6, 138.6, 138.1, 133.1, 132.4, 130.4, 130.3, 129.0, 128.6, 128.5, 128.1, 127.8, 127.7, 126.5, 121.7, 116.2, 112.3, 111.0, 68.6, 56.1, 56.0, 50.2, 47.8, 39.7, 33.3, 16.7.

Scheme S2. General procedure for the synthesis of monomers.



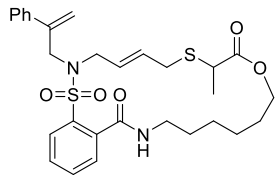
S3 **1-3**

Following a slightly modified procedure,[1,2] in a 250 mL flask, **S3** (1.0 eq.) and *N*-Boc-protected amine alcohol (1.5 eq.) were dissolved in dry DCM (50 mL). To this solution were added *N*-ethyl-*N*'-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC•HCl, 1.5 eq.) and 4-dimethylaminopyridine (DMAP, 0.05 eq.). After stirring at room temperature for 14 h, the reaction mixture was diluted with DCM (100 mL), washed with 1 M HCl (2×50 mL) and brine (50 mL), dried by Na_2SO_4, filtered, and concentrated *in vacuo* to afford a yellow oil, which was then directly subjected to the subsequent reaction. The yellow oil (1.0 eq.) was dissolved in DCM (50 mL). To this solution, triethylsilane (10 eq.) was added via a syringe, followed by the addition of trifluoroacetic acid (TFA, 13.0 eq.). After stirring at room temperature for 2 h, the reaction mixture was diluted with toluene (50 mL) and concentrated *in vacuo* to give the intermediated amino acid, which was directly dissolved in DMF (1500 mL). 1-[Bis(dimethylamino)methylene]-1*H*-1,2,3-triazolo[4,5-*b*]pyridinium 3-oxide hexafluorophosphate (HATU, 2.0 eq) was then added to the reaction mixture at room temperature. The mixture was stirred for 30 min, and diisopropylethylamine (DIPEA, 5.0 eq.) was slowly added. After stirring for an additional 36 h at room temperature, the reaction mixture was concentrated *in vacuo* and diluted with ethyl acetate (150 mL). The organic layer was washed with 1 M HCl (3×50 mL), 0.5 M NaOH (2×50 mL), and brine (50 mL) and dried over Na_2SO_4. The filtrate was concentrated and purified by column chromatography to afford the monomers.



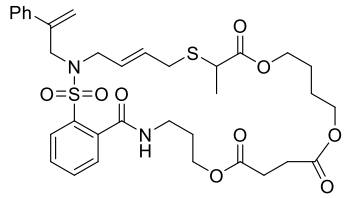
1

Following the general procedure, the reaction of **S3** (6.26 g, 10 mmol) and *tert*-Butyl (3-hydroxypropyl)carbamate (2.63 g, 15 mmol) afforded macrocyclic monomer **1** as a white solid (2.06 g, 40 % yield, CAS: 2969136-45-4). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.0 Hz, 2H), 7.30–7.21 (m, 5H), 6.17 (t, *J* = 5.8 Hz, 1H), 5.53–5.42 (m, 1H), 5.39 (s, 1H), 5.36–5.27 (m, 1H), 5.20 (s, 1H), 4.38 – 4.20 (m, 3H), 4.18–4.10 (m, 1H), 3.99–3.90 (m, 1H), 3.74–3.57 (m, 2H), 3.48–3.34 (m, 2H), 3.22–3.13 (m, 1H), 3.06–2.97 (m, 1H), 2.01–1.85 (m, 2H), 1.40 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.0, 168.3, 142.7, 138.6, 136.9, 136.8, 132.8, 130.0, 129.7, 129.6, 129.6, 128.6, 128.3, 128.2, 126.6, 116.9, 63.2, 52.6, 47.8, 40.9, 37.1, 33.0, 28.3, 17.3.



2

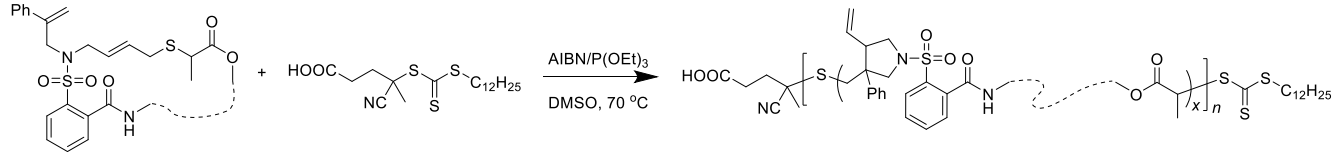
Following the general procedure, the reaction of **S3** (6.26 g, 10 mmol) and *tert*-Butyl (6-hydroxyhexyl)carbamate (3.26 g, 15 mmol) afforded macrocyclic monomer **2** as a white solid (2.62 g, 47% yield, CAS: 2969136-48-7). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.26–7.21 (m, 5H), 5.91–5.81 (m, 1H), 5.67 – 5.49 (m, 2H), 5.36 (s, 1H), 5.18 (s, 1H), 4.32–4.22 (m, 2H), 4.21–4.14 (m, 1H), 4.13–4.06 (m, 1H), 3.95–3.87 (m, 1H), 3.82–3.75 (m, 1H), 3.55–3.45 (m, 1H), 3.41–3.23 (m, 3H), 3.12–3.04 (m, 1H), 1.77–1.45 (m, 8H), 1.39 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.9, 168.6, 142.4, 138.8, 137.2, 136.9, 132.5, 130.5, 129.6, 129.3, 129.2, 129.1, 128.5, 128.1, 126.5, 116.7, 65.5, 50.7, 48.0, 39.7, 39.6, 33.5, 28.7, 28.4, 25.6, 25.5, 17.2.



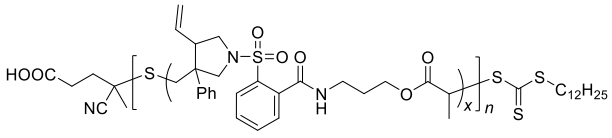
3

Following the general procedure, the reaction of **S3** (6.26 g, 10 mmol) and 3-((tert-butoxycarbonyl)amino)propyl (4-hydroxybutyl) succinate (5.21 g, 15 mmol) afforded macrocyclic monomer **3** as a yellowish oil (1.92 g, 28% yield, CAS: 2969136-54-5). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.9 Hz, 1H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.26–7.20 (m, 5H), 6.08 (t, *J* = 5.9 Hz, 1H), 5.59–5.44 (m, 2H), 5.40 (s, 1H), 5.24 (s, 1H), 4.35–4.24 (m, 2H), 4.23–4.11 (m, 6H), 3.81 (d, *J* = 5.6 Hz, 2H), 3.45 (q, *J* = 6.6 Hz, 2H), 3.31 (q, *J* = 7.1 Hz, 1H), 3.27–3.20 (m, 1H), 3.11–3.05 (m, 1H), 2.63 (s, 4H), 1.91 (p, *J* = 6.5 Hz, 2H), 1.77–1.69 (m, 4H), 1.36 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.5, 172.3, 172.2, 168.2, 142.6, 138.8, 137.2, 136.6, 132.6, 130.5, 129.7, 129.5, 129.0, 128.6, 128.3, 128.2, 126.5, 116.9, 64.8, 64.4, 62.1, 50.2, 47.9, 39.7, 37.1, 33.4, 29.7, 29.6, 28.5, 25.4, 25.4, 17.0.

Scheme S3. General procedure for controlled radical polymerization.



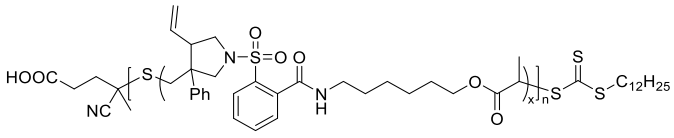
All polymerization reactions were performed under a nitrogen atmosphere using a standard Schlenk technique. The stock solution 4-cyano-4-(((dodecylthio)carbonothioyl)thio)pentanoic acid (**CTA1**) and stock solution of AIBN were prepared in degassed DMSO at 0.04 M and 0.04 M, respectively. A typical procedure for the preparation of **P1** is given below as an example. A 10 mL Schlenk vial equipped with a stir bar was charged with macrocyclic monomer **1** (0.1 mmol), followed by the stock solution of **CTA1** (0.04 M, 125 μL), AIBN (0.04 M, 125 μL), triethyl phosphite (0.12 mmol) and DMSO (750 μL). The vial was sealed. The solution was deoxygenated via three freeze-pump-thaw cycles, backfilled with nitrogen, and then heated at 70 °C for a given time. After the reaction, the vial was cooled by the ice bath and opened to air to stop the polymerization. The reaction mixture was diluted with a minimum amount of DCM and precipitated in diethyl ether. The obtained solid was re-dissolved with a minimum amount of DCM for further precipitation, yielding the polymer that was then characterized using SEC and NMR.



P1

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.79 (m, 1H), 7.67–7.41 (m, 3H), 7.32–7.01 (m, 5H), 6.85–6.58 (m, 1H), 5.88–5.65 (m, 1H), 5.23–4.86 (m, 2H), 4.28–3.92 (m, 1H), 3.92–3.61 (m, 1H), 3.61–3.17 (m, 4H), 3.13–2.61 (m, 2H), 2.36–1.77 (m, 3H), 1.76–1.34 (m, 2H), 1.34–1.00 (m, 2H), 0.88 (d, *J* = 27.2 Hz, 2H).

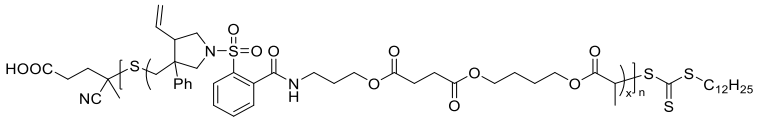
^{13}C NMR (100 MHz, $CDCl_3$): δ 176.9, 176.8, 176.5, 168.7, 142.6, 142.1, 136.8, 135.5, 135.0, 134.5, 132.7, 129.8, 129.3, 128.6, 128.2, 128.0, 127.9, 127.0, 126.9, 126.6, 119.1, 118.6, 118.3, 62.3, 61.8, 54.4, 53.7, 52.4, 52.2, 51.9, 50.8, 42.2, 41.0, 38.8, 37.1, 36.7, 36.6, 36.6, 36.3, 32.0, 30.1, 29.8, 28.1, 22.8, 19.8, 19.6, 19.1, 16.9, 14.2.



P2

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02–7.70 (m, 1H), 7.66–7.40 (m, 3H), 7.38–7.05 (m, 5H), 6.47–6.13 (m, 1H), 5.91–5.62 (m, 1H), 5.24–4.89 (m, 2H), 4.15–3.94 (m, 1H), 3.94–3.79 (m, 1H), 3.78–3.49 (m, 1H), 3.49–3.21 (m, 4H), 3.19–2.65 (m, 2H), 2.25–2.01 (m, 1H), 1.70–1.49 (m, 4H), 1.49–1.04 (m, 7H), 1.02–0.80 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 176.7, 176.6, 176.2, 172.9, 168.2, 142.5, 141.9, 136.8, 135.6, 135.4, 135.0, 134.9, 134.4, 133.8, 132.7, 129.7, 129.6, 128.9, 128.5, 128.4, 128.3, 128.2, 128.1, 127.9, 127.8, 127.1, 126.9, 126.8, 126.7, 126.6, 126.5, 119.3, 118.9, 118.3, 65.8, 65.0, 64.5, 64.2, 64.1, 56.0, 55.7, 55.1, 54.8, 54.4, 54.0, 53.8, 53.2, 53.0, 52.7, 52.5, 52.3, 52.2, 51.9, 51.0, 50.8, 50.4, 49.9, 42.1, 41.4, 40.9, 40.4, 40.3, 39.8, 38.6, 36.7, 36.6, 36.5, 36.2, 31.9, 29.6, 29.3, 29.1, 28.4, 28.3, 28.2, 26.6, 25.6, 25.5, 22.7, 19.7, 19.7, 19.4, 18.9, 16.9, 15.3.

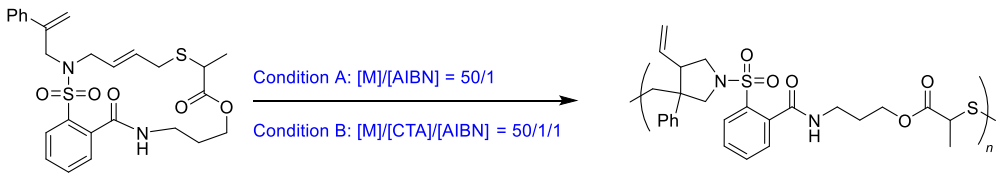


P3

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03–7.75 (m, 1H), 7.64–7.42 (m, 3H), 7.38–7.06 (m, 5H), 6.60–6.37 (m, 1H), 5.89–5.65 (m, 1H), 5.24–4.90 (m, 2H), 4.23 (s, 2H), 4.11–3.94 (m, 3H), 3.94–3.81 (m, 1H), 3.71–3.22 (m, 5H), 3.20–2.96 (m, 1H), 2.96–2.73 (m, 1H), 2.73–2.50 (m, 1H), 2.40–2.02 (m, 2H), 2.02–1.83 (m, 4H), 1.78–1.56 (m, 3H), 1.55–1.35 (m, 2H), 1.34–1.11 (m, 2H), 1.00–0.82 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 176.6, 176.3, 172.7, 172.5, 168.6, 168.6, 142.6, 142.1, 138.7, 138.2, 136.8, 135.7, 135.5, 135.1, 134.6, 133.9, 132.8, 132.6, 129.8, 129.4, 129.2, 129.0, 128.6, 128.4, 128.3, 128.2, 128.0, 127.9, 127.3, 127.0, 126.9, 126.8, 126.6, 119.0, 118.5, 118.4, 64.6, 64.4, 64.3, 64.1, 63.6, 62.4, 55.7, 54.5, 54.3, 54.0, 53.8, 53.6, 53.2, 52.8, 52.4, 52.2, 52.2, 51.9, 50.8, 50.5, 50.0, 42.1, 41.0, 39.8, 38.7, 37.1, 36.8, 36.5, 36.3, 29.1, 28.3, 25.3, 25.2, 25.1, 25.0, 19.8, 19.5, 19.1, 17.0.

Scheme S4. Effect of RAFT reagent on the polymerization of monomer **1**.



Two 5 mL vials were charged with monomer **1** (51.5 mg, 0.1 mmol), respectively. One vial (condition A) was added DMSO (950 μL) and AIBN (0.04 M in DMSO, 50 μL); the other vial (condition B) was added DMSO (900 μL), **CTA1** (0.04 M in DMSO, 50 μL) and AIBN (0.04 M in DMSO, 50 μL). The vials were sealed. The solution was deoxygenated via three freeze-pump-thaw cycles, backfilled with nitrogen, and then heated at 70 °C for 48 h. After the reaction, the vials were cooled and opened to air to stop the polymerization. The monomer conversion was determined by ^{1}H NMR analysis of the crude reaction mixture (condition A: 88%, condition B: 85%). Next, the reaction mixture was diluted with a minimum amount of DCM and precipitated in diethyl ether. The resulting solid was re-dissolved with a minimum amount of DCM for further precipitation. The obtained polymers were then characterized using SEC. Condition A: M_n = 12600, $Đ$ =1.73; Condition B: M_n = 10400, $Đ$ =1.64.

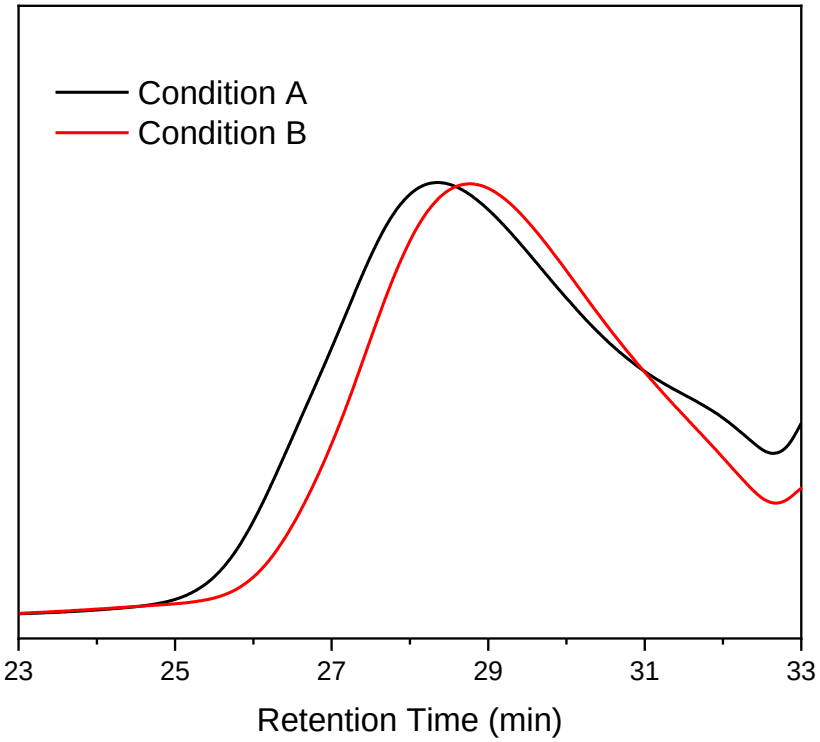
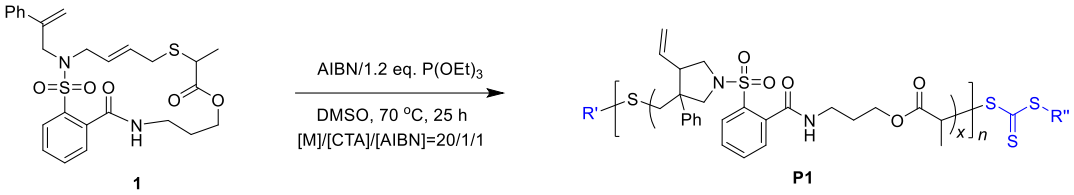
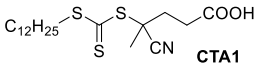
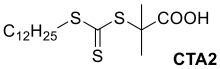
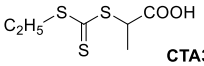
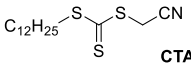


Figure S1. SEC traces showed that the RAFT reagent could not directly control the polymerization of monomer **1**.

Table S1. Effect of different CTAs on the polymerization of monomer **1**.



1 **P1**

Entry	CTA[a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	 **CTA1**	80%	8400	7900	1.42
2	 **CTA2**	80%	8300	6700	1.38
3	 **CTA3**	81%	8300	6600	1.42
4	 **CTA4**	81%	8400	6700	1.39

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index ($Đ$) were determined by SEC analysis calibrated to polystyrene standards.

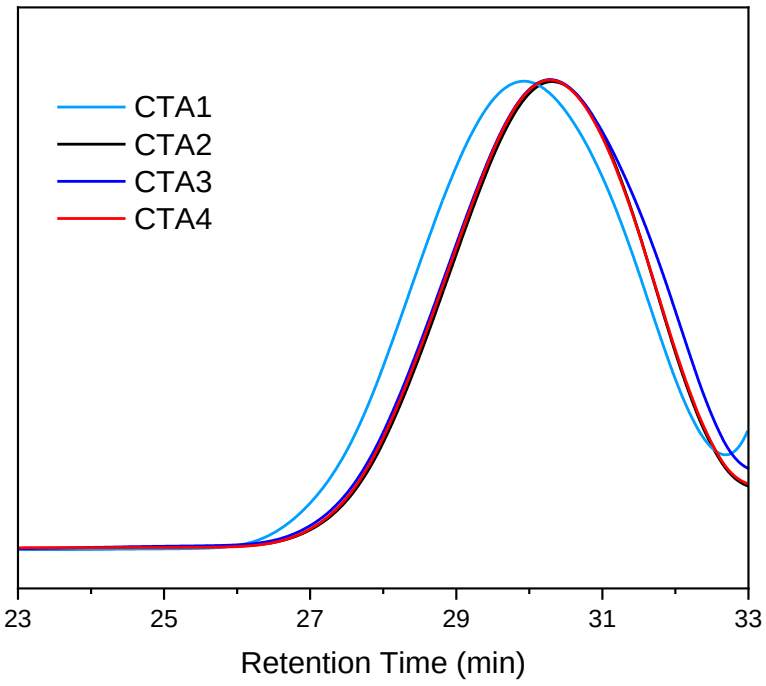
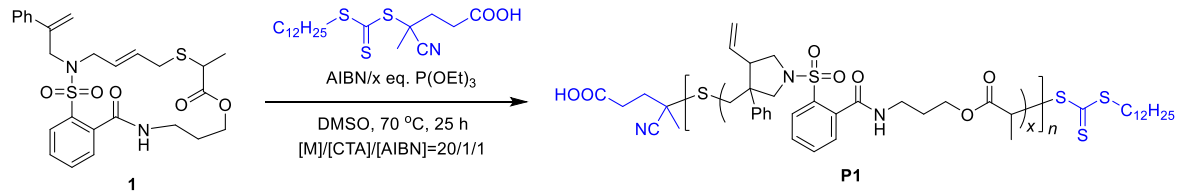


Figure S2. SEC traces for the polymerization of monomer **1** in the presence of different CTAs.

Table S2. Effect of different amounts of $P(OEt)_3$ on the polymerization of monomer **1**.



Entry	Equivalent of $P(OEt)_3$[a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	0.8 eq.	84%	8800	7700	1.40
2[e]	1.2 eq.	80%	8400	7900	1.42
3	1.5 eq.	79%	8300	7600	1.44

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x $MW^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, $MW^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index (*Đ*) were determined by SEC analysis calibrated to polystyrene standards. [e] Data taken from Table S1, entry 1.

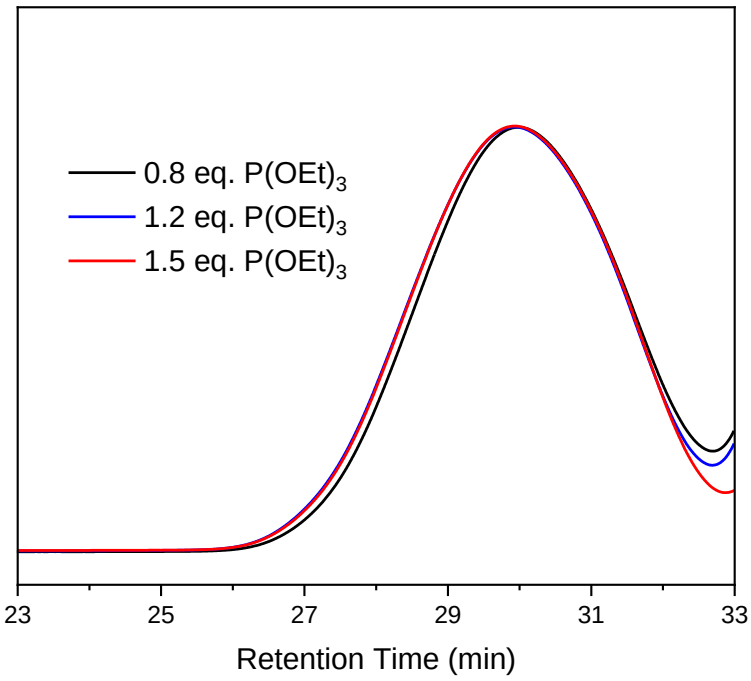
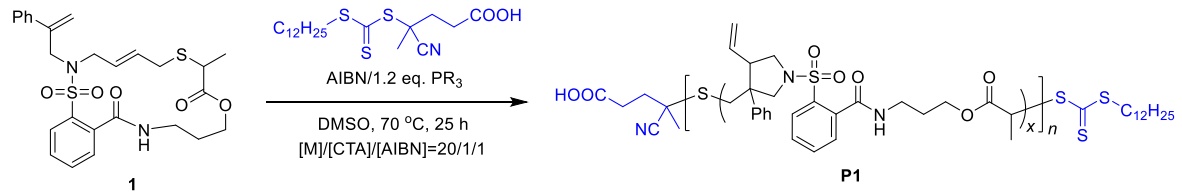


Figure S3. SEC traces for the polymerization of monomer **1** at different amounts of $P(OEt)_3$.

Table S3. Effect of different trivalent phosphorus on the polymerization of monomer **1**.



Entry	Equivalent of PR_3[a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1[e]	$P(OEt)_3$	80%	8400	7900	1.42
2	PPh_3	82%	8600	6300	1.43
3	PPh_2Pr	78%	8200	6800	1.44
4	$PPhMe_2$	67%	7100	6500	1.36

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x $MW^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, $MW^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index (*Đ*) were determined by SEC analysis calibrated to polystyrene standards. [e] Data taken from Table S1, entry 1.

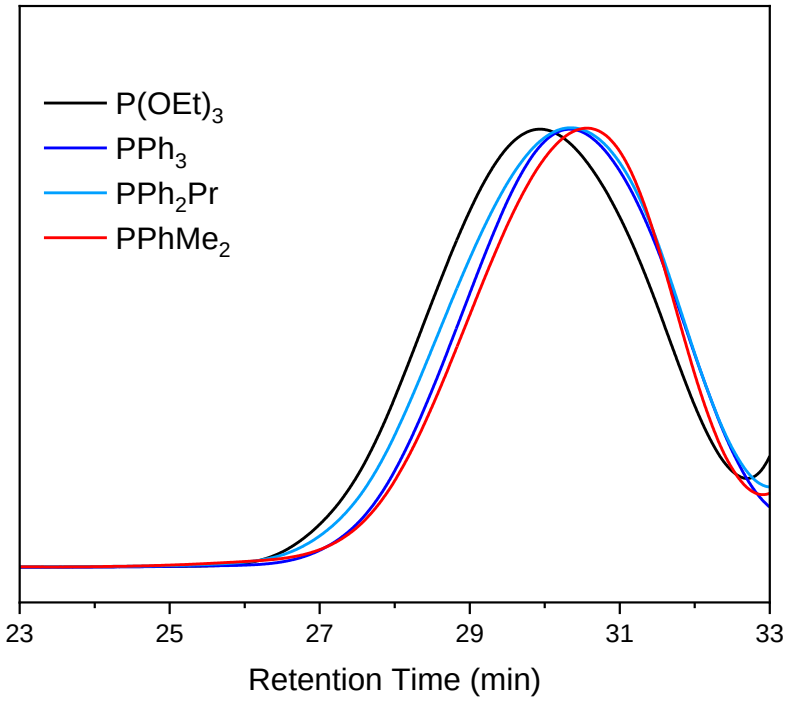
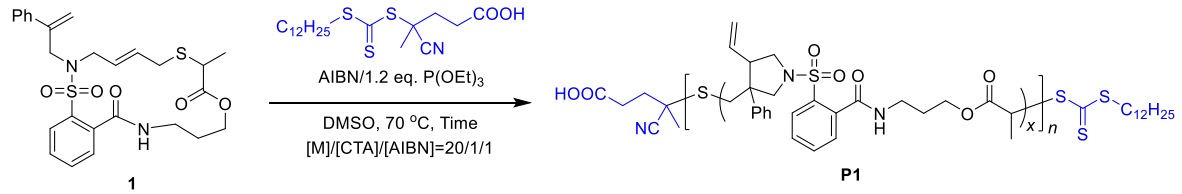


Figure S4. SEC traces for the polymerization of monomer **1** with different trivalent phosphorus.

Table S4. Effect of different reaction time on the polymerization of monomer **1**.



Entry	Time[a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	9 h	77%	8100	7700	1.39
2	12 h	79%	8300	7800	1.41
3	15 h	83%	8700	8200	1.46
4[e]	25 h	80%	8400	7900	1.42

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index ($Đ$) were determined by SEC analysis calibrated to polystyrene standards. [e] Data taken from Table S1, entry 1.

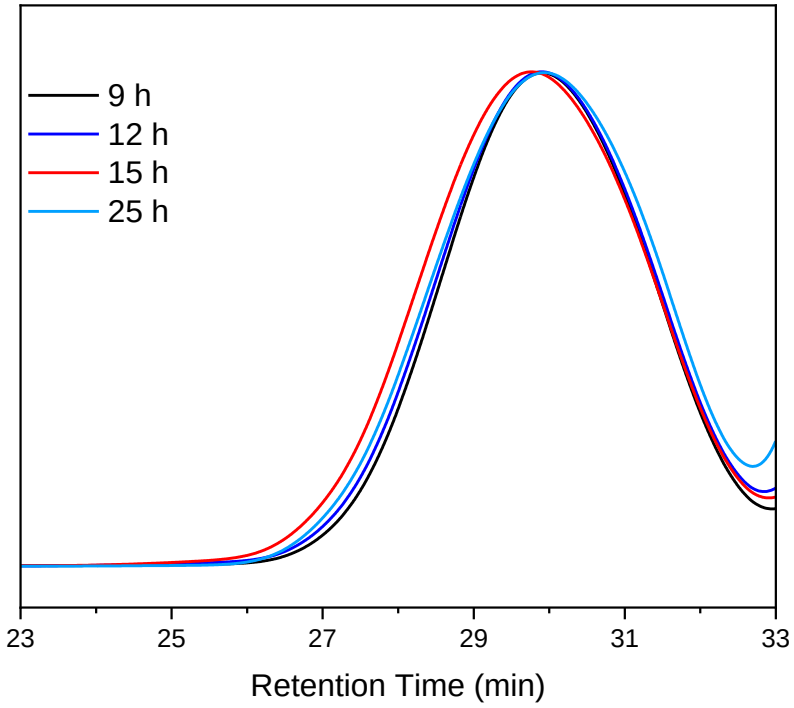
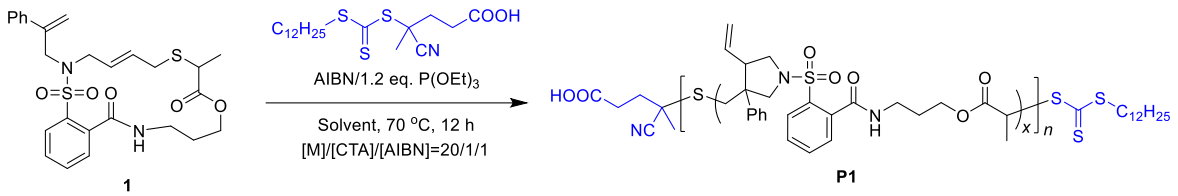


Figure S5. SEC traces for the polymerization of monomer **1** at different reaction time.

Table S5. Effect of different solvents on the polymerization of monomer **1**.



Entry	Solvents[a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1[e]	DMSO	79%	8300	7800	1.41
2	DMF	62%	6600	6000	1.40
3	Toluene	<5%	/	/	/
4	Dioxane	68%	7200	7900	1.40
5	THF	57%	6100	5900	1.33

[a] Experimental conditions: [**M**] = 0.1 M at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index (*Đ*) were determined by SEC analysis calibrated to polystyrene standards. [e] Data taken from Table S4, entry 2.

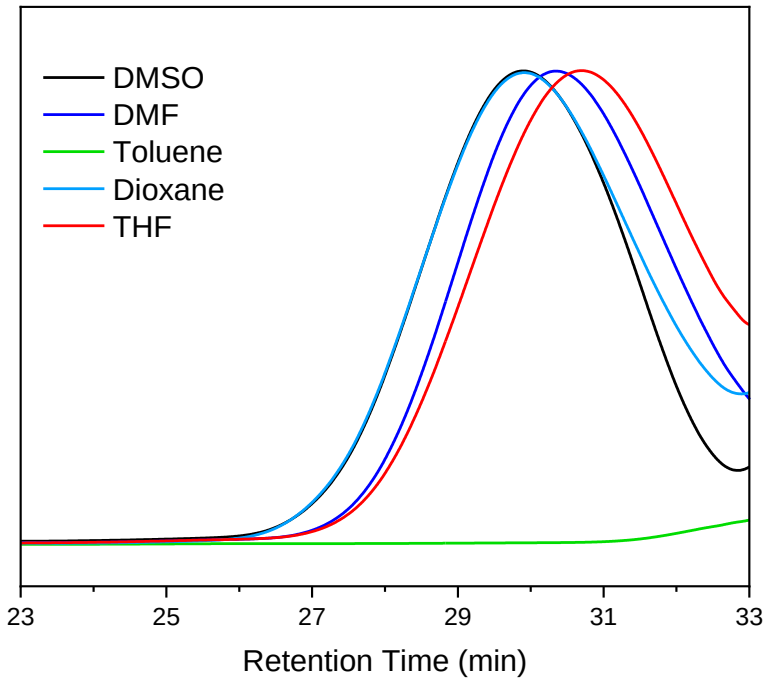
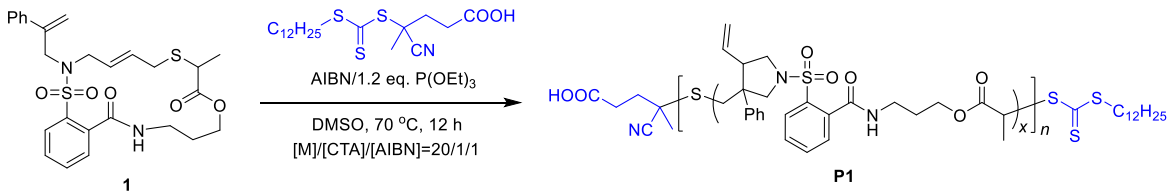


Figure S6. SEC traces for the polymerization of monomer **1** in different solvents.

Table S6. Effect of different concentrations on the polymerization of monomer **1**.



Entry	Monomer concentration[a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	0.05 M	58%	6200	6100	1.20
2[e]	0.1 M	79%	8300	7800	1.41
3	0.2 M	94%	9800	11100	1.63

[a] Experimental conditions: carried out in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index ($Đ$) were determined by SEC analysis calibrated to polystyrene standards. [e] Data taken from Table S4, entry 2.

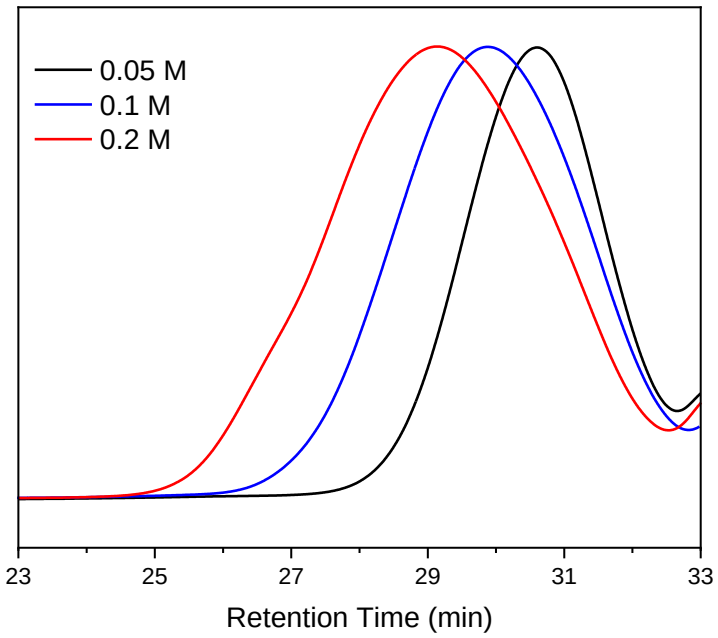
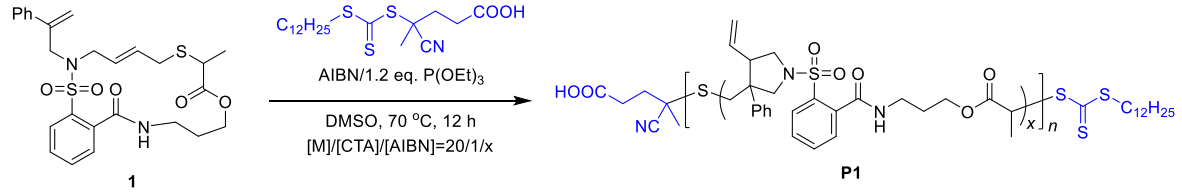


Figure S7. SEC traces for the polymerization of monomer **1** at different concentrations.

Table S7. Effect of different amount of AIBN on the polymerization of monomer **1**.



Entry	[M]/[CTA]/[AIBN][a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1[e]	20/1/1	79%	8300	7800	1.41
2	20/1/0.5	63%	6700	8100	1.32
3	20/1/0.3	50%	5400	8100	1.27
4	20/1/0.1	37%	4100	6300	1.17

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index ($Đ$) were determined by SEC analysis calibrated to polystyrene standards. [e] Data taken from Table S4, entry 2.

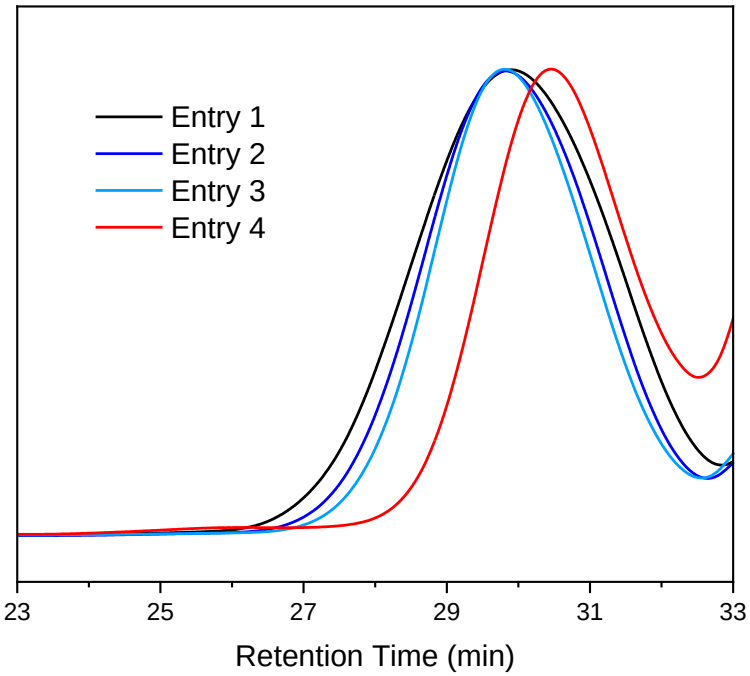
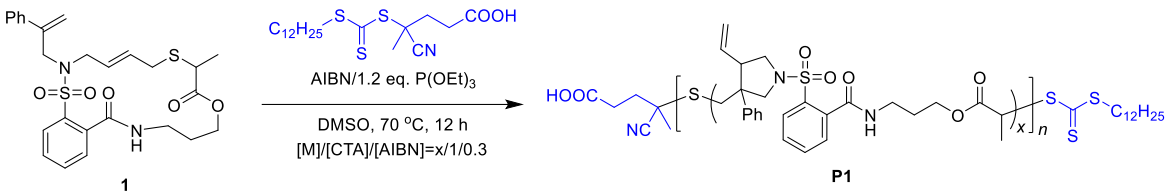


Figure S8. SEC traces for the polymerization of monomer **1** at different amount of AIBN.

Table S8. Polymerization of monomer **1** at different monomer/CTA ratios.



Entry	[M]/[CTA]/[AIBN][a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	10/1/0.3	69%	3800	6100	1.22
2[e]	20/1/0.3	50%	5400	8100	1.27
3	50/1/0.3	36%	9400	9000	1.33
4[f]	50/1/0.3	46%	11900	9900	1.40
5	100/1/0.3	29%	14900	9300	1.37
6[f]	100/1/0.5	41%	21500	13500	1.54

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index ($Đ$) were determined by SEC analysis calibrated to polystyrene standards. [e] Data taken from Table S7, entry 3. [f] 24 h.

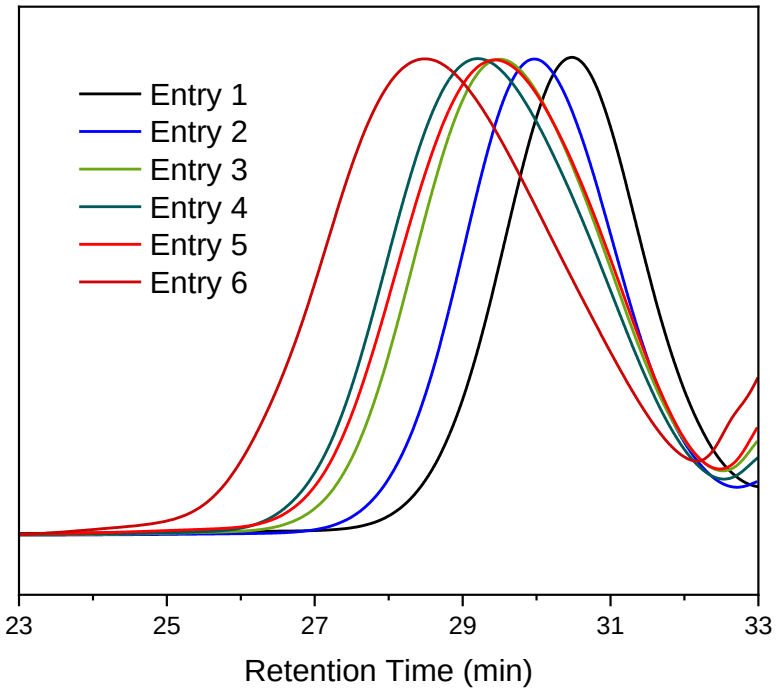
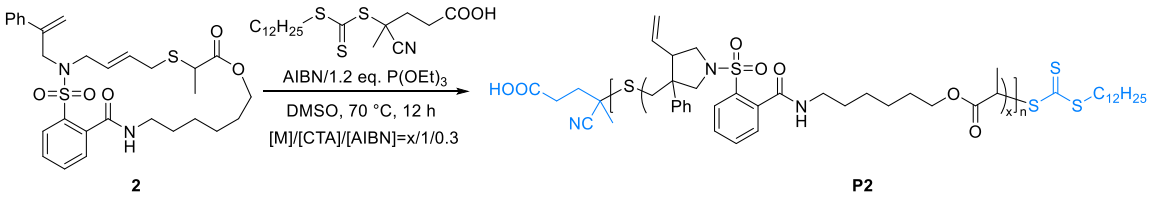


Figure S9. SEC traces for the polymerization of monomer **1** at different monomer/CTA ratios.

Table S9. Polymerization of monomer **2** at different monomer/CTA ratios.



2 **P2**

Entry	[M]/[CTA][a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	10/1	65%	4000	8000	1.26
2	20/1	55%	6500	10400	1.33
3	50/1	32%	9300	13600	1.38
4	100/1	23%	13200	14700	1.48

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index (*Đ*) were determined by SEC analysis calibrated to polystyrene standards.

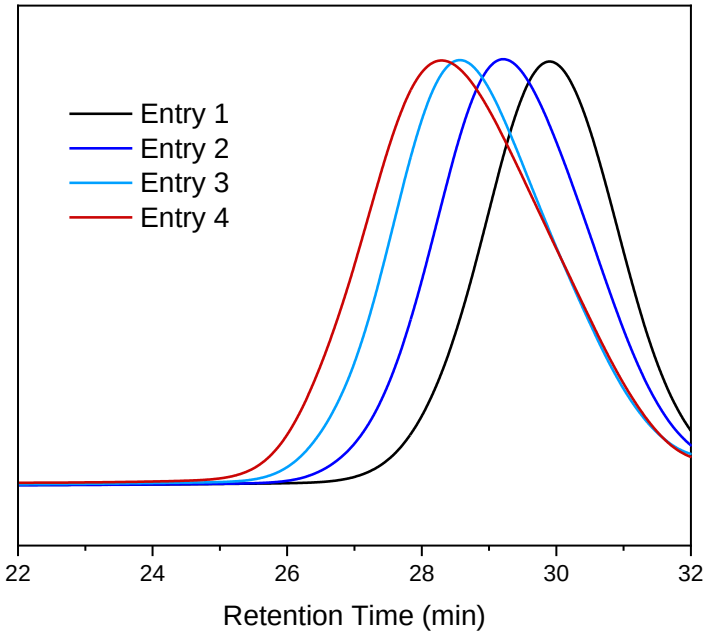
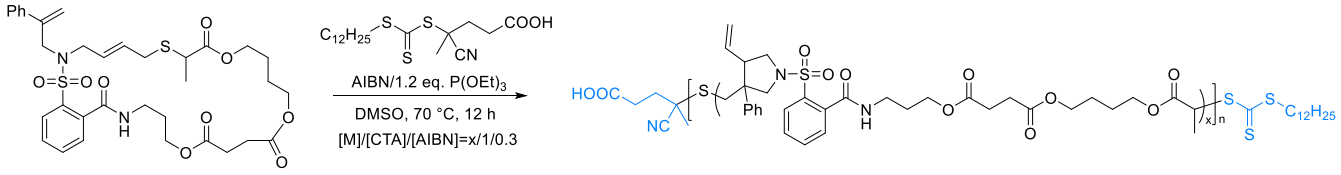


Figure S10. SEC traces for the polymerization of monomer **2** at different monomer/CTA ratios.

Table S10. Polymerization of monomer **3** at different monomer/CTA ratios.



3 **P3**

Entry	[M]/[CTA][a]	Conversion[b]	$M_{n\ (Theo)}$[c]	$M_{n\ (SEC)}$[d]	$Đ$[d]
1	10/1	77%	5600	11200	1.30
2	20/1	61%	8600	14300	1.39
3	50/1	49%	16800	17900	1.42
4	100/1	42%	28600	18300	1.49
5[e]	100/1	47%	32000	18100	1.55

[a] Experimental conditions: [**M**] = 0.1 M in DMSO at 70 °C under a nitrogen atmosphere unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Theoretical molecular weight was calculated using the following equation: $M_{n\ theo}$= ([M]$_0$/[CTA]$_0$) x MW$^{M'}$ x conversion + MW^{CTA}, where [M]$_0$, [CTA]$_0$, MW$^{M'}$ and MW^{CTA} correspond to initial monomer concentration, initial CTA concentration, average molar mass of the monomer and desulfurization unit, and molar mass of CTA, respectively. [d] Molecular weight and polydispersity index ($Đ$) were determined by SEC analysis calibrated to polystyrene standards. [e] 24 h.

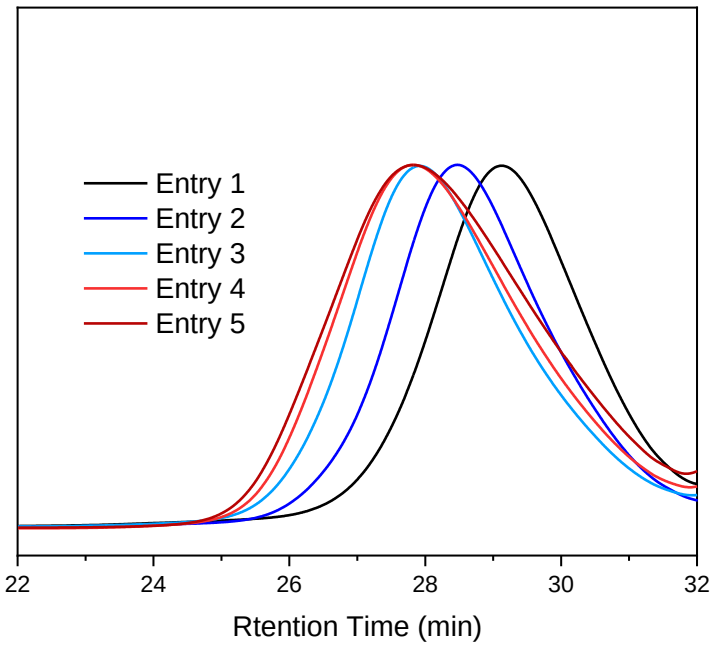


Figure S11. SEC traces for the polymerization of monomer **3** at different monomer/CTA ratios.

Scheme S5. Kinetic study of polymerization of monomer **1**.

A 10 mL vial was charged with macrocyclic monomer **1** (257.3 mg, 0.5 mmol), followed by followed by the addition of **CTA1** (0.04 M in DMSO, 625 μL, 25 μmol), AIBN (0.01 M in DMSO, 750 μL, 7.5 μmol), $P(OEt)_3$ (0.6 mmol) and DMSO (3.625 mL).The solution was divided into five Schlenk vials. The vials were sealed. The solution was deoxygenated via three freeze-pump-thaw cycles, backfilled with nitrogen. Five identical reactions were carried out in parallel at 70 °C and stopped at different reaction times (t = 3, 4, 5, 7, 9 h). The vial was cooled and opened to air to stop the polymerization. The monomer conversion was determined by ^{1}H NMR analysis of the crude reaction mixture. The reaction mixture was diluted with a minimum amount of DCM and precipitated with hexane twice, yielding the polymer **P1**. The resulting polymer was then characterized using SEC to determine its molecular weight and dispersity.

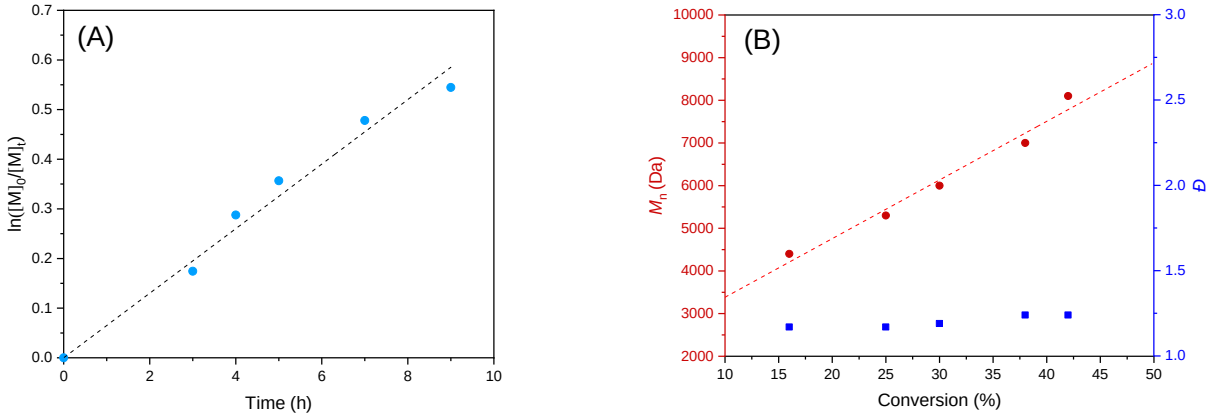


Figure S12. (A) Plot of $\ln([M]_0/[M]_t)$ versus time. (B) Plots of M_n and $Đ$ versus monomer conversion.

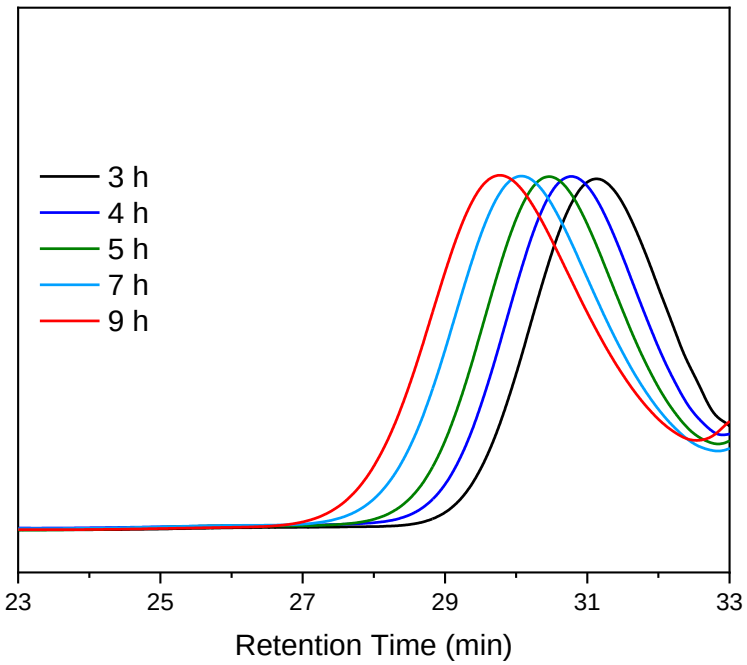


Figure S13. SEC traces for the kinetic study of the polymerization of monomer **1**.

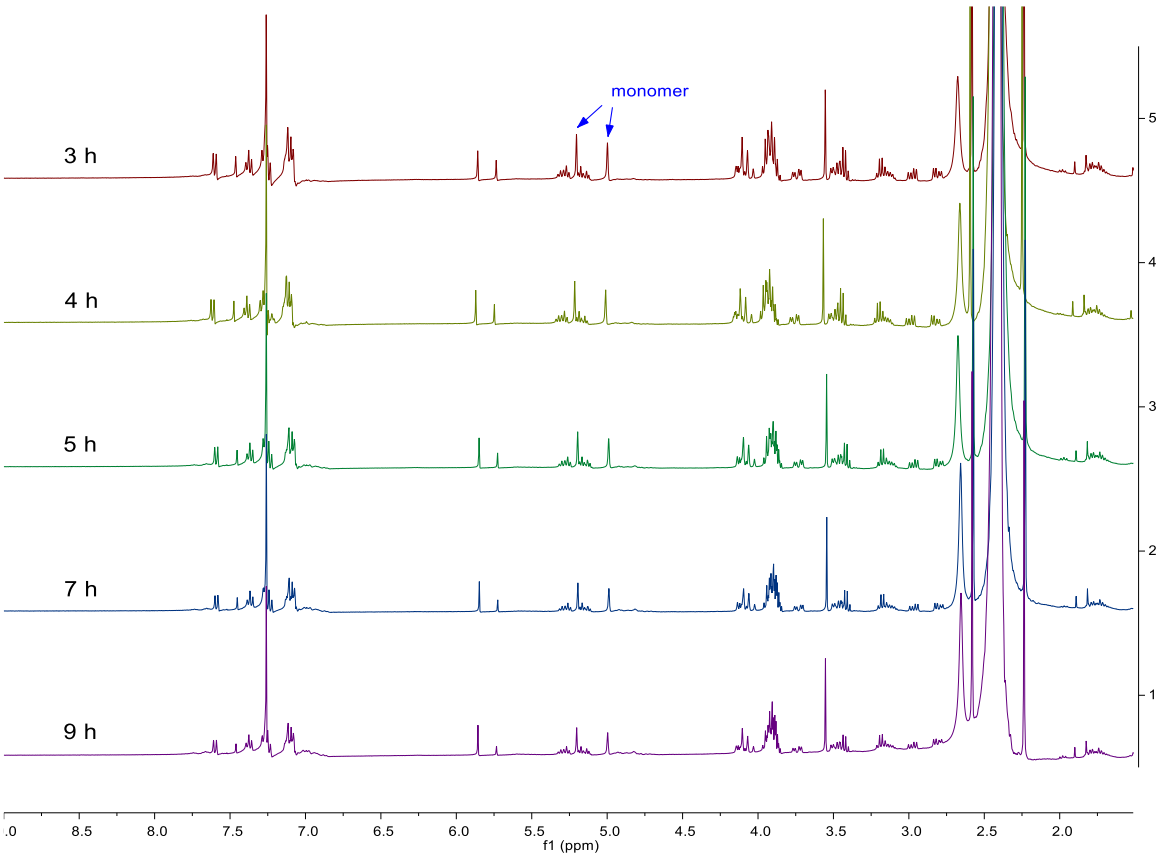
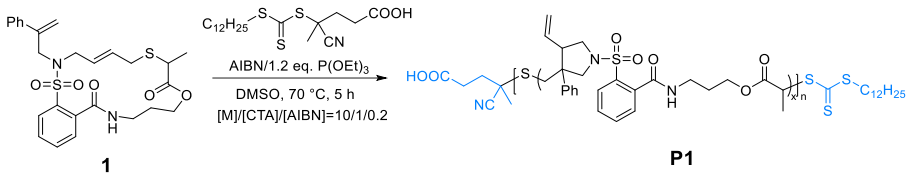


Figure S14. NMR traces for the kinetic study of the polymerization of monomer **1**.

Scheme S6. Polymer synthesis for MALDI-TOF analysis.



Following the general polymerization procedure, a 10 mL Schlenk vial was charged with macrocyclic monomer **1** (51.5 mg, 0.1 mmol), followed by the addition of **CTA1** (0.04 M in DMSO, 250 μL, 10 μmol), AIBN (0.01 M in DMSO, 200 μL, 2 μmol), $P(OEt)_3$ (0.12 mmol) and DMSO (550 μL). The vial was sealed, and the solution was deoxygenated via three freeze-pump-thaw cycles, backfilled with nitrogen, then heated at 70 °C for 5 h. The vial was cooled and opened to air to stop the polymerization. The reaction mixture was precipitated twice with diethyl ether, yielding the polymer **P1** (M_n = 4800, $Đ$ =1.08) for the MALDI-TOF analysis.

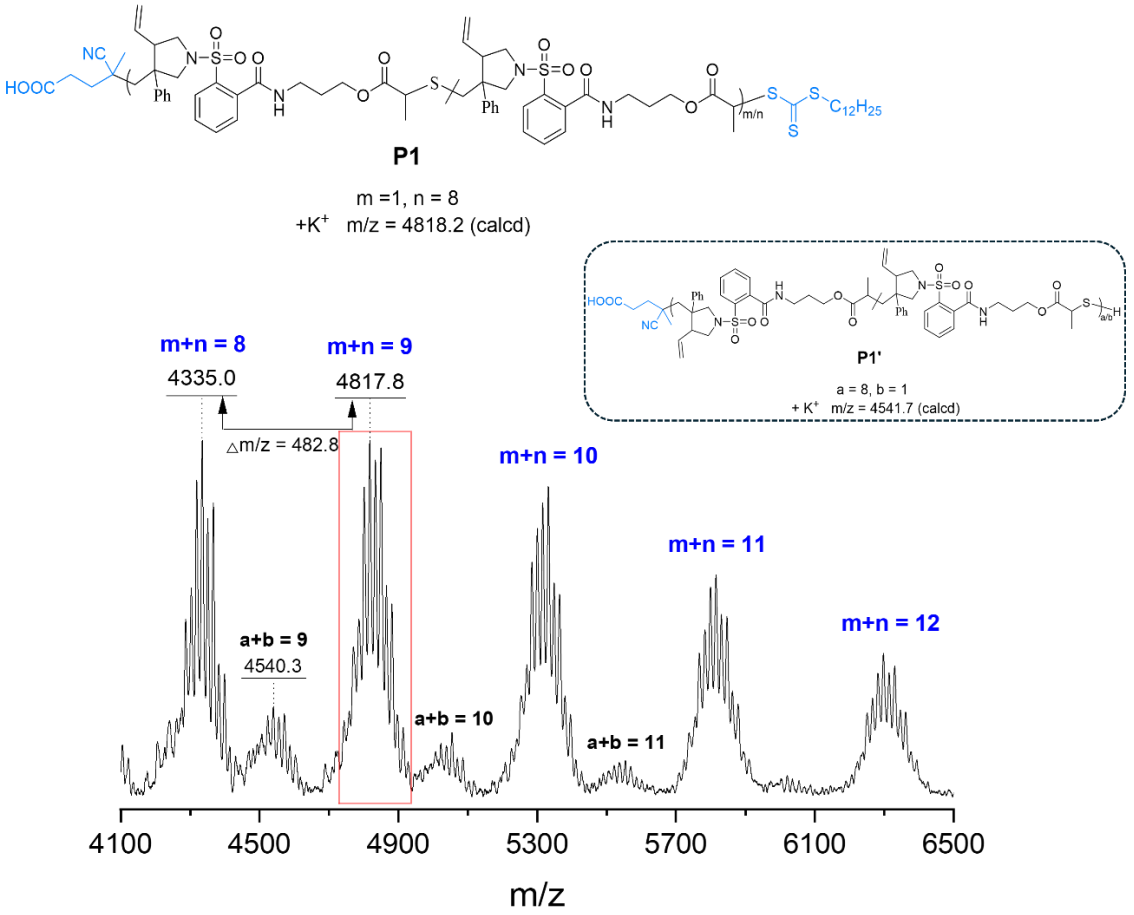


Figure S15. MALDI-TOF analysis of polymer **P1**.

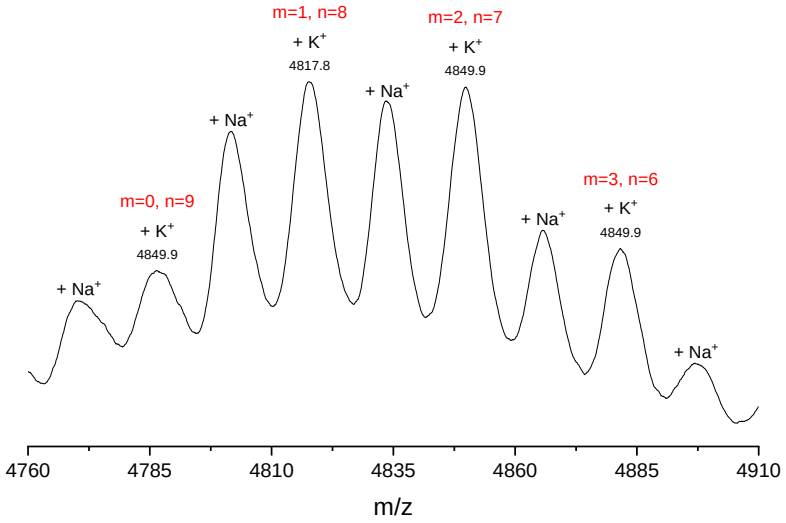


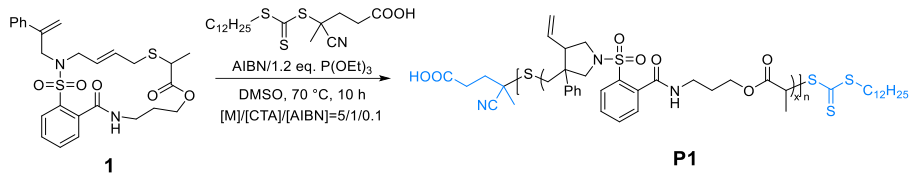
Figure S16. The zoom-in image of the 9-mers in the MALDI-TOF spectrum of polymer **P1**.

Organic Elemental Analysis (EA) Report					
Basic information about the experiment					
Test item	Organic Elemental Analysis (EA)				
Order number	2411120267				
Number of samples	1				
Test mode	CHNS mode				
Date of detection	2024.11.17				
CHNS mode	Elementar UNICUBE (Germany)				
Description of Special Circumstances	None				
Experimental results					
Sample name	N(%)	C(%)	H(%)	S(%)	O(%)
HHJ-04-070	5.19	61.71	6.28	8.97	\
HHJ-04-070	5.35	61.86	6.37	8.80	\

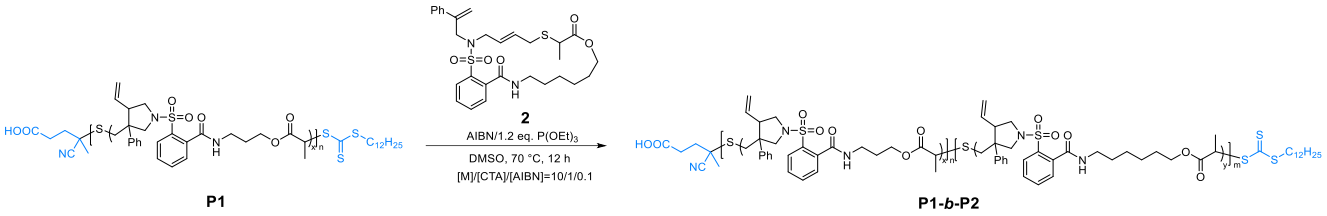
Figure S17. Elemental analysis of polymer **P1**.

Note: the desulfurization yield determined by elemental analysis is 61%.

Scheme S7. Synthesis of diblock copolymer **P1-*b*-P2**.



Following the general polymerization procedure, a 10 mL Schlenk vial was charged with macrocyclic monomer **1** (51.5 mg, 0.1 mmol), followed by the addition of **CTA1** (0.04 M in DMSO, 500 μL, 20 μmol), AIBN (0.01 M in DMSO, 200 μL, 2 μmol), $P(OEt)_3$ (0.12 mmol) and DMSO (300 μL). The vial was sealed, and the solution was deoxygenated via three freeze-pump-thaw cycles, backfilled with nitrogen, then heated at 70 °C for 10 h. The vial was cooled and opened to air to stop the polymerization. The monomer conversion was monitored by ^{1}H NMR spectroscopy (46% monomer conversion). The reaction mixture was precipitated twice with diethyl ether, yielding the macroinitiator **P1** (M_n = 5800, $Đ$ =1.11).



A 10 mL Schlenk vial was charged with monomer **2** (11.1 mg, 0.02 mmol), macroinitiator **P1** (2 μmol), AIBN (0.01 M in DMSO, 20 μL, 1 μmol), and DMSO (180 μL). The vial was sealed, and the solution was deoxygenated via three freeze-pump-thaw cycles, backfilled with nitrogen, then heated at 70 °C for 12 h. The vial was cooled and opened to air to stop the polymerization. The monomer conversion was monitored by ^{1}H NMR spectroscopy (47% monomer conversion). The reaction mixture was precipitated twice with ethyl ether, yielding the polymer **P1-*b*-P2** (M_n = 8000, $Đ$ =1.22).

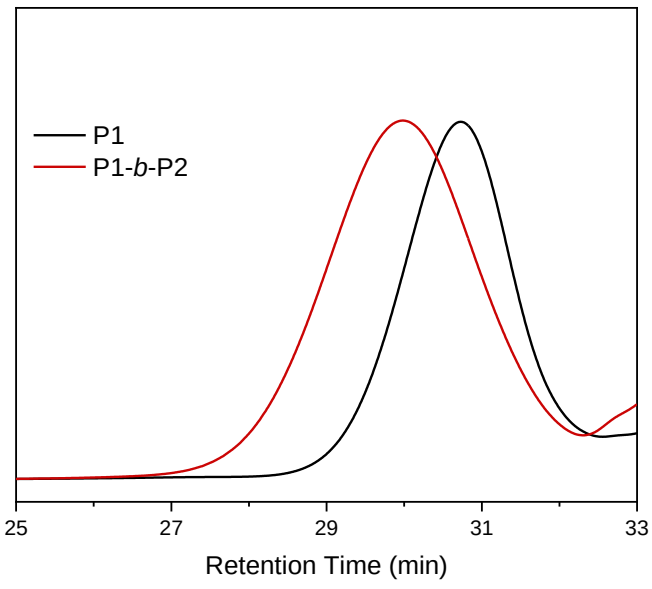
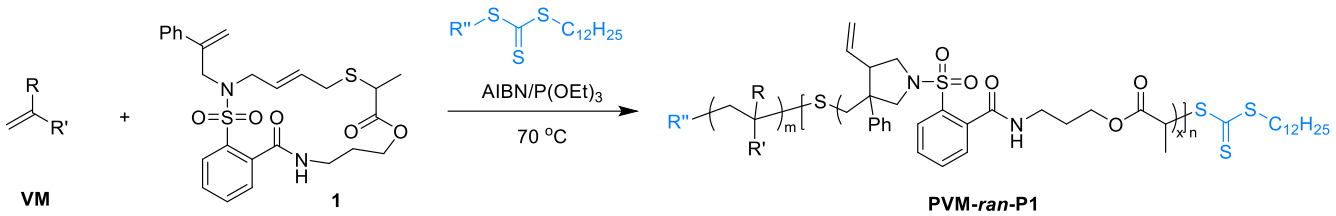


Figure S18. SEC traces for the synthesis of diblock copolymer **P1-*b*-P2**.

Table S11. Copolymerization of monomer **1** and vinyl monomers**.**



Entry[a]	**VM**	CTA	[**VM**]/[**1**]/[P(OEt)$_3$] /[CTA]/[AIBN]	solvent	Conc.	Time	Conver. of **VM**[b]	Conver. of **1**[b]	$M_{n,SEC}$[c]	$Đ$[c]
1	MMA	**CTA1**	300/0/0/1/0.27	benzene	7.0 M	10 h	98%	/	22000	1.18
2	MMA	**CTA1**	300/3/3.6/1/0.27	benzene	7.0 M	10 h	>99%	60%	27600	1.22
3	styrene	**CTA2**	1000/0/0/1/0.2	/	bulk	20 h	34%	/	34400	1.15
4	styrene	**CTA2**	1000/10/12/1/0.2	/	bulk	20 h	47%	14%	26400	1.15

[a] Experimental conditions: [**VM**]/[**1**]=100/1, reacted at 70ºC under a nitrogen atmosphere, unless otherwise noted. [b] Monomer conversion was determined by ^{1}H NMR spectroscopy. [c] Molecular weight and polydispersity index ($Đ$) were determined by SEC analysis calibrated to polystyrene standards.

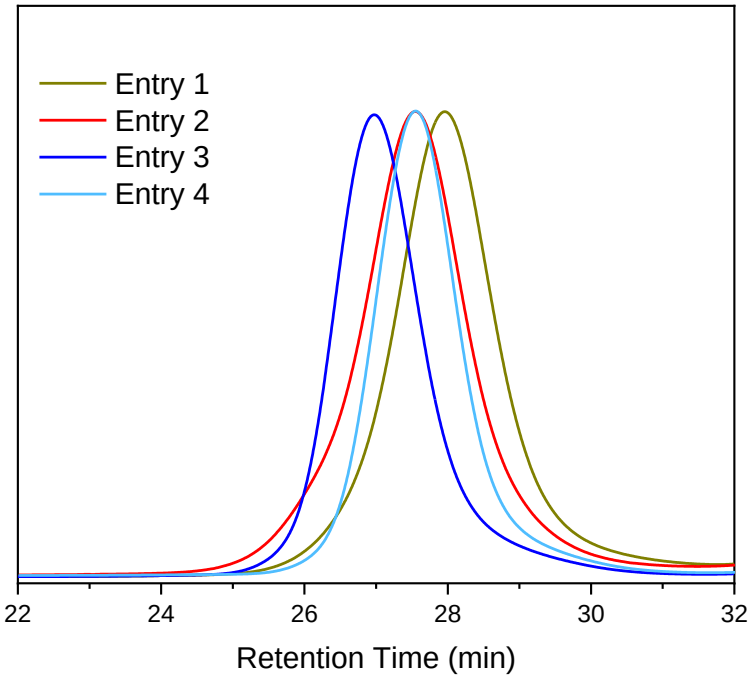


Figure S19. SEC traces for copolymerization of monomer **1** and vinyl monomers**.**

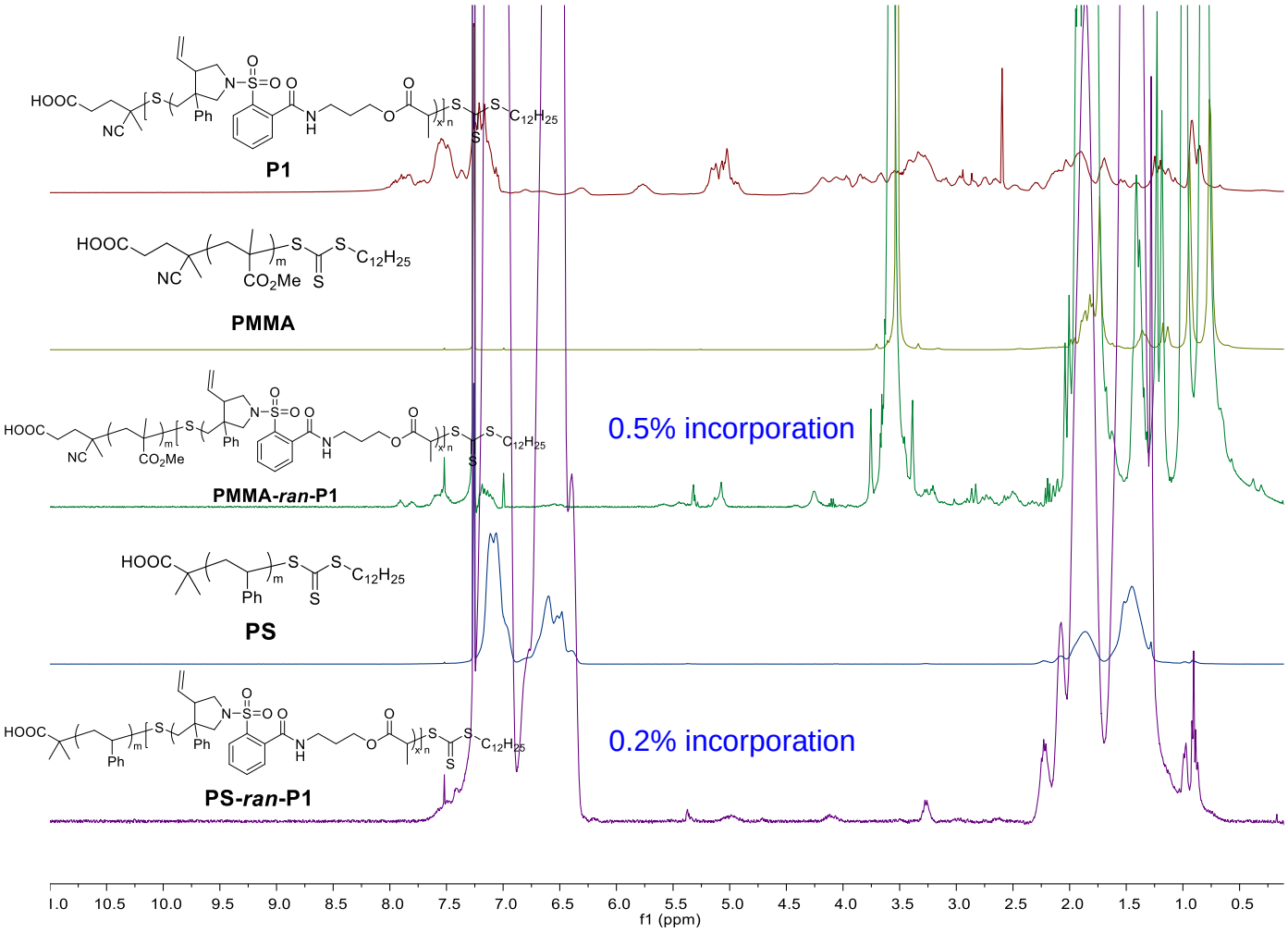
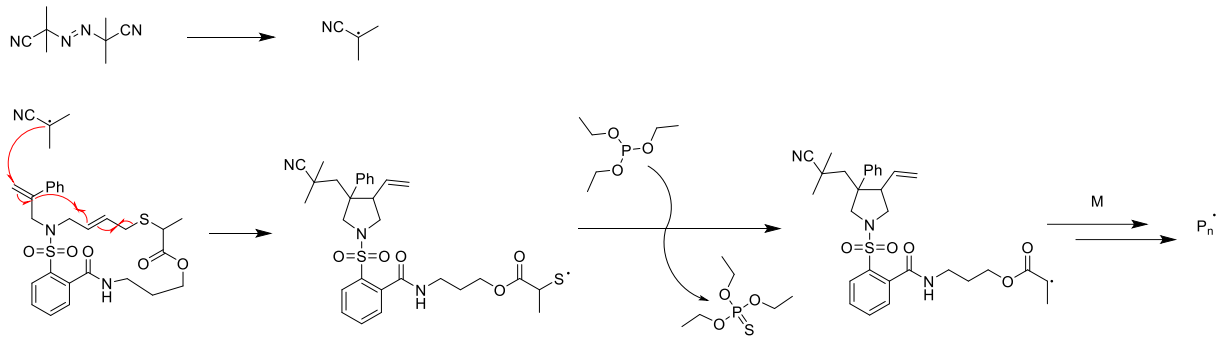
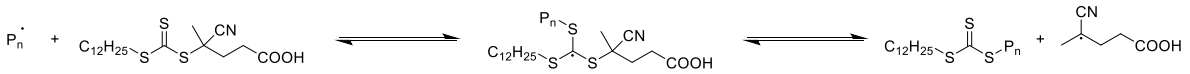


Figure S20. ^{1}H NMR analysis of the vinyl copolymers.

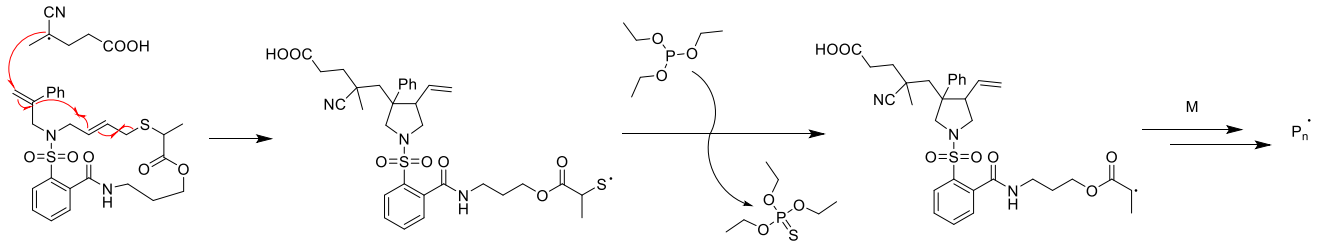
(1) Initiation



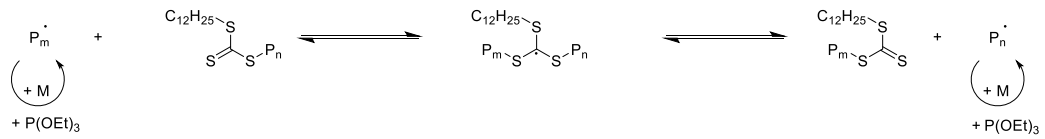
(2) Chain transfer to CTA



(3) Reinitiation



(4) Degenerative chain transfer propagation



(5) Temination

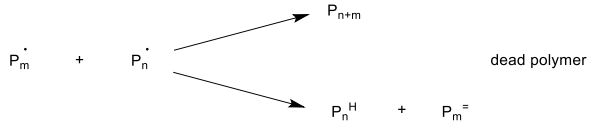


Figure S21. Proposed mechanism for the polymerization.

Table S12. Computed results for the chain-growth process.

	Thermal correction to *G* (Hartree)	Single point energy (Hartree)	Imaginary frequency
Int0	0.075222	-705.126967211734	
P(OEt)$_3$	0.171681	-804.573284659005	
TS1	0.271511	-1509.714552278729	355.0311i
S=P(OEt)$_3$	0.174810	-1202.790225324309	
Int1	0.071641	-306.960052554172	
M	0.466253	-2290.305800850286	
TS2	0.559666	-2597.263820661758	527.1335i
Int2	0.563335	-2597.307111852610	
TS3	0.566053	-2597.283789955884	600.5732i
Int3	0.568756	-2597.315336851205	
TS4	0.568463	-2597.299429094894	267.5393i
Int4	0.565929	-2597.304332031877	
TS5	0.562047	-2995.441233371177	149.3291i
Int5	0.561612	-2995.460238695563	
TS6	0.563570	-2995.438773740694	571.8135i
Int6	0.568007	-2995.466551546289	
TS7	0.566904	-2995.453310178335	272.7202i
Int7	0.563275	-2995.459178247476	
CTA	0.140975	-1618.755142037458	
TS8	0.234994	-1925.719465481299	280.3348i
Int8	0.240041	-1925.750304322839	

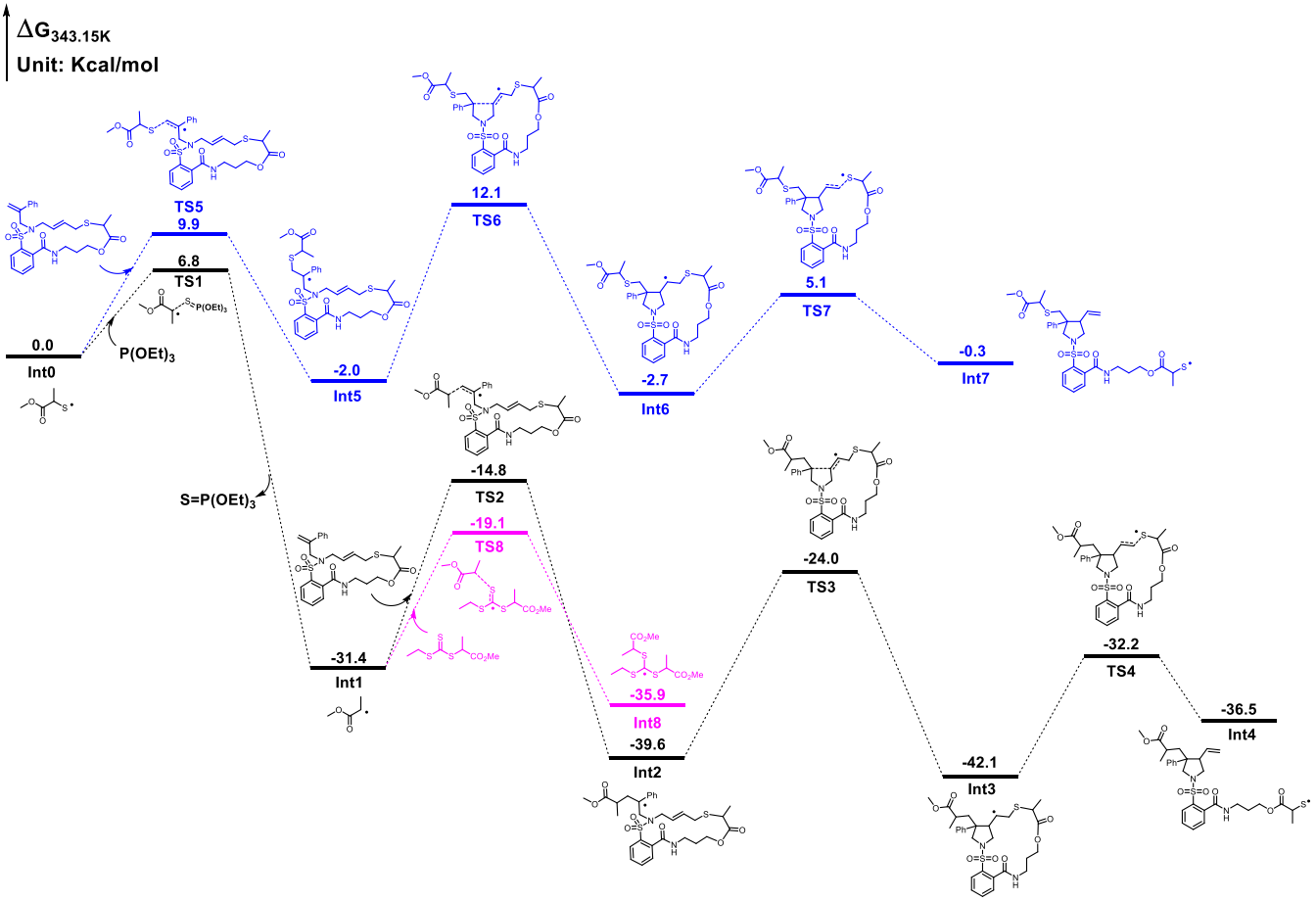


Figure S22. Calculated free energy profiles for the chain-growth process.

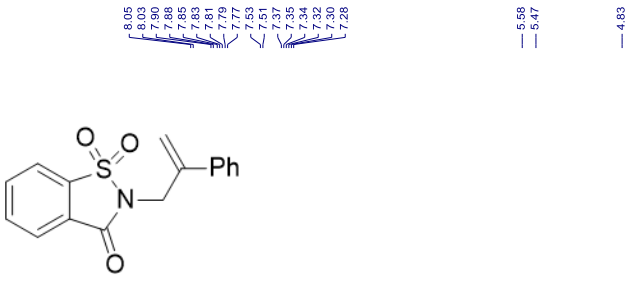
References

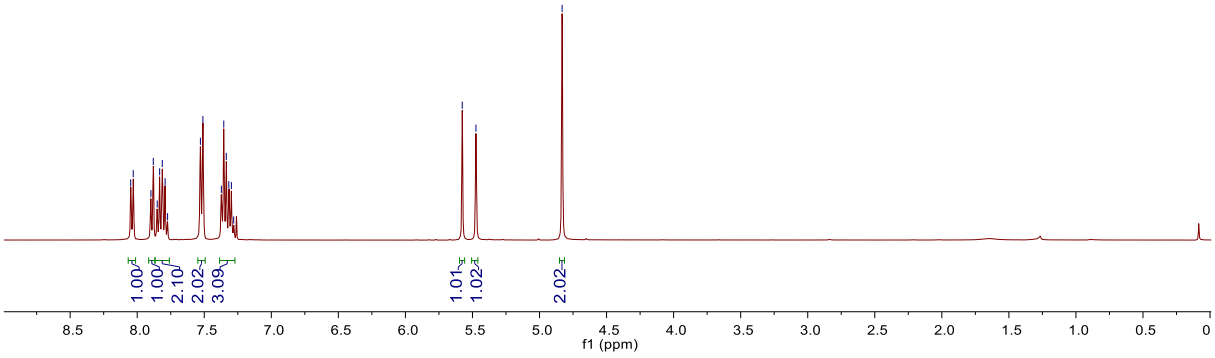
1 S. Zhang, C. Cao, S. Jiang and H. Huang, *Macromolecules*, 2022, **55**, 9411–9419.

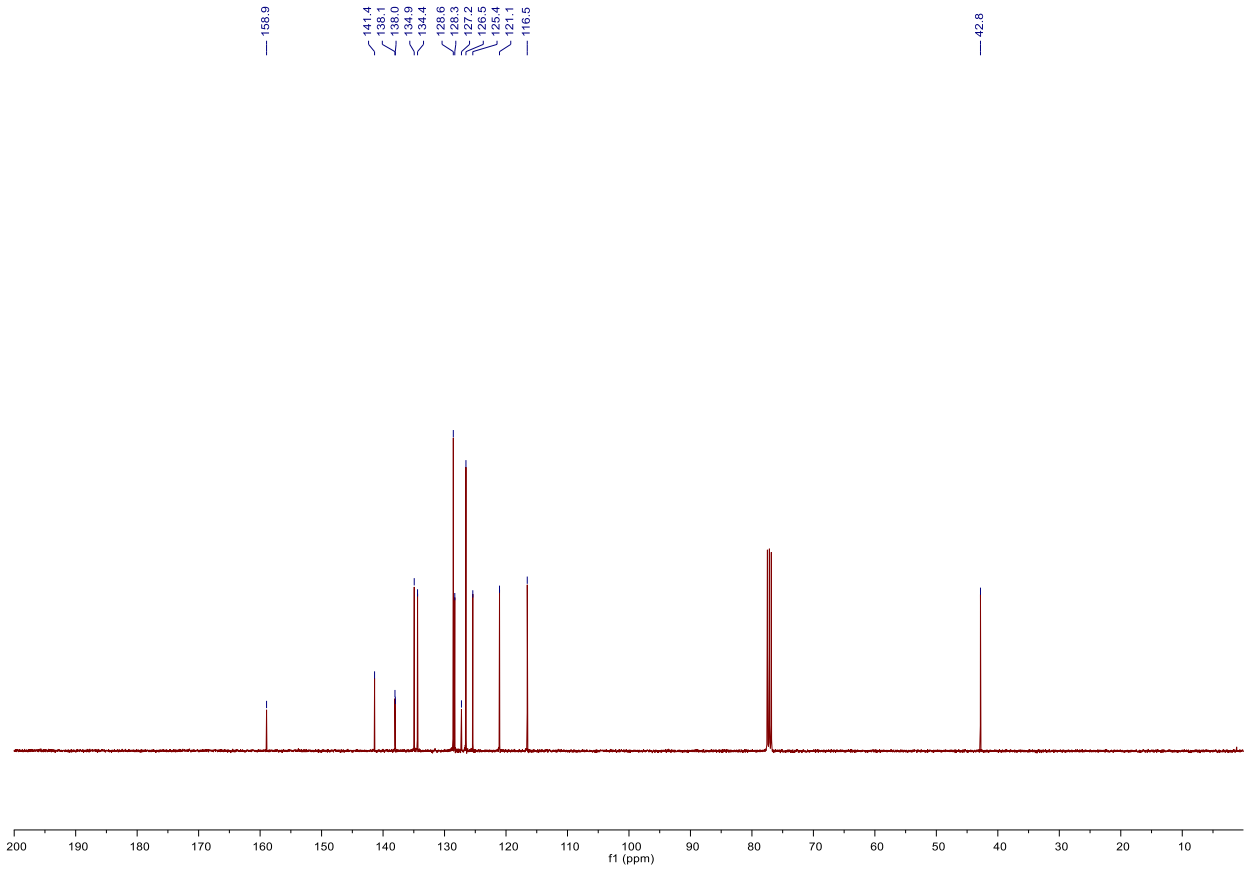
2 S. Zhang, Y. Wang, H. Huang and D. Cao, *Angew. Chem. Int. Ed.*, 2023, **62**, e202308524.

NMR spectra

NMR of S1







NMR of S2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7.58
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7.49
7.47
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7.34
7.33
7.28
7.27
7.27
7.26
7.02
7.00
6.99
6.98
6.97
6.83
6.81
5.76
5.74
5.72
5.70
5.68
5.51
5.50
5.48
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3.82
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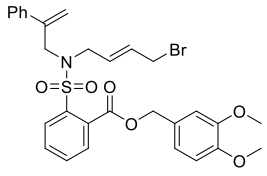
3.78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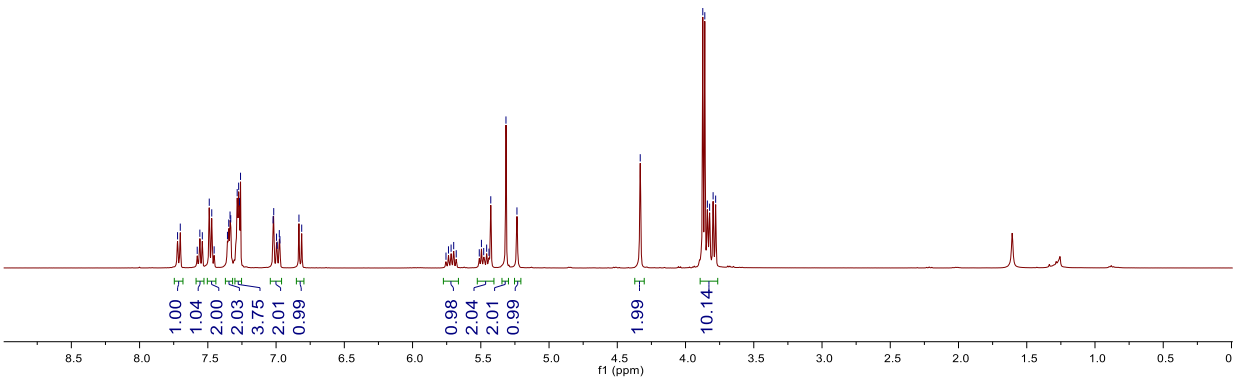
Br
O=S=O
O
O
O
O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2.01
0.99
1.99
10.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
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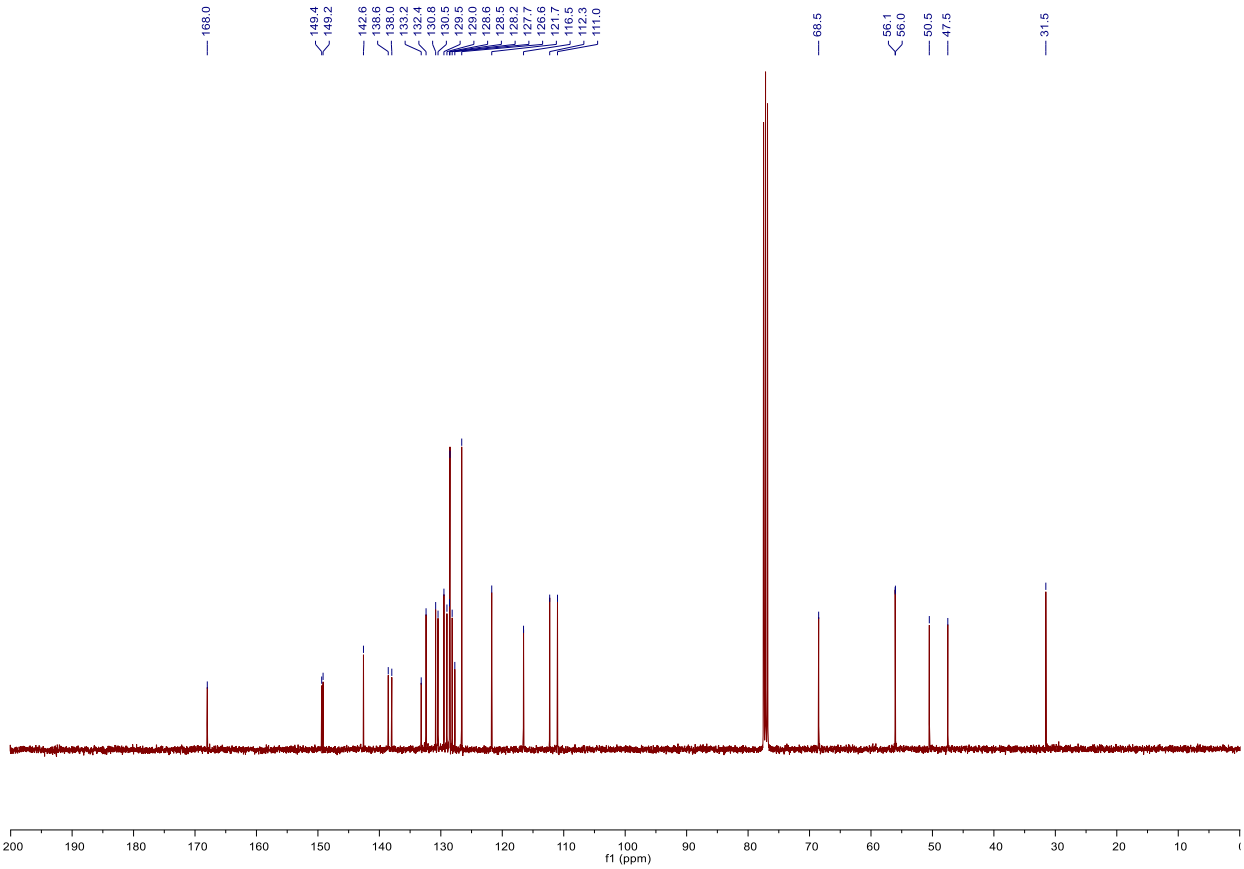
1.5
1.0
0.5
0
f1 (ppm)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138.6
138.0
133.2
132.4
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130.5
129.5
129.0
128.6
128.5
128.2
127.7
126.6
121.7
116.5
112.3
111.0
68.5
56.1
56.0
50.5
47.5
31.5
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

NMR of S3


7.74
7.72
7.57
7.55
7.53
7.49
7.47
7.46
7.35
7.34
7.33
7.29
7.28
7.27
7.26
7.02
6.99
6.97
6.97
6.83
6.80
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5.53
5.51
5.49
5.48
5.43
5.38
5.36
5.35
5.33
5.31
5.29
5.23
4.37
4.33
4.32
4.28
3.87
3.85
3.83
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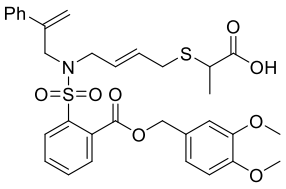
3.08
3.06
3.04
1.37
1.36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O
OH
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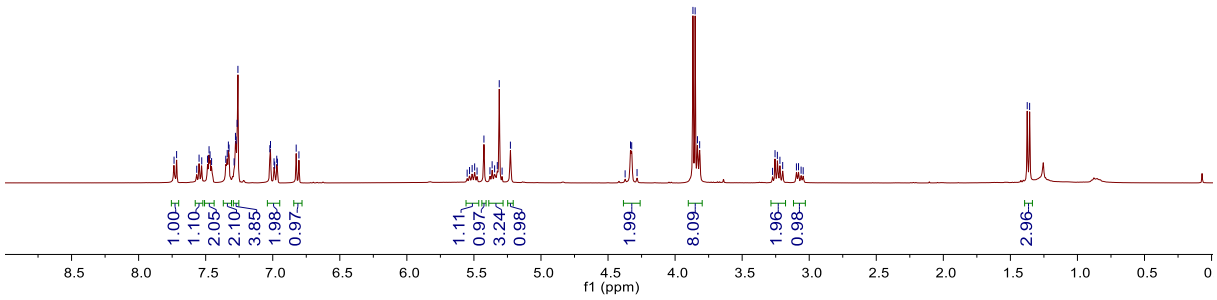
O
O
O
O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0.98
2.96
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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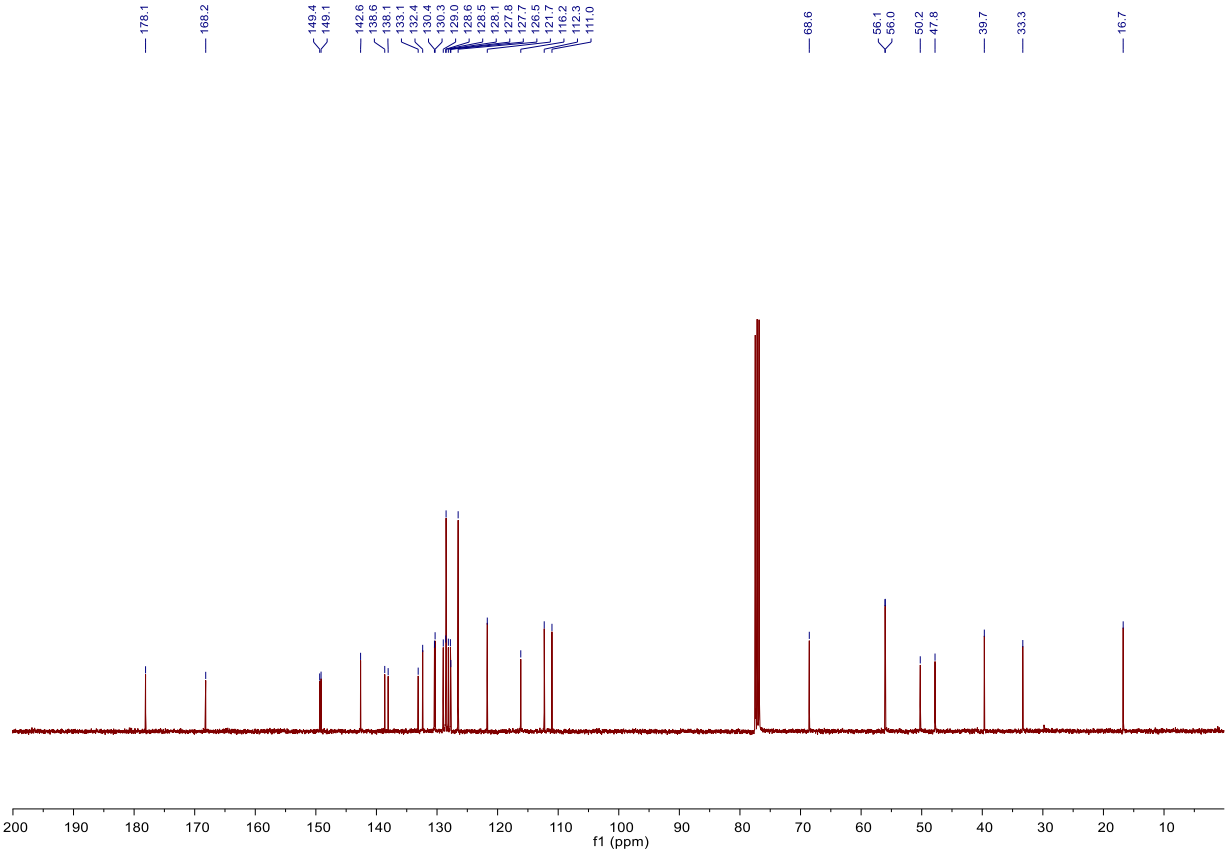
0.5
0
f1 (ppm)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128.5
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126.5
121.7
116.2
112.3
111.0
68.6
56.1
56.0
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47.8
39.7
33.3
16.7
200
190
180
170
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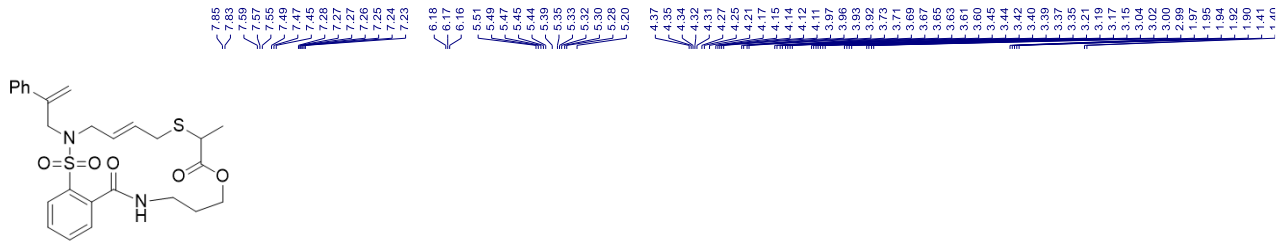
40
30
20
10
f1 (ppm)

NMR of 1



Ph
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S
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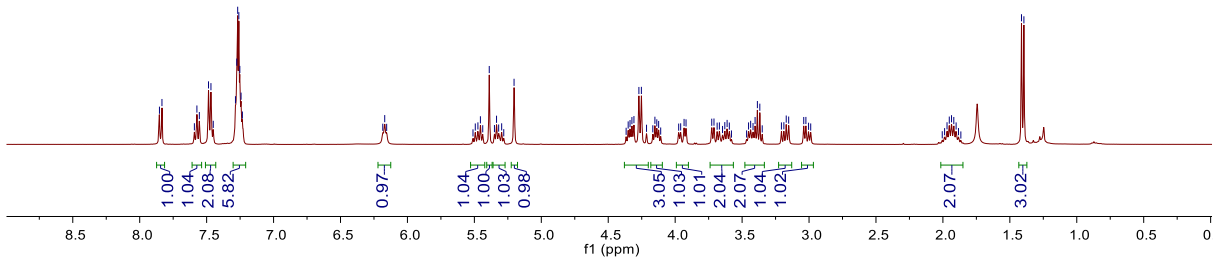
O
O
O
N
H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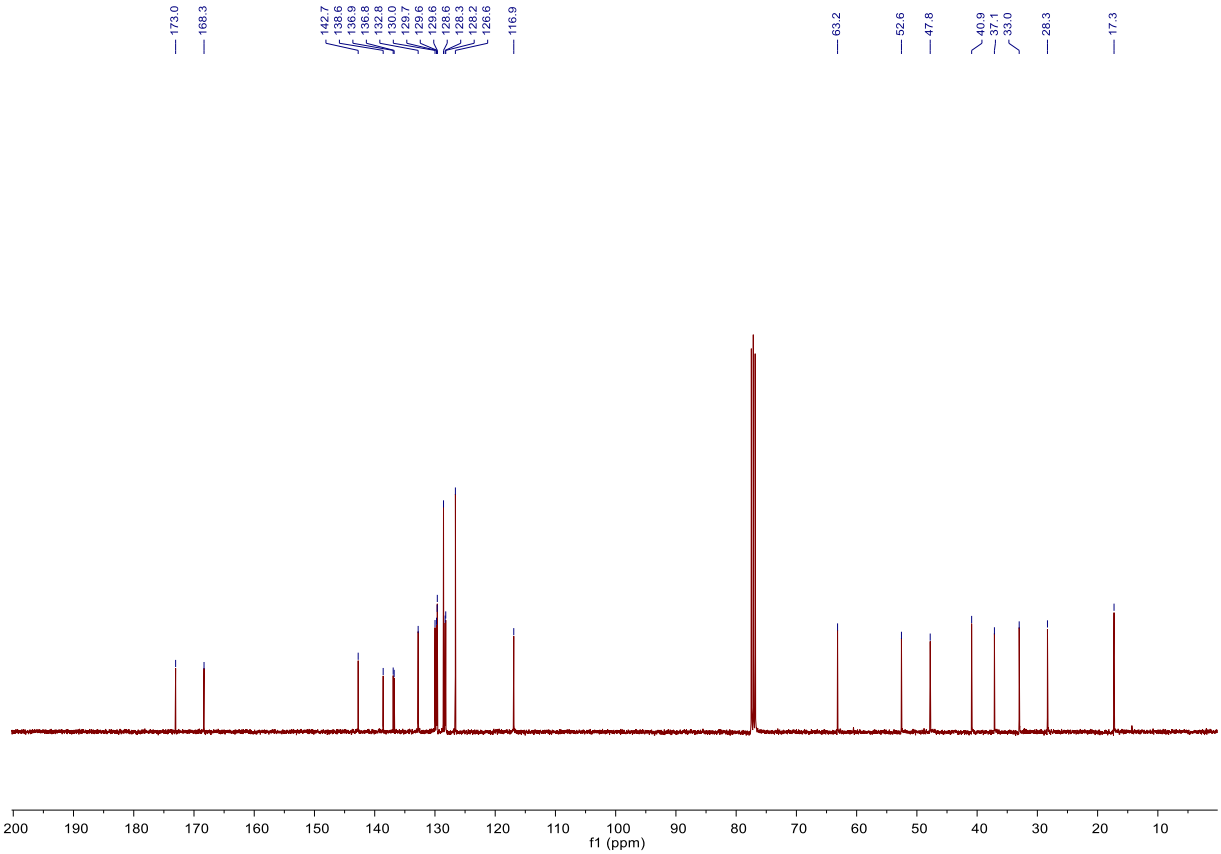
1.02
2.07
3.02
f1 (ppm)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128.2
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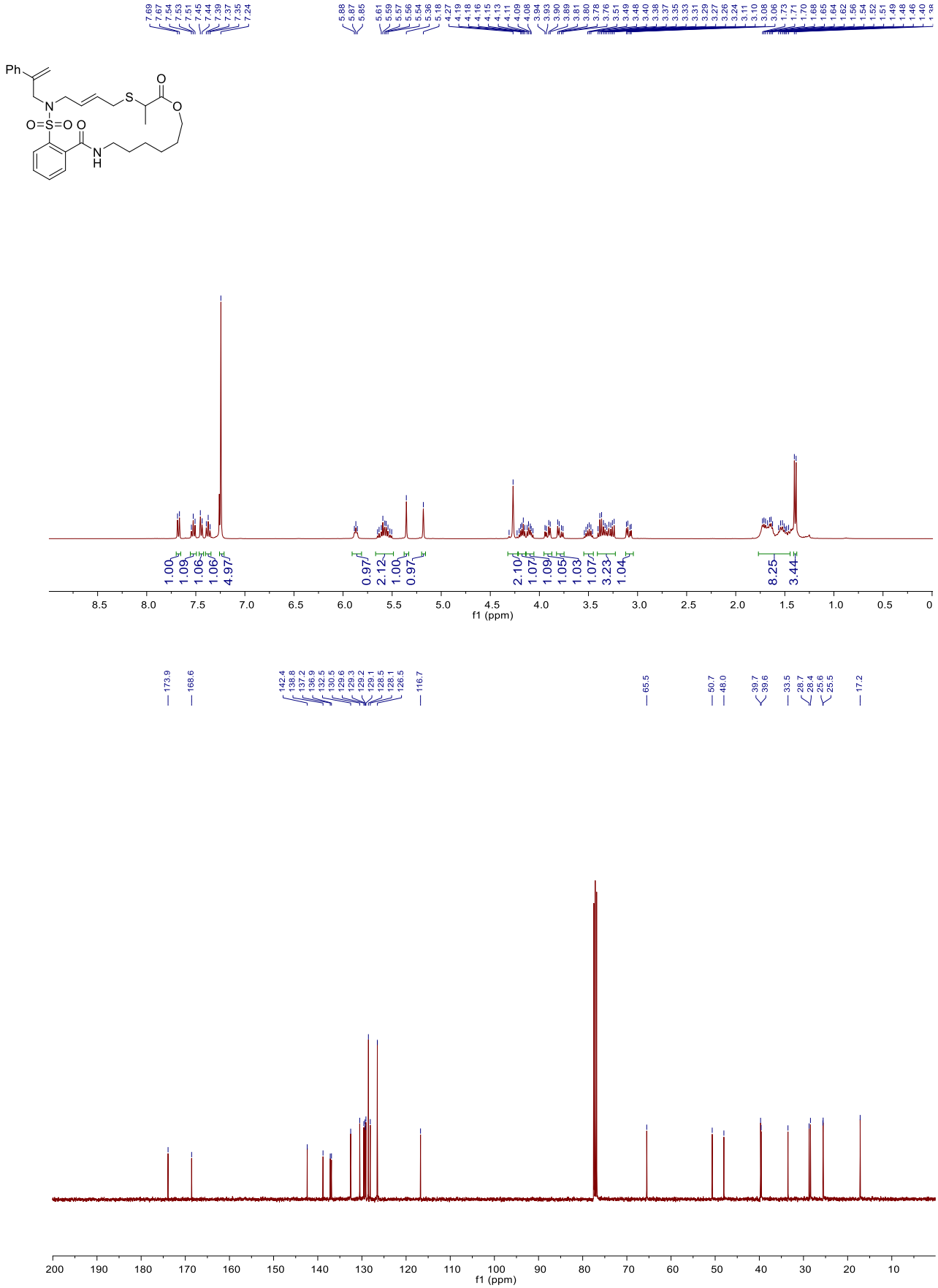
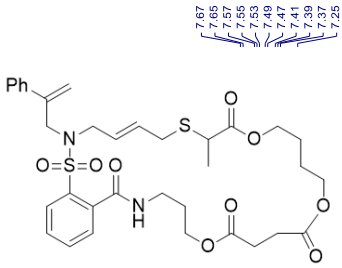
28.3
17.3
f1 (ppm)

NMR of 2



NMR of 3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O
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O
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O
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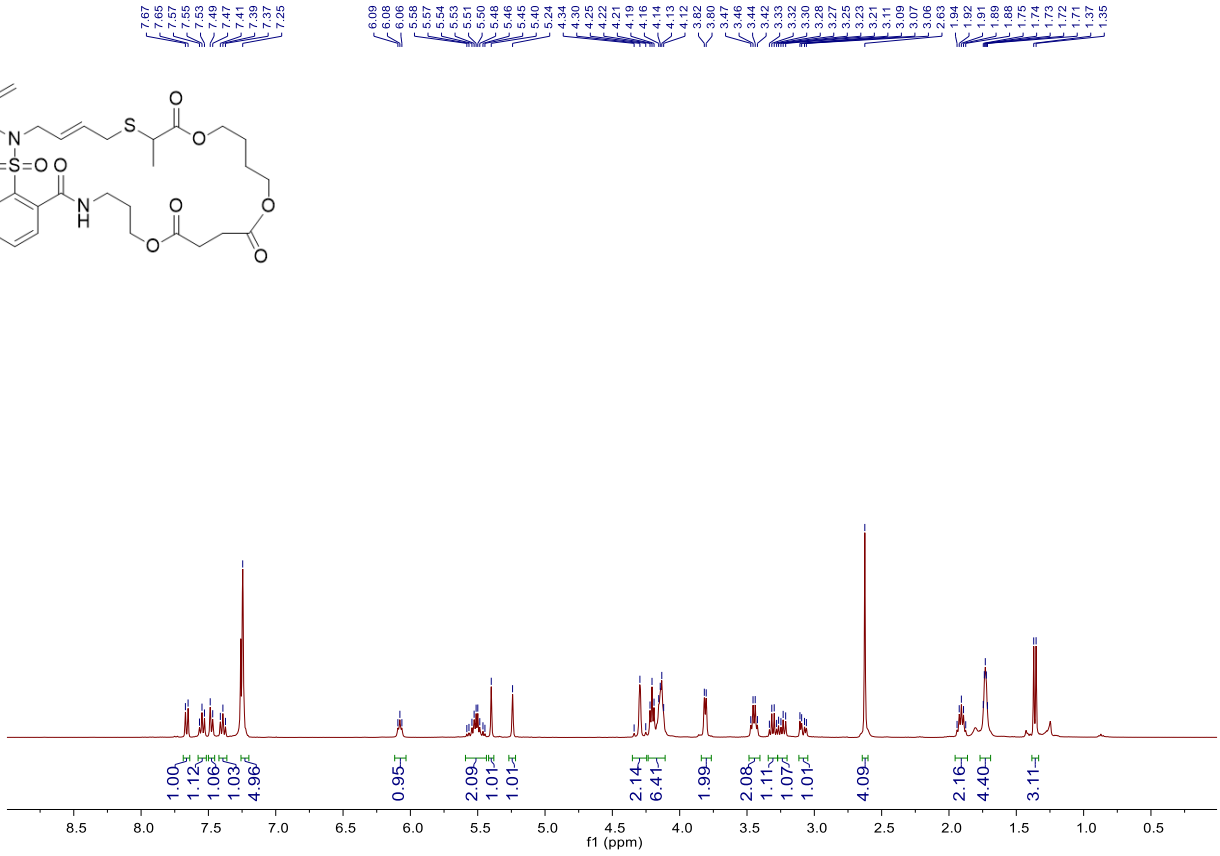
O
O
O
O
O
N
H


7.67 7.65 7.57 7.55 7.53 7.49 7.47 7.41 7.39 7.37 7.25
6.09 6.08 6.06 5.58 5.57 5.54 5.53 5.51 5.50 5.48 5.46 5.45 5.40 5.24 4.34 4.30 4.25 4.22 4.21 4.19 4.16 4.14 4.13 4.12 3.82 3.80 3.47 3.46 3.44 3.42 3.33 3.32 3.30 3.28 3.27 3.25 3.23 3.21 3.11 3.09 3.07 3.06 2.63 1.94 1.92 1.91 1.89 1.88 1.75 1.74 1.73 1.72 1.71 1.37 1.35
1.00 1.12 1.06 1.03 4.96 0.95 2.09 1.01 1.01 2.14 6.41 1.99 2.08 1.11 1.07 1.01 4.09 2.16 4.40 3.11
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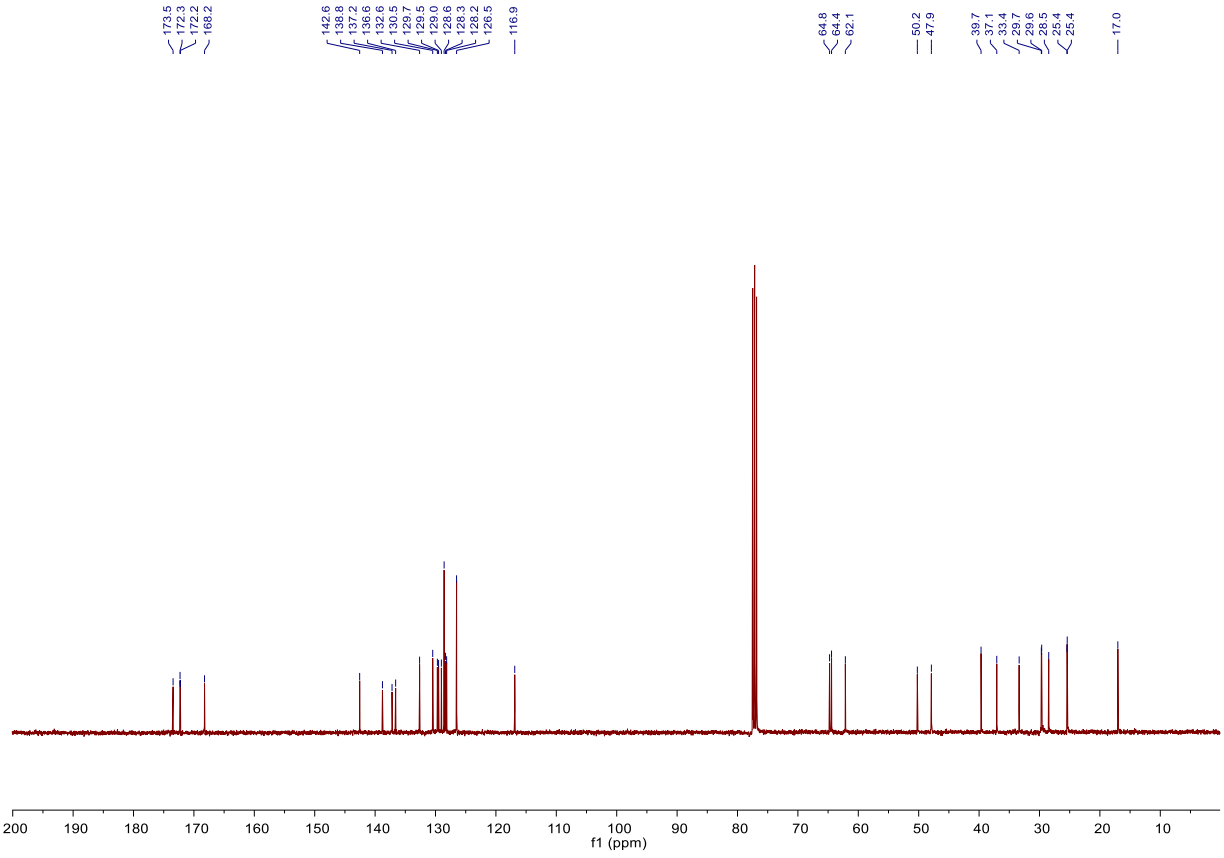
f1 (ppm)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142.6 138.8 137.2 136.6 132.6 130.5 129.7 129.5 129.0 128.6 128.3 128.2 126.5 116.9
64.8 64.4 62.1
50.2 47.9
39.7 37.1 33.4 29.7 29.6 28.5 25.4 25.4
17.0
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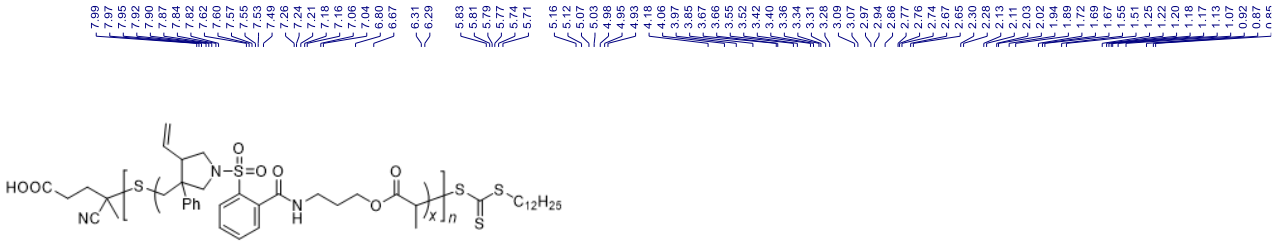
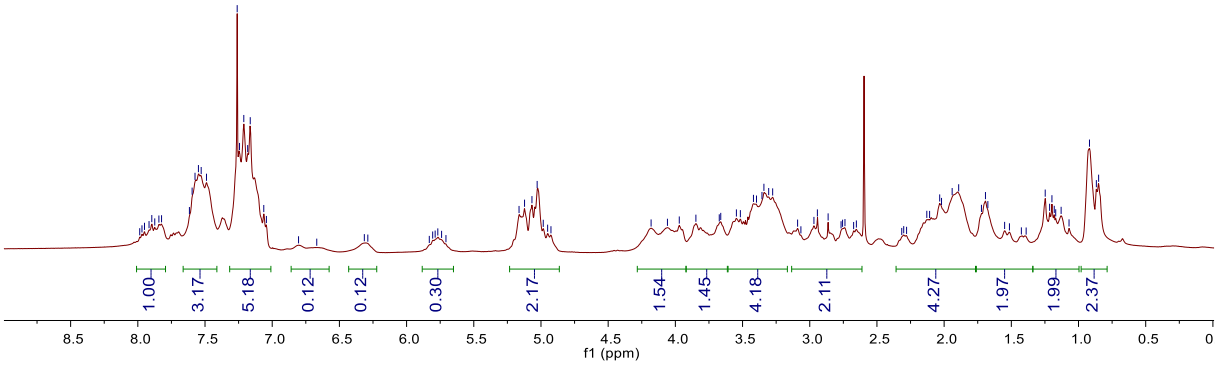
f1 (ppm)

NMR of P1

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0.12
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4.27
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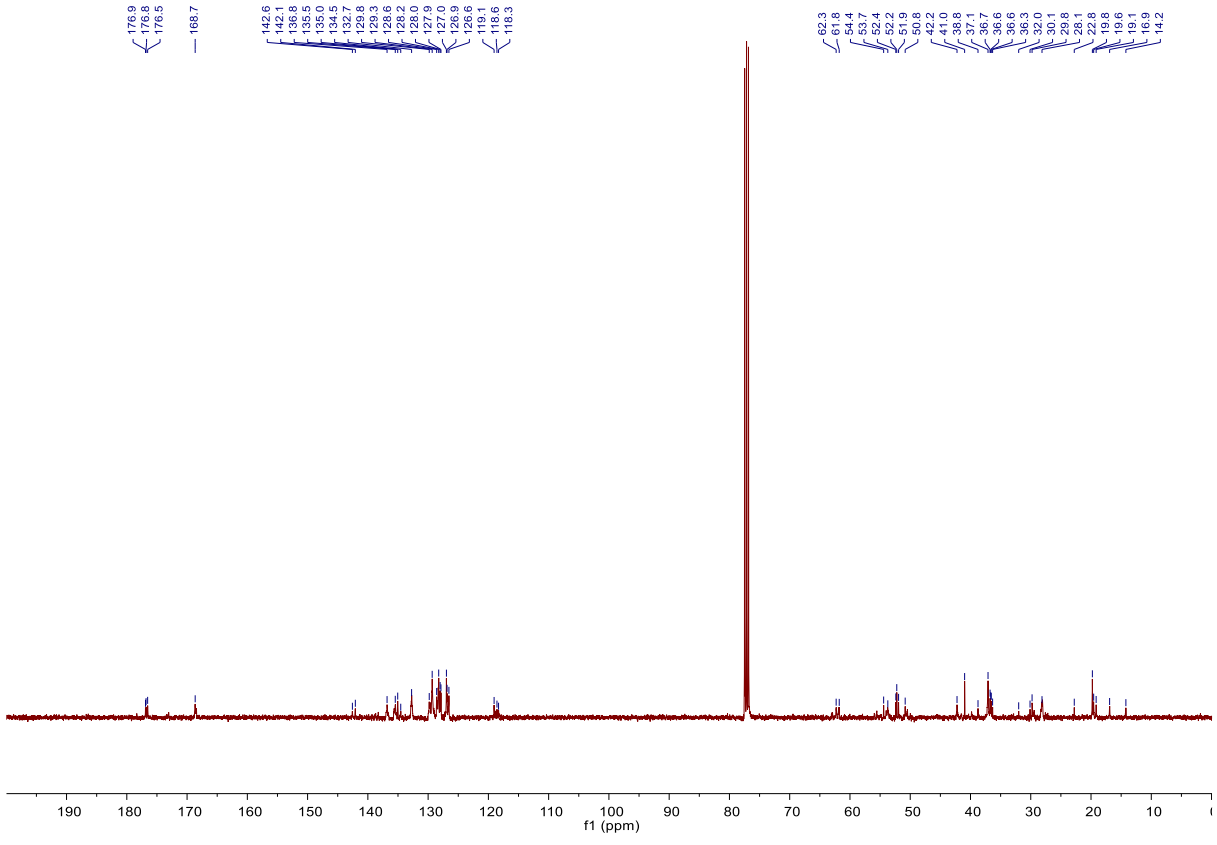
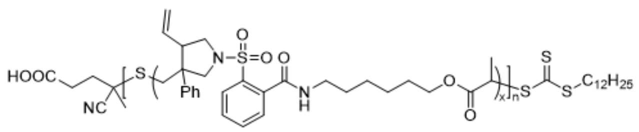
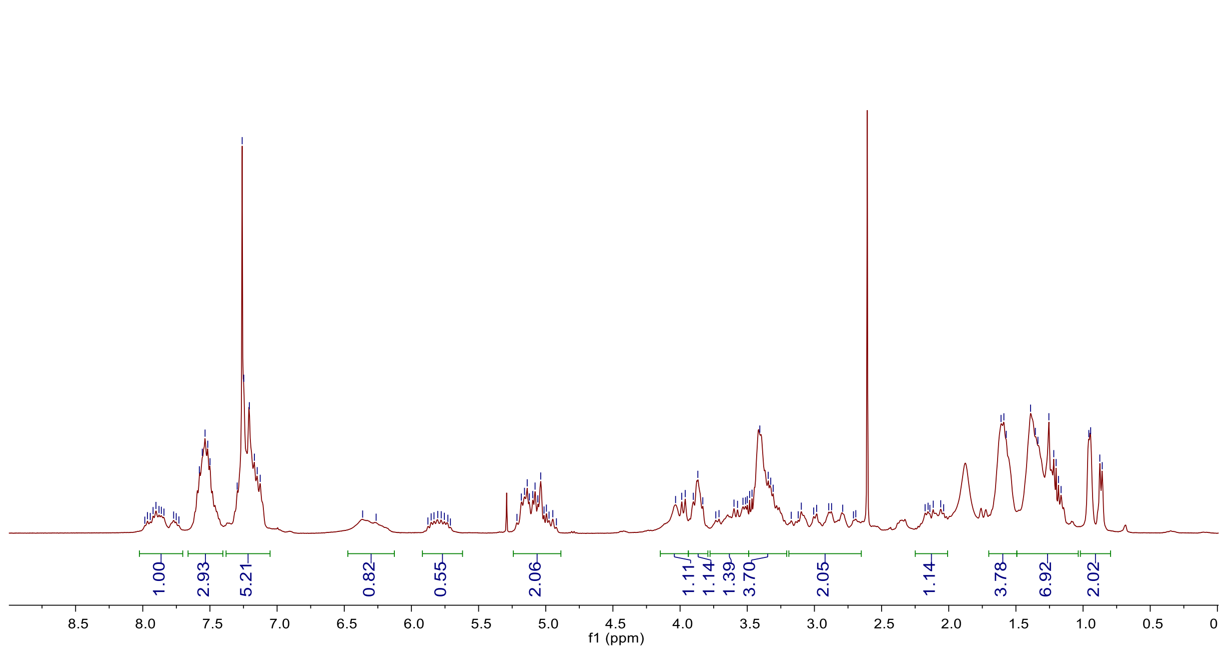
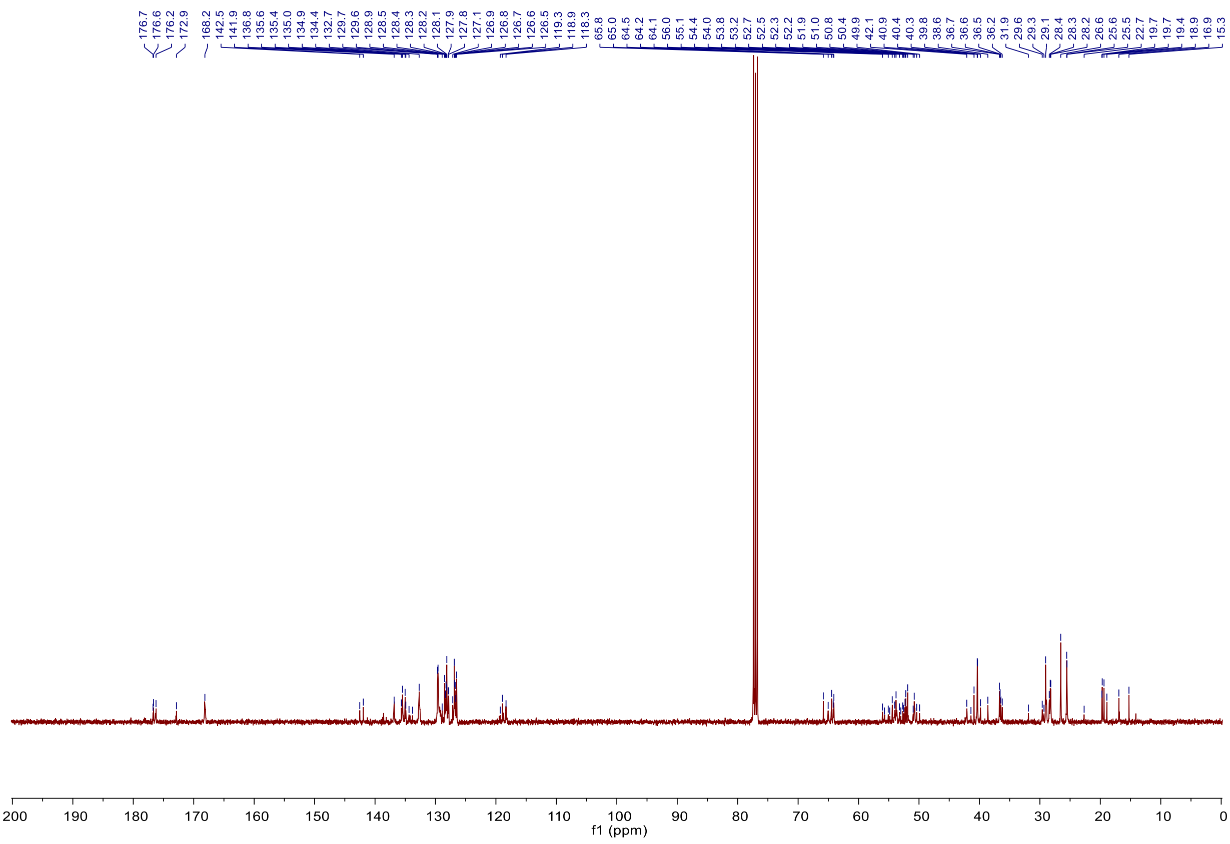
1.99
2.37
f1 (ppm)


f1 (ppm)

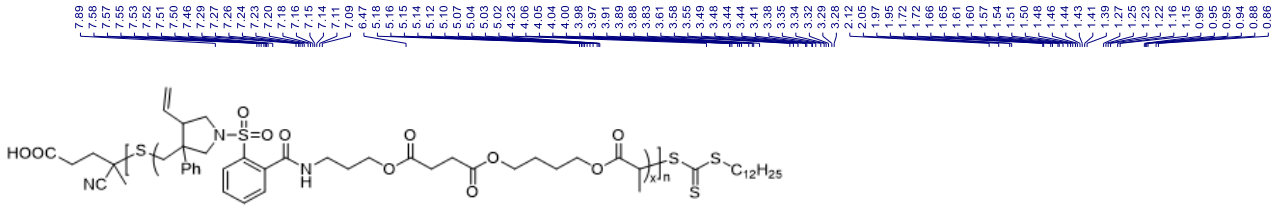
NMR of P2

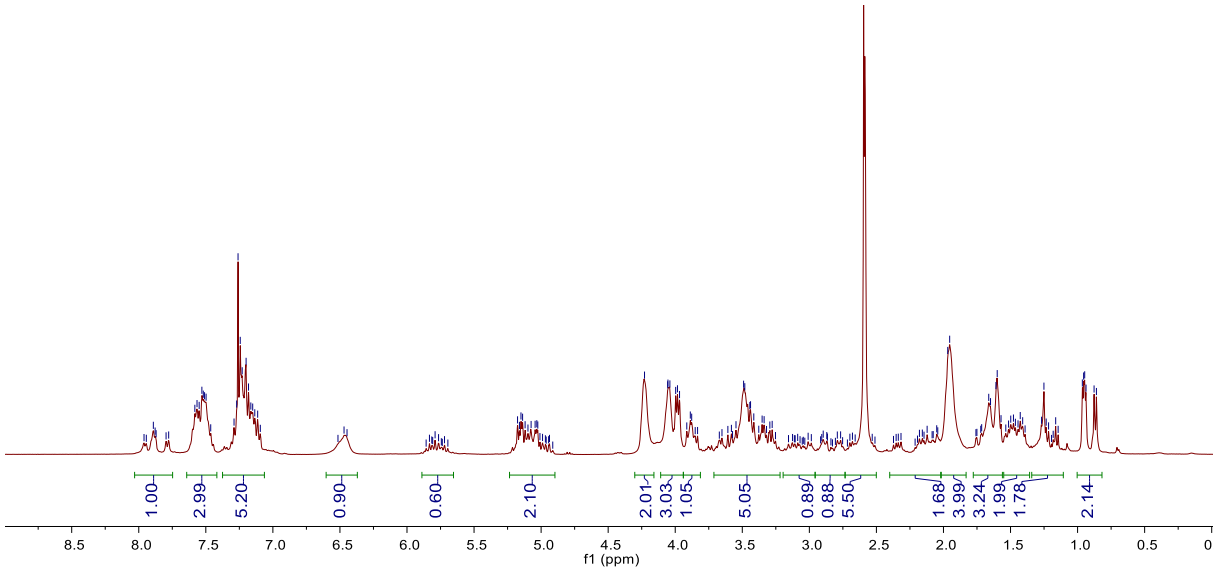






NMR of P3


HOOC
NC
Ph
$C_{12}H_{25}$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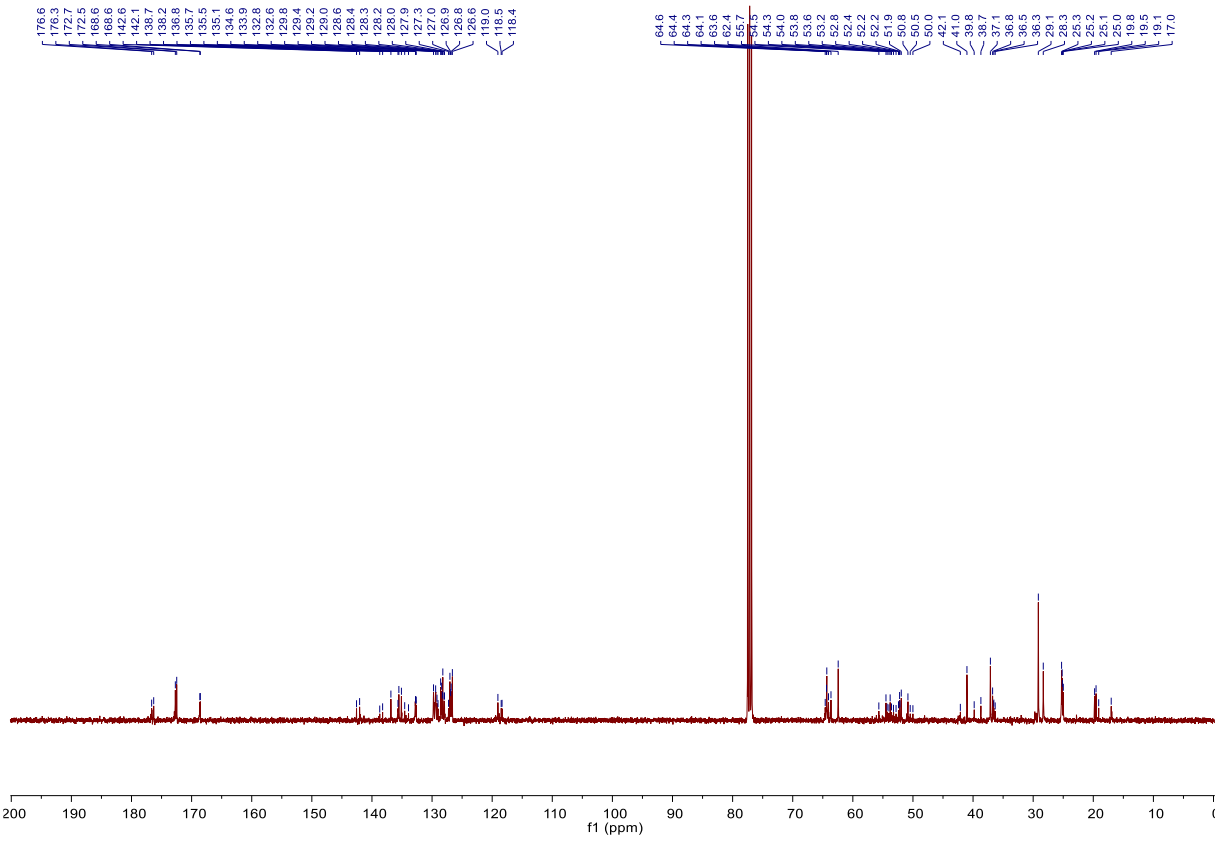
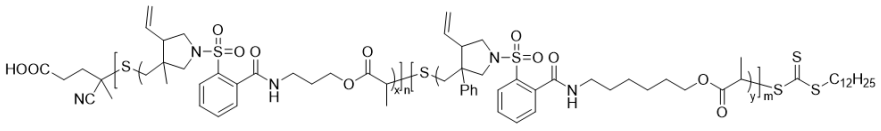
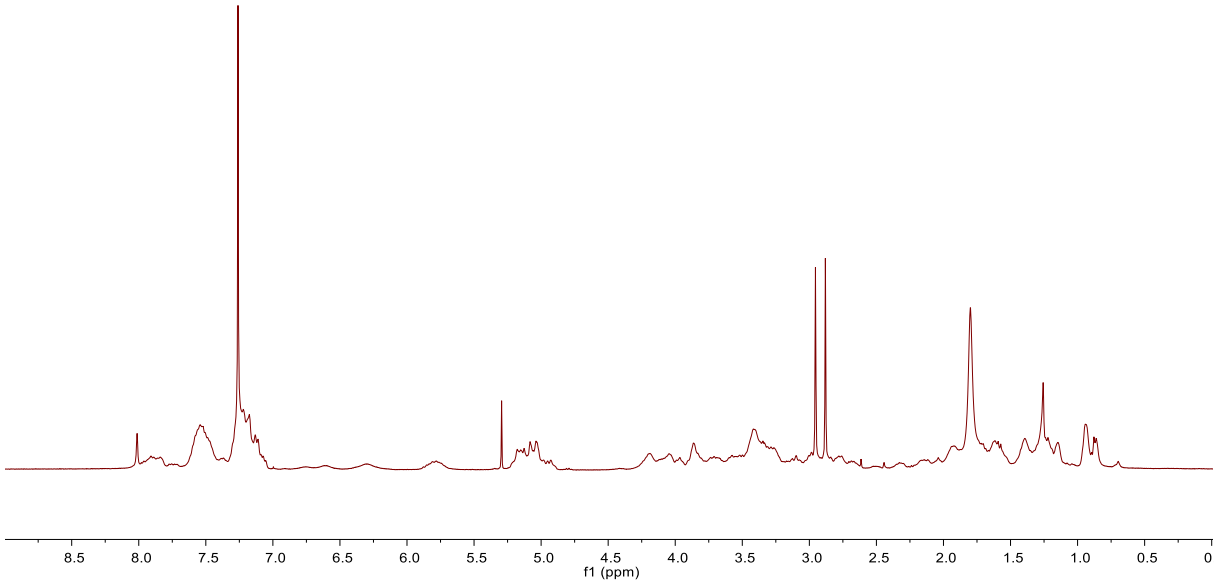
5.20
0.90
0.60
2.10
2.01
3.03
1.05
5.05
0.89
0.88
5.50
1.68
3.99
3.24
1.99
1.78
2.14
f1 (ppm)


f1 (ppm)

NMR of P1-*b*-P2


HOOC
NC
S
N
S
O
O
O
N
H
O
O
x
n
S
Ph
N
S
O
O
O
N
H
O
O
y
m
S
S
S
C12H25


8.5
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7.5
7.0
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4.5
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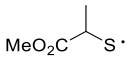
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

Cartesian coordinates of all optimized structures



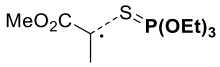
Int0

C	-2.23961400	0.23358800	-0.17348500
O	-0.90696200	-0.16241100	0.13775600
C	1.39036400	0.26442300	0.44627800
S	2.05937600	-0.46544500	-1.07477700
H	2.03485900	1.13799300	0.63759100
C	0.00541100	0.80738600	0.15562900
H	-2.28599400	0.66973900	-1.18059800
H	-2.60421100	0.96987500	0.55512400
O	-0.24656600	1.96355700	-0.05874500
C	1.43357400	-0.70485700	1.62187000
H	2.47117300	-0.99862600	1.82664200
H	1.01687900	-0.22438400	2.51940400
H	0.84456800	-1.60556300	1.40399500
H	-2.84944800	-0.67422200	-0.12851900

$P(OEt)_3$

P	0.14381500	-0.06027900	0.50759000
O	1.52349200	-0.69971400	-0.10320500
O	-0.80201900	-1.23668900	-0.12681500
O	-0.11980300	1.15603600	-0.57611800
C	2.71800300	0.04878500	0.09999000
C	3.90533800	-0.84771300	-0.15964400
H	2.75006400	0.44248600	1.13237300
H	2.72770900	0.91492700	-0.58286300
H	4.84065500	-0.28622000	-0.02685300
H	3.90458600	-1.69875600	0.53609000
H	3.87437800	-1.23667100	-1.18740600
C	-2.20528200	-1.12927100	0.09043700
C	-2.84250100	-2.47375200	-0.17040300
H	-2.62253600	-0.36395400	-0.58549500
H	-2.40663900	-0.80198300	1.12668400
H	-3.93035100	-2.41174500	-0.02739700
H	-2.64359000	-2.79851400	-1.20164900
H	-2.43996600	-3.23028600	0.51800700
C	-0.40415500	2.46641800	-0.09164600
C	-1.89432300	2.69448100	0.03908500
H	0.03763100	3.17050700	-0.81109400
H	0.09655000	2.63114700	0.87838200
H	-2.09680500	3.72896600	0.35243600

H	-2.39683000	2.51751300	-0.92305600
H	-2.32790600	2.01601600	0.79018700



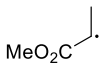
TS1

C	3.75060000	0.67038200	0.58570800
O	2.77923600	-0.28573500	0.18723700
C	1.46085700	-1.34669400	-1.44359300
S	-0.16014700	-0.15394500	-1.54171300
H	1.55198100	-1.68309600	-2.48343800
C	2.57741700	-0.41258400	-1.13357900
H	3.44974100	1.68220100	0.27780900
H	4.72928900	0.44143400	0.14215700
O	3.21408600	0.20825900	-1.95072600
P	-1.63934300	0.22829900	-0.02799400
O	-2.78076400	-0.89816400	0.03819300
O	-0.85633000	-0.01650800	1.35801500
O	-2.46872800	1.56538100	0.39866900
C	-2.58710100	-2.28328400	-0.28417900
C	-2.13617900	-3.06449600	0.92896600
H	-1.86753200	-2.36578900	-1.11297400
H	-3.56132900	-2.63903500	-0.64431300
H	-2.03115100	-4.12712400	0.66629000
H	-1.16812900	-2.69750000	1.29646100
H	-2.87432700	-2.97718300	1.73891200
C	0.16392100	0.90639500	1.76915700
C	0.98183700	0.26431000	2.86135100
H	-0.32408300	1.82769200	2.12231400
H	0.79681900	1.15443300	0.90173900
H	1.72429300	0.98236500	3.23747400
H	0.33726300	-0.03715400	3.69946900
H	1.51145700	-0.61906900	2.47753600
C	-3.14314700	2.32586600	-0.61509900
C	-2.22992500	3.38070800	-1.19681000
H	-4.01238500	2.77740200	-0.11905600
H	-3.52063000	1.65057400	-1.40006500
H	-2.77509400	3.98743000	-1.93368900
H	-1.85485700	4.04499400	-0.40525500
H	-1.37079700	2.91147800	-1.69929700
C	1.20332500	-2.44959900	-0.44648200
H	0.94619900	-2.02285300	0.53315900
H	0.37138500	-3.08387000	-0.78338500

H	2.09365000	-3.08704100	-0.32372100
H	3.81432500	0.61393600	1.67757400

$S{=}P(OEt)_3$

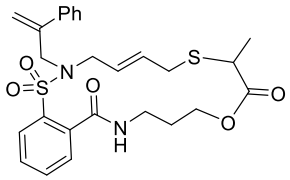
S	0.33098400	-0.63669500	1.80347300
P	0.05282500	-0.19393700	-0.06314300
O	-0.63908100	-1.32406500	-0.95312600
O	-0.86241900	1.08133200	-0.36177700
O	1.35799800	0.15607000	-0.91438600
C	-1.64113300	-2.21479300	-0.43391600
C	-2.93059000	-1.49415600	-0.11345400
H	-1.23539000	-2.72168800	0.45474700
H	-1.78710600	-2.96300600	-1.22263700
H	-3.69594300	-2.22692100	0.17891300
H	-2.79396100	-0.79156100	0.72173300
H	-3.29367100	-0.93818400	-0.98930100
C	-0.60818900	2.32839600	0.30709400
C	-1.54415000	3.36582500	-0.25898500
H	0.44403400	2.61198600	0.14765300
H	-0.76745400	2.18740500	1.38696900
H	-1.37462500	4.32824200	0.24311700
H	-1.37220800	3.49760300	-1.33622400
H	-2.59053500	3.06900600	-0.10128500
C	2.56319500	-0.62178200	-0.79390900
C	3.60721100	0.15485700	-0.02846000
H	2.89066700	-0.83609900	-1.81990400
H	2.34121800	-1.58033000	-0.30029600
H	4.54092100	-0.42297400	0.02093100
H	3.81543200	1.11338900	-0.52461500
H	3.26046500	0.35250600	0.99585600



Int1

C	1.69751100	0.29099200	-0.00026200
O	0.37734400	-0.22945400	-0.00020300
C	-1.93896700	0.09386500	-0.00002500
H	-2.75620900	0.81658200	0.00005500
C	-0.61233100	0.68105200	-0.00013000
H	1.87686700	0.90587900	0.89290400
H	1.87686200	0.90568200	-0.89356600
O	-0.39678200	1.87735600	-0.00012800

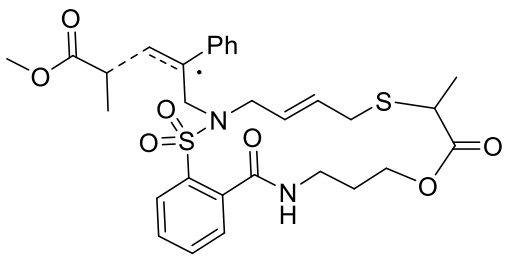
C	-2.22934400	-1.35683100	0.00000400
H	-2.83539300	-1.63009300	0.88062100
H	-2.83575800	-1.63005700	-0.88037100
H	-1.31334300	-1.95816400	-0.00019100
H	2.37150900	-0.57207400	-0.00017400



M

C	0.98849700	-3.56631300	-1.05717300
C	-0.40908400	-3.11533300	-0.69473500
N	-0.44135100	-1.68455800	-0.38369300
S	-1.42171900	-1.15213700	0.82638800
O	-1.41870500	-2.17461200	1.86497100
O	-1.02345700	0.21105100	1.14595000
C	-3.08769400	-1.08787500	0.17460500
C	-3.67447200	0.10418900	-0.26539200
C	-4.99457900	0.06025900	-0.72878300
C	-5.69716000	-1.14164500	-0.77361200
C	-5.09532200	-2.32233400	-0.33886000
C	-3.79134300	-2.29483100	0.14634900
C	-0.14975300	-0.75163100	-1.47296300
C	1.16549300	-0.03389600	-1.35128400
C	1.94986700	-0.02924000	-0.27290500
C	3.26836700	0.67941300	-0.13078300
H	-5.47121700	0.98555100	-1.05911800
H	-5.64503800	-3.26400100	-0.36248000
H	-3.32192600	-3.20487900	0.52314900
H	-0.95681900	-0.00363200	-1.56632700
H	-0.16805600	-1.32804500	-2.41147200
H	1.45652100	0.54480100	-2.23567500
H	1.63422100	-0.60169000	0.60538600
H	4.10057100	-0.02671400	-0.29112700
C	-2.98106000	1.45240000	-0.32375400
O	-2.27952600	1.76147200	-1.27542400
N	-3.30175100	2.28868800	0.67603700
H	-3.83349400	1.92387300	1.45958500
H	-1.09274900	-3.34212100	-1.52948700
H	-0.76044100	-3.66433300	0.18904800
H	-6.72356100	-1.15385200	-1.14323500

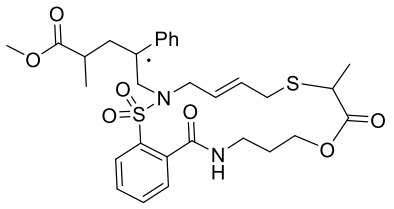
H	3.38682500	1.06000000	0.89478200
S	3.58516100	2.04508600	-1.28714700
C	2.18183800	3.13314800	-0.88317100
O	0.91912200	3.61935000	1.16129700
C	-0.30668800	3.33929600	0.46927200
C	-1.43176000	3.80282900	1.37374100
H	-1.26882700	4.86609700	1.60917200
H	-1.39532500	3.24540200	2.32253100
C	-2.81449300	3.65439100	0.74319300
H	-2.80922600	4.06354500	-0.27789000
H	1.26422000	2.63103300	-1.20657500
H	-3.54335800	4.22902700	1.32830900
C	2.06643600	-3.35458800	-0.05314400
C	1.76941500	-3.24833300	1.31429500
C	3.40331100	-3.21077400	-0.45773500
C	2.78070500	-3.01804700	2.24733100
H	0.73703800	-3.31423000	1.66115600
C	4.41287800	-2.98186100	0.47436600
H	3.65246100	-3.24781400	-1.52004600
C	4.10549900	-2.88273500	1.83309300
H	2.52771600	-2.93590700	3.30610200
H	5.44421300	-2.86461000	0.13601300
H	4.89444700	-2.69390000	2.56326000
H	-0.37346100	2.26114200	0.26600800
H	-0.34224900	3.89153400	-0.48221500
C	2.12332700	3.44799700	0.61056700
O	3.10282200	3.60971500	1.28803800
C	1.21198900	-4.13706500	-2.24834200
H	2.19304300	-4.52780800	-2.52762300
H	0.40158300	-4.24810700	-2.97313800
C	2.34632800	4.44651000	-1.65105600
H	3.26681900	4.95991200	-1.33909200
H	2.39500600	4.25159200	-2.73134400
H	1.49242100	5.11262700	-1.45929900



TS2

C	-2.64497600	-0.79848600	0.10887200
C	-2.05544600	0.56528300	0.37817400
N	-0.59168600	0.52863400	0.28279800
S	0.30152400	1.46938900	1.29475900
O	-0.39692400	1.50930700	2.57367300
O	1.67734800	0.99758600	1.23261200
C	0.27388500	3.13485800	0.64000000
C	1.33022100	3.65883100	-0.11417700
C	1.23118800	4.98112600	-0.56233700
C	0.10123200	5.74720500	-0.28559200
C	-0.94655500	5.20743900	0.46027000
C	-0.85696600	3.90179500	0.93336000
C	-0.01134700	0.20333600	-1.02094400
C	0.62299100	-1.15705200	-1.10250700
C	0.88074200	-1.95311100	-0.06421900
C	1.51117700	-3.31702300	-0.12048000
H	2.05507200	5.40822000	-1.13792100
H	-1.82913300	5.80658300	0.68754700
H	-1.65477800	3.47958700	1.54670200
H	0.73569500	0.96308400	-1.31087200
H	-0.81765600	0.27856600	-1.76752300
H	0.90951200	-1.47266500	-2.11253300
H	0.60147900	-1.61074000	0.93733300
H	0.73419300	-4.09934900	-0.08376900
C	2.57158500	2.89348500	-0.53323500
O	2.57190700	2.19297300	-1.53466500
N	3.66276300	3.14819000	0.20539600
H	3.55332100	3.68208000	1.06138500
H	-2.46544200	1.28930200	-0.34585400
H	-2.32146500	0.90896600	1.38746600
H	0.04258800	6.77429000	-0.64886500
H	2.14757700	-3.47890700	0.76221700
S	2.48893900	-3.69459000	-1.60559500
C	3.72688800	-2.36203300	-1.51401800
O	4.81294700	-1.15632300	0.32337300
C	4.43276800	0.09288600	-0.27252600
C	5.18402800	1.17602300	0.47689900
H	6.25975400	0.94622500	0.42608400
H	4.89280000	1.15853800	1.53851700
C	4.96249700	2.57520800	-0.09344000
H	5.08421800	2.56086200	-1.18655000
H	3.21166400	-1.41264400	-1.69301800
H	5.71802300	3.25692200	0.31674700
C	-2.29717600	-1.90784600	1.01705500

C	-1.73795000	-1.65675800	2.28437600
C	-2.49098300	-3.24935400	0.63549600
C	-1.39135100	-2.70593000	3.13411200
H	-1.54100300	-0.63286500	2.60582500
C	-2.14120300	-4.29513500	1.48515700
H	-2.89364700	-3.48138700	-0.35166000
C	-1.58858600	-4.02965500	2.74040900
H	-0.95624100	-2.48513700	4.11068000
H	-2.29235700	-5.32646000	1.16071400
H	-1.30929700	-4.85001400	3.40378600
H	3.34503500	0.22381400	-0.18430800
H	4.71649500	0.10917000	-1.33594600
C	4.43455200	-2.34160600	-0.16050600
O	4.71869800	-3.33797600	0.44868700
C	-3.54252800	-0.93637600	-0.91270000
C	-5.56702200	-0.61999400	0.07785200
H	-5.62490100	-1.64904400	0.43766900
C	-7.02641800	1.18610900	-2.73030600
H	-6.45271500	0.75630300	-3.56336000
H	-8.04787200	0.78182700	-2.75889400
C	-6.26249300	-0.40310600	-1.18589200
O	-6.63902900	-1.28647800	-1.92839200
O	-6.40351500	0.90061200	-1.48706300
H	-3.91298700	-1.91032400	-1.23419700
H	-3.67312200	-0.10947700	-1.61602900
C	-5.34942200	0.47342000	1.06421700
H	-4.63496900	0.15994100	1.83868100
H	-4.97796100	1.38628900	0.57806100
H	-6.29554400	0.73150400	1.57264800
C	4.77404300	-2.59221300	-2.60579500
H	5.29770700	-3.54418100	-2.43930900
H	4.29457400	-2.61642700	-3.59420600
H	5.51554600	-1.77976800	-2.60201100
H	-7.05483100	2.27720000	-2.82046600

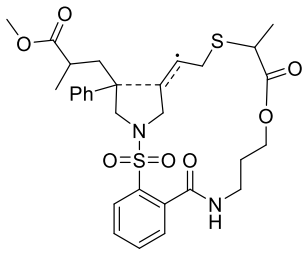


Int2

C	-2.69694200	0.09598300	0.59163700
C	-1.79162400	1.29242500	0.71438000

N	-0.39051200	0.91578400	0.46444600
S	0.81858500	1.61413700	1.33042300
O	0.28442400	1.90854400	2.65500200
O	1.99994800	0.77370100	1.19452900
C	1.19234000	3.18622200	0.56149300
C	2.27505300	3.35334400	-0.30956900
C	2.50315400	4.62649100	-0.84474000
C	1.66201100	5.69290600	-0.53587900
C	0.58232800	5.50762800	0.32772700
C	0.35125200	4.25392000	0.88549500
C	-0.05829400	0.40207100	-0.86412100
C	0.14760800	-1.08571000	-0.92565100
C	0.25755100	-1.89084600	0.13159300
C	0.47010200	-3.37884600	0.10402300
H	3.35325700	4.77543900	-1.51375600
H	-0.07346300	6.34205900	0.57912900
H	-0.47035300	4.10254000	1.58755400
H	0.84662600	0.90118800	-1.25267500
H	-0.87132900	0.69426500	-1.54798000
H	0.24196000	-1.49889400	-1.93658300
H	0.17784600	-1.45081500	1.13085200
H	-0.48834100	-3.90510300	0.24887100
C	3.20951400	2.24906900	-0.76738100
O	2.92369600	1.53583100	-1.71794400
N	4.38925400	2.21135100	-0.12906900
H	4.51179000	2.79083100	0.69492300
H	-2.10064800	2.06637400	-0.00772200
H	-1.84695500	1.72621400	1.72202700
H	1.85538300	6.67603000	-0.96773200
H	1.11446100	-3.68603300	0.94104300
S	1.15959600	-4.06807400	-1.42975800
C	2.72853500	-3.14569300	-1.51243100
O	4.26918300	-2.23844700	0.16583100
C	4.20871100	-0.95417700	-0.47244800
C	5.29827900	-0.10691900	0.15578800
H	6.25513600	-0.64031000	0.04399800
H	5.10478700	0.00085400	1.23424200
C	5.43994600	1.27381400	-0.48150400
H	5.46063100	1.18275000	-1.57751100
H	2.49115700	-2.09524500	-1.71037200
H	6.39083100	1.72159200	-0.16674200
C	-2.67256100	-0.93505900	1.59437900
C	-1.87068500	-0.81500700	2.76082300
C	-3.42455800	-2.13000400	1.44579600

C	-1.82405000	-1.83002400	3.70803300
H	-1.25699000	0.07417000	2.91238400
C	-3.36898400	-3.14013100	2.39931100
H	-4.05534300	-2.27240500	0.56743000
C	-2.56915500	-3.00128900	3.53709600
H	-1.19388900	-1.70951000	4.59145100
H	-3.95624600	-4.04870500	2.25245000
H	-2.52618400	-3.79709300	4.28243400
H	3.21497400	-0.51308900	-0.31233400
H	4.39180700	-1.05739600	-1.55286600
C	3.53020500	-3.28145600	-0.21908200
O	3.57330600	-4.29590600	0.42419100
C	-3.60158000	0.00041400	-0.59902500
H	-3.56343900	-1.01214000	-1.03404900
H	-3.26028600	0.69786700	-1.37863300
C	-5.07408600	0.34570600	-0.26162900
H	-5.43025600	-0.34378000	0.51663800
C	-6.44244000	0.72406300	-3.66309400
H	-6.20367300	-0.25525200	-4.09974800
H	-7.52258700	0.77588100	-3.47050200
C	-5.92768200	0.05644000	-1.47574000
O	-6.69925300	-0.86317200	-1.57770600
O	-5.70813400	0.93065300	-2.46158400
C	-5.22629400	1.78864300	0.21220300
H	-4.66287500	1.94336700	1.14432500
H	-4.84736800	2.48988900	-0.54505700
H	-6.28046300	2.03048600	0.41085200
C	3.56466100	-3.70846300	-2.66387300
H	3.80954300	-4.76387500	-2.47877100
H	3.01077900	-3.63095100	-3.60976900
H	4.50324900	-3.14434600	-2.76698400
H	-6.14487400	1.52347300	-4.34930200

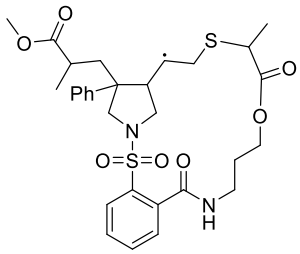


TS3

C	-2.31168500	0.26846400	0.34642400
C	-1.54999500	1.57116100	0.58160300
N	-0.15349000	1.41871100	0.17664500

S	1.13087900	1.70870500	1.13865000
O	0.60387700	2.14385500	2.42780100
O	2.05711700	0.58101600	1.08961100
C	1.98709800	3.10338600	0.41939200
C	3.12887400	2.94596000	-0.37345800
C	3.76742800	4.09707500	-0.84907300
C	3.26368600	5.36335100	-0.56085400
C	2.11631100	5.50105100	0.22093100
C	1.48043200	4.36886200	0.72076900
C	-0.03677700	0.67398200	-1.06762700
C	-0.76653600	-0.64286700	-0.89123100
C	-0.16396100	-1.64088000	-0.15268200
C	-0.64224900	-3.04948200	-0.13390100
H	4.66771200	3.99010400	-1.45773400
H	1.72216500	6.49113200	0.45344400
H	0.59948400	4.46104600	1.35829700
H	1.02453700	0.53413300	-1.31857100
H	-0.49821200	1.26742600	-1.87260800
H	-1.47425200	-0.94392200	-1.67031600
H	0.68857700	-1.37763100	0.48494200
H	-1.73111200	-3.10899900	-0.27799100
C	3.69469000	1.61014700	-0.81484500
O	3.19679100	0.99058200	-1.74290800
N	4.82094200	1.24419300	-0.18217600
H	5.11531300	1.78317200	0.62577300
H	-1.99509300	2.36241400	-0.04035700
H	-1.59054900	1.89457700	1.62906900
H	3.77300600	6.24796900	-0.94609000
H	-0.38013200	-3.55845500	0.80408000
S	0.03544800	-4.04688800	-1.53028200
C	1.78299700	-3.54776100	-1.45998200
O	3.36213600	-2.93600100	0.31071000
C	3.73026900	-1.76085400	-0.42551400
C	4.99861400	-1.22294900	0.20713000
H	5.76576900	-2.01170600	0.16487300
H	4.81477200	-0.99716700	1.26873800
C	5.53926700	0.02224500	-0.49510000
H	5.51558200	-0.11723900	-1.58591100
H	1.83689000	-2.49064300	-1.74494900
H	6.58504000	0.17873200	-0.20273200
C	-2.44662200	-0.66607200	1.47645600
C	-1.55482700	-0.61709600	2.56791700
C	-3.39990600	-1.70492300	1.46497100
C	-1.62133400	-1.55287000	3.59757300

H	-0.78858000	0.15858700	2.61698300
C	-3.46657700	-2.63766600	2.49827300
H	-4.10184600	-1.79637100	0.63489200
C	-2.57785100	-2.56964200	3.57185300
H	-0.91537100	-1.48721800	4.42788000
H	-4.21958600	-3.42731400	2.46006500
H	-2.62918900	-3.30123900	4.38000500
H	2.91338700	-1.02789700	-0.37266500
H	3.92228100	-2.01188600	-1.47940900
C	2.37940000	-3.75799800	-0.07011000
O	2.05312700	-4.65476500	0.66015500
C	-3.44930100	0.35297000	-0.64553900
H	-3.65441300	-0.64177500	-1.07050400
H	-3.14166900	0.99757800	-1.48505500
C	-4.77553800	0.90487500	-0.06267600
H	-5.11052100	0.22961900	0.73642800
C	-6.67912800	1.71157300	-3.11814300
H	-6.50820100	0.80375200	-3.71272600
H	-7.71531800	1.71033300	-2.75386100
C	-5.82163700	0.77709100	-1.14804600
O	-6.59661700	-0.14014400	-1.25074600
O	-5.76444000	1.77827300	-2.02978300
C	-4.67097500	2.32532200	0.48242200
H	-4.01057400	2.35221800	1.36087600
H	-4.27634900	3.01544000	-0.27651400
H	-5.65837100	2.69218500	0.79858600
C	2.56966000	-4.39251800	-2.46514700
H	2.52098700	-5.45569700	-2.19037500
H	2.15373500	-4.26615800	-3.47433500
H	3.62552300	-4.08555800	-2.48656200
H	-6.49772300	2.60090800	-3.73028000



Int3

C	0.48385500	-1.38879200	0.46581300
C	-1.04413300	-1.21552200	0.35903600
N	-1.29630100	0.10388400	0.94946800

S	-2.75184000	0.44868100	1.59278500
O	-3.18194800	-0.58331900	2.53351100
O	-2.70126300	1.82720300	2.07220400
C	-3.81005700	0.29717100	0.15709700
C	-3.49159600	0.91643600	-1.06155900
C	-4.30101800	0.63784400	-2.16660500
C	-5.41329200	-0.19508600	-2.05331100
C	-5.72614200	-0.78336100	-0.83028000
C	-4.91117500	-0.54944000	0.27534100
C	-0.07388100	0.84877700	1.24227600
C	0.93811700	0.12426600	0.35124300
C	2.35216700	0.44836400	0.67602200
C	3.42825300	0.47361900	-0.34896000
H	-4.04991600	1.09144100	-3.12672000
H	-6.59096800	-1.44130400	-0.73666500
H	-5.10904700	-1.03634800	1.23025800
H	0.21656600	0.77075300	2.30433500
H	-0.19381200	1.90770700	0.98711100
H	0.73330700	0.40530200	-0.69817400
H	2.60983200	0.69179400	1.70810800
H	3.54427900	-0.49365900	-0.86504600
C	-2.34976000	1.88311900	-1.33170100
O	-1.58876400	1.69370100	-2.26654800
N	-2.35826000	3.00104300	-0.57780800
H	-2.98055200	3.03574800	0.22418100
H	-1.35262300	-1.21809500	-0.69953300
H	-1.61026600	-1.99362600	0.88723000
H	-6.03313100	-0.38899800	-2.93002700
H	4.40252500	0.71773100	0.09530800
S	3.11579600	1.63139100	-1.75372800
C	3.65226500	3.22994600	-1.02854700
O	1.75319600	3.61424500	0.50588200
C	0.80576100	3.67312200	-0.56186400
C	-0.39312900	4.45454800	-0.05690600
H	-0.15096300	5.52729100	-0.04380100
H	-0.61299200	4.16055600	0.98134500
C	-1.63168000	4.21351900	-0.91557200
H	-1.35858300	4.15090400	-1.97870500
H	3.21442000	3.98028600	-1.70238600
H	-2.32862200	5.05418300	-0.79858500
C	0.91953800	-1.94843600	1.81765800
C	0.06464800	-1.98247700	2.92788300
C	2.24130800	-2.39153000	1.99251800
C	0.51185900	-2.45288700	4.16557600

H	-0.96371200	-1.62430100	2.84926400
C	2.68803300	-2.86341300	3.22515200
H	2.93663200	-2.37165800	1.15047400
C	1.82255800	-2.89790300	4.31996200
H	-0.17559400	-2.46715000	5.01346000
H	3.71907600	-3.20638300	3.32991800
H	2.17006800	-3.26775600	5.28622800
H	0.52138900	2.65191800	-0.85835500
H	1.23236900	4.16797100	-1.44650100
C	3.06541400	3.40357900	0.36466300
O	3.75246700	3.35401900	1.35058700
C	1.05285300	-2.18737900	-0.71867500
H	2.13337600	-1.99700300	-0.79244000
H	0.60218100	-1.78415900	-1.64027000
C	0.85501500	-3.71441200	-0.69062900
H	1.44079200	-4.13056700	0.14048400
C	1.28837400	-4.58932300	-4.24905400
H	2.19258200	-4.01651900	-4.49615100
H	1.54472800	-5.65603500	-4.19563700
C	1.51464600	-4.25946600	-1.93990300
O	2.63045500	-4.71167300	-1.98851800
O	0.73325200	-4.14403900	-3.01668900
C	5.16373200	3.37716100	-1.00675000
H	5.44393100	4.36079900	-0.60284200
H	5.62774700	2.60859700	-0.37414000
H	5.55952300	3.28685500	-2.02644400
C	-0.59821300	-4.16397800	-0.56711300
H	-0.97576400	-3.95904000	0.44376700
H	-1.24016200	-3.64958200	-1.29609300
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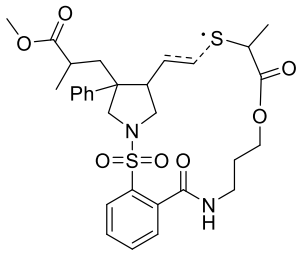
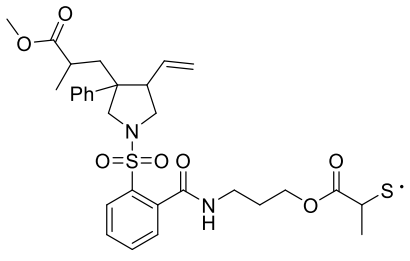


TS4

C	1.88227100	-0.27534000	0.14884900
C	1.23915700	-1.67196900	0.06352900
N	-0.17299300	-1.39895100	0.34664200

S	-1.15512200	-2.44016900	1.11791600
O	-0.32349800	-3.53534400	1.60028900
O	-1.95807000	-1.69914100	2.08653700
C	-2.24397000	-3.11094200	-0.15258900
C	-3.27129100	-2.39854100	-0.80681100
C	-3.91537900	-3.03217200	-1.87723800
C	-3.59670100	-4.32995000	-2.26631000
C	-2.59571000	-5.02579300	-1.59569200
C	-1.91303200	-4.40930700	-0.55103500
C	-0.55269700	-0.01477600	0.07097400
C	0.73813600	0.56565300	-0.52466500
C	0.81170400	2.04785000	-0.39168100
C	1.03778600	2.87907000	-1.45271800
H	-4.69218500	-2.47816600	-2.40523900
H	-2.33289700	-6.04363400	-1.88653100
H	-1.10931800	-4.93387500	-0.03581200
H	-0.84426500	0.50762200	0.99792700
H	-1.37690300	0.05388700	-0.65678100
H	0.77428500	0.30732300	-1.59543700
H	0.57752400	2.47967900	0.58554700
H	1.40819300	2.47782600	-2.39964300
C	-3.81319200	-0.99888400	-0.53844800
O	-4.03606400	-0.25320000	-1.48105500
N	-4.13613000	-0.71182300	0.73271400
H	-3.80456000	-1.33326200	1.46393700
H	1.36513000	-2.07571400	-0.95415100
H	1.63803100	-2.39719100	0.77843600
H	-4.13225600	-4.79360000	-3.09595400
H	1.13410100	3.95636700	-1.29654800
S	-1.22020500	2.89054700	-2.37236500
C	-1.88220100	4.27480000	-1.37356300
O	-2.06672500	3.13736400	0.80951000
C	-3.15933300	2.33803800	0.34596600
C	-3.72270000	1.60416800	1.54761600
H	-4.19368700	2.33342300	2.22362700
H	-2.90540900	1.11945800	2.10433400
C	-4.74392500	0.54006900	1.14379900
H	-5.37487900	0.89988500	0.31848000
H	-2.97457300	4.16862600	-1.45743000
H	-5.40024400	0.31800800	1.99489100
C	2.11344300	0.17615900	1.59187300
C	1.65329100	-0.54671100	2.70117800
C	2.81197400	1.37096600	1.83439300
C	1.87493800	-0.08780500	4.00231700

H	1.10839700	-1.48251000	2.57315500
C	3.03451500	1.83047000	3.13069300
H	3.19549400	1.95431500	0.99433700
C	2.56414000	1.10158900	4.22422700
H	1.50310800	-0.67243500	4.84579800
H	3.58190000	2.76197400	3.28624400
H	2.73699800	1.45835100	5.24107000
H	-2.81284000	1.64809500	-0.43507900
H	-3.94053100	2.97907700	-0.09108200
C	-1.47747600	4.08968000	0.08176300
O	-0.61649700	4.75921900	0.59224200
C	3.15061300	-0.15602600	-0.71470900
H	3.31376500	0.90801500	-0.95323000
H	2.94912500	-0.66128600	-1.67301900
C	4.45206000	-0.71981500	-0.11963900
H	4.74842000	-0.10567500	0.74145500
C	6.43286900	-1.23581700	-3.18821800
H	6.35599400	-0.24850000	-3.66379700
H	7.44708900	-1.36024300	-2.78527100
C	5.54699900	-0.50668200	-1.14376100
O	6.39014900	0.35195200	-1.08852600
O	5.46227400	-1.37341900	-2.15680900
C	-1.45087900	5.63440200	-1.89442200
H	-1.90202000	6.43785500	-1.29332400
H	-0.35896900	5.74107300	-1.84725000
H	-1.77264500	5.75064000	-2.93757300
C	4.36126000	-2.18460700	0.30375700
H	3.73993300	-2.28328200	1.20464900
H	3.92856000	-2.80414300	-0.49491100
H	5.35770000	-2.58254800	0.54554000
H	6.22094300	-2.02219800	-3.91980100

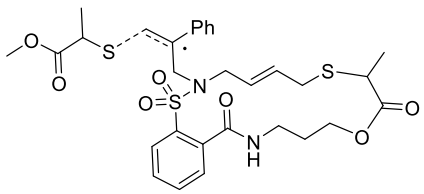


Int4

C	-1.07079000	-1.49008400	0.05786200
C	0.05377300	-2.28906200	-0.63988200
N	1.30841900	-1.61525900	-0.23384000
S	2.54957500	-1.54446600	-1.30245800

O	2.51683500	-2.79804400	-2.04308400
O	2.54059200	-0.31309300	-2.10243600
C	4.00904700	-1.51714100	-0.25488800
C	4.44379400	-0.43484700	0.53873400
C	5.58704500	-0.63768000	1.32329200
C	6.29833100	-1.83321500	1.30022600
C	5.85950700	-2.88424700	0.50107500
C	4.70867900	-2.72703500	-0.26486400
C	1.06648500	-0.54156800	0.72913600
C	-0.29781200	-0.91674500	1.30142800
C	-0.96574500	0.22227900	2.00618200
C	-1.56320400	0.12631600	3.19457600
H	5.91420700	0.18031200	1.96521000
H	6.40115900	-3.83048000	0.47516200
H	4.34050400	-3.54789100	-0.87935600
H	1.02609600	0.44472300	0.23743100
H	1.83845000	-0.52118900	1.51214200
H	-0.16751500	-1.75791100	2.00110300
H	-0.96671700	1.18581200	1.48320700
H	-1.58420300	-0.81799400	3.74796100
C	3.83349200	0.94918300	0.74068900
O	3.81021500	1.42159200	1.86737500
N	3.43604100	1.63228800	-0.34541500
H	3.38530800	1.15741600	-1.24278000
H	0.06603900	-3.32700800	-0.27861400
H	-0.05044500	-2.31000500	-1.73125300
H	7.19341800	-1.94180500	1.91434100
H	-2.04756800	0.99189400	3.65477400
S	-3.01874300	3.17365900	1.39206500
C	-2.63287700	4.70021100	0.49268600
O	-0.29524100	4.62324600	0.82646900
C	1.06436600	4.52360400	0.39453600
C	1.47707400	3.07591000	0.20317500
H	0.82998400	2.60382600	-0.55517200
H	1.34686000	2.53400900	1.15275500
C	2.93916900	2.98966100	-0.23114700
H	3.56648900	3.51988800	0.50059800
H	-2.58030000	5.44674800	1.30621900
H	3.07405300	3.47624100	-1.20680700
C	-1.59076300	-0.33143500	-0.79438300
C	-0.81344700	0.24516600	-1.80975500
C	-2.83914800	0.24961200	-0.52122100
C	-1.26637200	1.35337100	-2.52824000
H	0.17453600	-0.14885200	-2.04822500

C	-3.30149100	1.34855700	-1.24870200
H	-3.46869000	-0.15401200	0.27413700
C	-2.51430600	1.90833400	-2.25566500
H	-0.63228700	1.78391600	-3.30556200
H	-4.28481000	1.76740600	-1.02307400
H	-2.86801600	2.77155200	-2.82103200
H	1.65670000	4.99482700	1.18951500
H	1.19471200	5.09817000	-0.53323500
C	-1.23988800	4.62834900	-0.11270500
O	-1.01853000	4.60185100	-1.29470700
C	-2.19315800	-2.40902500	0.57012900
H	-2.76611600	-1.86218400	1.33699600
H	-1.71547400	-3.25574900	1.08854300
C	-3.18087400	-2.96596600	-0.47068400
H	-3.74661300	-2.13563300	-0.91310900
C	-4.64274900	-5.79647100	1.39067200
H	-4.91071400	-5.31045800	2.33873600
H	-5.55975900	-5.99693700	0.82020500
C	-4.21325800	-3.77381900	0.28711300
O	-5.31553700	-3.38482300	0.57947100
O	-3.75360300	-4.97715900	0.64022800
C	-3.68700700	5.09476800	-0.52704100
H	-3.42871100	6.06116900	-0.98314800
H	-3.75332000	4.34487900	-1.32654700
H	-4.66586100	5.18296000	-0.03898300
C	-2.52629700	-3.78384500	-1.58112200
H	-1.94856600	-3.13007800	-2.24837500
H	-1.85542700	-4.55087000	-1.16949800
H	-3.28865900	-4.28737300	-2.19341200
H	-4.11059700	-6.73301200	1.58644100

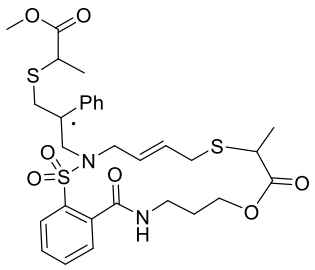


TS5

C	2.08451000	-1.65183200	0.14397400
C	1.84907400	-0.20536300	-0.21896700
N	0.42102900	0.11620100	-0.20679900
S	-0.15852100	1.17714200	-1.32545500
O	0.57351600	0.93918900	-2.56309600
O	-1.61038700	1.07912100	-1.30868200

C	0.28329400	2.81874100	-0.76848200
C	-0.62622000	3.65445200	-0.11047400
C	-0.19482300	4.92955200	0.27331700
C	1.11150500	5.34593300	0.02800800
C	2.00854900	4.49722600	-0.62075700
C	1.59214700	3.23394200	-1.02937000
C	-0.26946800	0.05768200	1.08313800
C	-1.24431300	-1.07824000	1.21915400
C	-1.65646300	-1.86741000	0.22639000
C	-2.62608000	-3.01083300	0.34000700
H	-0.89842900	5.59872000	0.77293600
H	3.03013100	4.82217600	-0.82151600
H	2.27534900	2.57289800	-1.56568600
H	-0.79773000	1.00708200	1.28183000
H	0.50179400	-0.02205200	1.86567300
H	-1.64804300	-1.22017000	2.22835100
H	-1.25274500	-1.69886700	-0.77710100
H	-2.08143100	-3.96752700	0.41045000
C	-2.04601200	3.27566000	0.26763500
O	-2.28313400	2.68391100	1.31023100
N	-2.99027300	3.74099400	-0.56463500
H	-2.69726300	4.16012800	-1.44120400
H	2.40311000	0.43973600	0.48370300
H	2.23315000	-0.01586700	-1.23237000
H	1.42844500	6.34213100	0.34026100
H	-3.24295700	-3.07852600	-0.56841800
S	-3.73194100	-2.99384700	1.78259800
C	-4.57472500	-1.40095100	1.51764500
O	-5.22080800	-0.11704500	-0.46873600
C	-4.56033900	1.03994100	0.06543600
C	-4.95913100	2.21062300	-0.81194300
H	-6.05856000	2.27113100	-0.82621300
H	-4.62526700	2.02660400	-1.84481700
C	-4.40920100	3.54979800	-0.32544500
H	-4.59043600	3.66249200	0.75368000
H	-3.84030000	-0.60247600	1.66588800
H	-4.93555400	4.36470300	-0.83788900
C	1.45776900	-2.70020100	-0.68761700
C	1.04481500	-2.42655200	-2.00298900
C	1.22066800	-3.98427900	-0.16648100
C	0.42396800	-3.40911200	-2.77210400
H	1.18035000	-1.43024700	-2.42702200
C	0.59668200	-4.96299800	-0.93532100
H	1.49804600	-4.21152800	0.86430100

C	0.19474800	-4.67947800	-2.24243900
H	0.10953500	-3.17662500	-3.79116100
H	0.41208100	-5.95004400	-0.50733400
H	-0.30062200	-5.44443700	-2.84298700
H	-3.47338900	0.87966700	0.05019300
H	-4.88729600	1.22032700	1.10092300
C	-5.18791900	-1.31405300	0.12120300
O	-5.69189300	-2.25269100	-0.43525200
C	2.90328100	-1.93607800	1.19389300
H	3.09133700	-2.96184400	1.51539400
H	3.25242700	-1.13354200	1.84736900
S	5.12187700	-1.96729600	-0.11505200
C	5.35012300	-0.16262500	-0.29901900
C	5.47485700	0.45006100	1.07755400
O	4.54851100	0.92175000	1.69395400
O	6.71026500	0.38796700	1.56129500
C	6.89747500	0.88104100	2.88464200
H	6.30147000	0.29800100	3.59994200
H	6.60572300	1.93764300	2.94906300
C	-5.69596800	-1.26544300	2.55017900
H	-6.44064600	-2.06229000	2.41345000
H	-5.28638200	-1.33027200	3.56778500
H	-6.19963800	-0.29355700	2.44278300
H	4.44791600	0.26255200	-0.75860600
C	6.56028100	0.09231100	-1.19324500
H	7.46306700	-0.36782300	-0.77059700
H	6.38101900	-0.32613100	-2.19235200
H	6.73306400	1.17448700	-1.29098100
H	7.96367900	0.77032800	3.10600600

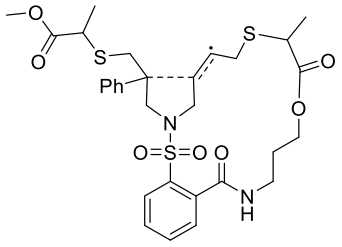


Int5

C	-2.17548900	-0.24481100	0.70899700
C	-1.37459800	1.02327700	0.83581100
N	0.04245900	0.78967400	0.51875400
S	1.21918600	1.54683600	1.38101600
O	0.70857400	1.73064500	2.73439800

O	2.46009900	0.81581300	1.16692900
C	1.43520000	3.18000500	0.68354000
C	2.47080900	3.47955900	-0.20928300
C	2.57994500	4.79386600	-0.67795100
C	1.66889500	5.77129900	-0.28402600
C	0.63723300	5.45382700	0.59943500
C	0.52453400	4.15755400	1.09272500
C	0.37432000	0.35268900	-0.83609000
C	0.68135900	-1.11350600	-0.95734400
C	0.88518900	-1.94014800	0.06901500
C	1.21518000	-3.40429400	-0.01451200
H	3.39222300	5.04622700	-1.36269100
H	-0.07282800	6.21817600	0.91735500
H	-0.25776700	3.90392800	1.81020500
H	1.23405900	0.92726100	-1.22226400
H	-0.46994200	0.61663200	-1.49272700
H	0.77560400	-1.48601400	-1.98392100
H	0.80338200	-1.53939300	1.08468300
H	0.30734100	-4.01195400	0.13671100
C	3.46955100	2.47746100	-0.75761100
O	3.19817300	1.78429100	-1.72715400
N	4.67643400	2.50855700	-0.17225400
H	4.78979700	3.05890500	0.67288400
H	-1.78769800	1.78629400	0.15420300
H	-1.42789800	1.41561000	1.85969400
H	1.76999400	6.78876700	-0.66465300
H	1.90657800	-3.68369600	0.79407800
S	1.91439000	-3.98471700	-1.58845700
C	3.39609300	-2.92982600	-1.68750000
O	4.92571900	-1.94396600	-0.04498700
C	4.73837100	-0.65159400	-0.64103900
C	5.77831800	0.26290000	-0.02267900
H	6.77068900	-0.18411100	-0.18974400
H	5.61959900	0.31587600	1.06549800
C	5.77980200	1.67288800	-0.60999500
H	5.75483300	1.62486200	-1.70860500
H	3.06538000	-1.89814000	-1.84609700
H	6.70636000	2.18415700	-0.32033600
C	-2.11929900	-1.26063100	1.72409700
C	-1.24221300	-1.14373000	2.83455100
C	-2.92628000	-2.42562600	1.64872400
C	-1.16965600	-2.14272000	3.79686100
H	-0.59686300	-0.26910300	2.92984400
C	-2.84797800	-3.41659700	2.61972500

H	-3.63589300	-2.54359900	0.82867600
C	-1.96742900	-3.28722900	3.69779600
H	-0.48013800	-2.02995900	4.63567100
H	-3.48335000	-4.30040400	2.53709400
H	-1.90588500	-4.06950500	4.45604000
H	3.71872800	-0.29784400	-0.43373200
H	4.89020600	-0.70887200	-1.72989300
C	4.24936600	-3.03073200	-0.42465800
O	4.38889400	-4.05068800	0.19568500
C	-3.06184200	-0.39065100	-0.47818200
H	-3.11115000	-1.42546900	-0.84495400
H	-2.71940700	0.25710100	-1.29703600
S	-4.76775700	0.15746800	-0.03472900
C	-5.46723600	0.23759800	-1.73389100
C	-6.94521300	-0.06944500	-1.61558000
O	-7.48072800	-1.05253400	-2.05501300
O	-7.59346000	0.88756900	-0.95240000
C	-8.99228900	0.69045800	-0.76770300
H	-9.18005500	-0.22816600	-0.19558000
H	-9.50337900	0.62147200	-1.73733200
C	4.23935700	-3.38788700	-2.87964700
H	4.57784800	-4.42339000	-2.73361100
H	3.65087600	-3.33194500	-3.80593200
H	5.12336800	-2.74350600	-2.99352500
H	-5.02751800	-0.59248900	-2.30167100
C	-5.19985200	1.57615000	-2.40714100
H	-5.64801900	2.39297000	-1.82650200
H	-4.11780900	1.75203200	-2.48609800
H	-5.62413600	1.58599300	-3.42286300
H	-9.35556700	1.56062500	-0.21198700

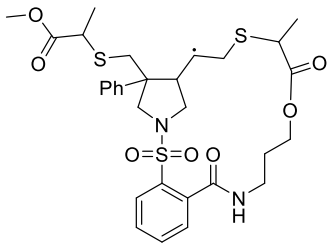


TS6

C	-1.85777700	-0.37560800	0.35394500
C	-1.38527100	1.03827900	0.67856200
N	-0.00553500	1.23299700	0.23193100
S	1.20839400	1.71638600	1.21564000
O	0.62074800	1.95141700	2.52968100

O	2.34775300	0.81017500	1.09762200
C	1.75032000	3.29739100	0.58310500
C	2.88914500	3.42473800	-0.21957400
C	3.27792800	4.70973500	-0.61528700
C	2.53495100	5.82719800	-0.24128500
C	1.39436100	5.67970900	0.54835700
C	1.00515800	4.41225400	0.97059200
C	0.25962400	0.55998600	-1.03168300
C	-0.12680300	-0.89832900	-0.88493700
C	0.66728300	-1.73960200	-0.13868500
C	0.49970600	-3.21905000	-0.12629700
H	4.17302500	4.82652900	-1.22975800
H	0.81367700	6.55297300	0.84810800
H	0.13339900	4.28338300	1.61428200
H	1.31726600	0.68700400	-1.30402700
H	-0.34731400	1.04246000	-1.81367200
H	-0.74332400	-1.34562100	-1.67192900
H	1.43348000	-1.30274800	0.51131900
H	-0.56055100	-3.50608500	-0.20322700
C	3.70403200	2.26179900	-0.75074000
O	3.31531400	1.60078600	-1.70220200
N	4.90268200	2.10740300	-0.16601400
H	5.10831700	2.65459300	0.66371500
H	-2.03014200	1.75391600	0.14243100
H	-1.45280100	1.25828600	1.75034400
H	2.85190500	6.81969400	-0.56513900
H	0.92189800	-3.66917200	0.78239800
S	1.28665300	-4.03025300	-1.58181400
C	2.89648900	-3.18208300	-1.57202000
O	4.39022200	-2.30130500	0.16098300
C	4.46931400	-1.05017200	-0.53675500
C	5.61928800	-0.27819100	0.08027300
H	6.53505700	-0.88002200	-0.02706700
H	5.43633600	-0.14497900	1.15765900
C	5.85049700	1.08497600	-0.57044000
H	5.80805700	0.99543200	-1.66579000
H	2.71621500	-2.12899300	-1.81792200
H	6.85088400	1.44873900	-0.30479900
C	-1.86798000	-1.37243300	1.43317400
C	-0.93394300	-1.28403400	2.48637400
C	-2.73590200	-2.48195300	1.41788700
C	-0.86682000	-2.26392100	3.47227800
H	-0.24297600	-0.43943200	2.53181600
C	-2.66934500	-3.45910300	2.41027000

H	-3.48367400	-2.58235700	0.62974700
C	-1.73253000	-3.36017500	3.43943000
H	-0.13051500	-2.17204400	4.27308900
H	-3.35782200	-4.30569700	2.37698900
H	-1.67885200	-4.12843800	4.21265200
H	3.51838900	-0.51042400	-0.42606200
H	4.66739600	-1.21813500	-1.60615300
C	3.59254100	-3.30425600	-0.21808900
O	3.50479200	-4.27593300	0.48339200
C	-2.93061100	-0.44683500	-0.69201900
H	-3.05276000	-1.46052500	-1.09681800
H	-2.68621000	0.23265800	-1.52175900
S	-4.53757100	0.11621800	0.01068800
C	-5.36793500	0.57863500	-1.56375600
H	-5.05375000	-0.15128800	-2.32060400
C	-6.85258600	0.36078800	-1.36104300
O	-7.50895000	-0.47176500	-1.92901300
O	-7.35503700	1.20739100	-0.46299800
C	-8.74517200	1.07510400	-0.18048400
H	-8.96441400	0.07450600	0.21598700
H	-9.34075400	1.24114200	-1.08811500
C	-5.03880800	2.00166000	-1.99125000
H	-5.36145200	2.71594900	-1.22246400
H	-3.95534400	2.11146700	-2.14208200
H	-5.54372400	2.24489400	-2.93878200
C	3.78876700	-3.81453100	-2.64234800
H	3.97568300	-4.87203300	-2.40800200
H	3.30532400	-3.74780600	-3.62684000
H	4.75562900	-3.29313800	-2.69722700
H	-8.98147700	1.83689700	0.56901100

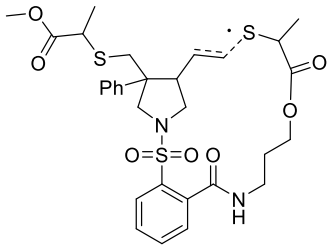


Int6

C	-1.48757100	-0.17606600	-0.00345800
C	-1.28865900	1.34252800	0.16263400
N	0.17824000	1.51255100	0.15430400
S	0.86260200	2.74177700	0.98735900
O	-0.16457700	3.76565800	1.11405100

O	1.48607500	2.27535200	2.23100300
C	2.15428100	3.35726600	-0.10942400
C	3.38994900	2.73824400	-0.40369900
C	4.21043400	3.37246800	-1.34705800
C	3.85997300	4.57508800	-1.95143700
C	2.64455700	5.17458600	-1.63959600
C	1.79238000	4.55760100	-0.72941100
C	0.89432000	0.27335400	-0.14798100
C	-0.20513100	-0.57499400	-0.81172700
C	0.08138300	-2.03274800	-0.89598700
C	0.56112600	-2.63157300	-2.15901700
H	5.15343200	2.88866000	-1.59997900
H	2.34847100	6.11569500	-2.10454900
H	0.82943100	5.00752200	-0.49164400
H	1.27925200	-0.21390700	0.76511400
H	1.73002700	0.44713500	-0.84360400
H	-0.34504900	-0.17729900	-1.83145300
H	0.15876500	-2.60735900	0.02925400
H	0.02908600	-2.22530400	-3.03215600
C	4.01234400	1.44530900	0.12108700
O	4.70223900	0.77626400	-0.63507000
N	3.85742900	1.15232600	1.42149900
H	3.21928900	1.71002100	1.98373900
H	-1.73394800	1.88159200	-0.68757300
H	-1.73843000	1.72783500	1.08589900
H	4.53888600	5.03834000	-2.66876400
H	0.47580900	-3.72634300	-2.17250400
S	2.34225000	-2.20322700	-2.49146800
C	3.20811500	-3.57420500	-1.62110800
O	2.79585800	-3.01940100	0.74901500
C	3.67419300	-1.89324300	0.65857400
C	3.73030900	-1.26369100	2.03583500
H	4.18660000	-1.97945500	2.73646500
H	2.70652500	-1.06574900	2.39325500
C	4.53390900	0.03355600	2.05314000
H	5.49990400	-0.11051400	1.54836700
H	4.22423000	-3.18455900	-1.47079600
H	4.73559100	0.32084400	3.09296500
C	-1.51615500	-0.90967400	1.33951400
C	-0.85138400	-0.40498200	2.46699300
C	-2.16349500	-2.14903100	1.46226600
C	-0.83204600	-1.11268400	3.67029400
H	-0.32627000	0.55010800	2.42407100
C	-2.14799500	-2.85590100	2.66401600

H	-2.69229100	-2.57824300	0.61019200
C	-1.48043300	-2.34158400	3.77533900
H	-0.30579200	-0.69321100	4.52975500
H	-2.66356000	-3.81576100	2.72963700
H	-1.46789500	-2.89435300	4.71626300
H	3.29892300	-1.19235200	-0.09916500
H	4.68027400	-2.22055100	0.35338900
C	2.54839500	-3.83733000	-0.27451200
O	1.78670000	-4.75617300	-0.11460100
C	-2.72290400	-0.45983800	-0.85762000
H	-2.77018500	-1.52014300	-1.14682000
H	-2.65314000	0.13591400	-1.77880200
S	-4.25339900	0.02196500	0.01318700
C	-5.31437100	0.30917600	-1.46040100
H	-5.06346200	-0.46333800	-2.19837400
C	-6.74195700	0.03600400	-1.03504800
O	-7.42555600	-0.85925700	-1.45637900
O	-7.15887900	0.91422700	-0.12398300
C	-8.48739200	0.73955500	0.35996600
H	-9.21100000	0.81920500	-0.46234600
H	-8.59618600	-0.24143300	0.84186700
C	-5.13898700	1.70717400	-2.03654800
H	-5.39424600	2.46523300	-1.28450300
H	-4.09710500	1.86012400	-2.35211700
H	-5.78700700	1.84386200	-2.91589700
C	3.24673900	-4.83840100	-2.46237900
H	3.78730300	-5.63463900	-1.92967200
H	2.23130700	-5.19971000	-2.67405000
H	3.75825900	-4.63720600	-3.41241200
H	-8.65715200	1.53781000	1.08930800

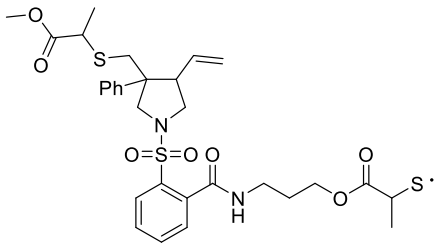


TS7

C	-1.49750000	-0.18041200	0.00586700
C	-1.30186100	1.34143200	0.14884000
N	0.16385900	1.51423000	0.14911200
S	0.84456500	2.74898800	0.97814900
O	-0.18767300	3.76744200	1.10444500

O	1.47110900	2.28562200	2.22118700
C	2.13218100	3.36926800	-0.12079800
C	3.37512400	2.76186400	-0.41034100
C	4.19034900	3.40270700	-1.35394100
C	3.82804600	4.59880200	-1.96413500
C	2.60513700	5.18565500	-1.65805500
C	1.75835200	4.56290200	-0.74687100
C	0.88593900	0.27566800	-0.14086500
C	-0.20697800	-0.58620900	-0.78632200
C	0.10200400	-2.04446400	-0.79792400
C	0.17294700	-2.77803000	-1.94884400
H	5.13923100	2.92857300	-1.60277500
H	2.29920600	6.12126500	-2.12768800
H	0.79023400	5.00352100	-0.51276900
H	1.28071800	-0.19473000	0.77740600
H	1.71742800	0.44452500	-0.84293000
H	-0.34825600	-0.23755900	-1.82198900
H	0.35786700	-2.51215100	0.15800600
H	-0.19611000	-2.36174100	-2.88981600
C	4.01282900	1.47679600	0.11749700
O	4.72333900	0.82359500	-0.63314400
N	3.84734200	1.17325900	1.41427300
H	3.19879900	1.72079800	1.97457200
H	-1.74212800	1.86537900	-0.71331600
H	-1.75994400	1.73913300	1.06261200
H	4.50369700	5.06666100	-2.68155100
H	0.32454700	-3.85900700	-1.90619900
S	2.46824600	-2.20795600	-2.51794600
C	3.29694200	-3.58477000	-1.63493800
O	2.84471700	-3.00593400	0.72319300
C	3.71518500	-1.87285500	0.64082600
C	3.75512600	-1.24644700	2.02044300
H	4.21827800	-1.95686000	2.72203500
H	2.72660700	-1.06498800	2.37304300
C	4.53785100	0.06340700	2.04676100
H	5.50914000	-0.06340500	1.54764300
H	4.31724300	-3.21591100	-1.45036600
H	4.72824700	0.35039700	3.08883200
C	-1.53224400	-0.89538200	1.35942500
C	-0.87715800	-0.37248800	2.48371500
C	-2.17171200	-2.13766900	1.49189400
C	-0.86103500	-1.06562000	3.69561200
H	-0.35655200	0.58450900	2.43186700
C	-2.15910900	-2.82981300	2.70211000

H	-2.69225400	-2.58056500	0.64166500
C	-1.50220800	-2.29728100	3.81127000
H	-0.34283100	-0.63261200	4.55320100
H	-2.66854100	-3.79229100	2.77613900
H	-1.49200500	-2.83847600	4.75890400
H	3.34147300	-1.17512200	-0.12043500
H	4.72612500	-2.19236000	0.34313100
C	2.61741000	-3.83785700	-0.29478800
O	1.86624000	-4.76417200	-0.12769500
C	-2.72597300	-0.48036900	-0.85268500
H	-2.76978100	-1.54416600	-1.12856300
H	-2.65189900	0.10354600	-1.78102100
S	-4.26195800	0.00888700	0.00402900
C	-5.31489300	0.27598900	-1.47924300
H	-5.05722300	-0.50420800	-2.20671500
C	-6.74429900	0.00346000	-1.05942900
O	-7.42349600	-0.89696500	-1.47676600
O	-7.16821900	0.88903300	-0.15884600
C	-8.49935100	0.71627900	0.31877700
H	-9.21806900	0.78730000	-0.50856500
H	-8.60922500	-0.26056300	0.80873300
C	-5.14039800	1.66785200	-2.07027600
H	-5.40203900	2.43368700	-1.32837300
H	-4.09732500	1.82035000	-2.38204900
H	-5.78406200	1.79233300	-2.95461200
C	3.33827800	-4.85506900	-2.46683600
H	3.87651400	-5.65057900	-1.93016400
H	2.32130100	-5.20954700	-2.68158400
H	3.85236100	-4.65999300	-3.41708600
H	-8.67484800	1.52070200	1.03992000

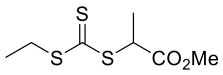


Int7

C	-1.35422800	-0.30017600	0.46237200
C	-1.13701700	-1.60594200	-0.33412900
N	0.27661700	-1.96241100	-0.08726600
S	1.11463500	-2.71870400	-1.27715100
O	0.16806500	-3.60822400	-1.93507500

O	1.83686000	-1.77663100	-2.14076800
C	2.31984300	-3.70251200	-0.37861300
C	3.45486600	-3.21053000	0.29886800
C	4.23831100	-4.14188400	0.99313500
C	3.94708300	-5.50244200	0.98861000
C	2.83012000	-5.96926300	0.30250600
C	2.01212700	-5.06595400	-0.36873700
C	0.93059600	-1.04186600	0.84406000
C	-0.25428600	-0.41317500	1.57615200
C	0.09021200	0.87525300	2.25649600
C	-0.26625400	1.18533300	3.50334400
H	5.10002300	-3.76909300	1.54711700
H	2.58402700	-7.03171100	0.29312100
H	1.12154700	-5.41298100	-0.89181600
H	1.51959700	-0.27284500	0.31590000
H	1.59005200	-1.57847400	1.54131200
H	-0.63014000	-1.13537100	2.31824800
H	0.65375800	1.60271200	1.66039400
H	-0.83258900	0.48458300	4.12514900
C	3.96630100	-1.78171600	0.45332200
O	4.37795800	-1.41765700	1.54454000
N	4.03646600	-1.01718900	-0.64858300
H	3.58655200	-1.33390700	-1.50303200
H	-1.79139200	-2.40343000	0.04875500
H	-1.34702500	-1.47954700	-1.40452400
H	4.59368800	-6.19560400	1.52859500
H	-0.00156300	2.15029000	3.94389500
S	0.47455400	4.42997400	1.33089300
C	1.73185600	5.33815200	0.38839700
O	3.45559400	3.73482500	0.49809200
C	4.32316100	2.73422900	-0.04037800
C	3.63802200	1.38121800	-0.09374700
H	2.75729300	1.43691200	-0.75495900
H	3.29276300	1.10870700	0.91571300
C	4.60573200	0.31487200	-0.60250300
H	5.48966700	0.28449400	0.05146600
H	2.34258500	5.79786500	1.18571400
H	4.94521100	0.56563400	-1.61692400
C	-1.11589700	0.94920900	-0.38901700
C	-0.15528600	0.95132800	-1.41342000
C	-1.79609500	2.14678900	-0.12755200
C	0.12422000	2.10921600	-2.13866600
H	0.39381200	0.04271100	-1.66432700
C	-1.53351500	3.30223700	-0.86854800

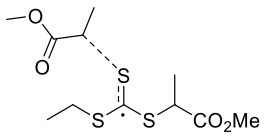
H	-2.55107600	2.19393200	0.65807900
C	-0.56582900	3.29095700	-1.87272400
H	0.88570500	2.08395200	-2.91984400
H	-2.08898400	4.21692900	-0.65162200
H	-0.35519800	4.19127700	-2.45174400
H	5.18768600	2.70545400	0.63557100
H	4.66312700	3.04515800	-1.03814200
C	2.63135600	4.35767600	-0.34334000
O	2.60892700	4.17343400	-1.53191800
C	-2.72977200	-0.31120800	1.12715400
H	-2.83453200	0.52215700	1.83736100
H	-2.83241900	-1.24787800	1.69269900
S	-4.07327100	-0.25677800	-0.10911800
C	-5.37574700	-1.08235100	0.89211600
H	-5.26993500	-0.72238700	1.92340600
C	-6.70848400	-0.55794500	0.40008300
O	-7.46465400	0.11438400	1.05013800
O	-6.94923500	-0.93050000	-0.85622100
C	-8.17421700	-0.47721500	-1.42512000
H	-9.02986000	-0.85691500	-0.85075700
H	-8.20924800	0.62045800	-1.44055900
C	-5.28660400	-2.60014800	0.81971000
H	-5.39587300	-2.94028700	-0.21844900
H	-4.31461900	-2.94269400	1.20264700
H	-6.07741600	-3.06057200	1.43167000
C	1.15803800	6.40337800	-0.52948900
H	1.97138500	6.95200300	-1.02608200
H	0.52576400	5.94958000	-1.30377100
H	0.55486300	7.11293700	0.05105600
H	-8.20329400	-0.86889400	-2.44670100



CTA

H	-4.46350200	-2.62450500	-0.02720200
C	-4.26517200	-1.58472900	0.27044100
H	-2.35185600	-1.44937400	-0.75769400
H	-2.24749400	-2.03925900	0.92553600
H	-4.78366900	-0.91595400	-0.43015900
C	-2.76495500	-1.34079700	0.25426200
H	-4.68727800	-1.43586400	1.27478500
S	-1.18012400	2.70637400	-0.40624900
S	-2.42571800	0.37176600	0.81534000

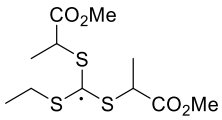
C	-1.26432400	1.07639800	-0.28109400
O	1.34793600	0.14001100	1.69709400
H	-0.28920000	-1.44266600	0.59355900
S	-0.22940400	0.06883400	-1.30842900
C	1.55106800	-0.41242200	0.64776400
C	0.48220600	-1.15770700	-0.12882500
H	3.98254400	-0.08138800	1.64471700
C	3.76813400	0.33005400	0.64941800
O	2.72127300	-0.40449400	0.01949300
C	0.98288800	-2.35699200	-0.91476300
H	0.13954500	-2.87660200	-1.38903100
H	1.48731300	-3.05684400	-0.23355900
H	3.48810000	1.38756000	0.74791900
H	1.70012900	-2.05437100	-1.68953300
H	4.64559400	0.23072000	0.00296600



TS8

H	-2.04239500	3.89254600	0.64951800
C	-2.07056800	2.94111100	0.09774800
H	-0.12979800	2.26563100	0.79964600
H	-0.06667100	3.19226400	-0.72098800
H	-2.63349400	2.20461100	0.68809900
C	-0.65072800	2.45915400	-0.14750700
H	-2.60508300	3.11403200	-0.84759300
S	-0.39766700	-1.88957100	-0.27839400
S	-0.66660400	0.89759800	-1.10809900
C	0.07315300	-0.32202400	-0.09907100
O	2.96755100	0.14110600	-1.81906700
H	1.84464400	1.89272000	-0.37211800
S	1.25947900	0.09107500	1.14563300
C	3.24439400	0.33616500	-0.66463100
C	2.42666800	1.21415900	0.26168100
H	5.49062200	-0.60038100	-1.69833100
C	5.06754300	-1.11918800	-0.82791100
O	4.27899500	-0.22545400	-0.04687100
C	3.23960300	1.97533000	1.29524600
H	2.58502800	2.63471500	1.88092300
H	3.99367900	2.59306200	0.78722600
H	4.45859100	-1.96569500	-1.17315500

H	3.76000900	1.28906600	1.97674300
C	-4.45989400	0.35443600	-0.74064200
O	-3.63785800	-0.16093800	0.29415800
C	-2.46718100	-1.91963500	1.28656700
H	-2.39462700	-3.00140400	1.40716800
C	-3.41626200	-1.48678900	0.26131100
H	-5.43065800	-0.15937600	-0.76237200
H	-3.97095600	0.23352000	-1.71858500
O	-3.95127700	-2.21995300	-0.54078600
C	-1.99213000	-1.01233800	2.36085200
H	-2.78045500	-0.87243400	3.12299900
H	-1.10926400	-1.42644800	2.86717000
H	-1.75271500	-0.01458900	1.96217200
H	5.86992500	-1.47416200	-0.17354000
H	-4.60641700	1.41824800	-0.52625300



Int8

H	-2.43313900	4.17184000	-0.12407300
C	-2.18599100	3.34839700	-0.80897000
H	-1.90521300	1.87247400	0.77854700
H	-0.42666700	2.75216800	0.31096500
H	-3.12765400	2.92432700	-1.18592600
C	-1.35858800	2.31144300	-0.06885200
H	-1.62891600	3.76895500	-1.65868600
S	-0.22612800	-1.88308000	-0.62061800
S	-0.95060600	0.93758600	-1.20285400
C	-0.10455600	-0.19111100	-0.19017100
O	2.81288900	0.18137000	-1.66457400
H	1.58588700	2.03962800	-0.43211700
S	0.91184100	0.32000400	1.13004100
C	3.03295900	0.49986500	-0.52446800
C	2.14284100	1.41843400	0.28133600
H	5.34389800	-0.45990300	-1.38148600
C	4.90375200	-0.90185300	-0.47758600
O	4.06234000	0.03804300	0.18276600
C	2.85516600	2.25347600	1.32949200
H	2.14001400	2.91694700	1.83432800
H	3.62815400	2.87237300	0.85190400
H	4.33266600	-1.79793600	-0.75694500
H	3.34156700	1.61607200	2.08023500

C	-4.26249600	0.31149800	0.02729800
O	-3.24301800	-0.55372800	0.51364700
C	-1.77172500	-2.39095200	0.27336900
H	-1.91631400	-3.42228600	-0.07797300
C	-2.93461000	-1.58609600	-0.27185300
H	-5.21301100	-0.23010200	-0.07409500
H	-3.97686100	0.71928400	-0.95259700
O	-3.51207300	-1.83459400	-1.29735600
C	-1.60286500	-2.32941900	1.77900900
H	-2.52075400	-2.67151900	2.28018400
H	-0.77079200	-2.97447100	2.09146500
H	-1.40083100	-1.30031900	2.10807900
H	5.69178100	-1.16501000	0.23521200
H	-4.36711100	1.11665200	0.76231900