

Vinyl polymers with fully degradable carbon backbones enabled by aromatization-driven C–C bond cleavage

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Materials, Reagents, and Methods.

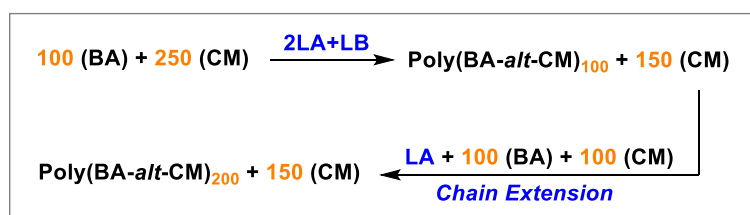
All synthesis and manipulations of air- and moisture-sensitive materials were carried out in flamed Schlenk-type glassware on a dual-manifold Schlenk line or in an argon-filled glovebox. HPLC-grade organic solvents were first sparged extensively with nitrogen during filling 20 L solvent reservoirs and then dried by passage through activated alumina [for dichloromethane (DCM), tetrahydrofuran (THF), Et₂O] followed by passage through Q-5 supported copper catalyst [for toluene (TOL), hexane] stainless steel columns. Acrylate monomers, including methyl acrylate (MA), ethyl acrylate (EA), *n*-butyl acrylate (BA), 2-ethylhexyl acrylate (EHA), and 1,4-butanediol diacrylate (BDA) were purchased from TCI Chemical Co, which were dried over CaH₂ overnight followed by vacuum distillation. Further purification of acrylate monomers involved titration with tri(*n*-octyl)aluminum (Sigma-Aldrich Co) to a yellow end point, followed by distillation under reduced pressure. Coumarin (CM, TCI Chemical Co) was purified by dissolving in DCM over CaH₂, filtering after stirring overnight, and removing the solvent. All purified monomers were stored in the brown bottles in a glovebox freezer at -30 °C for further use. Tri-*t*-butylphosphine (PtBu₃) was purchased from Strem Chemicals, which was purified by distillation over CaH₂. Literature procedures were employed to prepare tris(pentafluorophenyl)aluminum [Al(C₆F₅)₃],¹ methyl bis(2,6-*tert*-butyl-4-methylphenoxy)aluminum (MAD),² tris(pentafluorophenyl)borane [B(C₆F₅)₃],³ tris(2,4-difluorophenyl)borane [B(2,4-F₂Ph)₃],⁴ tetrahydrogeraniol acrylate (THGA),⁵ 7-allyloxycoumarin (ACM),⁶ 7-*n*-propoxycoumarin (PCM).⁶

General Polymerization Procedures.

Polymerizations were performed in 20 mL glass reactors inside the glovebox at room temperature (RT). A predetermined amount of Lewis acid (LA) was first dissolved in the predetermined amount of monomer and solvent inside a glovebox. The mixture was stirred for 10 minutes, and then the

polymerization was started by rapid addition of a predetermined amount of Lewis base (LB) in the solvent via a gastight syringe to the above mixture under vigorous stirring. After the measured time interval, a 0.2 mL aliquot was taken from the reaction mixture via syringe and quickly quenched into a 2 mL septum-sealed vial containing 0.4 mL of “wet” CDCl₃ mixed with by 250 ppm of benzoic acid; the quenched aliquots were later analyzed by quantitative ¹H NMR spectrum to obtain the percent monomer conversion data. After a desired period of time, the polymerization was immediately quenched by addition of 5 mL of methanol acidified with HCl (5%). The quenched mixture was precipitated into 100 mL methanol, filtered, washed with methanol to remove unreacted monomer, and dried in a vacuum oven at 80 °C to a constant weight.

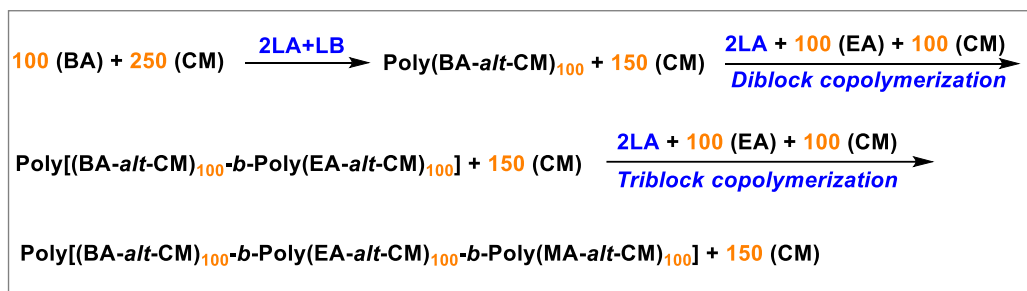
General Procedures for Chain Extension Experiment.



A 20 mL glass reactor was charged with B(2,4-F₂Ph)₃ (7.0 mg, 0.02 mmol), BA (128.0 mg, 1.0 mmol), CM (365.4 mg, 2.5 mmol), and DCM (0.3 mL) inside the glovebox at RT. The mixture was stirred for 10 minutes, and then the polymerization was started by rapid addition of PtBu₃ (2.0 mg, 0.01 mmol) in DCM (0.10 mL) via a gastight syringe to the above mixture under vigorous stirring. When the first batch of BA was consumed after 40 min, the resulting solution was kept stirring for another 30 min. Subsequently, the second batch of mixture B(2,4-F₂Ph)₃ (3.5 mg, 0.01 mmol), BA (128.0 mg, 1.0 mmol), CM (146.1 mg, 1.0 mmol), and DCM (0.2 mL) was added and the resulting mixture was stirred for an additional 60 min. The polymerization was immediately quenched by addition of 5 mL of methanol acidified with HCl (5%). The quenched mixture was precipitated into 100 mL methanol,

filtered, washed with methanol to remove unreacted monomer, and dried in a vacuum oven at 80 °C to a constant weight.

Synthesis of Poly(BA-*alt*-CM)-*b*-poly(EA-*alt*-CM) Diblock and Poly(BA-*alt*-CM)-*b*-poly(EA-*alt*-CM)-*b*-poly(MA-*alt*-CM) Triblock Copolymers.



A 20 mL glass reactor was charged with B(2,4-F₂Ph)₃ (7.0 mg, 0.02 mmol), BA (1.0 mmol), CM (365.4 mg, 2.5 mmol) and DCM (0.3 mL) inside the glovebox at RT. The mixture was stirred for 10 minutes, and then the polymerization was started by rapid addition of PtBu₃ (2.0 mg, 0.01 mmol) in DCM (0.10 mL) via a gastight syringe to the above mixture under vigorous stirring. When BA was consumed, the resulting solution was kept stirring for another 30 min, and the mixture of B(2,4-F₂Ph)₃ (7.0 mg, 0.02 mmol), EA (1.0 mmol), CM (146.1 mg, 1.0 mmol) and DCM (0.4 mL) was subsequently added. For the triblock copolymer, a mixture of B(2,4-F₂Ph)₃ (7.0 mg, 0.02 mmol), MA (1.0 mmol), CM (146.1 mg, 1.0 mmol) and DCM (0.4 mL) was subsequently added. After a desired period of time, the polymerization was immediately quenched by addition of 5 mL of methanol acidified with HCl (5%). The quenched mixture was precipitated into 100 mL methanol, filtered, washed with methanol to remove unreacted monomer, and dried in a vacuum oven at 80 °C to a constant weight. Triblock copolymer was prepared through the same procedure.

Characterizations.

NMR spectra were recorded on a Varian 400 MHz spectrometer. Chemical shifts for ^1H NMR and ^{13}C NMR spectra were referenced to internal solvent resonances and were reported as parts per million relative to SiMe_4 . Polymer number average molecular weight (M_n), and molecular weight distributions ($D = M_w/M_n$) were measured by gel permeation chromatography (GPC) analyses, carried out at 40 $^\circ\text{C}$ and a flow rate of 1.0 mL/min with THF as the eluent on a Waters E2695 GPC instrument equipped with a Wyatt OPTILAB[®] T-Rex refractive-index detector, one Agilent Plgel 5 μm guard column, and two Agilent Plgel 5 μm Mixed-C columns (Polymer Laboratories; linear range of MW = 200–2,000,000). The resultant chromatograms were processed with Wyatt ASTRA 7 software. Glass-transition temperatures (T_g) were measured by differential scanning calorimetry (DSC) on a DSC Q2500, TA Instrument. All T_g values were obtained from the second scan after the thermal history was removed from the first scan. The first heating rate was 10 $^\circ\text{C}/\text{min}$, while the cooling rate was 5 $^\circ\text{C}/\text{min}$ and the second heating rate was 10 $^\circ\text{C}/\text{min}$. The onset decomposition temperatures (T_d , defined at 5% weight loss) of the polymers were measured by thermal gravimetric analysis (TGA) on a TGA550, TA Instrument. Polymer samples were heated from ambient temperatures to 700 $^\circ\text{C}$ at a rate of 20 $^\circ\text{C}/\text{min}$. High resolution mass spectra (HRMS) were obtained on a Thermo Scientific Q Exactive HF Orbitrap-FTMS in positive electrospray ionization (ESI) method. FT-IR spectra were measured on a Bruker Tensor 27 FT-IR Spectrometer.

The polymer thin films for the tensile stress and strain testing were prepared by compression molding using a Carver Bench Top Laboratory Press (Model 4386) equipped with a two-column hydraulic unit (Carver, Model 3912, maximum force 24000 psi). Materials were loaded between non-stick Teflon paper sheets into a steel tile mold with inset dimensions 50×50×2 mm and compressed

between two 6" × 6" steel electrically heated platens at clamp force 5000 psi, temperature ($T_g + 45$) °C for 5 min. The obtained polymer thin films were cut into dumbbell-shaped samples, and the testing was carried out at 30 °C on the Instron 3367 tensile tester with a cross-head rate of 10 mm/min according to the ASTM standard. The data reported were averaged and from five determinations.

Table S1. Results of BA/CM copolymerizations by different polymerization methodologies.^a

Run	I./Cat.	Temp. (°C)	Time (min)	Conv. ^b (BA%)	Conv. ^b (CM%)	Incorp. ^b (CM mol%)	M_n ^c (kg/mol)	$\bar{D}$ ^c	I^* ^d
1	s-BuLi	25	1440	0	0	-	-	-	-
2	s-BuLi	0	1440	0	0	-	-	-	-
3	AIBN	80	1440	77.5	5.5	6.60	7.4	2.42	-
4	B(C ₆ F ₅) ₃ /PtBu ₃	25	20	>99	75.5	43.0	249.1	1.39	9.70
5	B(C ₆ F ₅) ₃	25	1440	0	0	-	-	-	-
6	PtBu ₃	25	1440	0	0	-	-	-	-
7	B(2,4-F ₂ Ph) ₃ /PiBu ₃	25	30	>99	82.0	45.0	38.5	1.17	64.3
8	Al(C ₆ F ₅) ₃ /PtBu ₃	25	5	>99	85.1	46.0	46.4	1.36	54.8
9	MAD/PtBu ₃	25	40	>99	92.5	48.1	40.9	1.17	64.8
10	B(2,4-F ₂ Ph) ₃ /PtBu ₃	25	80	>99	20.3	50.4	38.2	1.14	73.8

^a Runs 1–3: Initiator (I.) = 0.01 mol, [BA]₀: [CM]₀: [I.]₀ = 100:100:1, toluene = 0.4 mL; Runs 4, 7–9: LB = 0.01 mol, [BA]₀: [CM]₀: [LA]₀: [LB]₀ = 100:100:2:1, DCM = 0.4 mL; Runs 5–6: [BA]₀: [CM]₀: [LA]₀ or [LB]₀ = 100:100:1, DCM = 0.4 mL; Run 10: [BA]₀: [CM]₀: [LA]₀: [LB]₀ = 100:500:2:1, DCM = 0.7 mL. ^b Monomer conversion and CM incorporation of copolymer measured by quantitative ¹H NMR spectrum using ethylene carbonate as internal standard. ^c Number-average molecular weight (M_n) and molecular weight distribution ($\bar{D} = M_w/M_n$) determined by GPC at 40 °C in THF relative to PMMA standards. ^d Initiation efficiency (I^*)% = $M_n(\text{calcd})/M_n(\text{exptl}) \times 100$, where $M_n(\text{calcd}) = [\text{MW}(\text{BA})] \times [\text{BA}]_0/[\text{LB}]_0 \times \text{conversion\%} + [\text{MW}(\text{CM})] \times [\text{CM}]_0/[\text{LB}]_0 \times \text{conversion\%} + \text{MW}(\text{end groups: } -\text{PtBu}_3^+ \text{ or } -\text{PiBu}_3^+/-\text{H})$.

Stoichiometric Reaction of B(2,4-F₂Ph)₃ with PtBu₃ to Form B(2,4-F₂Ph)₃/PtBu₃ FLP.

In a typical procedure, a Teflon-valve-sealed J. Young-type NMR tube was charged with B(2,4-F₂Ph)₃ (35.0 mg, 0.1 mmol) in the glovebox. A solution of PtBu₃ (20.2 mg, 0.1 mmol) in 0.50 mL of benzene-*d*₆ was added to the above NMR tube *via* pipette at RT, and the resulting mixture was then taken out of the glovebox for NMR analysis, which indicated the formation of B(2,4-F₂Ph)₃/PtBu₃ FLP.

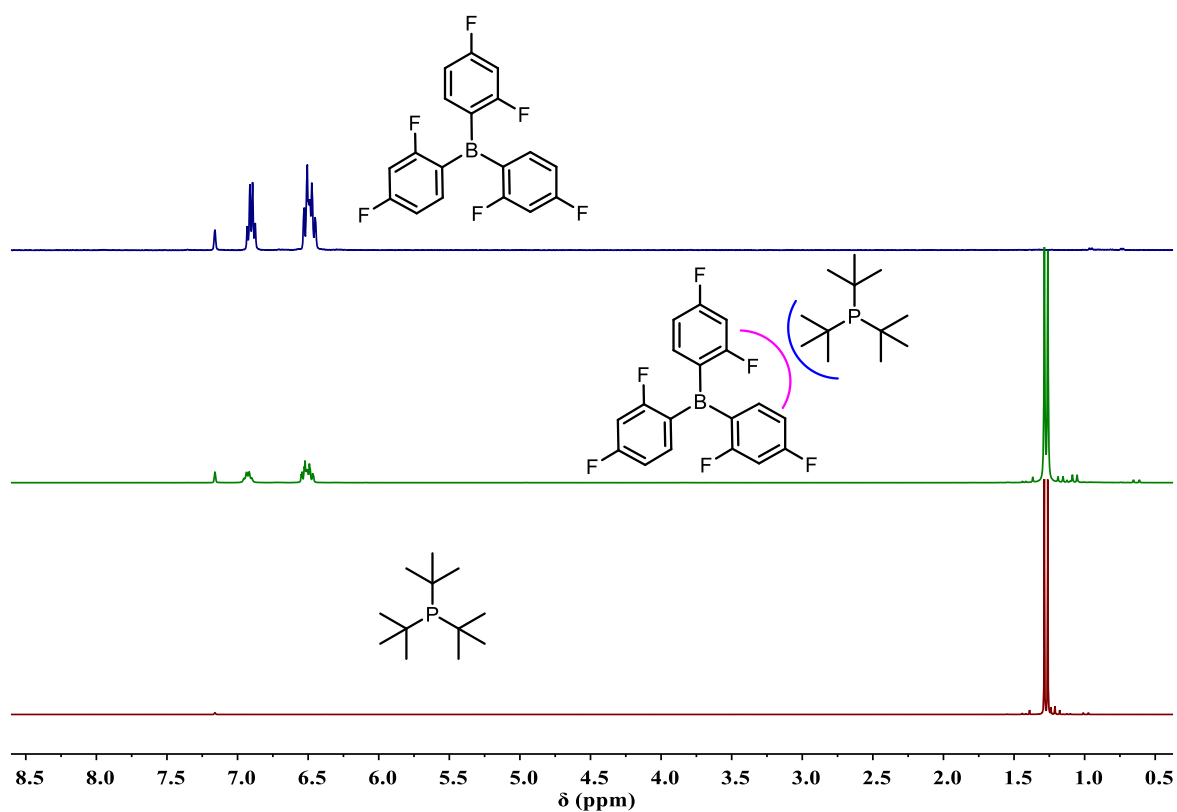


Figure S1. ^1H NMR spectra (benzene- d_6 , RT): (top) $\text{B}(2,4\text{-F}_2\text{Ph})_3$; (middle) $\text{B}(2,4\text{-F}_2\text{Ph})_3/\text{PtBu}_3$ FLP; (bottom) PtBu_3 .

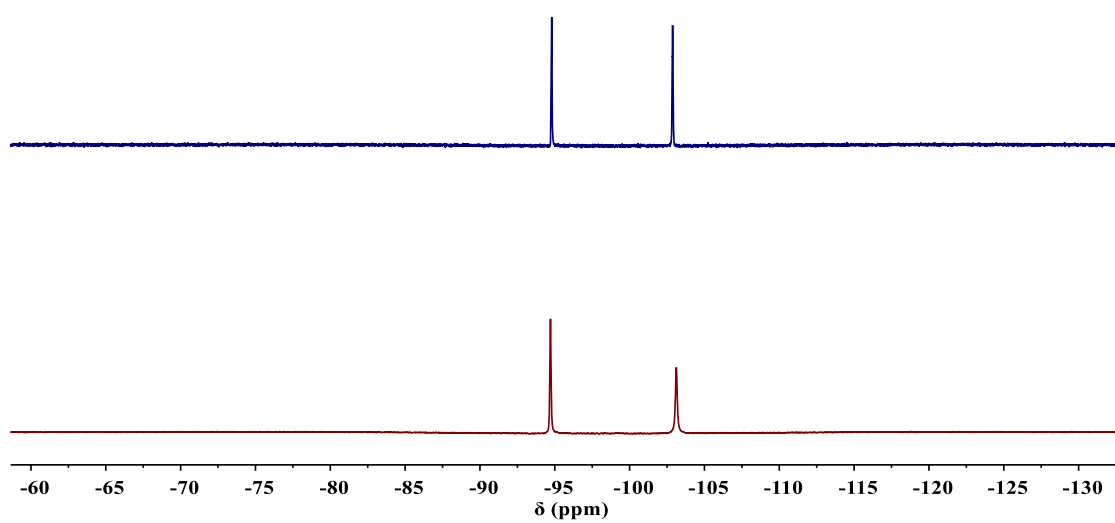


Figure S2. ^{19}F NMR spectra (benzene- d_6 , RT): (top) $\text{B}(2,4\text{-F}_2\text{Ph})_3$; (bottom) $\text{B}(2,4\text{-F}_2\text{Ph})_3/\text{PtBu}_3$ FLP.

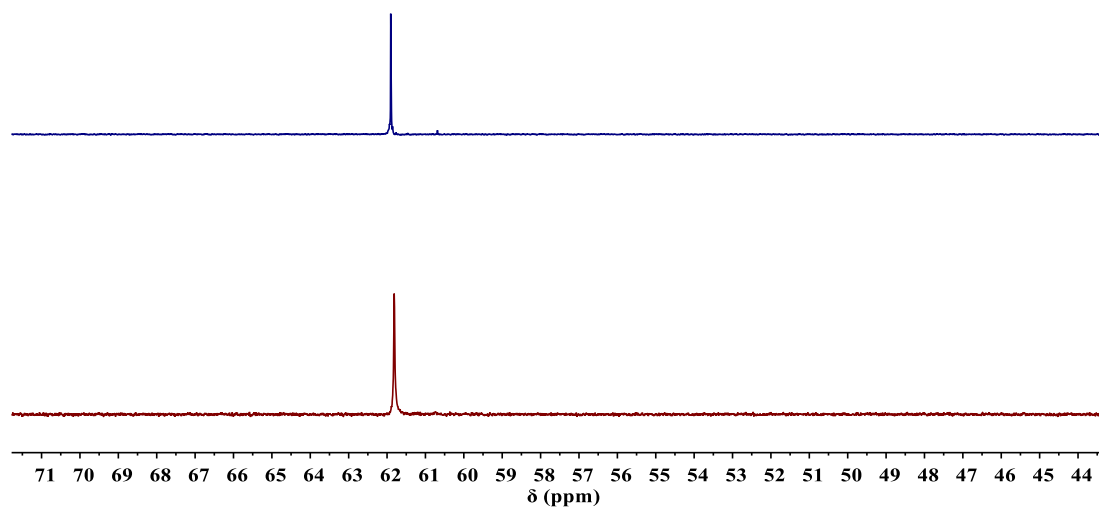


Figure S3. ^{31}P NMR spectra (benzene- d_6 , RT): (top) PtBu_3 ; (bottom) $\text{B}(2,4\text{-F}_2\text{Ph})_3/\text{PtBu}_3$ FLP.

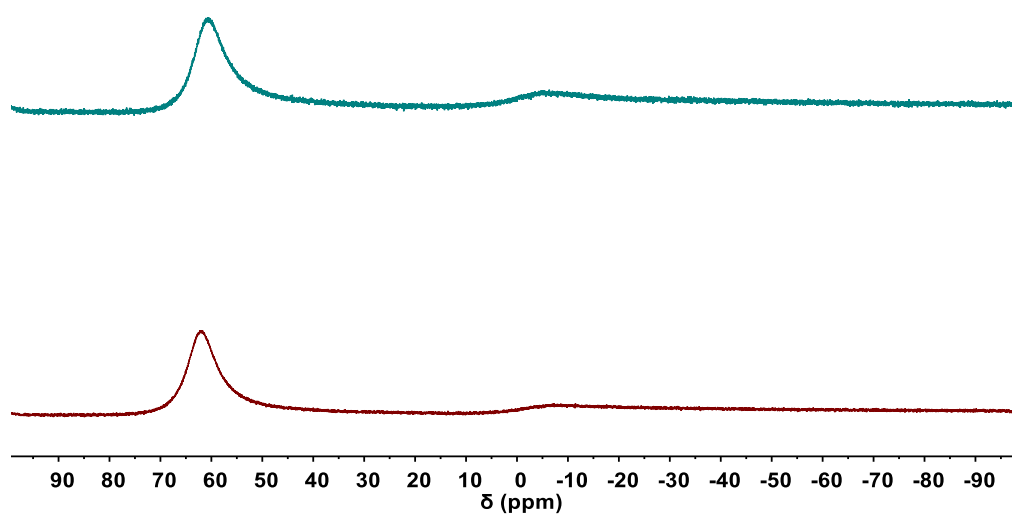


Figure S4. ^{11}B NMR spectra (benzene- d_6 , RT) of $\text{B}(2,4\text{-F}_2\text{Ph})_3/\text{PtBu}_3$ FLP (top) and $\text{B}(2,4\text{-F}_2\text{Ph})_3$ (bottom).

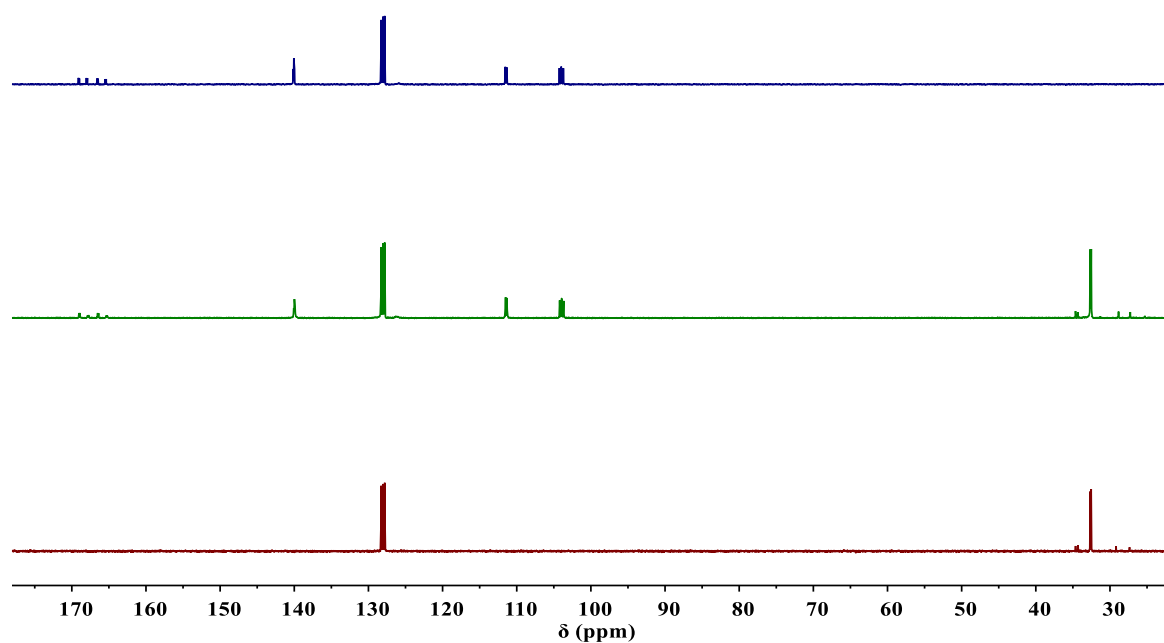


Figure S5. ^{13}C NMR spectra (benzene- d_6 , RT): (top) $\text{B}(2,4\text{-F}_2\text{Ph})_3$; (middle) $\text{B}(2,4\text{-F}_2\text{Ph})_3/\text{PtBu}_3$ FLP; (bottom) PtBu_3 .

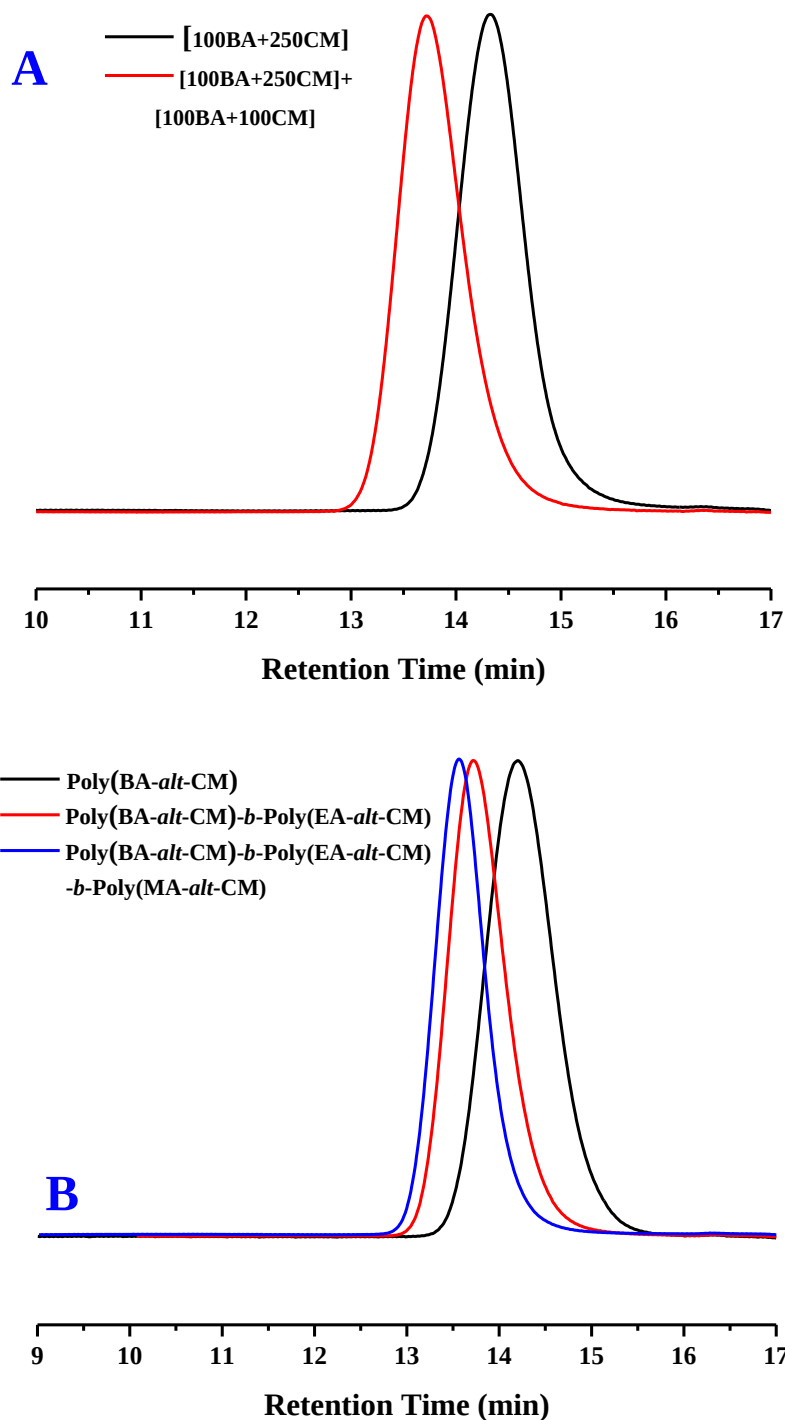


Figure S6. (A) GPC curves of poly(BA-*co*-CM) samples obtained from chain extension experiment by $\text{B(2,4-F}_2\text{C}_6\text{H}_3)_3/\text{PtBu}_3$ at RT: $M_n = 38.5$ kg/mol, $D = 1.09$ (first batch); $M_n = 67.5$ kg/mol, $D = 1.11$ (second batch after 60 min); (B) GPC curves for poly(BA-*co*-CM)-*b*-poly(EA-*co*-CM) diblock ($M_n = 70.6$ kg/mol, $D = 1.10$), poly(BA-*co*-CM)-*b*-poly(EA-*co*-CM)-*b*-poly(MA-*co*-CM) triblock ($M_n = 86.2$ kg/mol, $D = 1.08$) copolymers produced by $\text{B(2,4-F}_2\text{C}_6\text{H}_3)_3/\text{PtBu}_3$ through sequential monomer addition at RT.

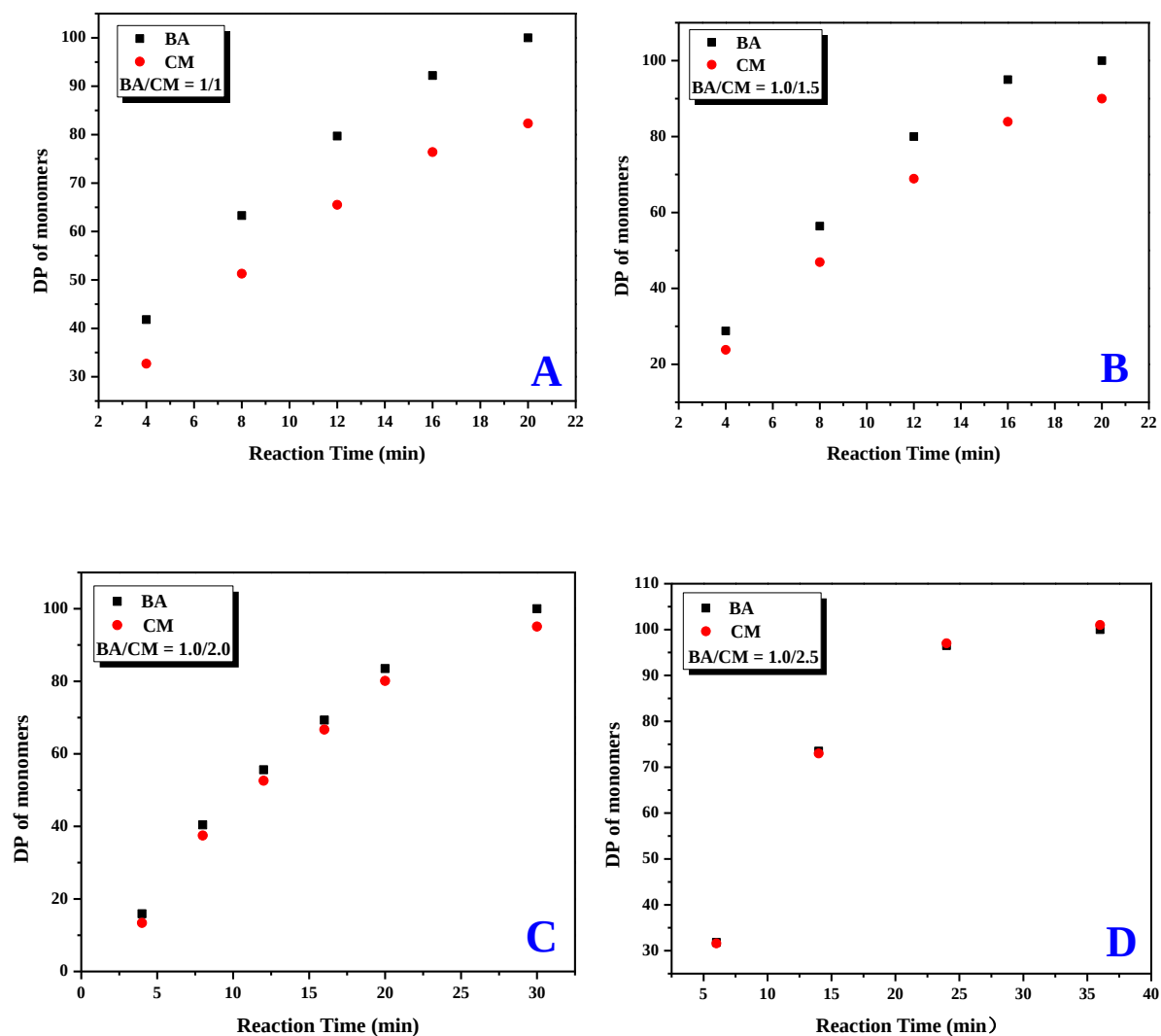


Figure S7. Degrees of polymerization [$DP = ([M]_0/[LB]_0) \times \text{conversion}\%$] of CM (red circle) and BA (black square) in the copolymerizations with different comonomer ratios: (A) $[BA]_0:[CM]_0 = 1:1$ (Table 1, Run 1); (B) $[BA]_0:[CM]_0 = 1:1.5$ (Table 1, Run 3); (C) $[BA]_0:[CM]_0 = 1:2$ (Table 1, Run 4); (D) $[BA]_0:[CM]_0 = 1:2.5$ (Table 1, Run 5).

Measurement of Reactivity ratios of CM and BA

The reactivity ratio of CM and BA were determined according to Meyer-Lowry model.⁷⁻⁸ Different from conventional Fineman-Ross or Kelen-Tüdös method which is only valid at low monomer conversion (approximately 5–10%), Meyer-Lowry model can be calculated from kinetic polymerization data that span the full range of conversion. Considering that a given copolymerization at low monomer conversion may not reach a steady state concentration of growing polymer and may not yet consume enough monomer to present a statistically meaningful and representative result, Meyer-Lowry model is thus a more suitable method to determine the reactivity ratios of alternating copolymerizations. The equation of Meyer-Lowry model is provided as follows:

$$X = 1 - \left(\frac{f_{BA,t}}{f_{BA,0}} \right)^{\frac{b}{1-b}} \times \left(\frac{1-f_{BA,t}}{1-f_{BA,0}} \right)^{\frac{a}{1-a}} \times \left(\frac{(2-a-b)f_{BA,t}+b-1}{(2-a-b)f_{BA,0}+b-1} \right)^{\frac{ab-1}{(1-a)(1-b)}} = 1 - \frac{n_{BA,t}+n_{CM,t}}{n_{BA,0}+n_{CM,0}}$$

where a and b are the reaction ratios of BA (r_{BA}) and CM (r_{CM}), respectively; $f_{BA,0}$ is the molar composition of BA in feed, $f_{BA,t}$ is the instantaneous molar composition of BA at the copolymerization time of t , which can be calculated based on the equations:

$$f_{BA,t} = \frac{n_{BA,0}[1 - \text{Conv.}(BA)_t]}{n_{BA,0}[1 - \text{Conv.}(BA)_t] + n_{CM,0}[1 - \text{Conv.}(CM)_t]}$$

$n_{BA,0}$ and $n_{CM,0}$ are the moles of BA and CM in feed, respectively. $n_{BA,t}$ and $n_{CM,t}$ are the instantaneous moles of BA and CM at the copolymerization time of t , respectively, which can be calculated based on the equations:

$$n_{BA,t} = n_{BA,0}[1 - \text{Conv.}(BA)_t]; n_{CM,t} = n_{CM,0}[1 - \text{Conv.}(CM)_t]$$

where $\text{Conv.}(BA)_t$ and $\text{Conv.}(CM)_t$ are the conversions of BA and CM at the copolymerization time of t , respectively.

Table S2. Copolymerization data used for calculating the reactivity ratios of BA and CM in the copolymerization with a $[BA]_0:[CM]_0$ feed ratio of 100:100 ($n_{BA,0} = 1$ mmol, $n_{CM,0} = 1$ mmol, $n_{BA,0}+n_{CM,0} = 2.0$ mmol, $f_{BA,0} = 0.5$).

Conv.% (BA)	Conv.% (CM)	$n_{BA,t}$ (mmol)	$n_{CM,t}$ (mmol)	$n_{BA,t}+n_{CM,t}$ (mmol)	$f_{BA,t}$	$X = 1 - \frac{n_{BA,t}+n_{CM,t}}{n_{BA,0}+n_{CM,0}}$
41.8	32.7	0.582	0.673	1.255	0.464	0.373
63.3	51.3	0.367	0.487	0.854	0.430	0.573
79.7	65.5	0.203	0.345	0.548	0.370	0.726
92.2	76.4	0.078	0.236	0.314	0.248	0.843

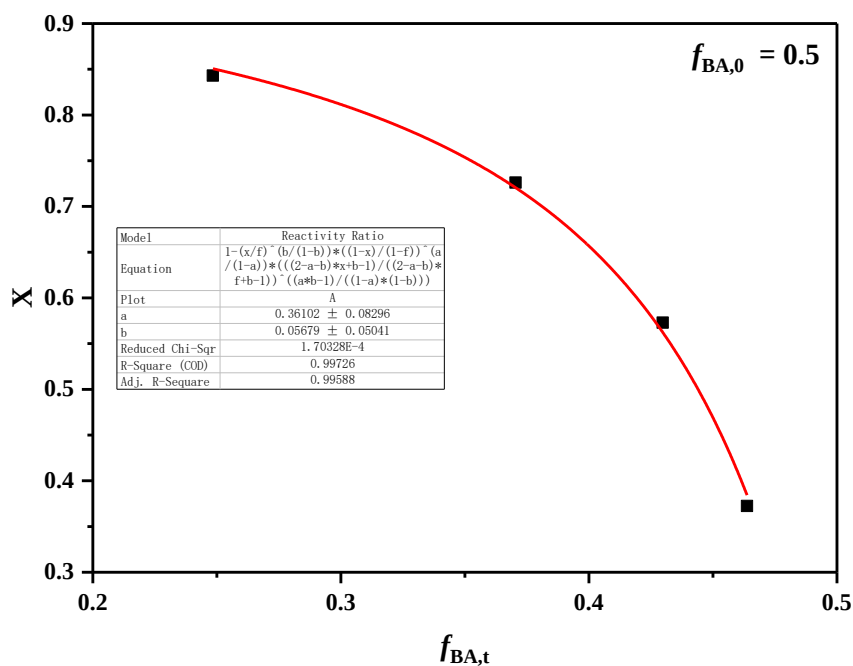


Figure S8. Non-linear fitting plots of Meyer-Lowry model in the copolymerization with a $[BA]_0:[CM]_0$ feed ratio of 100:100 ($r_{BA} = 0.361$, $r_{CM} = 0.057$).

Table S3. Copolymerization data used for calculating the reactivity ratios of BA and CM in the copolymerization with a $[BA]_0:[CM]_0$ feed ratio of 100:200 ($n_{BA,0} = 1.0$ mmol, $n_{CM,0} = 2.0$ mmol, $n_{BA,0} + n_{CM,0} = 3.0$ mmol, $f_{BA,0} = 0.333$).

Conv.% (BA)	Conv.% (CM)	$n_{BA,t}$ (mmol)	$n_{CM,t}$ (mmol)	$n_{BA,t}+n_{CM,t}$ (mmol)	$f_{BA,t}$	$X = 1 - \frac{n_{BA,t}+n_{CM,t}}{n_{BA,0}+n_{CM,0}}$
15.9	6.7	0.841	1.866	2.707	0.311	0.098
40.4	18.8	0.596	1.624	2.220	0.268	0.260
55.6	26.3	0.444	1.474	1.918	0.231	0.361
69.3	33.4	0.307	1.332	1.639	0.187	0.454
83.5	40.1	0.165	1.198	1.363	0.121	0.546

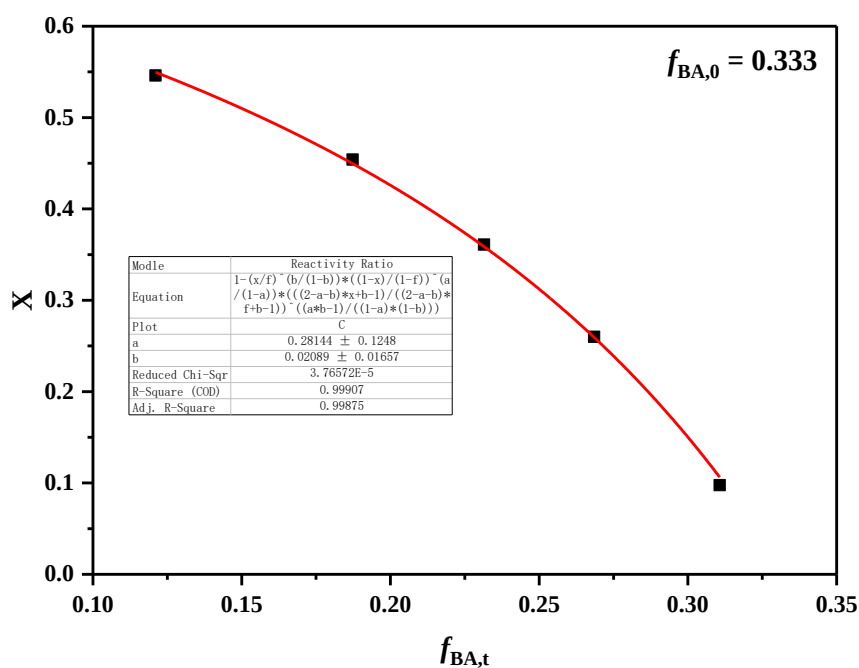


Figure S9. Non-linear fitting plots of Meyer-Lowry model in the copolymerization with a $[BA]_0:[CM]_0$ feed ratio of 100:200 ($r_{BA} = 0.281$, $r_{CM} = 0.021$).

Table S4. Copolymerization data used for calculating the reactivity ratios of BA and CM in the copolymerization with a $[BA]_0:[CM]_0$ feed ratio of 200:500 ($n_{BA,0} = 2.0$ mmol, $n_{CM,0} = 5.0$ mmol, $n_{BA,0} + n_{CM,0} = 7.0$ mmol, $f_{BA,0} = 0.286$).

Conv.% (BA)	Conv.% (CM)	$n_{BA,t}$ (mmol)	$n_{CM,t}$ (mmol)	$n_{BA,t}+n_{CM,t}$ (mmol)	$f_{BA,t}$	$X = 1 - \frac{n_{BA,t}+n_{CM,t}}{n_{BA,0}+n_{CM,0}}$
26.2	10.3	1.476	4.485	5.961	0.248	0.148
38.1	16.1	1.238	4.195	5.433	0.228	0.224
48.5	20.1	1.030	3.995	5.025	0.205	0.282
60.9	24.1	0.782	3.795	4.577	0.171	0.346
70.3	27.6	0.594	3.620	4.214	0.141	0.398
81.2	32.4	0.376	3.380	3.756	0.100	0.463
90.1	36.7	0.198	3.165	3.363	0.059	0.520

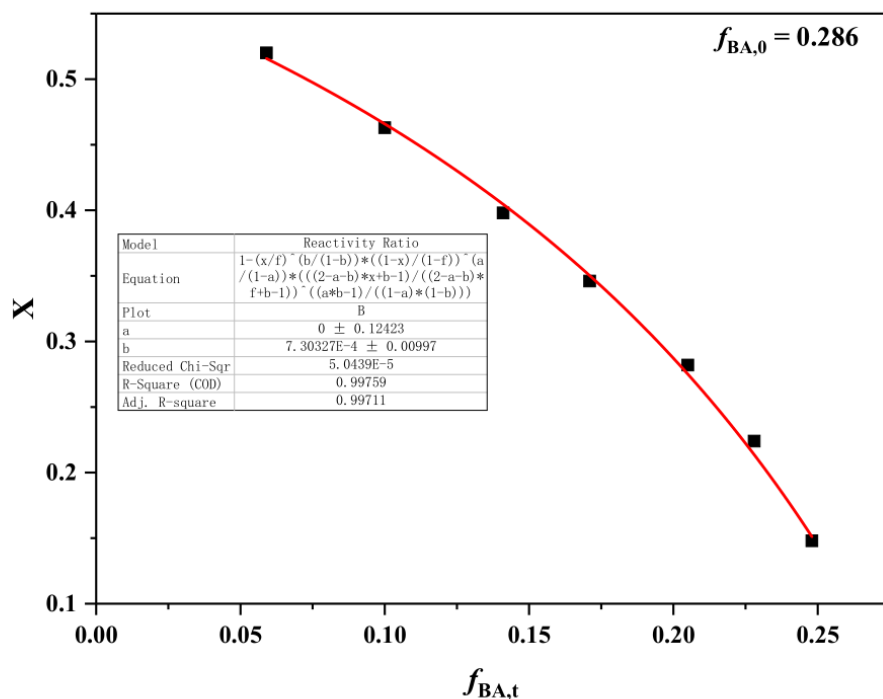


Figure S10. Non-linear fitting plots of Meyer-Lowry model in the copolymerization with a $[BA]_0:[CM]_0$ feed ratio of 200:500 ($r_{BA} = 0$, $r_{CM} = 0.00073$).

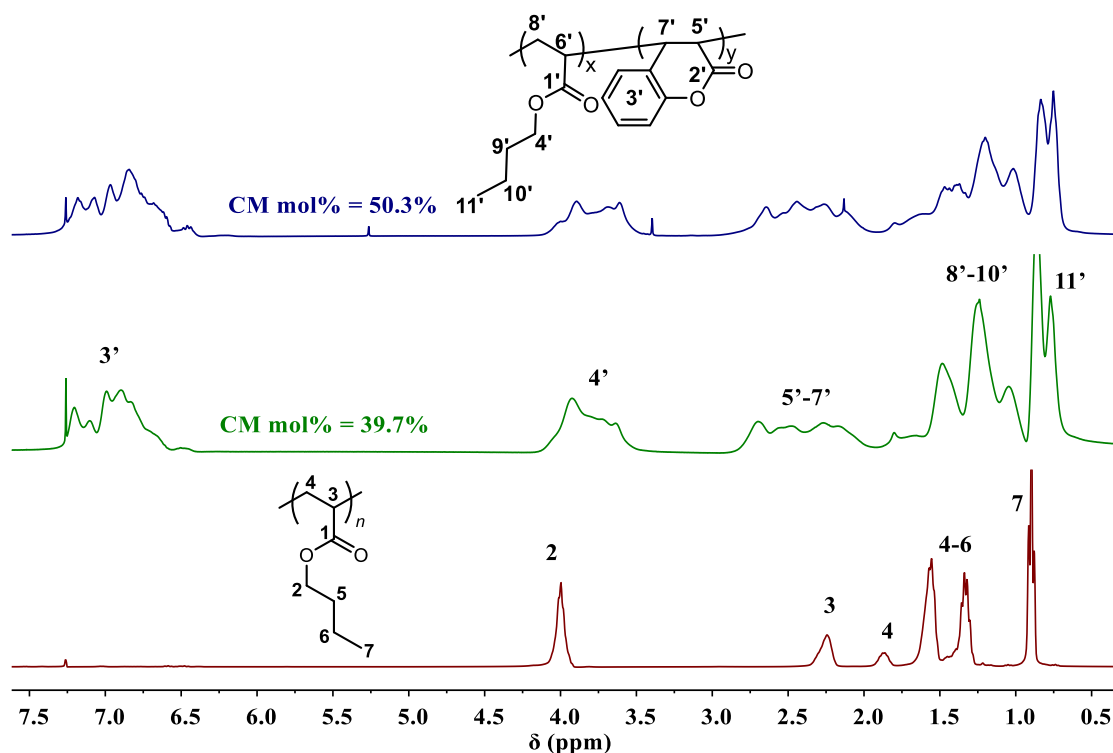


Figure S11. ^1H NMR spectra (CDCl₃, RT): (top) poly(BA-*alt*-CM) (CM mol% = 50.3%, Table 1, Run 8); (middle) poly(BA-*co*-CM) (CM mol% = 39.7%, Table 1, Run 9); (bottom) PBA.

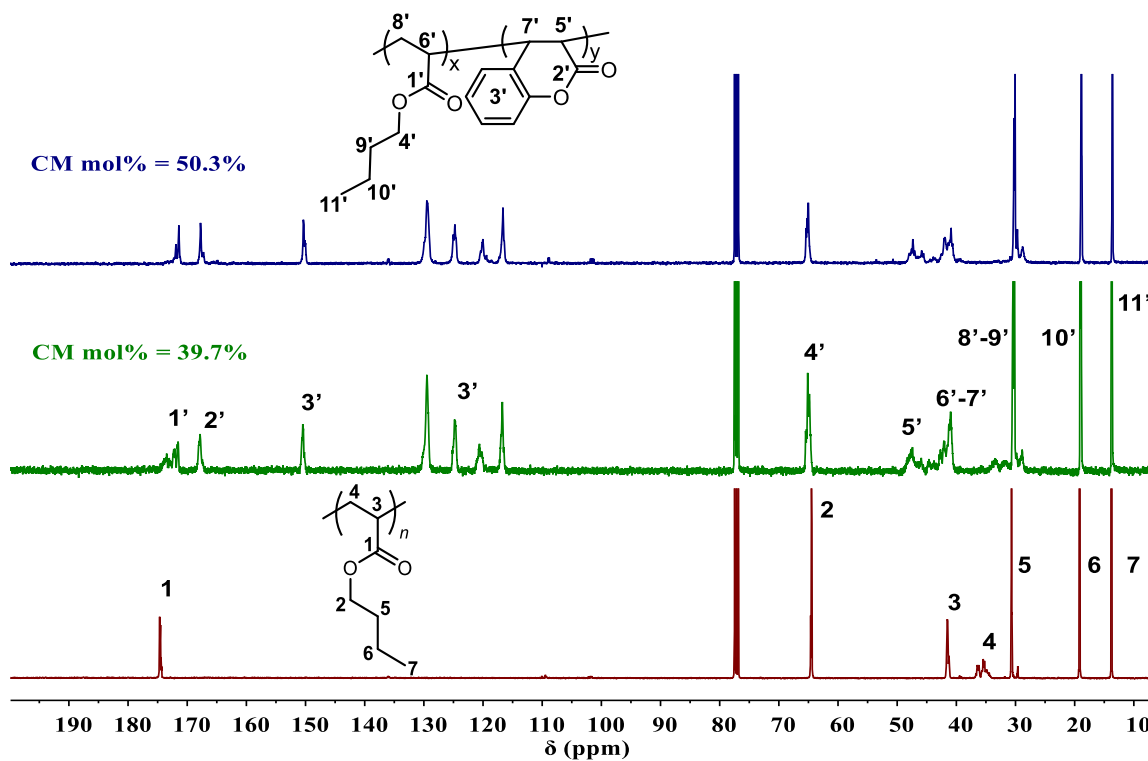


Figure S12. ^{13}C NMR spectra (CDCl₃, RT): (top) poly(BA-*alt*-CM) (CM mol% = 50.3%, Table 1, Run 8); (middle) poly(BA-*co*-CM) (CM mol% = 39.7%, Table 1, Run 9); (bottom) PBA.

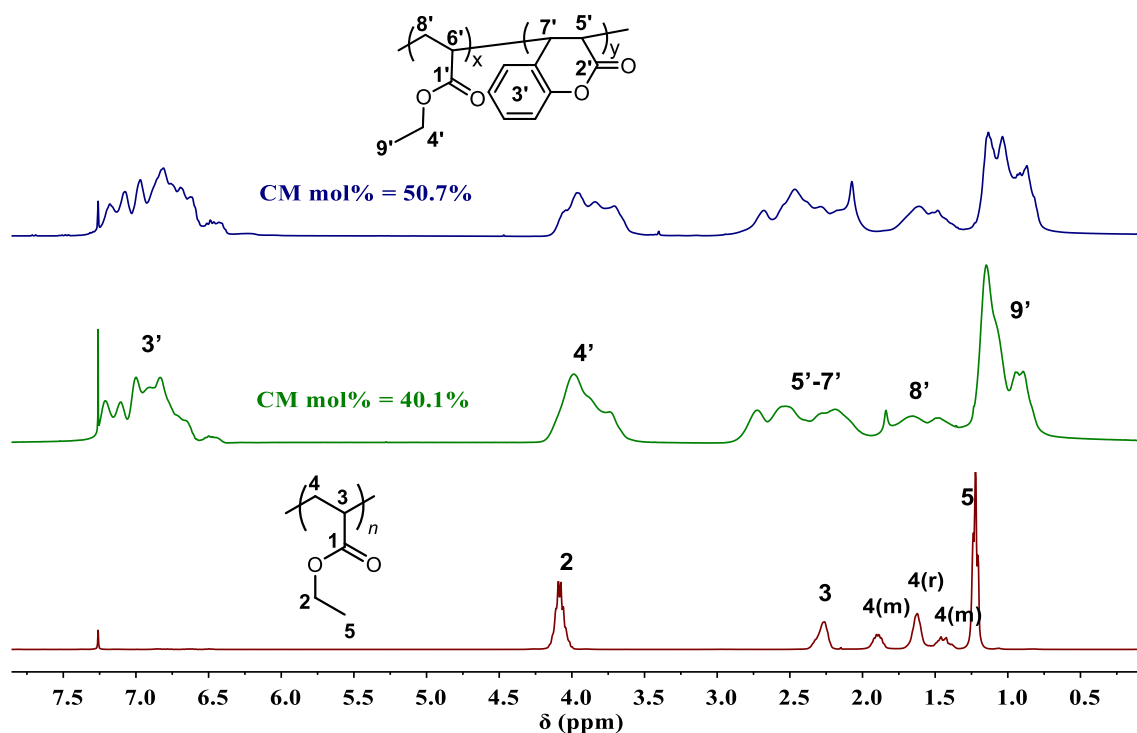


Figure S13. ^1H NMR spectra (CDCl₃, RT): (top) poly(EA-*alt*-CM) (CM mol% = 50.7%, Table 1, Run 11); (middle) poly(EA-*co*-CM) (CM mol% = 40.1%, Table 1, Run 10); (bottom) PEA.

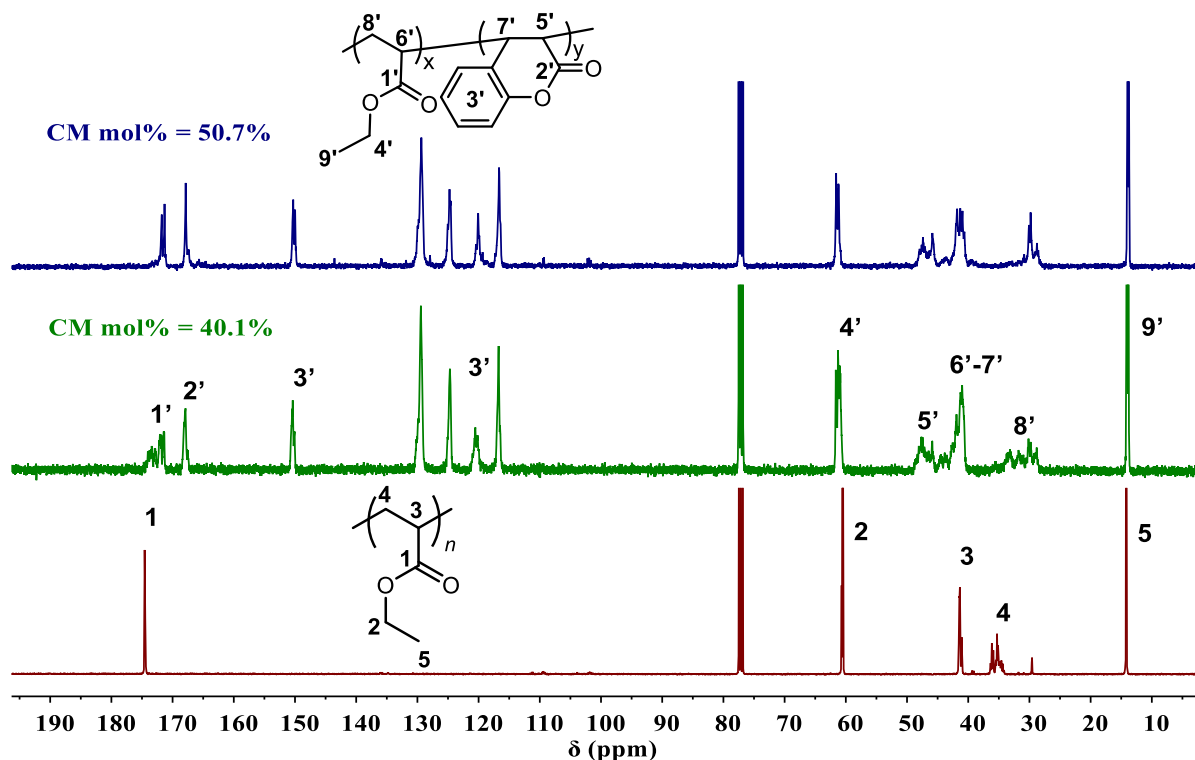


Figure S14. ^{13}C NMR spectra (CDCl₃, RT): (top) poly(EA-*alt*-CM) (CM mol% = 50.7%, Table 1, Run 11); (middle) poly(EA-*co*-CM) (CM mol% = 40.1%, Table 1, Run 10); (bottom) PEA.

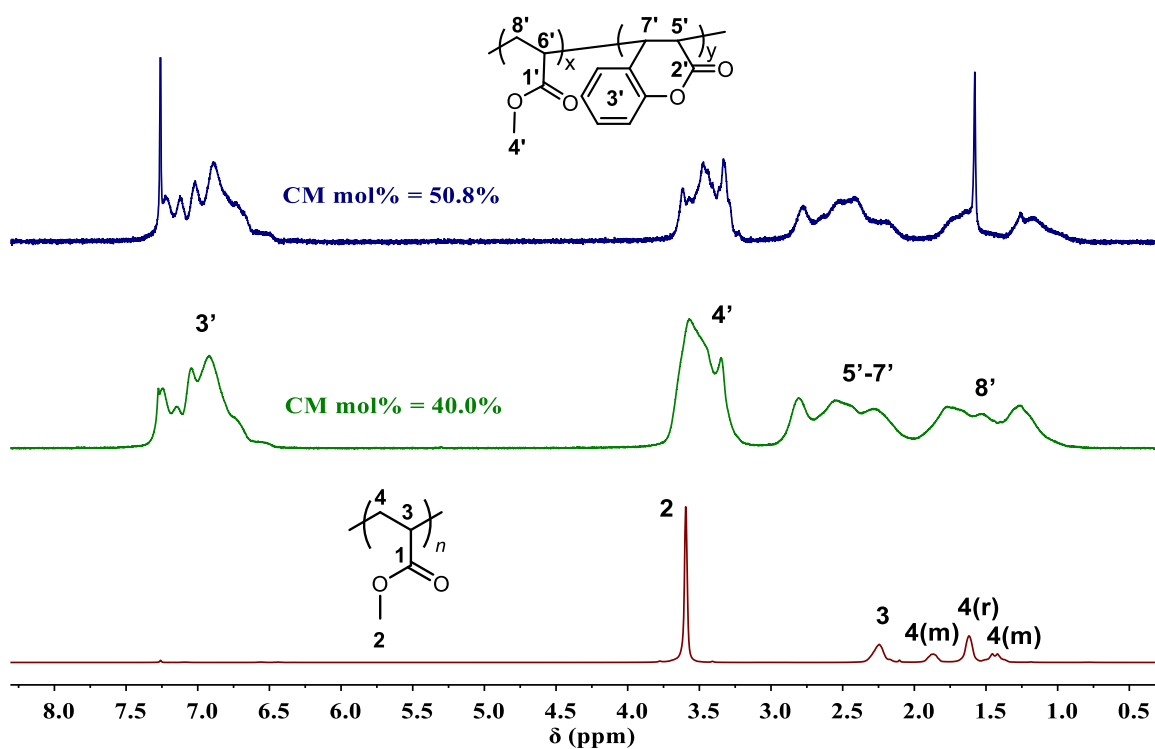


Figure S15. ^1H NMR spectra (CDCl₃, RT): (top) poly(MA-*alt*-CM) (CM mol% = 50.8%, Table 1, Run 13); (middle) poly(MA-*co*-CM) (CM mol% = 40.0%, Table 1, Run 12); (bottom) PMA.

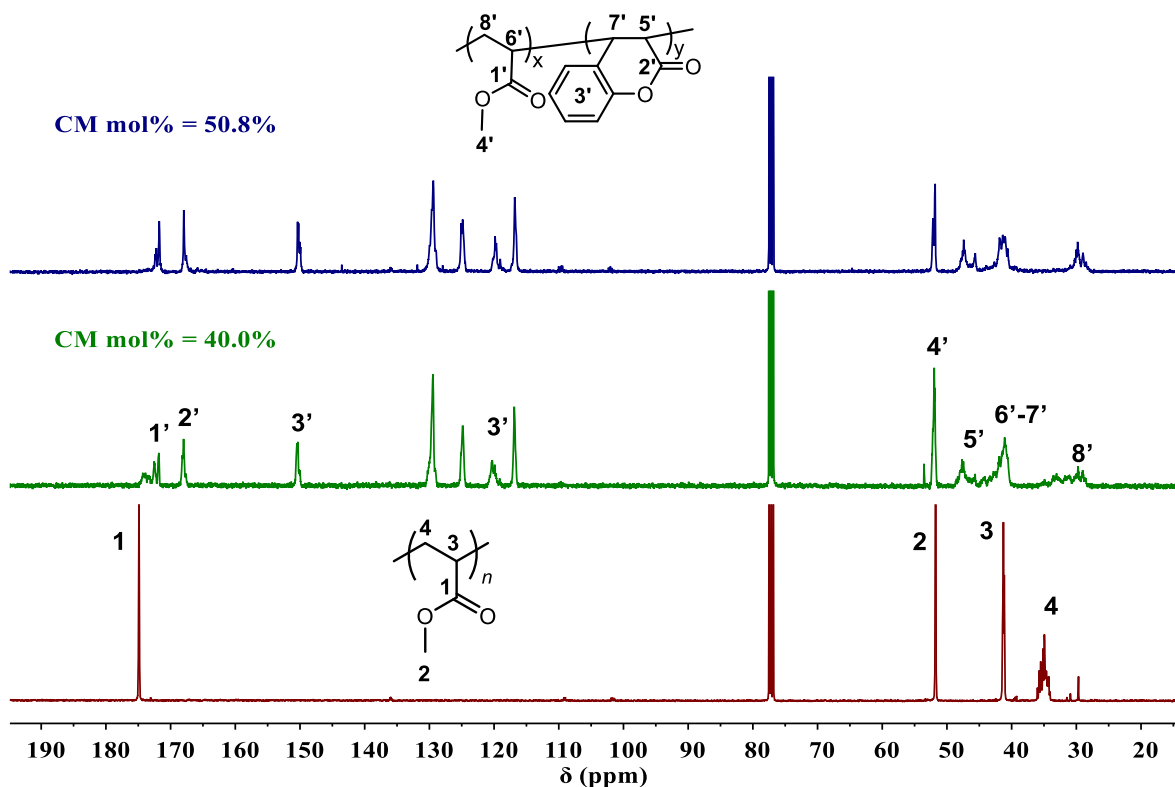


Figure S16. ^{13}C NMR spectra (CDCl₃, RT): (top) poly(MA-*alt*-CM) (CM mol% = 50.8%, Table 1, Run 13); (middle) poly(MA-*co*-CM) (CM mol% = 40.0%, Table 1, Run 12); (bottom) PMA.

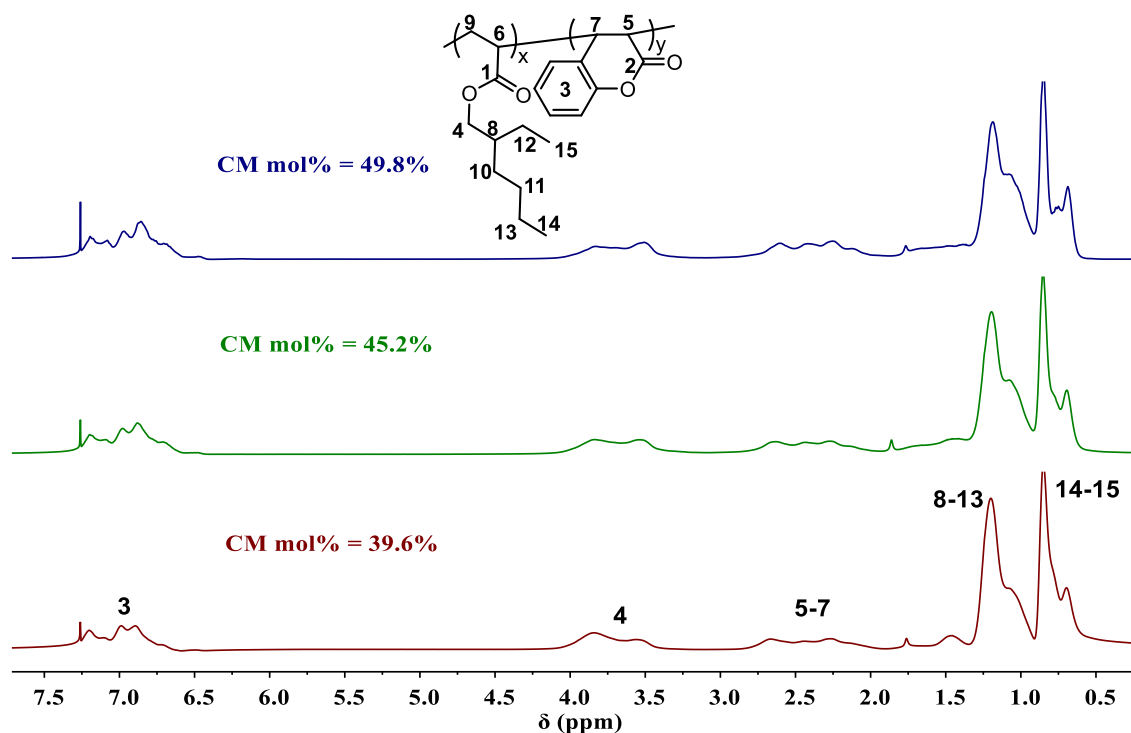


Figure S17. ^1H NMR spectra (CDCl_3 , RT) of poly(EHA-co-CM)s: (top) CM mol% = 49.8% (Table 1, Run 16); (middle) CM mol% = 45.2% (Table 1, Run 15); (bottom) CM mol% = 39.6% (Table 1, Run 14).

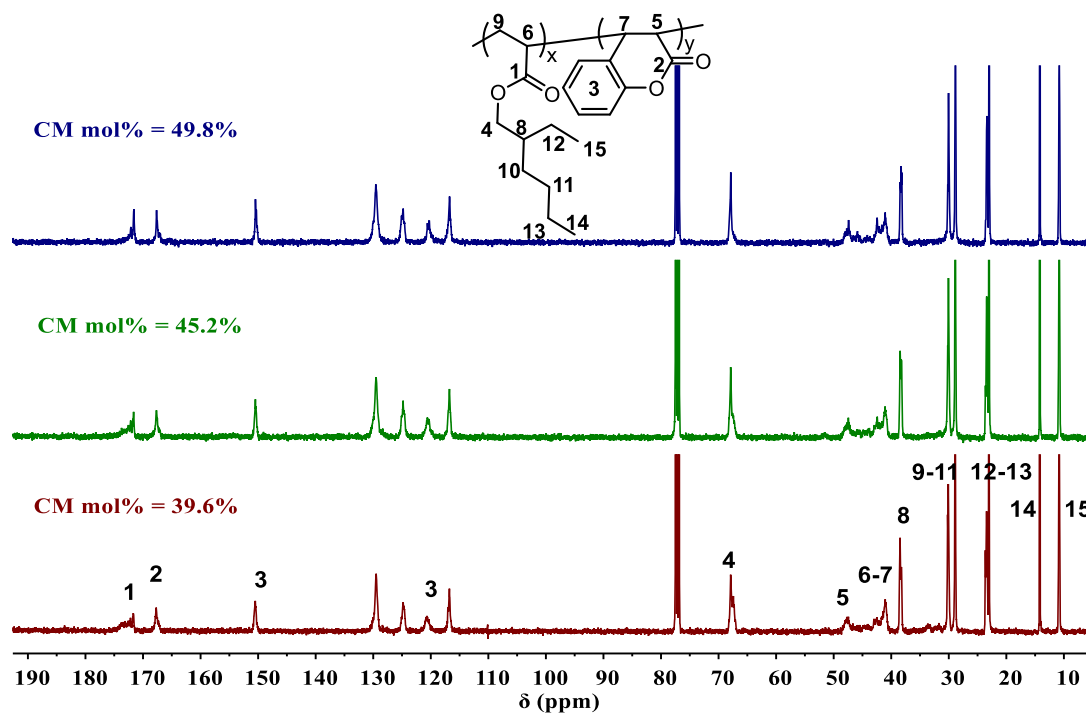


Figure S18. ^{13}C NMR spectra (CDCl_3 , RT) of poly(EHA-co-CM)s: (top) CM mol% = 49.8% (Table 1, Run 16); (middle) CM mol% = 45.2% (Table 1, Run 15); (bottom) CM mol% = 39.6% (Table 1, Run 14).

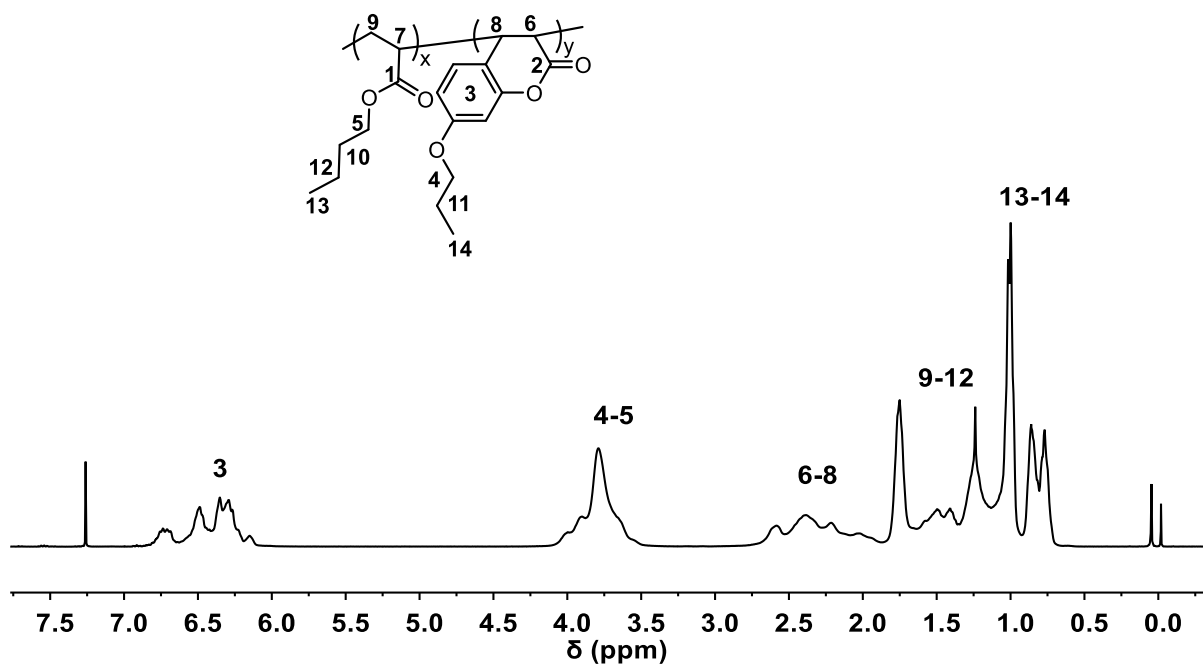


Figure S19. ^1H NMR spectrum (CDCl_3 , RT) of poly(BA-*alt*-PCM) (Table 1, Run 17).

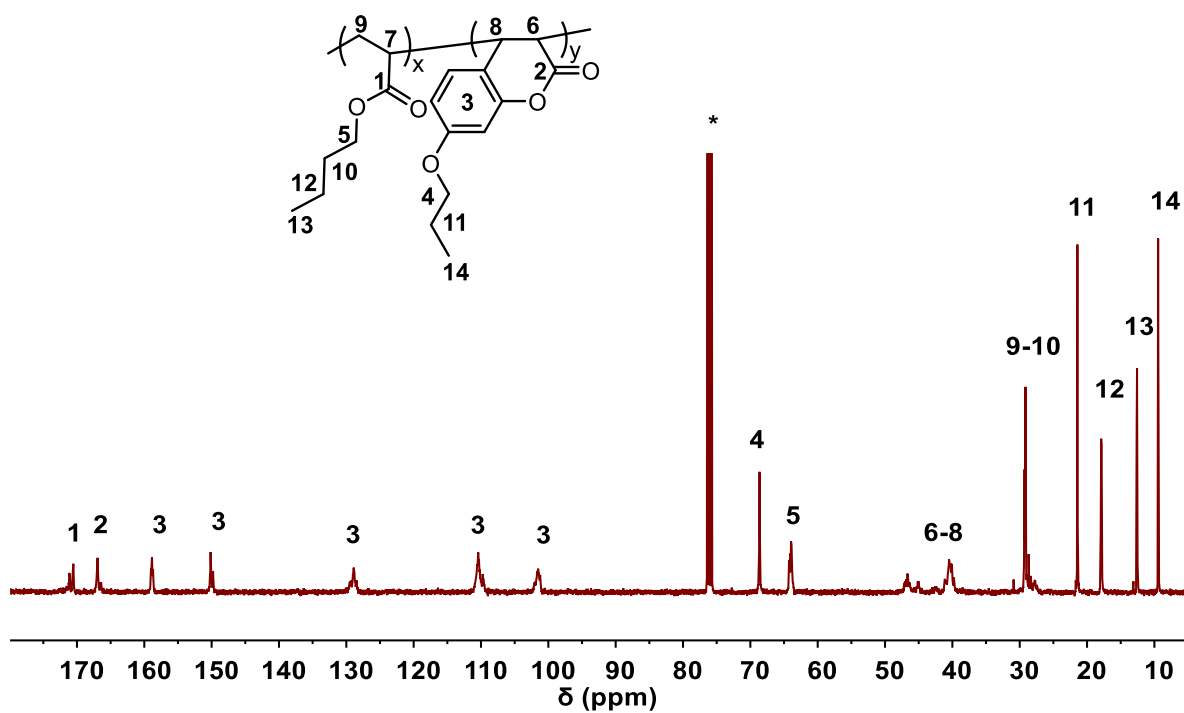


Figure S20. ^{13}C NMR spectrum (CDCl_3 , RT) of poly(BA-*alt*-PCM) (Table 1, Run 17).

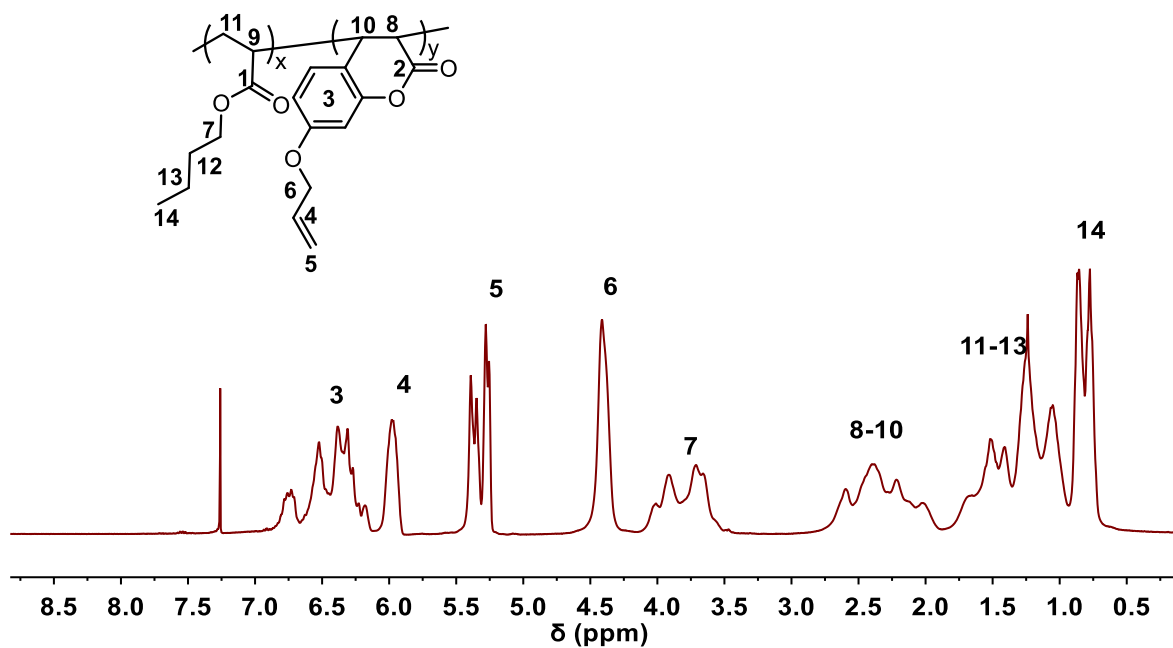


Figure S21. ^1H NMR spectrum (CDCl_3 , RT) of poly(BA-*alt*-ACM) (Table 1, Run 18).

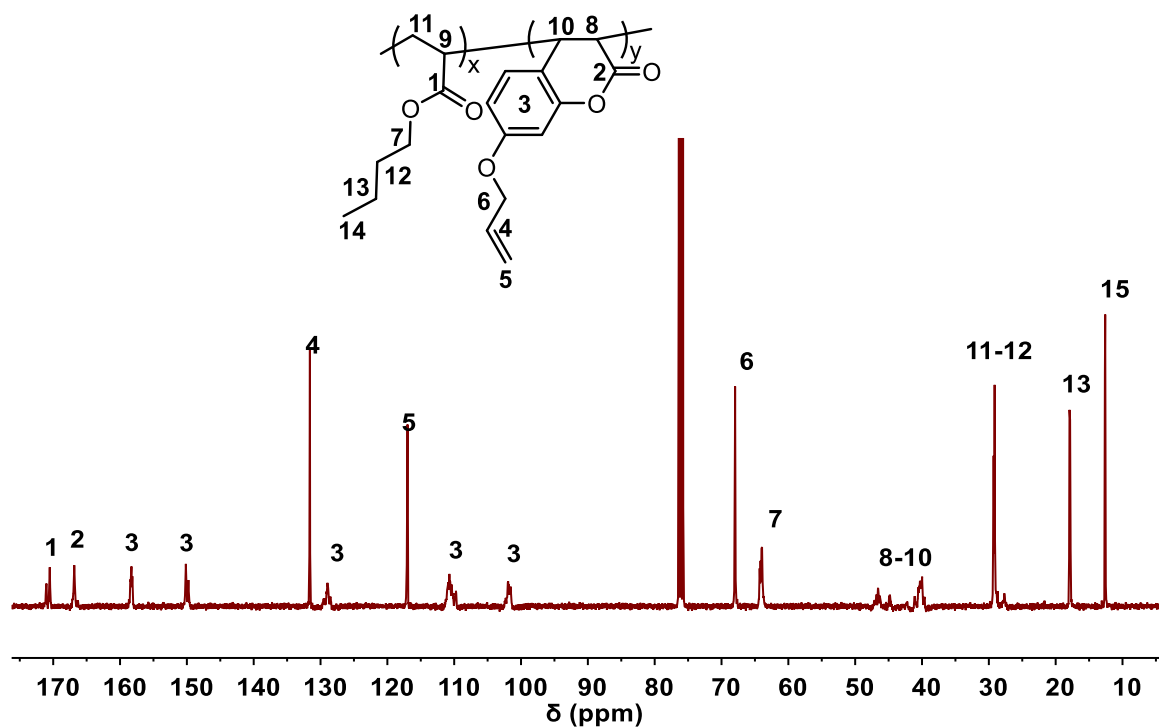


Figure S22. ^{13}C NMR spectrum (CDCl_3 , RT) of poly(BA-*alt*-ACM) (Table 1, Run 18).

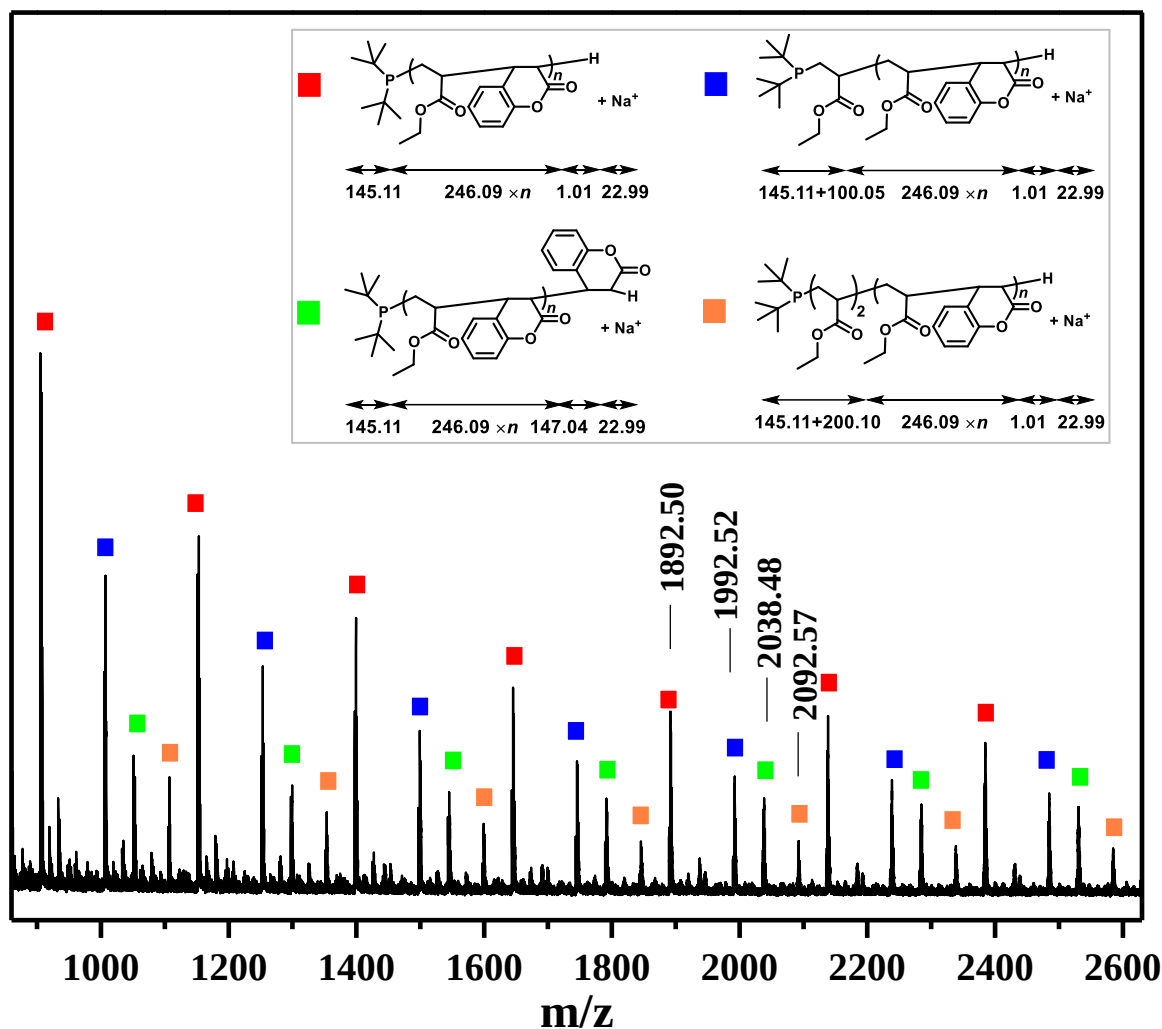


Figure S23. MALDI-TOF MS spectrum of poly(EA-*alt*-CM) oligomer produced by B(2,4-F₂Ph)₃/PtBu₃ FLP (Inset: exact masses for proposed structures). Different series of mass ions all show one type of chain ends, corresponding to H-terminated chain end derived from quenching process and *t*Bu₂P-initiated chain end formed by the conjugate addition of PtBu₃ LB onto LA-activated monomer and the subsequent elimination of one *tert*-butyl group from *t*Bu₃P⁺⁻ end during MALDI-TOF MS measurement (Figure S24).

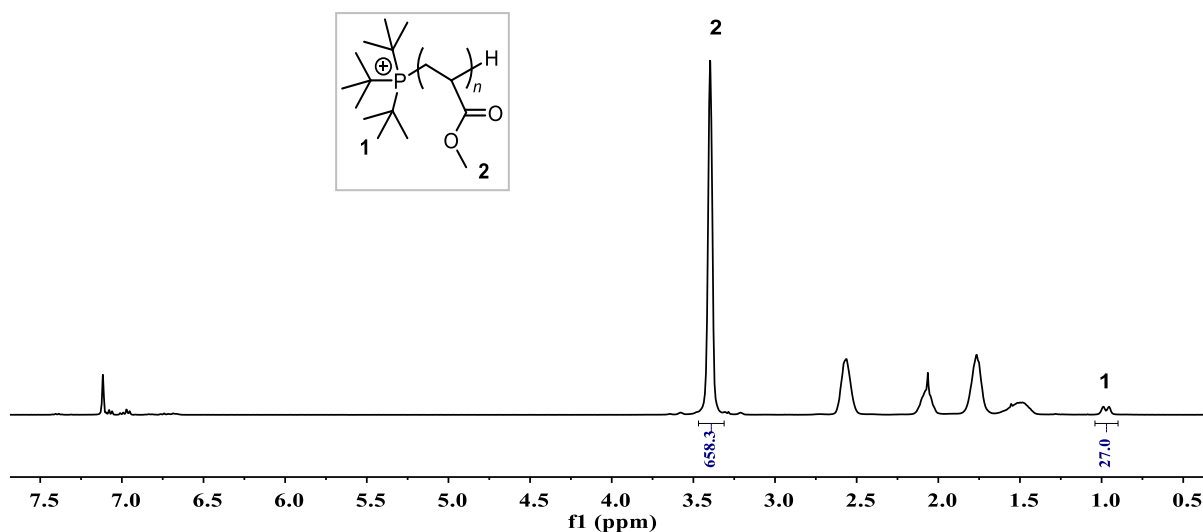


Figure S24. ^1H NMR spectrum of PMA produced by $\text{B}(2,4\text{-F}_2\text{Ph})_3/\text{PtBu}_3$ FLP (benzene- d_6 was used in place of CDCl_3 because the chemical resonances of P^+tBu_3 -initiated chain end are overlapped with those of main chains in CDCl_3). Based on $\text{tBu}_3\text{P}^+/\text{H}-$ ends, M_n calculated by ^1H NMR is 19.1 kg/mol, which is consistent with M_n (18.0 kg/mol) obtained by GPC [if M_n was calculated based on $\text{tBu}_2\text{P}-/\text{H}-$ ends, the resultant M_n (NMR) of 12.7 kg/mol severely deviated from M_n (GPC)]. This result thereby indicates that the elimination of one tert-butyl group from tBu_3P^+ - end to form $\text{tBu}_2\text{P}-$ end occurs during the MALDI-TOF MS measurement. The split of PtBu_3^+ - chemical signal into two peaks should be caused by $^{31}\text{P}-^1\text{H}$ coupling.

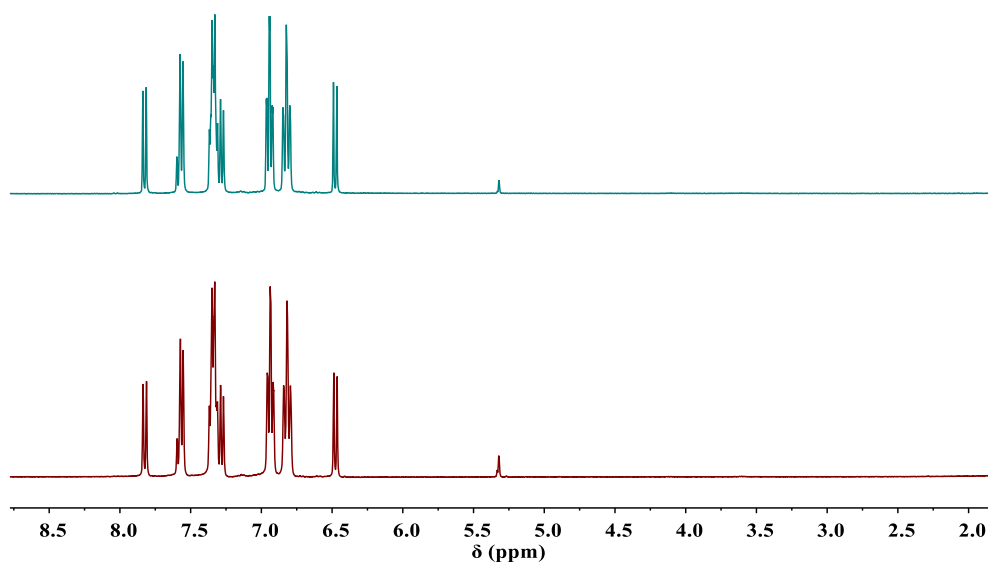


Figure S25. ^1H NMR spectra (CD_2Cl_2 , RT): (top) $[\text{B}(2,4\text{-F}_2\text{Ph})_3]_0:[\text{CM}]_0 = 1$, (bottom) $[\text{B}(2,4\text{-F}_2\text{Ph})_3]_0:[\text{PtBu}_3]_0:[\text{CM}]_0 = 1$.

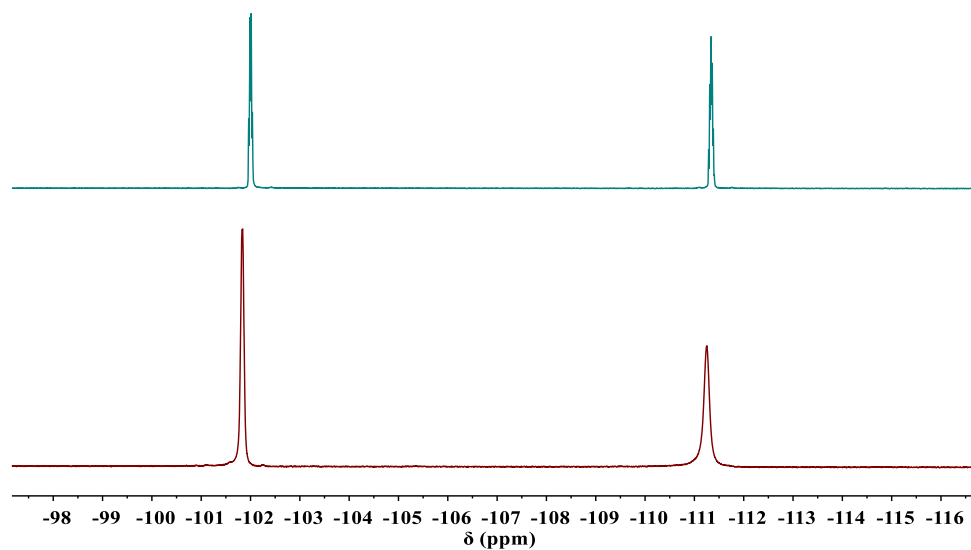


Figure S26. ^{19}F NMR spectra (CD_2Cl_2 , RT): (top) $[\text{B}(2,4\text{-F}_2\text{Ph})_3]_0:[\text{CM}]_0 = 1$, (bottom) $[\text{B}(2,4\text{-F}_2\text{Ph})_3]_0:[\text{PtBu}_3]_0:[\text{CM}]_0 = 1$.

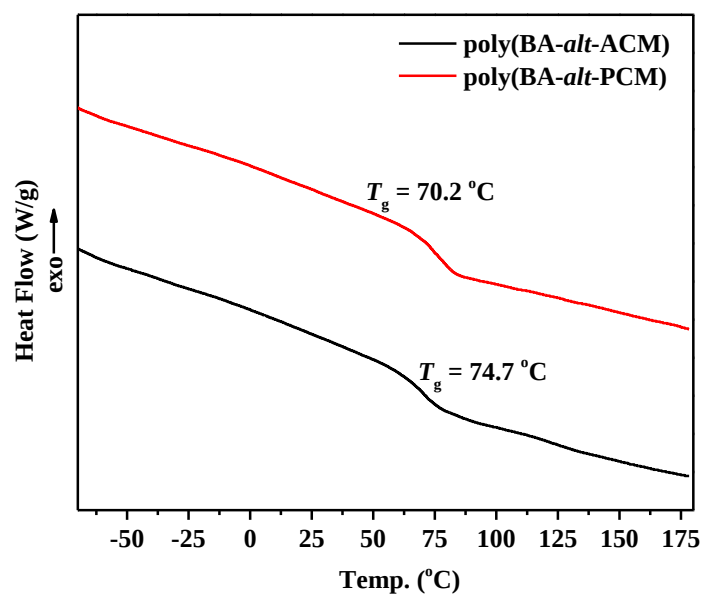


Figure S27. The second heating scans of DSC curves of poly(BA-*alt*-ACM) and poly(BA-*alt*-PCM). In contrast to poly(BA-*alt*-CM) (93.3 °C), low T_g values of coumarin derivatives-contained copolymers should be on account of the plasticizing effect of allyloxy and *n*-propoxy groups.

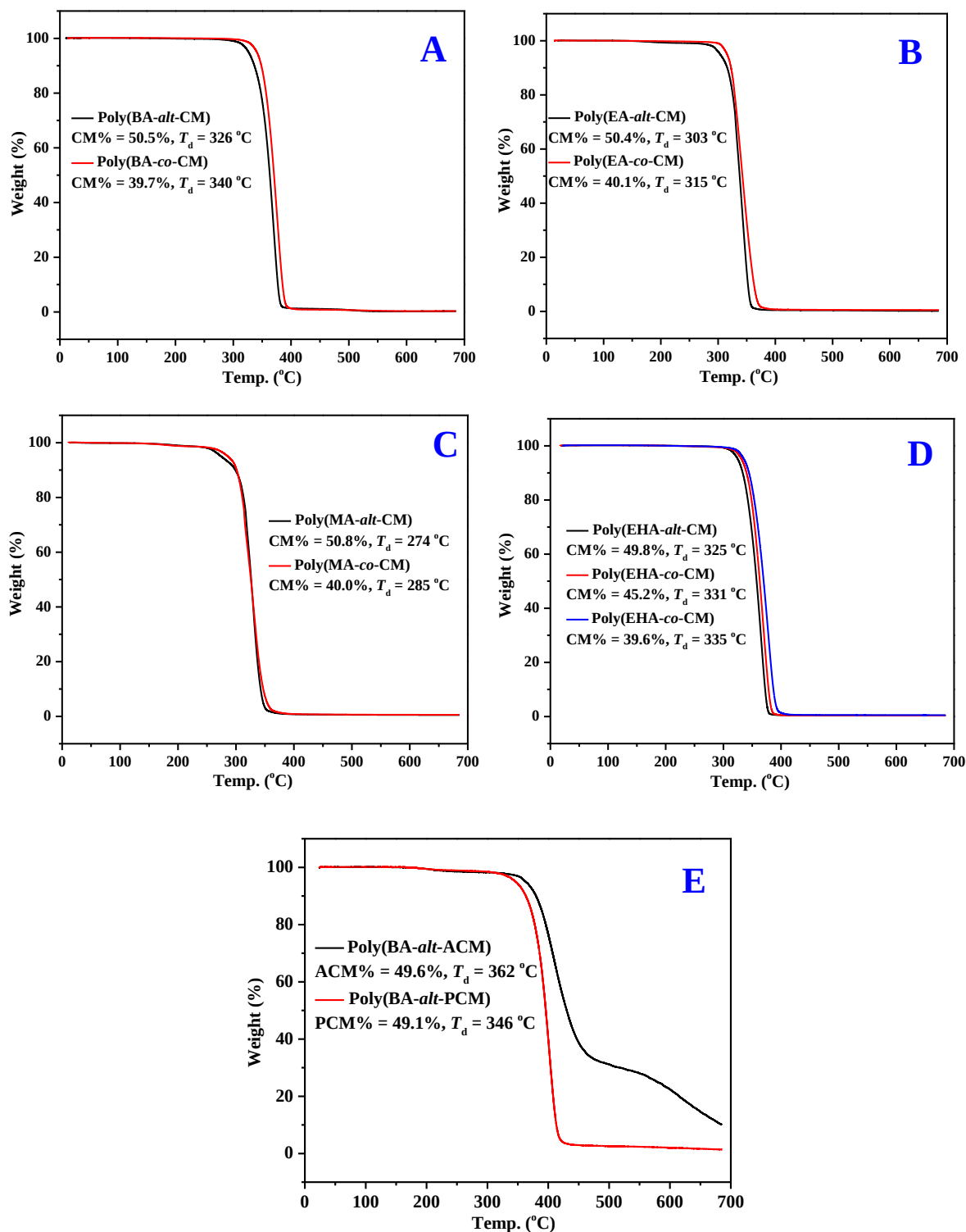


Figure S28. TGA curves of poly(MA-*alt*-CM), poly(MA-*co*-CM), poly(EA-*alt*-CM), poly(EA-*co*-CM), poly(BA-*alt*-CM), poly(BA-*co*-CM), poly(EHA-*alt*-CM), poly(EHA-*co*-CM), poly(BA-*alt*-ACM), and poly(BA-*alt*-PCM). Note: At similar level of CM incorporation (e.g. ~50%), acrylate structures influence T_d s which follow an order of MA (274 °C) < EA (303 °C) < EHA (325 °C) $\approx$ BA (326 °C). Poly(BA-*alt*-PCM) and poly(BA-*alt*-ACM) exhibit enhanced thermal stability as compared to

poly(BA-*alt*-CM). During TGA measurement of poly(BA-*alt*-ACM), some carbonaceous material remained after the heating (ca. 10% mass), which should be attributed to cross-linked network structure caused by allyl group.

Thin Film Preparation for Measurement of Optical Properties. In a 20 mL glass vial, the desired copolymer (10 wt%) was dissolved in THF, and the resultant solution was filtered using a filter. The filtrate was then casted on a glass plate, and the solvent was evaporated overnight at RT and further dried in an oven at 100 °C for 12h. After falling away from glass plate, and the thickness of obtained film was measured about 50 μm . The transparency of the copolymer film was recorded on Agilent Cary 6000i spectrophotometer. ATAGO DR-M4/1550 multi-wavelength Abbe refractometer was used to measure the refractive index of copolymers.

Table S5. The results of refractive index (n) and transmittance of copolymers.

Samples	RI (486 nm)	RI (589 nm)	RI (656 nm)	Transmittance (%)
poly(BA- <i>co</i> -CM) (CM = 39.7%)	1.5404	1.5317	1.5287	90.9
poly(BA- <i>alt</i> -CM) (CM = 50.3%)	1.5549	1.5450	1.5405	90.8
poly(EA- <i>co</i> -CM) (CM = 40.1%)	1.5495	1.5391	1.5351	90.3
poly(EA- <i>alt</i> -CM) (CM = 50.7%)	1.5632	1.5526	1.5478	90.8
poly(MA- <i>co</i> -CM) (CM = 40.0%)	1.5580	1.5478	1.5439	91.0
poly(MA- <i>alt</i> -CM) (CM = 50.8%)	1.5586	1.5481	1.5441	90.0
PMMA	—	1.4900	—	—

General Procedures for TBD-mediated Degradation.

Degradation experiment was performed in 5 mL glass reactors inside the glovebox at RT. 250 mg of poly(MA-*alt*-CM) ($M_n = 180.2$ kg/mol, $\bar{D} = 1.09$, CM mol% = 50.8%) was dissolved in DMF (1.5 mL). The degradation was triggered by the rapid addition of TBD (150 mg) [TBD:CM (mol:mol) = 1:1] in DMF (1.0 mL) to the above solution under vigorous stirring. After 24 h, a 0.4 mL aliquot was taken

from the reaction mixture via syringe and quickly quenched into a 2 mL septum-sealed vial containing 0.5 mL of “wet” CDCl_3 . The quenched aliquots were later analyzed by ^1H and ^{13}C NMR. The residual mixture was then quenched by the addition of 1 mL of dilute HCl. After removing the volatiles under the reduced pressure, the obtained mixture was analyzed by ESI-MS. To purify the crude product, 20 mL of ethyl acetate was added, and the resultant solution was washed by deionized water. The layers were then separated, and the aqueous layer was extracted with ethyl acetate (3×100 mL). The combined organic extracts were dried over anhydrous Na_2SO_4 , filtered, and concentrated. The crude product was purified by flash column chromatography (a short silica gel column with the height of ca. 2 cm), which afforded methyl-3-(2-oxo-2H-chromen-3-yl)propionate (MCP) as the white solid. ^1H NMR (400 MHz, CDCl_3 , RT): δ 7.54 (s, 1H, $-\text{CH}=\text{C}<$), 7.43–7.38 (m, 2H, $-\text{Ph}$), 7.24–7.17 (m, 2H, $-\text{Ph}$), 3.60 (s, 3H, $-\text{OCH}_3$), 2.82 (t, $J = 7.2$ Hz, 2H, $-\text{CH}_2-\text{COO}-$), 2.66 (t, $J = 6.8$ Hz, 2H, $-\text{CH}_2-\text{CH}_2\text{COO}-$). ^{13}C NMR (100 MHz, CDCl_3 , RT): δ 173.01, 161.46, 153.29, 140.03, 130.93, 127.70, 127.46, 124.39, 119.35, 116.43, 51.72, 32.03, 26.60. HRMS (ESI): Exact mass calcd. for $\text{C}_{13}\text{H}_{12}\text{O}_4\text{Na}$ ($[\text{M}+\text{Na}]^+$): 255.0630. Found: 255.0628.

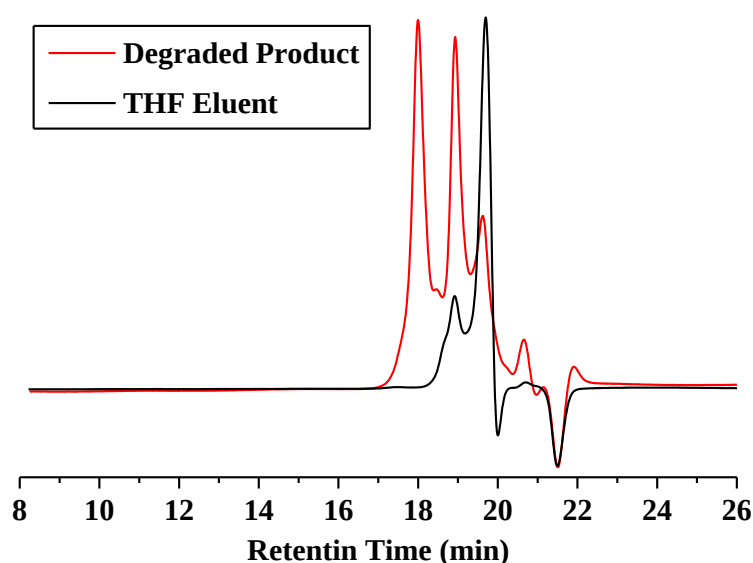


Figure S29. Overlay of GPC curves of the crude degradation mixture in TBD-triggered degradation of poly(MA-*alt*-CM) after 24 h (Red) and THF eluent as blank control (Black).

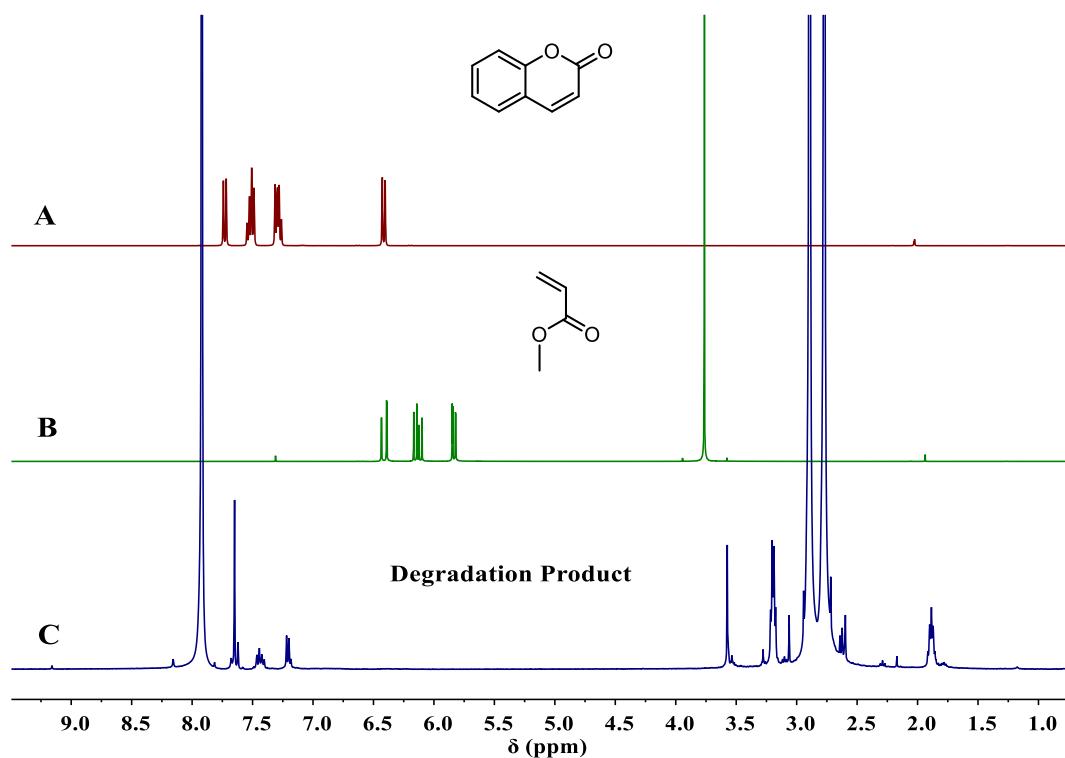


Figure S30. ^1H NMR spectra (CDCl₃, RT): (A) CM; (B) MA; (C) crude reaction mixture obtained by TBD-triggered degradation of poly(MA-*alt*-CM) ($M_n = 180.2$ kg/mol, Table 1, Run 13) after 24 h.

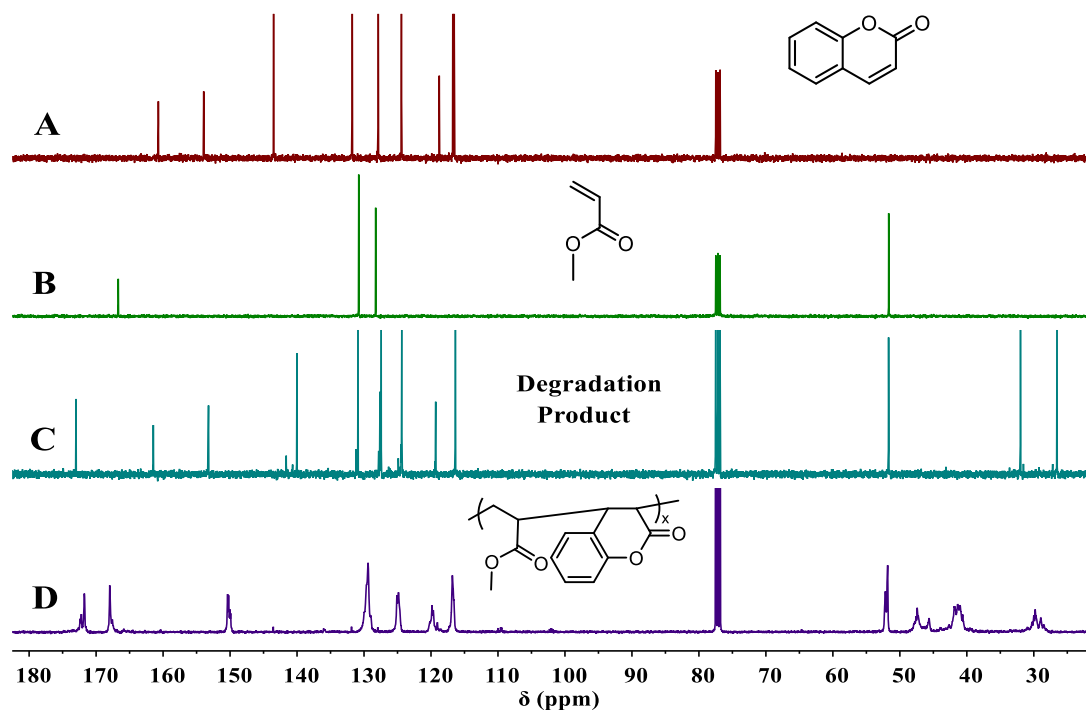


Figure S31. ^{13}C NMR spectra (CDCl₃, RT): (A) CM; (B) MA; (C) crude reaction mixture obtained by TBD-triggered degradation after 24 h; (D) poly(MA-*alt*-CM) ($M_n = 180.2$ kg/mol, $D = 1.09$).

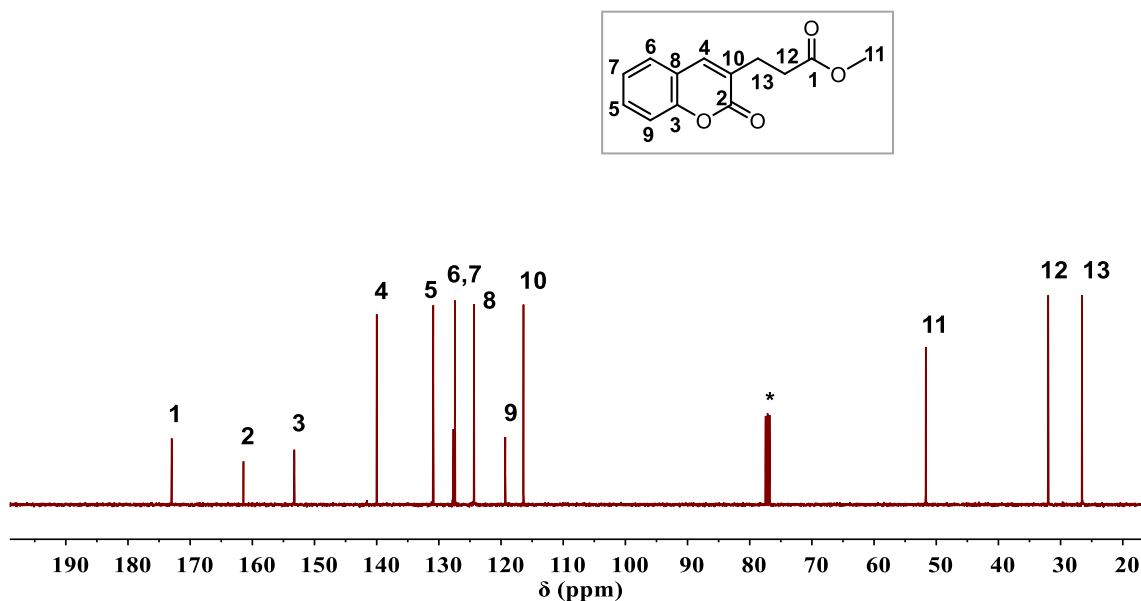


Figure S32. ^{13}C NMR spectrum (CDCl₃, RT) of purified MCP degradation product.

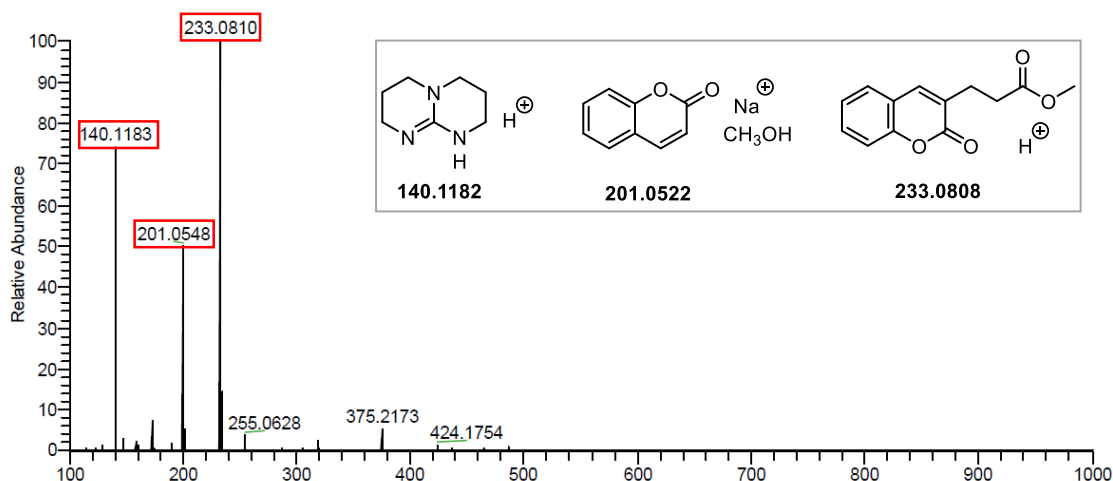


Figure S33. ESI-MS of crude reaction mixture produced by TBD-triggered degradation of poly(MA-*alt*-CM) ($M_n = 180.2$ kg/mol) [Inset: exact masses for proposed structures. In this ESI-MS spectrum, both CM and methyl-3-(2-oxo-2H-chromen-3-yl)propionate degradation product can be found. However, the intensity of mass ions in ESI-MS spectrum does not represent the actual amount. Because the characteristic peaks of CM are negligible in NMR spectra (Figures S30-31) of the crude degradation mixture, the content of CM should be in a very small amount which is presumably formed by the degradation of continuous CM units at the termination end of $t\text{Bu}_2\text{P}-(\text{EA-}i\text{alt-}\text{CM})_n\text{-CM-H}$].

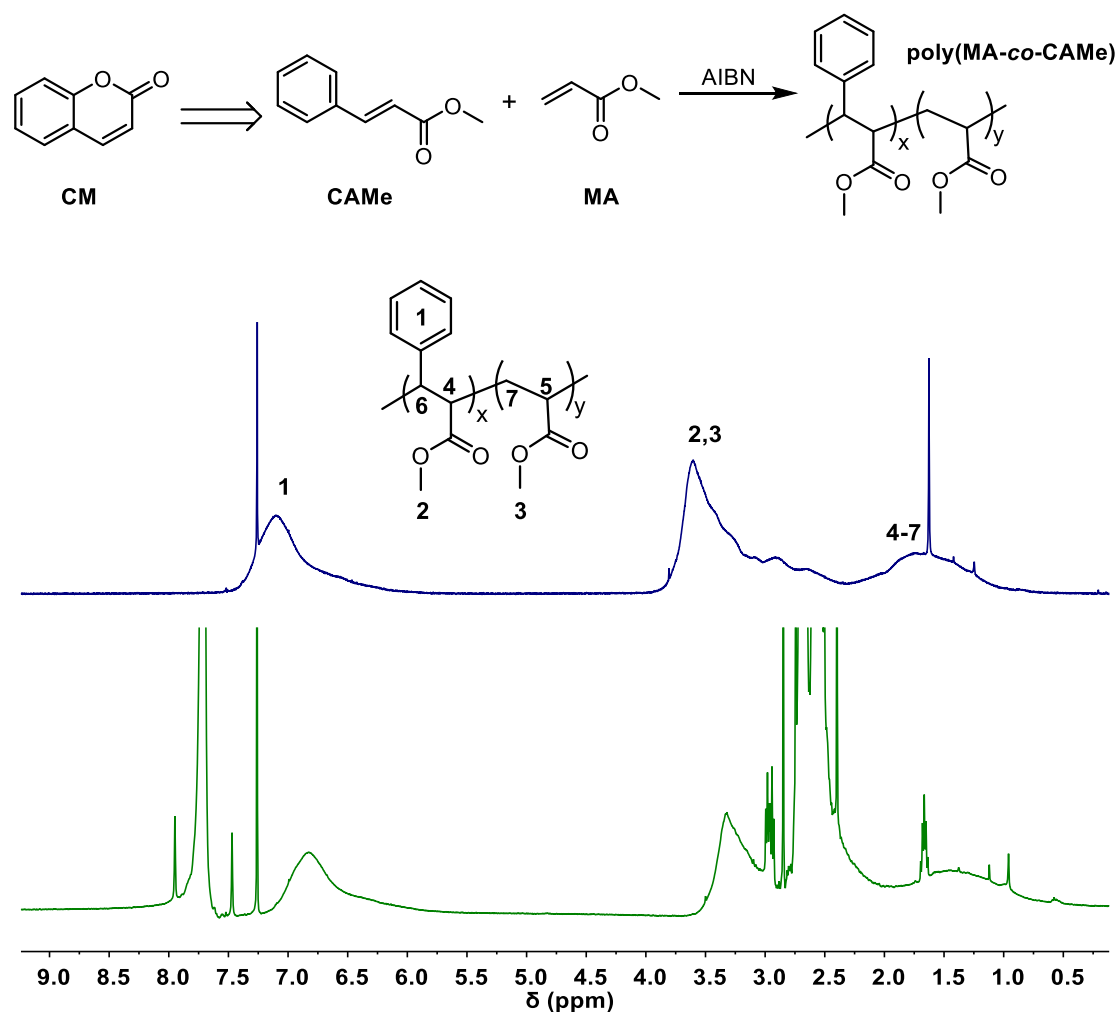


Figure S34. ¹H NMR spectra (CDCl₃, RT) of poly(MA-*co*-CAME) (top) and the crude reaction mixture obtained by TBD-mediated degradation of poly(MA-*co*-CAME) (bottom).

The copolymerization of CAME and MA was carried out according to modified literature procedure.⁹ Copolymerization conditions: CAME (16 mmol), MA (8 mmol), AIBN (0.01 mmol), toluene as the solvent (4.0 mL), Temp. = 80 °C, Time = 14 days. Monomer conversion and monomer composition of copolymer were measured by quantitative ¹H NMR spectrum using ethylene carbonate as internal standard: Conv.(CAME)% = 23.5%, Conv.(MA)% = 56.4%, Incorp.(CAME)% = 45.5%. Note: B(2,4-F₂Ph)₃/PtBu₃ FLP catalyst was inactive toward the copolymerization of CAME and MA.

Degradation conditions: Temp. = 80 °C, Time = 24 h, TBD:CAME unit (mol:mol) = 1:1, DMF as the solvent.

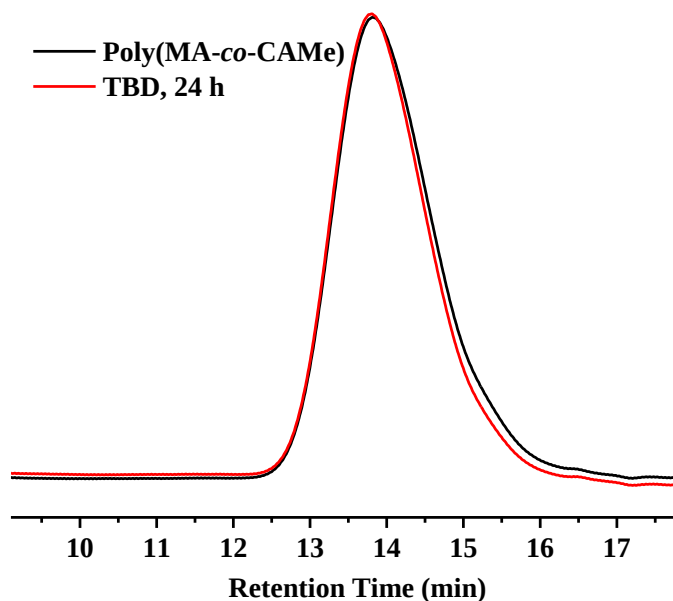


Figure S35. GPC curves of poly(MA-*co*-CAME) ($M_n = 52.8$ kg/mol, $D = 1.46$) before and after TBD-mediated degradation for 24 h ($M_n = 55.8$ kg/mol, $D = 1.44$).

General Procedure for Monitoring Cs_2CO_3 -triggered Degradation.

A predetermined amount of alternating copolymer [poly(MA-*alt*-CM), poly(EA-*alt*-CM), poly(BA-*alt*-CM), poly(EHA-*alt*-CM), 100~200 mg] and ethylene carbonate (internal standard) were dissolved in DMF (1.5 mL). The degradation was triggered by the rapid addition of Cs_2CO_3 solid powder to the above solution under vigorous stirring. After the measured time interval, a 0.2 mL aliquot was taken from the reaction mixture via syringe and quickly quenched into a 2 mL septum-sealed vial containing 0.5 mL of “wet” CDCl_3 . The quenched aliquots were later analyzed by ^1H NMR spectra to obtain conversion data.

Table S6. Results of Cs₂CO₃-triggered Degradations.^a

Sample	Cs ₂ CO ₃ :CM unit (mol:mol)	Temp. (°C)	Time (h)	Conversion ^b (%)
Poly(MA- <i>alt</i> -CM)	1:1	25	2	64.5
			6	76.3
			12	81.4
			24	92.4
Poly(EA- <i>alt</i> -CM)	1:1	25	2	68.2
			6	76.3
			12	80.4
			24	91.0
Poly(BA- <i>alt</i> -CM)	1:1	25	2	72.5
			6	76.8
			12	80.0
			24	91.4
Poly(EHA- <i>alt</i> -CM)	1:1	25	2	60.1
			6	71.5
			12	80.6
			24	94.5
Poly(BA- <i>alt</i> -PCM)	1:1	25	24	90.4
Poly(BA- <i>alt</i> -ACM)	1:1	25	24	91.0
Poly(EA- <i>alt</i> -CM)	0.1:1	25	24	40.1
			48	73.2
Poly(EA- <i>alt</i> -CM)	0.1:1	50	6	80.7
			12	86.1
			24	96.8

^a Conditions: Poly(MA-*alt*-CM): $M_n = 180.2$ kg/mol (Table 1, Run 13), Poly(EA-*alt*-CM): $M_n = 190.0$ kg/mol (Table 1, Run 11), Poly(BA-*alt*-CM): $M_n = 263.5$ kg/mol (Table 1, Run 8), Poly(EHA-*alt*-CM): $M_n = 164.1$ kg/mol (Table 1, Run 16), Poly(BA-*alt*-PCM): $M_n = 39.7$ kg/mol (Table 1, Run 17); Poly(BA-*alt*-ACM): $M_n = 50.5$ kg/mol (Table 1, Run 18), DMF as the solvent. ^b Conversions of degradation product measured by quantitative ¹H NMR spectrum using ethylene carbonate as internal standard.

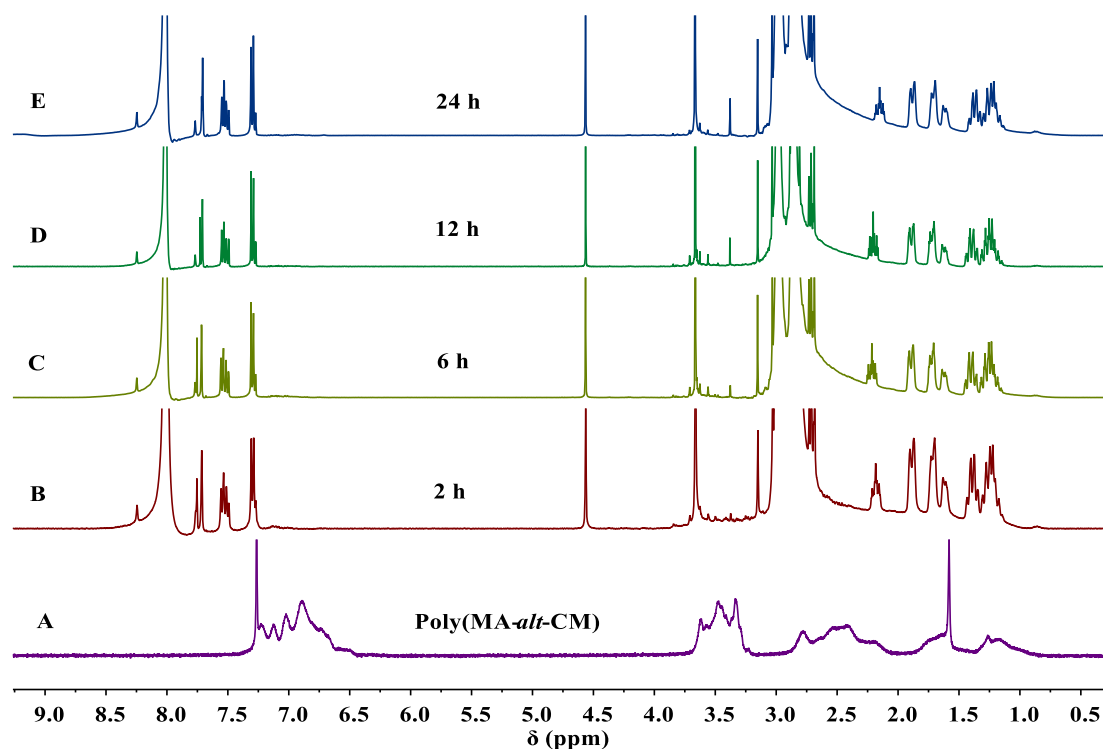


Figure S36. Degradation process of poly(MA-*alt*-CM) (Table S6) by Cs_2CO_3 monitored by ^1H NMR spectra (CDCl_3 , RT): (A) poly(MA-*alt*-CM); (B) 2 h; (C) 6 h; (D) 12 h; (E) 24 h.

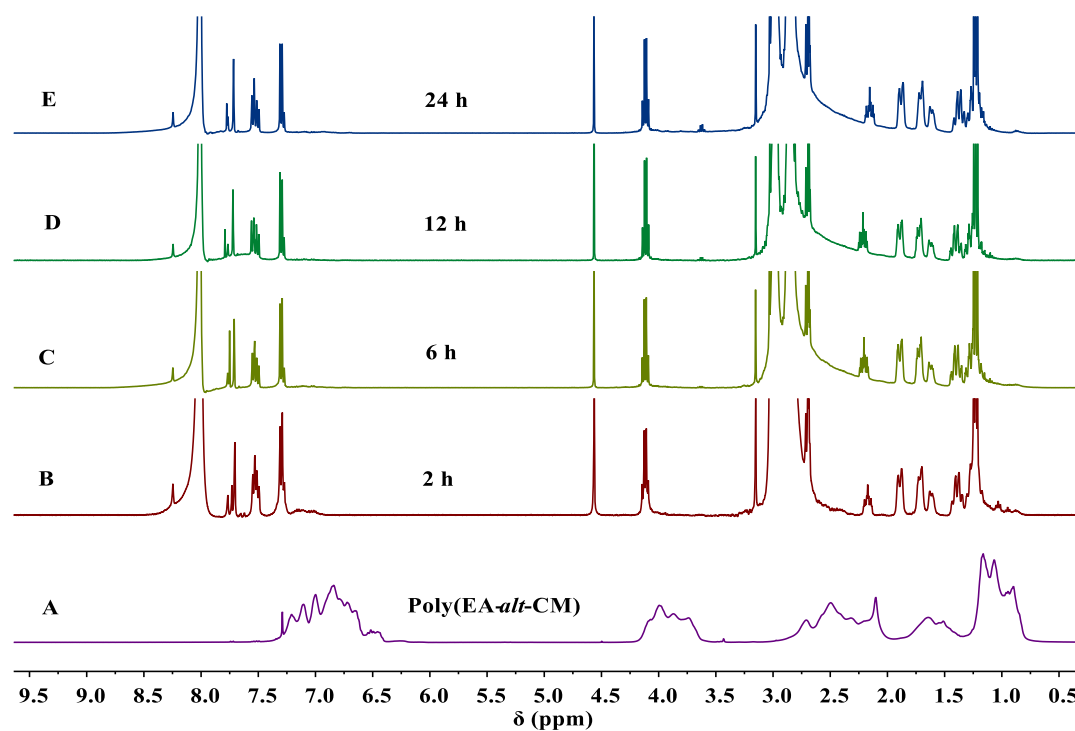


Figure S37. Degradation process of poly(EA-*alt*-CM) (Table S6) by Cs_2CO_3 monitored by ^1H NMR spectra (CDCl_3 , RT): (A) poly(EA-*alt*-CM); (B) 2 h; (C) 6 h; (D) 12 h; (E) 24 h.

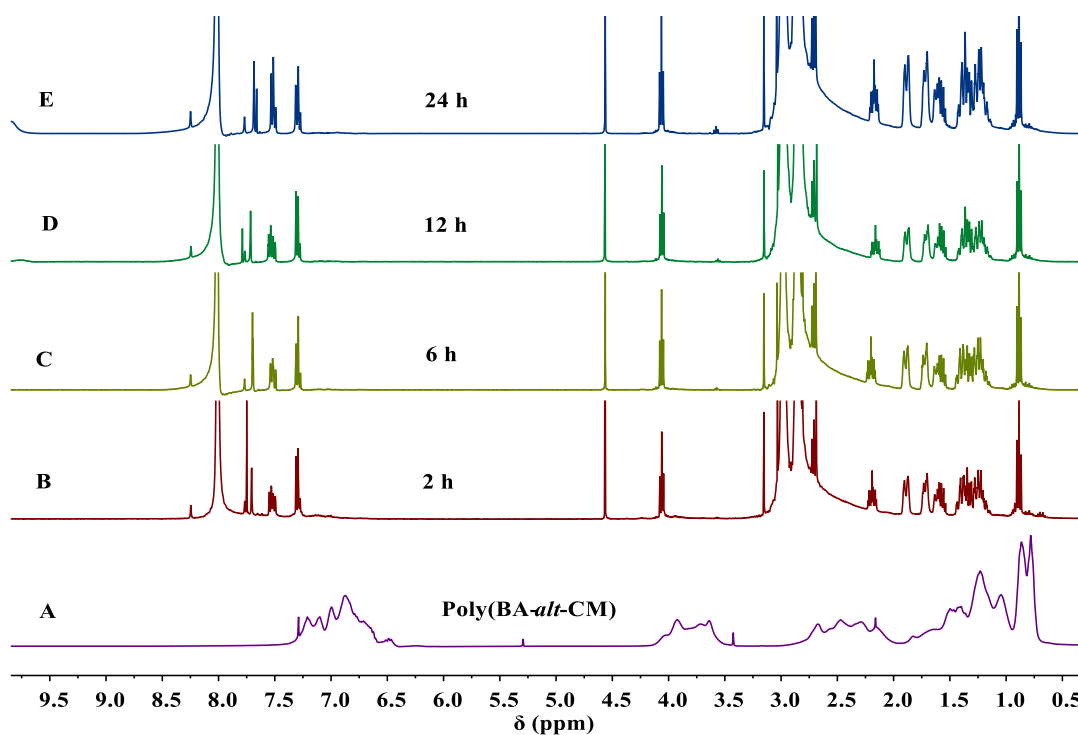


Figure S38. Degradation process of poly(BA-*alt*-CM) (Table S6) by Cs_2CO_3 monitored by ^1H NMR spectra (CDCl_3 , RT): (A) poly(BA-*alt*-CM); (B) 2 h; (C) 6 h; (D) 12 h; (E) 24 h.

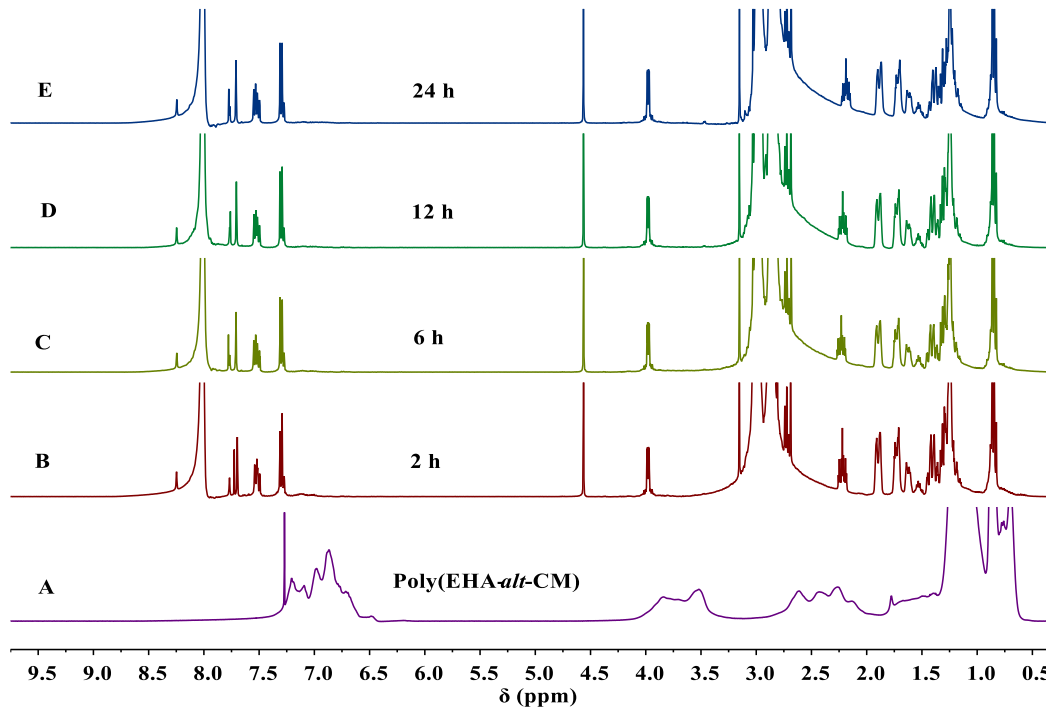


Figure S39. Degradation process of poly(EHA-*alt*-CM) (Table S6) by Cs_2CO_3 monitored by ^1H NMR spectra (CDCl_3 , RT): (A) poly(EHA-*alt*-CM); (B) 2 h; (C) 6 h; (D) 12 h; (E) 24 h.

General Procedures for Cs₂CO₃-triggered Degradation.

A predetermined amount of alternating copolymer [poly(MA-*alt*-CM), poly(EA-*alt*-CM), poly(BA-*alt*-CM), poly(EHA-*alt*-CM), ca. 500 mg] and ethylene carbonate (internal standard) were dissolved in DMF (5.0 mL). The degradation was triggered by the rapid addition of Cs₂CO₃ solid powder [Cs₂CO₃:CM (mol:mol) = 1:1] to the above solution under vigorous stirring. The mixture was reacted at RT for 24 h, and then quenched by the addition of 3 mL of dilute HCl. After removing the volatiles under the reduced pressure, 20 mL of ethyl acetate was added and the resultant solution was washed by deionized water. The layers were then separated, and the aqueous layer was extracted with ethyl acetate (3 × 100 mL). The combined organic extracts were dried over anhydrous Na₂SO₄, filtered, and concentrated. The crude product was purified by flash column chromatography (a short silica gel column with the height of ca. 2 cm): Methyl-3-(2-oxo-2H-chromen-3-yl)propionate (MCP): isolated yield = 83.0%.

Ethyl-3-(2-oxo-2H-chromen-3-yl)propionate (ECP, isolated yield = 81.5%) as colorless viscous oil. ¹H NMR (400 MHz, CDCl₃, RT): δ 7.53 (s, 1H, -CH=C<), 7.43–7.38 (m, 2H, -Ph), 7.24–7.17 (m, 2H, -Ph), 4.06 (q, *J* = 7.2 Hz, 2H, -OCH₂-), 2.82 (t, *J* = 7.2 Hz, 2H, -CH₂COO-), 2.64 (t, *J* = 7.2 Hz, 2H, -CH₂CH₂COO-), 1.16 (t, 3H, -OCH₂CH₃). ¹³C NMR (100 MHz, CDCl₃, RT): δ 172.52, 161.44, 153.24, 139.94, 130.88, 127.76, 127.41, 124.36, 119.33, 116.39, 60.52, 32.25, 26.58, 14.21. HRMS (ESI): Exact mass calcd. for C₁₄H₁₄O₄Na ([M+Na]⁺): 269.0783. Found: 269.0784.

n-Butyl-3-(2-oxo-2H-chromen-3-yl)propionate (BCP, isolated yield = 80.0%) as colorless viscous oil: ¹H NMR (400 MHz, CDCl₃, RT): δ 7.53 (s, 1H, -CH=C<), 7.43–7.37 (m, 2H, -Ph), 7.24–7.17 (m, 2H, -Ph), 4.00 (t, *J* = 6.8 Hz, 2H, -OCH₂-), 2.82 (t, *J* = 7.2 Hz, 2H, -CH₂COO-), 2.65 (t, *J* = 6.8 Hz, 2H, -CH₂CH₂COO-), 1.54–1.47 (m, 2H, -CH₂CH₂CH₃), 1.31–1.21 (m, 2H, -CH₂CH₃), 0.81 (t, *J* = 7.6 Hz,

3H, $-CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, RT): δ 172.65, 161.45, 153.27, 139.95, 130.89, 127.78, 127.41, 124.37, 119.35, 116.41, 64.46, 32.27, 30.64, 26.66, 19.11, 13.66. HRMS (ESI): Exact mass calcd. for $C_{16}H_{18}O_4Na$ ($[M+Na]^+$): 297.1095. Found: 297.1097.

Ethylhexyl-3-(2-oxo-2H-chromen-3-yl)propionate (EHCP, isolated yield = 84.0%) as colorless viscous oil: 1H NMR (400 MHz, $CDCl_3$, RT): δ 7.53 (s, 1H, $-CH=C<$), 7.43–7.37 (m, 2H, $-Ph$), 7.25–7.17 (m, 2H, $-Ph$), 3.91 (dd, $J = 5.6, 2.4$ Hz, 2H, $-OCH_2-$), 2.83 (t, $J = 7.2$ Hz, 2H, $-CH_2COO-$), 2.66 (t, $J = 6.8$ Hz, 2H, $-CH_2CH_2COO-$), 1.47–1.43 (m, 1H, $-CH<$), 1.27–1.17 (m, 8H, $-CH_2CH_3$, $-(CH_2)_3CH_3$), 0.81–0.75 (m, 6H, $-CH_2CH_3$, $-(CH_2)_3CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, RT): δ 172.80, 161.48, 153.32, 139.93, 130.92, 127.84, 127.43, 124.39, 119.38, 116.46, 67.05, 38.73, 32.32, 30.37, 28.92, 26.71, 23.74, 22.96, 14.07, 10.97. HRMS (ESI): Exact mass calcd. for $C_{20}H_{26}O_4Na$ ($[M+Na]^+$): 353.1719. Found: 353.1723.

Butyl 3-[7-(allyloxy)-2-oxo-2H-chromen-3-yl]propanoate (BACP, isolated yield = 85.0%) as yellowish viscous oil. 1H NMR (400 MHz, $CDCl_3$, RT): δ 7.53 (s, 1H, $-CH=C<$), 7.33 (d, $J = 8.5$ Hz, 1H, $-Ph$), 6.88–6.79 (m, 2H, $-Ph$), 6.04 (ddt, $J = 16.1, 10.6, 5.3$ Hz, 1H, $-OCH_2CH=CH_2$), 5.50–5.39 (m, 1H, $-OCH_2CH=CH_2$), 5.37–5.30 (m, 1H, $-OCH_2CH=CH_2$), 4.63–4.54 (m, 2H, $-OCH_2CH=CH_2$), 4.06 (t, $J = 6.8$ Hz, 2H, $-OCH_2-$), 2.85 (t, $J = 7.2$ Hz, 2H, $-CH_2CH_2(C=O)O-$), 2.69 (t, $J = 7.2$ Hz, 2H, $-CH_2CH_2(C=O)O-$), 1.57 (p, $J = 6.8$ Hz, 2H, $-CH_2CH_2CH_3$), 1.33 (h, $J = 7.4$ Hz, 2H, $-CH_2CH_2CH_3$), 0.89 (t, $J = 7.4$ Hz, 3H, $-CH_2CH_2CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, RT): δ 172.81, 161.82, 160.96, 154.84, 140.10, 132.17, 128.24, 124.11, 118.46, 113.03, 112.99, 101.31, 69.18, 64.40, 32.35, 30.57, 26.48, 19.06, 13.63. HRMS (ESI): Exact mass calcd. for $C_{19}H_{22}O_5Na$ ($[M+Na]^+$): 353.1360. Found: 353.1359.

Butyl 3-(2-oxo-7-propoxy-2H-chromen-3-yl)propanoate (BPCP, isolated yield = 83.0%) as

colorless viscous oil. ^1H NMR (400 MHz, CDCl_3 , RT): δ 7.53 (s, 1H, $-\text{CH}=\text{C}<$), 7.32 (d, $J = 8.5$ Hz, 1H, $-\text{Ph}$), 6.84 – 6.76 (m, 2H, $-\text{Ph}$), 4.06 (t, $J = 6.7$ Hz, $-\text{OCH}_2-$), 3.96 (t, $J = 6.5$ Hz, 2H, $-\text{OCH}_2\text{CH}_2\text{CH}_3$), 2.85 (t, $J = 7.2$ Hz, 2H, $-\text{CH}_2\text{CH}_2(\text{C}=\text{O})\text{O}-$), 2.69 (t, $J = 7.1$ Hz, 2H, $-\text{CH}_2\text{CH}_2(\text{C}=\text{O})\text{O}-$), 1.84 (h, $J = 7.1$ Hz, 2H, $-\text{OCH}_2\text{CH}_2\text{CH}_3$), 1.63 – 1.52 (m, 2H, $-\text{CH}_2\text{CH}_2\text{CH}_3$), 1.33 (h, $J = 7.4$ Hz, 2H, $-\text{CH}_2\text{CH}_2\text{CH}_3$), 1.05 (t, $J = 7.4$ Hz, 3H, $-\text{OCH}_2\text{CH}_2\text{CH}_3$), 0.89 (t, $J = 7.4$ Hz, 3H, $-\text{CH}_2\text{CH}_2\text{CH}_3$). ^{13}C NMR (100 MHz, CDCl_3 , RT): δ 172.80, 161.87, 161.62, 154.92, 140.14, 128.16, 123.80, 112.82, 112.72, 100.88, 69.97, 64.36, 32.36, 30.56, 26.46, 22.29, 19.04, 13.61, 10.40. HRMS (ESI): Exact mass calcd. for $\text{C}_{19}\text{H}_{24}\text{O}_5\text{Na}$ ($[\text{M}+\text{Na}]^+$): 355.1517. Found: 355.1516.

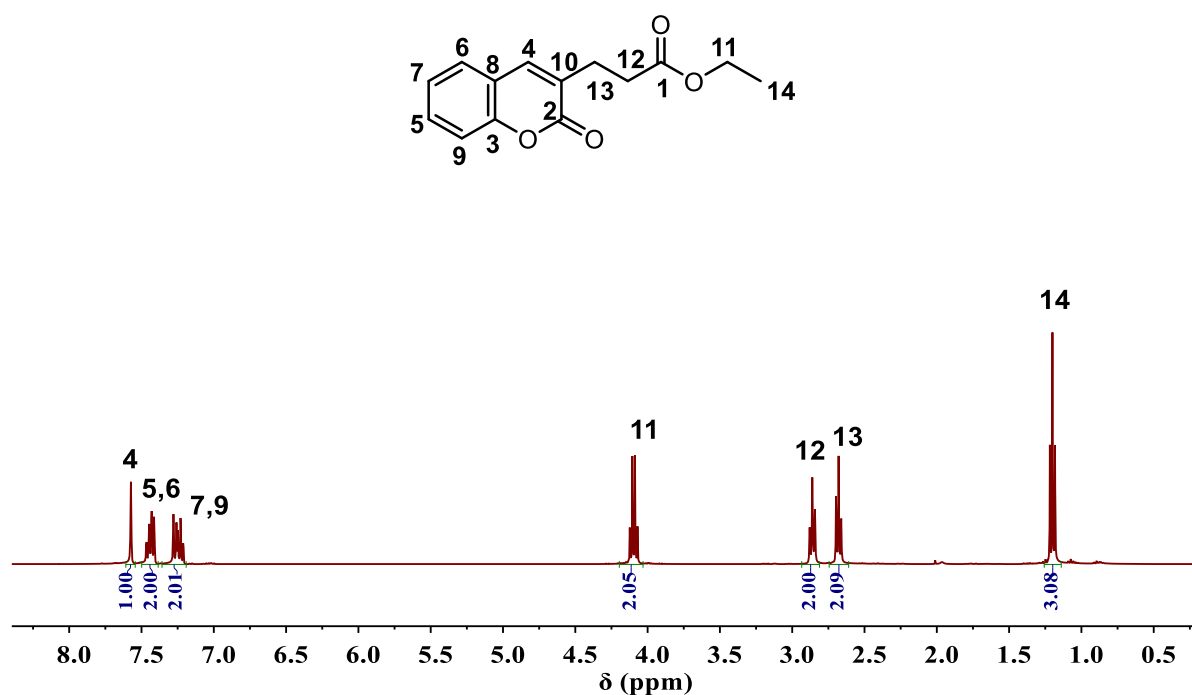


Figure S40. ^1H NMR spectrum (CDCl_3 , RT) of purified ECP degradation product.

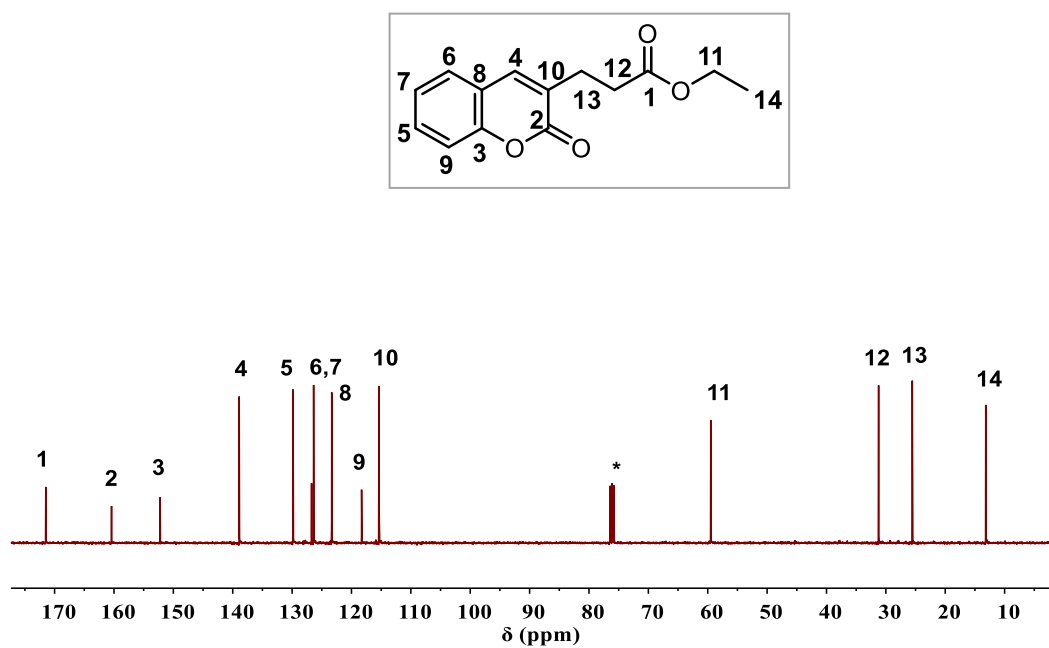


Figure S41. ^{13}C NMR spectrum (CDCl₃, RT) of purified ECP degradation product.

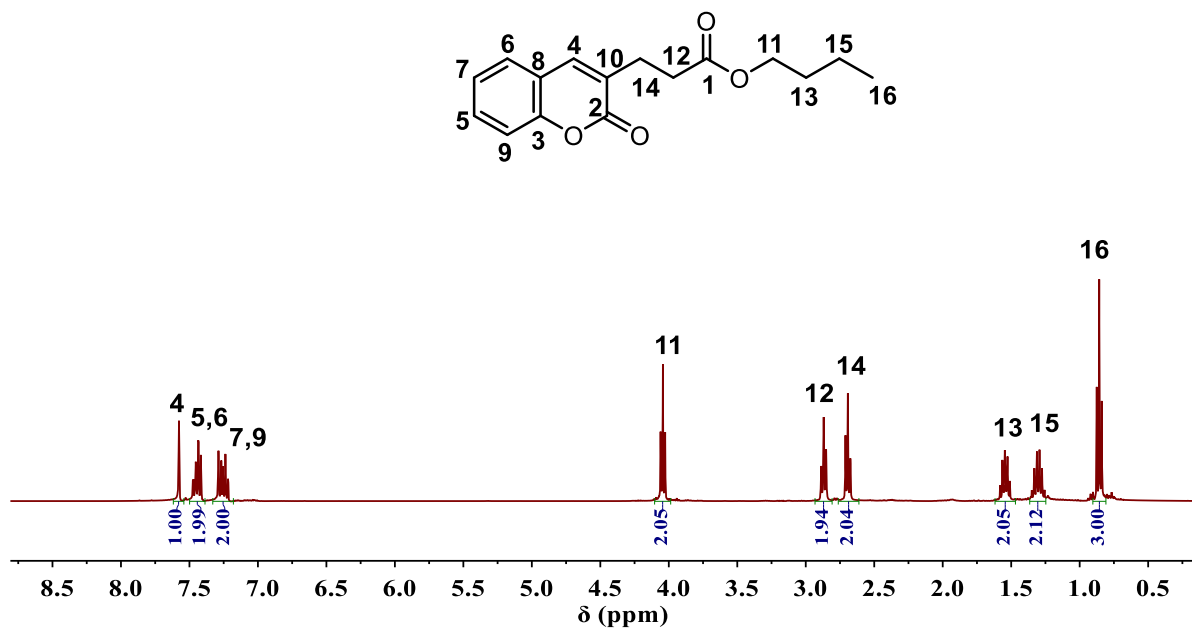


Figure S42. ^1H NMR spectrum (CDCl₃, RT) of purified BCP degradation product.

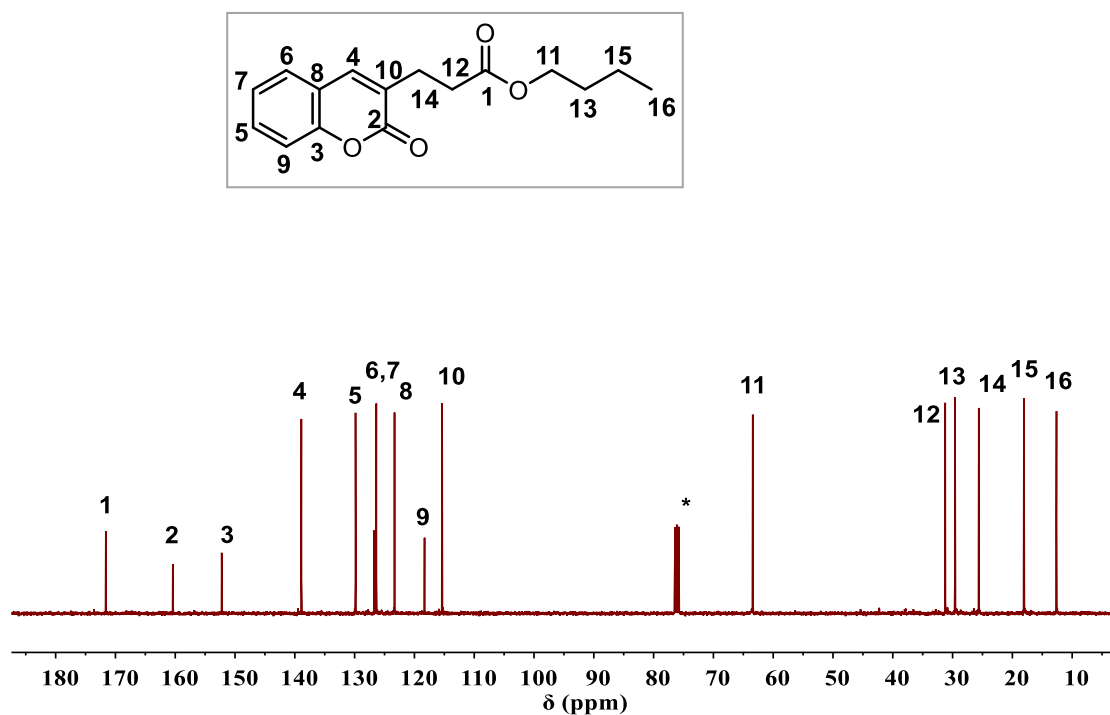


Figure S43. ^{13}C NMR spectrum (CDCl₃, RT) of purified BCP degradation product.

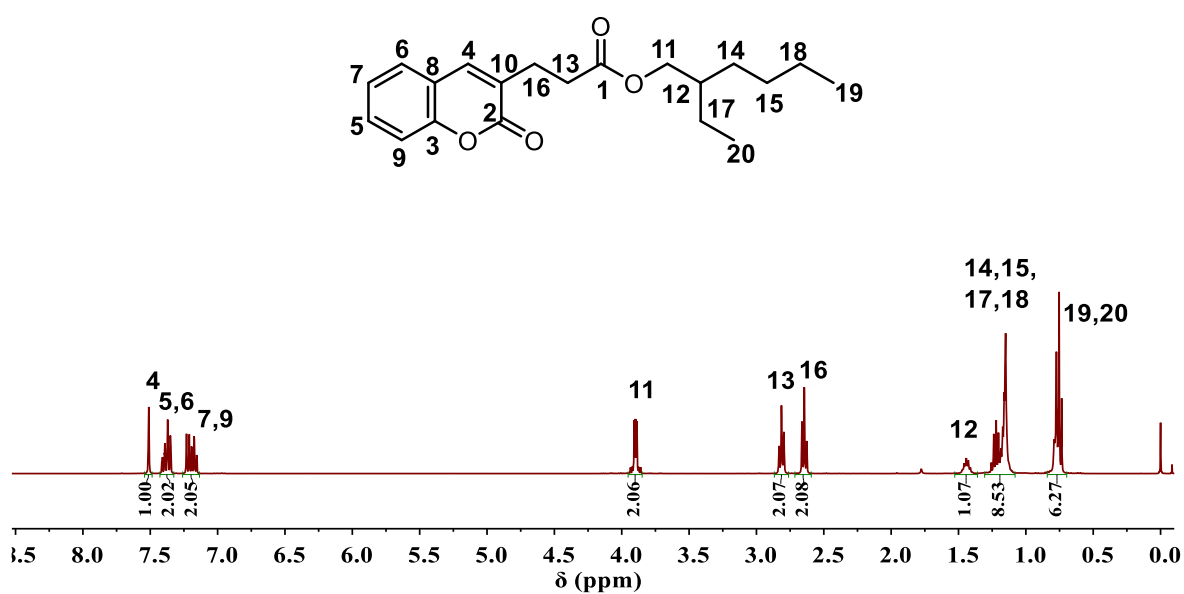


Figure S44. ^1H NMR spectrum (CDCl₃, RT) of purified EHCP degradation product.

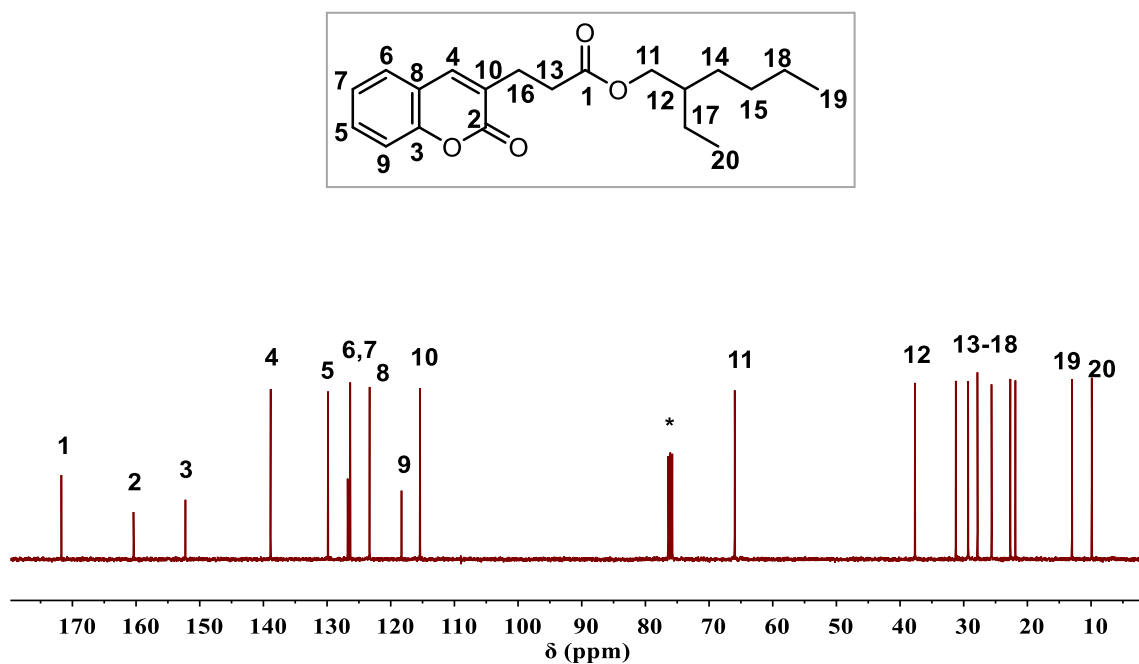


Figure S45. ^{13}C NMR spectrum (CDCl₃, RT) of purified EHCP degradation product.

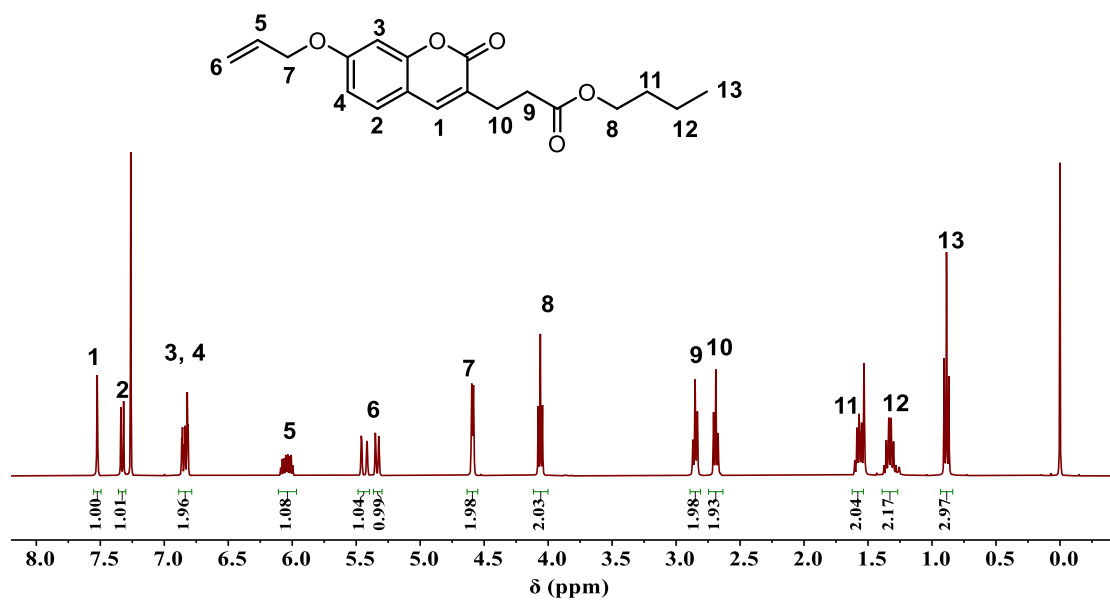


Figure S46. ^1H NMR spectrum (CDCl₃, RT) of purified BACP degradation product.

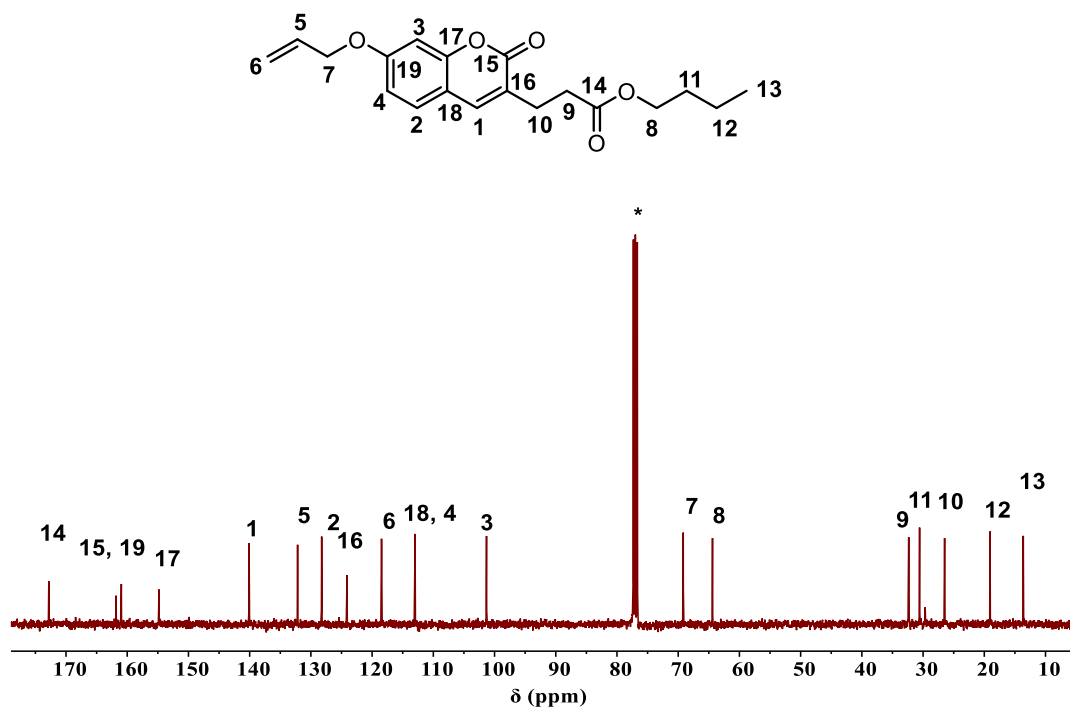


Figure S47. ¹³C NMR spectrum (CDCl₃, RT) of purified BACP degradation product.

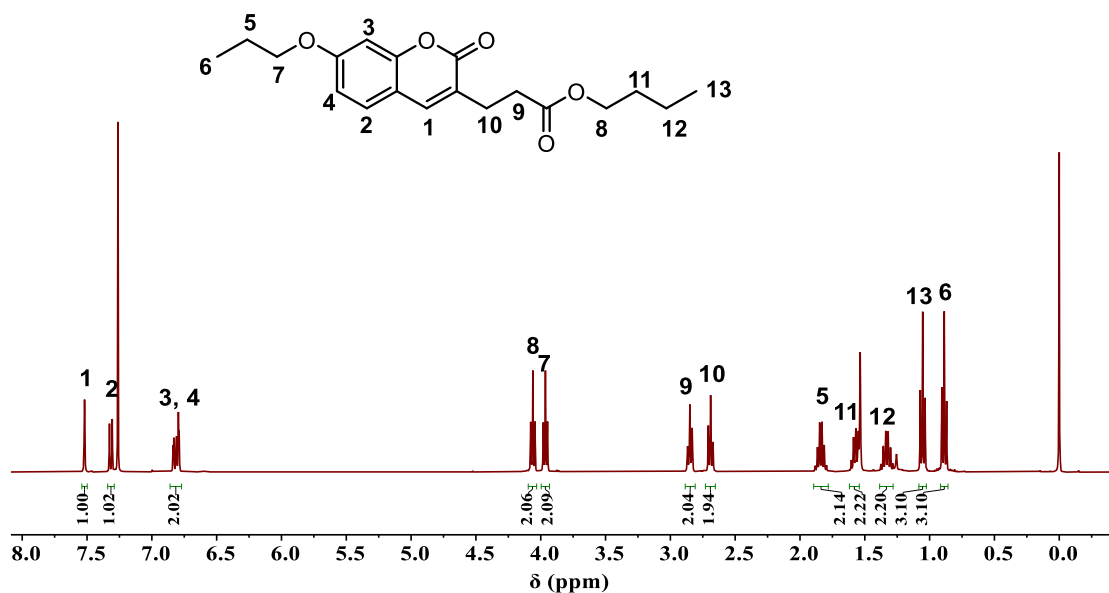


Figure S48. ¹H NMR spectrum (CDCl₃, RT) of purified BPCP degradation product.

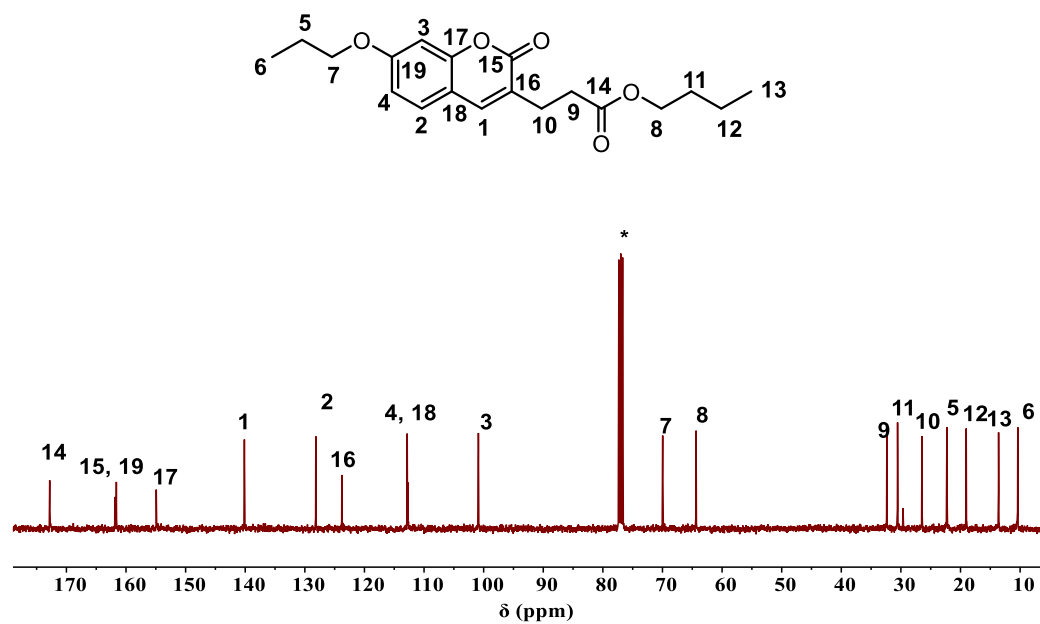


Figure S49. ^{13}C NMR spectrum (CDCl₃, RT) of purified BPCP degradation product.

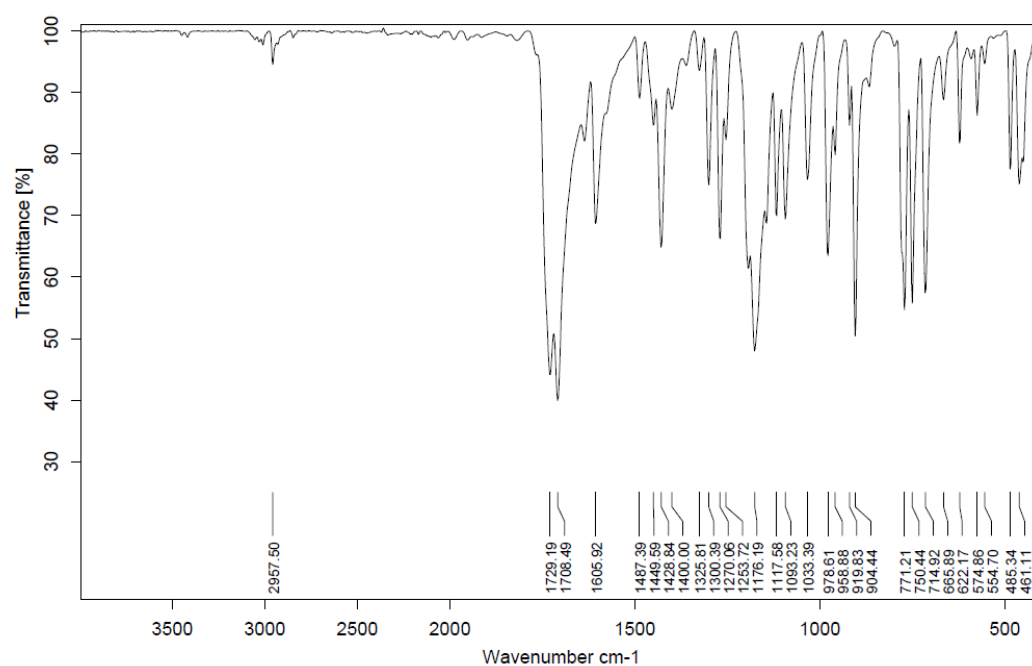


Figure S50. FT-IR spectrum of purified MCP degradation product.

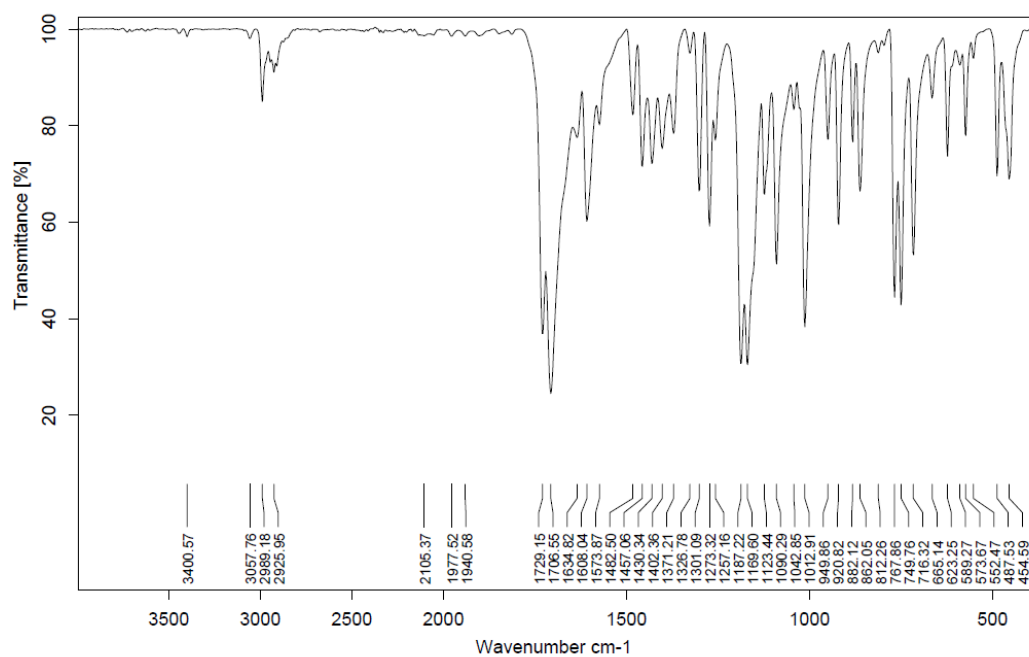


Figure S51. FT-IR spectrum of purified ECP degradation product.

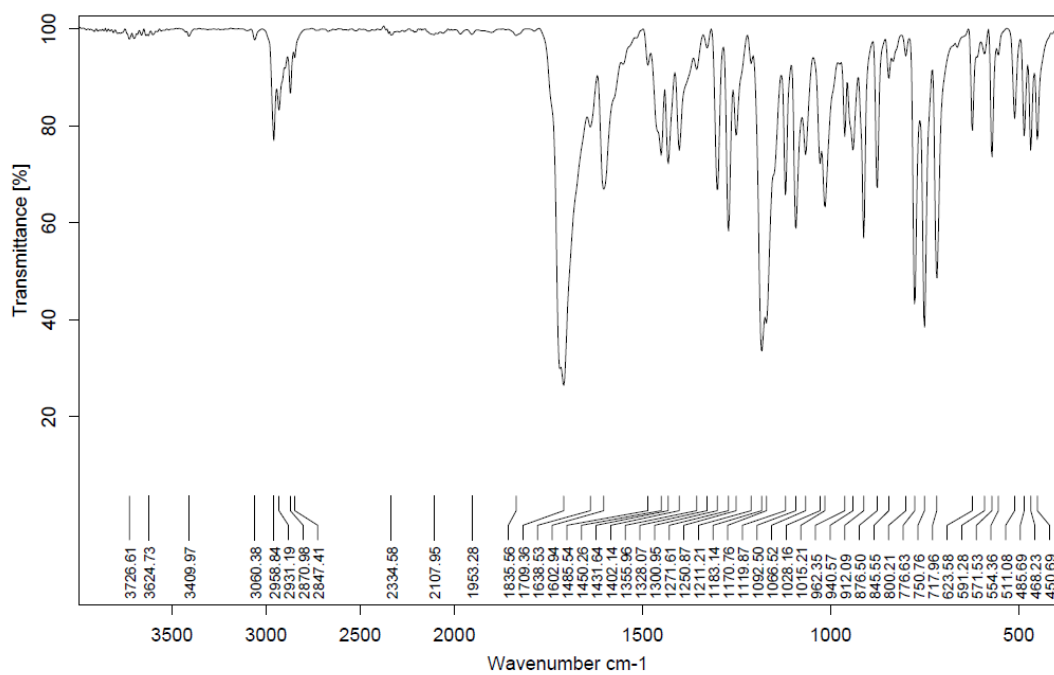


Figure S52. FT-IR spectrum of purified BCP degradation product.

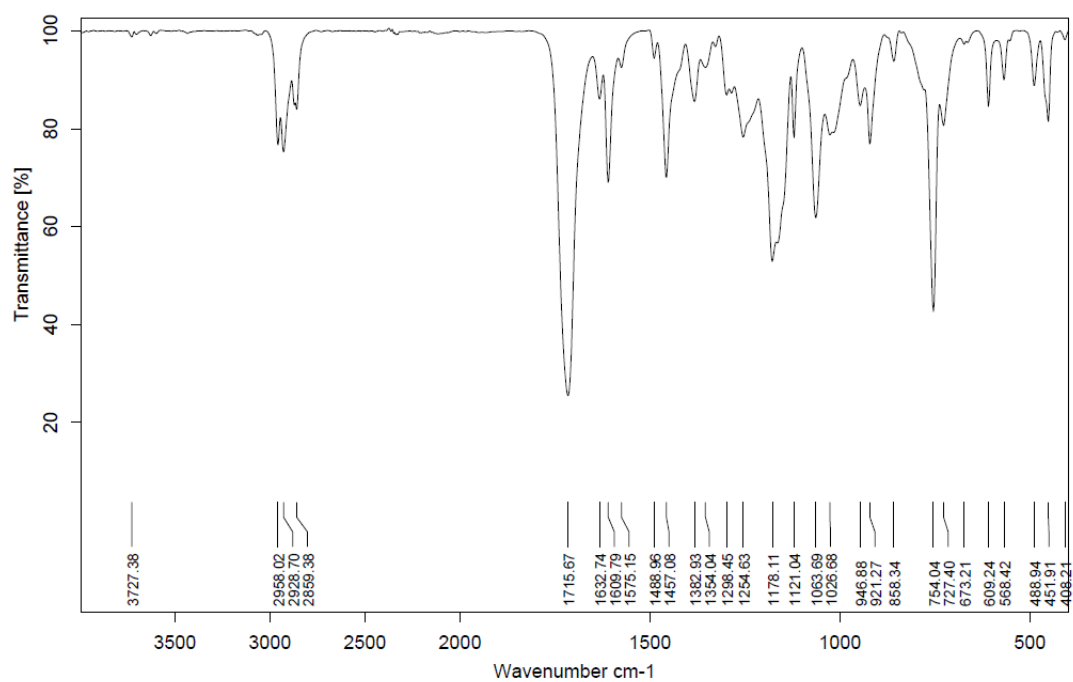


Figure S53. FT-IR spectrum of purified EHCP degradation product.

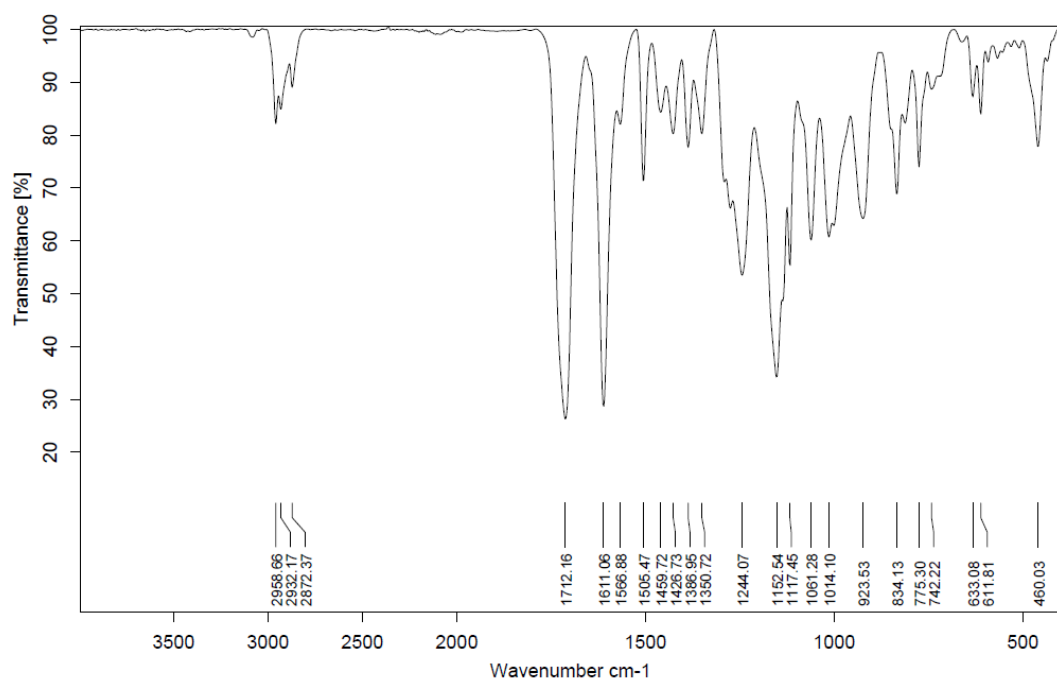


Figure S54. FT-IR spectrum of purified BACP degradation product.

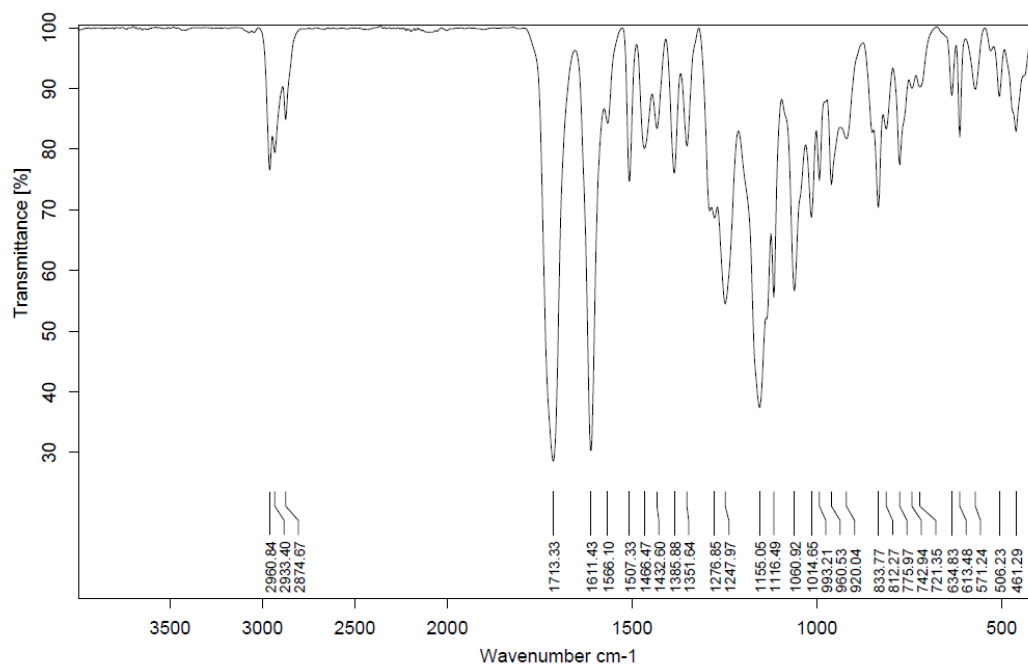


Figure S55. FT-IR spectrum of purified BPCP degradation product.

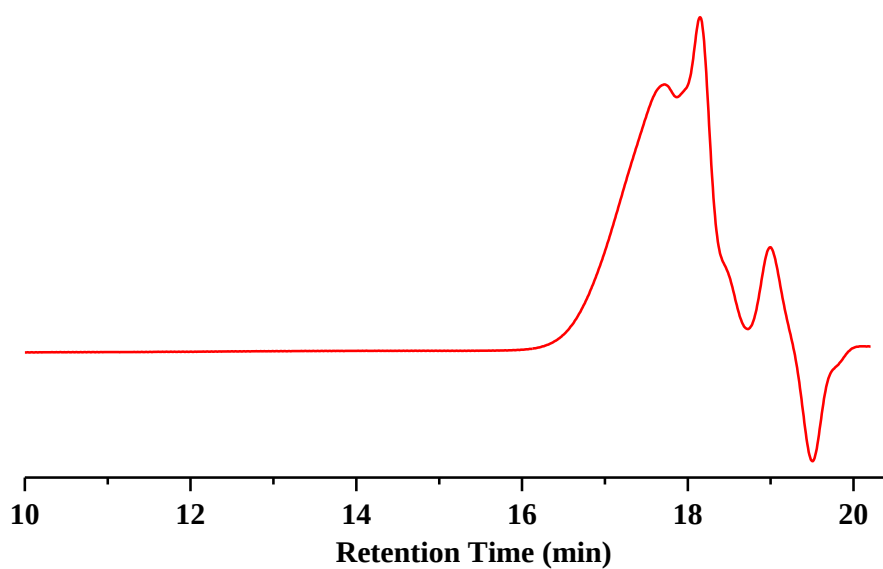


Figure S56. GPC curve of the crude reaction mixture ($M_n = 480$ g/mol, $D = 1.36$) after the Cs_2CO_3 -mediated degradation of poly(MA-*co*-CM) ($M_n = 151.8$ kg/mol, $D = 1.05$, CM mol% = 40.0%, Table 1, Run 12).

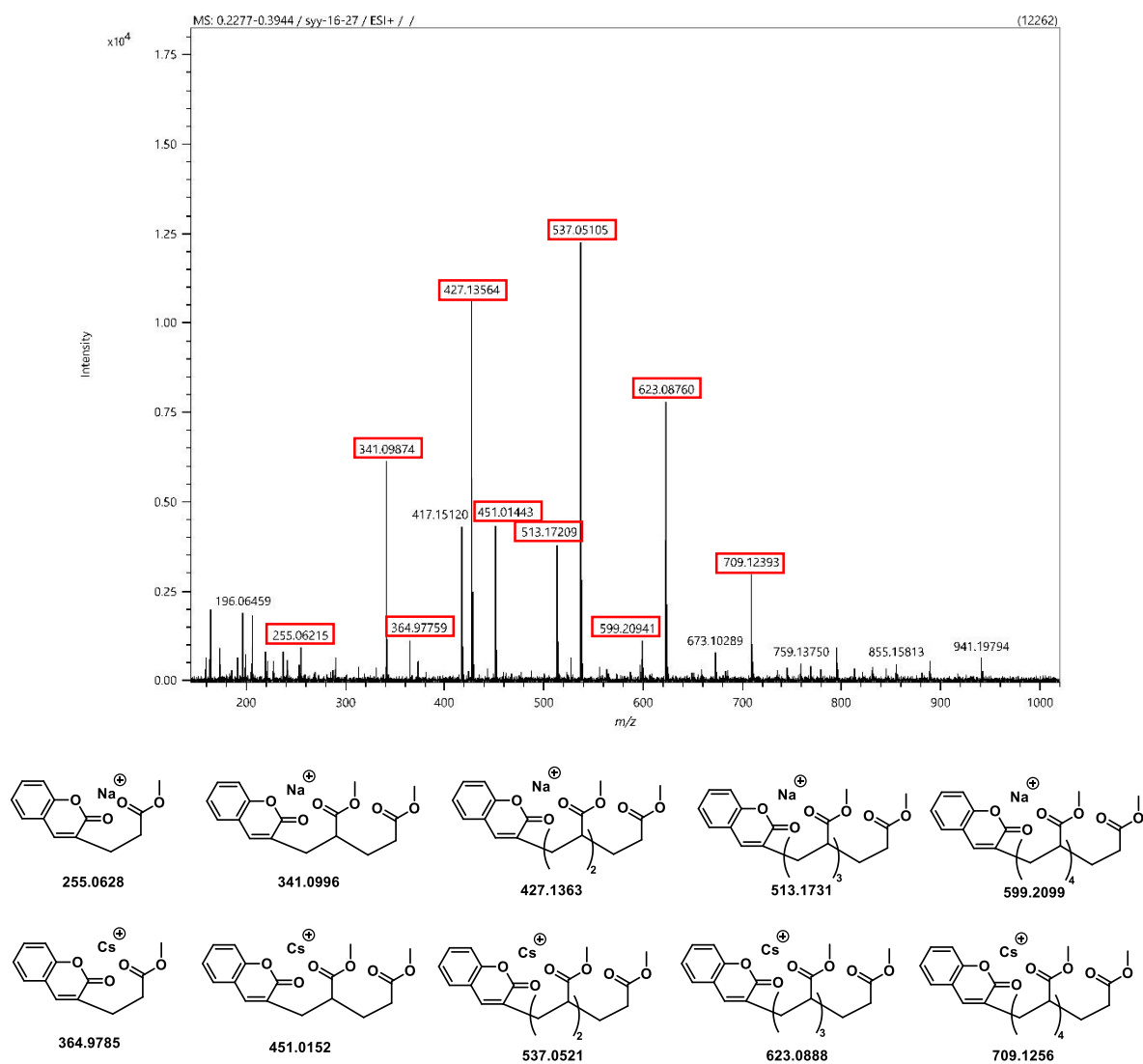


Figure S57. ESI-MS of crude reaction mixture produced by Cs_2CO_3 -triggered degradation of poly(MA-*co*-CM) (CM mol% = 40.0%, Table 1, Run 12). Exact masses for proposed structures are provided below (Note: the intensity of molecular ion peak does not represent the actual amount).

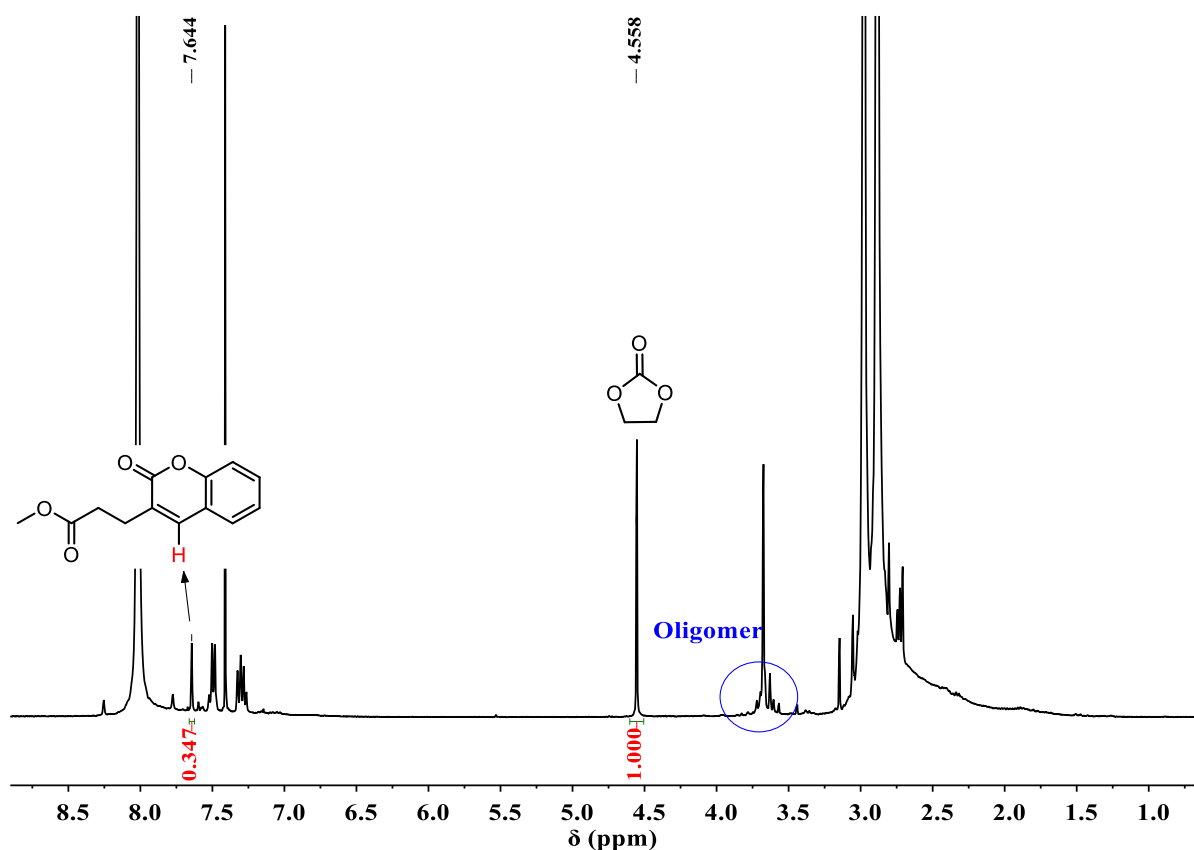


Figure S58. ^1H NMR spectrum (CDCl_3 , RT, 400 MHz) of reaction mixture obtained by Cs_2CO_3 -triggered degradation of poly(MA-*co*-CM) (CM mol% = 40.0%, Table 1, Run 12) after 24 h [Conv. (MCP) = $[(I_{7.64 \text{ ppm}}/I_{4.56 \text{ ppm}}) \times 4 \times n_{\text{internal standard}} \times M_{\text{MCP}} / m_{\text{copolymer}}] \times 100\% = 69.0\%$ ($I_{7.64 \text{ ppm}}$ and $I_{4.56 \text{ ppm}}$: Integrals of the peaks at 7.64 and 4.56 ppm, respectively; $n_{\text{internal standard}} = m_{\text{internal standard}}/88 = 18.8/88$ mmol, where $m_{\text{internal standard}}$ is the weight of internal standard; $M_{\text{MCP}} = 232 \text{ g/mol}$; $m_{\text{copolymer}} = 100 \text{ mg}$).

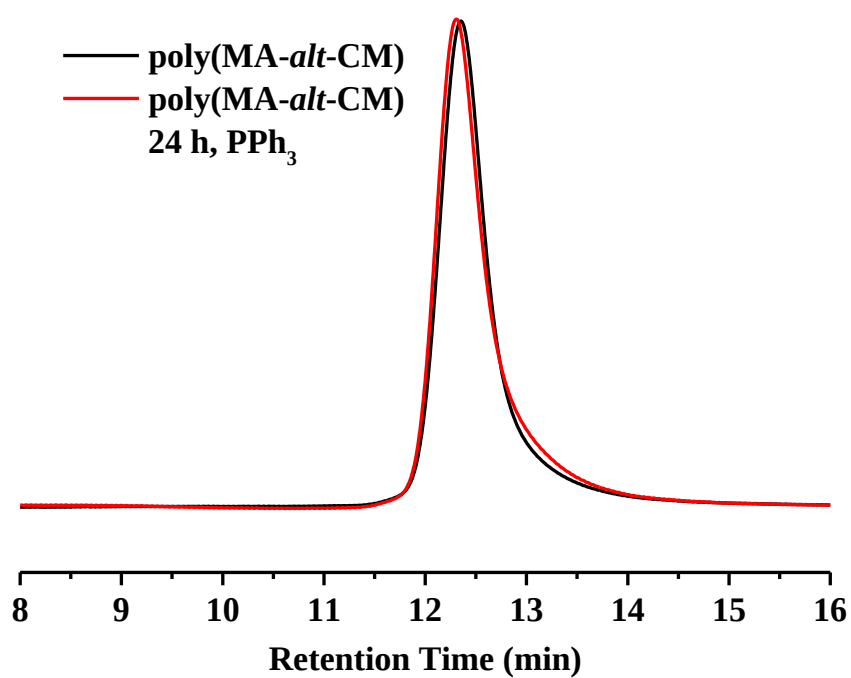


Figure S59. GPC curves of poly(MA-*alt*-CM) ($M_n = 180.2$ kg/mol, $D = 1.09$, Table 1, Run 13) before and after PPh₃-mediated degradation for 24 h ($M_n = 182.5$ kg/mol, $D = 1.10$) (Conditions: [MA unit]₀: [PPh₃]₀ = 2, DMF as the solvent, RT).

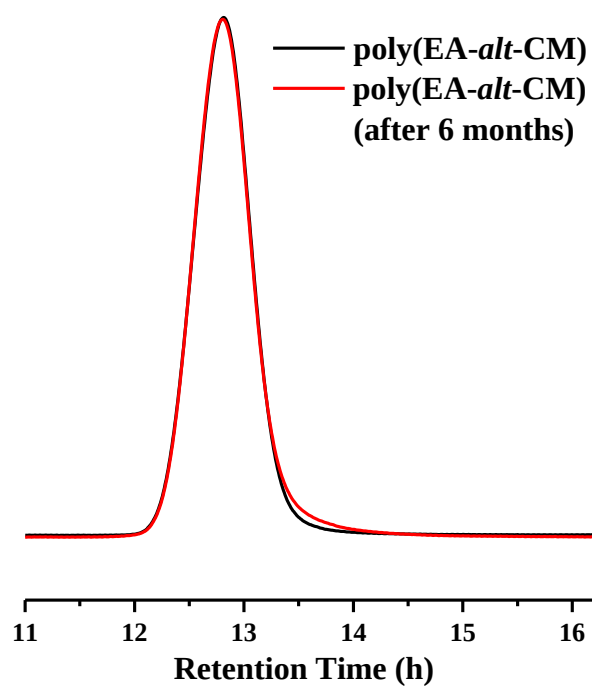


Figure S60. GPC curves of poly(EA-*alt*-CM) ($M_n = 200.4$ kg/mol, $D = 1.08$) before and after 6 months of storage under ambient conditions ($M_n = 202.3$ kg/mol, $D = 1.08$).



Figure S61. Thin films of poly(BA-*alt*-CM) (Table 1, Run 8) obtained by melt processing for once (A), twice (B), and three consecutive times (C).

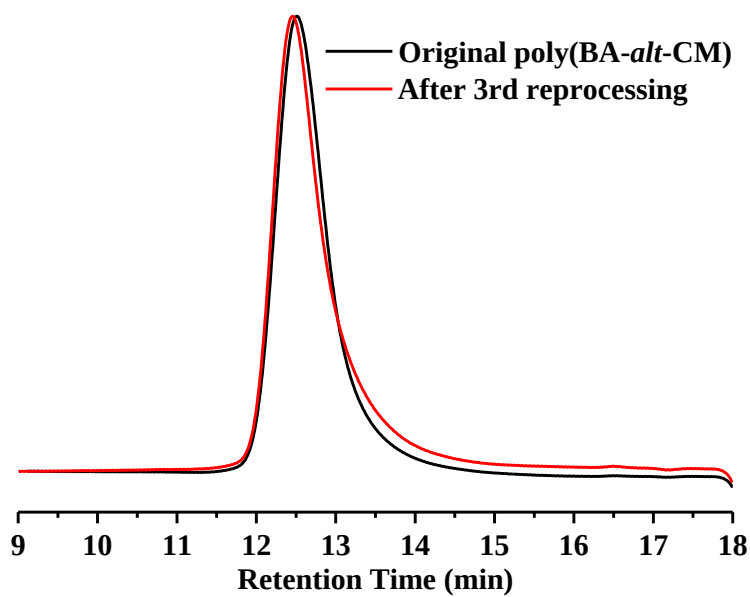


Figure S62. GPC curves of poly(BA-*alt*-CM) ($M_n = 236.5$ kg/mol, $D = 1.07$) before and after three consecutive melt processing ($M_n = 237.0$ kg/mol, $D = 1.08$).

Synthesis and Degradation of Thermoset

20 mL glass reactor was charged with B(2,4-F₂Ph)₃ (0.04 mmol), MA (4.0 mmol), BDA (0.1 mmol), CM (10.5 mmol) and DCM (2.8 mL) inside the glovebox at RT. The mixture was stirred for 10 minutes, and then the polymerization was started by rapid addition of PtBu₃ (0.02 mmol) in DCM (0.20 mL) via a gastight syringe to the above mixture under vigorous stirring. Cross-linked polymer gel was formed within 1.0 h, which was then repeatedly washed with DCM for five times to remove unreacted monomer and catalyst, and dried in a vacuum oven at 80 °C to a constant weight. The Cs₂CO₃-triggered degradation of cross-linking copolymer was performed under the same conditions used in the degradation of alternating copolymers.

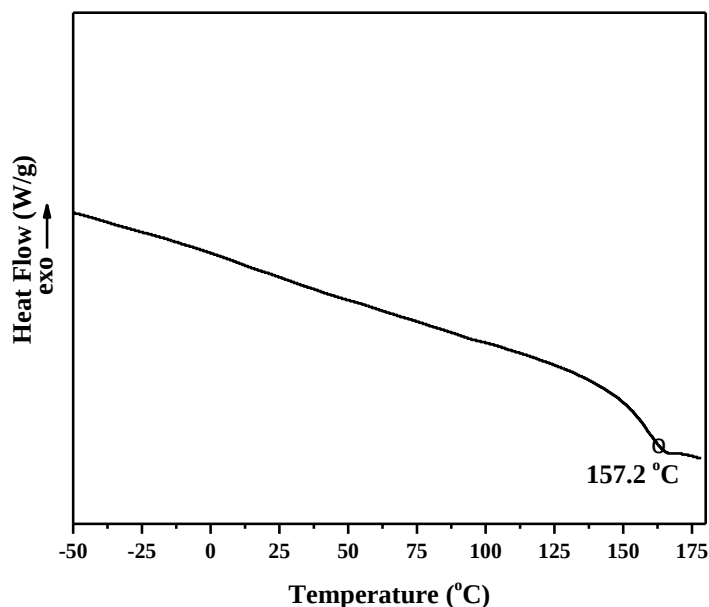


Figure S63. DSC curve of cross-linked poly(MA-*alt*-CM) which exhibits comparable T_g to uncrosslinked analogue ($T_g = 158.0$ °C).

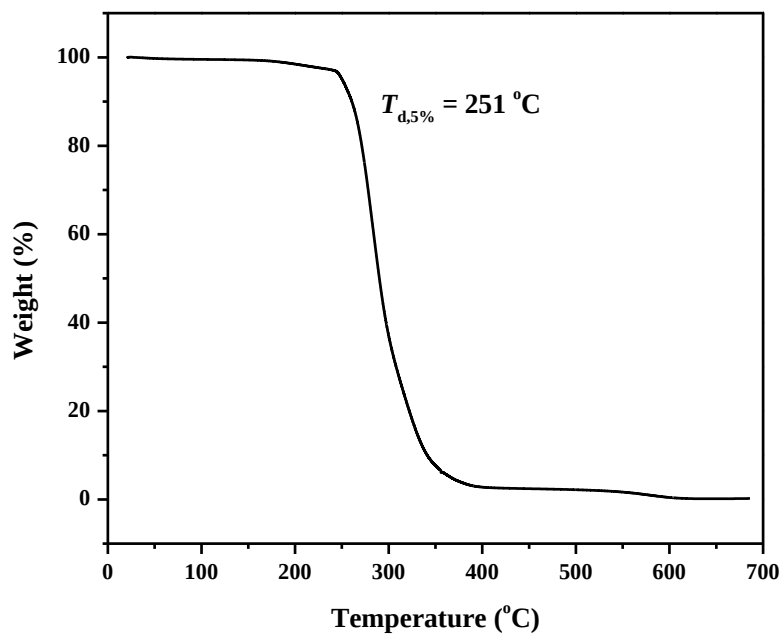


Figure S64. TGA curve of cross-linked poly(MA-*alt*-CM) which exhibits slightly lower thermal stability than uncrosslinked analogue ($T_d = 274\text{ }^{\circ}\text{C}$).

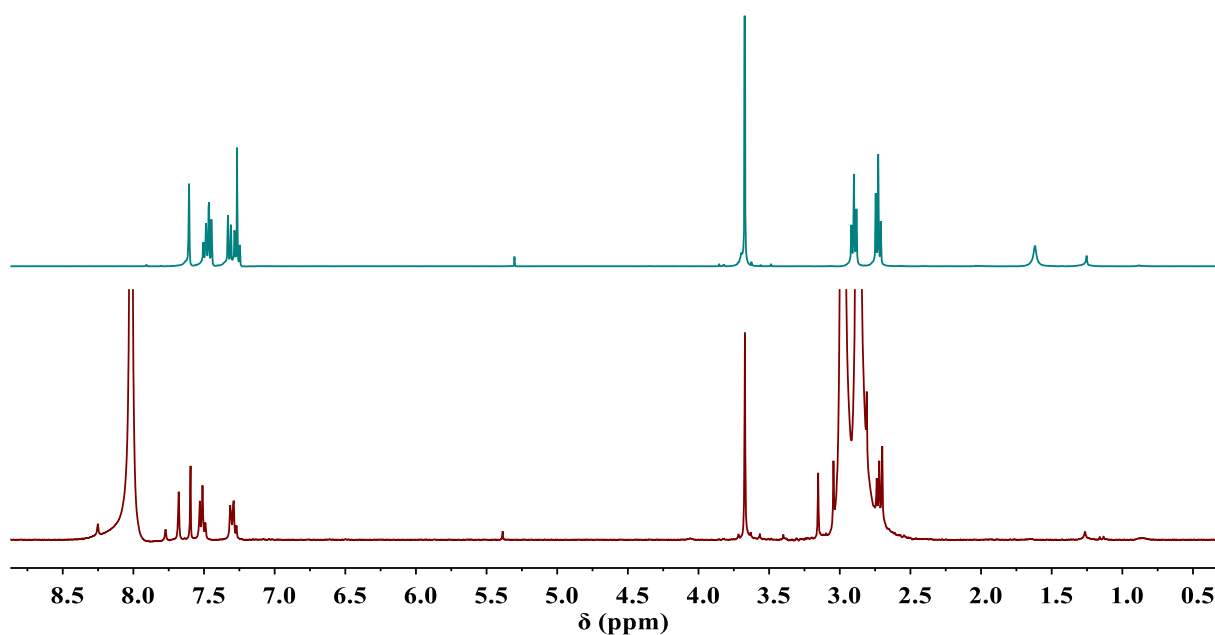


Figure S65. ^1H NMR spectra (CDCl_3 , RT): the crude reaction mixture obtained by Cs_2CO_3 -mediated degradation of cross-linked poly(MA-*alt*-CM) (bottom) and the isolated MCP degradation product (Conv. = 90.0%, Yield = 75%) after the purification of by flash column chromatography (top).

Degradation of Poly(EA-*alt*-CM) from Mixed Commodity Plastic

A 20 mL vial was charged with alternating copolymer [poly(EA-*alt*-CM), 300 mg], polymethyl methacrylate (PMMA, ca. 300 mg), polyethylene terephthalate (PET, ca. 300 mg), low-density polyethylene (LDPE, ca. 300 mg), high-density polyethylene (HDPE, ca. 300 mg), isotactic polypropylene (*i*PP, ca. 300 mg), ethylene carbonate (internal standard), and 4.0 mL of DMF. The degradation was triggered by the rapid addition of Cs₂CO₃ solid powder [Cs₂CO₃:CM (mol:mol) = 1:1] at RT under vigorous stirring. After 24 h, the degradation was then quenched by the addition of 3 mL of dilute HCl. Commodity plastic, including PET, LDPE, HDPE, *i*PP, which were insoluble in DMF during degradation, can be recovered by simple filtration and purified by washing with water. The combined filtrate was concentrated under reduced pressure and then precipitated into 100 mL of methanol, filtered, washed with methanol, and dried in a vacuum oven at 80 °C to recover PMMA (290 mg, 97.0 %). The methanol solution was concentrated and purified by flash column chromatography (a short silica gel column with the height of ca. 2 cm), affording pure ethyl-3-(2-oxo-2H-chromen-3-yl)propionate (ECP) with an isolated yield of 86.0%.

Computational Details

All the DFT calculations were performed using Gaussian09 suite of programs.¹⁰ Hybrid DFT functional (B3PW91)¹¹ including dispersion corrections using the GD3BJ approach along with SDD basis sets¹² for P atoms (with additional polarization¹³) and 6-31G** basis sets¹⁴⁻¹⁶ for rest of the atoms were employed for the computation. Frequency calculations were performed to locate minima for the optimized structures (maxima for transition state structures) and for obtaining thermal corrections over the energies. Single point calculations were carried to include solvent effects (dichloromethane) using the SMD approach and the standard state was set to 1M instead of 1atm by shifting all energies by 1.89

kcal/mol.

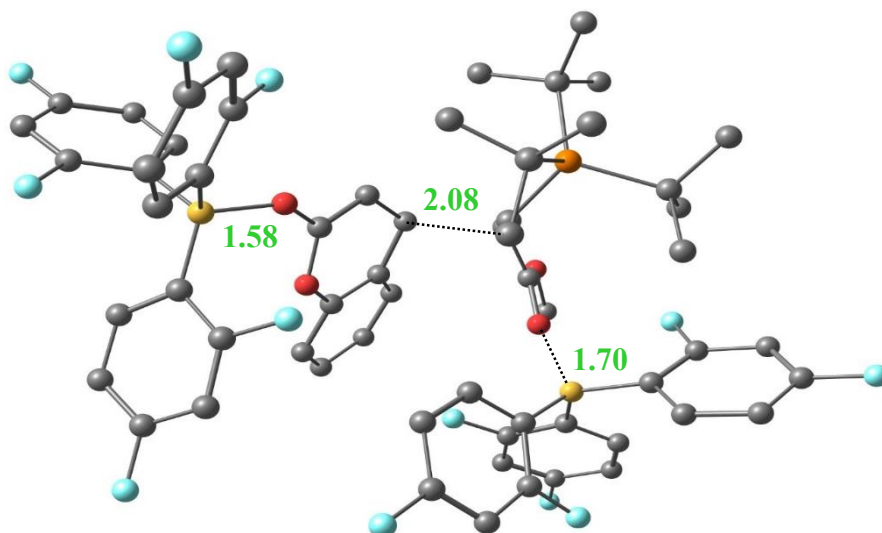


Figure S66. 3D depiction of **I_{TS2}** (The distances are given in Å).

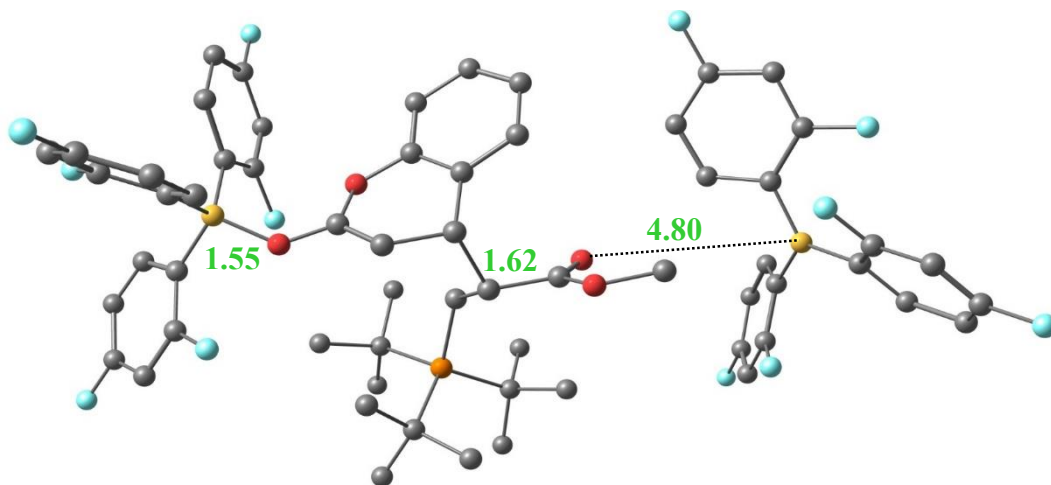


Figure S67. 3D depiction of **I_{IM3}** (The distances are given in Å).

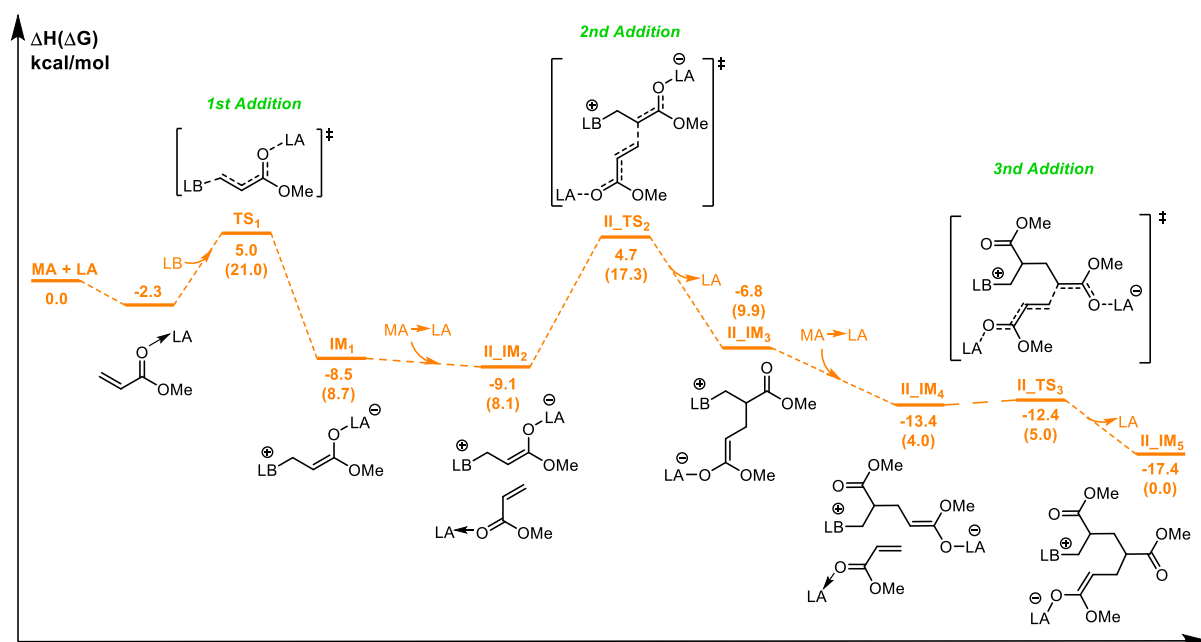


Figure S68. Energy profile of three conjugate-additions of MA to form MA-MA-MA continuous sequence [LA: B(2,4-F₂Ph)₃; LB: PtBu₃; the energies are given in kcal/mol and the Gibbs free energies (ΔG) are given in brackets]. The calculations reveal that the formation of MA-MA-MA continuous sequence is both thermodynamically and kinetically feasible, indicating that MA homopolymerization is possible when CM comonomer is absent.

Optimized Geometries

MA→LA

C	0.992421000	-0.029108000	2.622399000
O	0.167229000	0.168449000	1.715030000
O	1.064571000	0.822212000	3.624847000
C	0.235611000	2.001296000	3.539577000
H	0.582258000	2.624958000	2.713666000
H	-0.804728000	1.722895000	3.369427000
H	0.365103000	2.507727000	4.494249000
C	1.914876000	-1.153406000	2.777732000
H	2.653560000	-1.036790000	3.564242000
B	-0.042247000	-0.067887000	0.083870000
C	-0.716153000	1.330834000	-0.373896000
C	-1.819963000	1.888345000	0.275668000
C	-0.276537000	2.042511000	-1.500797000
C	-2.452469000	3.063331000	-0.109754000
C	-0.876541000	3.220737000	-1.943243000
C	-1.959795000	3.714697000	-1.231860000
H	0.567702000	1.651697000	-2.061115000
H	-3.304272000	3.448069000	0.438811000
H	-0.518855000	3.750523000	-2.819557000
C	1.437838000	-0.308324000	-0.528036000
C	2.499433000	0.561881000	-0.262398000
C	1.757972000	-1.366064000	-1.395898000
C	3.778097000	0.442566000	-0.789192000
C	3.021441000	-1.538161000	-1.960842000
C	4.014909000	-0.622311000	-1.647436000
H	0.986217000	-2.086586000	-1.645608000
H	4.557027000	1.153658000	-0.540319000
H	3.238551000	-2.360651000	-2.633832000
C	-1.074831000	-1.308658000	-0.036350000
C	-1.584859000	-1.689101000	-1.281241000
C	-1.598640000	-2.025129000	1.051498000
C	-2.509000000	-2.706314000	-1.481020000
C	-2.529601000	-3.055332000	0.914719000
C	-2.968860000	-3.381434000	-0.359468000
H	-1.281230000	-1.758888000	2.055296000
H	-2.861598000	-2.953569000	-2.475426000
H	-2.918907000	-3.591414000	1.773584000
F	-2.327654000	1.269648000	1.370977000
F	-2.554288000	4.853344000	-1.631110000
F	2.300775000	1.597441000	0.592276000
F	5.241524000	-0.765160000	-2.176261000

F	-1.155706000	-1.038696000	-2.385663000
F	-3.863765000	-4.371749000	-0.519956000
C	1.834699000	-2.263992000	2.037647000
H	2.530939000	-3.081594000	2.196352000
H	1.076812000	-2.392521000	1.272657000

LA

B	-0.048557000	-0.090475000	0.005225000
C	-1.452799000	-0.794039000	0.040002000
C	-2.562208000	-0.364296000	-0.702833000
C	-1.679185000	-1.909728000	0.872970000
C	-3.814292000	-0.960568000	-0.640770000
C	-2.919499000	-2.528073000	0.988353000
C	-3.969673000	-2.037978000	0.220994000
H	-0.849468000	-2.290476000	1.461733000
H	-4.636388000	-0.601131000	-1.248154000
H	-3.081194000	-3.374055000	1.647105000
C	1.211809000	-1.016021000	0.002278000
C	2.432961000	-0.693945000	0.614735000
C	1.181022000	-2.262929000	-0.658017000
C	3.551726000	-1.512801000	0.591013000
C	2.281227000	-3.109461000	-0.731874000
C	3.453031000	-2.714805000	-0.097589000
H	0.258707000	-2.564398000	-1.145633000
H	4.467717000	-1.223440000	1.091957000
H	2.244762000	-4.056092000	-1.259346000
C	0.021419000	1.467970000	0.039518000
C	1.042467000	2.226502000	-0.550627000
C	-0.969359000	2.212246000	0.712421000
C	1.111817000	3.610333000	-0.494369000
C	-0.934094000	3.597012000	0.819938000
C	0.112924000	4.273812000	0.205363000
H	-1.786274000	1.674771000	1.185193000
H	1.915503000	4.151020000	-0.979531000
H	-1.695630000	4.152578000	1.355676000
F	-2.422538000	0.661584000	-1.558698000
F	-5.171195000	-2.624245000	0.303929000
F	2.543298000	0.454326000	1.300899000
F	4.524025000	-3.517440000	-0.141346000
F	2.008249000	1.602747000	-1.245058000
F	0.163637000	5.610163000	0.282034000

LB

P	-0.000250000	0.000264000	-0.715512000
C	0.853458000	1.608514000	0.001759000
C	2.370901000	1.503195000	-0.219993000
C	0.597729000	1.952544000	1.473702000
H	-0.455459000	2.160254000	1.677890000
H	0.921314000	1.157316000	2.149481000
H	1.159042000	2.858958000	1.741300000
H	2.851323000	0.782793000	0.445457000
H	2.826784000	2.481252000	-0.016726000
H	2.613943000	1.239265000	-1.254483000
C	0.966101000	-1.543064000	0.001493000
C	0.117063000	-2.805546000	-0.219603000
C	1.393060000	-1.493832000	1.473287000
H	2.098976000	-0.685201000	1.677627000
H	0.542893000	-1.377835000	2.149713000
H	1.898617000	-2.432816000	1.739760000
H	-0.745678000	-2.863101000	0.447456000
H	0.737898000	-3.688567000	-0.018144000
H	-0.235058000	-2.884152000	-1.253419000
C	-1.819997000	-0.064969000	0.001725000
C	-1.991432000	-0.459420000	1.473426000
C	-2.597615000	-1.052722000	-0.890997000
H	-2.504187000	-0.786144000	-1.948663000
H	-2.273016000	-2.087339000	-0.776685000
H	-3.663198000	-1.015114000	-0.627336000
H	-1.641486000	-1.474071000	1.677922000
H	-3.057721000	-0.430427000	1.738997000
H	-1.468796000	0.220120000	2.150699000
C	0.388157000	2.777034000	-0.889876000
H	0.570498000	2.562958000	-1.947882000
H	-0.668890000	3.016144000	-0.774153000
H	0.956263000	3.679424000	-0.626617000
C	-2.488052000	1.301771000	-0.220543000
H	-2.380288000	1.644458000	-1.254846000
H	-3.563239000	1.206745000	-0.018515000
H	-2.105971000	2.078566000	0.445151000
C	2.210708000	-1.723469000	-0.890927000
H	2.943962000	-0.924748000	-0.778507000
H	2.711293000	-2.664251000	-0.624930000
H	1.933446000	-1.778662000	-1.948578000

TS₁

C	-0.265133000	-1.088502000	-1.687312000
O	-1.005327000	-0.159856000	-1.219831000
O	-0.552672000	-1.588202000	-2.891687000
C	-1.815835000	-1.238236000	-3.474088000
H	-2.628265000	-1.690546000	-2.902069000
H	-1.948024000	-0.156061000	-3.494789000
H	-1.787941000	-1.648018000	-4.483888000
C	0.878526000	-1.649648000	-1.090321000
H	1.278106000	-2.532967000	-1.575804000
B	-1.951845000	-0.030524000	0.079975000
C	-3.483961000	-0.053178000	-0.475216000
C	-3.915899000	0.769332000	-1.518807000
C	-4.500306000	-0.819007000	0.117563000
C	-5.221941000	0.835637000	-1.989256000
C	-5.830327000	-0.789881000	-0.302063000
C	-6.168694000	0.041160000	-1.358895000
H	-4.241748000	-1.460298000	0.954999000
H	-5.489573000	1.493239000	-2.808187000
H	-6.594075000	-1.393414000	0.176852000
C	-1.613718000	-1.267614000	1.081839000
C	-1.775085000	-2.601579000	0.697593000
C	-1.148089000	-1.101319000	2.396744000
C	-1.523050000	-3.703090000	1.505472000
C	-0.875287000	-2.164142000	3.259130000
C	-1.073599000	-3.455779000	2.794576000
H	-0.991366000	-0.092527000	2.765819000
H	-1.671691000	-4.712559000	1.140373000
H	-0.526295000	-2.002866000	4.273709000
C	-1.639000000	1.442535000	0.692605000
C	-2.317459000	1.931822000	1.812820000
C	-0.783296000	2.371199000	0.081892000
C	-2.157044000	3.206833000	2.343165000
C	-0.588241000	3.669088000	0.559773000
C	-1.279465000	4.063481000	1.695347000
H	-0.273182000	2.069088000	-0.826451000
H	-2.711246000	3.520499000	3.220097000
H	0.067691000	4.372820000	0.057541000
F	-3.019390000	1.568201000	-2.149786000
F	-7.444020000	0.086188000	-1.790465000
F	-2.194013000	-2.873362000	-0.562538000
F	-0.818897000	-4.500647000	3.604257000
F	-3.198431000	1.127383000	2.448400000
F	-1.105497000	5.307721000	2.181936000

C	1.466604000	-1.139713000	0.063398000
H	2.005820000	-1.808968000	0.723977000
H	0.984008000	-0.307058000	0.565233000
P	3.617451000	0.014615000	-0.281770000
C	3.988666000	1.288329000	1.143472000
C	3.156819000	2.559198000	0.917611000
C	5.463357000	1.682863000	1.301255000
H	6.101747000	0.842153000	1.582228000
H	5.873610000	2.135746000	0.395400000
H	5.544249000	2.427474000	2.104129000
H	3.516753000	3.161830000	0.081291000
H	3.235032000	3.183103000	1.816478000
H	2.094412000	2.345464000	0.770610000
C	3.668433000	0.903198000	-2.005371000
C	3.685236000	-0.153256000	-3.123366000
C	4.845083000	1.865936000	-2.205973000
H	4.819401000	2.705845000	-1.508657000
H	5.815467000	1.373755000	-2.113500000
H	4.785338000	2.287602000	-3.218018000
H	4.627607000	-0.701617000	-3.183659000
H	3.556691000	0.365219000	-4.081661000
H	2.860788000	-0.865170000	-3.027376000
C	4.957048000	-1.398919000	-0.243258000
C	6.319035000	-1.003141000	-0.831285000
C	4.405594000	-2.612981000	-1.016641000
H	3.486650000	-2.999894000	-0.569245000
H	4.210424000	-2.412552000	-2.069240000
H	5.150456000	-3.417346000	-0.971083000
H	6.265392000	-0.789047000	-1.900926000
H	7.015961000	-1.842636000	-0.707862000
H	6.759130000	-0.137593000	-0.331147000
C	3.470679000	0.665529000	2.455245000
H	2.403251000	0.433816000	2.400202000
H	4.002492000	-0.238142000	2.751467000
H	3.600914000	1.397510000	3.261955000
C	5.169558000	-1.881827000	1.201229000
H	4.233765000	-2.171694000	1.688822000
H	5.804652000	-2.775856000	1.172686000
H	5.677816000	-1.149698000	1.831118000
C	2.342563000	1.670592000	-2.158745000
H	2.252460000	2.517407000	-1.479197000
H	2.285560000	2.066529000	-3.180276000
H	1.480823000	1.016424000	-2.010157000

IM₁

C	-0.173973000	-1.048186000	-1.766681000
O	-0.979527000	-0.127394000	-1.310647000
O	-0.554329000	-1.714773000	-2.883608000
C	-1.913371000	-1.593204000	-3.297429000
H	-2.585412000	-2.060308000	-2.573769000
H	-2.197094000	-0.546992000	-3.424630000
H	-1.971443000	-2.120668000	-4.251539000
C	1.076452000	-1.350852000	-1.304390000
H	1.562213000	-2.202753000	-1.760224000
B	-1.824675000	-0.047546000	0.003647000
C	-3.399803000	-0.288284000	-0.369421000
C	-4.030063000	0.398368000	-1.410285000
C	-4.253444000	-1.117929000	0.374294000
C	-5.374792000	0.279672000	-1.742025000
C	-5.612539000	-1.273687000	0.098130000
C	-6.151508000	-0.568793000	-0.966695000
H	-3.838713000	-1.662063000	1.217949000
H	-5.799238000	0.838738000	-2.567932000
H	-6.246159000	-1.923880000	0.692262000
C	-1.262379000	-1.144267000	1.083300000
C	-1.274019000	-2.518651000	0.826147000
C	-0.718147000	-0.803964000	2.333059000
C	-0.789923000	-3.498265000	1.687049000
C	-0.219816000	-1.737199000	3.245547000
C	-0.263783000	-3.079860000	2.900102000
H	-0.682887000	0.245121000	2.611070000
H	-0.831751000	-4.547562000	1.418880000
H	0.178024000	-1.439731000	4.210455000
C	-1.668052000	1.500594000	0.512632000
C	-2.303894000	1.995179000	1.655222000
C	-0.986022000	2.474224000	-0.233805000
C	-2.251940000	3.317277000	2.084184000
C	-0.904387000	3.818844000	0.138271000
C	-1.539284000	4.216789000	1.304934000
H	-0.531202000	2.158352000	-1.166915000
H	-2.764397000	3.632087000	2.985902000
H	-0.384862000	4.553198000	-0.469395000
F	-3.305628000	1.247188000	-2.180661000
F	-7.460450000	-0.702661000	-1.262434000
F	-1.787714000	-2.966203000	-0.341309000
F	0.214388000	-4.004587000	3.756564000
F	-3.023378000	1.148918000	2.425865000
F	-1.472159000	5.506227000	1.694290000

C	1.682409000	-0.665282000	-0.135918000
H	1.792553000	-1.300733000	0.754415000
H	1.047338000	0.174282000	0.166322000
P	3.398758000	0.075076000	-0.349679000
C	3.608686000	1.305821000	1.130727000
C	2.799798000	2.585190000	0.860633000
C	5.076491000	1.686616000	1.376547000
H	5.683728000	0.841976000	1.708554000
H	5.553352000	2.131857000	0.500617000
H	5.104682000	2.435233000	2.177058000
H	3.221116000	3.195183000	0.059970000
H	2.828099000	3.192887000	1.772419000
H	1.745713000	2.392505000	0.643893000
C	3.505039000	0.972762000	-2.052332000
C	3.626481000	-0.056084000	-3.189526000
C	4.694153000	1.942244000	-2.121965000
H	4.604342000	2.773675000	-1.420064000
H	5.657716000	1.453346000	-1.960978000
H	4.714676000	2.376064000	-3.128710000
H	4.570677000	-0.604152000	-3.177146000
H	3.591009000	0.496734000	-4.135716000
H	2.789631000	-0.757872000	-3.186299000
C	4.662072000	-1.381581000	-0.219203000
C	6.060524000	-0.972720000	-0.705481000
C	4.162327000	-2.583266000	-1.042544000
H	3.230622000	-2.990767000	-0.644546000
H	4.019832000	-2.367484000	-2.100601000
H	4.920633000	-3.371853000	-0.968520000
H	6.083414000	-0.749775000	-1.773867000
H	6.742314000	-1.814933000	-0.538173000
H	6.465561000	-0.115123000	-0.164079000
C	3.020570000	0.673748000	2.407961000
H	1.957686000	0.442989000	2.310880000
H	3.540385000	-0.226693000	2.731786000
H	3.118615000	1.411036000	3.213421000
C	4.762789000	-1.872398000	1.235138000
H	3.791003000	-2.150029000	1.652379000
H	5.380866000	-2.777714000	1.237340000
H	5.244407000	-1.155491000	1.901781000
C	2.190608000	1.740612000	-2.279261000
H	2.046147000	2.568609000	-1.586734000
H	2.225064000	2.164122000	-3.289966000
H	1.325494000	1.076739000	-2.228880000

CA→LA

C	-4.031695000	-0.304991000	-1.974015000
C	-5.437233000	-0.290945000	-2.051837000
C	-3.429197000	0.106774000	-0.773713000
C	-6.189758000	0.120783000	-0.965918000
C	-4.172012000	0.524137000	0.326651000
C	-5.555742000	0.527056000	0.219189000
H	-5.918047000	-0.607264000	-2.973336000
H	-7.273208000	0.130450000	-1.028661000
H	-3.655687000	0.833833000	1.228923000
H	-6.153246000	0.849202000	1.066522000
O	-2.070420000	0.119292000	-0.643669000
C	-3.162340000	-0.711445000	-3.038154000
C	-1.815444000	-0.694712000	-2.874145000
C	-1.249198000	-0.268631000	-1.622946000
O	-0.018106000	-0.234841000	-1.443019000
H	-1.120018000	-1.000802000	-3.645487000
H	-3.596717000	-1.037856000	-3.979529000
B	0.973553000	-0.031550000	-0.110855000
C	1.314660000	-1.567223000	0.274229000
C	2.634654000	-2.027957000	0.402150000
C	0.341796000	-2.545658000	0.482384000
C	2.959362000	-3.344540000	0.728413000
C	0.597432000	-3.871995000	0.797308000
C	1.927200000	-4.249564000	0.921460000
H	3.447170000	-1.327828000	0.237186000
H	3.989229000	-3.669948000	0.828388000
H	-0.209096000	-4.580042000	0.946848000
C	0.191294000	0.915305000	0.945675000
C	-0.080931000	2.248704000	0.590085000
C	-0.249662000	0.552058000	2.219347000
C	-0.762286000	3.145408000	1.409552000
C	-0.928631000	1.405863000	3.086141000
C	-1.177524000	2.700459000	2.657439000
H	0.264677000	2.600214000	-0.379645000
H	-0.955619000	4.169052000	1.106706000
H	-1.234348000	1.068033000	4.069610000
C	2.233796000	0.751075000	-0.767040000
C	2.443302000	0.926426000	-2.143603000
C	3.217933000	1.315031000	0.050218000
C	3.533855000	1.620944000	-2.668878000
C	4.325598000	2.013636000	-0.414227000
C	4.460234000	2.157714000	-1.787536000
H	1.722666000	0.503299000	-2.836235000

H	3.671603000	1.745697000	-3.737726000
H	5.054233000	2.427058000	0.273165000
F	3.115144000	1.167004000	1.388419000
F	5.520920000	2.832204000	-2.268214000
F	-0.968828000	-2.205404000	0.362693000
F	2.210127000	-5.528255000	1.229759000
F	-0.025268000	-0.690544000	2.686770000
F	-1.833198000	3.542414000	3.478538000

I_IM₂

C	3.111521000	0.376829000	-2.081719000
O	3.009297000	-0.678752000	-1.315396000
O	3.106453000	0.148265000	-3.421905000
C	3.421045000	-1.167688000	-3.866149000
H	4.436021000	-1.451154000	-3.578131000
H	2.722009000	-1.904523000	-3.464478000
H	3.341033000	-1.131217000	-4.954369000
C	3.123406000	1.691485000	-1.716646000
H	3.326014000	2.394224000	-2.512981000
B	3.937377000	-1.244313000	-0.204218000
C	4.539826000	-2.678818000	-0.732207000
C	3.756561000	-3.684553000	-1.296220000
C	5.894389000	-3.029419000	-0.598972000
C	4.218844000	-4.919422000	-1.734127000
C	6.425074000	-4.253020000	-1.006381000
C	5.571346000	-5.183654000	-1.577455000
H	6.567750000	-2.309967000	-0.142992000
H	3.550298000	-5.648607000	-2.177240000
H	7.477719000	-4.486843000	-0.886820000
C	5.144014000	-0.187628000	0.135454000
C	6.037621000	0.268209000	-0.838951000
C	5.390599000	0.326140000	1.419360000
C	7.070370000	1.172668000	-0.616918000
C	6.414835000	1.230327000	1.712077000
C	7.239901000	1.644241000	0.676820000
H	4.751136000	0.003301000	2.235238000
H	7.723171000	1.484510000	-1.423964000
H	6.585385000	1.596388000	2.719288000
C	2.952001000	-1.506004000	1.077707000
C	3.354360000	-2.155688000	2.248242000
C	1.599124000	-1.134915000	1.064648000
C	2.528780000	-2.408903000	3.339653000
C	0.716485000	-1.363807000	2.123346000
C	1.206044000	-1.997963000	3.254518000

H	1.221532000	-0.658012000	0.165312000
H	2.909102000	-2.911468000	4.221533000
H	-0.322462000	-1.057005000	2.073103000
F	2.410913000	-3.484885000	-1.451204000
F	6.052761000	-6.372391000	-1.989004000
F	5.920058000	-0.187490000	-2.106699000
F	8.231771000	2.521530000	0.924689000
F	4.637508000	-2.562761000	2.366134000
F	0.383719000	-2.221097000	4.299950000
C	3.018364000	2.154250000	-0.304675000
H	3.978011000	2.455095000	0.140881000
H	2.640703000	1.341635000	0.325605000
P	1.911978000	3.624597000	0.061840000
C	1.605114000	3.557563000	1.972037000
C	0.572009000	2.467035000	2.302158000
C	1.105000000	4.900267000	2.526967000
H	1.851555000	5.694380000	2.457679000
H	0.187273000	5.243045000	2.045078000
H	0.881550000	4.764760000	3.591618000
H	-0.434361000	2.693479000	1.948137000
H	0.515923000	2.391406000	3.394347000
H	0.866173000	1.479928000	1.936978000
C	0.268498000	3.487542000	-0.929922000
C	0.496569000	3.845968000	-2.408717000
C	-0.826275000	4.398843000	-0.357695000
H	-1.130336000	4.118236000	0.651675000
H	-0.547565000	5.455328000	-0.359000000
H	-1.716114000	4.292931000	-0.987743000
H	0.748137000	4.896367000	-2.568221000
H	-0.447360000	3.663029000	-2.934894000
H	1.256579000	3.210160000	-2.867183000
C	2.924160000	5.200431000	-0.417202000
C	2.034464000	6.451220000	-0.474807000
C	3.601588000	4.985531000	-1.783026000
H	4.342874000	4.183880000	-1.749742000
H	2.902788000	4.777727000	-2.592339000
H	4.132411000	5.910331000	-2.038434000
H	1.287400000	6.398550000	-1.268950000
H	2.672785000	7.316378000	-0.689096000
H	1.520672000	6.652253000	0.467480000
C	2.908640000	3.156715000	2.689527000
H	3.265020000	2.169668000	2.388032000
H	3.721408000	3.869990000	2.560236000
H	2.688299000	3.106153000	3.762205000

C	4.057497000	5.438151000	0.594343000
H	4.717402000	4.572530000	0.698777000
H	4.672384000	6.262959000	0.215560000
H	3.699266000	5.734044000	1.581248000
C	-0.195428000	2.020135000	-0.896328000
H	-0.456991000	1.661406000	0.097599000
H	-1.105698000	1.950650000	-1.502884000
H	0.562642000	1.365470000	-1.335011000
C	-1.195566000	-3.744779000	-0.551251000
C	-0.482275000	-4.932379000	-0.299503000
C	-2.508993000	-3.639817000	-0.065173000
C	-1.084903000	-5.964922000	0.397200000
C	-3.127716000	-4.668673000	0.636454000
C	-2.403801000	-5.832360000	0.860085000
H	0.542481000	-5.004575000	-0.649317000
H	-0.534234000	-6.879111000	0.594394000
H	-4.140981000	-4.535094000	0.998742000
H	-2.866000000	-6.646755000	1.409697000
O	-3.233156000	-2.492192000	-0.260917000
C	-0.662662000	-2.629434000	-1.272917000
C	-1.415332000	-1.513332000	-1.462378000
C	-2.724012000	-1.431951000	-0.894431000
O	-3.414856000	-0.391630000	-0.973924000
H	-1.054760000	-0.642662000	-1.993794000
H	0.354977000	-2.677942000	-1.646043000
B	-4.760247000	0.047530000	-0.190281000
C	-4.705767000	1.669573000	-0.265434000
C	-4.924434000	2.489756000	0.851086000
C	-4.528326000	2.356215000	-1.469357000
C	-4.960579000	3.883381000	0.785191000
C	-4.551928000	3.741144000	-1.598641000
C	-4.773849000	4.487145000	-0.448885000
H	-5.088170000	2.015160000	1.814333000
H	-5.141640000	4.493294000	1.663979000
H	-4.424853000	4.215198000	-2.565249000
C	-4.651441000	-0.530972000	1.327149000
C	-5.691326000	-1.233974000	1.958229000
C	-3.513100000	-0.364440000	2.118663000
C	-5.608888000	-1.719962000	3.262727000
C	-3.359922000	-0.834572000	3.416506000
C	-4.436213000	-1.510389000	3.973857000
H	-6.605311000	-1.414624000	1.403025000
H	-6.432415000	-2.252981000	3.726062000
H	-2.435462000	-0.697745000	3.965580000

C	-6.003923000	-0.539339000	-1.054268000
C	-5.875818000	-1.376419000	-2.172623000
C	-7.318732000	-0.172008000	-0.755025000
C	-6.961582000	-1.829761000	-2.921952000
C	-8.440193000	-0.591982000	-1.459566000
C	-8.234610000	-1.427586000	-2.547335000
H	-4.884279000	-1.679343000	-2.494588000
H	-6.831326000	-2.474507000	-3.784557000
H	-9.434135000	-0.270899000	-1.170918000
F	-7.544083000	0.642272000	0.301765000
F	-9.299829000	-1.851474000	-3.251792000
F	-4.315044000	1.656127000	-2.604929000
F	-4.802196000	5.831161000	-0.544946000
F	-2.429941000	0.272198000	1.585005000
F	-4.327348000	-1.977718000	5.229330000

I_TS₂

C	-2.448046000	-0.283891000	-1.873368000
O	-2.854065000	0.177359000	-0.780312000
O	-2.997337000	-0.035749000	-3.059162000
C	-4.041208000	0.938573000	-3.210607000
H	-4.892198000	0.699328000	-2.578418000
H	-3.658928000	1.930185000	-2.967853000
H	-4.318861000	0.887586000	-4.263810000
C	-1.254887000	-1.097609000	-2.006730000
H	-1.289067000	-1.685006000	-2.917982000
B	-3.954111000	0.815976000	0.349987000
C	-4.840190000	2.003501000	-0.296305000
C	-4.265731000	3.208794000	-0.710556000
C	-6.242441000	1.970090000	-0.369650000
C	-4.977427000	4.301859000	-1.188635000
C	-7.012021000	3.034893000	-0.837413000
C	-6.359684000	4.189620000	-1.243156000
H	-6.761518000	1.080570000	-0.026652000
H	-4.471078000	5.209179000	-1.496221000
H	-8.094690000	2.983260000	-0.878721000
C	-4.848900000	-0.459290000	0.826942000
C	-5.621088000	-1.247680000	-0.027622000
C	-5.009854000	-0.774072000	2.189427000
C	-6.503853000	-2.243769000	0.373578000
C	-5.874311000	-1.762579000	2.659483000
C	-6.620442000	-2.480137000	1.736249000
H	-4.434187000	-0.215627000	2.919353000
H	-7.086484000	-2.801791000	-0.350351000

H	-5.982245000	-1.967397000	3.719263000	H	-2.395579000	-6.206202000	-0.966021000
C	-2.966290000	1.358271000	1.512952000	H	-3.542567000	-6.001506000	0.350692000
C	-3.471965000	2.084494000	2.595655000	H	-1.830511000	-6.198385000	0.713805000
C	-1.578975000	1.161301000	1.547668000	C	0.301524000	-2.616639000	2.007492000
C	-2.706630000	2.572791000	3.648587000	H	0.578910000	-1.635157000	1.619332000
C	-0.757798000	1.617047000	2.577185000	H	-0.723568000	-2.575062000	2.374378000
C	-1.342995000	2.320634000	3.617740000	H	0.949531000	-2.799238000	2.871749000
H	-1.110026000	0.653032000	0.713679000	C	-2.828079000	-3.638960000	1.335703000
H	-3.163253000	3.129475000	4.458516000	H	-2.768462000	-2.548799000	1.374476000
H	0.308835000	1.430140000	2.569842000	H	-3.878903000	-3.892239000	1.511567000
F	-2.923773000	3.333526000	-0.678605000	H	-2.250385000	-4.062638000	2.158730000
F	-7.075629000	5.230859000	-1.701299000	C	1.131399000	-3.741200000	-2.706585000
F	-5.519370000	-1.065841000	-1.370753000	H	1.957377000	-3.508322000	-2.036165000
F	-7.470067000	-3.432254000	2.157731000	H	1.537322000	-4.341986000	-3.528683000
F	-4.801958000	2.326192000	2.658627000	H	0.757624000	-2.812219000	-3.140358000
F	-0.573963000	2.776362000	4.625741000	C	-0.000001000	1.575261000	-2.506216000
C	-0.705863000	-1.762082000	-0.780265000	C	-0.846284000	2.326327000	-3.337278000
H	-1.199947000	-1.367303000	0.112784000	C	0.722742000	2.267829000	-1.524967000
H	0.365609000	-1.488231000	-0.694371000	C	-0.993384000	3.694792000	-3.161120000
P	-0.663402000	-3.608101000	-0.495166000	C	0.571871000	3.637394000	-1.320781000
C	0.570263000	-3.749714000	0.995765000	C	-0.294449000	4.347112000	-2.140028000
C	2.018879000	-3.569597000	0.513741000	H	-1.370735000	1.817393000	-4.140876000
C	0.438047000	-5.104026000	1.709426000	H	-1.644992000	4.259663000	-3.821003000
H	-0.523565000	-5.224174000	2.212542000	H	1.158312000	4.118055000	-0.545068000
H	0.596257000	-5.958885000	1.048799000	H	-0.411393000	5.416725000	-1.995542000
H	1.211518000	-5.148722000	2.484268000	O	1.668046000	1.641178000	-0.749469000
H	2.377899000	-4.391257000	-0.107879000	C	0.263620000	0.142048000	-2.709746000
H	2.660829000	-3.541793000	1.400774000	C	1.480701000	-0.298882000	-2.115842000
H	2.191690000	-2.625218000	-0.006906000	C	2.123055000	0.420788000	-1.114945000
C	0.002932000	-4.550217000	-2.048857000	O	3.137123000	-0.036629000	-0.496671000
C	-1.092750000	-4.732077000	-3.114521000	H	1.985283000	-1.198928000	-2.436321000
C	0.532017000	-5.941545000	-1.661454000	H	0.068294000	-0.190138000	-3.726334000
H	1.421700000	-5.894627000	-1.032445000	B	4.430231000	0.604135000	0.149217000
H	-0.216218000	-6.560413000	-1.162451000	C	5.016059000	-0.591149000	1.096749000
H	0.818434000	-6.459693000	-2.584007000	C	5.498254000	-0.361593000	2.394890000
H	-1.878826000	-5.425402000	-2.811943000	C	5.159376000	-1.908896000	0.657473000
H	-0.613937000	-5.158982000	-4.003355000	C	6.056131000	-1.354454000	3.200762000
H	-1.550441000	-3.788093000	-3.417951000	C	5.700871000	-2.944548000	1.413037000
C	-2.432178000	-4.210865000	-0.034258000	C	6.145925000	-2.640163000	2.691240000
C	-2.532440000	-5.743074000	0.013046000	H	5.441257000	0.647748000	2.791468000
C	-3.434309000	-3.665162000	-1.063550000	H	6.419567000	-1.141507000	4.200580000
H	-3.449671000	-2.576296000	-1.086821000	H	5.793019000	-3.945481000	1.006895000
H	-3.271170000	-4.033670000	-2.074613000	C	4.045090000	1.947394000	0.984501000
H	-4.433549000	-3.988755000	-0.753836000	C	4.604496000	3.207642000	0.722396000

C	3.126590000	1.936956000	2.035369000
C	4.286136000	4.357103000	1.446982000
C	2.767388000	3.040135000	2.799459000
C	3.369993000	4.250044000	2.482284000
H	5.314801000	3.297924000	-0.093426000
H	4.737896000	5.317733000	1.222711000
H	2.039996000	2.968332000	3.599785000
C	5.463868000	0.884121000	-1.083003000
C	5.146610000	0.714837000	-2.438764000
C	6.786530000	1.270575000	-0.844907000
C	6.058281000	0.921705000	-3.475701000
C	7.739225000	1.492636000	-1.832284000
C	7.348585000	1.309257000	-3.150478000
H	4.143234000	0.398793000	-2.706423000
H	5.782478000	0.783866000	-4.516038000
H	8.748395000	1.794011000	-1.576737000
F	7.192803000	1.462597000	0.430136000
F	8.249897000	1.515233000	-4.131286000
F	4.742800000	-2.253931000	-0.589035000
F	6.675340000	-3.625386000	3.445214000
F	2.497749000	0.767754000	2.341056000
F	3.046085000	5.342232000	3.200123000

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C	1.726743000	-0.020042000	-0.927900000
O	2.305400000	0.041132000	0.141206000
O	2.313839000	-0.412500000	-2.068253000
C	3.695629000	-0.789654000	-1.973428000
H	4.313980000	0.081494000	-1.741497000
H	3.838820000	-1.546264000	-1.200739000
H	3.960036000	-1.187594000	-2.952025000
C	0.263211000	0.266622000	-1.155502000
H	0.163295000	0.730363000	-2.139085000
B	7.059608000	-0.601054000	0.318548000
C	7.977673000	-0.724204000	-0.937717000
C	7.761782000	-1.629535000	-1.985304000
C	9.122820000	0.087567000	-1.069825000
C	8.595344000	-1.759095000	-3.085037000
C	10.004783000	-0.017387000	-2.138517000
C	9.719894000	-0.945130000	-3.133609000
H	9.335175000	0.812968000	-0.289608000
H	8.377301000	-2.467274000	-3.875415000
H	10.891606000	0.601584000	-2.216066000
C	6.902623000	0.803601000	1.005315000

C	6.697890000	1.993489000	0.295289000
C	7.000694000	0.942347000	2.404503000
C	6.616630000	3.246467000	0.886804000
C	6.944788000	2.175901000	3.045798000
C	6.753227000	3.311120000	2.267664000
H	7.141679000	0.047095000	3.003445000
H	6.455101000	4.138634000	0.293414000
H	7.040972000	2.268837000	4.121862000
C	6.308244000	-1.804871000	0.964508000
C	6.773779000	-3.129420000	0.957244000
C	5.044694000	-1.609537000	1.563376000
C	6.067887000	-4.199741000	1.484329000
C	4.285266000	-2.652481000	2.080870000
C	4.818117000	-3.934426000	2.030884000
H	4.623871000	-0.609623000	1.579371000
H	6.473308000	-5.204225000	1.463723000
H	3.298542000	-2.488522000	2.498031000
F	6.661075000	-2.405805000	-1.965244000
F	10.546256000	-1.057458000	-4.180548000
F	6.527293000	1.938986000	-1.039562000
F	6.683930000	4.510717000	2.861492000
F	7.981717000	-3.397843000	0.436731000
F	4.103691000	-4.958718000	2.518086000
C	-0.361963000	1.102318000	-0.035855000
H	0.132406000	0.861227000	0.909455000
H	-1.406326000	0.784153000	0.044097000
P	-0.569883000	2.957919000	-0.028265000
C	-1.985214000	3.184626000	1.285388000
C	-3.348116000	2.838186000	0.664979000
C	-2.037230000	4.623814000	1.820831000
H	-1.164622000	4.892285000	2.419943000
H	-2.164508000	5.370308000	1.033674000
H	-2.911439000	4.699444000	2.476924000
H	-3.688635000	3.573974000	-0.064461000
H	-4.085425000	2.828352000	1.473508000
H	-3.395860000	1.842922000	0.217848000
C	-1.117176000	3.594169000	-1.769549000
C	0.093665000	3.680910000	-2.715173000
C	-1.756547000	4.988868000	-1.674341000
H	-2.684651000	4.985937000	-1.101657000
H	-1.087137000	5.743149000	-1.256022000
H	-2.011241000	5.307623000	-2.691639000
H	0.800851000	4.463110000	-2.432152000
H	-0.285431000	3.936954000	-3.711043000

H	0.633652000	2.735955000	-2.812910000
C	1.067431000	3.801300000	0.556402000
C	1.005425000	5.328485000	0.392081000
C	2.270344000	3.261623000	-0.234532000
H	2.463248000	2.214401000	-0.004190000
H	2.183029000	3.382147000	-1.313299000
H	3.152425000	3.830149000	0.083106000
H	0.997910000	5.635120000	-0.656279000
H	1.912518000	5.750829000	0.839773000
H	0.152661000	5.787186000	0.894274000
C	-1.764664000	2.206777000	2.457843000
H	-1.944441000	1.169919000	2.170478000
H	-0.785284000	2.286712000	2.930118000
H	-2.516199000	2.445158000	3.218094000
C	1.331821000	3.459239000	2.032944000
H	1.391637000	2.381000000	2.204067000
H	2.310734000	3.875763000	2.297017000
H	0.602157000	3.892638000	2.718064000
C	-2.131234000	2.617333000	-2.388618000
H	-3.080147000	2.553911000	-1.860952000
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H	-1.744956000	1.601885000	-2.480239000
C	-0.430764000	-2.022123000	-0.088028000
C	0.662691000	-2.859515000	0.161823000
C	-1.495992000	-2.057371000	0.818139000
C	0.711706000	-3.670603000	1.292077000
C	-1.462143000	-2.856155000	1.961304000
C	-0.350845000	-3.655643000	2.198771000
H	1.482051000	-2.881419000	-0.552484000
H	1.568294000	-4.314769000	1.465068000
H	-2.321426000	-2.852133000	2.624215000
H	-0.324496000	-4.288204000	3.081545000
O	-2.631981000	-1.315443000	0.627428000
C	-0.532750000	-1.134624000	-1.306084000
C	-1.969614000	-0.886894000	-1.618326000
C	-2.926410000	-0.879307000	-0.650778000
O	-4.113284000	-0.391985000	-0.794771000
H	-2.269348000	-0.600825000	-2.619497000
H	-0.029586000	-1.626893000	-2.146990000
B	-5.533089000	-0.771201000	-0.287643000
C	-6.337128000	0.659216000	-0.222363000
C	-7.253116000	0.961683000	0.798545000
C	-6.233949000	1.649008000	-1.203148000
C	-7.984655000	2.148069000	0.862602000

C	-6.928057000	2.856317000	-1.192403000
C	-7.804286000	3.084960000	-0.142670000
H	-7.406428000	0.224867000	1.581432000
H	-8.684935000	2.344933000	1.667788000
H	-6.803909000	3.578384000	-1.991607000
C	-5.484278000	-1.518400000	1.168996000
C	-5.907801000	-2.842614000	1.362046000
C	-5.020980000	-0.897094000	2.330479000
C	-5.884655000	-3.493090000	2.597674000
C	-4.977387000	-1.481278000	3.590276000
C	-5.422339000	-2.792415000	3.699784000
H	-6.264665000	-3.397171000	0.499422000
H	-6.221127000	-4.518395000	2.710351000
H	-4.613176000	-0.934610000	4.452575000
C	-6.202289000	-1.715443000	-1.443113000
C	-5.493632000	-2.181359000	-2.560816000
C	-7.548716000	-2.088780000	-1.417071000
C	-6.069292000	-2.955729000	-3.570052000
C	-8.179644000	-2.855944000	-2.389978000
C	-7.413182000	-3.278716000	-3.466013000
H	-4.442374000	-1.925909000	-2.646355000
H	-5.495410000	-3.303428000	-4.422973000
H	-9.230080000	-3.110036000	-2.307959000
F	-8.317463000	-1.701910000	-0.372587000
F	-7.996990000	-4.024241000	-4.427339000
F	-5.402059000	1.473328000	-2.261584000
F	-8.489540000	4.247938000	-0.108051000
F	-4.548539000	0.375874000	2.258875000
F	-5.394967000	-3.386424000	4.910483000

I_IM₄

C	-0.586424000	3.856968000	1.242110000
O	-1.108862000	4.794106000	1.819461000
O	0.733684000	3.748578000	1.058251000
C	1.545672000	4.779988000	1.639692000
H	1.240176000	5.762717000	1.273362000
H	1.457677000	4.763609000	2.728680000
H	2.565080000	4.554541000	1.330898000
C	-1.301880000	2.649124000	0.674640000
H	-0.810243000	2.404459000	-0.270147000
B	5.598147000	0.096440000	-0.051611000
C	5.448284000	1.708601000	-0.281825000
C	6.399974000	2.626427000	0.176166000
C	4.378959000	2.295735000	-0.977927000

C	6.333653000	4.003353000	-0.005005000	C	-1.958219000	2.654146000	-3.131872000
C	4.256777000	3.668865000	-1.196218000	C	-4.409046000	2.634364000	-3.579513000
C	5.244472000	4.506168000	-0.699525000	H	-5.415228000	2.391356000	-3.235315000
H	3.603578000	1.650435000	-1.377316000	H	-4.416537000	3.641696000	-4.001383000
H	7.111103000	4.652832000	0.379946000	H	-4.180045000	1.939154000	-4.394857000
H	3.421844000	4.086589000	-1.749029000	H	-1.861057000	3.612350000	-3.646461000
C	6.622333000	-0.570382000	-1.130542000	H	-1.828192000	1.868505000	-3.884150000
C	6.466404000	-1.827471000	-1.721397000	H	-1.137034000	2.545738000	-2.419245000
C	7.778117000	0.114633000	-1.545878000	C	-2.995629000	5.413068000	-1.380870000
C	7.332641000	-2.381765000	-2.655570000	C	-3.544581000	5.894333000	-2.735662000
C	8.692695000	-0.394358000	-2.466410000	C	-1.457809000	5.468743000	-1.437309000
C	8.448703000	-1.643231000	-3.015507000	H	-1.025833000	5.425796000	-0.440565000
H	7.987939000	1.089301000	-1.121619000	H	-1.002168000	4.703903000	-2.062594000
H	7.144415000	-3.363916000	-3.073124000	H	-1.182740000	6.440849000	-1.862978000
H	9.576327000	0.163012000	-2.758249000	H	-3.106923000	5.352975000	-3.577179000
C	5.831662000	-0.301587000	1.507431000	H	-3.262832000	6.947047000	-2.852417000
C	6.311073000	-1.541831000	1.945230000	H	-4.630338000	5.839492000	-2.815278000
C	5.559873000	0.609569000	2.546351000	C	-5.592352000	4.139275000	1.019196000
C	6.521846000	-1.880580000	3.278526000	H	-5.213876000	3.402792000	1.731158000
C	5.742294000	0.324716000	3.897610000	H	-5.099177000	5.092226000	1.209689000
C	6.230504000	-0.928467000	4.241620000	H	-6.657460000	4.274992000	1.238145000
H	5.179564000	1.592082000	2.281548000	C	-3.430818000	6.383308000	-0.270231000
H	6.898527000	-2.860355000	3.547625000	H	-3.069672000	6.069362000	0.712999000
H	5.525677000	1.052717000	4.672098000	H	-2.970798000	7.355425000	-0.483919000
F	7.485037000	2.173480000	0.844103000	H	-4.509721000	6.543125000	-0.234313000
F	5.148800000	5.835745000	-0.892119000	C	-3.386510000	0.992424000	-1.977929000
F	5.401737000	-2.605906000	-1.394749000	H	-4.342315000	0.703412000	-1.549708000
F	9.306567000	-2.156903000	-3.915992000	H	-3.211768000	0.327359000	-2.829701000
F	6.584696000	-2.510015000	1.052488000	H	-2.610592000	0.773861000	-1.239695000
F	6.421933000	-1.232360000	5.536379000	C	-1.896490000	1.295161000	2.836497000
C	-2.804417000	2.896845000	0.521451000	C	-1.961624000	2.324255000	3.788507000
H	-3.119970000	3.543165000	1.343566000	C	-2.659447000	0.144444000	3.087042000
H	-3.324209000	1.938104000	0.640122000	C	-2.771167000	2.235040000	4.915789000
P	-3.618952000	3.623807000	-0.995449000	C	-3.482664000	0.044841000	4.213366000
C	-5.484369000	3.649008000	-0.439139000	C	-3.541758000	1.089363000	5.123850000
C	-6.083895000	2.232180000	-0.470268000	H	-1.369358000	3.221242000	3.642613000
C	-6.336384000	4.556462000	-1.340702000	H	-2.794627000	3.051977000	5.630944000
H	-6.092097000	5.615164000	-1.233717000	H	-4.054332000	-0.867541000	4.348375000
H	-6.275889000	4.286583000	-2.397094000	H	-4.179022000	1.005153000	5.999560000
H	-7.383202000	4.439608000	-1.038125000	O	-2.636479000	-0.963779000	2.294354000
H	-6.205808000	1.836649000	-1.479394000	C	-1.014163000	1.376553000	1.604560000
H	-7.086133000	2.297526000	-0.030370000	C	-1.119666000	0.117817000	0.803727000
H	-5.524248000	1.504874000	0.119900000	C	-1.848586000	-0.966586000	1.166433000
C	-3.340775000	2.436656000	-2.491874000	O	-1.794682000	-2.117271000	0.576118000

H	-0.493136000	-0.001302000	-0.073281000
H	0.029076000	1.525555000	1.923472000
B	-2.867947000	-3.038317000	-0.054918000
C	-3.054148000	-2.585083000	-1.625268000
C	-4.303847000	-2.539164000	-2.264920000
C	-1.973530000	-2.319483000	-2.470753000
C	-4.476973000	-2.243508000	-3.618435000
C	-2.077732000	-2.014363000	-3.825966000
C	-3.349211000	-1.982705000	-4.381469000
H	-5.186769000	-2.768389000	-1.675073000
H	-5.458710000	-2.230682000	-4.080852000
H	-1.196267000	-1.833279000	-4.430842000
C	-4.280092000	-2.997369000	0.781941000
C	-4.792511000	-4.122203000	1.450310000
C	-5.083099000	-1.864824000	0.903942000
C	-5.989321000	-4.122598000	2.168476000
C	-6.282975000	-1.791055000	1.598465000
C	-6.721307000	-2.947905000	2.228032000
H	-4.218462000	-5.042749000	1.414254000
H	-6.352316000	-5.012417000	2.672006000
H	-6.854145000	-0.871587000	1.652960000
C	-2.191499000	-4.524992000	-0.004402000
C	-1.030638000	-4.806402000	0.730896000
C	-2.716973000	-5.620459000	-0.693642000
C	-0.425543000	-6.063404000	0.767973000
C	-2.162259000	-6.895637000	-0.697899000
C	-1.005441000	-7.092407000	0.041733000
H	-0.587680000	-3.996338000	1.301024000
H	0.474731000	-6.250257000	1.344282000
H	-2.620388000	-7.702781000	-1.257601000
F	-3.859823000	-5.466710000	-1.402302000
F	-0.443006000	-8.317627000	0.054782000
F	-0.709812000	-2.356488000	-1.979317000
F	-3.478800000	-1.690811000	-5.693799000
F	-4.674703000	-0.700610000	0.310694000
F	-7.882656000	-2.911829000	2.911102000
C	1.585225000	-1.650119000	1.687118000
H	1.326569000	-1.700857000	2.740341000
C	2.733486000	-1.074875000	1.302821000
H	3.437018000	-0.650092000	2.006745000
C	3.104226000	-0.975535000	-0.106742000
O	4.144908000	-0.463065000	-0.569213000
O	2.207773000	-1.450721000	-0.940210000
H	0.883750000	-2.081211000	0.980063000

C	2.509878000	-1.478345000	-2.347452000
H	1.634898000	-1.939231000	-2.799517000
H	2.656246000	-0.463041000	-2.723012000
H	3.412114000	-2.065919000	-2.515679000

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C	-0.677100000	-3.369826000	0.956652000
O	-0.358957000	-4.260657000	1.722272000
O	-1.936102000	-3.127430000	0.583897000
C	-2.950085000	-3.959129000	1.174262000
H	-2.727427000	-5.013669000	0.996637000
H	-3.002187000	-3.784194000	2.251461000
H	-3.880189000	-3.669333000	0.688544000
C	0.278980000	-2.373400000	0.320885000
H	-0.024856000	-2.258463000	-0.723810000
B	-5.351400000	0.557752000	-0.244979000
C	-5.854613000	-0.999901000	-0.374906000
C	-6.923414000	-1.528231000	0.356714000
C	-5.271437000	-1.912966000	-1.269221000
C	-7.395901000	-2.832763000	0.253193000
C	-5.703026000	-3.232193000	-1.425607000
C	-6.767270000	-3.672980000	-0.652427000
H	-4.439755000	-1.570424000	-1.875744000
H	-8.231818000	-3.170603000	0.854624000
H	-5.238149000	-3.905855000	-2.138400000
C	-6.329942000	1.547873000	-1.105208000
C	-5.904021000	2.681095000	-1.802280000
C	-7.712491000	1.311503000	-1.199005000
C	-6.725157000	3.514051000	-2.552313000
C	-8.591866000	2.117178000	-1.921740000
C	-8.076993000	3.211940000	-2.597379000
H	-8.132442000	0.463634000	-0.670815000
H	-6.319990000	4.377149000	-3.067531000
H	-9.654547000	1.903540000	-1.965469000
C	-5.102319000	0.990404000	1.307420000
C	-5.109078000	2.307169000	1.781167000
C	-4.848245000	0.025457000	2.299357000
C	-4.898540000	2.670222000	3.108474000
C	-4.620670000	0.327133000	3.640703000
C	-4.655379000	1.660131000	4.024685000
H	-4.829393000	-1.019200000	2.001253000
H	-4.920720000	3.711556000	3.407679000
H	-4.433476000	-0.443778000	4.380783000
F	-7.580103000	-0.736972000	1.235037000

F	-7.202746000	-4.941669000	-0.779263000	C	3.474994000	-1.542354000	-1.870098000
F	-4.592927000	3.039560000	-1.778771000	H	4.300951000	-1.515665000	-1.163646000
F	-8.898201000	4.003909000	-3.313442000	H	3.805099000	-0.992980000	-2.758260000
F	-5.309615000	3.329374000	0.929022000	H	2.644099000	-0.976773000	-1.444162000
F	-4.446148000	1.985010000	5.313637000	C	0.428564000	-0.806372000	2.410364000
C	1.724851000	-2.863193000	0.471663000	C	-0.231815000	-1.484911000	3.444593000
H	1.783642000	-3.397882000	1.421521000	C	1.448503000	0.073916000	2.784920000
H	2.405173000	-2.006995000	0.529958000	C	0.137244000	-1.328739000	4.775788000
P	2.567969000	-3.999324000	-0.763102000	C	1.836815000	0.244590000	4.113152000
C	4.137496000	-4.575047000	0.236494000	C	1.182676000	-0.466304000	5.110034000
C	5.168251000	-3.438157000	0.326876000	H	-1.064875000	-2.136457000	3.203070000
C	4.814561000	-5.793316000	-0.412780000	H	-0.397679000	-1.868118000	5.551381000
H	4.215244000	-6.703397000	-0.345164000	H	2.639891000	0.940266000	4.332656000
H	5.085353000	-5.626298000	-1.457048000	H	1.476989000	-0.334534000	6.146920000
H	5.745495000	-5.985278000	0.132656000	O	2.136346000	0.851530000	1.878869000
H	5.633321000	-3.195108000	-0.629298000	C	0.028662000	-0.940582000	0.957824000
H	5.969871000	-3.783893000	0.990345000	C	0.648769000	0.152245000	0.144752000
H	4.768063000	-2.522149000	0.761990000	C	1.783137000	0.845221000	0.575937000
C	3.059649000	-2.950648000	-2.317514000	O	2.459125000	1.587751000	-0.202860000
C	1.859797000	-2.788025000	-3.265436000	H	0.527672000	0.109797000	-0.932265000
C	4.213070000	-3.604843000	-3.094331000	H	-1.067064000	-0.817939000	0.885950000
H	5.145951000	-3.625097000	-2.529384000	B	3.821980000	2.391529000	-0.141868000
H	3.987565000	-4.616953000	-3.434905000	C	4.585628000	1.899610000	-1.503453000
H	4.399393000	-2.995396000	-3.985642000	C	5.916648000	1.457099000	-1.531259000
H	1.576031000	-3.712647000	-3.771786000	C	3.959822000	1.931968000	-2.753794000
H	2.156675000	-2.074329000	-4.041682000	C	6.573265000	1.053579000	-2.695516000
H	0.982490000	-2.364893000	-2.769855000	C	4.559379000	1.540249000	-3.948049000
C	1.480876000	-5.528920000	-1.261241000	C	5.874505000	1.099863000	-3.891936000
C	2.131661000	-6.289236000	-2.429855000	H	6.472951000	1.440955000	-0.598331000
C	0.069129000	-5.106940000	-1.706954000	H	7.607021000	0.723841000	-2.685248000
H	-0.539250000	-4.730066000	-0.888294000	H	4.022701000	1.601197000	-4.888056000
H	0.058023000	-4.379394000	-2.515972000	C	4.676909000	2.053559000	1.207966000
H	-0.432552000	-6.008252000	-2.078463000	C	5.162830000	3.050958000	2.069088000
H	2.106627000	-5.723150000	-3.363110000	C	5.024765000	0.761562000	1.595345000
H	1.548063000	-7.202162000	-2.595418000	C	5.930400000	2.785737000	3.204344000
H	3.159287000	-6.595834000	-2.236510000	C	5.781858000	0.422378000	2.707267000
C	3.743362000	-4.929616000	1.685245000	C	6.232846000	1.466892000	3.503703000
H	3.523824000	-4.040283000	2.280107000	H	4.919467000	4.084998000	1.847558000
H	2.903500000	-5.618565000	1.770885000	H	6.290901000	3.581778000	3.847180000
H	4.610480000	-5.412904000	2.149480000	H	6.010451000	-0.608671000	2.950516000
C	1.319024000	-6.474611000	-0.060529000	C	3.415251000	3.963566000	-0.240464000
H	0.884435000	-5.971014000	0.806166000	C	2.116054000	4.451929000	-0.042995000
H	0.623329000	-7.267889000	-0.358337000	C	4.361121000	4.944096000	-0.550749000
H	2.251745000	-6.962927000	0.225890000	C	1.775316000	5.800634000	-0.149100000

C	4.085576000	6.301263000	-0.670511000
C	2.775024000	6.707542000	-0.466662000
H	1.329009000	3.744429000	0.195582000
H	0.759234000	6.148117000	0.005263000
H	4.866979000	7.011077000	-0.915556000
F	5.650232000	4.575959000	-0.734792000
F	2.476537000	8.015934000	-0.578103000
F	2.684313000	2.362069000	-2.850170000
F	6.478394000	0.711657000	-5.034091000
F	4.567619000	-0.289783000	0.844223000
F	6.972142000	1.176845000	4.590704000
C	-0.840927000	1.778569000	0.286959000
H	-0.465356000	2.185866000	1.220669000
C	-2.117980000	1.240251000	0.286424000
H	-2.652375000	1.068860000	1.209393000
C	-2.787977000	0.912139000	-0.916324000
O	-3.989307000	0.543190000	-1.077636000
O	-2.032636000	0.970649000	-2.020709000
H	-0.430005000	2.217427000	-0.615389000
C	-2.694954000	0.880325000	-3.287256000
H	-1.918732000	1.073348000	-4.028166000
H	-3.121144000	-0.114913000	-3.437978000
H	-3.485068000	1.628468000	-3.354374000

I_IM5

C	0.956366000	2.975183000	1.570915000
O	0.583166000	3.917158000	2.244979000
O	2.223021000	2.582461000	1.468713000
C	3.200981000	3.321265000	2.221067000
H	3.110189000	4.389656000	2.015427000
H	3.059959000	3.148550000	3.290891000
H	4.165923000	2.943454000	1.888830000
C	0.041509000	2.074956000	0.744734000
H	0.546976000	1.903755000	-0.210331000
B	5.011231000	-0.853874000	-0.256704000
C	5.441470000	0.743728000	-0.203801000
C	6.506455000	1.274170000	0.531062000
C	4.762690000	1.700000000	-0.978729000
C	6.889197000	2.614254000	0.538455000
C	5.102479000	3.053235000	-1.026966000
C	6.169997000	3.491711000	-0.257975000
H	3.929466000	1.350790000	-1.579671000
H	7.732080000	2.947854000	1.132870000
H	4.568354000	3.757048000	-1.657795000

C	6.037161000	-1.660140000	-1.257712000
C	5.657638000	-2.693300000	-2.120284000
C	7.407856000	-1.353136000	-1.314236000
C	6.513256000	-3.359429000	-2.991559000
C	8.318767000	-1.993362000	-2.154705000
C	7.848665000	-2.990946000	-2.993182000
H	7.794481000	-0.582257000	-0.657846000
H	6.143918000	-4.151468000	-3.632699000
H	9.370494000	-1.726780000	-2.164237000
C	4.904271000	-1.511106000	1.240907000
C	4.916078000	-2.886933000	1.495727000
C	4.765780000	-0.720854000	2.395112000
C	4.814401000	-3.460508000	2.760421000
C	4.652017000	-1.233837000	3.687002000
C	4.682961000	-2.611149000	3.846717000
H	4.740117000	0.358054000	2.273499000
H	4.832884000	-4.537148000	2.883035000
H	4.552876000	-0.590723000	4.555492000
F	7.260900000	0.455163000	1.300858000
F	6.519134000	4.795522000	-0.279911000
F	4.372506000	-3.127000000	-2.146954000
F	8.699902000	-3.623262000	-3.827333000
F	5.010802000	-3.758994000	0.474742000
F	4.578851000	-3.140526000	5.082112000
C	-1.325552000	2.755215000	0.575834000
H	-1.514206000	3.319843000	1.490864000
H	-2.125919000	2.016021000	0.479144000
P	-1.687699000	3.972640000	-0.815696000
C	-3.284164000	4.870084000	-0.154755000
C	-4.504160000	3.939011000	-0.239989000
C	-3.593567000	6.148876000	-0.951443000
H	-2.857906000	6.939621000	-0.793952000
H	-3.694795000	5.971444000	-2.023642000
H	-4.556263000	6.534640000	-0.597611000
H	-4.816989000	3.726272000	-1.263096000
H	-5.339464000	4.456161000	0.246906000
H	-4.363217000	2.994603000	0.286301000
C	-2.060220000	2.949323000	-2.420275000
C	-0.755388000	2.520426000	-3.111879000
C	-2.903857000	3.760556000	-3.417477000
H	-3.907823000	3.973310000	-3.047315000
H	-2.436057000	4.698273000	-3.721248000
H	-3.023982000	3.151311000	-4.320146000
H	-0.204904000	3.351648000	-3.555981000

H	-1.031678000	1.846685000	-3.930431000	C	-6.187884000	-0.394230000	-3.210455000
H	-0.088131000	1.953707000	-2.457095000	C	-4.164743000	-1.343566000	-4.147574000
C	-0.263762000	5.259110000	-1.122141000	C	-5.366547000	-0.664412000	-4.294880000
C	-0.535110000	6.046017000	-2.417085000	H	-6.427443000	-0.626222000	-1.100929000
C	1.107685000	4.576098000	-1.271806000	H	-7.130201000	0.121861000	-3.361557000
H	1.487552000	4.157469000	-0.342932000	H	-3.535835000	-1.572976000	-5.000163000
H	1.138276000	3.803668000	-2.037839000	C	-5.044185000	-1.474205000	0.956837000
H	1.819791000	5.353148000	-1.572821000	C	-5.843908000	-2.328174000	1.734837000
H	-0.427647000	5.429895000	-3.311948000	C	-5.175772000	-0.127404000	1.284875000
H	0.220369000	6.837162000	-2.483667000	C	-6.700744000	-1.877267000	2.739355000
H	-1.510766000	6.531191000	-2.441598000	C	-6.000541000	0.392049000	2.271280000
C	-3.108906000	5.235260000	1.334509000	C	-6.767846000	-0.515369000	2.990137000
H	-3.196661000	4.361330000	1.983839000	H	-5.786503000	-3.396208000	1.553099000
H	-2.176639000	5.747112000	1.571176000	H	-7.307563000	-2.563392000	3.320409000
H	-3.929625000	5.909926000	1.603139000	H	-6.045637000	1.454701000	2.478490000
C	-0.169487000	6.240263000	0.057277000	C	-3.882098000	-3.629991000	-0.201324000
H	0.000340000	5.731727000	1.008770000	C	-2.722406000	-4.267466000	0.263578000
H	0.695805000	6.888113000	-0.125417000	C	-4.887289000	-4.498241000	-0.636162000
H	-1.041452000	6.890788000	0.139650000	C	-2.565004000	-5.652862000	0.288208000
C	-2.813775000	1.663697000	-2.050019000	C	-4.791097000	-5.884264000	-0.634295000
H	-3.727611000	1.812898000	-1.479434000	C	-3.610040000	-6.442387000	-0.167732000
H	-3.103111000	1.166733000	-2.981884000	H	-1.891654000	-3.663678000	0.614332000
H	-2.184678000	0.956023000	-1.509133000	H	-1.652430000	-6.117008000	0.646199000
C	-0.600615000	0.571120000	2.792768000	H	-5.609152000	-6.501472000	-0.986642000
C	-0.013136000	1.149387000	3.927383000	F	-6.056722000	-3.977748000	-1.073589000
C	-1.751096000	-0.185791000	3.013633000	F	-3.486151000	-7.781150000	-0.155819000
C	-0.574253000	1.010916000	5.192251000	F	-2.640086000	-2.409828000	-2.752097000
C	-2.333481000	-0.347315000	4.266000000	F	-5.736582000	-0.262223000	-5.525901000
C	-1.741015000	0.264875000	5.363283000	F	-4.406856000	0.784843000	0.607353000
H	0.916153000	1.698192000	3.821360000	F	-7.582061000	-0.050163000	3.953302000
H	-0.090489000	1.471934000	6.047778000	C	0.403699000	-1.762415000	0.582982000
H	-3.230793000	-0.950238000	4.355083000	H	0.197362000	-2.262652000	1.535952000
H	-2.180388000	0.146925000	6.348887000	C	1.845595000	-1.438436000	0.482731000
O	-2.414531000	-0.840225000	1.978771000	H	2.470954000	-1.511129000	1.358764000
C	0.012781000	0.654740000	1.416077000	C	2.423775000	-1.078504000	-0.704449000
C	-0.525926000	-0.446355000	0.492442000	O	3.655689000	-0.829708000	-1.005905000
C	-1.916606000	-0.872418000	0.755226000	O	1.557909000	-0.919797000	-1.756934000
O	-2.600650000	-1.388878000	-0.151452000	H	0.051604000	-2.408780000	-0.227079000
H	-0.453157000	-0.158732000	-0.558682000	C	2.117386000	-0.961312000	-3.069340000
H	1.084732000	0.405464000	1.499328000	H	1.263502000	-1.025593000	-3.747385000
B	-4.104478000	-2.025077000	-0.251143000	H	2.699583000	-0.060622000	-3.289290000
C	-4.570543000	-1.501695000	-1.717815000	H	2.763747000	-1.831568000	-3.191567000
C	-5.774171000	-0.819016000	-1.947138000				
C	-3.807782000	-1.746889000	-2.864444000				

II_IM₂

C	3.385835000	-0.330888000	-1.973684000
O	2.631174000	-1.069062000	-1.200732000
O	3.460991000	-0.673638000	-3.285258000
C	3.046762000	-1.984917000	-3.656016000
H	3.721166000	-2.741267000	-3.248045000
H	2.031809000	-2.192907000	-3.312322000
H	3.086661000	-2.003105000	-4.746990000
C	4.030056000	0.822862000	-1.633361000
H	4.682727000	1.246962000	-2.383885000
B	3.015696000	-2.018065000	-0.021998000
C	2.851152000	-3.566391000	-0.533479000
C	1.695363000	-4.022393000	-1.168966000
C	3.810143000	-4.566456000	-0.306502000
C	1.474626000	-5.327329000	-1.592781000
C	3.648522000	-5.896279000	-0.696910000
C	2.475991000	-6.254879000	-1.343450000
H	4.725017000	-4.294083000	0.211385000
H	0.554998000	-5.609592000	-2.092463000
H	4.410753000	-6.644492000	-0.506404000
C	4.537318000	-1.685386000	0.490033000
C	5.656344000	-1.811488000	-0.338505000
C	4.838534000	-1.236745000	1.787190000
C	6.964441000	-1.517482000	0.031230000
C	6.128787000	-0.927975000	2.224314000
C	7.177315000	-1.073977000	1.328063000
H	4.023016000	-1.121253000	2.494811000
H	7.783378000	-1.638706000	-0.668296000
H	6.326602000	-0.597866000	3.239004000
C	1.890550000	-1.746115000	1.133995000
C	1.845610000	-2.474401000	2.326890000
C	0.838928000	-0.830455000	0.976791000
C	0.884453000	-2.314387000	3.319433000
C	-0.160552000	-0.626293000	1.933386000
C	-0.113535000	-1.375626000	3.100010000
H	0.795330000	-0.273931000	0.045136000
H	0.914604000	-2.906812000	4.226677000
H	-0.965442000	0.086378000	1.783651000
F	0.679091000	-3.147227000	-1.410528000
F	2.292756000	-7.529833000	-1.739559000
F	5.491012000	-2.250382000	-1.607429000
F	8.433148000	-0.779119000	1.717368000
F	2.799185000	-3.401480000	2.566590000
F	-1.057092000	-1.197637000	4.045301000

C	3.957916000	1.408831000	-0.269337000
H	4.893817000	1.330086000	0.301813000
H	3.199424000	0.879568000	0.317632000
P	3.511869000	3.230102000	-0.128090000
C	2.955244000	3.486486000	1.706754000
C	1.537707000	2.927412000	1.913853000
C	2.961779000	4.967392000	2.113341000
H	3.961096000	5.407527000	2.113069000
H	2.310085000	5.579867000	1.486174000
H	2.582421000	5.039554000	3.139381000
H	0.763295000	3.512178000	1.416497000
H	1.324865000	2.974028000	2.988230000
H	1.443403000	1.877067000	1.625860000
C	2.102260000	3.643975000	-1.375778000
C	2.660353000	3.708230000	-2.808290000
C	1.408732000	4.975255000	-1.048424000
H	0.824572000	4.938738000	-0.127802000
H	2.099779000	5.819741000	-0.997241000
H	0.700585000	5.188249000	-1.857953000
H	3.347926000	4.541240000	-2.967075000
H	1.809263000	3.864745000	-3.481554000
H	3.140234000	2.770729000	-3.096746000
C	5.127597000	4.225685000	-0.504284000
C	4.834299000	5.709030000	-0.774505000
C	5.838491000	3.610846000	-1.723804000
H	6.179445000	2.592204000	-1.526334000
H	5.232074000	3.602967000	-2.628546000
H	6.727990000	4.217877000	-1.930296000
H	4.246229000	5.861528000	-1.681475000
H	5.789754000	6.226767000	-0.920084000
H	4.322014000	6.200463000	0.055238000
C	3.885467000	2.684257000	2.637245000
H	3.861336000	1.612758000	2.427824000
H	4.922348000	3.016190000	2.618496000
H	3.520429000	2.820389000	3.661812000
C	6.116328000	4.118937000	0.669037000
H	6.357089000	3.083349000	0.924276000
H	7.052859000	4.594655000	0.355437000
H	5.779829000	4.638045000	1.567627000
C	1.076323000	2.497612000	-1.342216000
H	0.549266000	2.414213000	-0.393252000
H	0.321124000	2.707397000	-2.108592000
H	1.540572000	1.539740000	-1.585614000
O	-2.300468000	-2.446030000	-0.797327000

C	-1.563647000	-0.801894000	-2.839974000
C	-2.678812000	-0.568377000	-2.137746000
C	-3.034479000	-1.378624000	-0.971834000
O	-3.969662000	-1.136248000	-0.177044000
H	-3.367356000	0.228628000	-2.387407000
H	-1.322140000	-0.188054000	-3.702433000
B	-4.981811000	0.144985000	0.013937000
C	-4.022547000	1.450062000	0.248999000
C	-3.508610000	1.738525000	1.528177000
C	-3.638062000	2.371580000	-0.729956000
C	-2.675115000	2.820197000	1.809489000
C	-2.816968000	3.474102000	-0.513434000
C	-2.342372000	3.674493000	0.770947000
H	-3.764797000	1.081363000	2.349759000
H	-2.303413000	3.005643000	2.811439000
H	-2.572978000	4.149862000	-1.324487000
C	-5.821240000	-0.292060000	1.343254000
C	-7.203925000	-0.051614000	1.435439000
C	-5.282587000	-0.927166000	2.465247000
C	-7.980403000	-0.406696000	2.536554000
C	-6.003186000	-1.319052000	3.586813000
C	-7.362177000	-1.046148000	3.600480000
H	-7.701538000	0.432860000	0.602175000
H	-9.045289000	-0.203467000	2.571897000
H	-5.514360000	-1.811817000	4.419034000
C	-5.944646000	0.148449000	-1.293924000
C	-6.143068000	-0.982652000	-2.102241000
C	-6.723162000	1.253426000	-1.647133000
C	-7.012020000	-1.006469000	-3.193478000
C	-7.605073000	1.291531000	-2.719353000
C	-7.729274000	0.143096000	-3.487571000
H	-5.606762000	-1.897616000	-1.867244000
H	-7.141570000	-1.895260000	-3.801573000
H	-8.174949000	2.186021000	-2.941761000
F	-6.645349000	2.373777000	-0.894857000
F	-8.573194000	0.150746000	-4.534613000
F	-4.053082000	2.221740000	-2.011931000
F	-1.521854000	4.725495000	1.007918000
F	-3.946238000	-1.183234000	2.519521000
F	-8.087349000	-1.411040000	4.672416000
H	-0.868270000	-1.590143000	-2.569116000
C	-2.529642000	-3.276168000	0.360130000
H	-1.628782000	-3.879309000	0.447108000
H	-2.688010000	-2.660651000	1.243745000

H	-3.405316000	-3.904752000	0.181624000
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II_TS₂

C	-2.276373000	-0.043739000	1.645698000
O	-2.804417000	-0.577908000	0.617254000
O	-2.616932000	-0.323591000	2.908972000
C	-3.120729000	-1.620411000	3.267915000
H	-4.133646000	-1.765483000	2.903458000
H	-2.465792000	-2.399798000	2.874936000
H	-3.103996000	-1.633799000	4.358212000
C	-1.160218000	0.815182000	1.562390000
H	-0.879529000	1.274169000	2.500176000
B	-4.156904000	-1.117977000	-0.064285000
C	-4.617147000	-2.546205000	0.558141000
C	-3.725105000	-3.606027000	0.737135000
C	-5.959995000	-2.866805000	0.814275000
C	-4.079387000	-4.880851000	1.158234000
C	-6.380539000	-4.129238000	1.232590000
C	-5.425263000	-5.120515000	1.399097000
H	-6.712925000	-2.098718000	0.665741000
H	-3.334610000	-5.657891000	1.285221000
H	-7.425655000	-4.349651000	1.421971000
C	-5.268601000	0.079060000	0.065423000
C	-5.885398000	0.461607000	1.260884000
C	-5.702311000	0.814816000	-1.052667000
C	-6.845858000	1.460236000	1.385297000
C	-6.662288000	1.825594000	-0.997589000
C	-7.225446000	2.131171000	0.232909000
H	-5.268853000	0.581933000	-2.019959000
H	-7.286482000	1.692197000	2.347895000
H	-6.986154000	2.355266000	-1.887577000
C	-3.708840000	-1.369609000	-1.614475000
C	-4.631364000	-1.815908000	-2.567352000
C	-2.400854000	-1.224702000	-2.100535000
C	-4.336828000	-2.069232000	-3.902026000
C	-2.044334000	-1.460135000	-3.431053000
C	-3.026991000	-1.878074000	-4.315365000
H	-1.621227000	-0.945847000	-1.399561000
H	-5.104510000	-2.407412000	-4.588141000
H	-1.026419000	-1.331363000	-3.784047000
F	-2.400951000	-3.396563000	0.520091000
F	-5.801623000	-6.346467000	1.805771000
F	-5.551915000	-0.162071000	2.413998000
F	-8.156842000	3.097582000	0.318907000

F	-5.915988000	-2.005947000	-2.195280000	H	0.939303000	2.303355000	2.337712000
F	-2.709611000	-2.106935000	-5.603222000	O	0.996262000	-1.625107000	-0.696924000
C	-0.724653000	1.426630000	0.278283000	C	0.334248000	-0.840389000	1.848322000
H	-1.310741000	1.010658000	-0.546728000	C	1.572745000	-0.546258000	1.295074000
H	0.331469000	1.157559000	0.086051000	C	1.964924000	-1.069640000	0.039609000
P	-0.736830000	3.275212000	0.003859000	O	3.129873000	-1.103580000	-0.459130000
C	0.386679000	3.477950000	-1.557968000	H	2.334264000	-0.025658000	1.860113000
C	1.868940000	3.312983000	-1.186067000	H	0.200814000	-0.743680000	2.920208000
C	0.196273000	4.847850000	-2.227921000	B	4.614532000	-0.758742000	-0.000854000
H	-0.798302000	4.975613000	-2.659755000	C	4.779935000	0.869581000	0.141505000
H	0.393924000	5.684242000	-1.553760000	C	5.240079000	1.650619000	-0.935396000
H	0.914356000	4.921922000	-3.052682000	C	4.588583000	1.601195000	1.316847000
H	2.262113000	4.138087000	-0.591407000	C	5.485602000	3.021789000	-0.861403000
H	2.442937000	3.296519000	-2.118654000	C	4.825629000	2.965121000	1.461933000
H	2.089320000	2.373259000	-0.673746000	C	5.277100000	3.660595000	0.351065000
C	0.026884000	4.150529000	1.546729000	H	5.435992000	1.158308000	-1.880574000
C	-1.001423000	4.253523000	2.687364000	H	5.854698000	3.582039000	-1.714133000
C	0.507924000	5.569165000	1.202340000	H	4.688149000	3.454404000	2.419152000
H	1.338815000	5.573217000	0.495717000	C	5.485136000	-1.348901000	-1.257886000
H	-0.287702000	6.205645000	0.809737000	C	6.678763000	-2.064024000	-1.058927000
H	0.871483000	6.035459000	2.125280000	C	5.125116000	-1.213152000	-2.601350000
H	-1.817825000	4.942643000	2.464085000	C	7.445133000	-2.597202000	-2.094412000
H	-0.477075000	4.651617000	3.563735000	C	5.836713000	-1.730086000	-3.677669000
H	-1.426029000	3.289278000	2.972572000	C	7.004082000	-2.423891000	-3.397294000
C	-2.541947000	3.851501000	-0.333217000	H	7.022723000	-2.220122000	-0.041491000
C	-2.668042000	5.382400000	-0.298543000	H	8.361858000	-3.144356000	-1.902044000
C	-3.473364000	3.230813000	0.720625000	H	5.493743000	-1.587733000	-4.695914000
H	-3.491896000	2.142891000	0.658048000	C	4.923778000	-1.616233000	1.349100000
H	-3.236996000	3.520597000	1.742921000	C	4.201930000	-2.769897000	1.694961000
H	-4.491326000	3.574643000	0.507497000	C	5.987072000	-1.327075000	2.207842000
H	-2.476572000	5.798185000	0.692817000	C	4.485056000	-3.552574000	2.814339000
H	-3.701594000	5.639676000	-0.556918000	C	6.320304000	-2.065895000	3.336823000
H	-2.018592000	5.885324000	-1.018370000	C	5.545848000	-3.179233000	3.625345000
C	0.059087000	2.362636000	-2.571394000	H	3.381137000	-3.083938000	1.057138000
H	0.329725000	1.373076000	-2.197600000	H	3.905134000	-4.437177000	3.055125000
H	-0.981955000	2.339445000	-2.890263000	H	7.157944000	-1.780813000	3.962513000
H	0.669618000	2.543870000	-3.463141000	F	6.782958000	-0.267058000	1.937688000
C	-3.014426000	3.340003000	-1.704685000	F	5.842182000	-3.913336000	4.714197000
H	-2.934602000	2.254177000	-1.802142000	F	4.141131000	0.980498000	2.437828000
H	-4.079769000	3.578380000	-1.791907000	F	5.510989000	4.982844000	0.462074000
H	-2.503840000	3.816887000	-2.543386000	F	4.006062000	-0.508121000	-2.932520000
C	1.216548000	3.321089000	2.059534000	F	7.716788000	-2.934752000	-4.418197000
H	2.046081000	3.265677000	1.357298000	H	-0.287125000	-1.583198000	1.358743000
H	1.595588000	3.811612000	2.963650000	C	1.393574000	-2.373442000	-1.856710000

H	0.461466000	-2.723842000	-2.297711000
H	1.953720000	-1.744312000	-2.549536000
H	2.016983000	-3.222993000	-1.566477000

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C	2.210544000	-0.109975000	-1.459901000
O	3.032064000	-0.330212000	-0.560169000
O	2.375877000	-0.293328000	-2.751653000
C	3.529391000	-0.941036000	-3.323113000
H	4.416754000	-0.775665000	-2.719973000
H	3.313800000	-2.006227000	-3.407471000
H	3.643625000	-0.502052000	-4.314185000
C	0.798881000	0.329644000	-1.177966000
H	0.406587000	0.761262000	-2.097861000
B	4.512940000	-0.947768000	0.188610000
C	5.059051000	-2.179193000	-0.685176000
C	4.236414000	-3.228060000	-1.102234000
C	6.430412000	-2.377822000	-0.915410000
C	4.682821000	-4.384956000	-1.725136000
C	6.940201000	-3.521571000	-1.527102000
C	6.051469000	-4.510440000	-1.924295000
H	7.129498000	-1.616099000	-0.585222000
H	3.991725000	-5.161028000	-2.032545000
H	8.003945000	-3.655809000	-1.690523000
C	5.417763000	0.390902000	0.273445000
C	6.112250000	0.971726000	-0.792345000
C	5.585048000	1.063790000	1.498691000
C	6.916841000	2.101459000	-0.699233000
C	6.375689000	2.200049000	1.658252000
C	7.036994000	2.701376000	0.545733000
H	5.074236000	0.667565000	2.370975000
H	7.437244000	2.489036000	-1.567229000
H	6.496553000	2.681885000	2.622654000
C	3.983280000	-1.474070000	1.621447000
C	4.923765000	-1.984680000	2.523805000
C	2.652930000	-1.557901000	2.055316000
C	4.618644000	-2.528790000	3.763710000
C	2.284773000	-2.101174000	3.286690000
C	3.279764000	-2.579753000	4.124888000
H	1.862913000	-1.197041000	1.408209000
H	5.397688000	-2.905582000	4.415878000
H	1.245541000	-2.169044000	3.587409000
F	2.896400000	-3.110978000	-0.933322000
F	6.517462000	-5.619366000	-2.520553000

F	6.021711000	0.430793000	-2.030966000
F	7.809385000	3.792593000	0.666891000
F	6.232638000	-1.942966000	2.187387000
F	2.949450000	-3.105039000	5.316676000
C	0.619526000	1.258321000	0.025700000
H	1.394635000	1.070095000	0.774553000
H	-0.336756000	0.971293000	0.476807000
P	0.449941000	3.113563000	-0.082619000
C	-0.566468000	3.513887000	1.516514000
C	-2.043841000	3.139893000	1.307105000
C	-0.471382000	5.001738000	1.885899000
H	0.530866000	5.298909000	2.200943000
H	-0.791823000	5.662934000	1.078337000
H	-1.140764000	5.180552000	2.734885000
H	-2.563851000	3.818142000	0.629454000
H	-2.544902000	3.211234000	2.278443000
H	-2.195382000	2.115814000	0.958243000
C	-0.513708000	3.609862000	-1.680634000
C	0.410700000	3.522346000	-2.909299000
C	-1.057505000	5.045844000	-1.592873000
H	-1.794530000	5.167722000	-0.797698000
H	-0.278131000	5.800757000	-1.471100000
H	-1.575189000	5.259067000	-2.535067000
H	1.202162000	4.274148000	-2.900370000
H	-0.205851000	3.716420000	-3.793838000
H	0.864402000	2.538629000	-3.046645000
C	2.206684000	3.904737000	-0.027551000
C	2.169928000	5.396207000	-0.391480000
C	3.125946000	3.152309000	-1.002942000
H	3.299741000	2.126669000	-0.675520000
H	2.771667000	3.146228000	-2.033005000
H	4.102191000	3.649658000	-0.996204000
H	1.887906000	5.568698000	-1.431817000
H	3.180607000	5.800161000	-0.262980000
H	1.503802000	5.977038000	0.249668000
C	-0.048363000	2.656226000	2.688215000
H	-0.236443000	1.591914000	2.533966000
H	1.008267000	2.800185000	2.911337000
H	-0.611302000	2.954743000	3.579716000
C	2.827199000	3.747704000	1.370426000
H	2.875091000	2.705702000	1.697022000
H	3.863542000	4.097396000	1.311952000
H	2.325616000	4.342154000	2.135404000
C	-1.698223000	2.648740000	-1.884391000

H	-2.540102000	2.864386000	-1.228550000
H	-2.060924000	2.780156000	-2.908695000
H	-1.459500000	1.591061000	-1.756977000
O	-1.216607000	-0.842007000	1.611900000
C	-0.035588000	-1.011351000	-0.934534000
C	-1.491926000	-0.796006000	-0.713518000
C	-2.064180000	-0.800225000	0.525247000
O	-3.314564000	-0.749298000	0.862971000
H	-2.156613000	-0.783108000	-1.566651000
H	0.129799000	-1.634019000	-1.820935000
B	-4.640789000	-0.783493000	0.075109000
C	-4.758300000	0.500912000	-0.961056000
C	-5.260608000	1.740951000	-0.523267000
C	-4.478999000	0.470715000	-2.330643000
C	-5.477979000	2.841102000	-1.355988000
C	-4.691195000	1.521860000	-3.219446000
C	-5.198783000	2.704728000	-2.707150000
H	-5.513715000	1.850765000	0.525139000
H	-5.887308000	3.772319000	-0.977338000
H	-4.477906000	1.406006000	-4.276001000
C	-5.763769000	-0.644666000	1.276605000
C	-6.964497000	-1.376279000	1.263843000
C	-5.623482000	0.174827000	2.399186000
C	-7.930195000	-1.309544000	2.267822000
C	-6.539911000	0.279623000	3.440014000
C	-7.696254000	-0.479278000	3.352542000
H	-7.153733000	-2.039463000	0.426649000
H	-8.843739000	-1.892819000	2.219260000
H	-6.357484000	0.936894000	4.282412000
C	-4.773195000	-2.252453000	-0.633247000
C	-3.979661000	-3.338656000	-0.232096000
C	-5.711052000	-2.566231000	-1.618373000
C	-4.086409000	-4.619149000	-0.776443000
C	-5.869334000	-3.818377000	-2.200743000
C	-5.035092000	-4.836003000	-1.763555000
H	-3.242634000	-3.177132000	0.548127000
H	-3.453772000	-5.436332000	-0.445812000
H	-6.618488000	-3.988352000	-2.965256000
F	-6.561042000	-1.602365000	-2.049763000
F	-5.160566000	-6.061963000	-2.311495000
F	-3.951869000	-0.644810000	-2.890413000
F	-5.409477000	3.742486000	-3.543999000
F	-4.525342000	0.979502000	2.526508000
F	-8.604618000	-0.398515000	4.345264000

H	0.419296000	-1.531225000	-0.086613000
C	-1.814805000	-1.112050000	2.880194000
H	-0.998452000	-1.054963000	3.603395000
H	-2.588865000	-0.381738000	3.120279000
H	-2.256003000	-2.113366000	2.906453000

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C	-0.429900000	-3.351584000	0.879859000
O	-0.340088000	-3.832450000	1.992485000
O	-1.499732000	-3.490913000	0.086177000
C	-2.625683000	-4.174198000	0.662401000
H	-2.412090000	-5.242378000	0.756625000
H	-2.855222000	-3.761924000	1.646069000
H	-3.453878000	-4.003189000	-0.022770000
C	0.598378000	-2.441454000	0.249243000
H	0.460235000	-2.450850000	-0.833610000
C	2.035113000	-2.781440000	0.661691000
H	2.030190000	-3.083145000	1.714151000
H	2.614226000	-1.850287000	0.593637000
P	3.101962000	-4.036182000	-0.224762000
C	4.883797000	-3.600971000	0.412511000
C	5.422773000	-2.350207000	-0.300820000
C	5.878898000	-4.750016000	0.184904000
H	5.662808000	-5.635009000	0.785900000
H	5.956143000	-5.047297000	-0.863519000
H	6.869237000	-4.393503000	0.489965000
H	5.643886000	-2.518276000	-1.355214000
H	6.369452000	-2.087600000	0.185058000
H	4.778990000	-1.476092000	-0.202731000
C	2.947104000	-3.775500000	-2.131136000
C	1.653221000	-4.415460000	-2.665643000
C	4.134997000	-4.399306000	-2.882118000
H	5.085120000	-3.921033000	-2.642367000
H	4.232052000	-5.473511000	-2.714233000
H	3.967062000	-4.250856000	-3.954817000
H	1.673837000	-5.506446000	-2.629716000
H	1.560372000	-4.131363000	-3.720000000
H	0.752323000	-4.063700000	-2.157779000
C	2.625745000	-5.843902000	0.288218000
C	3.347293000	-6.876431000	-0.594475000
C	1.109452000	-6.079365000	0.175060000
H	0.568625000	-5.577002000	0.975438000
H	0.679857000	-5.790934000	-0.783028000
H	0.938342000	-7.155961000	0.293107000

H	2.972399000	-6.877103000	-1.620335000	C	2.033865000	6.234929000	-0.501718000
H	3.140434000	-7.870119000	-0.180505000	C	4.286302000	6.202492000	-1.386981000
H	4.430681000	-6.757207000	-0.620499000	C	3.094175000	6.865282000	-1.135184000
C	4.815342000	-3.267724000	1.916678000	H	1.363445000	4.398675000	0.372034000
H	4.288683000	-2.330994000	2.103304000	H	1.115264000	6.781588000	-0.314852000
H	4.377476000	-4.055574000	2.529794000	H	5.116721000	6.696990000	-1.877378000
H	5.845895000	-3.125846000	2.262106000	F	5.559388000	4.259188000	-1.228468000
C	2.989482000	-6.081204000	1.763335000	F	2.974226000	8.153446000	-1.514236000
H	2.508027000	-5.360065000	2.429600000	F	1.779431000	2.130509000	-2.298960000
H	2.607513000	-7.070331000	2.041234000	F	5.007425000	-0.010483000	-4.924975000
H	4.063580000	-6.087095000	1.952722000	F	4.237780000	0.031487000	1.394266000
C	2.893289000	-2.268174000	-2.433110000	F	7.241177000	1.870284000	4.481447000
H	3.794071000	-1.727480000	-2.150063000	H	0.271803000	-1.010331000	1.853016000
H	2.782692000	-2.151597000	-3.516797000	C	1.583909000	2.118325000	3.163724000
H	2.044997000	-1.767774000	-1.964912000	H	1.508135000	1.770565000	4.195596000
O	1.449142000	0.951101000	2.360334000	H	2.543579000	2.613706000	3.006922000
C	0.224045000	-1.007551000	0.760045000	H	0.776073000	2.831764000	2.963409000
C	1.053726000	0.109053000	0.221494000	O	-2.350515000	0.193217000	-2.253886000
C	1.578934000	1.092293000	1.011411000	C	-1.106574000	1.984124000	-0.591752000
O	2.101971000	2.210818000	0.585098000	C	-2.339539000	1.517515000	-0.316103000
H	1.170329000	0.229804000	-0.848223000	C	-3.036037000	0.608837000	-1.200909000
H	-0.835531000	-0.867591000	0.494480000	O	-4.211801000	0.195716000	-1.072893000
B	3.502548000	2.585361000	0.061941000	H	-2.880952000	1.821605000	0.569364000
C	3.895532000	1.739570000	-1.288017000	H	-0.574832000	1.734575000	-1.501150000
C	5.176681000	1.210767000	-1.512154000	B	-5.447762000	0.391224000	-0.016708000
C	3.039864000	1.637493000	-2.387629000	C	-4.969118000	-0.132702000	1.454072000
C	5.575728000	0.620578000	-2.714741000	C	-5.189841000	-1.460986000	1.862821000
C	3.371387000	1.060424000	-3.609676000	C	-4.387868000	0.665664000	2.444414000
C	4.656695000	0.558049000	-3.751081000	C	-4.850931000	-1.956680000	3.120880000
H	5.909359000	1.292473000	-0.713957000	C	-4.021560000	0.233767000	3.713255000
H	6.582976000	0.243438000	-2.860953000	C	-4.264428000	-1.091995000	4.033327000
H	2.658691000	1.030676000	-4.426061000	H	-5.672208000	-2.140361000	1.169908000
C	4.588983000	2.381133000	1.283036000	H	-5.056572000	-2.983469000	3.405193000
C	5.284994000	3.452823000	1.871498000	H	-3.577066000	0.917757000	4.426377000
C	4.867010000	1.148778000	1.872575000	C	-6.576884000	-0.575237000	-0.696166000
C	6.174993000	3.311094000	2.936814000	C	-7.920543000	-0.171772000	-0.789641000
C	5.738965000	0.933032000	2.932354000	C	-6.330517000	-1.841399000	-1.230904000
C	6.389761000	2.042573000	3.452177000	C	-8.925945000	-0.951218000	-1.359220000
H	5.111375000	4.451036000	1.482220000	C	-7.282068000	-2.662711000	-1.822732000
H	6.693186000	4.163047000	3.364310000	C	-8.585748000	-2.192388000	-1.874999000
H	5.898063000	-0.055848000	3.346241000	H	-8.192552000	0.805346000	-0.403976000
C	3.358407000	4.160955000	-0.350113000	H	-9.952963000	-0.606277000	-1.412577000
C	2.188093000	4.900760000	-0.123295000	H	-7.015890000	-3.634890000	-2.221086000
C	4.377211000	4.874173000	-0.985852000	C	-5.877465000	1.953841000	-0.126194000

C	-5.548244000	2.770100000	-1.220118000
C	-6.682530000	2.574050000	0.833069000
C	-5.952944000	4.099651000	-1.339942000
C	-7.118890000	3.891367000	0.769840000
C	-6.733922000	4.642135000	-0.330976000
H	-4.954970000	2.353680000	-2.028942000
H	-5.676312000	4.706579000	-2.195316000
H	-7.736816000	4.312108000	1.554347000
F	-7.097728000	1.858442000	1.901565000
F	-7.138773000	5.921734000	-0.418459000
F	-4.140385000	1.976704000	2.195038000
F	-3.930339000	-1.539675000	5.255652000
F	-5.067185000	-2.362716000	-1.178883000
F	-9.531096000	-2.964502000	-2.440332000
H	-0.616427000	2.686781000	0.071320000
C	-3.026318000	-0.663964000	-3.188563000
H	-2.262482000	-0.955068000	-3.908474000
H	-3.446284000	-1.530473000	-2.677996000
H	-3.829505000	-0.116753000	-3.688201000

II_TS₃

C	0.769529000	-3.118908000	-1.162846000
O	0.533047000	-3.665572000	-2.223916000
O	1.966341000	-3.110880000	-0.575854000
C	3.037256000	-3.710985000	-1.328242000
H	2.853171000	-4.780323000	-1.460508000
H	3.122018000	-3.232447000	-2.304998000
H	3.935974000	-3.535453000	-0.742332000
C	-0.244715000	-2.304925000	-0.381423000
H	0.055758000	-2.273239000	0.668853000
C	-1.666671000	-2.844151000	-0.602668000
H	-1.728524000	-3.180324000	-1.642810000
H	-2.372734000	-2.014195000	-0.495147000
P	-2.457906000	-4.209036000	0.396580000
C	-4.306417000	-4.091681000	-0.191548000
C	-5.006402000	-2.881139000	0.447808000
C	-5.101781000	-5.358982000	0.157766000
H	-4.766623000	-6.239812000	-0.393143000
H	-5.094960000	-5.588248000	1.225540000
H	-6.145562000	-5.184622000	-0.126165000
H	-5.140585000	-2.970284000	1.525924000
H	-6.008708000	-2.822482000	0.007422000
H	-4.520969000	-1.929066000	0.227606000
C	-2.289780000	-3.809455000	2.278066000

C	-0.912637000	-4.233928000	2.816267000
C	-3.370616000	-4.525681000	3.104263000
H	-4.378859000	-4.182073000	2.871696000
H	-3.339065000	-5.612246000	3.001586000
H	-3.191694000	-4.293682000	4.160168000
H	-0.778914000	-5.316734000	2.849946000
H	-0.840616000	-3.869115000	3.847413000
H	-0.081986000	-3.791344000	2.261867000
C	-1.711945000	-5.942253000	-0.027450000
C	-2.244547000	-7.013446000	0.939945000
C	-0.173969000	-5.928873000	0.054059000
H	0.258996000	-5.425940000	-0.808577000
H	0.229974000	-5.492687000	0.965671000
H	0.160653000	-6.972338000	0.019771000
H	-1.865256000	-6.880818000	1.955139000
H	-1.882232000	-7.986699000	0.589753000
H	-3.332515000	-7.069931000	0.980300000
C	-4.346635000	-3.865386000	-1.717251000
H	-3.999207000	-2.867167000	-1.987548000
H	-3.793888000	-4.604479000	-2.296701000
H	-5.396238000	-3.931974000	-2.025576000
C	-2.061875000	-6.331639000	-1.474197000
H	-1.713200000	-5.587805000	-2.196192000
H	-1.530947000	-7.263850000	-1.699665000
H	-3.124583000	-6.523689000	-1.630829000
C	-2.411150000	-2.289786000	2.472867000
H	-3.328454000	-1.856727000	2.077545000
H	-2.406104000	-2.088954000	3.549516000
H	-1.562840000	-1.754046000	2.043970000
O	-0.747161000	1.490617000	-2.175583000
C	-0.125235000	-0.866030000	-0.958913000
C	-0.970051000	0.174538000	-0.287221000
C	-1.361839000	1.303286000	-0.992290000
O	-2.132890000	2.255702000	-0.589721000
H	-1.546849000	-0.054390000	0.599504000
H	0.940021000	-0.584468000	-0.890178000
B	-3.624387000	2.344299000	-0.148096000
C	-3.965065000	1.451765000	1.180001000
C	-5.167378000	0.740850000	1.324807000
C	-3.195943000	1.517780000	2.345086000
C	-5.567316000	0.130669000	2.516843000
C	-3.532434000	0.926143000	3.558788000
C	-4.733634000	0.234679000	3.620362000
H	-5.839613000	0.691791000	0.472747000

H	-6.516140000	-0.389187000	2.603429000
H	-2.892758000	1.031091000	4.427707000
C	-4.507931000	1.939073000	-1.472813000
C	-5.228442000	2.894837000	-2.212826000
C	-4.563543000	0.657463000	-2.018429000
C	-5.943074000	2.602407000	-3.374066000
C	-5.255744000	0.293831000	-3.166794000
C	-5.947134000	1.294520000	-3.833733000
H	-5.220804000	3.922217000	-1.862756000
H	-6.487900000	3.367830000	-3.916474000
H	-5.250580000	-0.725053000	-3.535897000
C	-3.811903000	3.911675000	0.264735000
C	-2.757728000	4.837581000	0.279363000
C	-5.038050000	4.423174000	0.696498000
C	-2.906856000	6.164433000	0.684530000
C	-5.251115000	5.733194000	1.108641000
C	-4.160666000	6.590811000	1.095708000
H	-1.776509000	4.497550000	-0.035162000
H	-2.072974000	6.858595000	0.687892000
H	-6.230900000	6.067158000	1.429519000
F	-6.119814000	3.607736000	0.710619000
F	-4.334354000	7.866678000	1.491503000
F	-2.034498000	2.210226000	2.330127000
F	-5.087846000	-0.351987000	4.782992000
F	-3.882617000	-0.360003000	-1.401030000
F	-6.627535000	0.977097000	-4.950446000
H	-0.350521000	-0.908292000	-2.031526000
C	-1.055353000	2.676561000	-2.909537000
H	-0.550691000	2.557789000	-3.868889000
H	-2.131797000	2.785758000	-3.056517000
H	-0.672239000	3.563483000	-2.397658000
O	2.130838000	-0.649010000	2.044692000
C	0.631528000	1.411301000	0.999014000
C	1.914461000	1.163930000	0.574047000
C	2.727103000	0.159908000	1.158350000
O	3.965378000	-0.035666000	0.972937000
H	2.380806000	1.779940000	-0.181382000
H	0.234474000	0.916353000	1.876020000
B	5.091676000	0.656768000	0.071885000
C	4.728685000	0.390880000	-1.503859000
C	5.193202000	-0.759571000	-2.167185000
C	3.993179000	1.249008000	-2.327424000
C	4.941423000	-1.045873000	-3.508771000
C	3.705178000	1.022644000	-3.668724000

C	4.191870000	-0.139633000	-4.243657000
H	5.801065000	-1.463393000	-1.610204000
H	5.334827000	-1.936861000	-3.987318000
H	3.131505000	1.741439000	-4.241545000
C	6.442090000	-0.154255000	0.535483000
C	7.669854000	0.513954000	0.694418000
C	6.513481000	-1.521669000	0.808194000
C	8.851671000	-0.110739000	1.089337000
C	7.653185000	-2.204254000	1.217610000
C	8.821807000	-1.471379000	1.353178000
H	7.701519000	1.581902000	0.505800000
H	9.778473000	0.442053000	1.199965000
H	7.627726000	-3.269558000	1.415562000
C	5.194210000	2.211574000	0.546200000
C	4.758262000	2.641907000	1.809786000
C	5.803970000	3.207466000	-0.220040000
C	4.882473000	3.954483000	2.264816000
C	5.957435000	4.530984000	0.175631000
C	5.480189000	4.884960000	1.428483000
H	4.304025000	1.917382000	2.479166000
H	4.529057000	4.256416000	3.244967000
H	6.435849000	5.254854000	-0.473605000
F	6.314924000	2.886677000	-1.430213000
F	5.612827000	6.160469000	1.838496000
F	3.500492000	2.410229000	-1.829624000
F	3.934054000	-0.383707000	-5.541788000
F	5.402527000	-2.306134000	0.659611000
F	9.943212000	-2.103142000	1.747692000
H	0.132674000	2.330619000	0.721798000
C	2.971877000	-1.557632000	2.764557000
H	2.293786000	-2.144039000	3.385483000
H	3.532832000	-2.194772000	2.081669000
H	3.675697000	-1.010069000	3.397247000

II_IM₅

C	-0.802751000	-2.774418000	1.750605000
O	-0.384541000	-3.451158000	2.673730000
O	-2.078629000	-2.466450000	1.560832000
C	-3.018672000	-2.919427000	2.548877000
H	-2.884414000	-3.987041000	2.738629000
H	-2.881254000	-2.361424000	3.476959000
H	-3.996677000	-2.707817000	2.123023000
C	0.075423000	-2.143390000	0.673366000
H	-0.501559000	-2.126248000	-0.255703000

C	1.407454000	-2.907127000	0.595565000	C	0.307812000	-0.677687000	1.131588000
H	1.601063000	-3.284049000	1.603985000	C	0.874111000	0.257005000	0.049874000
H	2.224254000	-2.223654000	0.353198000	C	1.163240000	1.608287000	0.629976000
P	1.749976000	-4.363750000	-0.513555000	O	2.206880000	2.283564000	0.508784000
C	3.542050000	-4.858613000	0.071396000	H	1.831425000	-0.104549000	-0.335247000
C	4.587080000	-3.856314000	-0.450819000	H	-0.662053000	-0.270100000	1.430979000
C	3.922896000	-6.267802000	-0.407009000	B	3.801393000	2.079367000	0.213951000
H	3.332003000	-7.049126000	0.074712000	C	4.084486000	1.168678000	-1.095620000
H	3.847431000	-6.388752000	-1.489243000	C	5.182876000	0.295954000	-1.168936000
H	4.969370000	-6.444637000	-0.134111000	C	3.429846000	1.382507000	-2.310791000
H	4.717101000	-3.882265000	-1.533116000	C	5.582786000	-0.332450000	-2.349048000
H	5.550118000	-4.137204000	-0.008327000	C	3.770259000	0.777273000	-3.514703000
H	4.389228000	-2.827879000	-0.140463000	C	4.860835000	-0.080484000	-3.507522000
C	1.759077000	-3.782968000	-2.354223000	H	5.768973000	0.127412000	-0.270948000
C	0.330740000	-3.705163000	-2.919820000	H	6.449309000	-0.984570000	-2.384454000
C	2.581710000	-4.735707000	-3.237315000	H	3.220521000	0.990619000	-4.424053000
H	3.645105000	-4.735333000	-2.993436000	C	4.339847000	1.517364000	1.644292000
H	2.217825000	-5.764591000	-3.210013000	C	4.877820000	2.391702000	2.606975000
H	2.493702000	-4.388132000	-4.272710000	C	4.257006000	0.193294000	2.071792000
H	-0.137220000	-4.684563000	-3.034078000	C	5.306923000	1.985313000	3.867933000
H	0.405088000	-3.269719000	-3.922954000	C	4.671345000	-0.281400000	3.309486000
H	-0.326884000	-3.049150000	-2.343552000	C	5.199640000	0.642390000	4.199230000
C	0.495709000	-5.806510000	-0.227280000	H	4.960862000	3.443164000	2.349279000
C	0.687779000	-6.917772000	-1.273156000	H	5.719861000	2.687217000	4.584397000
C	-0.953814000	-5.298031000	-0.321491000	H	4.581834000	-1.327907000	3.575807000
H	-1.220086000	-4.650660000	0.510204000	C	4.304863000	3.586054000	-0.118274000
H	-1.191037000	-4.783444000	-1.249764000	C	3.461332000	4.667805000	-0.411755000
H	-1.608203000	-6.175449000	-0.259286000	C	5.670160000	3.864252000	-0.229186000
H	0.410699000	-6.597880000	-2.279941000	C	3.933682000	5.931980000	-0.764749000
H	0.016890000	-7.742387000	-1.006431000	C	6.200341000	5.101382000	-0.570592000
H	1.699851000	-7.323058000	-1.301888000	C	5.304810000	6.127864000	-0.835231000
C	3.627707000	-4.807058000	1.610709000	H	2.388387000	4.513109000	-0.377946000
H	3.617345000	-3.780897000	1.983331000	H	3.259121000	6.751514000	-0.988260000
H	2.851053000	-5.373085000	2.124046000	H	7.271382000	5.253689000	-0.633174000
H	4.591703000	-5.241930000	1.898217000	F	6.558370000	2.872595000	0.014335000
C	0.679073000	-6.387952000	1.184720000	F	5.787143000	7.337477000	-1.170191000
H	0.573136000	-5.626513000	1.962378000	F	2.387324000	2.244422000	-2.345102000
H	-0.120331000	-7.120914000	1.343901000	F	5.218221000	-0.684348000	-4.657032000
H	1.624928000	-6.918251000	1.311388000	F	3.719858000	-0.749524000	1.235460000
C	2.348636000	-2.367149000	-2.431184000	F	5.608991000	0.216479000	5.404887000
H	3.353890000	-2.269162000	-2.025076000	H	0.963173000	-0.686945000	2.011027000
H	2.405080000	-2.088300000	-3.488541000	C	0.268891000	3.468676000	1.793607000
H	1.704575000	-1.632676000	-1.946191000	H	-0.716334000	3.692795000	2.191777000
O	0.151869000	2.129485000	1.273879000	H	1.040366000	3.503387000	2.564801000

H	0.519374000	4.160631000	0.988943000
O	-2.186291000	-1.443077000	-1.673287000
C	-0.133044000	0.442127000	-1.158332000
C	-1.563528000	0.646722000	-0.792953000
C	-2.544247000	-0.249906000	-1.065433000
O	-3.828718000	-0.161884000	-0.866866000
H	-1.867052000	1.580062000	-0.341303000
H	-0.041756000	-0.454333000	-1.779332000
B	-4.713968000	0.896549000	-0.187654000
C	-4.353519000	1.007032000	1.424303000
C	-4.976915000	0.161092000	2.360108000
C	-3.477944000	1.921800000	2.014497000
C	-4.749864000	0.197944000	3.736689000
C	-3.205943000	2.014645000	3.376679000
C	-3.855846000	1.135744000	4.227036000
H	-5.696458000	-0.561579000	1.994237000
H	-5.270564000	-0.465337000	4.420083000
H	-2.529049000	2.766477000	3.765556000
C	-6.233398000	0.278387000	-0.396651000
C	-7.323076000	1.090768000	-0.757798000
C	-6.570007000	-1.071290000	-0.265576000
C	-8.616411000	0.615785000	-0.975147000
C	-7.833568000	-1.612941000	-0.477016000
C	-8.850761000	-0.742757000	-0.835657000
H	-7.149503000	2.153885000	-0.886903000
H	-9.427847000	1.279729000	-1.254458000
H	-8.014027000	-2.675019000	-0.356857000
C	-4.591874000	2.302835000	-1.018528000
C	-4.106451000	2.332254000	-2.335739000
C	-5.021926000	3.542132000	-0.541594000
C	-4.027497000	3.492825000	-3.106661000
C	-4.970454000	4.733928000	-1.257271000
C	-4.460720000	4.684272000	-2.545629000
H	-3.772659000	1.399362000	-2.778756000
H	-3.642690000	3.481821000	-4.121261000
H	-5.321996000	5.662316000	-0.822184000
F	-5.554221000	3.623258000	0.701403000
F	-4.394288000	5.824464000	-3.264633000
F	-2.818333000	2.830263000	1.245988000
F	-3.612947000	1.207680000	5.551748000
F	-5.624912000	-1.980368000	0.123723000
F	-10.087160000	-1.237781000	-1.048213000
H	0.256752000	1.264024000	-1.770624000
C	-3.252580000	-2.212305000	-2.219937000

H	-2.784954000	-3.104812000	-2.645542000
H	-3.982184000	-2.489982000	-1.458640000
H	-3.770367000	-1.667311000	-3.016279000

III_IM₄

C	1.567371000	-4.349423000	0.489158000
O	2.290288000	-5.070202000	1.150793000
O	0.325479000	-4.693358000	0.118388000
C	-0.146765000	-5.969772000	0.581461000
H	0.529480000	-6.764706000	0.258572000
H	-0.207423000	-5.978494000	1.672242000
H	-1.134153000	-6.093996000	0.140729000
C	1.914264000	-2.959207000	-0.002355000
H	1.569680000	-2.881808000	-1.037296000
B	-5.402954000	-0.603017000	0.175348000
C	-4.794293000	-2.061199000	-0.225023000
C	-5.600370000	-3.203485000	-0.175832000
C	-3.455426000	-2.310387000	-0.557373000
C	-5.157368000	-4.497673000	-0.425182000
C	-2.949528000	-3.585302000	-0.819707000
C	-3.817797000	-4.660736000	-0.742537000
H	-2.755450000	-1.481182000	-0.597541000
H	-5.835255000	-5.340975000	-0.364100000
H	-1.904810000	-3.744699000	-1.062960000
C	-6.414479000	0.032379000	-0.914780000
C	-6.909109000	1.331797000	-0.786127000
C	-6.857777000	-0.655106000	-2.052881000
C	-7.776198000	1.941465000	-1.683350000
C	-7.731786000	-0.099782000	-2.989312000
C	-8.179352000	1.197074000	-2.783051000
H	-6.504348000	-1.668396000	-2.219477000
H	-8.125257000	2.955308000	-1.526256000
H	-8.071984000	-0.656435000	-3.856358000
C	-5.902141000	-0.610706000	1.722185000
C	-7.236669000	-0.633118000	2.130257000
C	-4.967152000	-0.662818000	2.769628000
C	-7.648645000	-0.683932000	3.458782000
C	-5.319895000	-0.710986000	4.116537000
C	-6.669630000	-0.719628000	4.438118000
H	-3.910278000	-0.659809000	2.517429000
H	-8.702256000	-0.694940000	3.711994000
H	-4.574797000	-0.743917000	4.904405000
F	-6.904486000	-3.064641000	0.132649000
F	-3.347456000	-5.910767000	-0.971162000

F	-6.504914000	2.078042000	0.266229000	H	4.983436000	0.007134000	-1.211872000
F	-9.020349000	1.758642000	-3.673010000	H	4.174083000	0.411586000	-2.711092000
F	-8.222384000	-0.608306000	1.211206000	H	3.258875000	-0.313553000	-1.396347000
F	-7.043703000	-0.767910000	5.731738000	C	1.310000000	-1.784947000	2.254677000
C	3.415495000	-2.696836000	0.149462000	C	0.920021000	-2.798034000	3.140937000
H	3.759292000	-3.264446000	1.016214000	C	1.926133000	-0.654489000	2.804251000
H	3.569134000	-1.630711000	0.354624000	C	1.179899000	-2.718801000	4.504301000
P	4.667491000	-3.058610000	-1.192221000	C	2.202720000	-0.560796000	4.169925000
C	6.353795000	-2.917006000	-0.231226000	C	1.837412000	-1.598636000	5.016608000
C	6.687405000	-1.444341000	0.056291000	H	0.382689000	-3.658445000	2.752728000
C	7.516038000	-3.535753000	-1.024120000	H	0.864405000	-3.520821000	5.164589000
H	7.443212000	-4.621626000	-1.108567000	H	2.687758000	0.337239000	4.538524000
H	7.625543000	-3.111684000	-2.024213000	H	2.047527000	-1.524113000	6.079667000
H	8.442650000	-3.319797000	-0.480228000	O	2.277909000	0.438286000	2.057736000
H	6.944754000	-0.874036000	-0.837476000	C	1.037586000	-1.859401000	0.768801000
H	7.573469000	-1.435466000	0.702267000	C	1.227127000	-0.520771000	0.142336000
H	5.899040000	-0.914211000	0.591830000	C	1.861373000	0.517867000	0.750627000
C	4.520080000	-1.693510000	-2.561238000	O	2.129601000	1.633626000	0.158179000
C	3.347113000	-2.011869000	-3.503030000	H	0.867375000	-0.347624000	-0.866003000
C	5.806913000	-1.590742000	-3.395681000	H	0.008062000	-2.215175000	0.623337000
H	6.658550000	-1.236803000	-2.812913000	B	2.670788000	3.022187000	0.594266000
H	6.084157000	-2.524143000	-3.889677000	C	3.414114000	3.536832000	-0.774953000
H	5.632258000	-0.847164000	-4.181495000	C	4.766779000	3.904046000	-0.832959000
H	3.519509000	-2.889317000	-4.129410000	C	2.758143000	3.601986000	-2.004501000
H	3.227243000	-1.155048000	-4.175405000	C	5.418265000	4.287390000	-2.007765000
H	2.400241000	-2.128479000	-2.969934000	C	3.344983000	3.964521000	-3.210159000
C	4.459673000	-4.836299000	-1.938215000	C	4.690874000	4.304215000	-3.186141000
C	5.351718000	-5.013266000	-3.179062000	H	5.340569000	3.899306000	0.089172000
C	3.005199000	-5.110974000	-2.362863000	H	6.465642000	4.571021000	-2.014350000
H	2.331650000	-5.206900000	-1.514280000	H	2.773303000	3.996010000	-4.130647000
H	2.595412000	-4.378032000	-3.055176000	C	3.739892000	2.956376000	1.833542000
H	2.998316000	-6.078887000	-2.877860000	C	3.732290000	3.900281000	2.873970000
H	5.019341000	-4.401924000	-4.020555000	C	4.774470000	2.027286000	1.926588000
H	5.275906000	-6.060082000	-3.495329000	C	4.662216000	3.914910000	3.915531000
H	6.406790000	-4.808388000	-2.996330000	C	5.727473000	1.977260000	2.934888000
C	6.248189000	-3.616301000	1.139900000	C	5.649910000	2.943343000	3.929213000
H	5.631440000	-3.050761000	1.841706000	H	2.955113000	4.658764000	2.871441000
H	5.877480000	-4.640239000	1.101471000	H	4.625363000	4.659806000	4.703446000
H	7.257795000	-3.650917000	1.564876000	H	6.502524000	1.219743000	2.947477000
C	4.827641000	-5.892458000	-0.882783000	C	1.362588000	3.905998000	1.038260000
H	4.235464000	-5.786329000	0.029893000	C	0.409241000	3.353959000	1.915172000
H	4.597949000	-6.877021000	-1.307147000	C	1.097850000	5.225539000	0.664885000
H	5.889923000	-5.894527000	-0.633260000	C	-0.720417000	4.036943000	2.366602000
C	4.222477000	-0.334075000	-1.909775000	C	-0.015532000	5.956743000	1.075124000

C	-0.916419000	5.339722000	1.927390000
H	0.573638000	2.344249000	2.281515000
H	-1.428837000	3.586684000	3.054674000
H	-0.161587000	6.978263000	0.743465000
F	1.960310000	5.884802000	-0.137993000
F	-1.997472000	6.025887000	2.341388000
F	1.430842000	3.299771000	-2.066984000
F	5.291004000	4.657524000	-4.341626000
F	4.884217000	1.066805000	0.960697000
F	6.560318000	2.923639000	4.922269000
C	-1.595624000	2.423780000	-1.202172000
H	-0.679751000	2.952398000	-0.953188000
C	-2.285665000	1.762393000	-0.235956000
H	-1.970841000	1.753398000	0.798978000
C	-3.461636000	1.021654000	-0.575516000
O	-4.090484000	0.354370000	0.274901000
O	-3.885650000	1.008519000	-1.842873000
C	-2.068395000	2.419577000	-2.555893000
C	-3.244951000	1.704276000	-2.832602000
C	-1.436919000	3.095623000	-3.617976000
C	-3.809472000	1.655029000	-4.103452000
C	-1.985418000	3.054596000	-4.888360000
C	-3.169992000	2.340056000	-5.127704000
H	-0.516602000	3.633497000	-3.416043000
H	-1.500053000	3.580749000	-5.704494000
H	-3.596229000	2.320623000	-6.126284000
H	-4.727613000	1.098098000	-4.256841000

III_TS₃

C	-0.850257000	-3.035845000	0.577344000
O	-0.915696000	-3.779083000	1.539766000
O	-1.838076000	-2.836151000	-0.287988000
C	-3.099358000	-3.474103000	0.000913000
H	-2.984195000	-4.560068000	-0.026398000
H	-3.462221000	-3.162706000	0.981847000
H	-3.777614000	-3.129611000	-0.777228000
C	0.345560000	-2.172257000	0.216193000
H	0.329446000	-2.073509000	-0.871356000
B	-5.358085000	0.648951000	0.145897000
C	-5.549507000	-0.389217000	1.394008000
C	-6.805938000	-0.882281000	1.759497000
C	-4.501730000	-0.796185000	2.233909000
C	-7.043044000	-1.731986000	2.834613000
C	-4.677173000	-1.641982000	3.333244000

C	-5.955399000	-2.100994000	3.612227000
H	-3.504814000	-0.414174000	2.032421000
H	-8.044375000	-2.080525000	3.059440000
H	-3.850222000	-1.927215000	3.975492000
C	-5.705602000	-0.006204000	-1.301157000
C	-5.618174000	0.730044000	-2.484720000
C	-6.123787000	-1.332027000	-1.472294000
C	-5.909678000	0.237669000	-3.750142000
C	-6.429720000	-1.890581000	-2.717080000
C	-6.319866000	-1.086338000	-3.840497000
H	-6.223988000	-1.960438000	-0.591652000
H	-5.826688000	0.866513000	-4.628993000
H	-6.766625000	-2.917201000	-2.818505000
C	-6.135785000	2.044776000	0.489126000
C	-7.385263000	2.415218000	-0.010758000
C	-5.584483000	2.952461000	1.409111000
C	-8.055716000	3.585053000	0.335561000
C	-6.206862000	4.139173000	1.792689000
C	-7.444650000	4.436103000	1.241551000
H	-4.616356000	2.716202000	1.841134000
H	-9.023657000	3.816479000	-0.093434000
H	-5.752835000	4.821698000	2.503644000
F	-7.882382000	-0.530775000	1.027428000
F	-6.153292000	-2.921715000	4.663912000
F	-5.191900000	2.010147000	-2.422301000
F	-6.612259000	-1.594357000	-5.055854000
F	-8.023194000	1.618147000	-0.893604000
F	-8.073911000	5.576576000	1.592300000
C	1.681420000	-2.736319000	0.719298000
H	1.542435000	-3.105975000	1.739562000
H	2.395310000	-1.907595000	0.779311000
P	2.695492000	-4.069966000	-0.143781000
C	4.418753000	-3.852346000	0.745066000
C	5.185356000	-2.651906000	0.165775000
C	5.305676000	-5.098351000	0.599211000
H	4.916517000	-5.968836000	1.130017000
H	5.490376000	-5.372228000	-0.441788000
H	6.278586000	-4.862526000	1.044527000
H	5.525301000	-2.804781000	-0.858586000
H	6.084115000	-2.521498000	0.779113000
H	4.643389000	-1.708368000	0.226310000
C	2.836179000	-3.702038000	-2.036004000
C	1.565383000	-4.158625000	-2.773649000
C	4.042938000	-4.430822000	-2.650971000

H	4.998297000	-4.063998000	-2.274559000	B	4.064456000	2.477683000	0.040190000
H	4.007174000	-5.512824000	-2.516080000	C	4.987359000	1.666403000	-1.036354000
H	4.031329000	-4.238313000	-3.729659000	C	6.189207000	1.024061000	-0.703467000
H	1.472230000	-5.244939000	-2.822932000	C	4.641784000	1.582146000	-2.388482000
H	1.636911000	-3.795078000	-3.804694000	C	6.976284000	0.332930000	-1.627538000
H	0.645804000	-3.740671000	-2.355703000	C	5.377218000	0.903124000	-3.354191000
C	1.982123000	-5.844801000	0.184513000	C	6.548510000	0.281009000	-2.945679000
C	2.756388000	-6.904729000	-0.620062000	H	6.536240000	1.081349000	0.324362000
C	0.495643000	-5.962449000	-0.197558000	H	7.910859000	-0.139747000	-1.343499000
H	-0.144101000	-5.427700000	0.500597000	H	5.058954000	0.885137000	-4.390270000
H	0.266985000	-5.646338000	-1.213854000	C	4.574602000	2.275201000	1.574625000
H	0.233466000	-7.024863000	-0.127927000	C	5.105085000	3.338597000	2.325314000
H	2.542026000	-6.845135000	-1.689561000	C	4.595852000	1.053356000	2.243620000
H	2.408817000	-7.888185000	-0.283771000	C	5.614706000	3.195434000	3.615883000
H	3.836190000	-6.879667000	-0.477740000	C	5.079018000	0.837542000	3.525878000
C	4.192928000	-3.560617000	2.243109000	C	5.595333000	1.937516000	4.197903000
H	3.781056000	-2.564035000	2.409813000	H	5.111406000	4.327505000	1.878876000
H	3.567821000	-4.293588000	2.753608000	H	6.018416000	4.038921000	4.165553000
H	5.175617000	-3.581398000	2.727704000	H	5.051460000	-0.141870000	3.988491000
C	2.072180000	-6.157220000	1.687766000	C	3.862472000	4.037578000	-0.353348000
H	1.536452000	-5.422053000	2.294685000	C	2.614543000	4.678925000	-0.362562000
H	1.576675000	-7.120668000	1.852931000	C	4.939276000	4.856171000	-0.700934000
H	3.094751000	-6.257199000	2.054356000	C	2.442202000	6.019370000	-0.706071000
C	2.984593000	-2.189361000	-2.266632000	C	4.832325000	6.196756000	-1.052164000
H	3.823167000	-1.729545000	-1.747724000	C	3.564046000	6.758292000	-1.052080000
H	3.148445000	-2.033696000	-3.338393000	H	1.732980000	4.106435000	-0.089445000
H	2.074537000	-1.647424000	-2.010319000	H	1.464082000	6.488327000	-0.709486000
C	0.288091000	-0.448904000	2.226931000	H	5.708500000	6.777651000	-1.315327000
C	-0.361206000	-1.194115000	3.224154000	F	6.188951000	4.338436000	-0.682113000
C	1.044989000	0.640529000	2.667772000	F	3.428327000	8.053127000	-1.390506000
C	-0.237299000	-0.879552000	4.574049000	F	3.516775000	2.194030000	-2.825141000
C	1.177145000	0.979635000	4.011346000	F	7.281287000	-0.387103000	-3.858637000
C	0.532433000	0.212699000	4.972078000	F	4.076856000	-0.053444000	1.616023000
H	-0.980734000	-2.036318000	2.943076000	F	6.076457000	1.765646000	5.441668000
H	-0.758276000	-1.480767000	5.312955000	C	-0.437769000	1.479941000	-1.001731000
H	1.785706000	1.838822000	4.271961000	H	0.238834000	2.330047000	-1.075339000
H	0.625723000	0.471453000	6.022334000	C	-1.614836000	1.654458000	-0.216148000
O	1.733346000	1.476440000	1.801844000	H	-1.633717000	2.332052000	0.628554000
C	0.090967000	-0.700096000	0.740148000	C	-2.792009000	0.966871000	-0.484350000
C	0.862044000	0.292386000	-0.103001000	O	-3.830396000	1.065085000	0.242421000
C	1.800044000	1.170680000	0.506370000	O	-2.875767000	0.134165000	-1.556355000
O	2.632067000	1.799665000	-0.201977000	C	-0.670454000	0.797517000	-2.292055000
H	1.281814000	-0.097408000	-1.022226000	C	-1.882271000	0.129372000	-2.495528000
H	-0.980037000	-0.510685000	0.540716000	C	0.275071000	0.780738000	-3.330315000

C	-2.154749000	-0.558168000	-3.679269000
C	0.013914000	0.109615000	-4.517935000
C	-1.201147000	-0.565742000	-4.687955000
H	1.217499000	1.304854000	-3.190911000
H	0.747625000	0.121436000	-5.318721000
H	-1.412340000	-1.083709000	-5.619203000
H	-3.119491000	-1.042009000	-3.790768000

III_IM₅

C	-0.683443000	-3.165554000	0.616166000
O	-0.669956000	-3.908703000	1.582025000
O	-1.702139000	-3.030998000	-0.219021000
C	-2.923499000	-3.725748000	0.108683000
H	-2.756482000	-4.805063000	0.091699000
H	-3.279285000	-3.414112000	1.092063000
H	-3.633305000	-3.424664000	-0.658661000
C	0.451093000	-2.231512000	0.220825000
H	0.422810000	-2.162760000	-0.869703000
B	-5.280231000	0.642067000	0.098940000
C	-5.371682000	-0.526356000	1.247894000
C	-6.559215000	-1.190659000	1.571444000
C	-4.286704000	-0.857250000	2.074456000
C	-6.692382000	-2.137473000	2.582285000
C	-4.359752000	-1.788585000	3.115518000
C	-5.571229000	-2.422523000	3.346764000
H	-3.345616000	-0.338594000	1.913535000
H	-7.645266000	-2.617488000	2.773295000
H	-3.508542000	-2.003762000	3.753576000
C	-5.658132000	0.136522000	-1.403231000
C	-5.606127000	1.004052000	-2.496512000
C	-6.035370000	-1.174502000	-1.721956000
C	-5.895414000	0.647505000	-3.808518000
C	-6.340581000	-1.597245000	-3.018916000
C	-6.266731000	-0.667978000	-4.045716000
H	-6.098479000	-1.904627000	-0.920512000
H	-5.837345000	1.373290000	-4.611338000
H	-6.648332000	-2.615827000	-3.233609000
C	-6.140669000	1.934841000	0.616329000
C	-7.451719000	2.231792000	0.241059000
C	-5.591270000	2.818232000	1.560203000
C	-8.186203000	3.308353000	0.731710000
C	-6.276085000	3.912862000	2.085967000
C	-7.575646000	4.138596000	1.657103000
H	-4.571393000	2.640499000	1.888517000

H	-9.200509000	3.486963000	0.394228000
H	-5.821945000	4.579981000	2.811542000
F	-7.675982000	-0.918579000	0.866234000
F	-5.669607000	-3.330883000	4.340440000
F	-5.227996000	2.284800000	-2.295090000
F	-6.557143000	-1.046217000	-5.309177000
F	-8.088613000	1.455234000	-0.661191000
F	-8.266911000	5.189509000	2.147865000
C	1.816601000	-2.704223000	0.740549000
H	1.687770000	-3.055892000	1.768362000
H	2.488431000	-1.840994000	0.788198000
P	2.909606000	-4.008151000	-0.070407000
C	4.583624000	-3.710034000	0.889911000
C	5.319195000	-2.476409000	0.340149000
C	5.531740000	-4.914986000	0.786056000
H	5.162508000	-5.798917000	1.309054000
H	5.766382000	-5.185883000	-0.245476000
H	6.475786000	-4.633017000	1.265331000
H	5.689366000	-2.604188000	-0.676866000
H	6.196993000	-2.318978000	0.977252000
H	4.739743000	-1.555105000	0.396457000
C	3.119190000	-3.648424000	-1.957394000
C	1.915256000	-4.179679000	-2.754091000
C	4.392792000	-4.314002000	-2.507424000
H	5.308800000	-3.887053000	-2.098500000
H	4.413818000	-5.394419000	-2.356512000
H	4.415753000	-4.138187000	-3.588682000
H	1.887754000	-5.269705000	-2.803367000
H	2.016424000	-3.813237000	-3.781511000
H	0.954103000	-3.812675000	-2.386394000
C	2.257411000	-5.809960000	0.237364000
C	3.119855000	-6.834306000	-0.522606000
C	0.799201000	-6.003842000	-0.219618000
H	0.097117000	-5.513061000	0.450031000
H	0.603219000	-5.694235000	-1.244506000
H	0.594119000	-7.079722000	-0.168353000
H	2.948502000	-6.792949000	-1.600657000
H	2.808896000	-7.831803000	-0.192057000
H	4.189543000	-6.752543000	-0.335075000
C	4.286650000	-3.426237000	2.377009000
H	3.831971000	-2.445395000	2.525180000
H	3.668312000	-4.180633000	2.864016000
H	5.248954000	-3.410879000	2.900965000
C	2.288152000	-6.107739000	1.745453000

H	1.689475000	-5.392984000	2.316833000	C	4.887030000	1.192384000	3.525784000
H	1.829677000	-7.091785000	1.895497000	C	5.285503000	2.344057000	4.191984000
H	3.295849000	-6.159117000	2.160588000	H	4.698475000	4.644545000	1.805864000
C	3.190993000	-2.130802000	-2.193403000	H	5.536521000	4.472196000	4.131682000
H	3.939806000	-1.608805000	-1.600019000	H	4.920455000	0.223124000	4.008836000
H	3.453671000	-1.971562000	-3.244759000	C	3.559624000	4.189024000	-0.488480000
H	2.220964000	-1.654510000	-2.044930000	C	2.267677000	4.723714000	-0.606876000
C	0.278185000	-0.474333000	2.191575000	C	4.590625000	5.076735000	-0.804796000
C	-0.297246000	-1.254777000	3.207455000	C	2.015694000	6.031448000	-1.019662000
C	0.914361000	0.693691000	2.614044000	C	4.403191000	6.389169000	-1.219798000
C	-0.219298000	-0.890029000	4.548488000	C	3.097084000	6.845263000	-1.324371000
C	0.998862000	1.088975000	3.943985000	H	1.414840000	4.094054000	-0.371699000
C	0.425088000	0.288162000	4.922142000	H	1.006135000	6.417925000	-1.107890000
H	-0.824072000	-2.164267000	2.949185000	H	5.246596000	7.028587000	-1.452366000
H	-0.681701000	-1.522472000	5.300104000	F	5.871647000	4.658226000	-0.685150000
H	1.516177000	2.011965000	4.182081000	F	2.883785000	8.110097000	-1.725906000
H	0.477718000	0.585435000	5.964772000	F	3.316061000	2.041888000	-2.848191000
O	1.555138000	1.560604000	1.728606000	F	7.392133000	-0.080653000	-3.726723000
C	0.100108000	-0.772836000	0.711327000	F	4.026590000	0.189849000	1.600149000
C	0.772944000	0.272788000	-0.195422000	F	5.729955000	2.235692000	5.455318000
C	1.661156000	1.252270000	0.454365000	C	-0.334970000	1.100192000	-1.105888000
O	2.477856000	1.870352000	-0.254379000	H	0.236387000	1.965127000	-1.463749000
H	1.410076000	-0.197610000	-0.944366000	C	-1.546184000	1.498809000	-0.360616000
H	-0.977640000	-0.651449000	0.523005000	H	-1.523677000	2.347896000	0.312216000
B	3.875680000	2.673625000	-0.022092000	C	-2.746063000	0.857818000	-0.502552000
C	4.858800000	1.876642000	-1.047999000	O	-3.806409000	1.160431000	0.156876000
C	6.136184000	1.426059000	-0.680656000	O	-2.884621000	-0.196367000	-1.377365000
C	4.518310000	1.633417000	-2.382332000	C	-0.691689000	0.239711000	-2.289479000
C	7.003649000	0.771603000	-1.556711000	C	-1.944525000	-0.375144000	-2.348233000
C	5.335439000	0.981024000	-3.299808000	C	0.194641000	0.041655000	-3.357253000
C	6.581491000	0.556937000	-2.860336000	C	-2.305105000	-1.192519000	-3.422771000
H	6.475208000	1.611255000	0.334559000	C	-0.149853000	-0.768852000	-4.434176000
H	7.992387000	0.448398000	-1.248248000	C	-1.402257000	-1.392061000	-4.458791000
H	5.017678000	0.834775000	-4.325832000	H	1.154856000	0.554436000	-3.341939000
C	4.344661000	2.548761000	1.528512000	H	0.540382000	-0.894270000	-5.263698000
C	4.755515000	3.667196000	2.273615000	H	-1.687378000	-2.012542000	-5.303857000
C	4.438156000	1.344037000	2.222454000	H	-3.301717000	-1.622687000	-3.434636000
C	5.224431000	3.589030000	3.584762000				

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