Supporting information

Free Radical Copolymerization of 1,3-Cyclooctadiene with Maleic Anhydride or *N*-Substituted Maleimides: A Simple Way to High-Performance Transparent Plastic

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1. Experimental

Materials. 1,3-cyclooctadiene (COD) was purchased from TCI (Shanghai) and passed through an alkaline aluminum oxide (Al_2O_3) column without further purification before use. Maleic anhydride (MA) was purchased from Sinopharm Chemical Reagent Co., Ltd. and sublimated once before use. All *N*-substituted maleimides (maleimide, MI; *N*-methyl maleimide, Me; *N*-ethyl maleimide, Et; *N*-propyl maleimide, Pr; *N*-tert-butyl maleimide, ^{t}Bu; *N*-hexyl maleimide, Hex; *N*-dodecyl maleimide, Doc; *N*-cyclohexyl maleimide, Cy; *N*-phenyl maleimide, Ph; *N*-benzyl maleimide, Bn) were purchased from Macklin Biochemical Co., Ltd. and sublimated once before use. 2,2'-azobis(2-methylpropionitrile) (AIBN) was purchased from Macklin Biochemical Co., Ltd. and recrystallization from methanol before use. All solvents (tetrahydrofuran, THF; dichloromethane, CH_2Cl_2; diethyl ether; anhydrous methanol; anhydrous alcohol and dimethyl sulphoxide) were purchased from Sinopharm Chemical Reagent Co., Ltd. and used as received.

Polymer Synthesis and Characterizations. All copolymerization of COD with MA or RMIs were carried out in the glovebox under Ar atmosphere. A 10 mL vial with a magnetic stirrer was first dried in an oven at 110 °C overnight, and then immediately placed into the glovebox. Taken the copolymerization of COD with MA for example, COD, MA, AIBN and THF (2 mL) were added into the reactor. Then, the vial was sealed with a Teflon-lined cap and removed from the glovebox. The reactor was placed in a preheated oil bath at design temperature and stirred for 12 hours. After that, the reactor was transferred to an ice-water bath. To obtain purified copolymer, the crude product was dissolved in THF and then precipitated from an ethanol or diethyl ether

solution for three times. Finally, the obtained polymer was dried in vacuum at 50 °C overnight. The yield of copolymer was determined gravimetrically and was calculated by the formula as Yield = m(product)/m(COD)*M(COD)/M(copolymer)*100 (n(COD)/n(MA) < 1) or Yield = m(product)/m(MA)*M(MA)/M(copolymer)*100 (n(COD)/n(MA) > 1). For poly(COD-*alt*-MA), poly(COD-*alt*-MI), poly(COD-*alt*-Me), poly(COD-*alt*-Et), poly(COD-*alt*-Pr), poly(COD-*alt*-^{t}Bu), poly(COD-*alt*-Cy), poly(COD-*alt*-Ph), poly(COD-*alt*-Bn), poly(COD-*alt*-Hex), poly(COD-*alt*-Doc), the M(copolymer) was 206.1 g/mol, 205.1 g/mol, 219.1 g/mol, 233.1 g/mol, 247.2 g/mol, 261.2 g/mol, 287.2 g/mol, 281.1 g/mol, 295.2 g/mol, 289.2 g/mol, 373.3 g/mol respectively.

^{1}H, and ^{13}C NMR spectra were performed on a Bruker Advance DMX 400 MHz. Chemical shifts values for ^{1}H, and ^{13}C NMR spectra were referenced to internal solvent resonances (to $CDCl_3$ at 7.26 ppm, to CD_3COCD_3 at 2.05 ppm and to CD_3SOCD_3 at 2.50 ppm for ^{1}H NMR; to $CDCl_3$ at 77.06 ppm, to CD_3COCD_3 at 206.03 and 29.82 ppm and to CD_3SOCD_3 at 39.53 ppm for ^{13}C NMR).

The number-average molecular weight (M_n) and dispersity ($Đ = M_w/M_n$) of the resultant copolymers were measured by GPC at 35 °C using a Waters 1515 isocratic pump, a model 2414 differential refractometer GPC instrument with THF as the mobile phase and Waters Styragel HR3 and HR4 7.8×300mm columns. The flow rate of THF was 1.0 mL/min. Linear polystyrene polymers with narrow molar mass distributions were used as standards to calibrate the apparatus.

Matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometric measurements were performed on a Bruker Ultraflex MALDI TOF mass spectrometer, equipped with a nitrogen laser delivering 3 ns laser pulses at 337 nm. trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) or 2,5-dihydroxybenzoic acid (DHB) were used as the matrix.

The decomposition temperature of the polymers was determined by using TA Q50 instrument. The sample was heated from room temperature to 500 °C at a rate of 10 °C/min under nitrogen atmosphere. Temperature when the mass loss is five percent was taken as $T_{d,5\%}$.

Differential scanning calorimetry measurements of polymers were carried out on a TA Q200 instrument with a heating/cooling rate of 10 °C/min. Data reported are from second heating cycles.

The transparency was evaluated by UV–VIS measurement using a SHIMADZU UV-2600i UV–VIS spectrophotometer. The thin films with specific thickness were prepared by the Thermo Universal Film Maker.

2. Supplementary experimental data

Table S1. (co)Polymerization of COD and MA under various reaction conditions.

entry	COD	MA	AIBN	T/ ℃	Solvent	Polymer
1	+	-	+	80	-	-
2	+	+	-	R.T.	-	-
3	+	+	-	60	-	-
4	+	+	-	60	THF	-

Polymerization conditions: n(MA)/n(COD) = 1.5, T = 60 ℃, t = 12 h, 2 mL THF, +/- indicated the presence/ absence of chemical reactant.

Table S2. Copolymerization of MA and COD under different concentrations of AIBN.

entry	n(COD)/n(AIBN)	Yield/ %	M_n/ kDa	$Đ$
1	100	56	9.9	1.80
2	200	41	12.6	1.61
3	400	11	12.4	1.44

Conditions: AIBN as initiator, n(MA)/n(COD) = 1.5, T = 60 ℃, t = 12 h, 2 mL THF.

Table S3. Copolymerization of COD and MA under different temperatures.

entry	n(COD)/n(AIBN)	T/℃	Yield/%	M_n /kDa	$Đ$
1	200	70	73	9.8	1.79
2	200	80	83	10.0	1.68
3	400	70	63	10.7	1.81
4	400	80	69	9.1	1.83
5[a]	200	70	80	31.5	2.54
6[b]	200	70	90	22.0	2.23

Conditions: AIBN as initiator, n(MA)/n(COD) = 1.5, t = 12 h, 2 mL THF, [a] bulk polymerization, [b] 2 mL CH_2Cl_2.

Table S4. Copolymerization of COD with MA under different molar ratio of COD to MA.

entry	n(COD)/n(MA)	Yield/ %	M_n/ kDa	$Đ$
1	0.7	37	6.4	1.78
2	0.8	42	6.5	1.78
3	1.0	66	7.0	1.81
4	1.2	66	8.1	1.85
5	1.5	63	10.7	1.81

Conditions: AIBN as initiator, n(COD)/n(AIBN) = 200, T = 70 °C, t = 12 h, 2 mL THF.

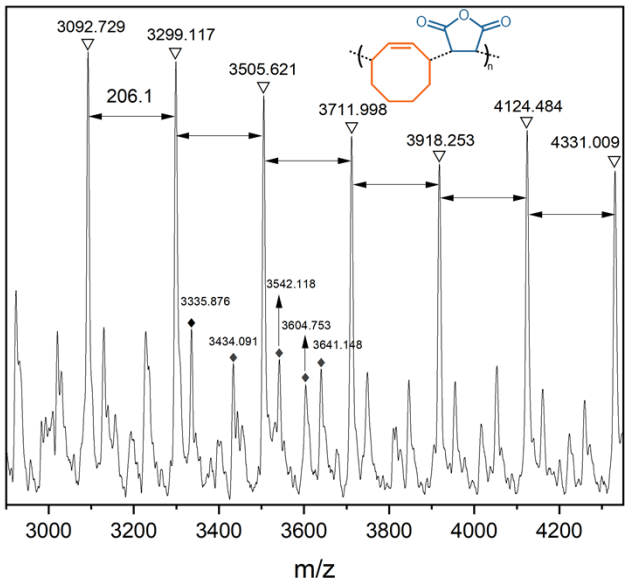


Figure S1. MALDI-TOF MS of copolymer in entry 2, Table S3.

Table S5. Free radical Copolymerization of COD and *N*-substituted maleimides (RMIs).

entry	MI	n(COD)/n(MI)	T/ ℃	Solvent	Yield/ %	M_n / kDa	*Đ*
1	MI	1.5	70	CH_2Cl_2	93	11.1	1.90
2	MI	1.5	70	THF	67	5.3	1.75
3	Me	1.5	80	THF	71	11.9	1.57
4	Ph	1.5	80	THF	80	19.6	5.57
5	Et	1.0	70	THF	63	3.2	2.02
6	Et	1.0	70	CH_2Cl_2	67	8.8	1.68
7	Pr	1.0	70	THF	63	11.0	1.71
8	^{t}Bu	1.0	70	THF	66	9.2	1.68
9	Cy	1.0	70	CH_2Cl_2	61	11.6	1.73
10	Cy	1.0	70	THF	59	4.7	1.81
11	Bn	1.0	70	CH_2Cl_2	64	8.6	1.67
12	Bn	1.0	70	THF	61	14.3	1.78
13	Hex	1.0	70	THF	57	10.0	1.38
14	Doc	1.0	70	THF	55	11.8	1.65

Conditions: AIBN as initiator, n(COD)/n(AIBN) = 200, t = 12 h, solvent: 2 mL.

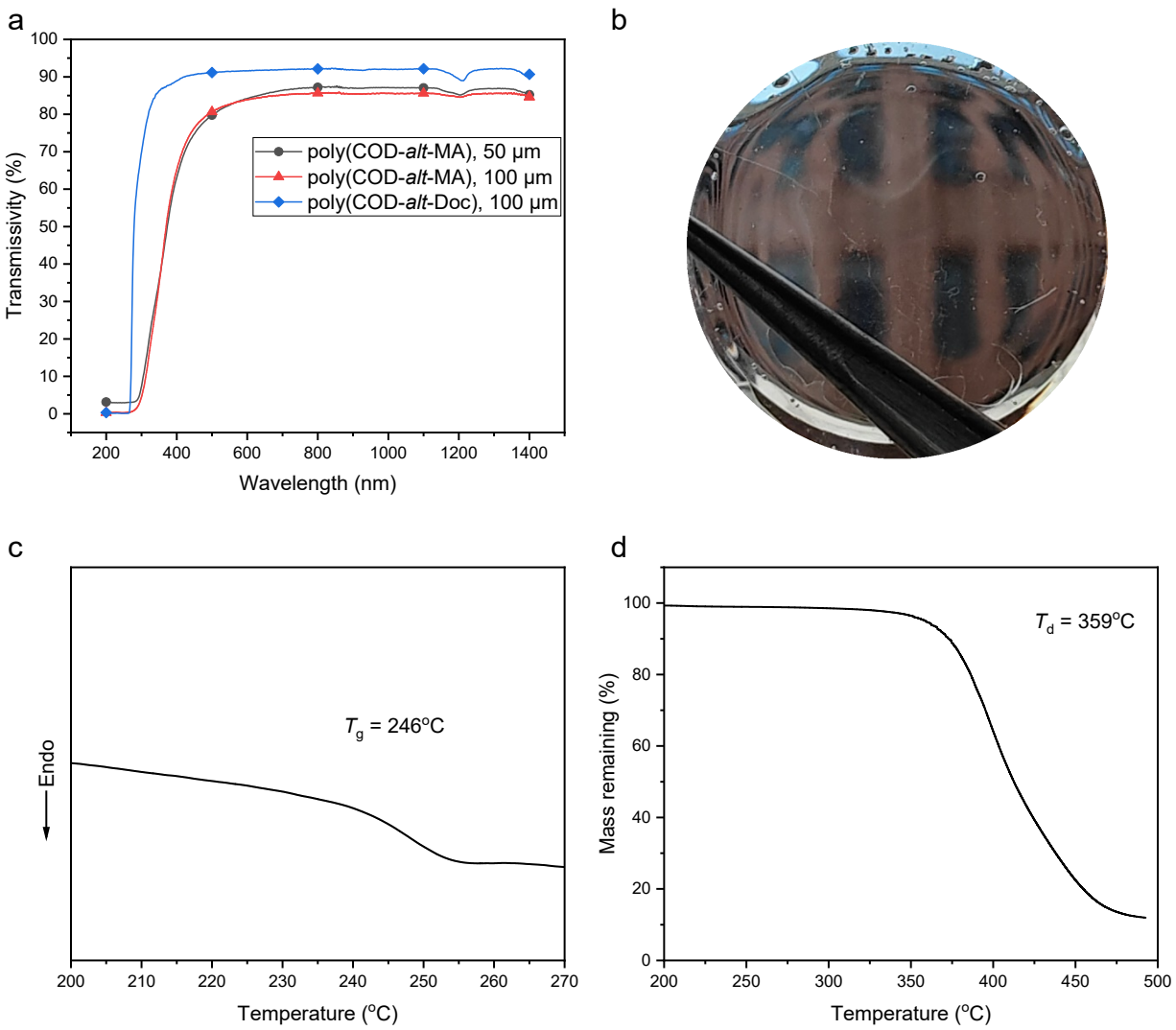
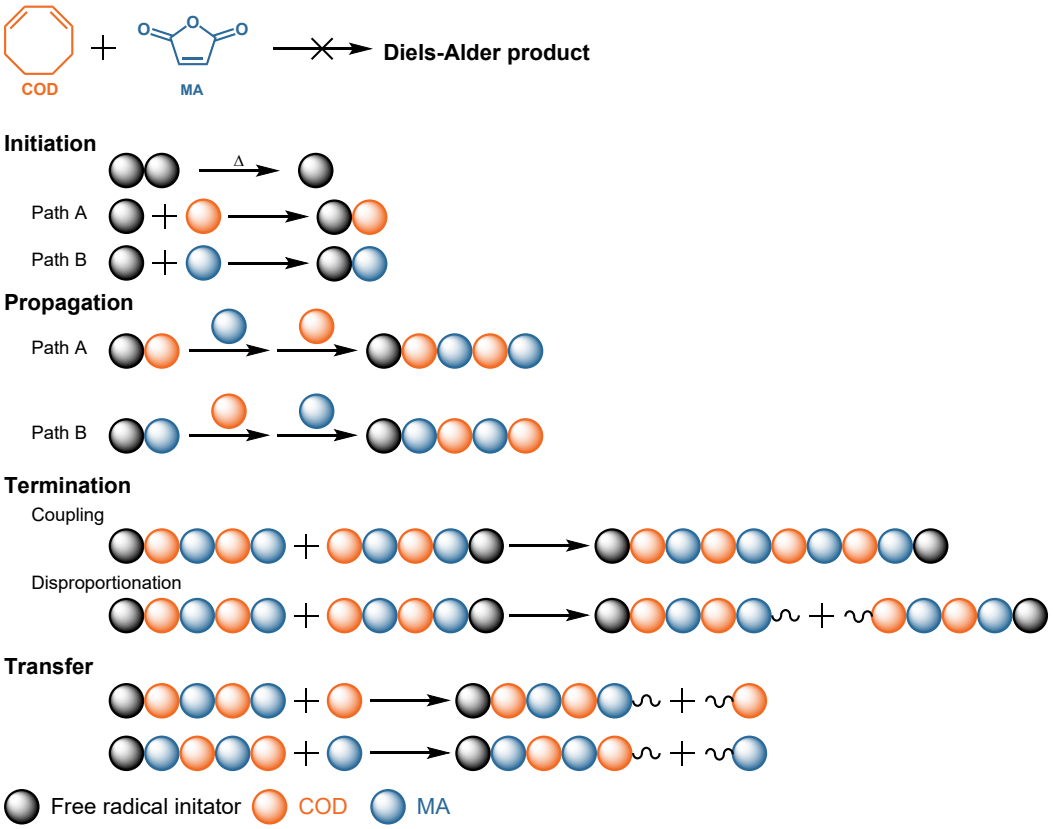


Figure S2. The properties of the obtained alternating copolymer. (a) the transmissivity of alternating copolymer ranged from 200 to 1400 nm wavelength, (b) vision under sunlight of poly(COD-*alt*-MA), (c & d) DSC curve and TGA curve of poly(COD-*alt*-MA), respectively.



Scheme S1. Proposed mechanism of copolymerization between COD and MA by AIBN as initiator (chain transfer to same monomer was ignored).

3. Possible structure of poly(MA-*alt*-COD)

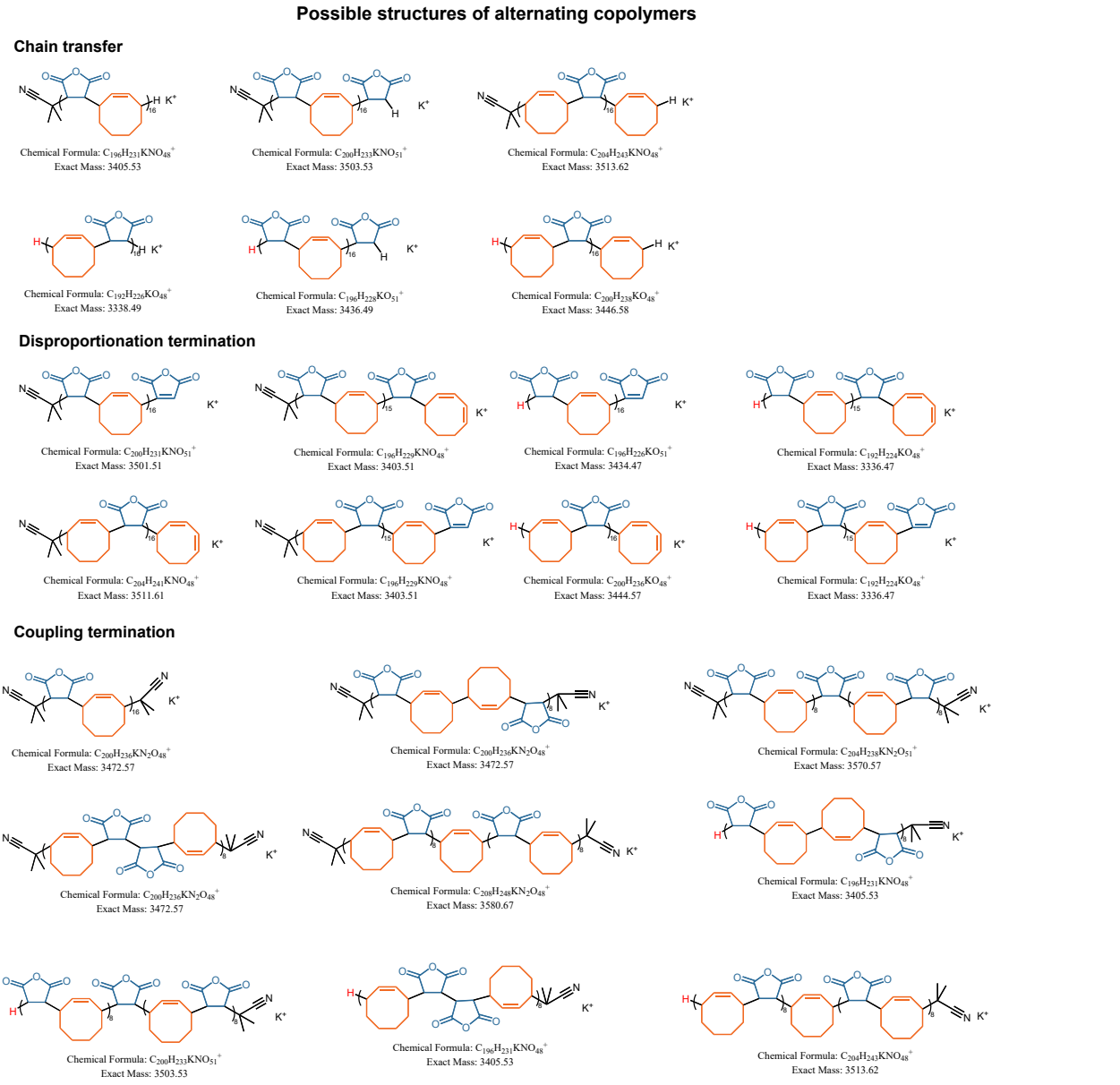
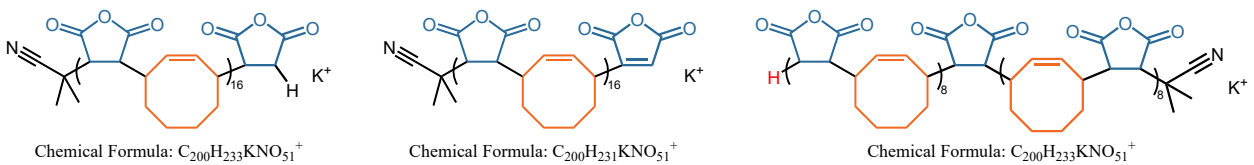


Figure S3. Possible structures of poly(COD-*alt*-MA) copolymer by chain transfer, disproportionation termination and coupling termination.



(*a*) (*b*) (*c*)

Figure S4. Possible structures of prepared poly(COD-*alt*-MA).

4. Computational Details

All DFT calculations were performed using Gaussian 09 program.[1] Calculations were performed using the M06-2X[2]/6-311+G(d,p) level of theory and the ultrafine integration grid.[3] All reactants, intermediates, transition states and products were subjected to geometry optimizations and stationary points were characterized as minima (0 imaginary frequencies for ground states) or first-order saddle points (1 imaginary frequency for transition states). Transition states were verified by performing intrinsic reaction coordinate calculations, followed by geometry optimizations to generate the prereactive and product complexes. The effects of solvation (THF) were included using the CPCM implicit solvent model. The 3D diagrams of molecules were generated by CYLView.[4]

4.1 Computations for DA reaction of cyclic conjugated dienes and maleic anhydride.

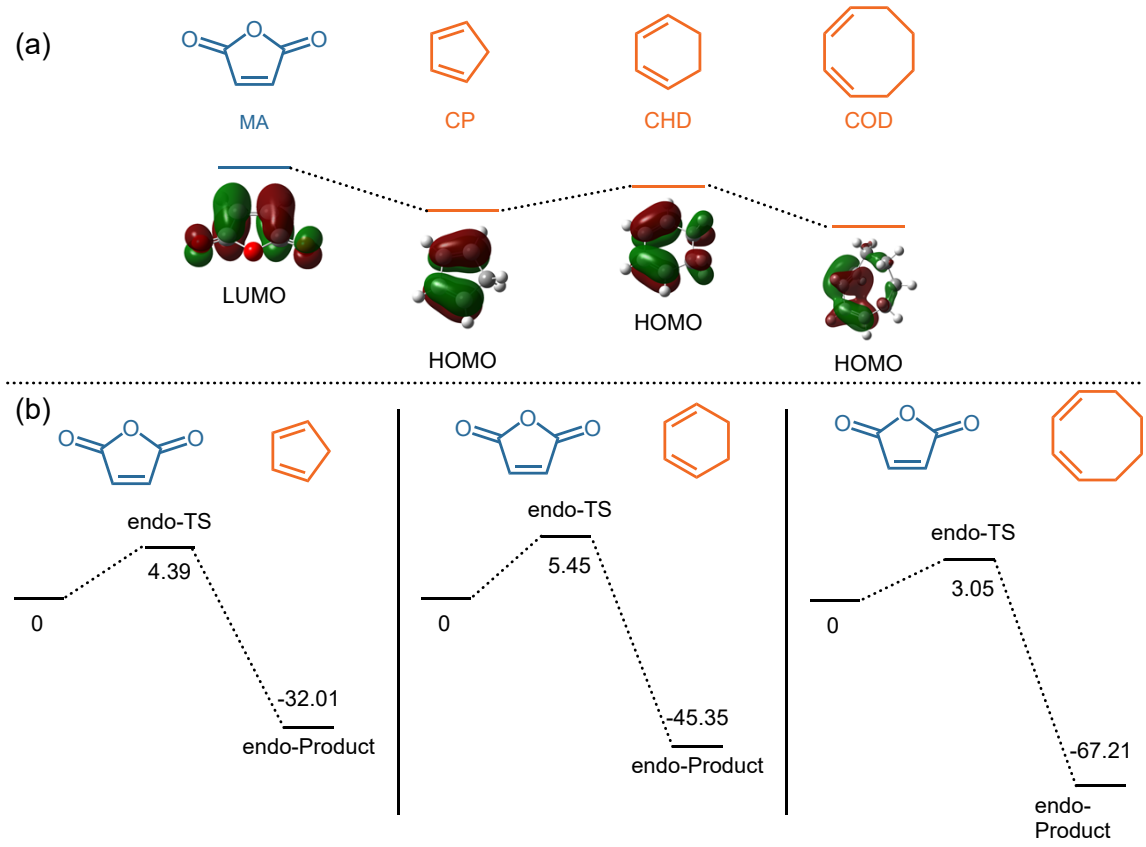


Figure S5. (a), FMOs of MA, CP, CHD and COD; (b), selected transition states of endo-DA products between CP, CHD, COD and MA.

4.1.1 Computations for DA reaction of cyclopentadiene and maleic anhydride.

The IRC (intrinsic reaction coordinate) calculation results.

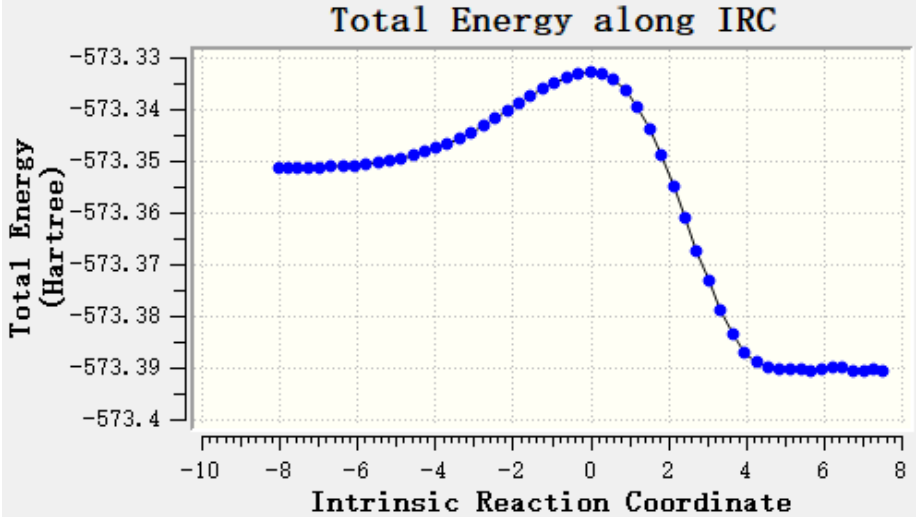


Figure S6. IRC/path for endo-TS in Figure S5.

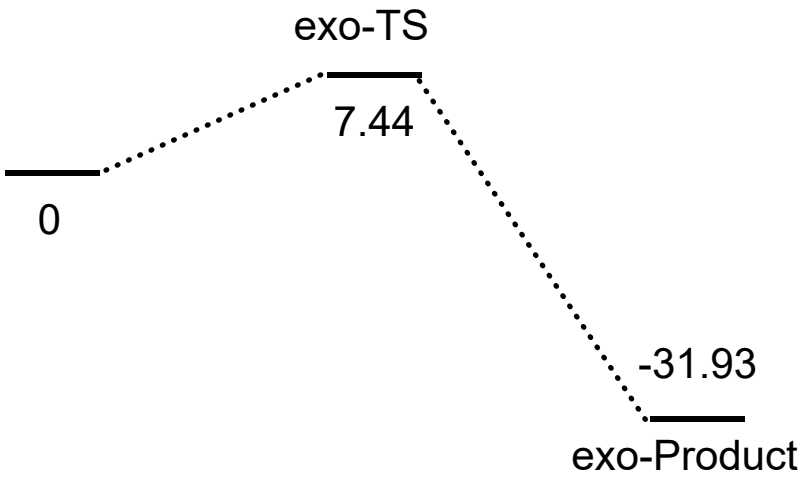


Figure S7. Free energy diagram for exo-DA product of cyclopentadiene and maleic anhydride.

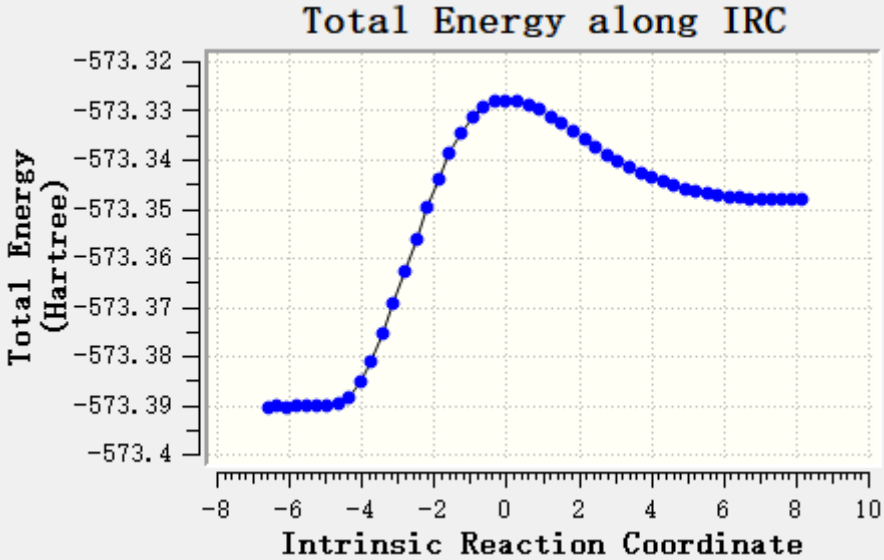


Figure S8. IRC/path for exo-TS in Figure S7.

4.1.2 Computations for DA reaction of cyclohexadiene and maleic anhydride.

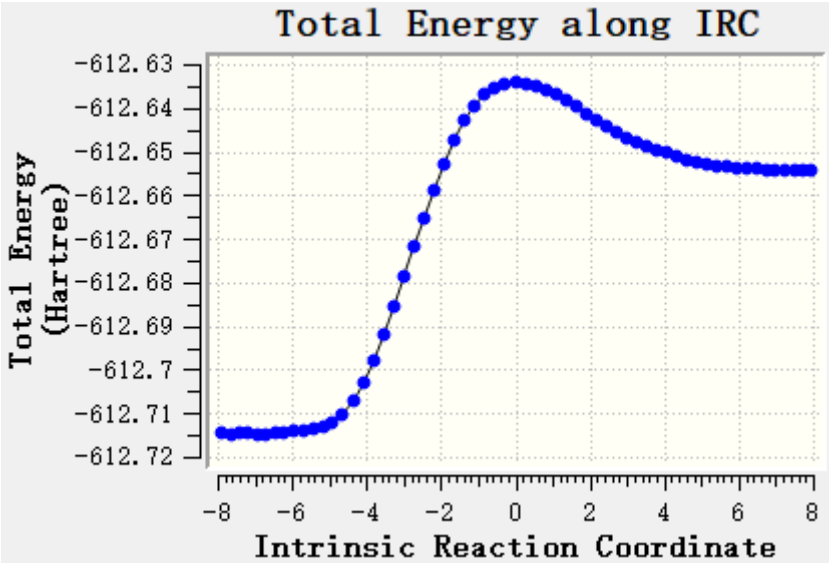


Figure S9**.** IRC/path for endo-TS in Figure S5.

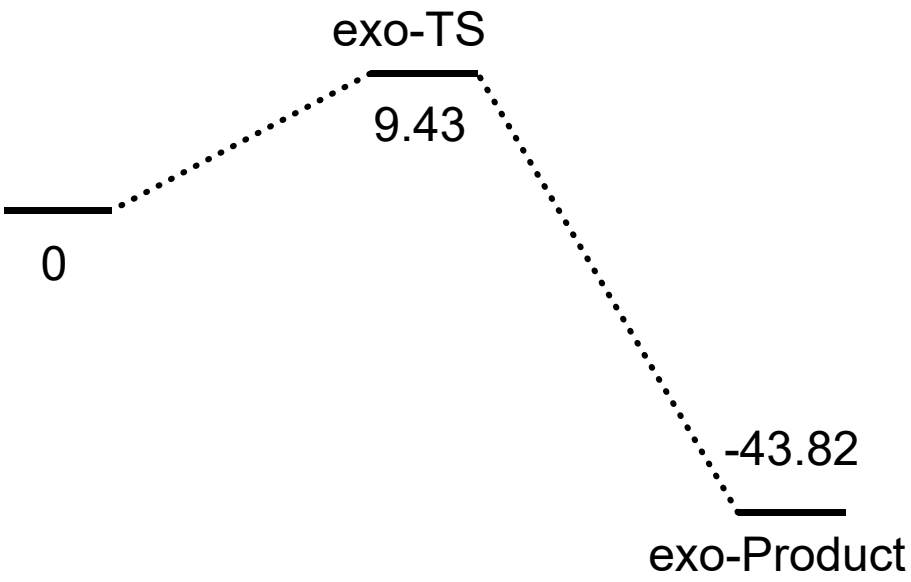


Figure S10. Free energy diagram for exo-DA product of cyclohexadiene and maleic anhydride.

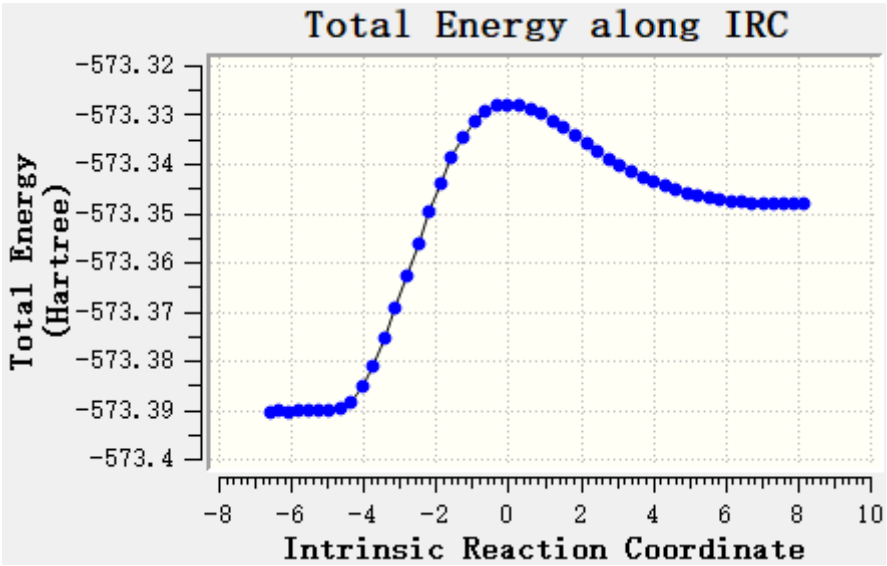


Figure S11 IRC/path for exo-TS in Figure S10.

4.1.3 Computations for DA reaction of cyclooctadiene and maleic anhydride.

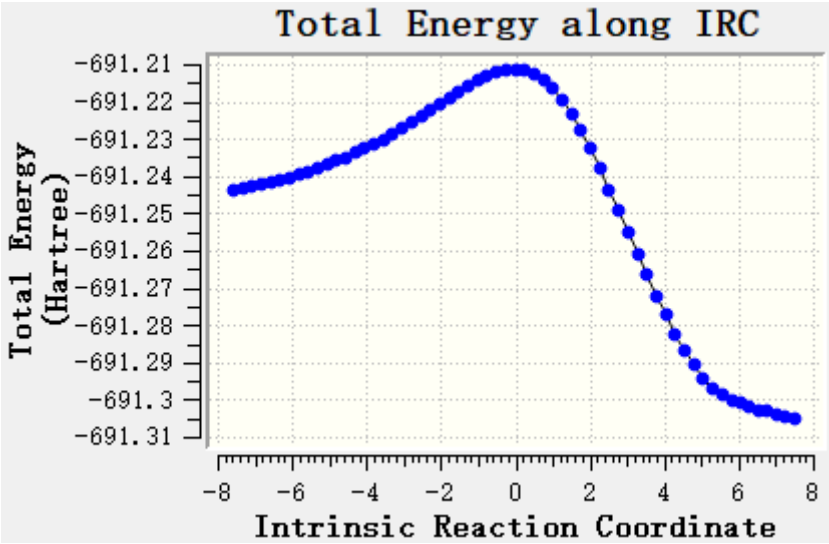


Figure S12. IRC/path for endo-TS in Figure S5.

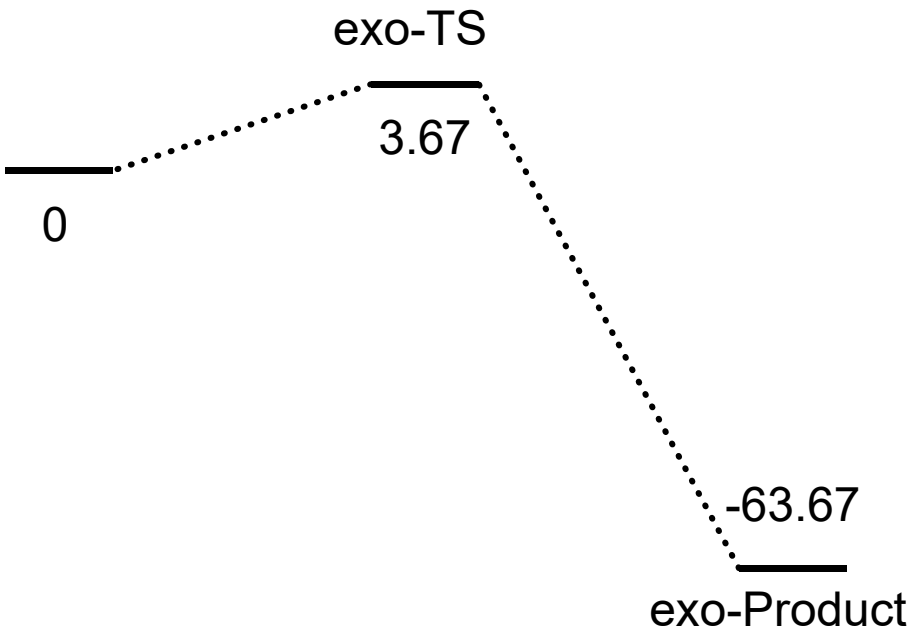


Figure S13. Free energy diagram for exo-DA product of cyclooctadiene and maleic anhydride.

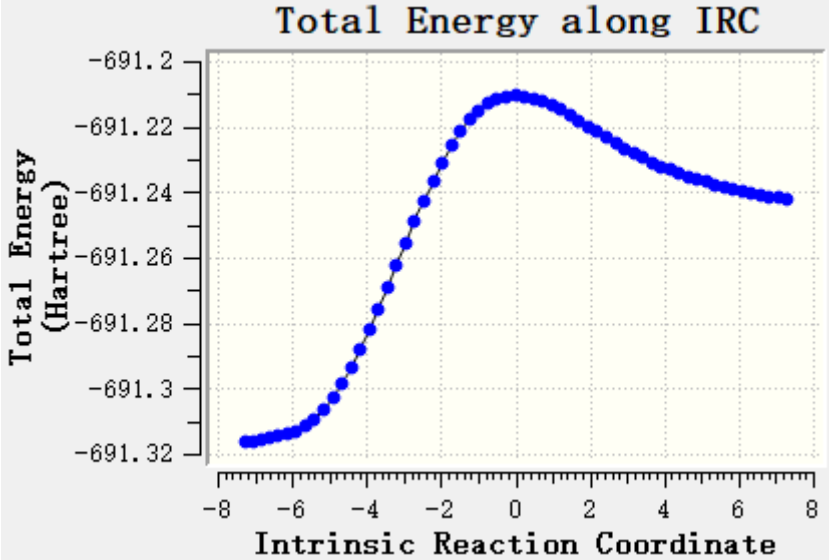


Figure S14. IRC/path for exo-TS in Figure S13.

4.1.4 The IRC (intrinsic reaction coordinate) calculation results for polymerization.

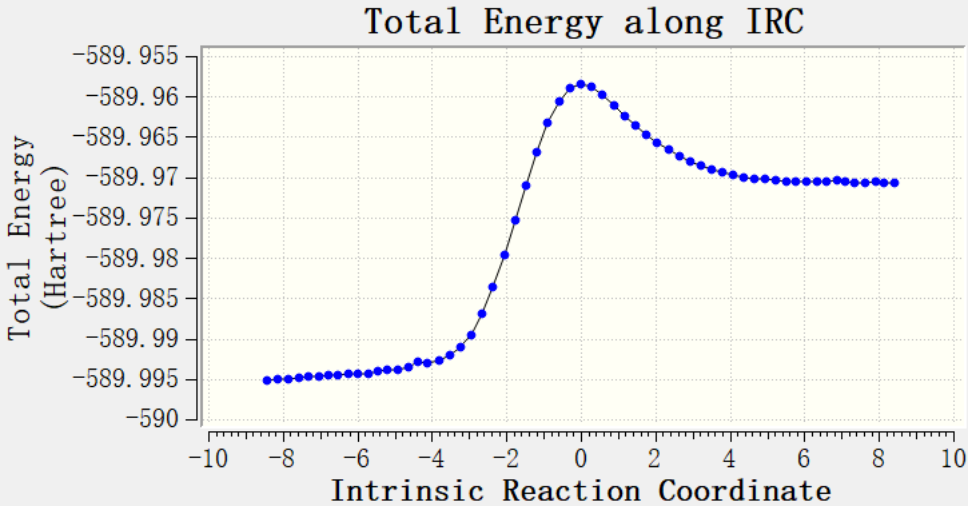


Figure S15. IRC/path for TS1 in Fig. 3.

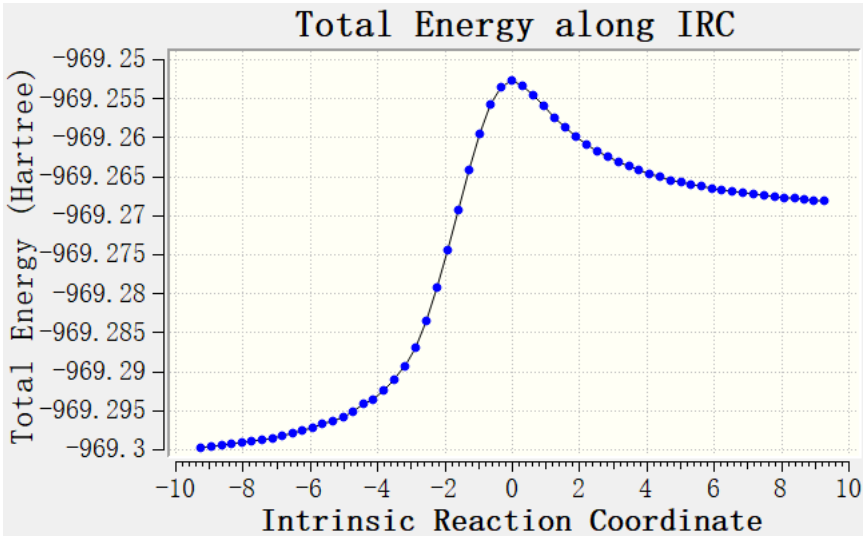


Figure S16. IRC/path for TS2 in Fig. 3.

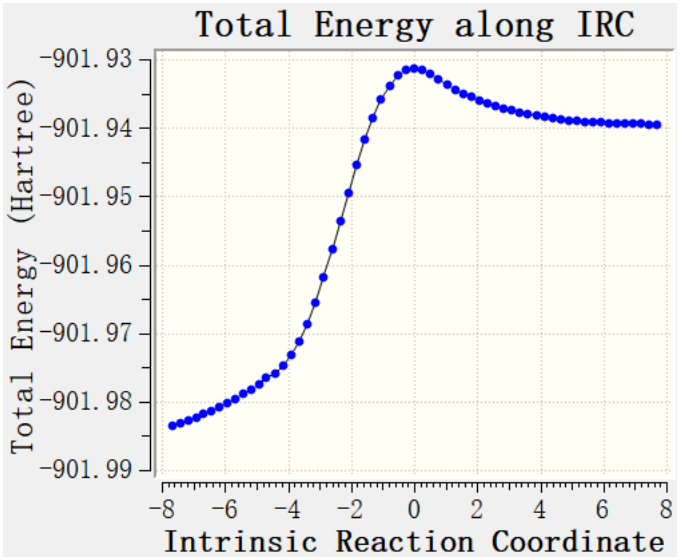


Figure S17. IRC/path for TS3 in Fig. 3.

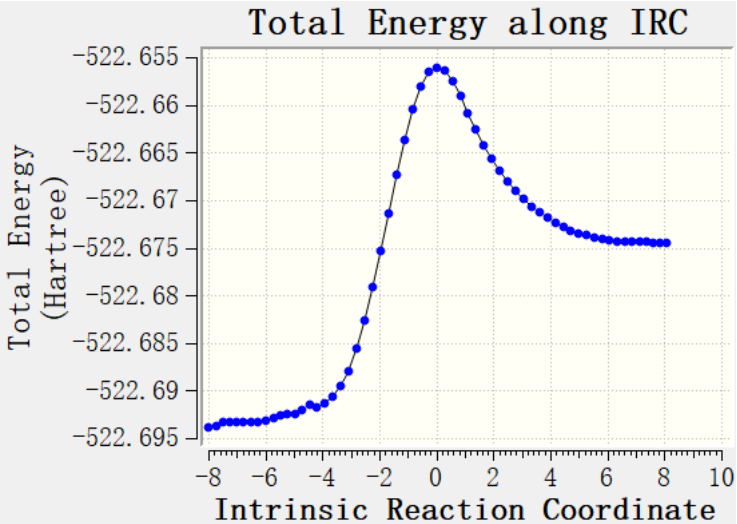


Figure S18. IRC/path for TS4 in Fig. 3.

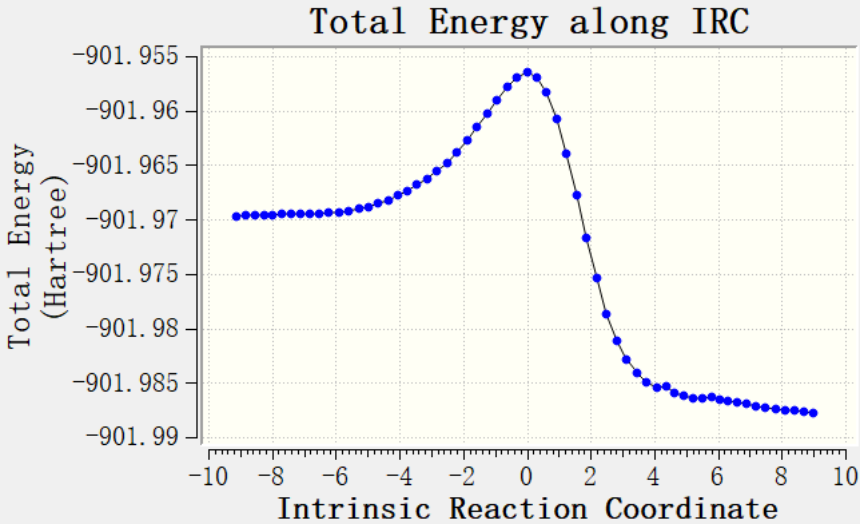


Figure S19. IRC/path for TS5 in Fig. 3.

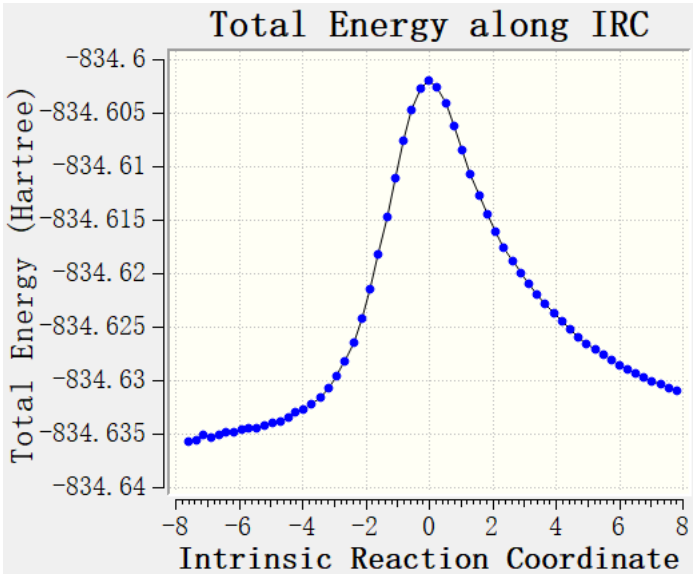


Figure S20. IRC/path for TS6 in Fig. 3.

4.2 Cartesian coordinates of the calculated species

MA

C	0.00103700	1.25997600	0.66384000
C	0.00103700	1.25997600	-0.66384000
H	0.00265600	2.08932200	1.35595800
H	0.00265600	2.08932200	-1.35595800
O	-0.00091000	-0.96305000	0.00000000
C	-0.00037400	-0.15642400	-1.12032200
C	-0.00037400	-0.15642400	1.12032200
O	-0.00037400	-0.60730500	-2.21891200
O	-0.00037400	-0.60730500	2.21891200

CP

C	0.00001900	-1.21375200	0.00019400

H	0.00003200	-1.87345800	-0.87652500
H	0.00002600	-1.87310500	0.87718700
C	1.17547000	-0.28184000	-0.00018900
H	2.20671400	-0.60949900	-0.00028300
C	0.73516300	0.98905000	0.00006100
H	1.34904100	1.88100600	0.00011600
C	-1.17546200	-0.28187600	-0.00020100
H	-2.20669500	-0.60956900	-0.00030300
C	-0.73519400	0.98902800	0.00008000
H	-1.34909700	1.88096700	0.00014500

CHD

C	1.27940600	0.73557700	-0.00002100
C	1.27943300	-0.73553100	0.00005000
C	0.13679900	-1.42477400	0.00000500
C	-1.22288100	-0.77503100	-0.00006900
C	-1.22290900	0.77498700	0.00008000
C	0.13674600	1.42477900	-0.00004700
H	2.23304400	1.25265600	-0.00007600
H	2.23309000	-1.25257500	0.00008700
H	0.15571200	-2.51092100	-0.00001300
H	-1.77416500	-1.14897200	-0.86861400
H	-1.77442200	1.14906300	-0.86825900

H	0.15562000	2.51092700	-0.00012400
H	-1.77430800	-1.14910100	0.86832800
H	-1.77413700	1.14888300	0.86868100

COD

C	-1.87399000	-0.86373700	-0.01682800
C	-1.88663800	0.47066100	0.12418800
C	1.82294600	-0.92521700	0.09665700
C	-0.78054800	1.47478800	-0.20888800
C	1.72138300	0.55216000	-0.38953300
C	0.68145600	1.44679400	0.33234300
H	-0.70974400	1.50288200	-1.30523600
H	2.18721700	-1.55660500	-0.71705700
H	1.46544000	0.53728800	-1.45416700
H	2.51635800	-1.00558800	0.93667100
H	-1.18140000	2.45138300	0.07374900
H	2.70500400	1.02315600	-0.30299000
H	1.03378600	2.47507000	0.20804900
H	0.68707700	1.26150600	1.41066900
C	-0.57909200	-1.48619200	-0.34326600
C	0.42521500	-1.24360800	0.50087600
H	0.14671100	-0.88647200	1.48928800
H	-0.39657000	-1.86205700	-1.35006900

H	-2.79721400	-1.43079000	0.07235600
H	-2.84106800	0.93633400	0.36544500

endo-TS-CPMA

O	-1.72200000	-0.00039100	0.52264800
C	-1.24909300	1.12951600	-0.12742900
C	-1.24852100	-1.12998400	-0.12758300
O	-1.65599100	2.21528100	0.15698700
O	-1.65462800	-2.21604000	0.15686700
C	-0.25401200	-0.69458200	-1.12164700
H	0.02624800	-1.34973000	-1.93255000
C	-0.25404800	0.69496200	-1.12145600
H	0.02546000	1.35040400	-1.93236200
C	1.22711700	-0.69926900	1.26147600
H	0.87885500	-1.32544400	2.07302800
C	1.22693300	0.70023200	1.26105400
H	0.87811400	1.32681800	2.07205100
C	2.25498800	-0.00003200	-0.71433400
C	1.59928300	-1.15254000	-0.00635700
H	1.76549300	-2.19171500	-0.26098500
C	1.59946500	1.15288400	-0.00697600
H	1.76555300	2.19205000	-0.26173900
H	3.31710800	0.00010900	-0.42965300

H	2.19144500	-0.00041000	-1.80029200

endo-CPMA

O	1.87066000	-0.00012100	0.26725300
C	1.20970900	-1.14131200	-0.13923900
C	1.20992700	1.14111000	-0.13915900
O	1.64127600	-2.21759900	0.12718000
O	1.64174700	2.21737600	0.12699600
C	-0.04209500	0.76808200	-0.88868000
H	-0.02227600	1.22026300	-1.87984800
C	-0.04213800	-0.76799400	-0.88883700
H	-0.02233600	-1.22008800	-1.88003600
C	-1.18433700	0.66824300	1.30850800
H	-0.98516100	1.32400600	2.14710800
C	-1.18409100	-0.66800400	1.30842200
H	-0.98486600	-1.32369100	2.14706600
C	-2.26770400	0.00004600	-0.67097600
C	-1.36868000	1.12955000	-0.12685400
H	-1.68854800	2.15723100	-0.27485600
C	-1.36891600	-1.12939000	-0.12684600
H	-1.68876300	-2.15704400	-0.27503900
H	-3.25737900	0.00008600	-0.21355500
H	-2.35018300	0.00001400	-1.76030300

exo-TS-CPMA

C	0.22801700	-0.69491500	-0.98246800
C	0.22774500	0.69428400	-0.98293900
C	-2.44646100	-0.70017700	-0.37806500
H	-3.05493000	-1.32831600	-1.01569100
C	-2.44699300	0.69895300	-0.37806100
H	-3.05630300	1.32668300	-1.01528300
C	-1.03214700	-0.00001700	1.33320500
C	-1.42639600	-1.15382200	0.46030200
H	-1.24851900	-2.19140700	0.71457800
C	-1.42731600	1.15339800	0.46035100
H	-1.24943100	2.19114100	0.71393800
O	1.96075100	0.00059900	0.39713800
C	1.36105800	1.12854300	-0.14496000
C	1.36194200	-1.12793600	-0.14458200
O	1.78588400	-2.21714400	0.09647300
O	1.78388100	2.21816200	0.09621900
H	-0.14258400	-1.35290200	-1.75171800
H	-0.14325100	1.35197500	-1.75226600
H	-0.02393600	0.00047800	1.74090800
H	-1.72186900	-0.00045900	2.19020300

exo-CPMA

C	0.03574900	0.76937800	-0.68563000
C	0.03579000	-0.76931100	-0.68568100
C	2.45564100	0.66753600	-0.36111100
H	3.16405400	1.32815000	-0.84459600
C	2.45570000	-0.66741500	-0.36110600
H	3.16414900	-1.32797400	-0.84461900
C	1.00464500	-0.00008600	1.36246000
C	1.18097200	1.12732200	0.32672900
H	1.15034800	2.15616500	0.67633100
C	1.18099300	-1.12730300	0.32661400
H	1.15042900	-2.15616400	0.67615800
O	-2.04301200	-0.00008700	0.15412200
C	-1.32418500	-1.13906800	-0.14715500
C	-1.32423900	1.13907700	-0.14716700
O	-1.79215100	2.21601700	0.04204700
O	-1.79202400	-2.21603400	0.04200100
H	0.17652700	1.24310400	-1.65582500
H	0.17643600	-1.24295000	-1.65594600
H	0.03256900	-0.00015000	1.86508800
H	1.79658200	-0.00013200	2.11033000

endo-TS-CHMA

O	2.01903900	0.00004900	0.37322600

C	1.47165800	-1.12931800	-0.21555300
C	1.47158800	1.12937400	-0.21555200
O	1.91669700	-2.21470900	0.00762000
O	1.91657100	2.21479400	0.00759000
C	0.35921400	0.69169500	-1.07555300
H	-0.04149400	1.34963200	-1.83155200
C	0.35931500	-0.69168300	-1.07562200
H	-0.04134600	-1.34971700	-1.83155400
C	-0.86406300	0.70228600	1.44807600
H	-0.32430700	1.23833600	2.22165700
C	-0.86424500	-0.70288300	1.44783300
H	-0.32460600	-1.23932800	2.22122400
C	-2.38232200	-0.77402400	-0.54994600
H	-2.31509900	-1.17223300	-1.56371500
H	-3.33024100	-1.13694100	-0.14201600
C	-2.38224100	0.77448500	-0.54952000
H	-3.32998900	1.13729800	-0.14110200
H	-2.31524100	1.17323900	-1.56308600
C	-1.29376100	1.36395000	0.31366900
H	-1.14077200	2.43644400	0.23854300
C	-1.29414300	-1.36408400	0.31323900
H	-1.14136700	-2.43657900	0.23769400

endo-CHMA

O	2.17005100	0.00021200	0.11749900
C	1.45661200	-1.13712600	-0.18985200
C	1.45616800	1.13737200	-0.18989100
O	1.91053800	-2.21516700	0.02765500
O	1.90970600	2.21551100	0.02783900
C	0.11654200	0.76690200	-0.78035900
H	0.05296900	1.19617900	-1.78217800
C	0.11668900	-0.76719100	-0.78003800
H	0.05287900	-1.19689200	-1.78166200
C	-0.92503200	0.66804400	1.46350700
H	-0.84951100	1.27294200	2.36011600
C	-0.92464000	-0.66718000	1.46393500
H	-0.84887700	-1.27145300	2.36094800
C	-2.35073000	-0.77487800	-0.55961200
H	-2.41728100	-1.16720900	-1.57740400
H	-3.20440100	-1.16225700	-0.00193500
C	-2.35085900	0.77378400	-0.56056900
H	-3.20506900	1.16170000	-0.00409400
H	-2.41669000	1.16481100	-1.57890700
C	-1.05022300	1.29399900	0.09622100
H	-1.02843100	2.38226100	0.12853100

C	-1.04959800	-1.29409300	0.09706300
H	-1.02751100	-2.38232800	0.13020800

exo-TS-CHMA

C	-0.40048400	0.69322200	-1.14060400
C	-0.40064200	-0.69330400	-1.14058400
C	2.30085600	0.70232500	-0.68473600
H	2.82678300	1.23655200	-1.46897000
C	2.30079300	-0.70275900	-0.68459800
H	2.82664500	-1.23714700	-1.46877200
C	0.98584500	-0.77481400	1.44342300
H	0.02889100	-1.18032300	1.77691800
H	1.71963800	-1.13323500	2.17091800
C	0.98598700	0.77493500	1.44332400
H	1.71988600	1.13330100	2.17074100
H	0.02912800	1.18068300	1.77681600
C	1.39314600	1.36664500	0.11632900
H	1.26367700	2.43867300	0.00221700
C	1.39295200	-1.36678600	0.11654900
H	1.26332800	-2.43881600	0.00264400
O	-1.97418600	0.00013500	0.41678800
C	-1.44731400	-1.12590400	-0.19781000
C	-1.44708600	1.12604100	-0.19783900

O	-1.85323200	2.21517900	0.07220900
O	-1.85368800	-2.21495000	0.07226100
H	-0.10661500	1.34584900	-1.94669600
H	-0.10684500	-1.34605600	-1.94660300

exo-CHMA

C	-0.11245700	0.76719100	-0.84302200
C	-0.11243900	-0.76727900	-0.84294500
C	2.33234600	0.66693700	-0.65499600
H	3.14085300	1.27379000	-1.04640100
C	2.33233600	-0.66699500	-0.65500700
H	3.14083500	-1.27386500	-1.04640100
C	0.99393800	-0.77441300	1.41749700
H	0.08760700	-1.16878900	1.88659700
H	1.83658600	-1.16104300	1.99165500
C	0.99376700	0.77448400	1.41743100
H	1.83618400	1.16136400	1.99175900
H	0.08723100	1.16870200	1.88628300
C	1.10576100	1.29424000	-0.03625600
H	1.12754200	2.38255000	-0.06428800
C	1.10576300	-1.29426800	-0.03620400
H	1.12757100	-2.38257500	-0.06415300
O	-2.10761300	0.00005000	0.18097500

C	-1.42318600	-1.13909200	-0.19050600
C	-1.42314800	1.13907000	-0.19054700
O	-1.87912200	2.21621800	0.02497900
O	-1.87928300	-2.21617700	0.02498900
H	-0.10611700	1.19161100	-1.84766900
H	-0.10623400	-1.19172200	-1.84759300

endo-TS-CODMA

C	2.76039000	-0.74610500	-0.75847800
C	2.27150000	-1.14660200	0.62742100
H	2.43742800	-1.47800400	-1.50434700
H	2.59724800	-0.39171100	1.34585900
H	3.85190600	-0.79979200	-0.73176500
H	2.78021100	-2.07378100	0.91370100
C	2.34079200	0.67429000	-1.18587100
H	1.57298000	0.63580300	-1.95775600
H	3.19949100	1.14608700	-1.67155700
C	1.91618600	1.64393400	-0.07084400
H	2.69869300	1.67574400	0.69562700
H	1.91611900	2.63703500	-0.52648300
C	-0.64911600	0.78344100	-0.90679100
C	-0.45144500	-0.58547500	-1.03155900
O	-2.48696200	-0.27280200	0.01945500

H	-0.26021200	1.56047400	-1.54840700
H	0.22102400	-1.10649500	-1.69490600
C	-1.98862600	0.96958900	-0.30228000
C	-1.64617600	-1.25232900	-0.51082200
O	-1.97525800	-2.40159600	-0.49419500
O	-2.61632400	1.96390300	-0.09325300
C	0.05945400	-0.64415700	1.73384600
H	-0.75637100	-1.10480400	2.28527700
C	0.07103300	0.75570700	1.70156000
H	-0.66803900	1.23834400	2.33603300
C	0.57527600	1.57441800	0.68203300
H	0.16380900	2.57955800	0.75996600
C	0.80453300	-1.42328300	0.87330400
H	0.49126800	-2.45506100	0.73359600

endo- CODMA

C	-0.51506000	-0.78531800	-0.60037400
C	-0.44018000	0.74908600	-0.60170900
C	0.47645900	1.40612700	0.46773800
C	0.47247000	-1.51403400	0.32806600
C	0.58535500	-0.77277100	1.63911200
C	0.55035500	0.55645900	1.70845800
C	1.88719600	1.74900800	-0.06178400

C	2.89361900	0.60474000	-0.20319800
C	2.46661400	-0.57013600	-1.09589400
C	1.82218500	-1.75911600	-0.37410400
H	0.01457100	2.36491900	0.71575600
H	0.70724400	-1.36623100	2.54047100
H	0.65194700	1.06251600	2.66397500
H	2.31702200	2.49031900	0.61964100
H	1.76589200	2.25004700	-1.02871800
H	3.16313200	0.22377400	0.78708300
H	3.80548500	1.04615400	-0.61588100
H	1.80823500	-0.21218500	-1.89721600
H	3.35365700	-0.96245000	-1.60132300
H	2.52784000	-2.14973900	0.36673500
H	1.66383900	-2.55606300	-1.10843400
H	0.04740600	-2.49967100	0.53345600
O	-2.66718900	0.08182000	-0.10096100
C	-1.93996100	-1.08174000	-0.17945700
C	-1.87159000	1.17592200	-0.34252400
O	-2.44835600	-2.13075900	0.05799400
O	-2.32952100	2.27379200	-0.31700500
H	-0.17531300	1.14199800	-1.58560300
H	-0.41519600	-1.18157400	-1.61614500

exo-TS- CODMA

C	0.89511200	-0.61352700	-1.27239800
C	0.96123200	0.77129800	-1.17889900
C	1.76734400	1.09294900	0.00838300
O	2.08527400	-0.08778900	0.65624000
C	1.64648900	-1.15073600	-0.12328400
C	-1.03054500	1.71681900	-0.44799300
C	-1.23380500	-1.42779300	-0.88179700
C	-1.82878500	-0.38110500	-1.58251200
C	-1.72039200	1.00369800	-1.41785800
O	1.91708200	-2.27397300	0.17740400
O	2.14914600	2.14298400	0.43218200
C	-1.12085300	1.60418500	1.05104100
C	-1.83886400	0.41208700	1.67014600
C	-0.99918000	-0.86251300	1.71992600
C	-1.22131300	-1.83831800	0.57102300
H	0.84645200	-1.19227300	-2.18077800
H	0.92900900	1.47137400	-1.99808900
H	-0.76275200	2.72738300	-0.75144800
H	-2.14927400	-0.66103500	-2.58356800
H	-1.94412200	1.56416800	-2.32294600
H	-1.67048600	2.51312400	1.32881000

H	-0.13816600	1.73465500	1.51897800
H	-2.78626300	0.22902700	1.15130700
H	-2.09697800	0.70153100	2.69195400
H	0.05688200	-0.59632800	1.81160800
H	-1.23730400	-1.41786900	2.63125300
H	-2.21670800	-2.28635400	0.70590200
H	-0.51960000	-2.67036200	0.66807600
H	-1.18135000	-2.32907400	-1.49234600

exo- CODMA

C	0.63359400	0.69644600	1.02968700
C	0.38434400	-0.81825200	1.02498800
C	1.45314800	-1.36897100	0.11136400
O	2.28183300	-0.35132900	-0.31240800
C	1.83194200	0.87714600	0.12829800
C	-1.06172900	-1.30622700	0.74154100
C	-0.57836900	1.58993000	0.67999800
C	-1.81586400	0.98653200	1.30706500
C	-2.02683400	-0.32615500	1.35974300
O	2.39303000	1.87576200	-0.19308700
O	1.65866700	-2.49244600	-0.22289000
C	-1.44369200	-1.57817700	-0.73452600
C	-1.79541000	-0.38453900	-1.62627900

C	-0.70706900	0.68328100	-1.79665300
C	-0.75708900	1.87045500	-0.82734400
H	0.97688400	0.99834100	2.02258200
H	0.64500300	-1.21302100	2.01129100
H	-1.15681100	-2.26669600	1.25156900
H	-2.56052200	1.67746600	1.69159200
H	-2.94798700	-0.72010700	1.77899900
H	-2.31620000	-2.23889600	-0.71007800
H	-0.64299100	-2.15779500	-1.20379600
H	-2.71424400	0.09162600	-1.27068500
H	-2.02871500	-0.79980100	-2.61103200
H	0.28049200	0.20581000	-1.78886900
H	-0.79539600	1.11090200	-2.79944400
H	-1.71773000	2.38068600	-0.95374700
H	0.01365800	2.58587200	-1.12776100
H	-0.40552300	2.56091500	1.14917200

AIBN-Free Radical

C	-0.31133700	0.00000200	-0.00031600
C	1.08455000	0.00005300	-0.00003700
N	2.24701900	0.00001300	0.00007500
C	-1.06092000	-1.29178400	0.00004400
H	-1.71166400	-1.34538700	-0.87899700

H	-0.39685400	-2.15411300	-0.00093100
H	-1.70978900	-1.34597800	0.88045900
C	-1.06099800	1.29174200	0.00004600
H	-0.39698300	2.15411100	-0.00078600
H	-1.71163200	1.34536900	-0.87907600
H	-1.70998200	1.34582800	0.88038100

TS1

C	-1.37972600	-0.71167400	0.25968900
C	-2.37289500	0.28792900	0.03273900
N	-3.16381000	1.10154600	-0.17912300
C	-1.61041200	-2.03351700	-0.41450700
H	-2.40716100	-2.56621600	0.11617300
H	-1.91277500	-1.91768800	-1.45533800
H	-0.70615300	-2.64129700	-0.35948100
C	-0.74180500	-0.72647400	1.61771700
H	-0.54741800	0.27517100	2.00184600
H	-1.41895400	-1.22977300	2.31693500
H	0.18487100	-1.30503200	1.59146100
O	1.73046700	0.93712500	0.44103900
C	1.23479000	-0.74733900	-1.06231900
C	0.18502100	0.12733300	-1.08745400
C	0.56741100	1.27520300	-0.21065900

C	2.19006200	-0.28228500	-0.05235700
O	0.02061500	2.31518400	-0.02718300
O	3.20850200	-0.76010600	0.34326600
H	-0.54809600	0.24658500	-1.87249400
H	1.39101200	-1.64525300	-1.63930600

IN1

C	-1.25927600	-0.56928100	0.11508300
C	-2.33382200	0.40566800	-0.14583700
N	-3.20712300	1.12505200	-0.34565400
C	-1.72948800	-1.93897700	-0.40169200
H	-2.67158200	-2.20954400	0.07574300
H	-1.87401700	-1.92427000	-1.48293600
H	-0.98843000	-2.69873300	-0.14895200
C	-0.98534900	-0.62249400	1.62607900
H	-0.69275000	0.35369700	2.01700800
H	-1.88140500	-0.94909300	2.15411200
H	-0.18772900	-1.34213500	1.82434100
O	1.91134800	1.01719100	0.16126000
C	1.17145500	-1.03354500	-0.57382800
C	0.00833600	-0.12028000	-0.67529900
C	0.59183900	1.19095500	-0.15161700
C	2.31265100	-0.29908500	-0.08026900

O	0.04094600	2.23207600	0.00182400
O	3.43979300	-0.64240200	0.12452200
H	-0.27721100	0.03049500	-1.72468200
H	1.22821500	-2.06847300	-0.87164000

TS2

C	1.98927300	-0.86058600	-0.54060200
C	2.60895600	-1.58408700	0.58500000
N	3.11015100	-2.18584800	1.42540000
C	1.53472800	-1.90773600	-1.57149400
H	2.38726600	-2.51593100	-1.87477700
H	0.76691600	-2.56291100	-1.15602100
H	1.14123900	-1.41289800	-2.46025100
C	3.02528300	0.09945600	-1.14532000
H	3.38442300	0.82120600	-0.40878600
H	3.88091800	-0.46543900	-1.51551700
H	2.58283100	0.63744000	-1.98636300
O	0.77430500	2.22150400	0.56214000
C	0.01727200	0.71127900	-1.02612200
C	0.74491000	-0.08963200	0.00680300
C	1.13841600	0.98188400	1.02459200
C	0.12205400	2.13074500	-0.65317700
O	1.69676400	0.84100500	2.06056500

O	-0.27837800	3.09858800	-1.22211000
H	0.11138300	-0.82291400	0.51941600
H	-0.02588800	0.45797200	-2.07549100
C	-2.52133800	-0.78185500	-1.20307100
C	-2.18764700	0.48450900	-0.82961300
H	-2.68644700	-1.18204400	-2.19138900
H	-2.28518000	1.39027700	-1.41287600
O	-2.42136000	-0.76858100	1.11176800
C	-2.20463600	0.51053900	0.66800200
C	-2.63095800	-1.60453600	0.01422200
O	-2.01443600	1.42070900	1.40910200
O	-2.86269400	-2.76118800	0.15465300
IN2			
C	1.74193500	-1.17122200	-0.44757800
C	2.42562800	-1.83025800	0.68181500
N	2.95349400	-2.39539200	1.53133100
C	0.89528800	-2.24352700	-1.15421800
H	1.53582500	-3.06742800	-1.46988300
H	0.12156700	-2.63850200	-0.49306300
H	0.43074000	-1.82236700	-2.04763900
C	2.80696600	-0.60878800	-1.40340500
H	3.45472000	0.11362800	-0.90436500

H	3.42747500	-1.42251800	-1.77943300
H	2.32893900	-0.12960400	-2.25984400
O	1.26840200	2.27961300	0.23254500
C	-0.06798700	0.66993500	-0.88378600
C	0.82371900	-0.05723200	0.13185600
C	1.64465000	1.06495100	0.75586800
C	0.25180300	2.14500600	-0.67235400
O	2.50872400	0.98490900	1.56299200
O	-0.25827700	3.08082700	-1.19229900
H	0.23363300	-0.49481400	0.94399300
H	0.21156900	0.44531500	-1.91615400
C	-2.16615900	-0.85967200	-1.03165700
C	-1.58609700	0.47171200	-0.74162100
H	-2.10059300	-1.42235200	-1.94936800
H	-2.07273400	1.23369300	-1.36895000
O	-2.92116800	-0.25896100	1.06487000
C	-2.03958500	0.70598900	0.69564000
C	-3.02579200	-1.24224500	0.06627600
O	-1.66946000	1.56504000	1.43193900
O	-3.73719700	-2.18832900	0.21800100

TS3

C	-2.44520100	-0.97090000	0.61379100

C	-3.61006500	-1.37941100	-0.19269300
N	-4.51913900	-1.74114100	-0.79547200
C	-1.70348800	-2.24980000	1.03962900
H	-2.38631200	-2.91644000	1.56739300
H	-1.29690700	-2.77485700	0.17343800
H	-0.88745500	-1.99551800	1.71709900
C	-2.93959900	-0.18983700	1.84077100
H	-3.49988700	0.70169400	1.55091700
H	-3.58998900	-0.82069900	2.44723200
H	-2.08484300	0.10885800	2.45124600
O	-1.48138200	2.26056700	-0.18173000
C	-0.27221500	0.38110300	0.39679100
C	-1.50967300	-0.10478600	-0.28797200
C	-2.17475600	1.20596500	-0.69898500
C	-0.37435700	1.81099800	0.55854300
O	-3.15738100	1.35968500	-1.35305700
O	0.30181600	2.59914400	1.15703800
H	-1.30059800	-0.67935200	-1.19496200
H	0.30453600	-0.18867400	1.10623000
C	1.40616000	-0.94230800	-1.69711800
C	1.33111800	0.38042300	-1.33000400
C	4.12971100	-1.50303400	0.74273800

C	2.46640900	1.24180200	-0.76409700
C	4.45761900	0.00742600	0.51737200
C	3.25951900	0.99193000	0.55096000
H	3.20165800	1.30477100	-1.57785900
H	4.88474000	-2.12318300	0.25647000
H	4.93865900	0.10069200	-0.46126800
H	4.11326900	-1.73554300	1.80905700
H	2.05218600	2.24777000	-0.67717400
H	5.18715000	0.32452900	1.26705800
H	3.68257900	1.97001900	0.79558300
H	2.57850300	0.76340300	1.37628100
C	2.51379600	-1.73270000	-1.17881700
C	2.78484200	-1.62481600	0.12707700
H	1.98619500	-1.23850600	0.74963700
H	3.21670200	-2.18527900	-1.87674500
H	0.70829600	-1.33395200	-2.43210200
H	0.60214200	0.97076400	-1.88514900

IN3

C	1.92682000	0.98773700	0.56551000
C	3.23081200	1.40207200	0.01264900
N	4.24219000	1.76982600	-0.39020700
C	1.08022300	2.26197300	0.72886100

H	1.60862100	2.97332200	1.36482900
H	0.87978400	2.72651200	-0.23756300
H	0.12704900	2.02401400	1.20275800
C	2.16732100	0.31451700	1.92736800
H	2.81244700	-0.56241500	1.83939200
H	2.64393000	1.01930000	2.60907700
H	1.21428200	0.01442500	2.36915300
O	1.49461400	-2.29033700	-0.00994000
C	-0.10169900	-0.54331300	0.00545900
C	1.25057900	0.02103700	-0.45400200
C	2.09847000	-1.22622200	-0.63573200
C	0.26171700	-1.92994200	0.49947700
O	3.14572200	-1.34756800	-1.18260000
O	-0.34829400	-2.68311800	1.18635500
H	1.17819500	0.53301000	-1.41509000
H	-0.54575200	0.01197800	0.82854200
C	-1.34310100	0.68494600	-1.82924000
C	-1.12055800	-0.65494800	-1.17034800
C	-2.89116800	1.41425100	1.01380900
C	-2.40048600	-1.44297300	-0.81073700
C	-3.80811100	0.23376200	0.62716100
C	-3.12996000	-1.13117100	0.49733300

H	-3.09536100	-1.32075200	-1.64755300
H	-3.44725900	2.07980700	1.67662500
H	-4.34700000	0.47609600	-0.29472000
H	-2.06615200	1.03786400	1.63455300
H	-2.13374300	-2.50328300	-0.78800700
H	-4.56349700	0.14434300	1.41168700
H	-3.90566300	-1.89674200	0.59393500
H	-2.45922500	-1.28624700	1.34847900
C	-1.82396000	1.88573500	-1.33248900
C	-2.39564800	2.25805100	-0.12217800
H	-2.57733700	3.32262200	-0.01646600
H	-1.72706200	2.70851800	-2.03784200
H	-1.01448200	0.72364500	-2.86264900
H	-0.62094100	-1.25970400	-1.93562400

TS4

C	2.11146500	-0.13013700	-0.03913700
C	1.68378800	0.64197500	-1.15709200
N	1.30074600	1.28441900	-2.03956100
C	3.05423100	0.58339300	0.89916700
H	3.17702400	0.00359000	1.81659400
H	4.04218400	0.68640200	0.43632100
H	2.69641400	1.58108900	1.15461500

C	2.44994900	-1.56687600	-0.34029600
H	1.72405400	-2.03133000	-1.00857600
H	3.43553000	-1.62098700	-0.81883600
H	2.50532200	-2.14156600	0.58727700
C	0.23589500	-0.18179300	1.20415100
C	-0.17571400	1.13559900	1.09499800
C	-2.65464800	-1.13732800	-0.56184700
C	-1.15598700	1.76788100	0.22832800
C	-3.01089200	0.05446500	0.34088400
C	-2.37893700	1.33105700	-0.12348900
H	-3.13290800	-2.03525600	-0.15742800
H	-2.68565700	-0.15553100	1.36405700
H	-3.06817700	-0.97802800	-1.56237300
H	-4.09671300	0.17213300	0.36858900
H	-2.96117900	1.95505900	-0.79637200
C	-0.45829000	-1.43503500	0.71408900
C	-1.14395400	-1.36587500	-0.66056000
H	-0.68844200	-0.57369700	-1.25982700
H	-0.96850500	-2.30124200	-1.19835800
H	0.27656600	-2.23990100	0.72157500
H	-1.18751700	-1.72684300	1.48011700
H	0.90415700	-0.37117900	2.04227000

H	0.44591700	1.84667700	1.63486700
H	-0.86472700	2.75571600	-0.12276100

IN4

C	1.88476000	0.09137300	-0.18470500
C	1.71239000	-0.22737400	1.24477600
N	1.62225500	-0.47452700	2.36495900
C	2.95633600	-0.86540100	-0.74595000
H	3.13452200	-0.61316300	-1.79339300
H	3.89189600	-0.74599600	-0.19736500
H	2.65778300	-1.91081800	-0.68220700
C	2.42320200	1.52962300	-0.28226500
H	1.78214100	2.24208900	0.23678800
H	3.42056800	1.58053100	0.15726700
H	2.49324100	1.81580100	-1.33424600
C	0.52038900	-0.08904300	-0.96083300
C	-0.08779800	-1.41924400	-0.59213400
C	-2.59142400	1.29902100	0.44210500
C	-1.31727700	-1.82932400	-0.08782500
C	-3.12509300	0.06806200	-0.31468700
C	-2.56884200	-1.25187800	0.12924000
H	-2.96558600	2.19640000	-0.06168600
H	-2.94016800	0.19253200	-1.38578700

H	-3.00002400	1.30719300	1.45652200
H	-4.21069900	0.03855600	-0.20138800
H	-3.27320200	-1.90498700	0.63436700
C	-0.40932600	1.12241800	-0.86734800
C	-1.06422200	1.33174400	0.51090500
H	-0.73827500	0.55146500	1.20215700
H	-0.74189000	2.28035000	0.94820000
H	0.13862100	2.01406600	-1.17275400
H	-1.17394100	0.99206300	-1.63448000
H	0.84451600	-0.16045700	-2.00879200
H	0.62136500	-2.23696400	-0.67362100
H	-1.29522900	-2.87684800	0.20802800

TS5

C	3.48013900	0.61122000	-0.11058000
C	3.73763100	-0.70771600	-0.71910500
N	3.96973400	-1.72660900	-1.20025100
C	4.00138700	1.68977700	-1.08182500
H	3.89293700	2.66598900	-0.60497800
H	5.05813000	1.52452100	-1.29612300
H	3.46186600	1.70206100	-2.02803300
C	4.30583300	0.69338400	1.18544600
H	4.10054600	-0.14096600	1.85588600

H	5.36921100	0.68424100	0.94183000
H	4.07659100	1.62920500	1.70001000
C	1.93294400	0.80303200	0.14773400
C	1.18686900	0.37537600	-1.09224200
C	-0.11851600	-1.80921800	1.69448000
C	0.10570500	-0.39816100	-1.36040800
C	-1.17555300	-1.04207200	0.87825300
C	-0.95011300	-1.03221000	-0.60334400
H	-0.38353200	-1.68414900	2.74883800
H	-1.24748100	-0.01565100	1.24639500
H	-0.19234700	-2.87701700	1.47313600
H	-2.14152100	-1.51279000	1.07706400
H	-1.39399200	-1.87201700	-1.13371000
C	1.44218300	0.20138000	1.46590300
C	1.31683200	-1.33338500	1.45766800
H	1.66493300	-1.73295300	0.50259100
H	1.96244700	-1.77303300	2.22160300
H	2.09754600	0.53180200	2.27070600
H	0.48173500	0.66557700	1.69136700
H	1.82473800	1.89354200	0.22499700
H	1.68328600	0.70636100	-2.00062400
H	-0.03197600	-0.56089600	-2.42770300

C	-2.54168200	1.45396200	-0.69196100
C	-2.59351500	0.24338000	-1.33869600
H	-1.93226900	2.31644600	-0.91099600
H	-2.30535200	0.03572900	-2.35777500
O	-4.12214200	0.17263700	0.39965600
C	-3.69021300	-0.53154600	-0.69632300
C	-3.45133100	1.40200900	0.44178700
O	-4.15380800	-1.59177200	-0.98809800
O	-3.69470500	2.19225900	1.30676100

IN5

C	2.70481800	-0.91380600	0.42416500
C	1.40969500	-1.29389800	1.01694700
N	0.41591600	-1.63498800	1.48658200
C	3.26069800	-2.18560700	-0.24964300
H	4.23904300	-1.95871500	-0.67848300
H	3.37845600	-2.98426700	0.48425300
H	2.59921800	-2.53653600	-1.04222500
C	3.65232300	-0.48283500	1.55577900
H	3.24950300	0.35033600	2.13244100
H	3.83224500	-1.31876200	2.23353000
H	4.60673400	-0.17875200	1.11946700
C	2.53974900	0.21642100	-0.64879200

C	1.54895900	-0.17956200	-1.72988900
C	0.16996000	2.80763300	0.43455000
C	0.22906900	-0.00306800	-1.79159900
C	-0.44235700	2.24641000	-0.85325700
C	-0.63780200	0.71037200	-0.78403800
H	0.47102600	3.84316500	0.24924400
H	-0.59412500	2.83916300	1.21908000
C	2.44495000	1.65921000	-0.08651600
C	1.37506700	2.01588100	0.96588500
H	1.02849500	1.11894900	1.48412700
H	1.84643000	2.62254000	1.74359400
H	3.42571700	1.87565400	0.34213600
H	2.35498400	2.32953800	-0.94664700
H	3.51490100	0.20227200	-1.14837600
H	1.99881600	-0.68390700	-2.58104100
H	-0.27775600	-0.36746900	-2.68183200
C	-2.13143900	0.32023900	-0.95873200
C	-3.00453400	0.90043500	0.08788000
O	-3.13314500	-1.37592700	0.36179200
C	-3.56444800	-0.15954000	0.88889700
C	-2.34095500	-1.17445400	-0.74041900
O	-4.28396300	-0.12784200	1.84732700

O	-1.91516400	-2.08923200	-1.37007400
H	-1.39036300	2.75310900	-1.05469000
H	0.20446100	2.47646600	-1.70157700
H	-0.36376200	0.37613200	0.21651400
H	-2.45359400	0.58408900	-1.97308900
H	-3.20618600	1.94293000	0.27783100

TS6

C	4.08484200	-0.83388300	-0.06109100
C	3.78052700	-0.86142200	1.38171800
N	3.58354500	-0.90465100	2.51458700
C	4.39459100	-2.28037600	-0.49873800
H	4.67916400	-2.27117200	-1.55300900
H	5.22877300	-2.67864200	0.08100100
H	3.54421100	-2.94837200	-0.37119000
C	5.36135000	0.00549400	-0.24976900
H	5.26672800	0.99874500	0.18884900
H	6.20712900	-0.49864100	0.22042700
H	5.56918800	0.10731000	-1.31746100
C	2.86085600	-0.25627100	-0.87527300
C	1.59711600	-0.94742800	-0.41033500
C	1.12329800	2.78138700	0.23453900
C	0.39010500	-0.55103600	0.04525600

C	-0.01308400	2.01190000	-0.45658400
C	-0.37006600	0.69159200	0.17051100
H	1.33778800	3.67703500	-0.35911400
H	0.22571600	1.85241100	-1.51136000
H	0.78308800	3.12458900	1.21624900
H	-0.90093000	2.65190000	-0.44789800
H	-0.84659800	0.77164500	1.14651100
C	2.81942600	1.27245300	-0.91975300
C	2.39665100	1.94928500	0.39752300
H	2.21853300	1.19371400	1.16616200
H	3.20039500	2.58682200	0.77527200
H	3.79024700	1.64370900	-1.24838000
H	2.13426300	1.54803000	-1.72238400
H	3.06303400	-0.59989500	-1.89873600
H	1.72492800	-2.02581500	-0.35946700
H	-0.20410200	-1.38952300	0.40954500
C	-2.35893700	-1.07610700	-1.01332000
C	-2.26032300	0.29178900	-0.78079700
C	-5.75284000	-1.29905200	0.44888300
C	-3.16616500	0.98448900	0.24666800
C	-5.60882100	0.20139400	0.88602900
C	-4.70666900	1.12888900	0.02472100

H	-3.02844600	0.47418000	1.20527200
H	-5.66752700	-1.94905200	1.32199100
H	-5.20724900	0.22350700	1.90357900
H	-6.72953100	-1.46758000	-0.00833200
H	-2.76430600	1.99084400	0.38814200
H	-6.60425000	0.64971900	0.93722900
H	-4.96985600	2.14771200	0.32188900
H	-4.96009200	1.05955100	-1.03558200
C	-3.37353400	-1.79170900	-0.21232700
C	-4.64224800	-1.51696100	-0.52139800
H	-4.81077400	-1.06836100	-1.49768000
H	-3.11595200	-2.24290600	0.74740700
H	-1.70016900	-1.56369200	-1.72510400
H	-1.88466700	0.90823100	-1.59472300

IN6

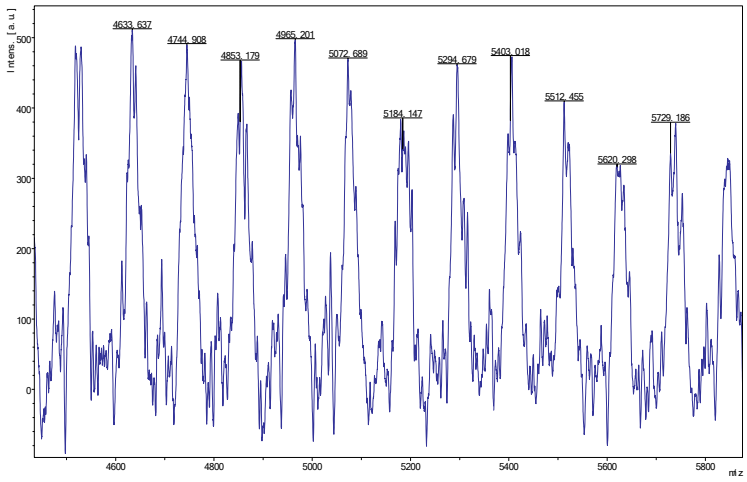
C	-3.46525500	-0.86659200	-0.19614600
C	-2.41257100	-1.15252500	-1.18774500
N	-1.62514800	-1.42594300	-1.98120600
C	-3.91120200	-2.23265000	0.36542100
H	-4.72065700	-2.07231600	1.08080800
H	-4.27788600	-2.87382900	-0.43768900
H	-3.08930200	-2.74167200	0.86959600

C	-4.64881500	-0.20703800	-0.92299900
H	-4.35466300	0.71210600	-1.43063500
H	-5.06617200	-0.89336500	-1.66159200
H	-5.42520600	0.02910900	-0.19139100
C	-2.93200600	0.02992700	0.97263100
C	-1.69957500	-0.57400100	1.62164000
C	-0.79772400	2.77110700	-0.20419100
C	-0.40247400	-0.40338500	1.35509100
C	0.12231500	1.97943600	0.73252900
C	0.26948000	0.48838400	0.33417800
H	-1.01188100	3.74221000	0.25432200
H	-0.25948700	2.03723800	1.75446900
H	-0.27111000	2.97851900	-1.14216400
H	1.10379500	2.46311600	0.75308000
H	-0.20744000	0.33533700	-0.63864700
C	-2.90327700	1.54891900	0.67813700
C	-2.12074000	2.07188600	-0.54219300
H	-1.93579600	1.26678800	-1.25645500
H	-2.74797500	2.78941100	-1.07861900
H	-3.94576500	1.85974300	0.57996700
H	-2.54112600	2.04027100	1.58626800
H	-3.72365800	-0.07437700	1.72371400

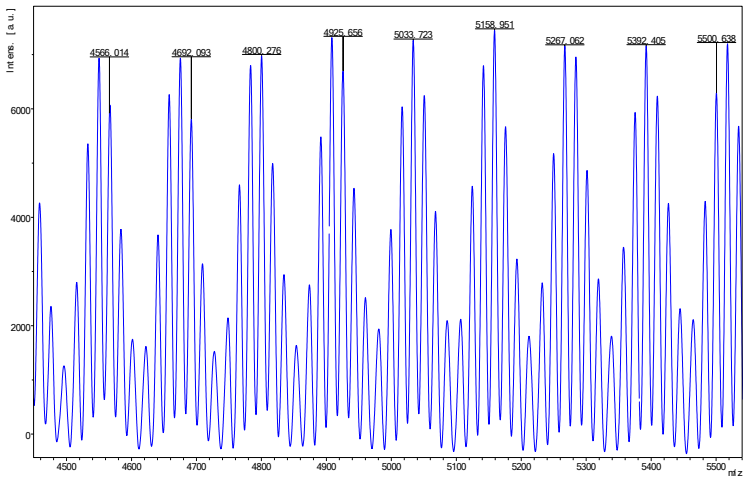
H	-1.92571900	-1.25487300	2.43878300
H	0.28660300	-0.95589400	1.99389300
C	1.82159300	-1.39700800	-0.16580900
C	1.74440600	0.06955400	0.15722600
C	4.81952800	-0.59298000	0.69048200
C	2.44675100	0.91960300	-0.93892700
C	4.96144300	0.47523100	-0.42397700
C	3.81369100	1.48135300	-0.54173600
H	2.54701400	0.32087800	-1.85006100
H	5.81366300	-0.79606800	1.09321900
H	5.10499300	-0.02891500	-1.38566900
H	4.24233800	-0.17297600	1.52006300
H	1.80041900	1.76225900	-1.20105200
H	5.87606200	1.04364700	-0.23324100
H	4.10444800	2.22965100	-1.28592300
H	3.71157900	2.01703100	0.41061500
C	2.94638000	-2.20841500	-0.13445200
C	4.24777200	-1.90778000	0.23789400
H	4.96062500	-2.72246300	0.15758800
H	2.78614600	-3.23312900	-0.46160600
H	0.90153600	-1.84712900	-0.53089900
H	2.24233300	0.26312600	1.11536500

5. MALDI-TOF Mass Spectrum

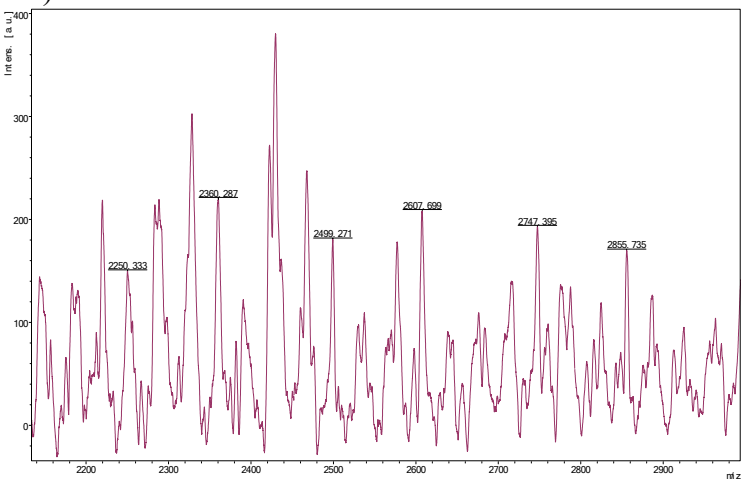
poly(COD-*alt*-Me):



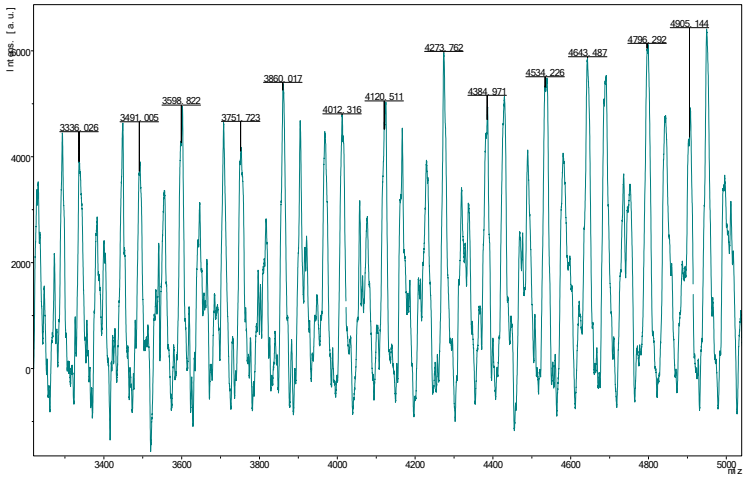
poly(COD-*alt*-Et):



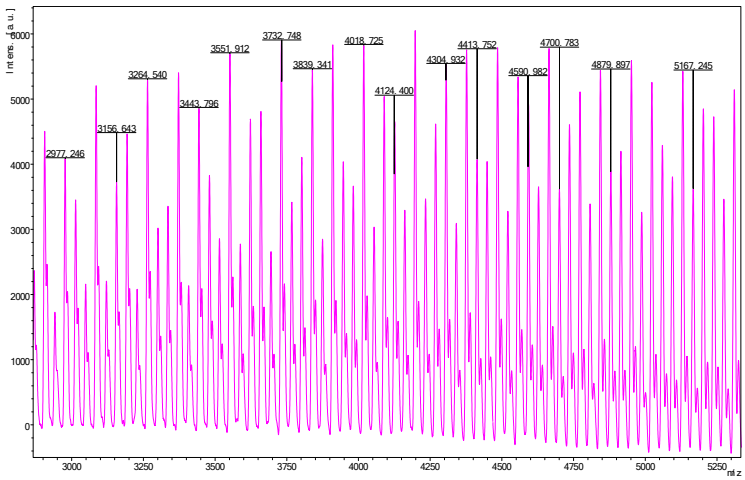
poly(COD-*alt*-Pr):



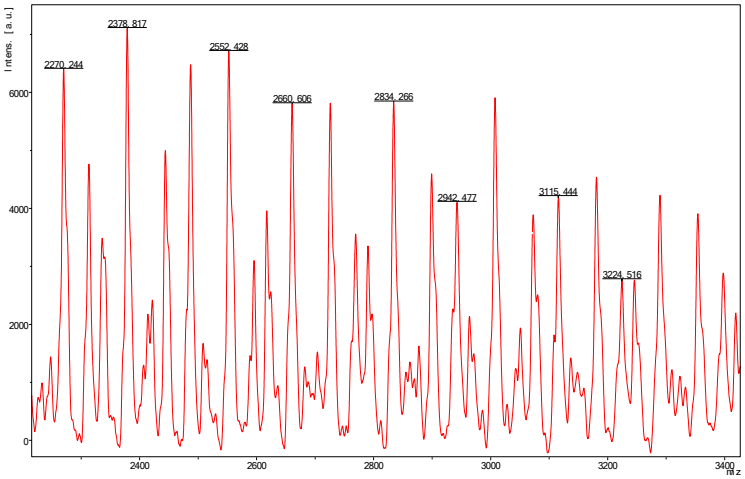
poly(COD-*alt*-^{t}Bu):



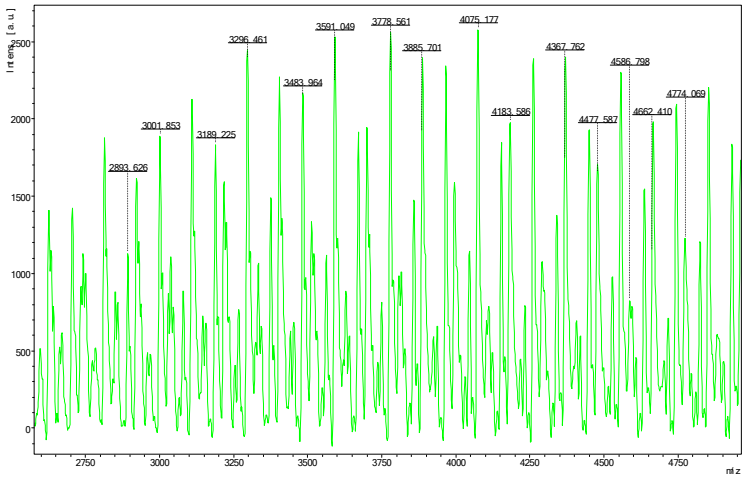
poly(COD-*alt*- Cy):



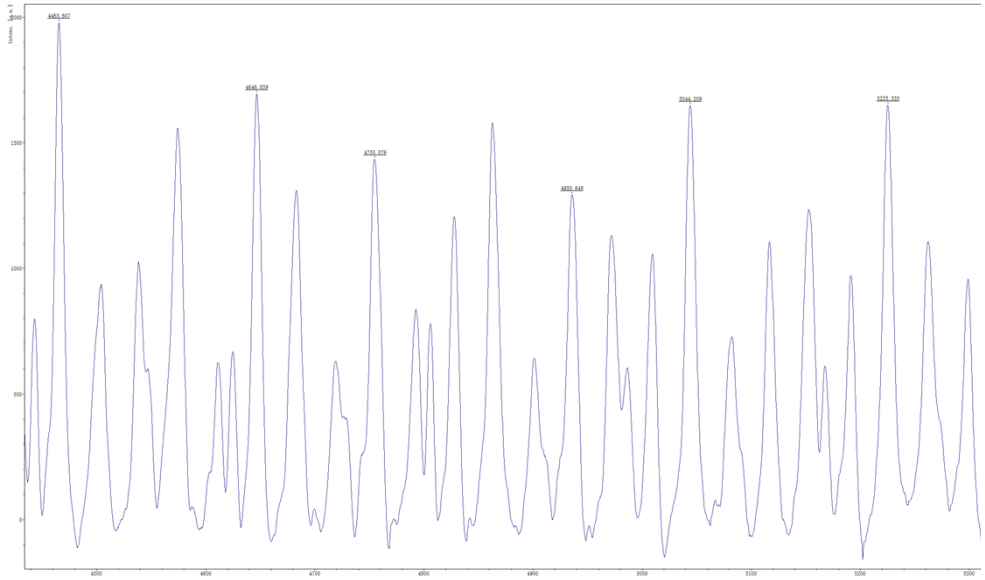
poly(COD-*alt*-Ph):



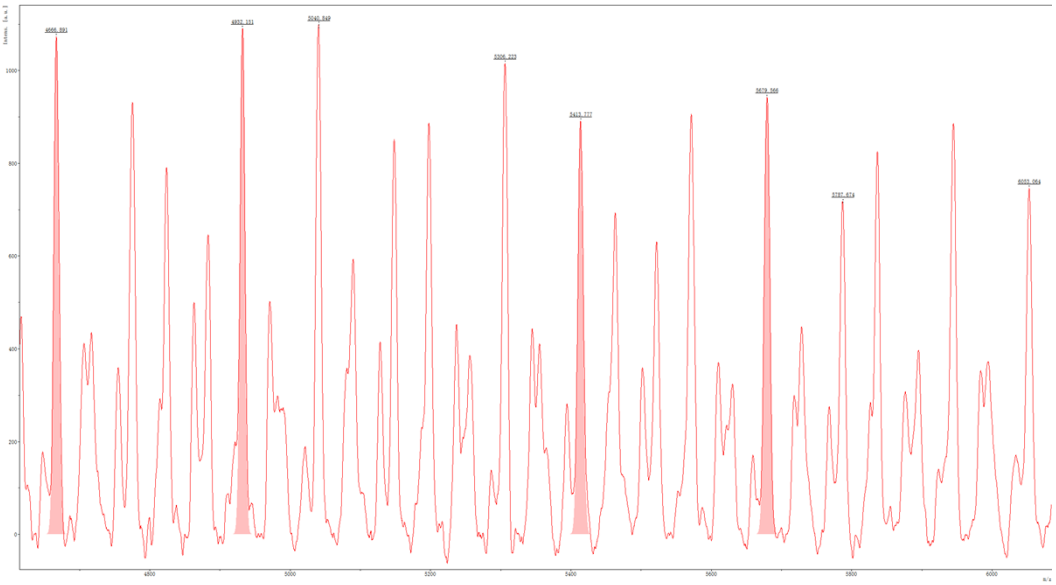
poly(COD-*alt*-Bn):



poly(COD-*alt*-Hex).



poly(COD-*alt*-Doc):



6. NMR spectra

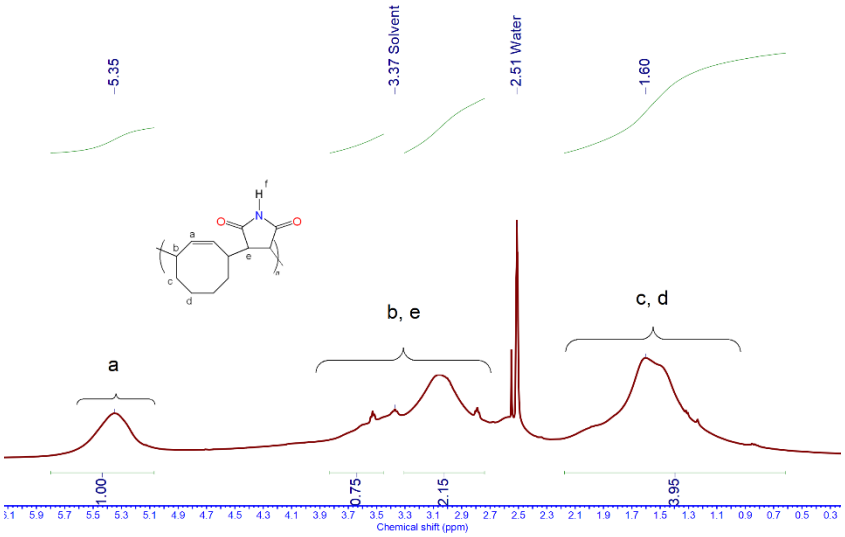


Figure S21. ^{1}H NMR spectrum of the poly(COD-*alt*-MI) in DMSO-d_6.

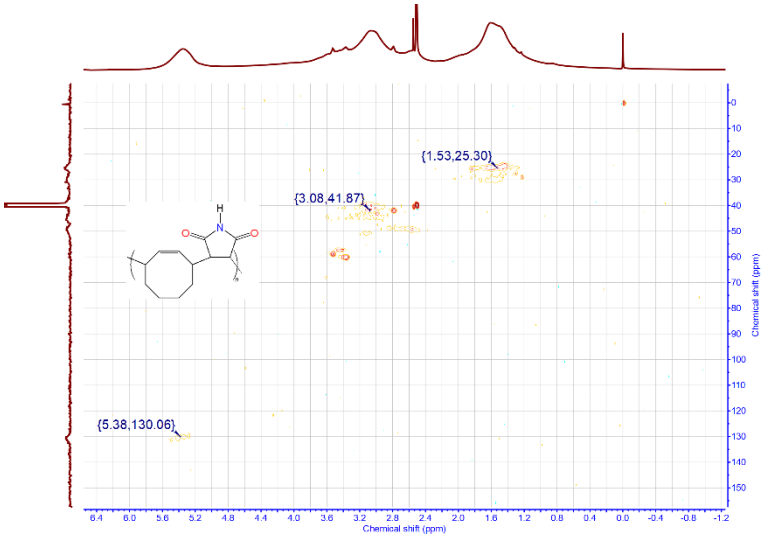


Figure S22. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-MI) in DMSO-d_6.

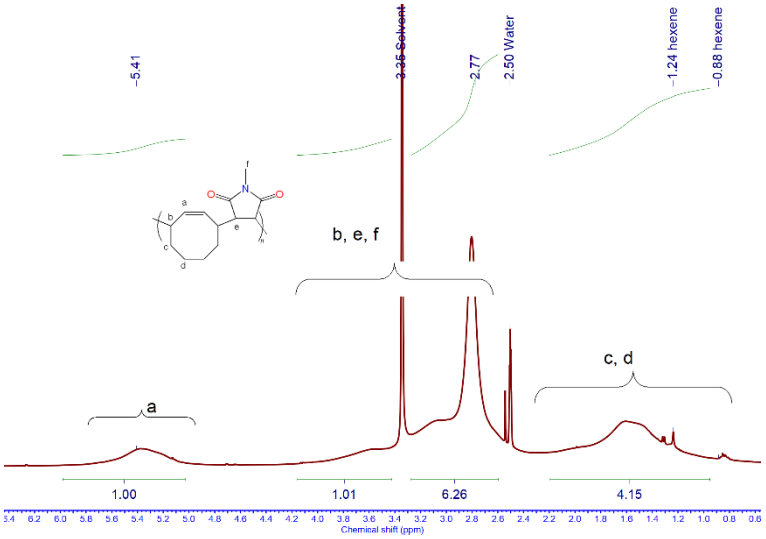


Figure S23. ^{1}H NMR spectrum of the poly(COD-*alt*-Me) in DMSO-d_6.

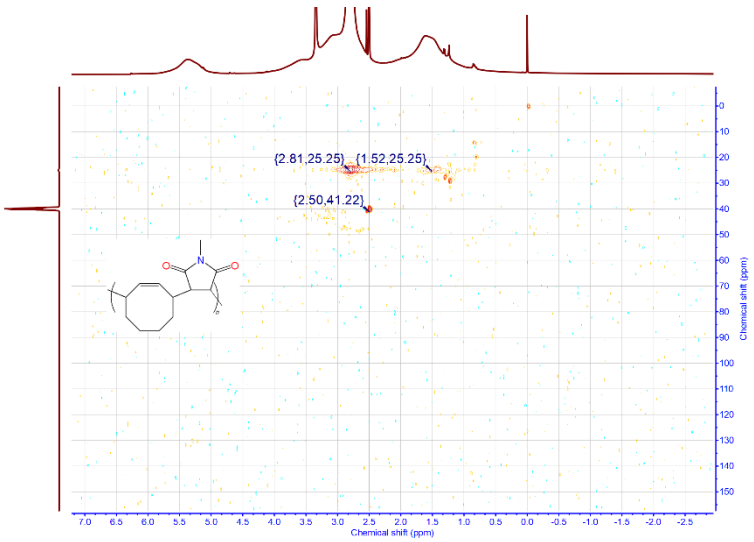


Figure S24. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Me) in DMSO-d_6.

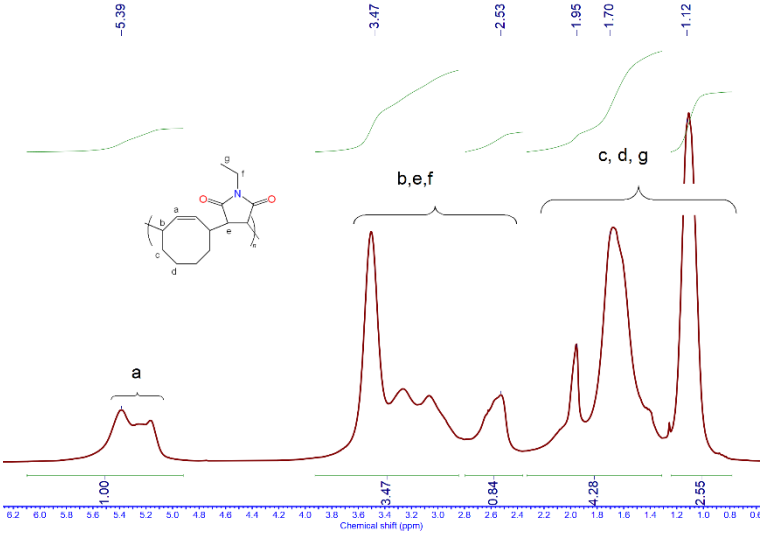


Figure S25. ^{1}H NMR spectrum of the poly(COD-*alt*-Et) in Chloroform-d.

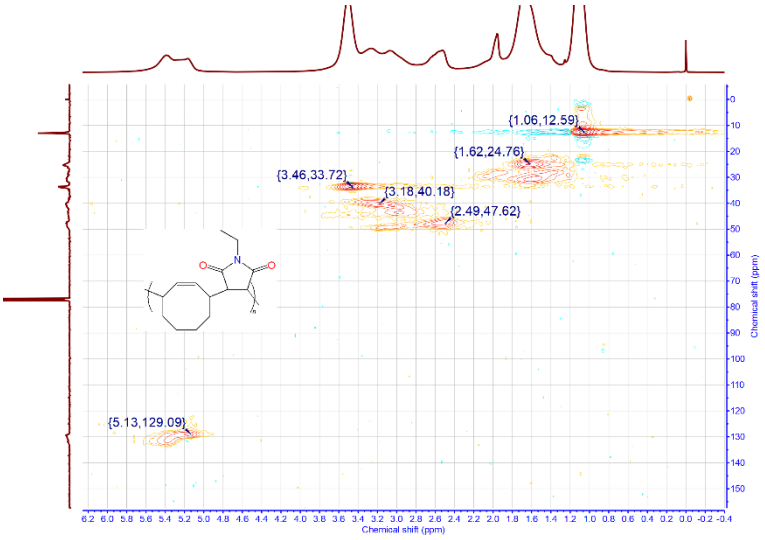


Figure S26. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Et) in Chloroform-d.

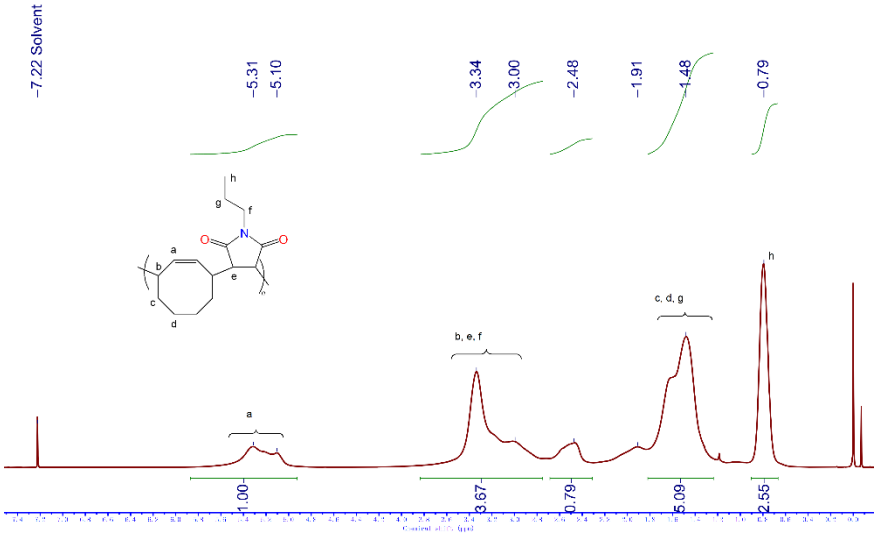


Figure S27. ^{1}H NMR spectrum of the poly(COD-*alt*-Pr) in Chloroform-d.

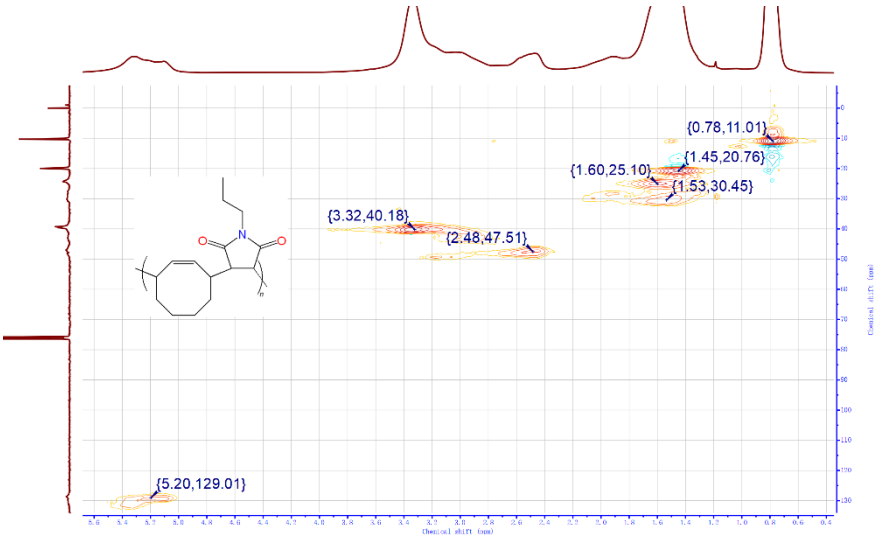


Figure S28. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Pr) in Chloroform-d.

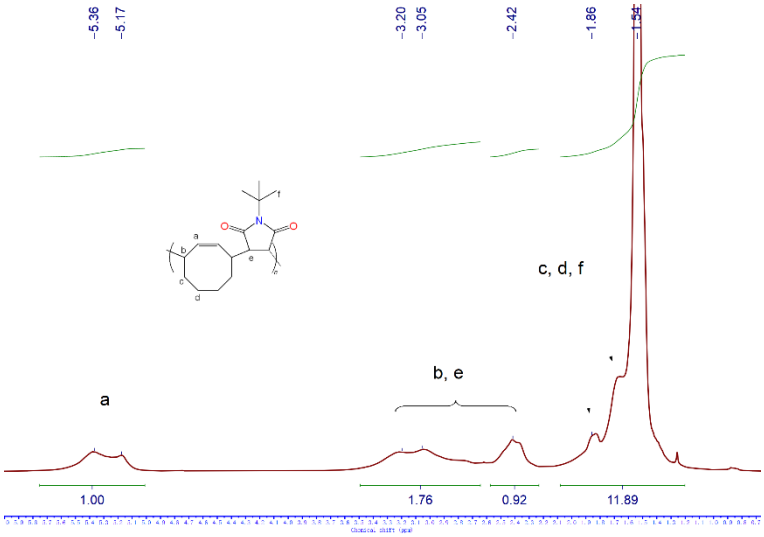


Figure S29. ^{1}H NMR spectrum of the poly(COD-*alt*-^{t}Bu) in Chloroform-d.

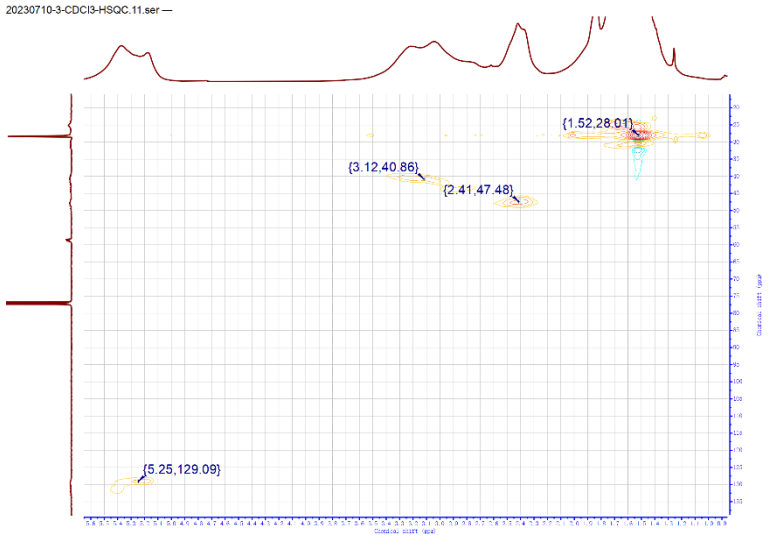


Figure S30. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-^{t}Bu) in Chloroform-d.

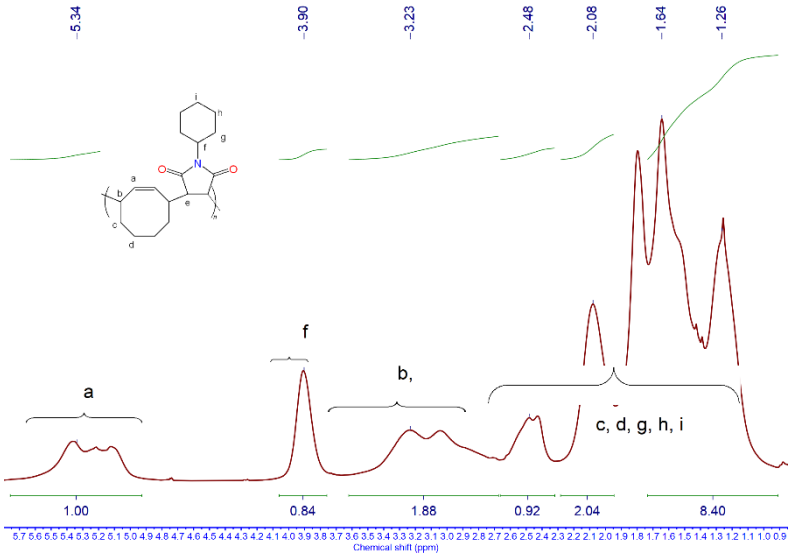


Figure S31. ^{1}H NMR spectrum of the poly(COD-*alt*-Cy) in Chloroform-d.

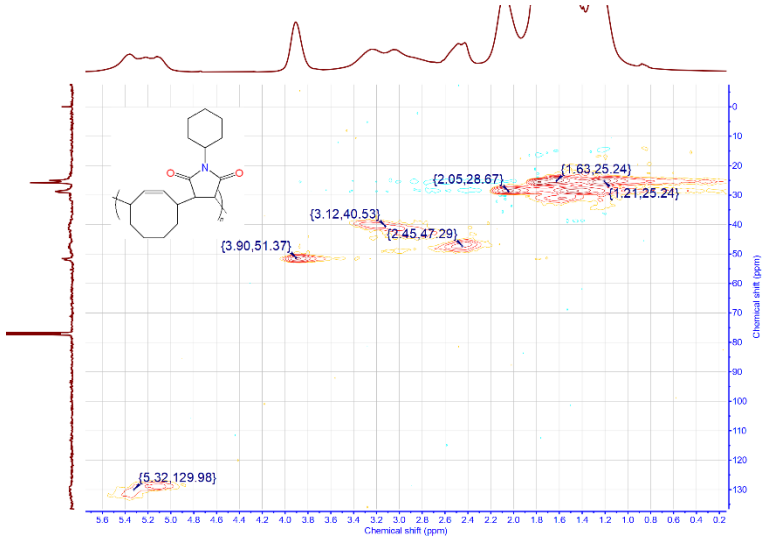


Figure S32. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Cy) in Chloroform-d.

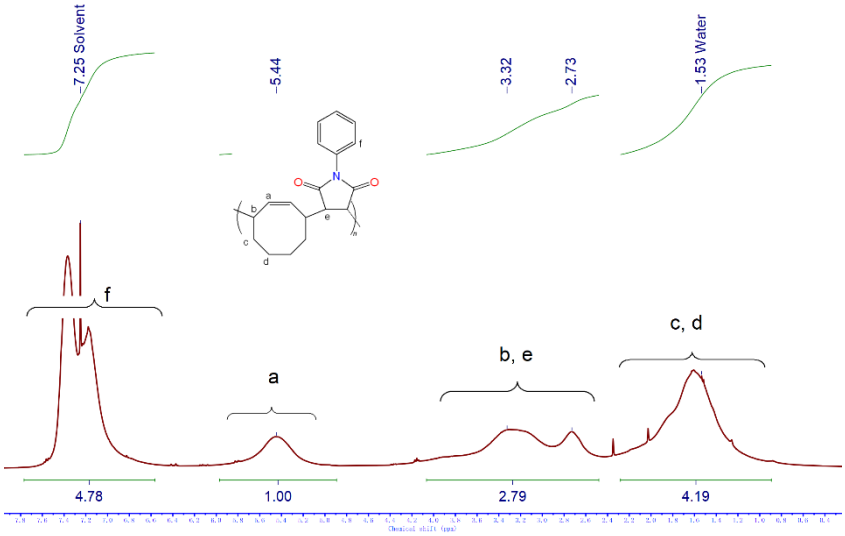


Figure S33. ^{1}H NMR spectrum of the poly(COD-*alt*-Ph) in Chloroform-d.

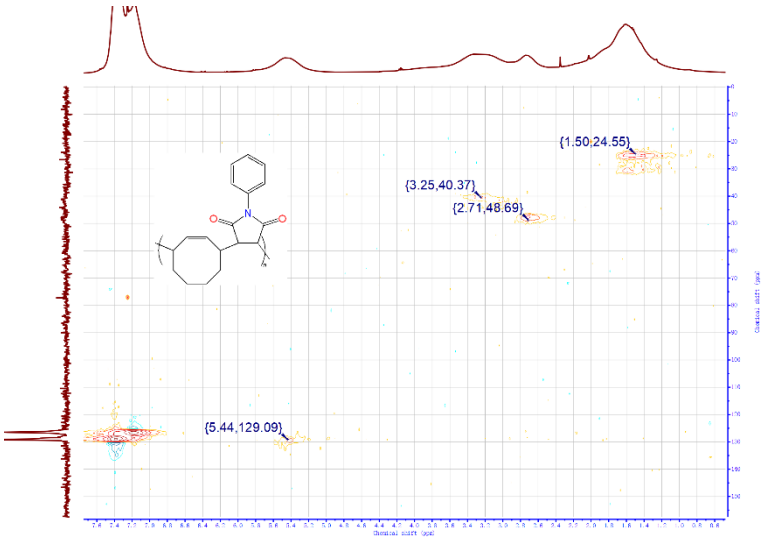


Figure S34. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Ph) in Chloroform-d.

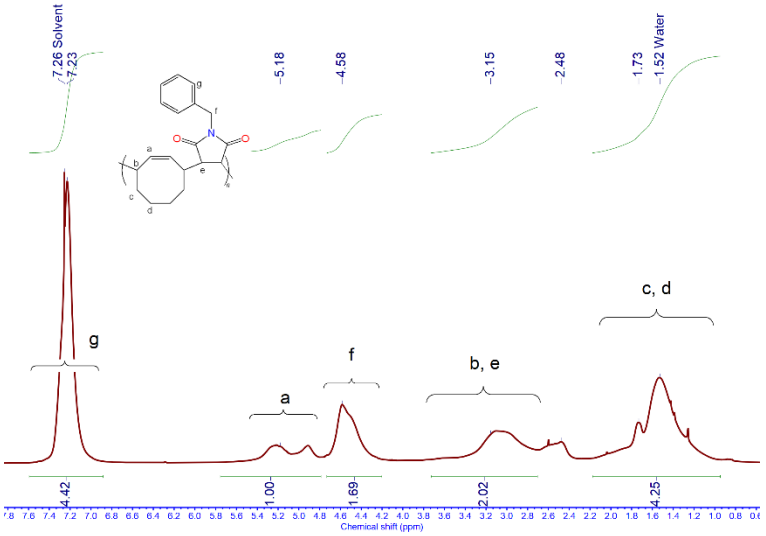


Figure S35. ^{1}H NMR spectrum of the poly(COD-*alt*-Bn) in Chloroform-d.

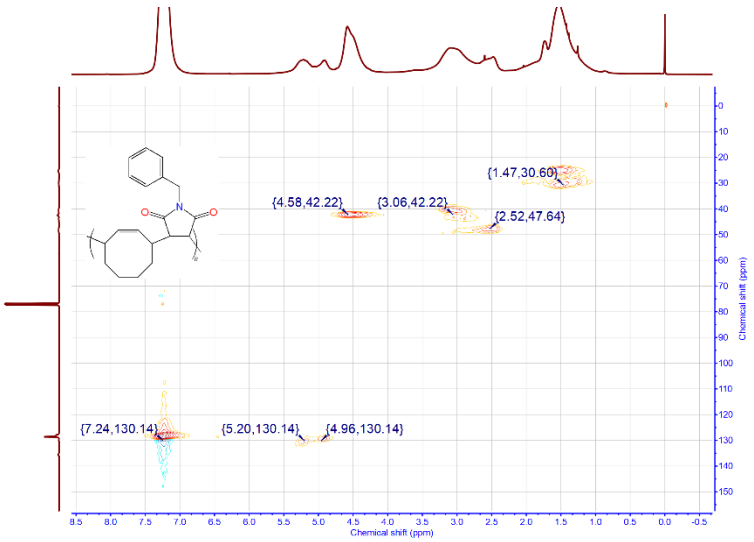


Figure S36. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Bn) in Chloroform-d.

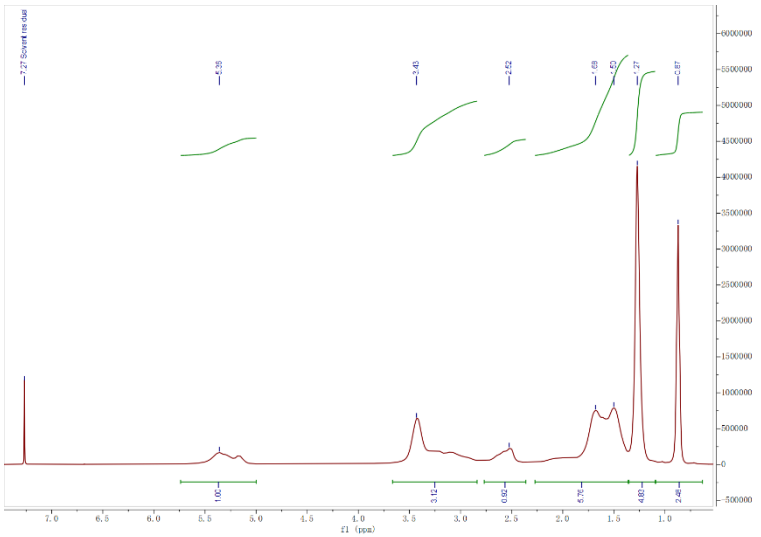


Figure S37. ^{1}H NMR spectrum of the poly(COD-*alt*-Hex) in Chloroform-d.

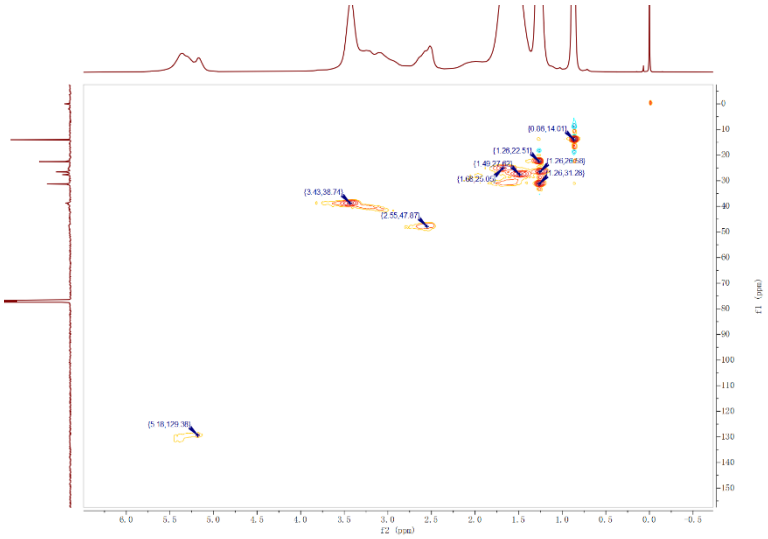


Figure S38. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Hex) in Chloroform-d.

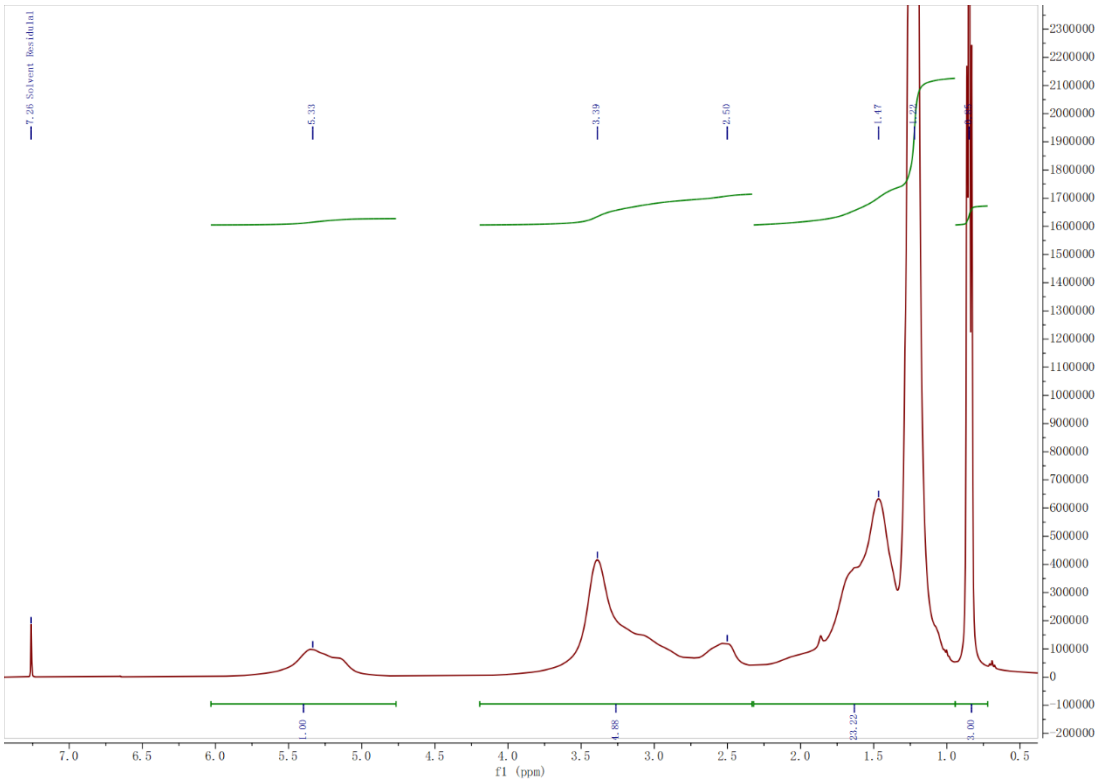


Figure S39. ^{1}H NMR spectrum of the poly(COD-*alt*-Doc) in Chloroform-d.

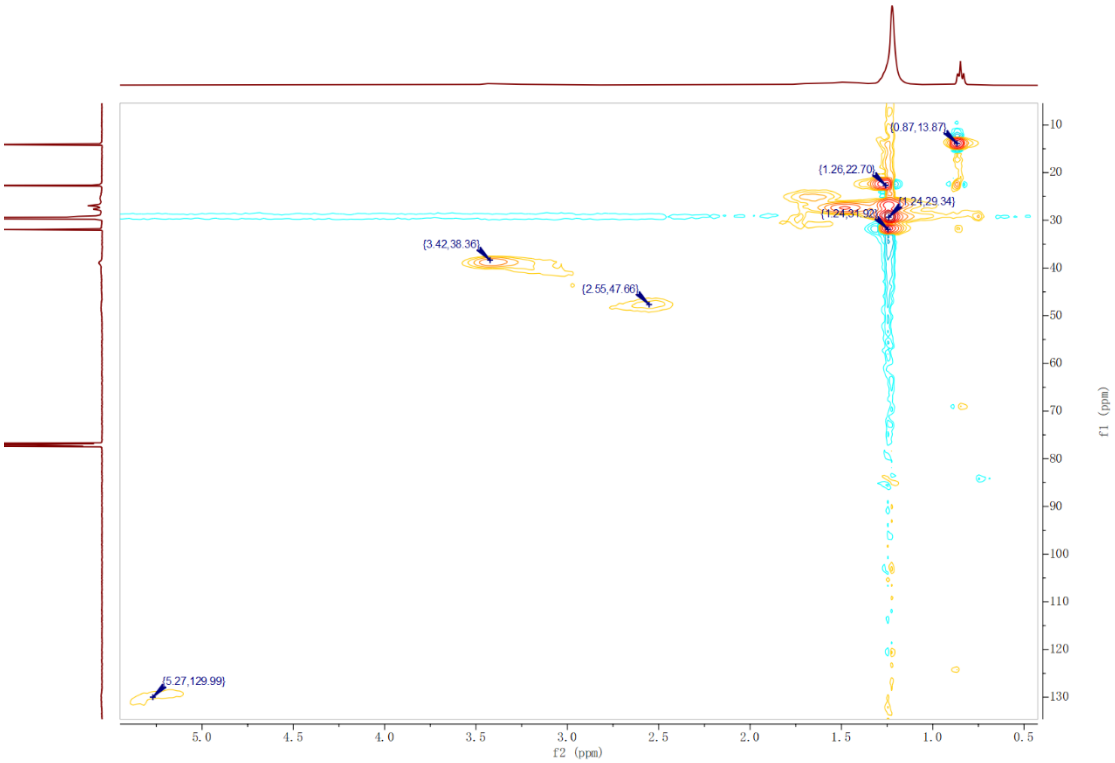


Figure S40. ^{1}H-^{13}C HSQC NMR spectrum of the poly(COD-*alt*-Doc) in Chloroform-d.

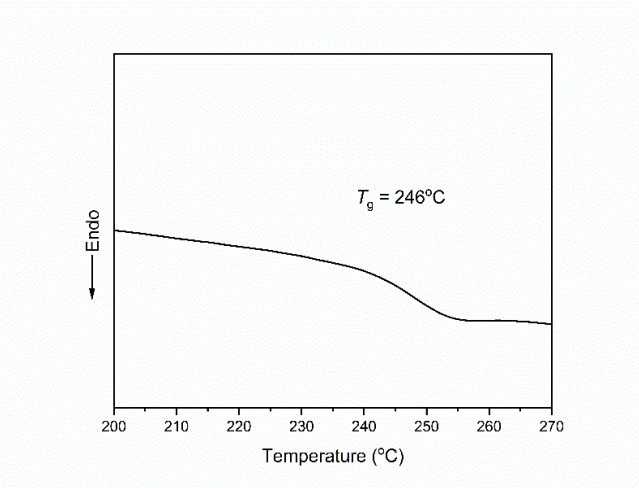
7. DSC and TGA curves of copolymers

Table S6. DSC and TGA results of copolymer.

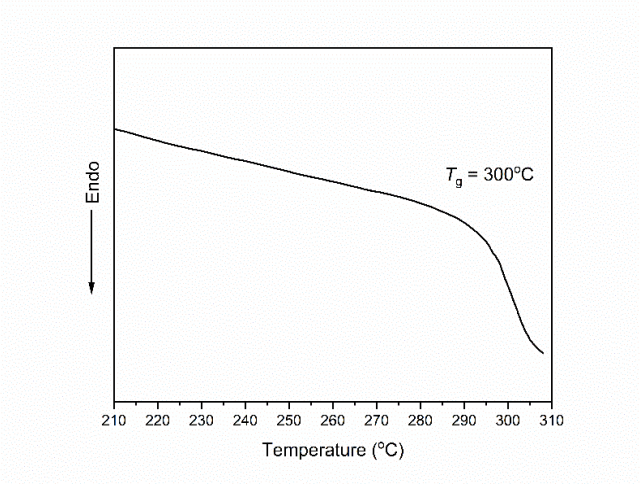
Polymer	T_g /°C	$T_{d,\ 5\%}$ /°C
poly(COD-*alt*-MA)	246	359
poly(COD-*alt*-MI)	300	378
poly(COD-*alt*-Me)	246	388
poly(COD-*alt*-Et)	193	385
poly(COD-*alt*-Pr)	168	388
poly(COD-*alt*-^{t}Bu)	204	341
poly(COD-*alt*-Cy)	240	394
poly(COD-*alt*-Ph)	258	395
poly(COD-*alt*-Bn)	165	397
poly(COD-*alt*-Hex)	98	365
poly(COD-*alt*-Dod)	62	373

DSC curves:

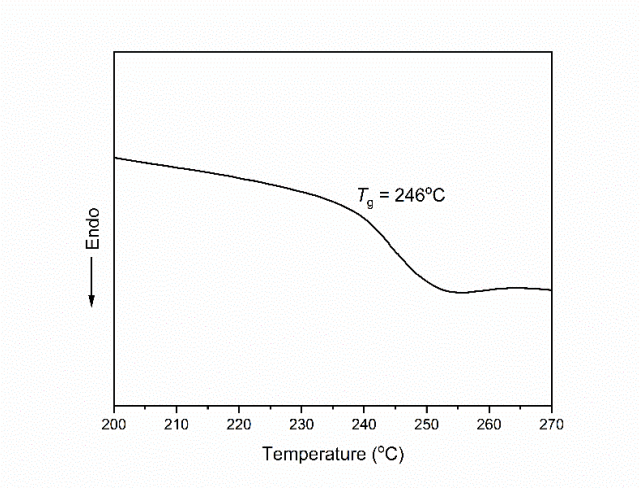
poly(COD-*alt*-MA)



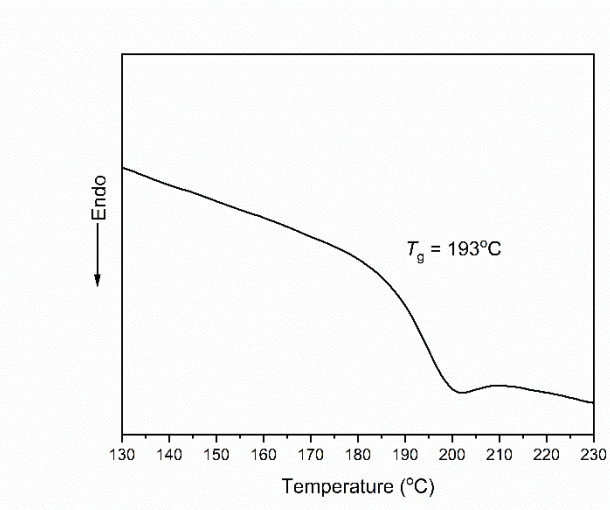
poly(COD-*alt*-MI)



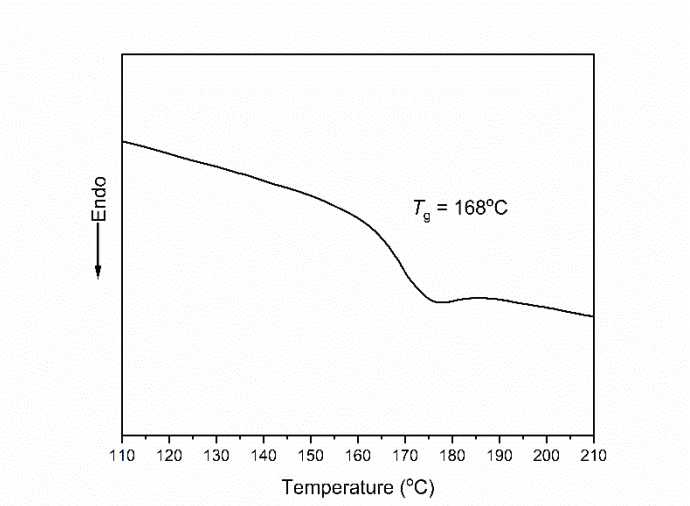
poly(COD-*alt*-Me)



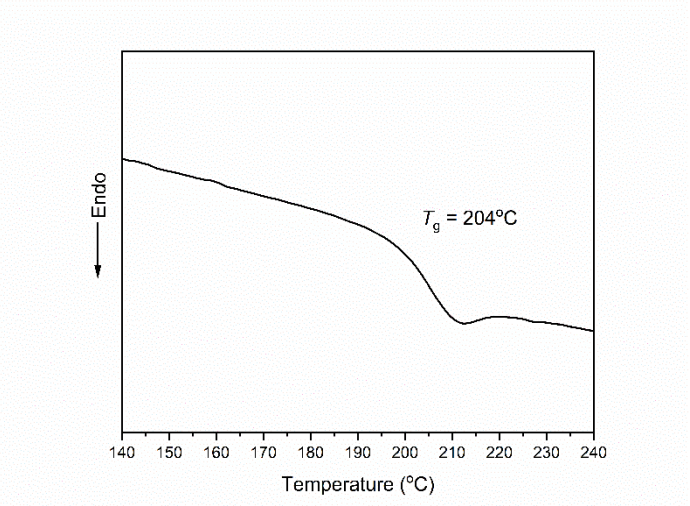
poly(COD-*alt*-Et)



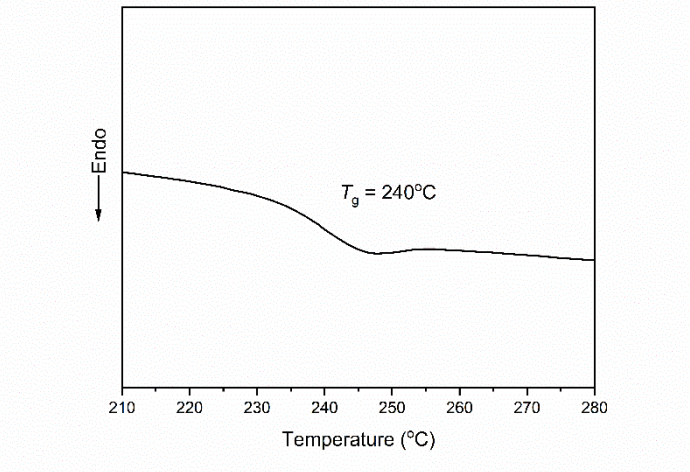
poly(COD-*alt*-Pr)



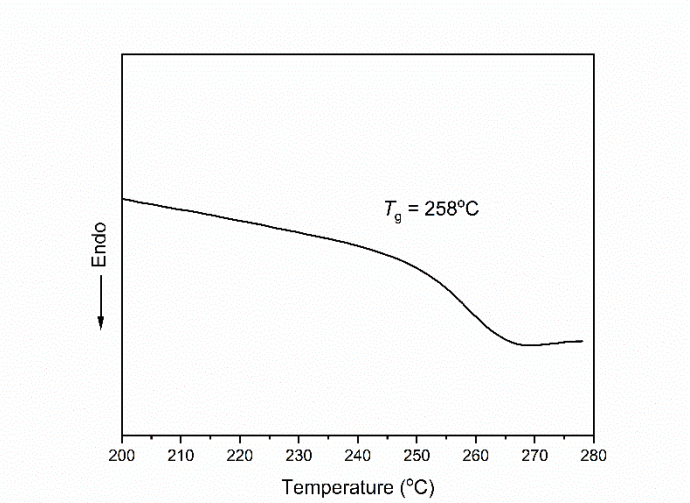
poly(COD-*alt*-^{t}Bu)



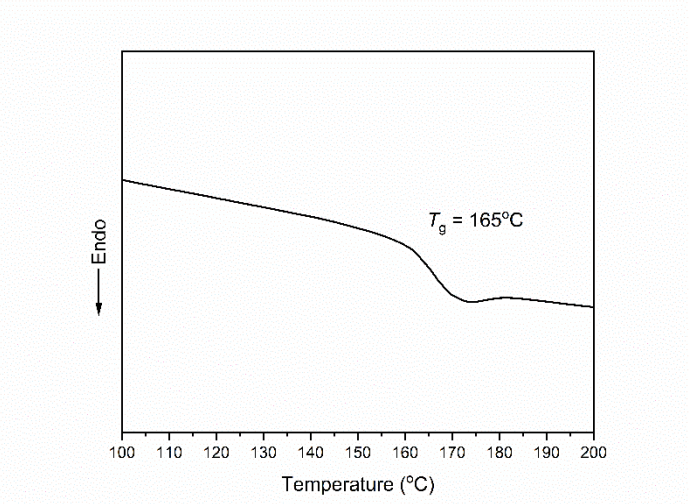
poly(COD-*alt*-Cy)



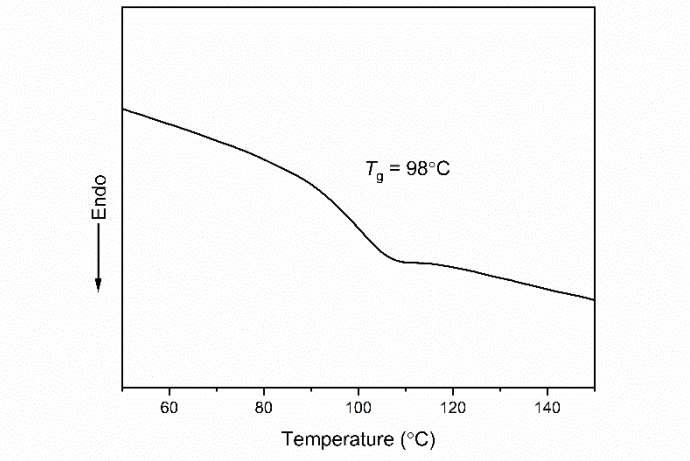
poly(COD-*alt*-Ph)



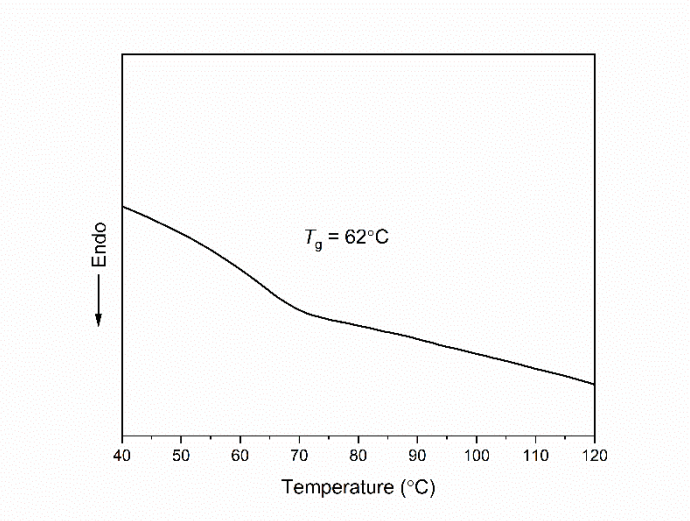
poly(COD-*alt*-Bn)



poly(COD-*alt*-Hex)

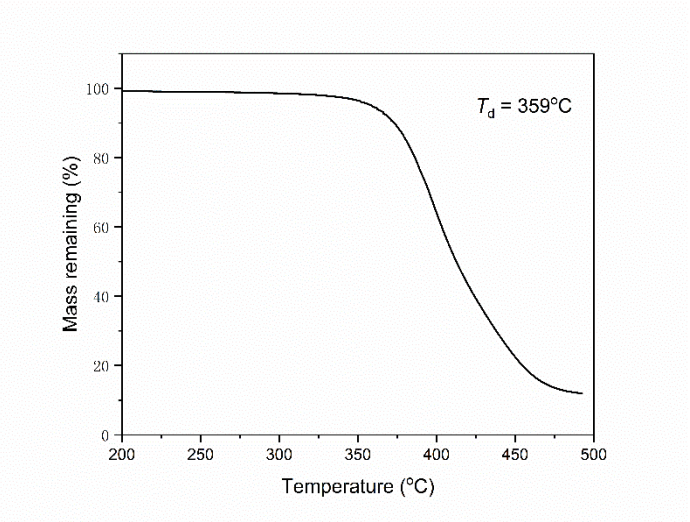


poly(COD-*alt*-Doc)

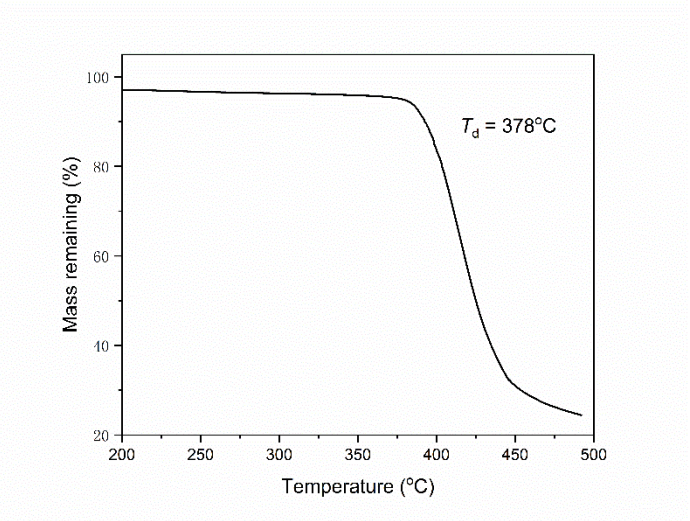


TGA curves:

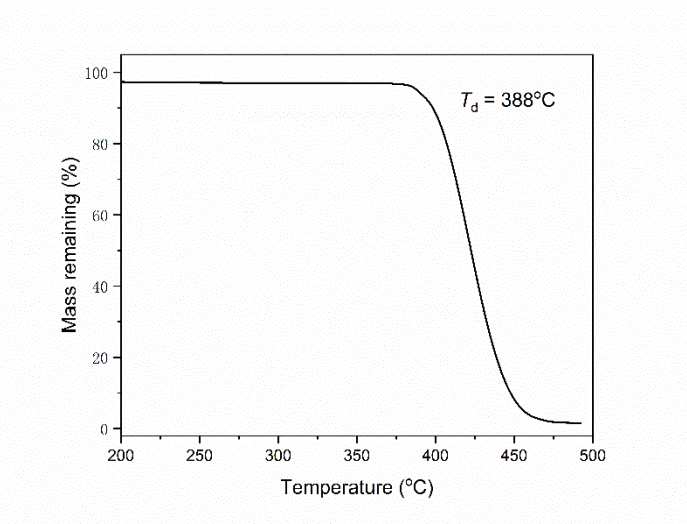
poly(COD-*alt*-MA)



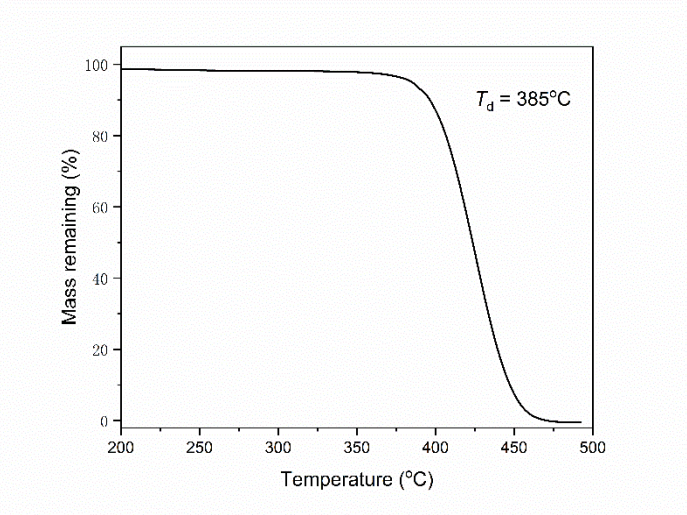
poly(COD-*alt*-MI)



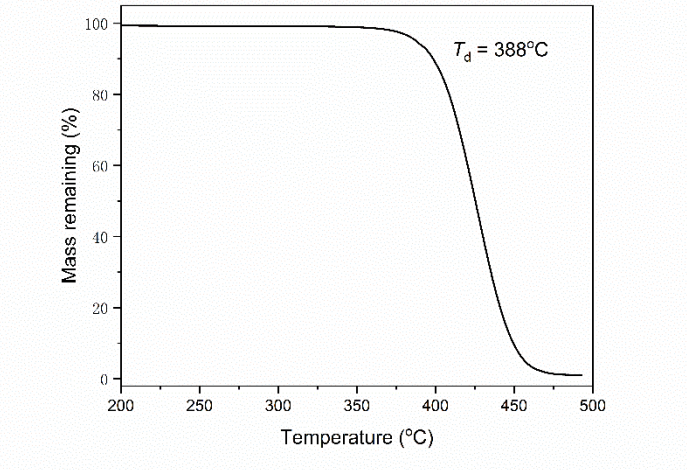
poly(COD-*alt*-Me)



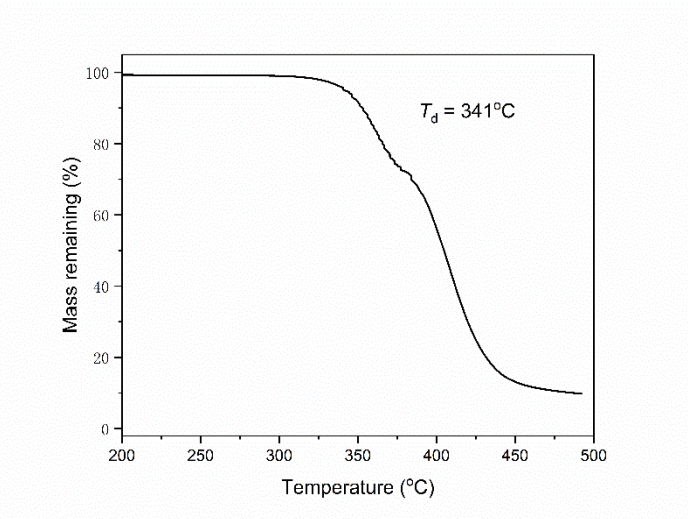
poly(COD-*alt*-Et)



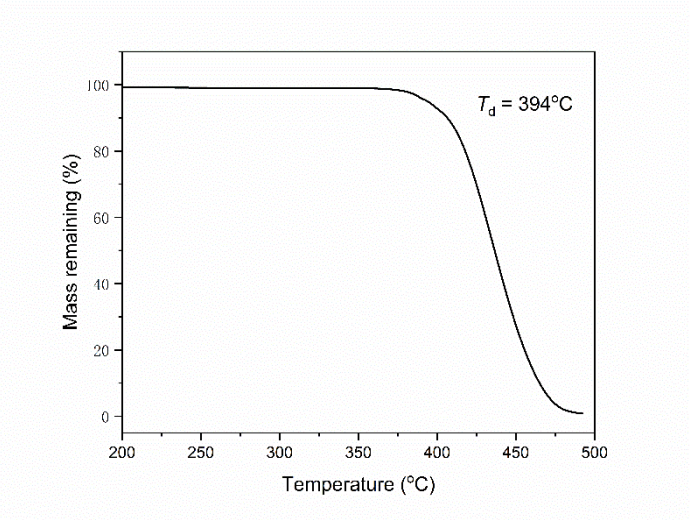
poly(COD-*alt*-Pr)



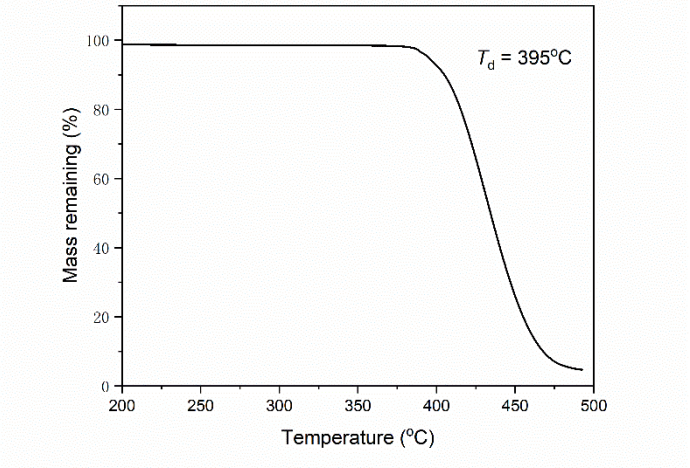
poly(COD-*alt*-^{t}Bu)



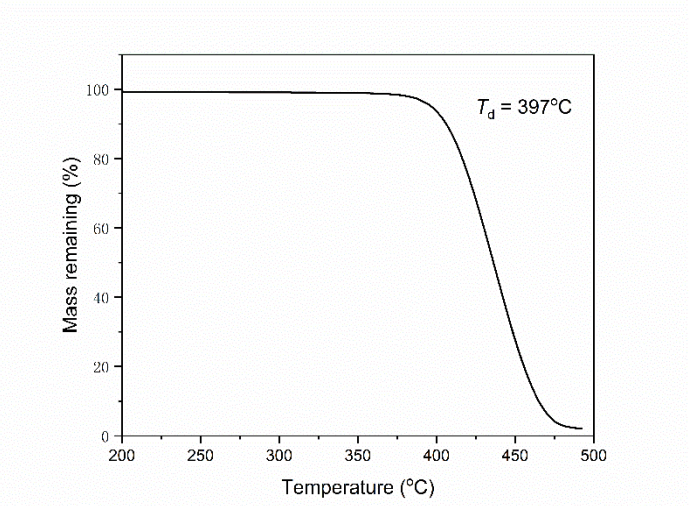
poly(COD-*alt*-Cy)



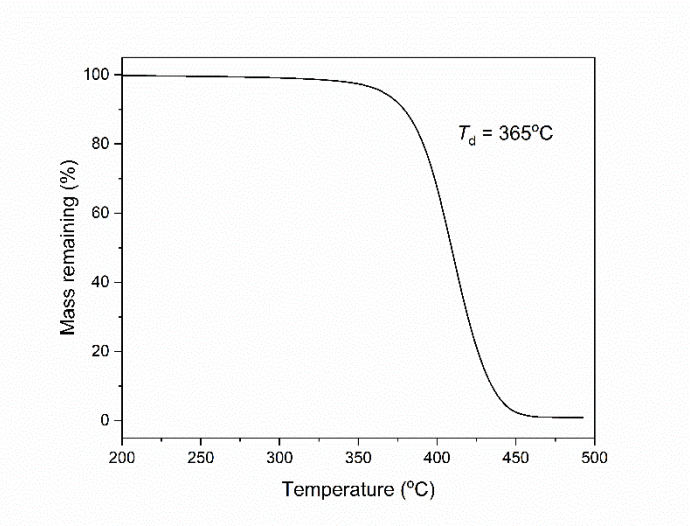
poly(COD-*alt*-Ph)



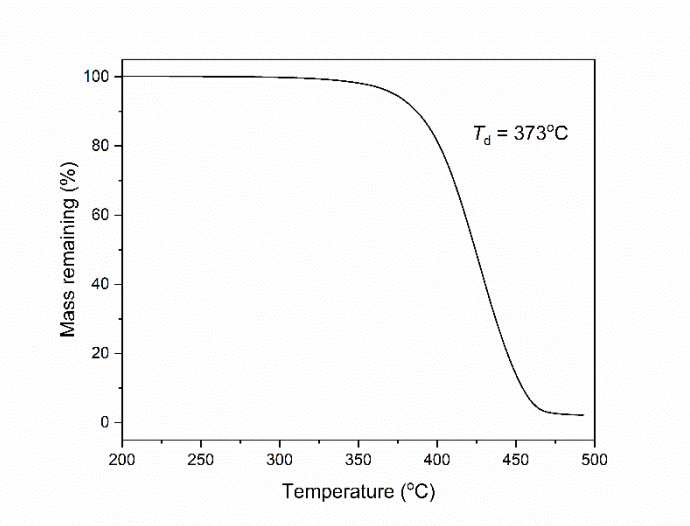
poly(COD-*alt*-Bn)



poly(COD-*alt*-Hex)



poly(COD-*alt*-Doc)



References

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian 09, revision C.01; Gaussian Inc.: Wallingford, CT, 2010.
(2) Y. Zhao, D. G. Truhlar, Theor. Chem. Acc. 2008, 120, 215–241.
(3) E. H. Krenske, R. C. Petter, K. N. Houk, J. Org. Chem. 2016, 81, 11726–11733.

(4) Legault, C. Y. CYLview, 1.0b; Université de Sherbrooke, ***2009*** (http://www.cylview.org).