Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Amphiphilic block copolymer from renewable ε-decalactone monomer: prediction and characterization of micelles core effects on indomethacin encapsulation and release

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Supporting Information

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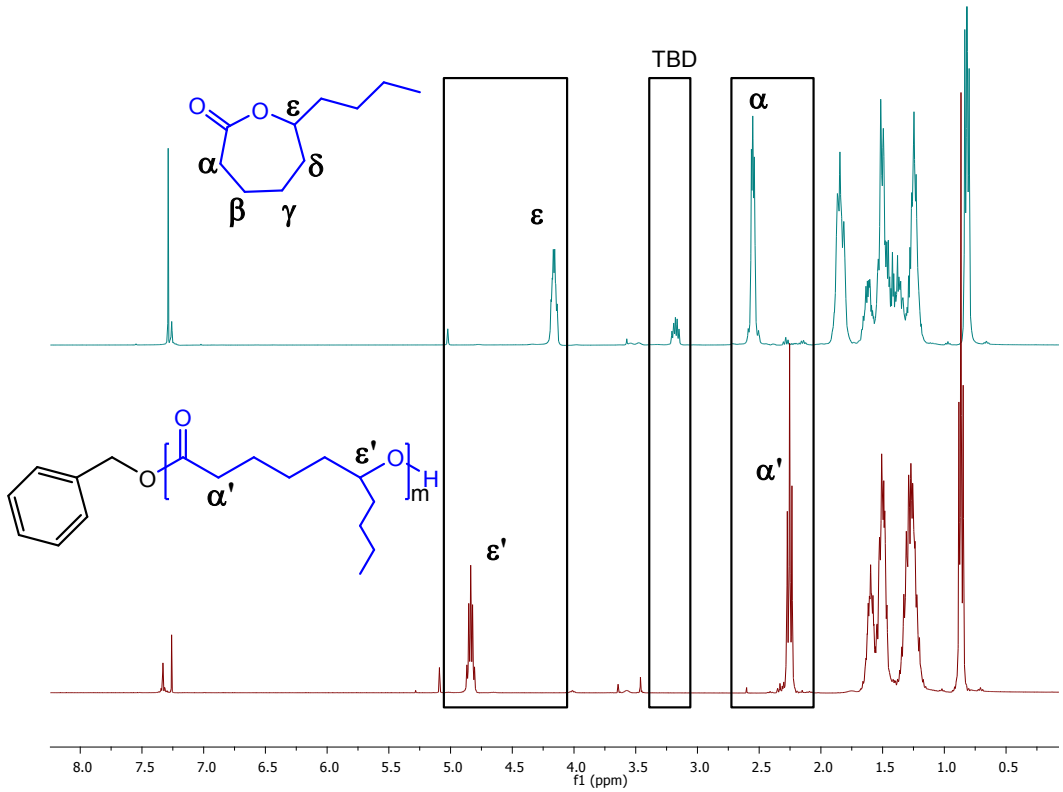


Figure S1 Peak positions in comparative ^{1}H NMR spectra before ε-DL polymerization and after ε-DL polymerization.

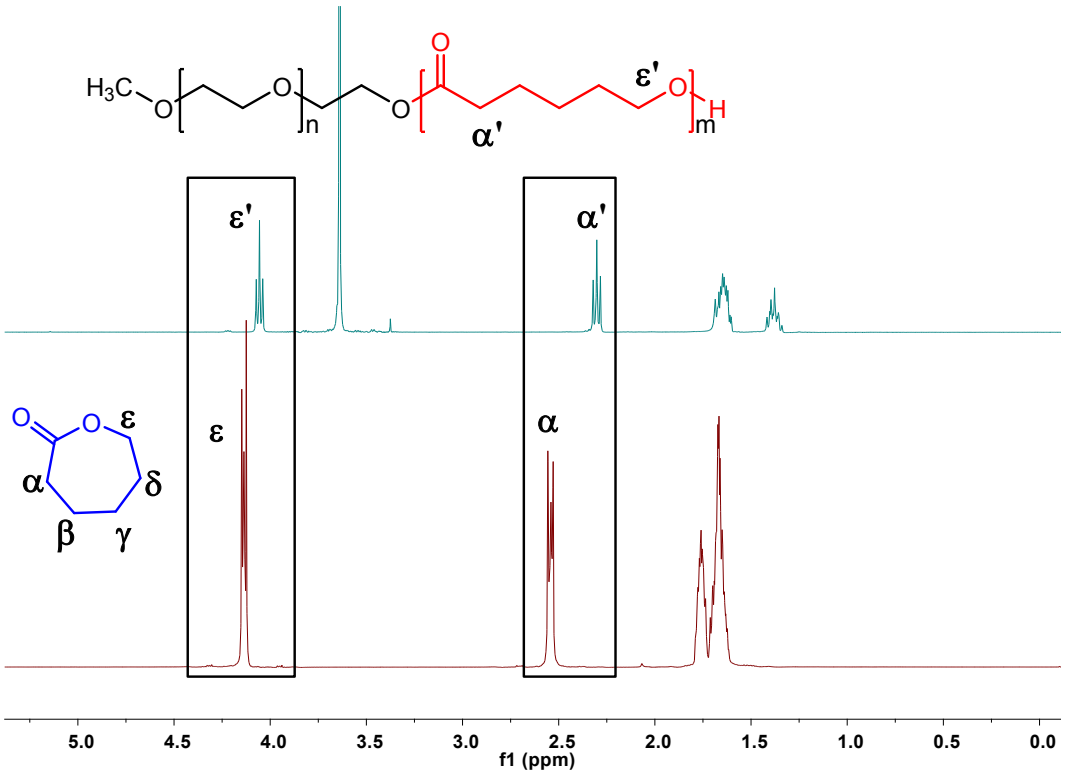


Figure S2 Peak positions in comparative ^{1}H NMR spectra before ε-CL polymerization and after ε-CL polymerization.

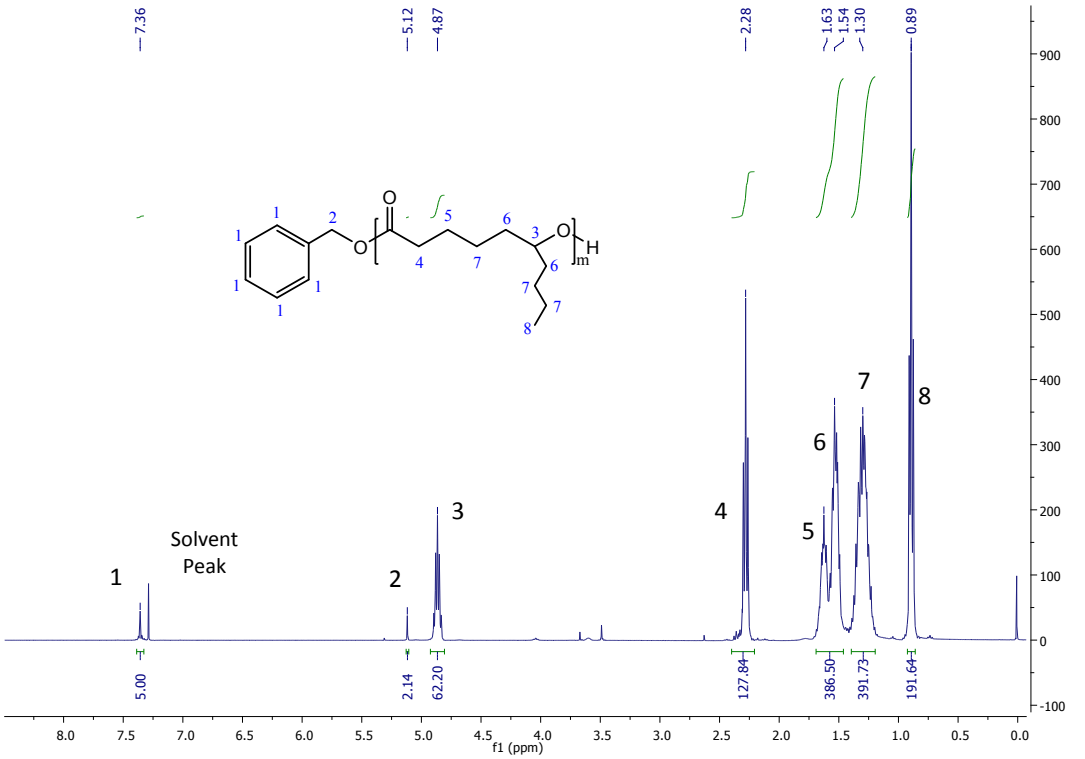


Figure S3 ^{1}H NMR spectrum with peak assignments of poly(ε-decalactone) (PεDL) homopolymer in $CDCl_3$

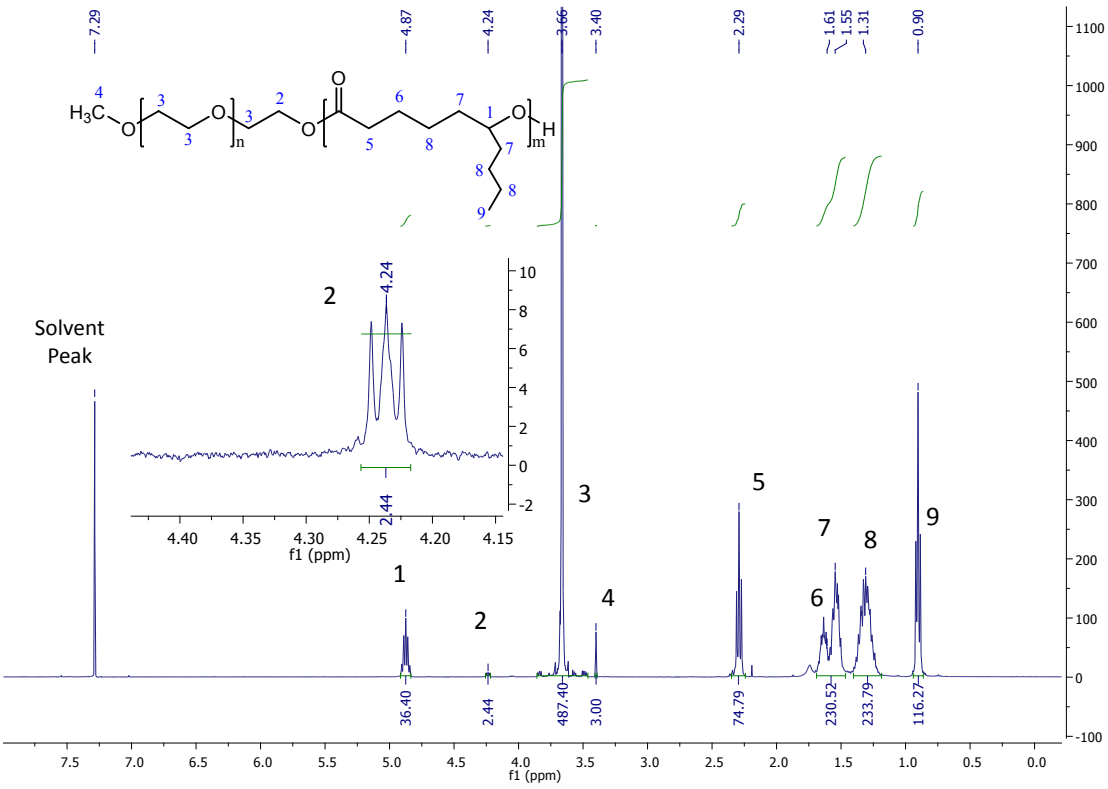


Figure S4 ^{1}H NMR spectrum with peak assignments of methoxy poly(ethyleneglycol)-*b*-poly(ε-decalactone) (mPEG-*b*-PεDL) copolymer in $CDCl_3$

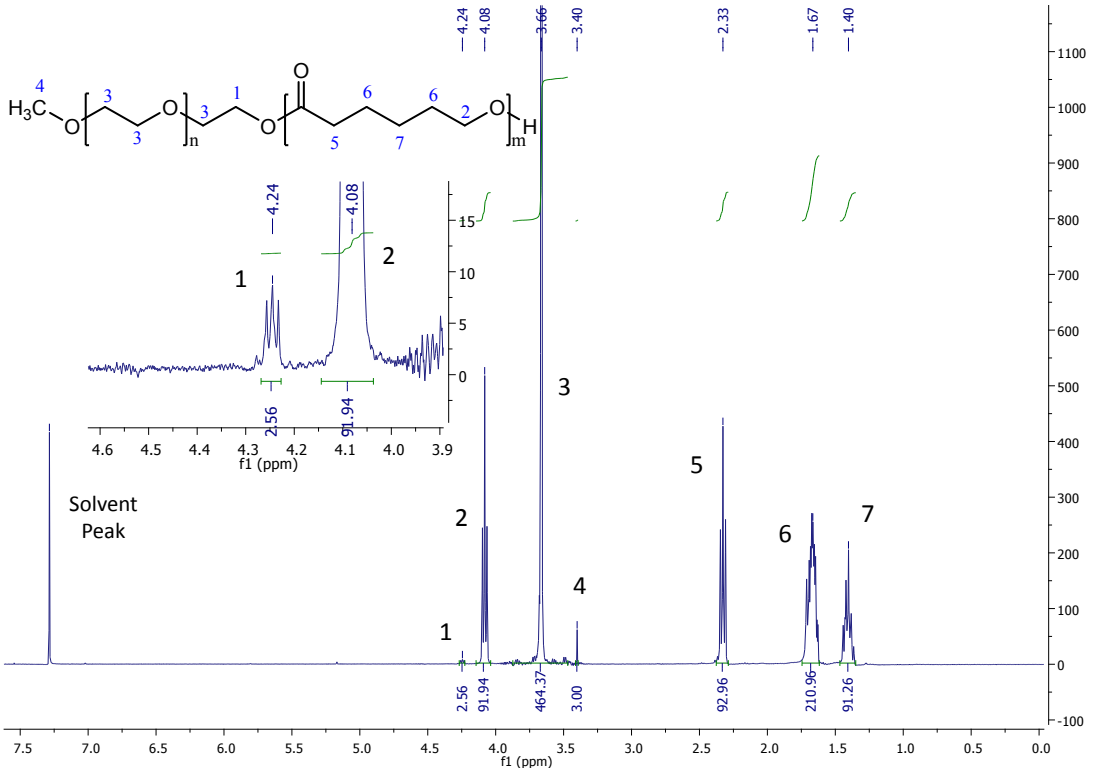


Figure S5 ^{1}H NMR spectrum with peak assignments of methoxy poly(ethyleneglycol)-*b*-poly(ε-caprolactone) (mPEG-*b*-PCL) copolymer in $CDCl_3$

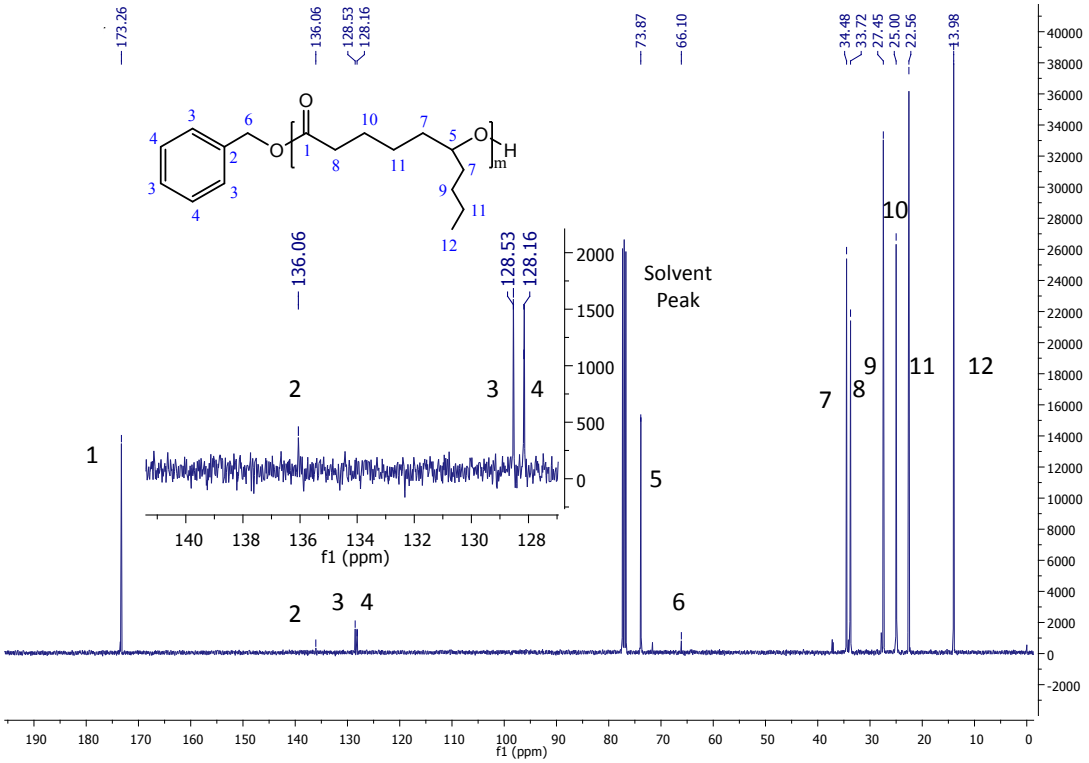


Figure S6 ^{13}C NMR spectrum with peak assignments of poly(ε-decalactone) (PεDL) homopolymer in $CDCl_3$

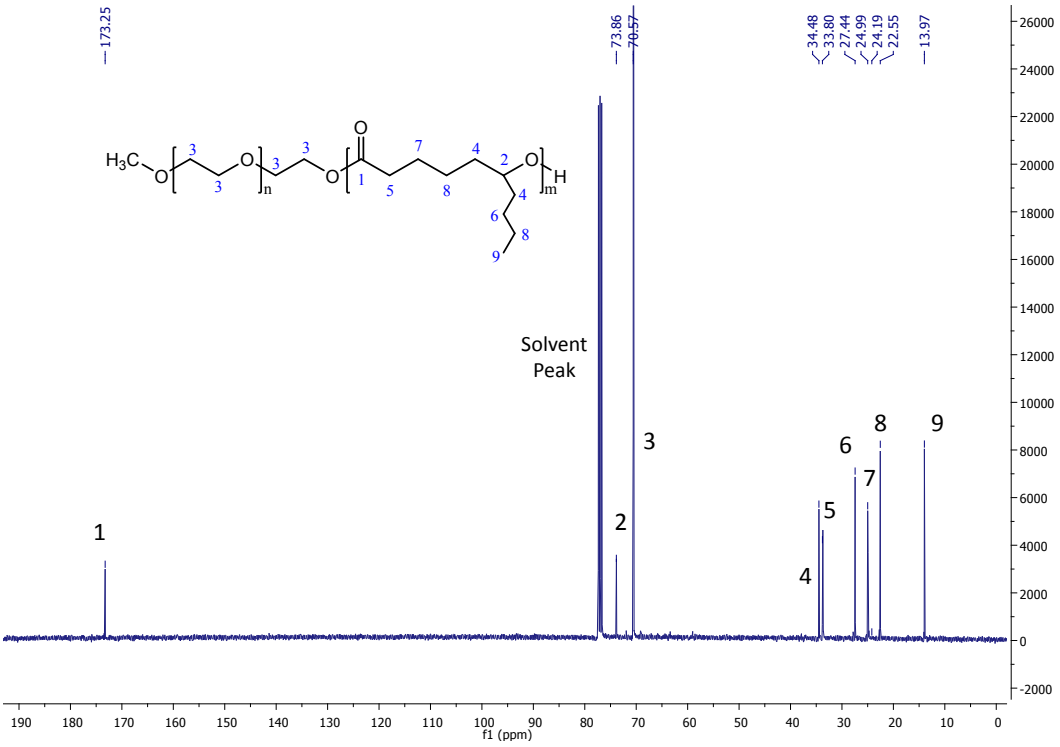


Figure S7 ^{13}C NMR spectrum with peak assignments of methoxy poly(ethyleneglycol)-*b*-poly(ε-decalactone) (mPEG-*b*-PεDL) copolymer in $CDCl_3$

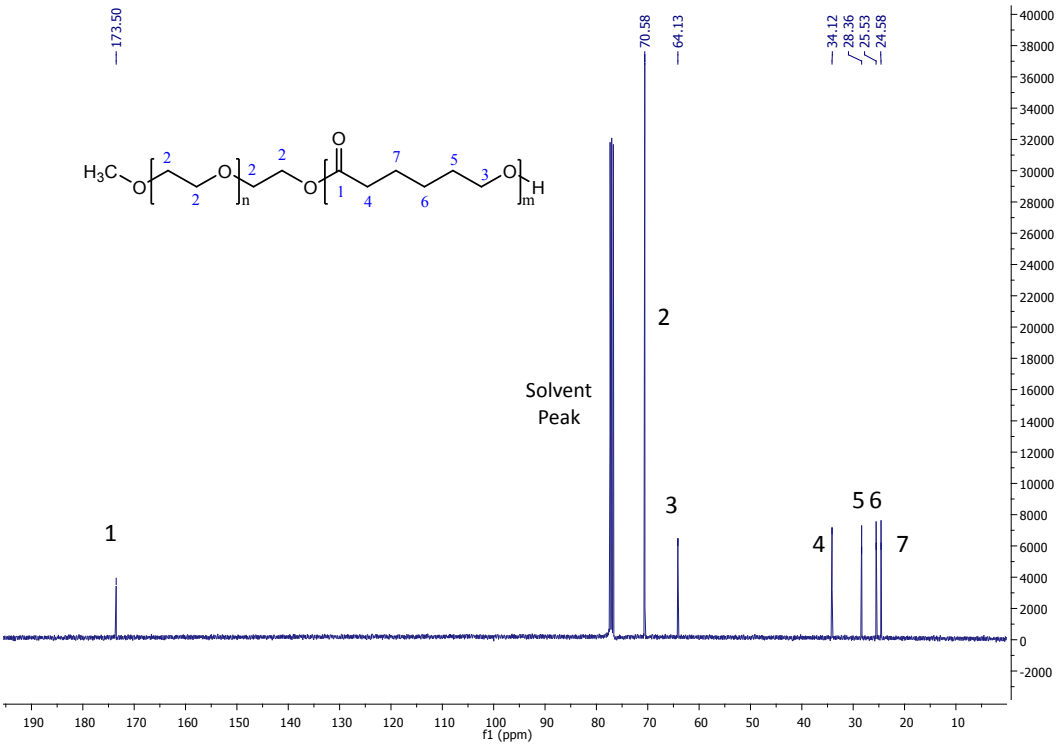


Figure S8 ^{13}C NMR spectrum with peak assignments of methoxy poly(ethyleneglycol)-b-poly(ε-caprolactone) (mPEG-*b*-PCL) copolymer in $CDCl_3$

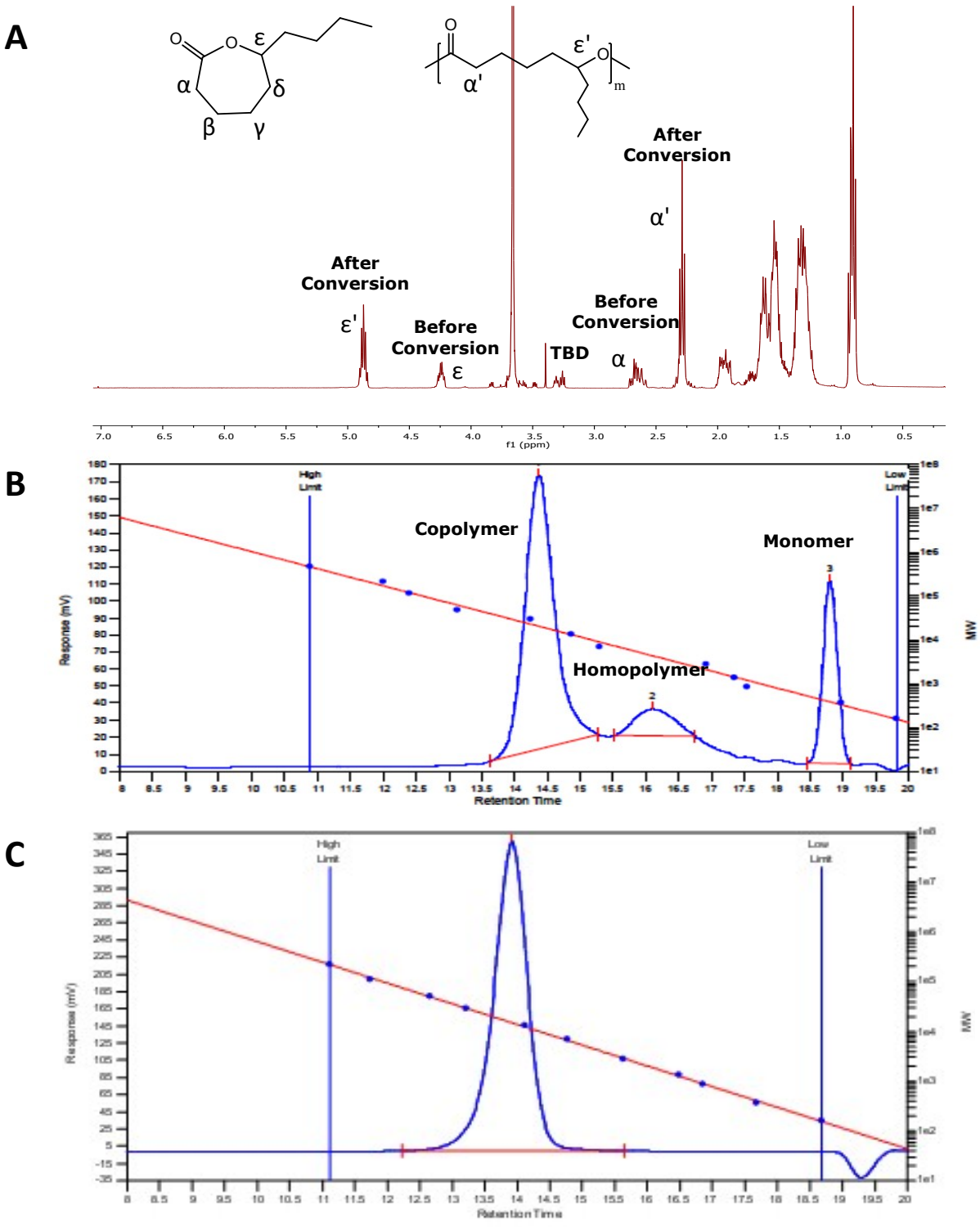


Figure S9 Position of peaks before and after conversion of ε-DL monomer in ^{1}H NMR of unpurified methoxy poly(ethyleneglycol)-*b*-poly(ε-decalactone) (mPEG-*b*-PεDL) copolymer (A), GPC of unpurified copolymer (B), GPC of purified copolymer (C).

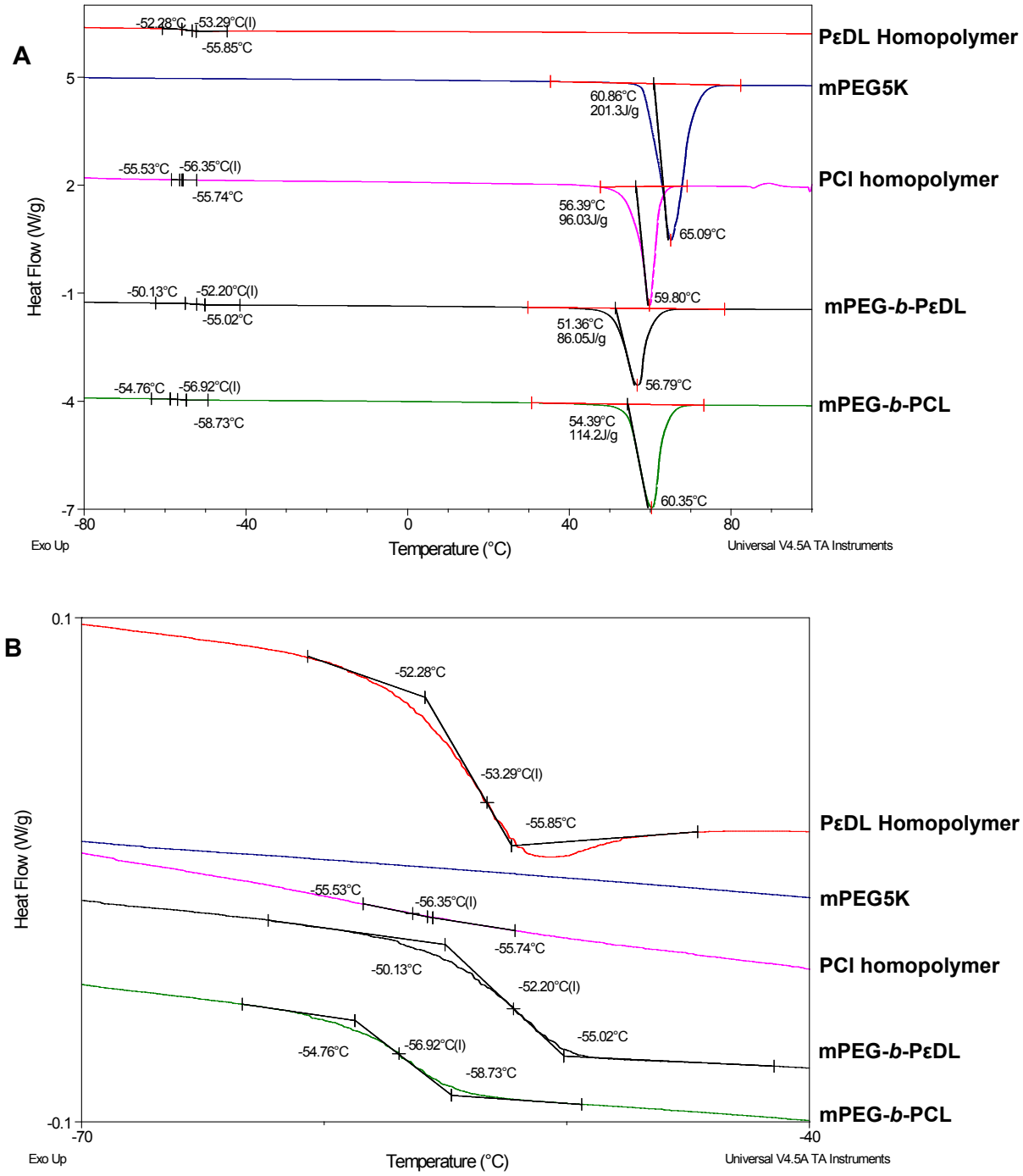
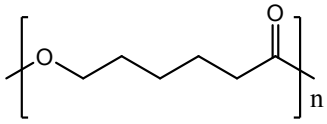


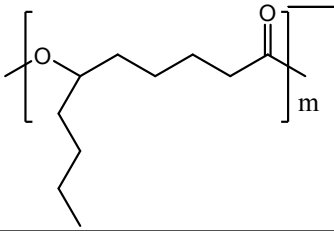
Figure S10 DSC graphs of homopolymers and copolymers (A) Graph shows glass transition (T_g) and melting temperature (T_m) (B) Expended view of glass transition (T_g) temperatures.

Table S1 Determination of Hansen partial solubility parameters and total solubility parameter of polymer segments and indomethacin (The values for molar volume (V) was taken from Fedors method[1] and the values for F_d (dispersion forces), F_p (polar or electrostatic interactions), and E_h (hydrogen bonding) for specific functional groups were taken from Barton[2]).

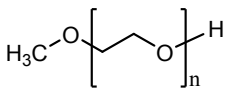
PCL Polymer

Fragments	Frequency	V (cm^3 mol^{-1})	Hansen solubility parameter					
			F_d ($J^{1/2}$ $cm^{3/2}$ mol^{-1})		F_p^2 ($J^{1/2}$ $cm^{3/2}$ mol^{-1})		E_h (J mol^{-1})	
COO	1	1x18	1x390	390	$(1x490)^2$	240100	1x7000	7000
CH_2	5	5x16.1	5x270	1350	$(5x0)^2$	0	5x0	0
		98.5		1740		240100		7000
			$\delta_d = F_d/V$		$\delta_p = (F_{pi}^2)^{1/2}/V)$		$\delta_h = (E_h/V)^{1/2}$	
			$\delta_d = (1740/98.5)$		$\delta_p = (240100)^{1/2}/98.5)$		$\delta_h = (7000/98.5)^{1/2}$	
			17.66 $MPa^{1/2}$		4.97 $MPa^{1/2}$		8.42 $MPa^{1/2}$	
			$\delta_T = (\delta_d^2+\delta_p^2+\delta_h^2)^{1/2}$		$(17.66^2+4.97^2+8.42^2)^{1/2}$		20.18 $MPa^{1/2}$	

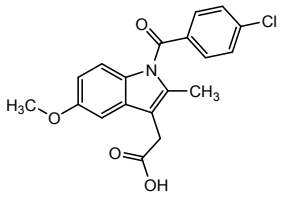
PεDL Polymer

Fragments	Frequency	V (cm^3 mol^{-1})	Hansen solubility parameter					
			F_d ($J^{1/2}$ $cm^{3/2}$ mol^{-1})		F^2_p($J^{1/2}$ $cm^{3/2}$ mol^{-1})		E_h (J mol^{-1})	
COO	1	18	1x390	390	$(1x490)^2$	240100	1x7000	7000
CH	1	-1	1x84	84	$(1x0)^2$	0	1x0	0
CH_2	7	7X16.1= 112.7	7x270	1890	$(7x0)^2$	0	7x0	0
CH_3	1	33.5	1x420	420	$(1x0)^2$	0	1x0	0
		163.2		2784		240100		7000
			$\delta_d = \sum F_d/V$		$\delta_p = (\sum F^2_p)^{1/2}/V)$		$\delta_h = (\sum E_h/V)^{1/2}$	
			$\delta_d = (2784/163.2)$		$\delta_p = (240100)^{1/2}/163.2)$		$\delta_h = (7000/163.2)^{1/2}$	
			17.05 $MPa^{1/2}$		3.00 $MPa^{1/2}$		6.54 $MPa^{1/2}$	
			$\delta_T = (\delta_d^2+\delta_p^2+\delta_h^2)^{1/2}$		$(17.05^2+3.00^2+6.54^2)^{1/2}$		18.5 $MPa^{1/2}$	

PEG Polymer

Fragments	Frequency	V (cm^3 mol^{-1})	Hansen solubility parameter					
			F_d ($J^{1/2}$ $cm^{3/2}$ mol^{-1})		F^2_p($J^{1/2}$ $cm^{3/2}$ mol^{-1})		E_h (J mol^{-1})	
O	1	1X3.8	1X100	100	$1X(400)^2$	160000	1X3000	3000
CH_2	2	2X16.1	2X270	540	$2X(0)^2$	0	2X0	0
		36.0		640		160000		3000
			$\delta_d = \sum F_d/V$		$\delta_p = (\sum F^2_p)^{1/2}/V)$		$\delta_h = (\sum E_h/V)^{1/2}$	
			$\delta_d = (640/36.0)$		$\delta_p = (160000)^{1/2}/36.0)$		$\delta_h = (3000/36.0)^{1/2}$	
			17.77 $MPa^{1/2}$		11.11 $MPa^{1/2}$		9.12 $MPa^{1/2}$	
			$\delta_T = (\delta_d^2+\delta_p^2+\delta_h^2)^{1/2}$		$(17.77^2+11.11^2+9.12^2)^{1/2}$		22.85 $MPa^{1/2}$	

Indomethacin

Fragments	Frequency	V (cm^3 mol^{-1})	Hansen solubility parameter					
			F_d ($J^{1/2}$ $cm^{3/2}$ mol^{-1})		F^2_p($J^{1/2}$ $cm^{3/2}$ mol^{-1})		E_h (J mol^{-1})	
Cl	1	1X24.0	1X450	450	$1X(550)^2$	302500	1X400	400
N	1	1X5.0	1X20	20	$1X(800)^2$	640000	1X5000	5000
O	1	1X3.8	1X100	100	$1X(400)^2$	160000	1X3000	3000
C=O	1	1X10.8	1X290	290	$1X(770)^2$	592900	1X2000	2000
COOH	1	1X28.5	1X530	530	$1X(420)^2$	176400	1X10000	10000
CH_3	2	2X33.5	2X420	840	$2X(0)^2$	0	2X0	0
CH_2	1	1X16.1	1X270	270	$1X(0)^2$	0	1X0	0
›C=	2	2X-5.5	2X70	140	$2X(0)^2$	0	2X0	0
Disubstituted phenyl ring	1	1X52.4	1X1270	1270	$1X(110)^2$	12100	1X0	0
Trisubstituted phenyl ring	1	1X33.4	1X1110	1110	$1X(110)^2$	12100	1X0	0
		230.0		5020		1896000		20400
			$\delta_d = \sum F_d / V$		$\delta_p = (\sum F^2_p)^{1/2} / V)$		$\delta_h = (\sum E_h / V)^{1/2}$	
			δ_d = (5020/230.0)		$\delta_p = (1896000)^{1/2}/230.0)$		$\delta_h = (20400/230.0)^{1/2}$	
			21.8 $MPa^{1/2}$		6.0 $MPa^{1/2}$		9.4 $MPa^{1/2}$	
			$\delta_T = (\delta_d^2 + \delta_p^2 + \delta_h^2)^{1/2}$		$(21.8^2+6.0^2+9.4^2)^{1/2}$		24.5 $MPa^{1/2}$	

References

1. R. F. Fedors, *Polymer Engineering and Science*, 1974, **14**, 147-154.
2. A. Barton, *Handbook of Solubility Parameters and Other Cohesion Parameters*, CRC Press, Boca Raton, Florida, 2nd ed edn., 1991.