Supporting Information

Green Synthesis of Novel Polyesterurethane Materials from Epoxides and Carbon dioxide by New set of 1D Coordination Polymer Catalyst

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Contents

Table S1Important bond distance and bond angles for 1a……PageS2-S4
Table S2 Important bond lengths and angles for 1b……..PageS4-S5
Figure S1: Crystal packing diagram of 1b.....PageS6
FigureS2: TGA data of the 1D coordination polymer 1a……...PageS7
FigureS3: TGA data of the 1D coordination polymer 1b……PageS7
Figure S4: The UV vis titration experiment of 1a with epoxide 2 in DMSO…....PageS8
Figure S5: 1H NMR spectra of the ring opened diol 6……PageS8
FigureS6: 13C NMR of the ring opened diol 6……PageS8
Figure S7 : ESI MS data of the ring opened diol 6……..PageS9
Figure S8: 1H NMR of the ring opened diol 7……PageS9
Figure S9: 13C NMR of the ring opened diol 7……PageS10
Figure S10: ESI MS of the ring opened diol 7……..PageS11
Figure S11: 1H NMR of the polyesterurethane PEU1……PageS12
Figure S12: 13C NMR of PEU1……PageS12
Figure S13: 1H NMR of PEU2……....PageS13
FigureS14: 13C NMR of PEU2……PageS13
Figure S15: TGA data of PEU2……PageS14
Figure S16: DSC data of PEU2…….....PageS14
Figure S17: GPC result of PEU1……PageS15
Figure S18: GPC Result of PEU2……PageS15
Figure S19: SEM image and EDX spectra of the polyestrerurethane PEU1……PageS16
Figure S20-S21: FT-IR data for the proof of involvement of catalyst 1a in catalysis reaction ……..PageS16-S17
FigureS22: FTIR of catalyst 1a and regenerated catalyst 1a……..Page S17

FigureS23: Bar diagram representating yield of catalysis by 1a and regenerated 1a pageS18

FigureS24: FT-IR of the polyesterurethane PEU2……page S18

FigureS25-26: HPLC data of ring opened diols 6-7……page S19

Table S1. Bond lengths [Å] and angles [°] for 1a.

Co(1)-N(7)#1	2.0289(17)	N(1)-C(1)	1.376(3)
Co(1)-N(1)	2.0299(17)	C(14)-C(15)	1.382(3)
Co(1)-Cl(1)	2.2301(6)	C(14)-C(19)	1.400(3)
Co(1)-Cl(2)	2.2395(6)	C(15)-C(16)	1.401(3)
N(4)-C(8)	1.333(2)	C(8)-C(9)	1.387(3)
N(4)-C(12)	1.337(2)	C(8)-C(7)	1.512(3)
N(7)-N(6)	1.315(2)	C(12)-C(11)	1.387(3)
N(7)-C(15)	1.382(3)	C(12)-C(13)	1.507(3)
N(7)-Co(1)#2	2.0289(17)	C(7)-H(7A)	1.05(3)
N(5)-N(6)	1.336(2)	C(7)-H(7B)	0.97(3)
N(5)-C(14)	1.363(2)	C(13)-H(13A)	0.89(3)
N(5)-C(13)	1.455(2)	C(13)-H(13B)	0.95(2)
N(3)-N(2)	1.337(2)	C(2)-C(1)	1.396(3)
N(3)-C(2)	1.352(3)	C(2)-C(3)	1.399(3)
N(3)-C(7)	1.456(3)	C(16)-C(17)	1.368(3)
N(1)-N(2)	1.313(2)	C(16)-H(16)	1.02(2)
C(1)-C(6)	1.403(3)	C(6)-H(6)	1.05(4)
C(11)-C(10)	1.378(3)	C(18)-C(17)	1.414(4)
C(11)-H(11)	1.01(3)	C(18)-H(18)	0.98(3)
C(19)-C(18)	1.366(3)	C(3)-C(4)	1.366(4)
C(19)-H(19)	0.92(3)	C(3)-H(3)	0.93(3)
C(9)-C(10)	1.376(3)	C(17)-H(17)	0.93(3)
C(9)-H(9)	0.96(2)	C(5)-C(4)	1.412(4)
C(10)-H(10)	0.93(3)	C(5)-H(5)	1.04(3)
C(6)-C(5)	1.364(4)	C(4)-H(4)	0.96(3)

N(7)#1-Co(1)-N(1)	111.64(7)	N(7)#1-Co(1)-Cl(2)	105.35(5)
N(7)#1-Co(1)-Cl(1)	109.88(5)	N(1)-Co(1)-Cl(2)	111.45(5)
N(1)-Co(1)-Cl(1)	107.18(5)	Cl(1)-Co(1)-Cl(2)	111.41(3)
C(8)-N(4)-C(12)	117.43(16)	C(12)-C(13)-H(13A)	109.1(16)
N(6)-N(7)-C(15)	109.13(16)	N(5)-C(13)-H(13B)	105.7(13)
N(6)-N(7)-Co(1)#2	125.03(14)	C(12)-C(13)-H(13B)	109.5(13)

C(15)-N(7)-Co(1)#2	125.15(13)	H(13A)-C(13)-H(13B)	114(2)
N(6)-N(5)-C(14)	111.27(16)	N(3)-C(2)-C(1)	104.60(18)
N(6)-N(5)-C(13)	120.73(16)	N(3)-C(2)-C(3)	133.2(2)
C(14)-N(5)-C(13)	128.00(17)	C(1)-C(2)-C(3)	122.2(2)
N(7)-N(6)-N(5)	107.59(16)	C(17)-C(16)-C(15)	116.1(2)
N(2)-N(3)-C(2)	111.39(17)	C(17)-C(16)-H(16)	121.9(13)
N(2)-N(3)-C(7)	120.08(19)	C(15)-C(16)-H(16)	121.8(13)
C(2)-N(3)-C(7)	128.33(19)	N(1)-C(1)-C(2)	107.02(18)
N(2)-N(1)-C(1)	109.31(16)	N(1)-C(1)-C(6)	131.7(2)
N(2)-N(1)-Co(1)	123.68(14)	C(2)-C(1)-C(6)	121.3(2)
C(1)-N(1)-Co(1)	126.25(14)	C(10)-C(11)-C(12)	118.77(19)
N(1)-N(2)-N(3)	107.67(17)	C(10)-C(11)-H(11)	119.6(16)
N(5)-C(14)-C(15)	104.63(17)	C(12)-C(11)-H(11)	121.3(16)
N(5)-C(14)-C(19)	132.23(19)	C(18)-C(19)-C(14)	115.1(2)
C(15)-C(14)-C(19)	123.13(19)	C(18)-C(19)-H(19)	124.2(17)
C(14)-C(15)-N(7)	107.37(17)	C(14)-C(19)-H(19)	120.5(17)
C(14)-C(15)-C(16)	121.20(19)	C(10)-C(9)-C(8)	118.71(19)
N(7)-C(15)-C(16)	131.43(19)	C(10)-C(9)-H(9)	118.7(15)
N(4)-C(8)-C(9)	123.23(18)	C(8)-C(9)-H(9)	122.4(15)
N(4)-C(8)-C(7)	118.67(16)	C(9)-C(10)-C(11)	118.82(19)
C(9)-C(8)-C(7)	118.06(17)	C(9)-C(10)-H(10)	119.6(18)
N(4)-C(12)-C(11)	123.02(17)	C(11)-C(10)-H(10)	121.5(18)
N(4)-C(12)-C(13)	117.99(15)	C(5)-C(6)-C(1)	116.2(2)
C(11)-C(12)-C(13)	118.97(17)	C(5)-C(6)-H(6)	117.0(19)
N(3)-C(7)-C(8)	114.33(16)	C(1)-C(6)-H(6)	126.8(19)
N(3)-C(7)-H(7A)	108.6(14)	C(19)-C(18)-C(17)	122.4(2)
C(8)-C(7)-H(7A)	106.2(14)	C(19)-C(18)-H(18)	122.4(18)
N(3)-C(7)-H(7B)	107.2(17)	C(17)-C(18)-H(18)	115.2(18)
C(8)-C(7)-H(7B)	103.9(16)	C(4)-C(3)-C(2)	115.8(2)
H(7A)-C(7)-H(7B)	117(2)	C(4)-C(3)-H(3)	122.4(18)
N(5)-C(13)-C(12)	113.41(15)	C(2)-C(3)-H(3)	121.7(18)
N(5)-C(13)-H(13A)	105.3(16)	C(16)-C(17)-C(18)	122.1(2)
C(6)-C(5)-H(5)	121.1(17)	C(16)-C(17)-H(17)	118.1(17)
C(4)-C(5)-H(5)	116.4(17)	C(18)-C(17)-H(17)	119.7(17)

C(3)-C(4)-C(5)	122.4(3)	C(6)-C(5)-C(4)	122.2(3)
C(3)-C(4)-H(4)	121.6(19)	C(5)-C(4)-H(4)	115.8(19)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z

Table S2 Bond lengths [Å] and angles [°] for 1b.

Zn(1)-O(1)	1.980(2)	Zn(1)-O(1)#1	1.980(2)
Zn(1)-N(2)#1	2.0323(17)	Zn(1)-N(2)	2.0323(17)
N(5)-C(8)#2	1.331(2)	N(5)-C(8)	1.331(2)
N(2)-N(3)	1.319(3)	N(2)-C(1)	1.371(3)
N(4)-N(3)	1.323(3)	N(4)-C(2)	1.351(3)
N(4)-C(7)	1.466(3)	O(1)-N(1)	1.258(3)
N(1)-O(2)	1.189(3)	N(1)-O(3)	1.242(3)
C(8)-C(9)	1.388(3)	C(8)-C(7)	1.500(3)
C(2)-C(1)	1.394(3)	C(2)-C(3)	1.400(3)
C(1)-C(6)	1.412(3)	C(6)-C(5)	1.361(3)
C(6)-H(6)	1.03(3)	C(9)-C(10)	1.377(3)
C(9)-H(9)	0.91(4)	C(10)-H(10)	0.75(5)
C(3)-C(4)	1.357(4)	C(3)-H(3)	0.87(4)
C(7)-H(7A)	1.14(4)	C(7)-H(7B)	0.96(3)
C(5)-C(4)	1.420(4)	C(5)-H(5)	0.97(4)
C(4)-H(4)	0.81(5)		

O(1)-Zn(1)-O(1)#1	133.42(12)	O(1)-Zn(1)-N(2)#1	114.89(9)
O(1)#1-Zn(1)-N(2)#1	89.96(8)	O(1)-Zn(1)-N(2)	89.96(8)
O(1)#1-Zn(1)-N(2)	114.89(9)	N(2)#1-Zn(1)-N(2)	115.79(10)
C(8)#2-N(5)-C(8)	117.3(2)	N(3)-N(2)-C(1)	109.08(17)
N(3)-N(2)-Zn(1)	121.96(14)	C(1)-N(2)-Zn(1)	127.70(13)
N(3)-N(4)-C(2)	111.62(17)	N(3)-N(4)-C(7)	120.5(2)
C(2)-N(4)-C(7)	127.9(2)	N(1)-O(1)-Zn(1)	114.95(16)
N(2)-N(3)-N(4)	107.74(18)	O(2)-N(1)-O(3)	120.5(3)
O(2)-N(1)-O(1)	123.2(3)	O(3)-N(1)-O(1)	116.2(2)

N(5)-C(8)-C(9)	123.47(19)	N(5)-C(8)-C(7)	117.86(17)
C(9)-C(8)-C(7)	118.67(18)	N(4)-C(2)-C(1)	104.49(17)
N(4)-C(2)-C(3)	133.2(2)	C(1)-C(2)-C(3)	122.3(2)
N(2)-C(1)-C(2)	107.06(18)	N(2)-C(1)-C(6)	132.11(19)
C(2)-C(1)-C(6)	120.8(2)	C(5)-C(6)-C(1)	116.5(2)
C(5)-C(6)-H(6)	122.5(16)	C(1)-C(6)-H(6)	120.7(16)
C(10)-C(9)-C(8)	118.3(2)	C(10)-C(9)-H(9)	123(2)
C(8)-C(9)-H(9)	119(2)	C(9)#2-C(10)-C(9)	119.2(3)
C(9)#2-C(10)-H(10)	120.38(14)	C(9)-C(10)-H(10)	120.38(14)
C(4)-C(3)-C(2)	116.2(2)	C(4)-C(3)-H(3)	128(3)
C(2)-C(3)-H(3)	116(3)	N(4)-C(7)-C(8)	113.49(17)
N(4)-C(7)-H(7A)	106.5(18)	C(8)-C(7)-H(7A)	106.7(18)
N(4)-C(7)-H(7B)	97.5(19)	C(8)-C(7)-H(7B)	111.2(18)
H(7A)-C(7)-H(7B)	121(2)	C(6)-C(5)-C(4)	122.0(2)
C(6)-C(5)-H(5)	119(2)	C(4)-C(5)-H(5)	118(2)
C(3)-C(4)-C(5)	122.2(3)	C(3)-C(4)-H(4)	120(3)
C(5)-C(4)-H(4)	118(3)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2 #2 -x+1,y,-z+1/2

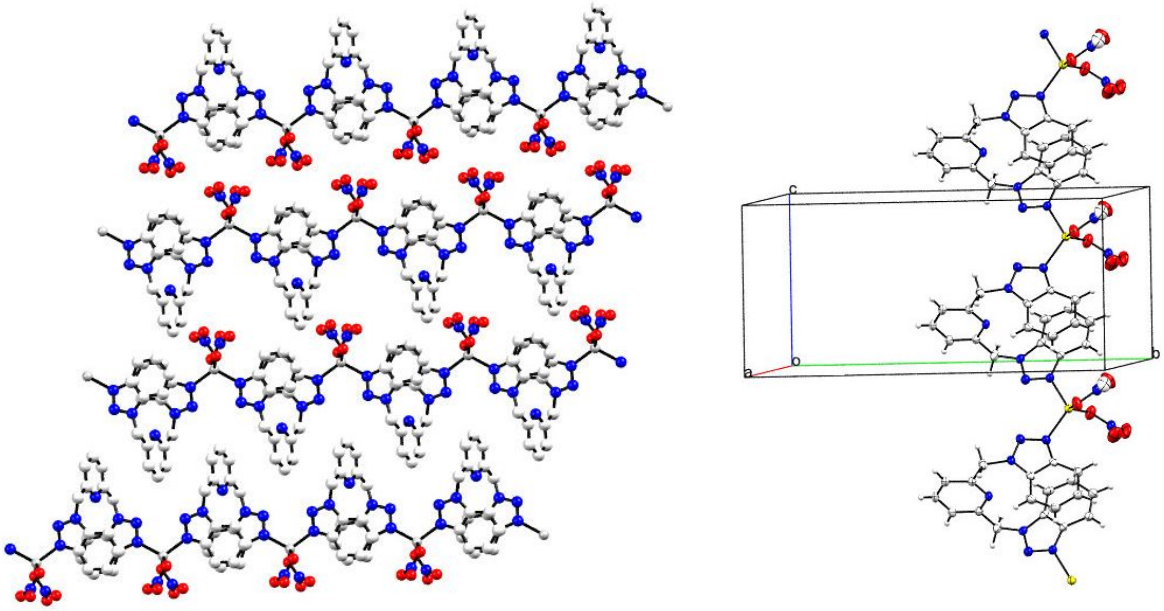
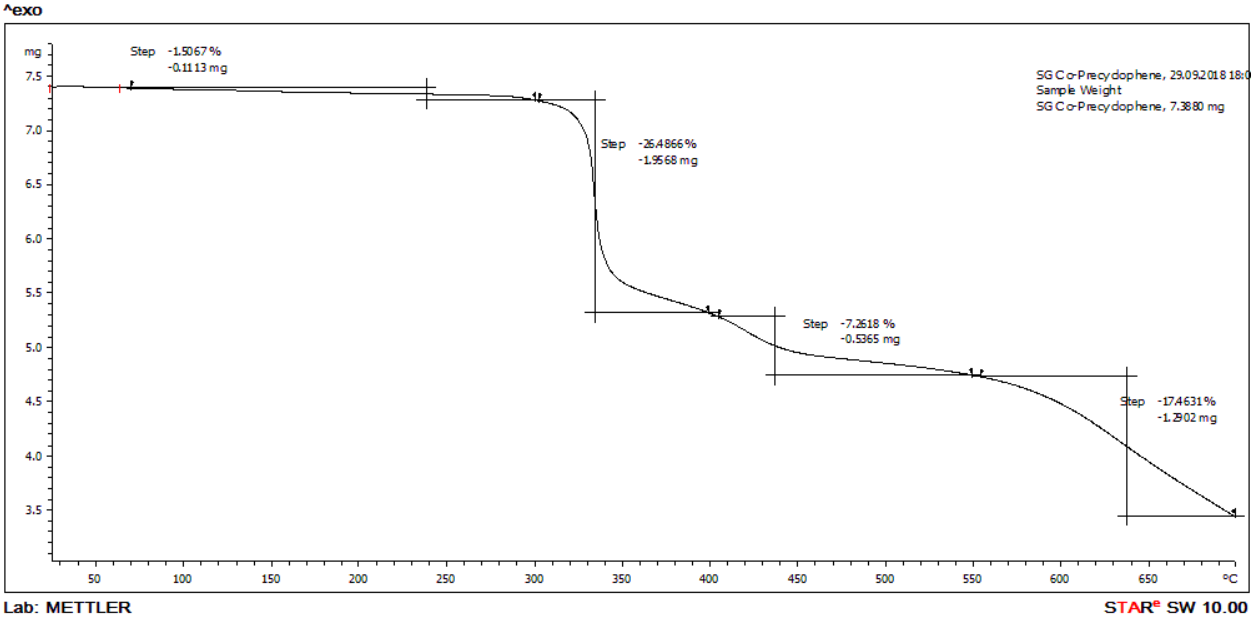
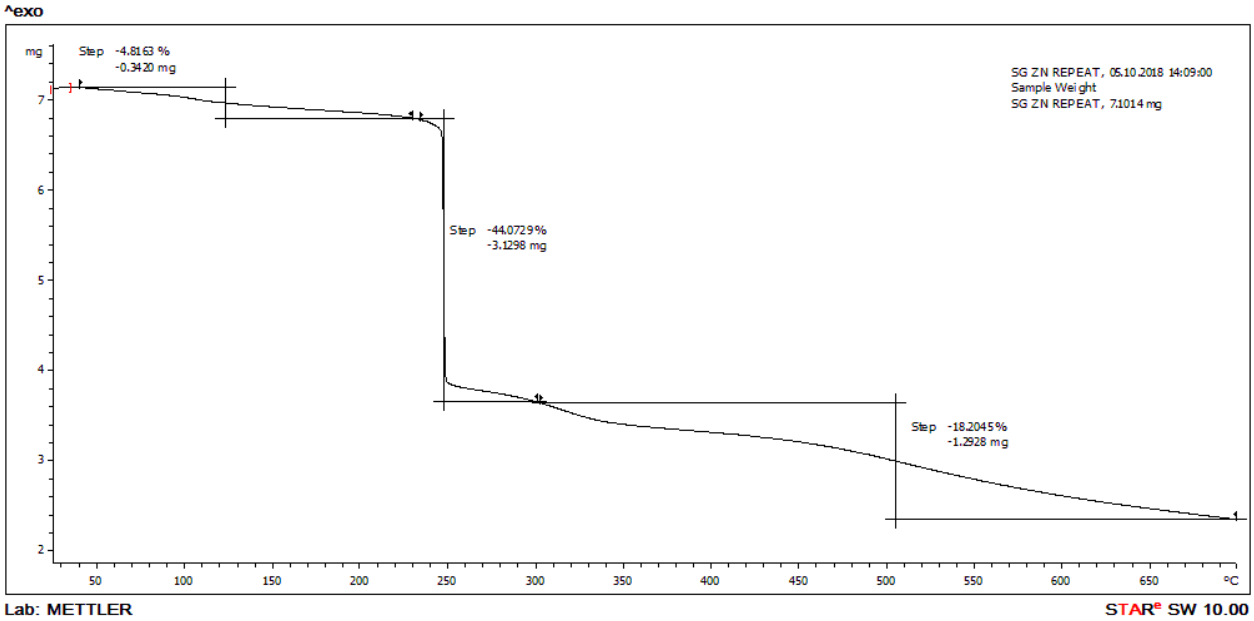


Figure S1: **Crystal packing diagram of 1b**.



FigureS2: TGA data of the 1D coordination polymer 1a.



FigureS3: TGA data of the 1D coordination polymer 1b.

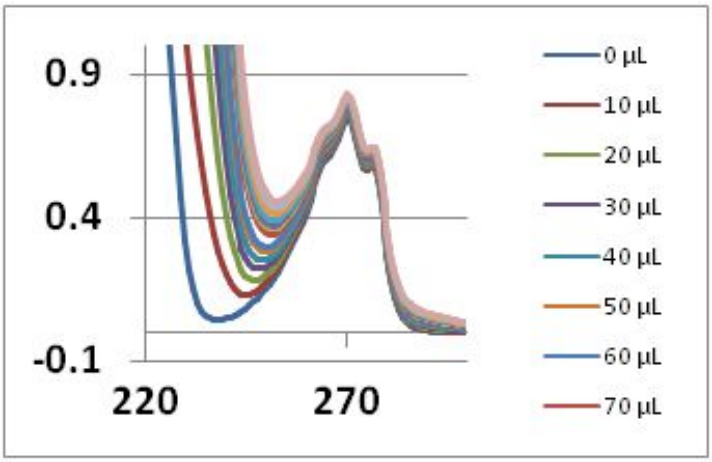


Figure S4: The UV vis titration experiment of 1a with epoxide 2 in DMSO.

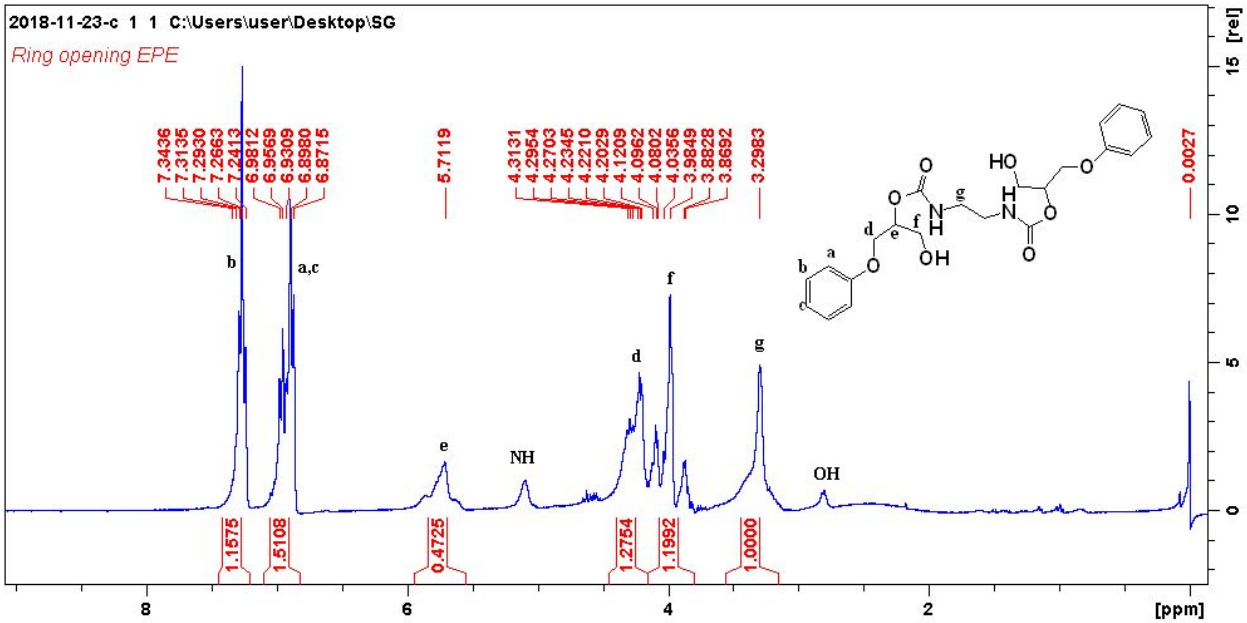
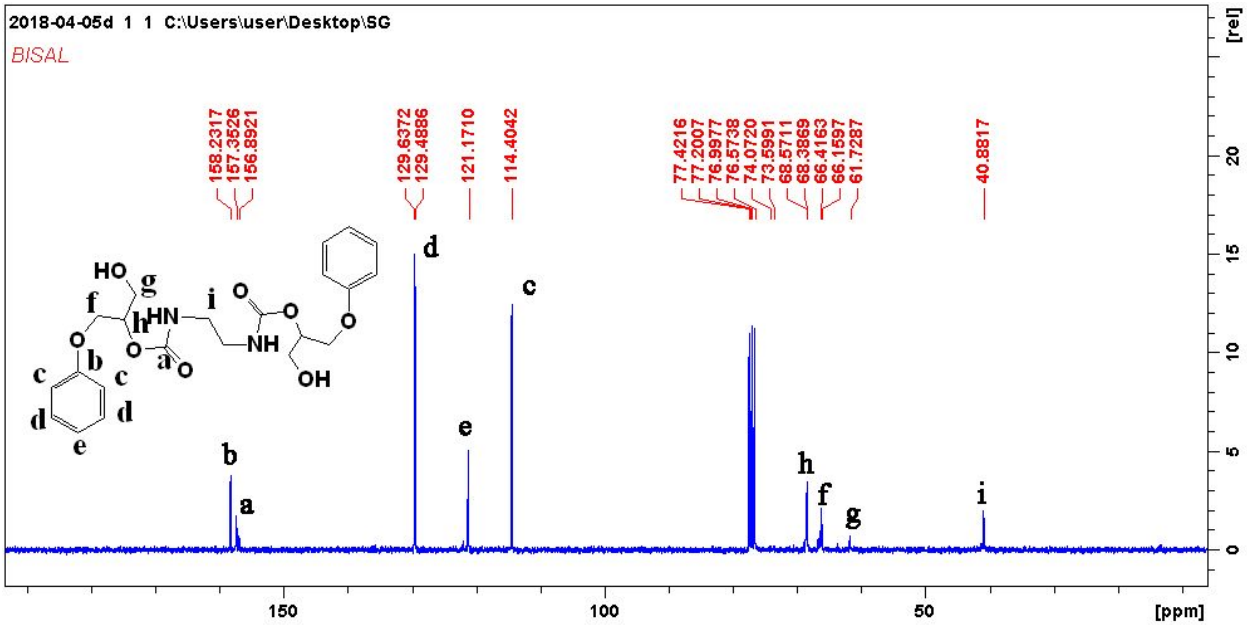


Figure S5: 1H NMR spectra of the ring opened diol 6.



FigureS6: 13C NMR of the ring opened diol 6.

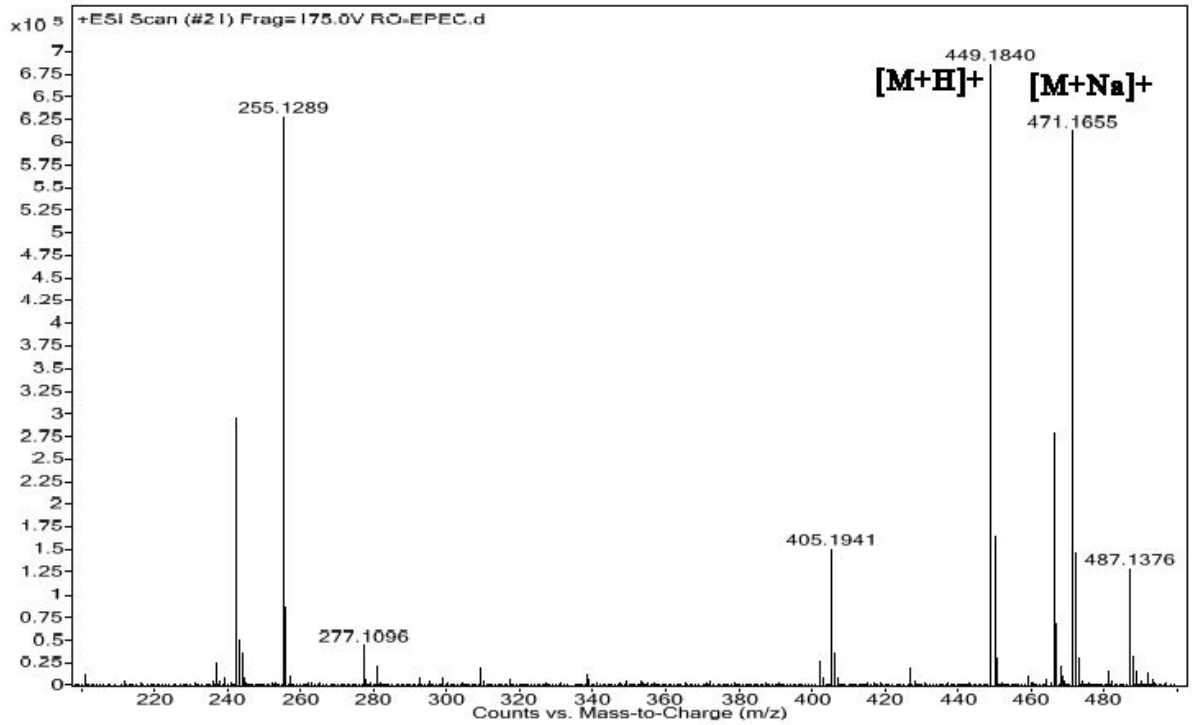


Figure S7 : ESI MS data of the ring opened diol 6.

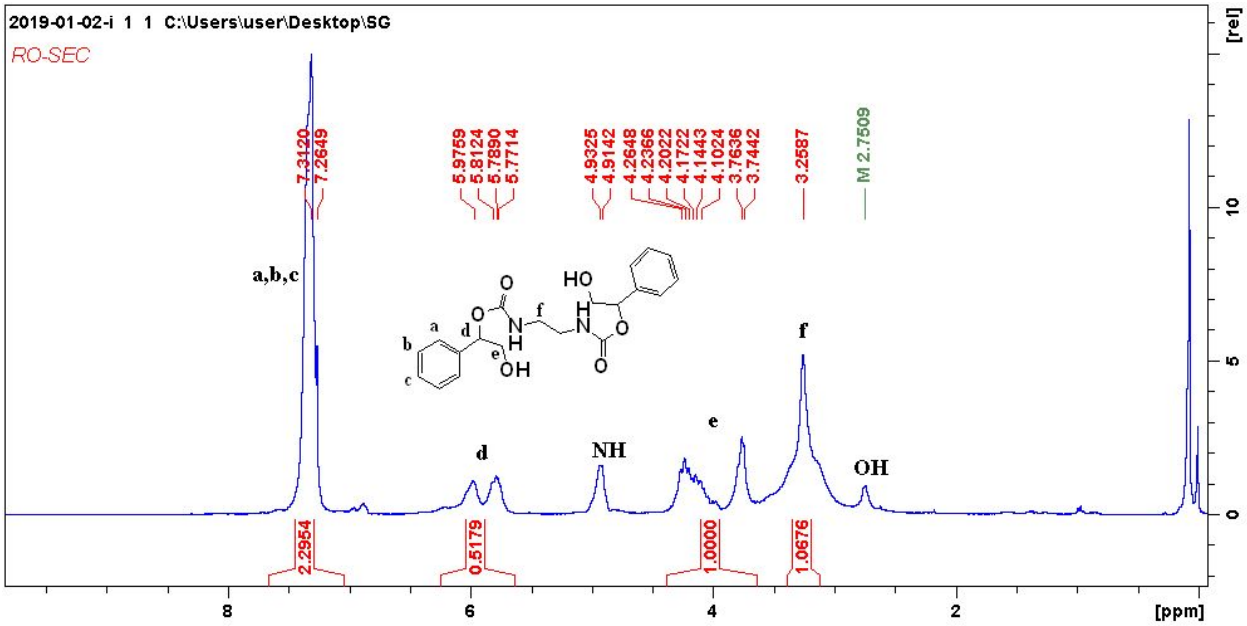


Figure S8: 1H NMR of the ring opened diol 7.

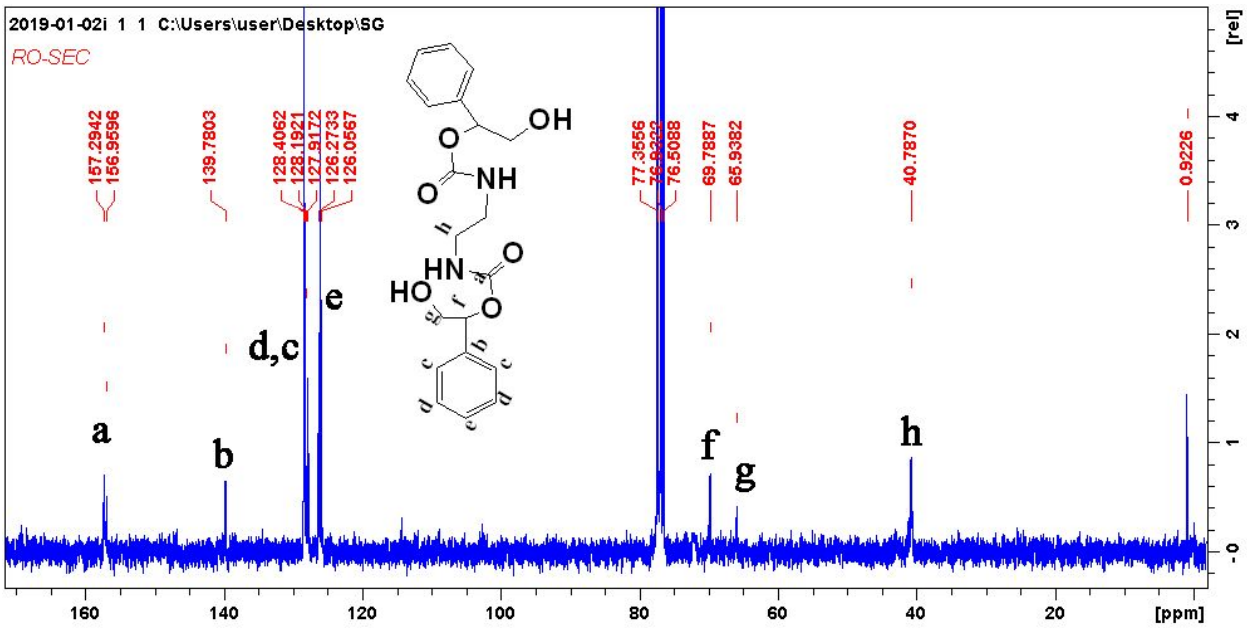


Figure S9: 13C NMR of the ring opened diol 7.

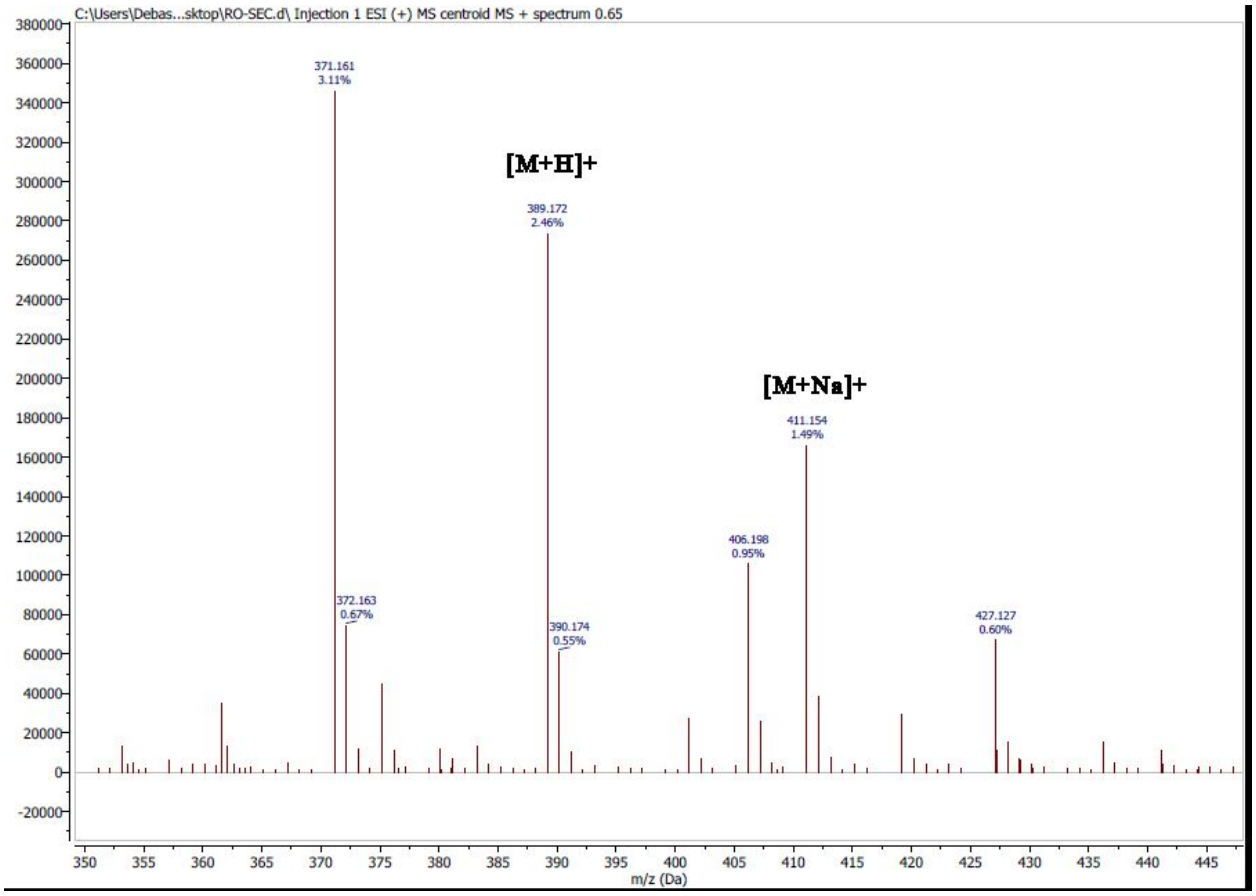


Figure S10: ESI MS of the ring opened diol 7.

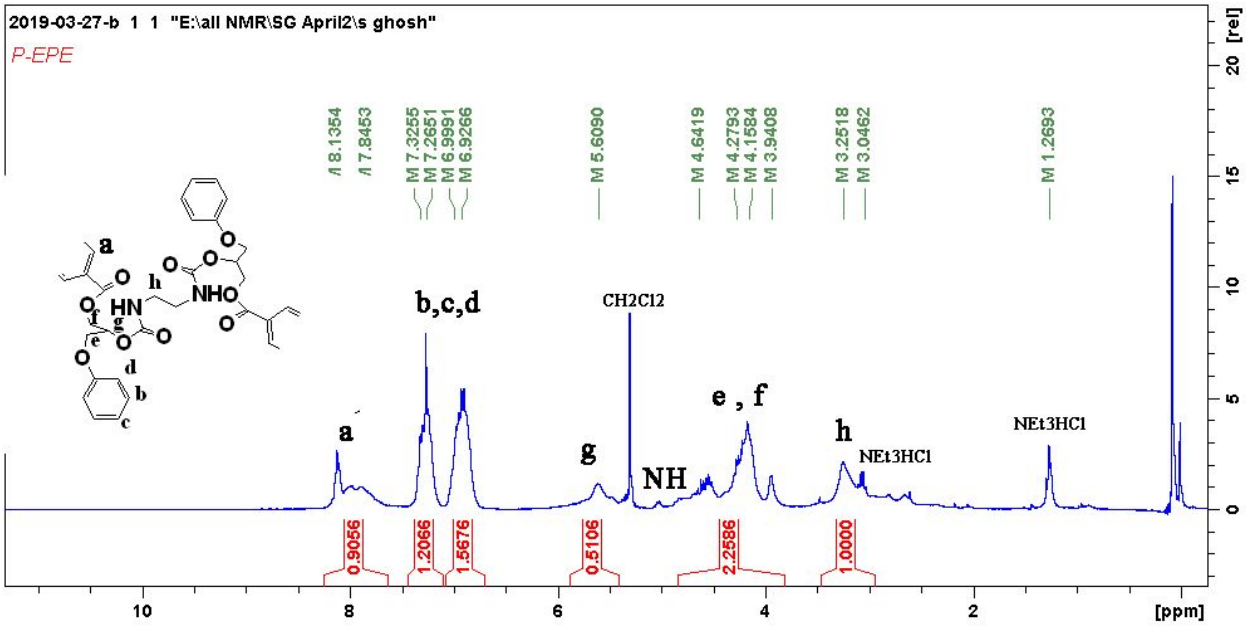


Figure S11: 1H NMR of the polyesterurethane PEU1.

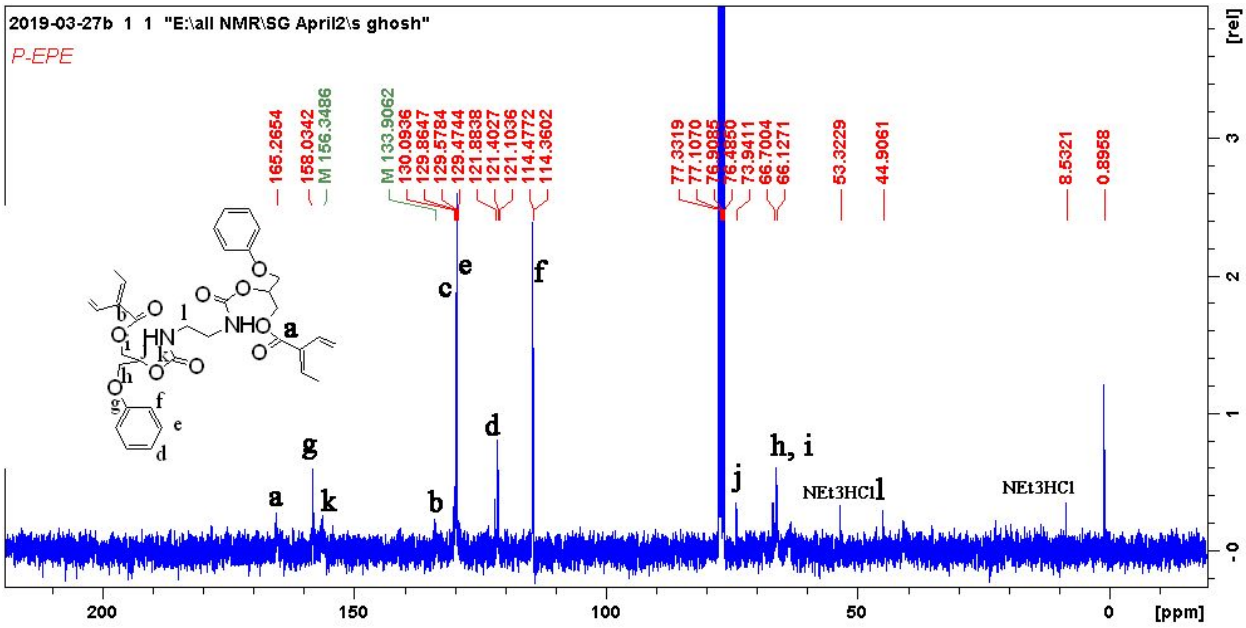


Figure S12: 13C NMR of PEU1.

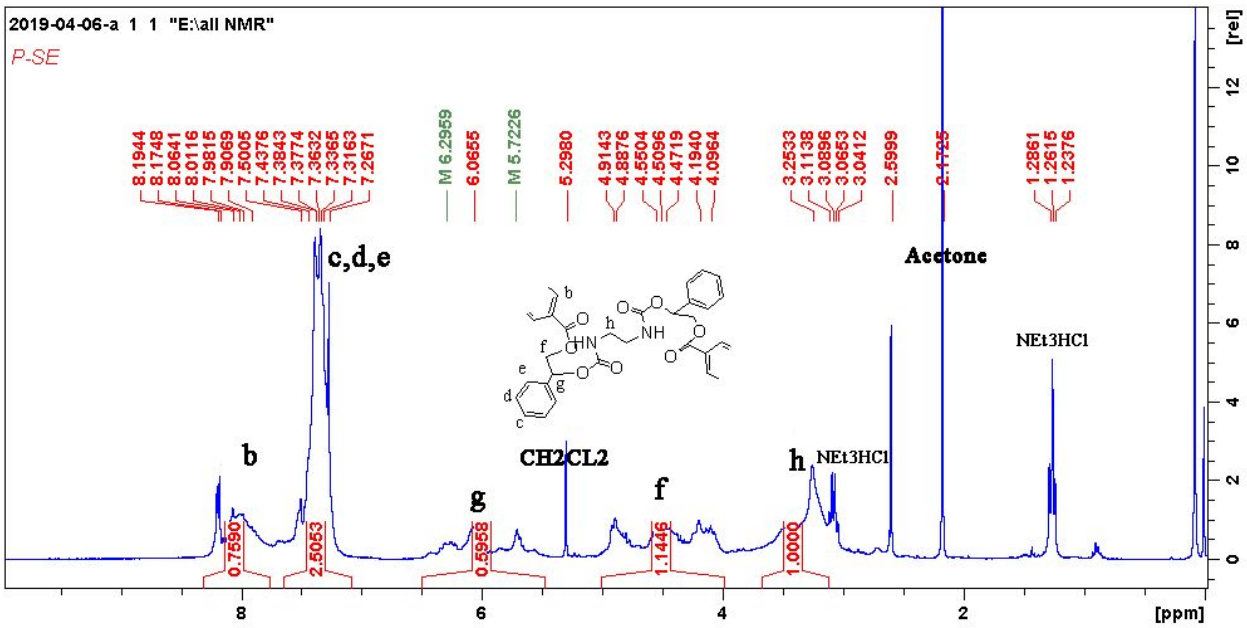
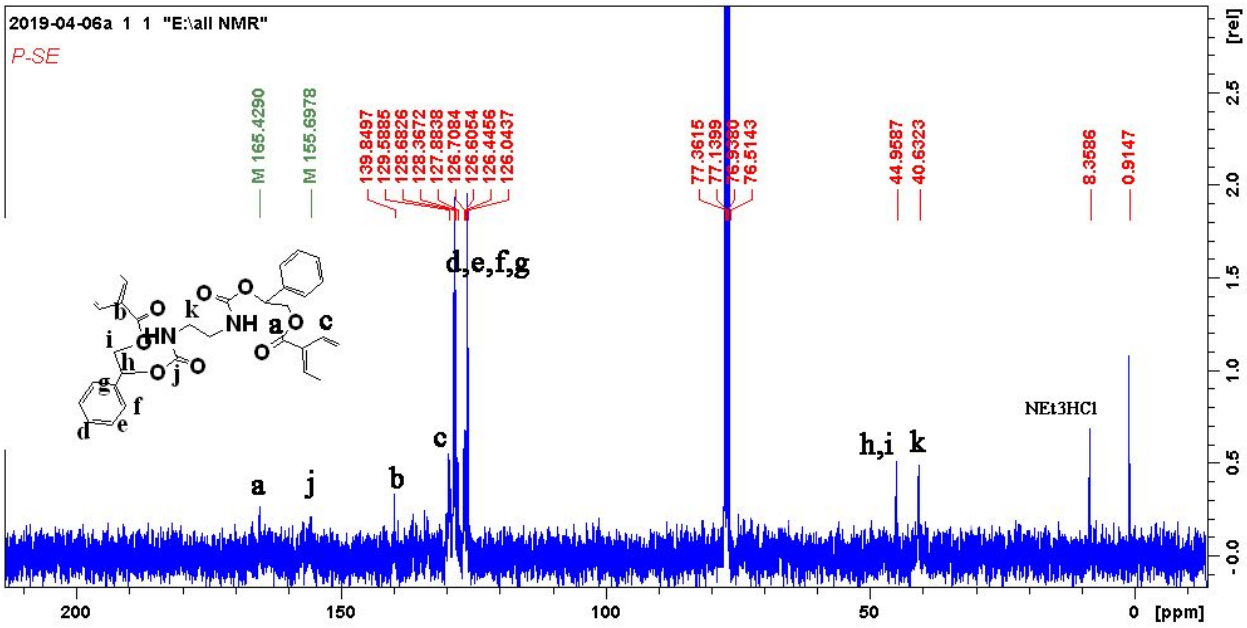


Figure S13: 1H NMR of PEU2.



FigureS14: 13C NMR of PEU2.

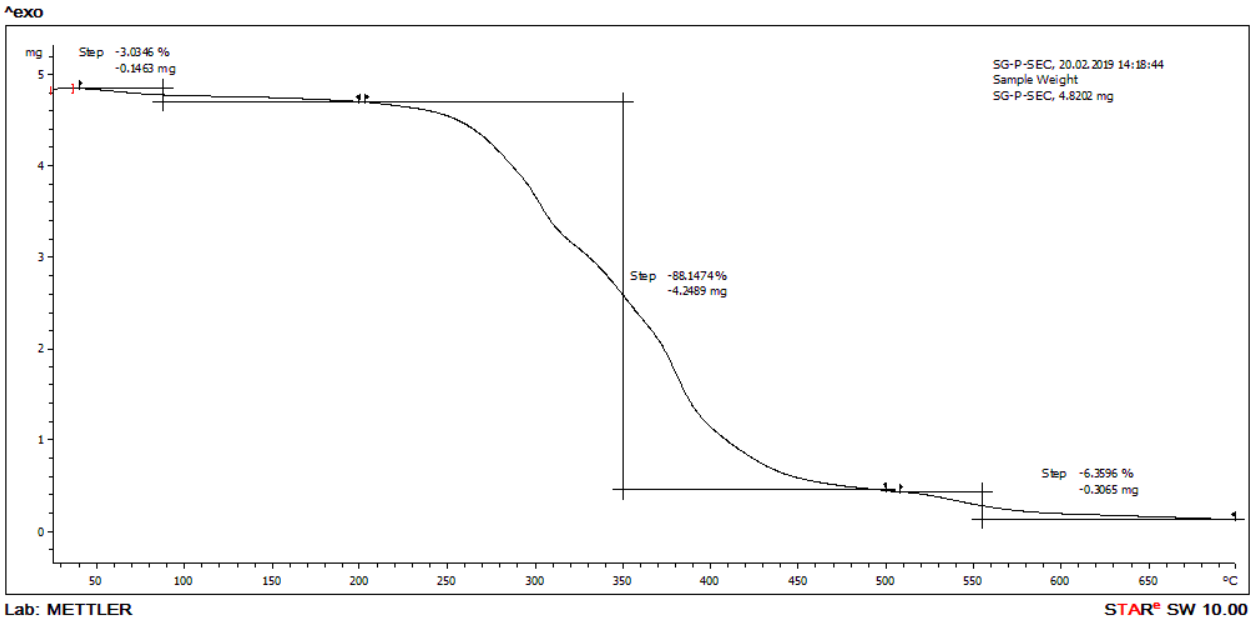


Figure S15: TGA data of PEU2.

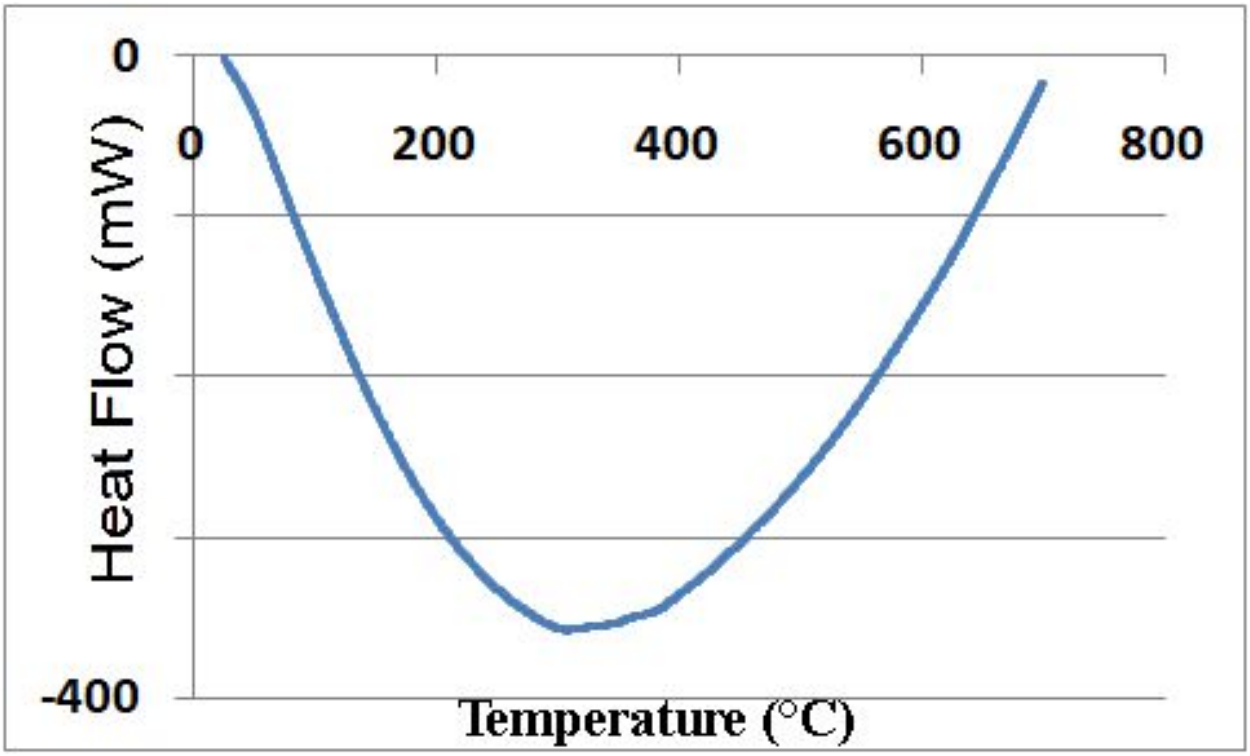
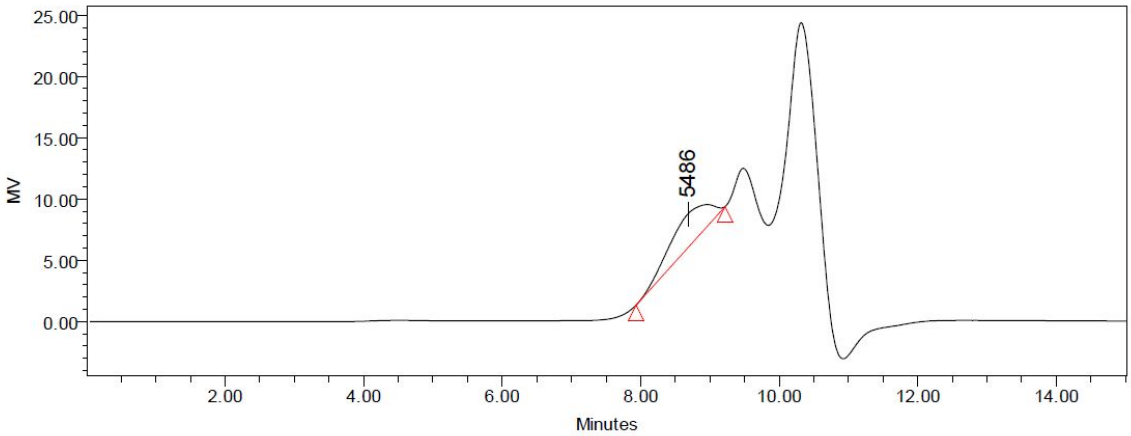
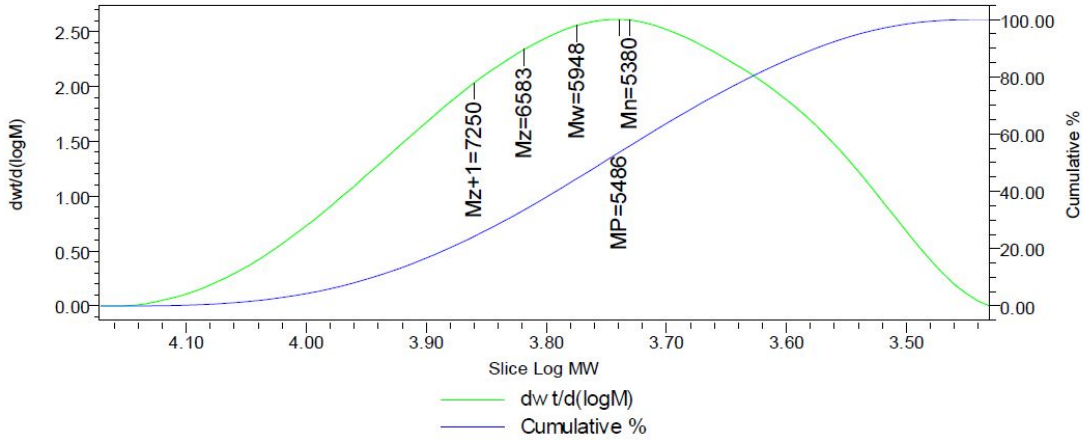


Figure S16: DSC data of PEU2.



GPC Results

	Retention Time (min)	% Area	Mn	Mw	MP	Mz	Mz+1	Poly dispersity
1	8.683	100.00	5380	5948	5486	6583	7250	1.105405



GPC Calibration Plot

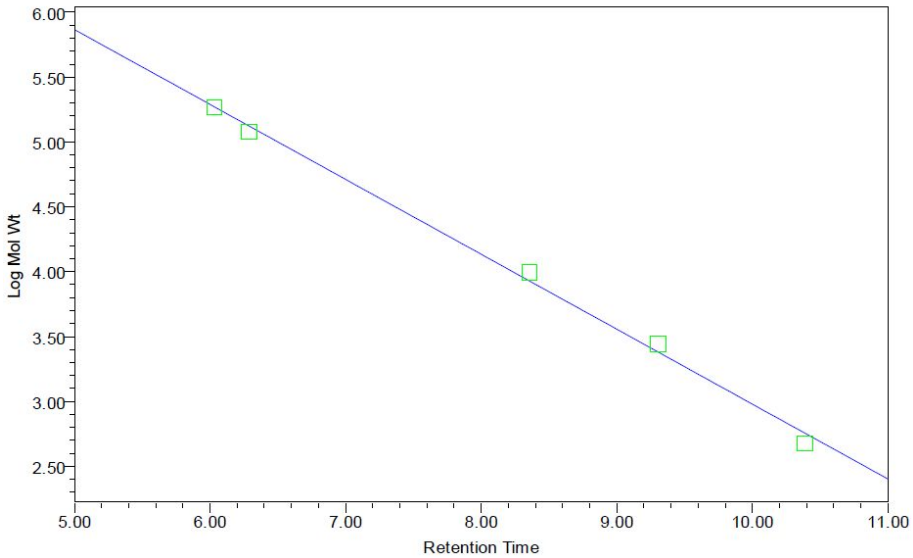
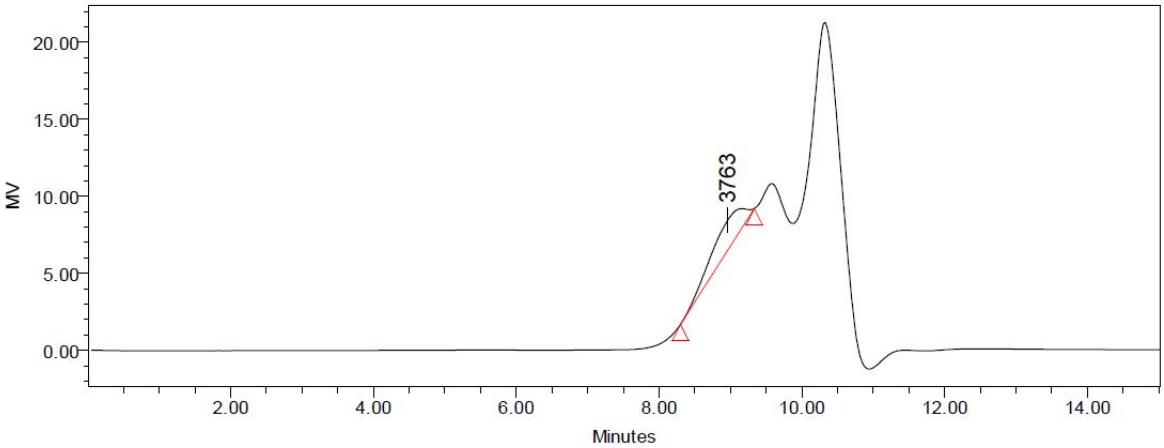
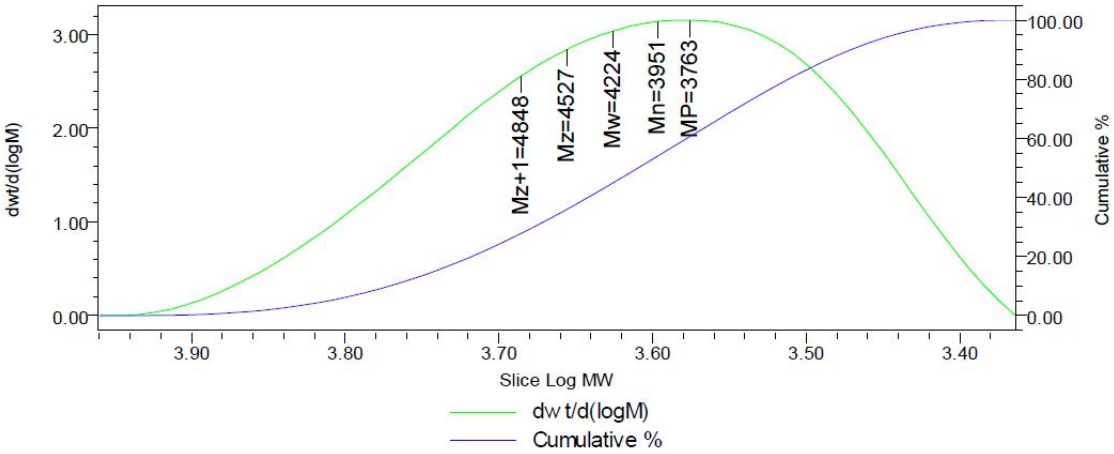


Figure S17: GPC result of PEU1



GPC Results

	Retention Time (min)	% Area	Mn	Mw	MP	Mz	Mz+1	Poly dispersity
1	8.967	100.00	3951	4224	3763	4527	4848	1.069042



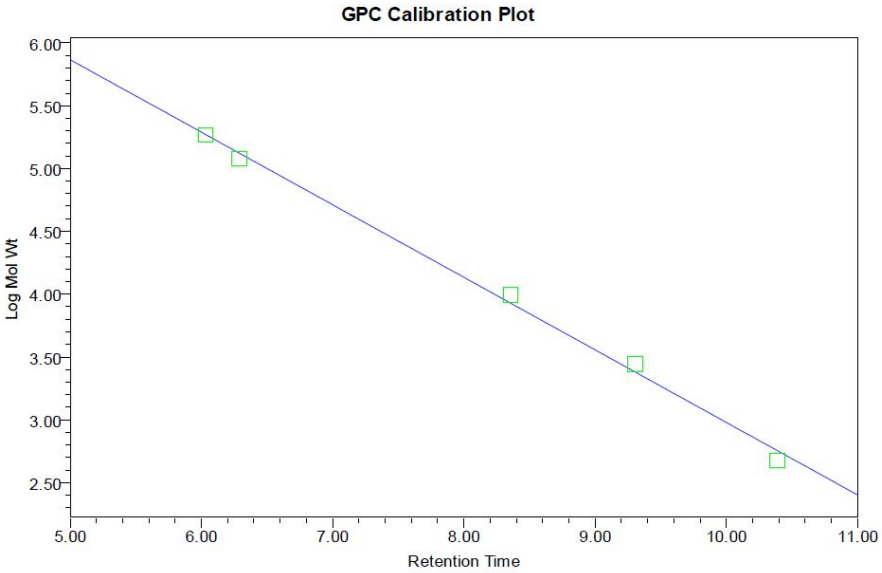


Figure S18: GPC Result of PEU2

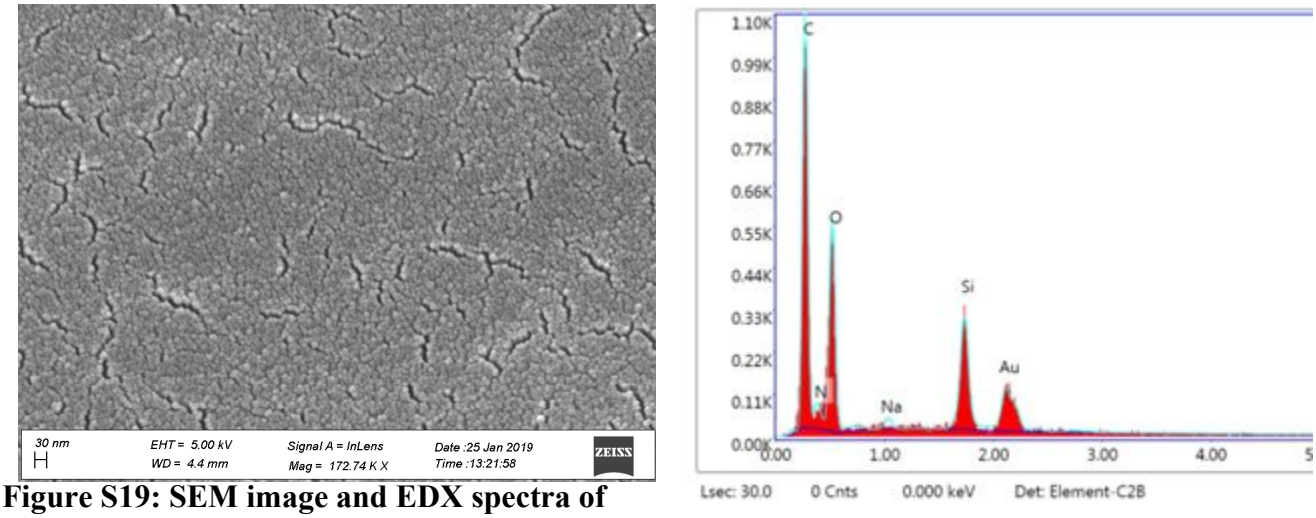


Figure S19: SEM image and EDX spectra of the polyestrerurethane PEU1.

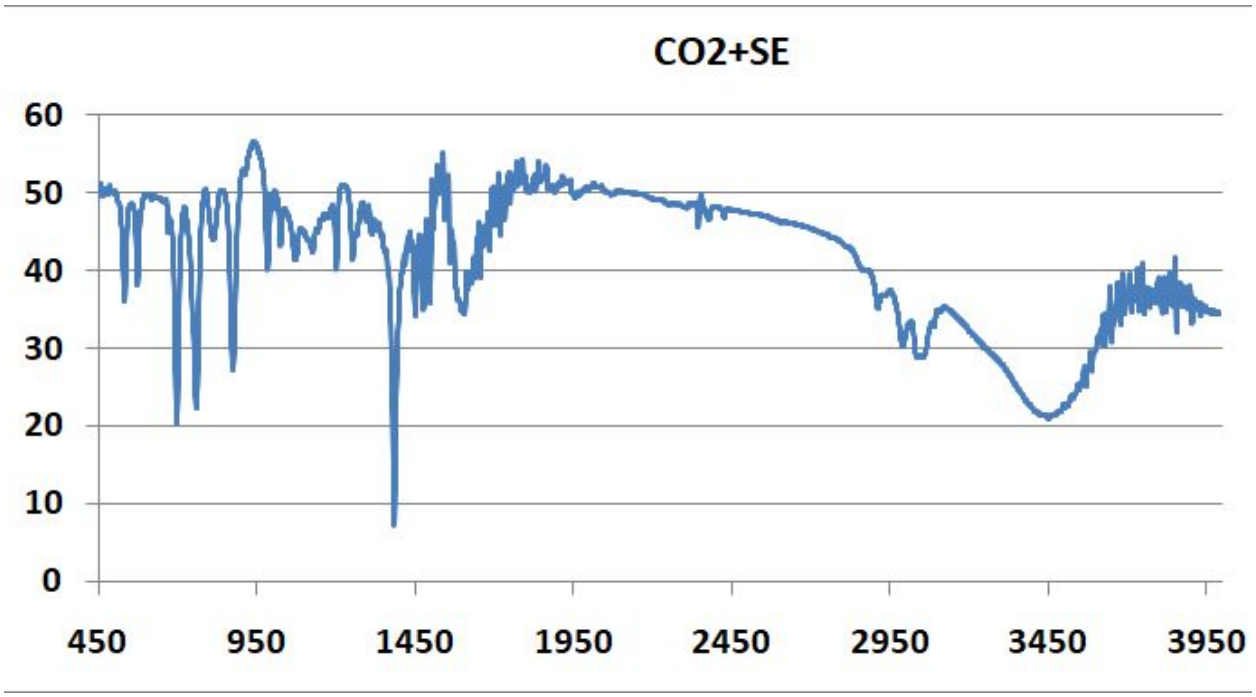


Figure S20: FT-IR of the reaction mixture of CO_2 and styrene oxide without any catalyst after 12 h.

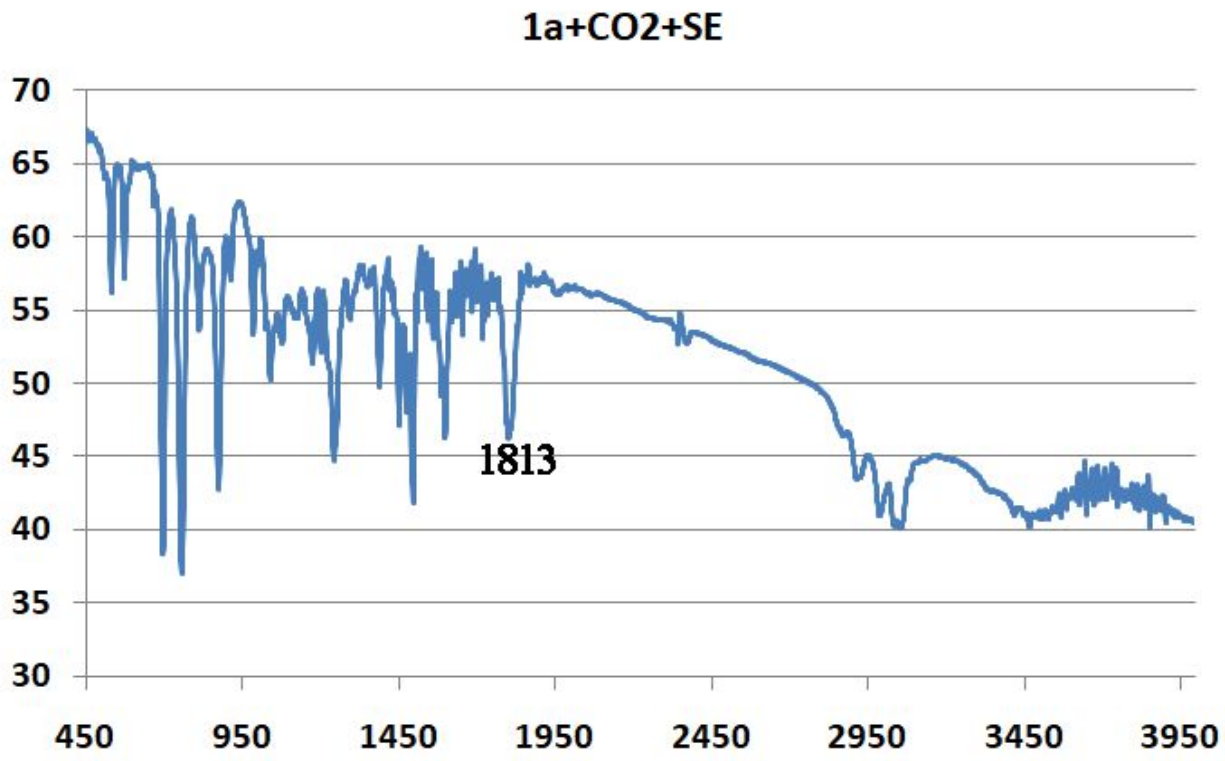


Figure S21: FT-IR of the reaction mixture of CO_2, styrene oxide and catalyst 1a after 12 h.

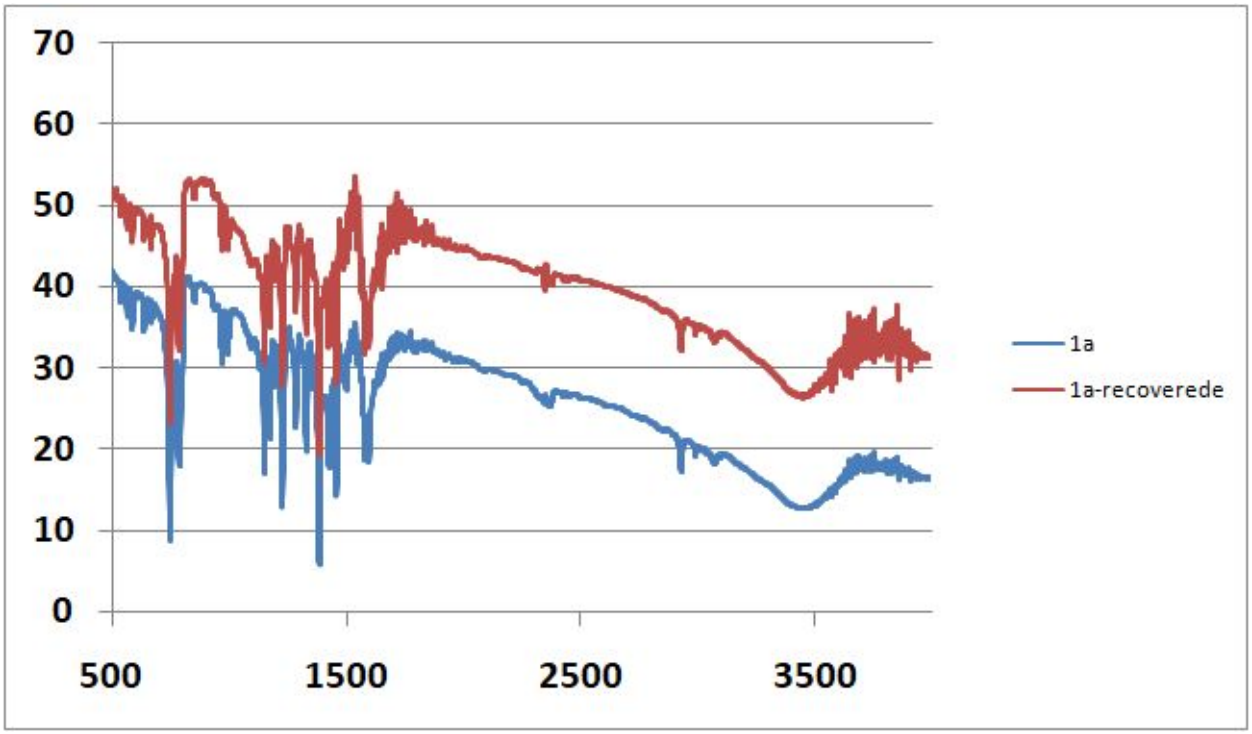


Figure S22: FT IR spectra of catalyst 1a before (brown) reaction with SE and CO_2 and after reaction with SE and CO_2 (blue) for 12 h.

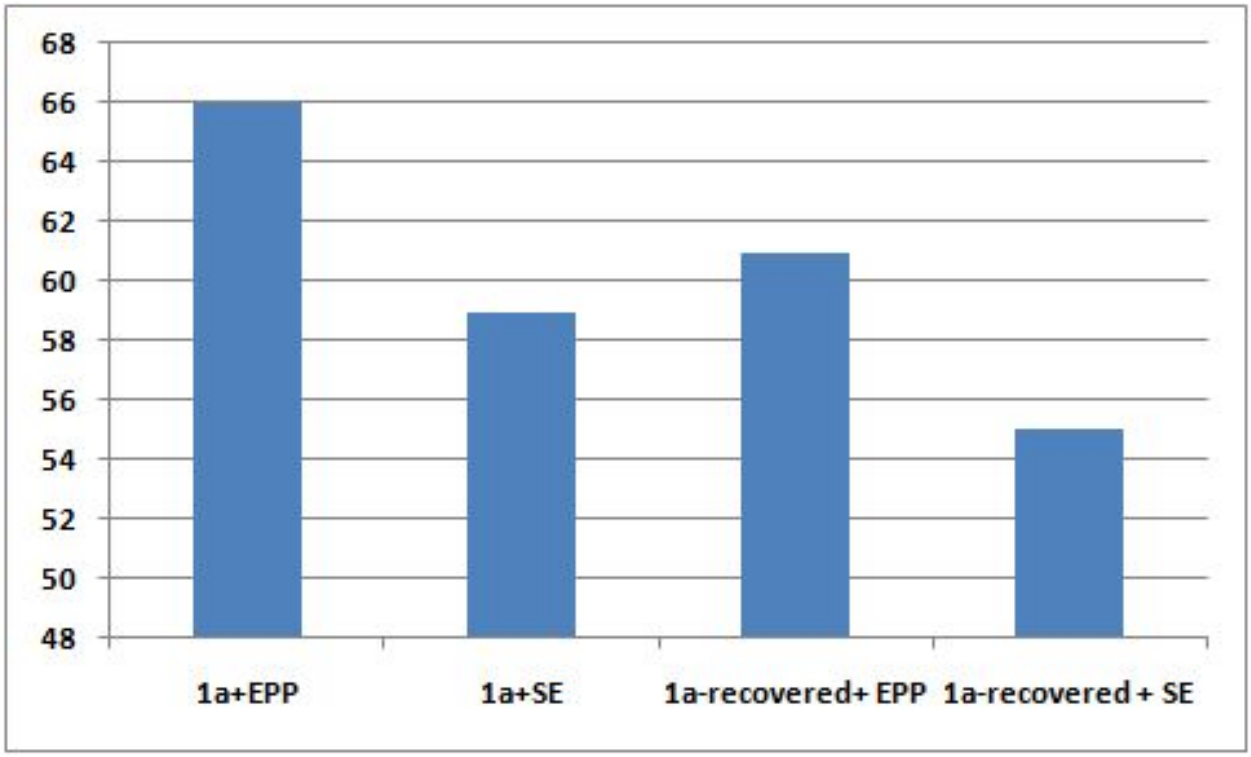


Figure S23: Bar diagram for the representating yield of the cyclic carbonates from the reaction with catalyst 1a and with recovered catalyst 1a from the respective reaction. Y axis represent the yield of the reaction. EPP represent epoxide 2 and SE represent epoxide 3.

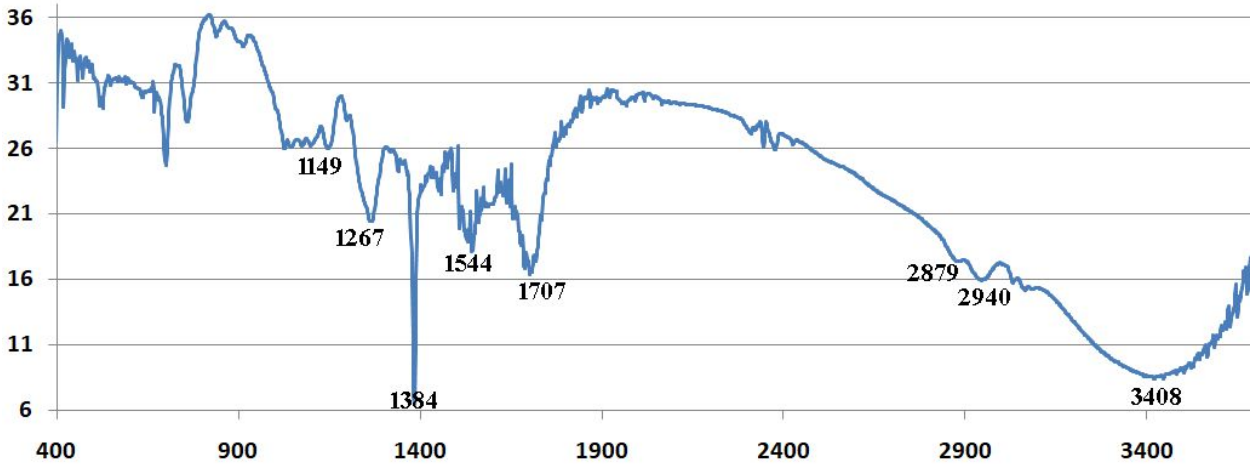


Figure S24: FT-IR spectra of the polyesterurethane PEU2.

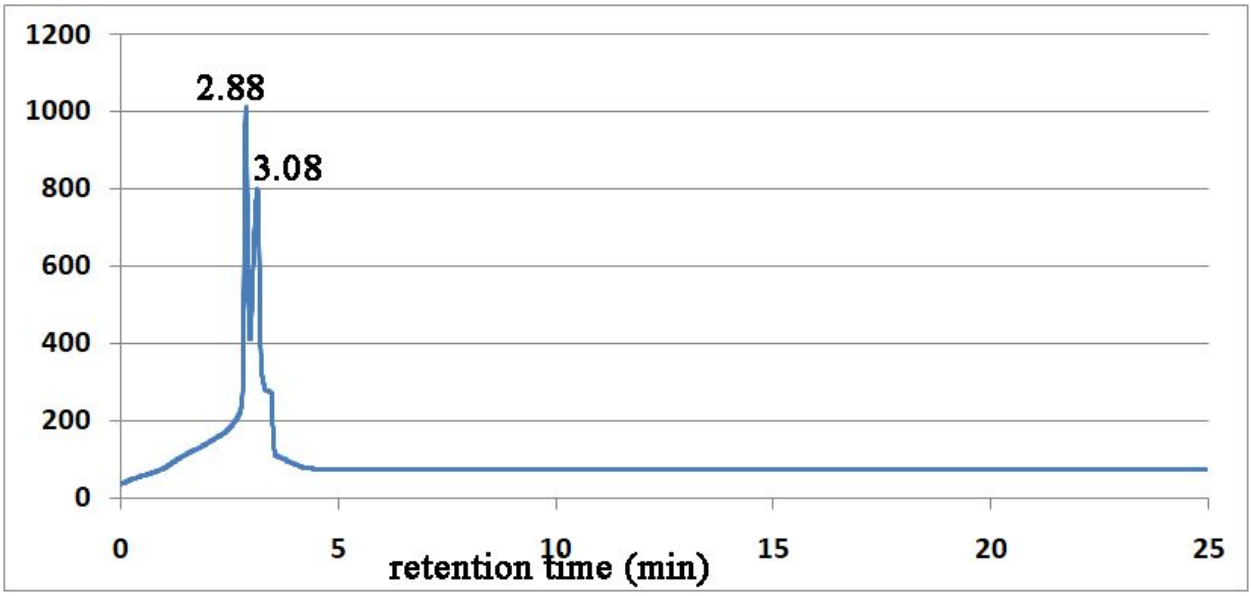


Figure S25: HPLC of the ring opening diol 6 collected with chiral column CHIRALPAK AD-H with HITACHI Primaide instrument. The two peaks appear due to two different enantiomers of the ring opened diol.

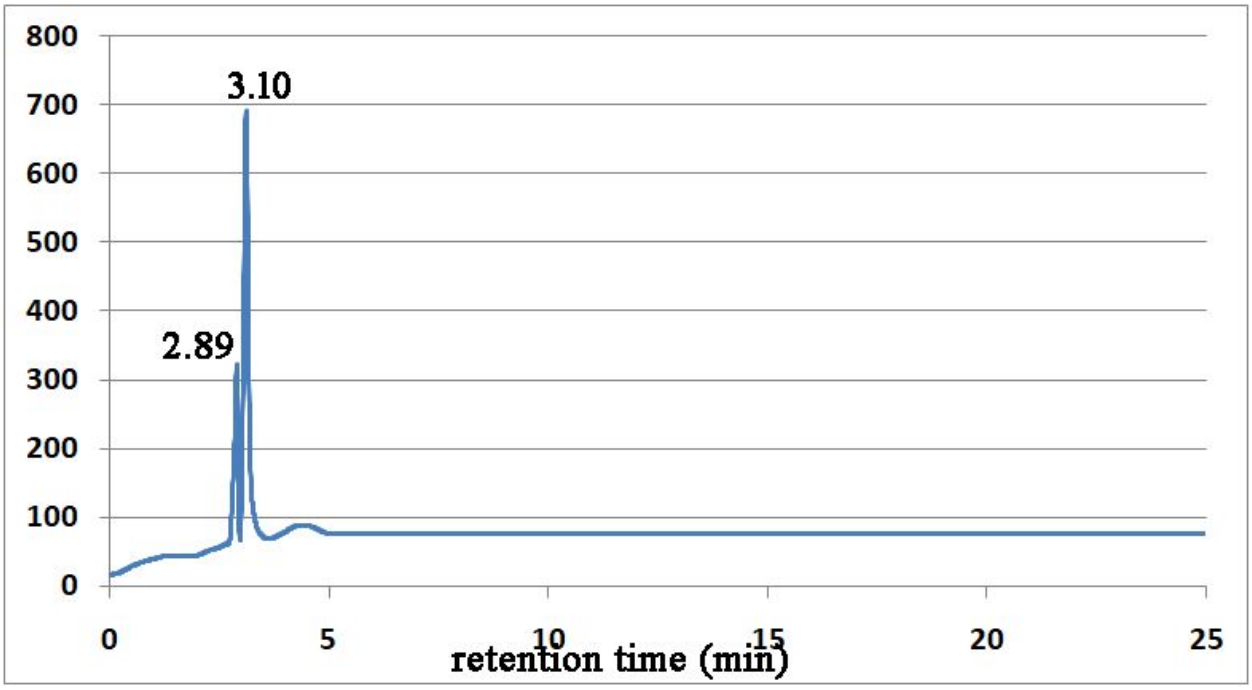


Figure S26: HPLC of the ring opening diol 7 collected with chiral column CHIRALPAK AD-H with HITACHI Primaide instrument. The two peaks appear due to two different enantiomers of the ring opened diol.