Supplementary Information

New insights into urethane alcoholysis enable chemical full recycling of blended fabric wastes

Wen-Hao Xu, Lin Chen*, Shun Zhang, Rong-Cheng Du, Xuehui Liu, Shimei Xu, Yu-Zhong Wang*

Collaborative Innovation Center for Eco-Friendly and Fire-Safety Polymeric Materials (MoE), State Key Laboratory of Polymer Materials Engineering, National Engineering Laboratory of Eco-Friendly Polymeric Materials (Sichuan), College of Chemistry, Sichuan University, Chengdu 610064, China

*Corresponding authors: linchen410@scu.edu.cn; yzwang@scu.edu.cn

Table S1. GPC data for unreacted spandex and formed sticky solid after glycolysis

Sample	M_n ($\times 10^4 g/mol$)	M_w ($\times 10^4 g/mol$)	M_w/M_n
Spandex	3.66	7.86	2.15
Sticky solid	0.30	0.74	2.47

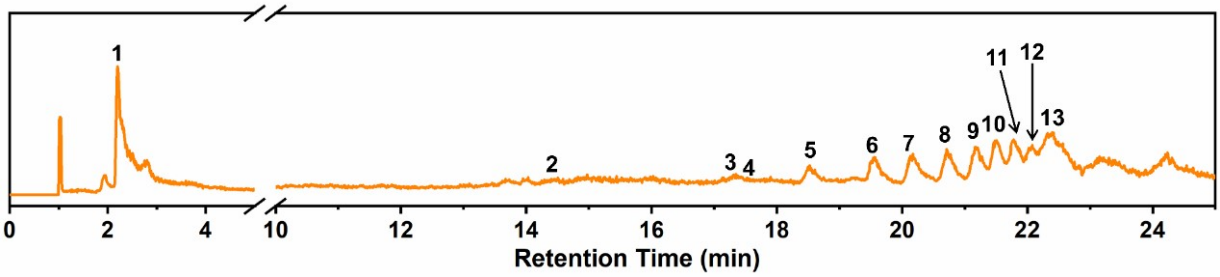


Fig. S1. High performance liquid chromatography mass spectrometer (LC-MS) chromatogram of the formed glycolysis solution for pure spandex after glycolysis process.

Detailed test conditions: separation was carried out on a Hypersil Gold column (150 mm × 2.1 mm, 5 um, Thermo), column temperature = 30 °C, detector temperature = 50 °C, electrospray ionization (ESI) source; Positive ion mode; Molecular weight range: 100-1200. Solvent acetonitrile/water (gradient: The proportion of acetonitrile in the mobile phase is 5% in 0-5 minutes, increases from 5% to 20% in 5-8 minutes, increases from 20% to 60% in 8-13 minutes, and increases from 60% in 13-18 minutes to 95%, in 18-23 min, the acetonitrile content is kept at 95%, in 23-23.1 min, the acetonitrile content is reduced from 95% to 5%, and in 23.1-30min, the acetonitrile content was 5%), flow rate of 0.5 mL/min, injection volume of 10 μL, and run time of 30 min.

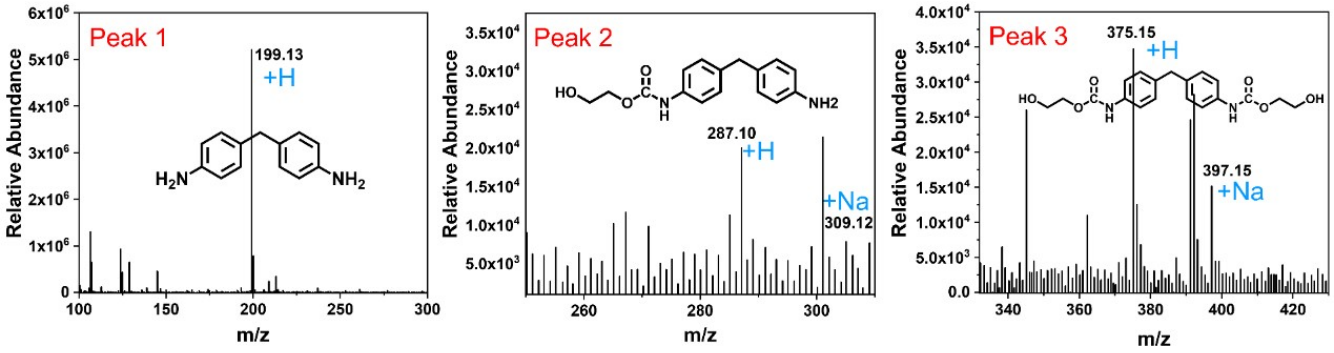


Fig. S2. Mass spectrum of peak 1-3 (containing diphenylmethane group) in the above Fig. S1

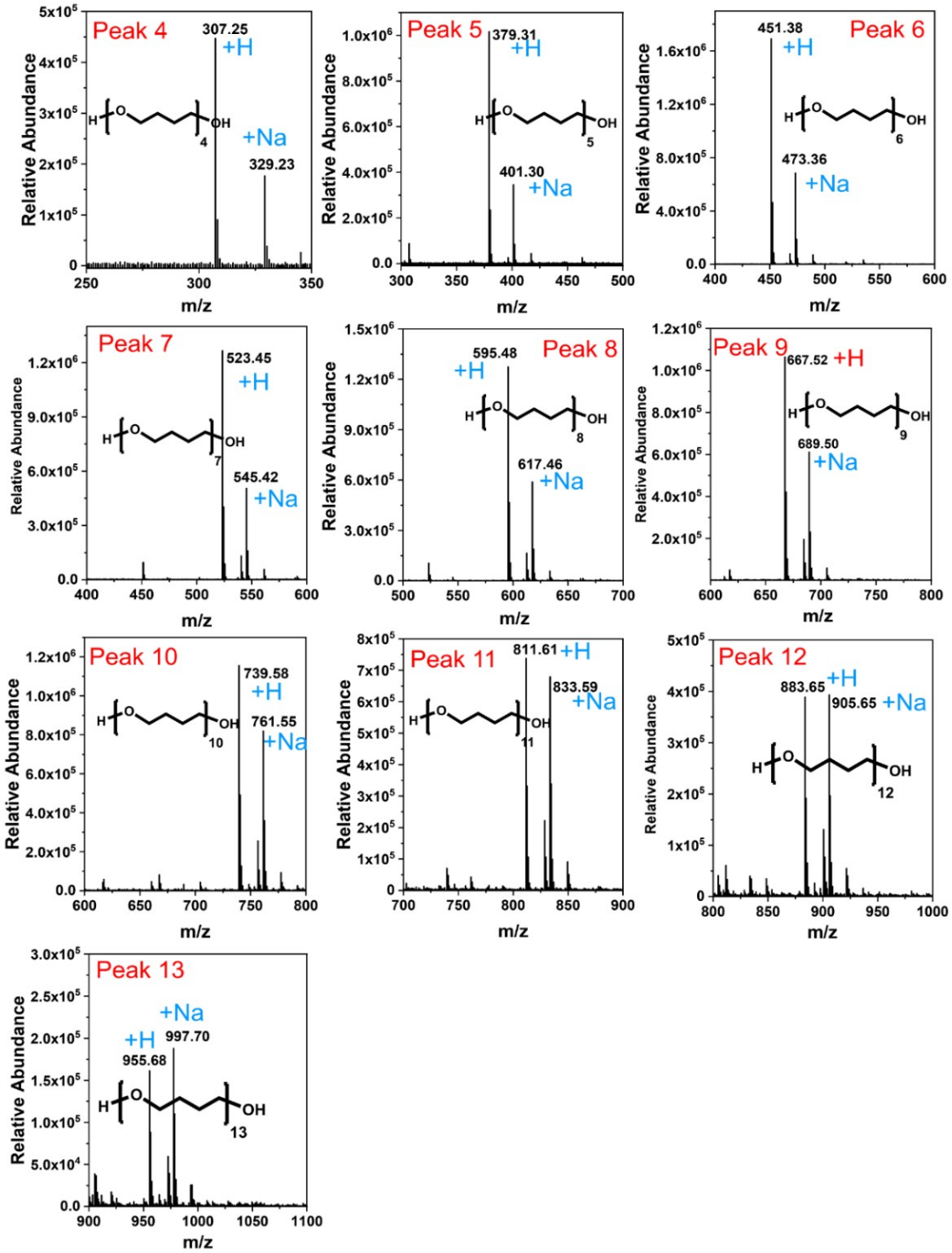
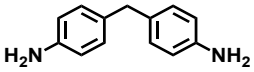
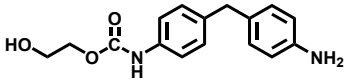
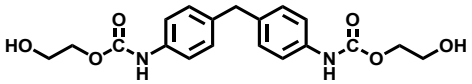
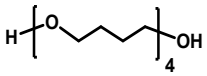
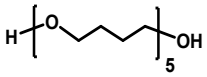
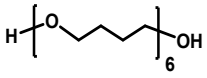
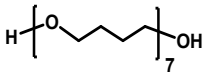
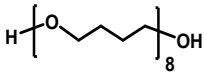
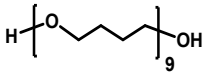
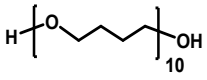
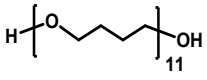
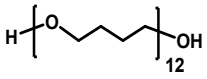
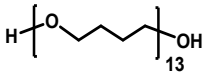


Fig. S3. Mass spectrum of peak 4-13 (polytetrahydrofuran diols) in the above Fig. S1

Table S2. Retention time, chemical structure and molecular weight of the peaks in above Fig. S1-S3

Peak number	Time (min)	Chemical structure	Molecular weight
1	2.18-2.48		198
2	14.27-15.31		286
3	17.17-17.54		374
4	17.41-17.54		306
5	18.36-18.73		378
6	19.43-19.69		450
7	19.93-20.30		522
8	20.50-20.83		594
9	20.96-21.29		666
10	21.46-21.62		738
11	21.74-21.91		810
12	22.00-22.16		882
13	22.24-22.49		954

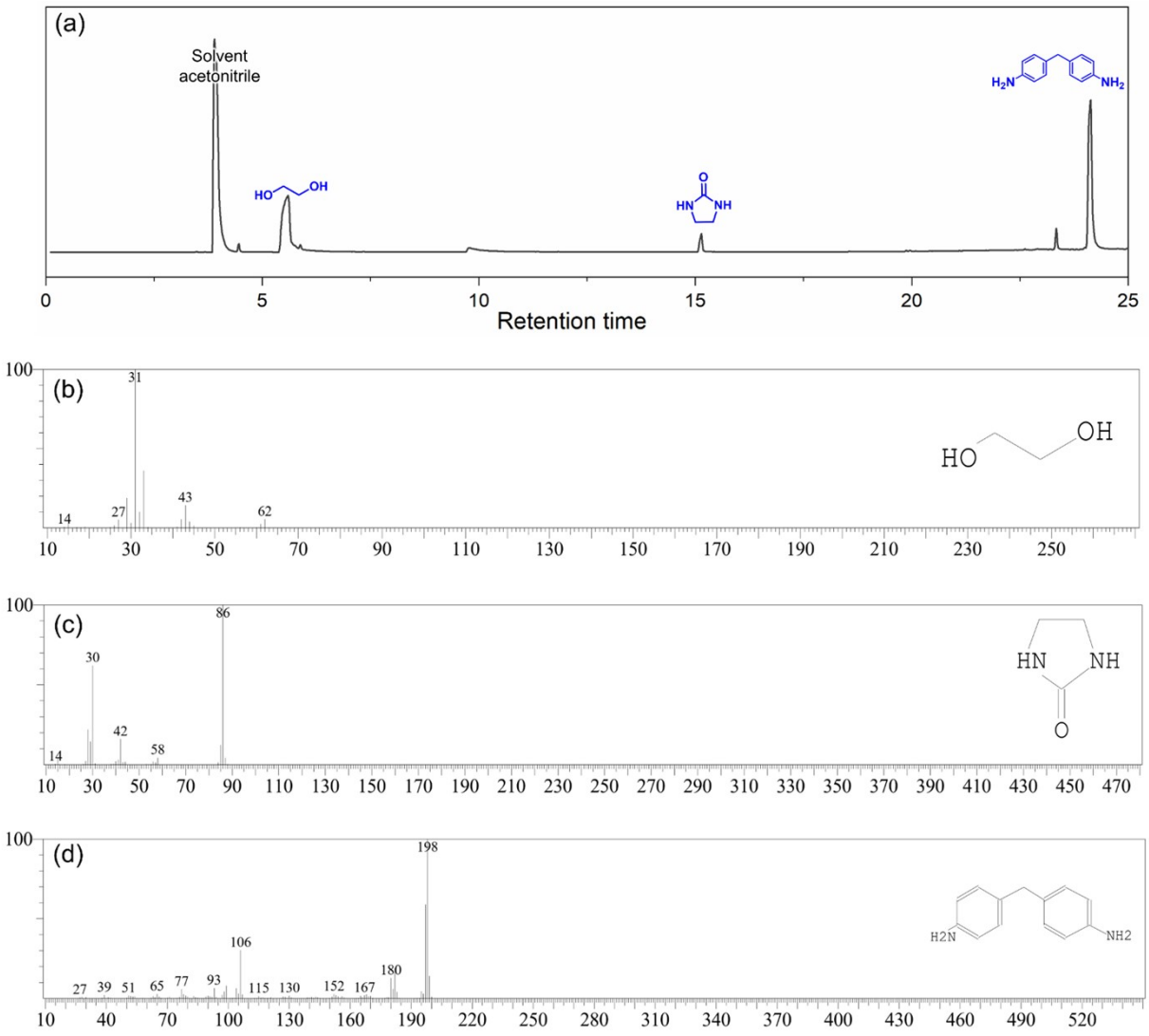


Fig. S4. (a) GC-MS chromatogram of the formed glycolysis solution for spandex, (b-d) Mass spectrum of the peaks.

The test conditions are as follows. The instrument model is GCMS-QP2010 Plus (chromatographic column model: DB-17MS; chromatographic column size: 60 m × 250 μm × 0.25 μm). The column temperature is 60 °C, the injection temperature is 300 °C, and the temperature is increased to 300 °C at 12 °C/min. Injection volume: 1 μL, split ratio: 10, solvent: acetonitrile. MS: Scan range 29-550, interval: 0.1 sec, scan speed 781 amu/s.

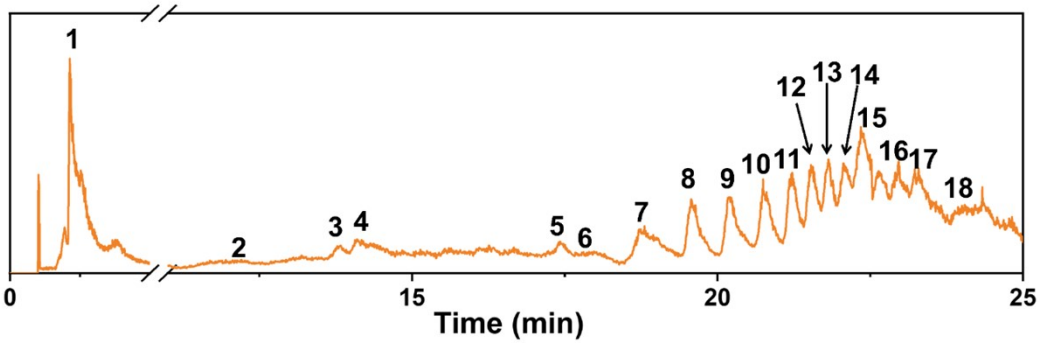


Fig. S5. LC-MS chromatogram of the formed solution for spandex after glycolysis and methanol transesterification process. The test conditions are the same as those in Fig. S1.

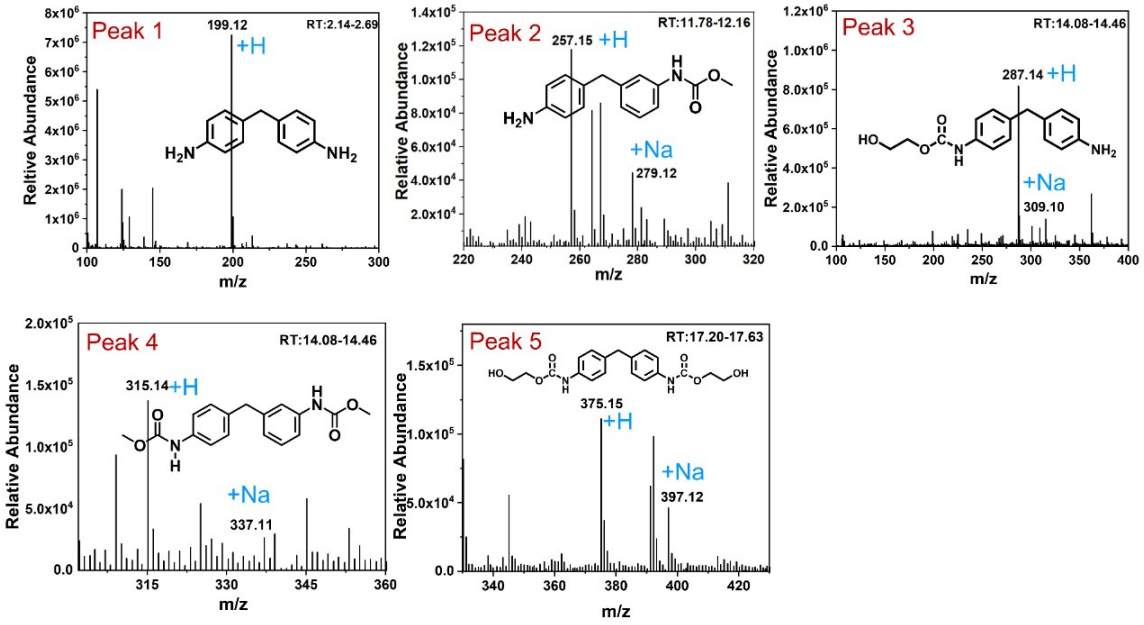


Fig. S6. Mass spectrum of peak 1-5 (containing diphenylmethane group) in the above Fig. S5

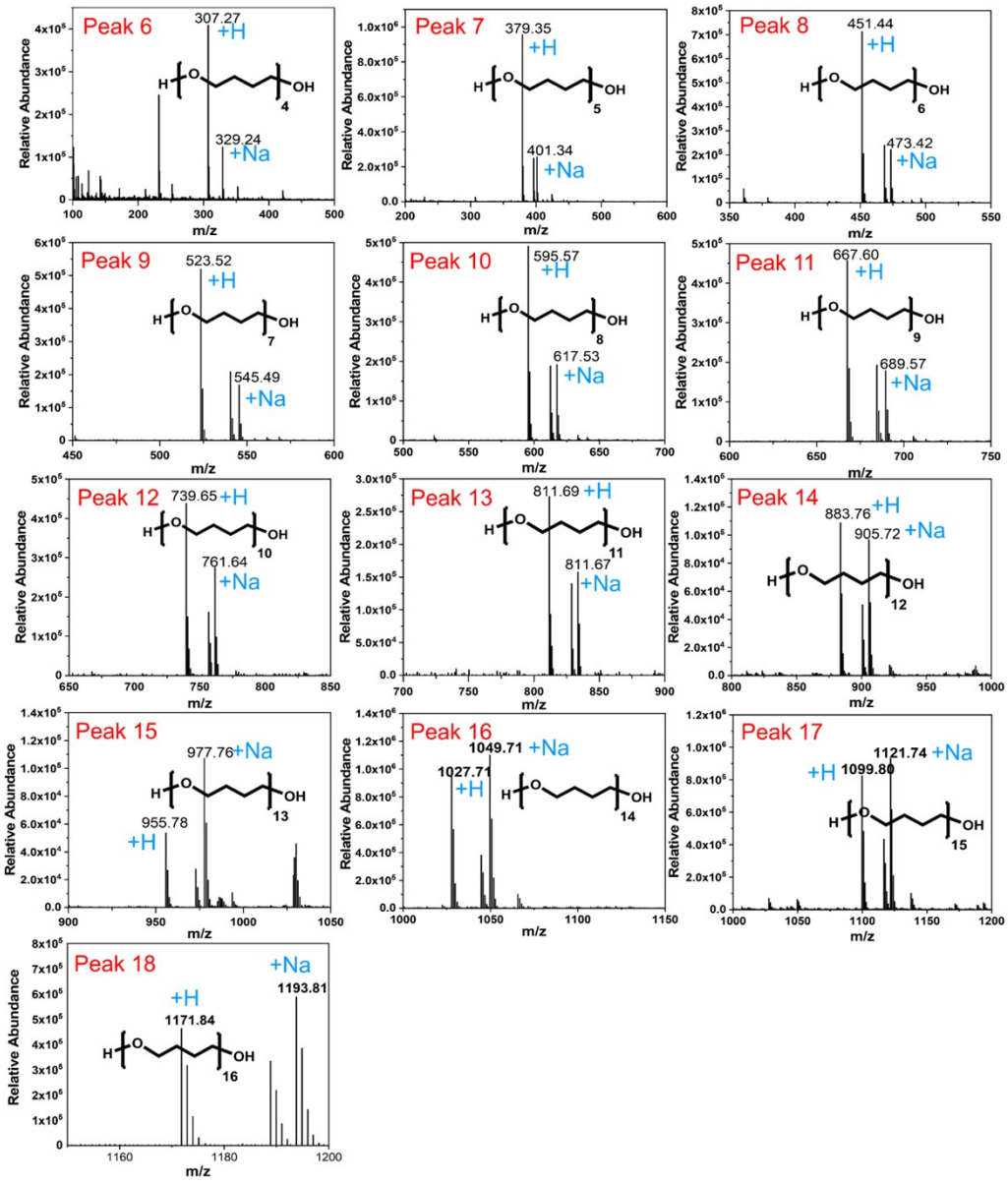
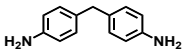
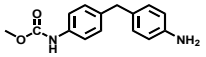
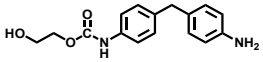
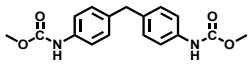
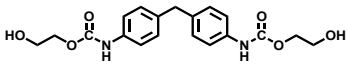
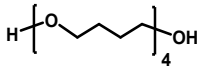
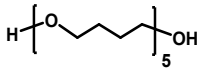
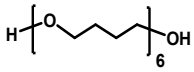
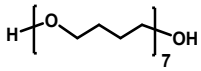
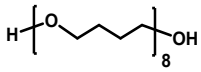
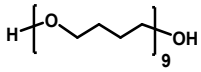
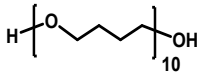
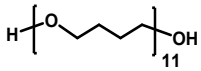
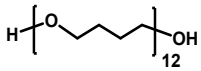
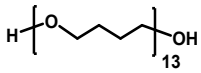
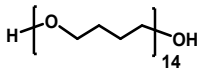
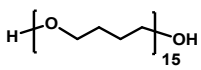
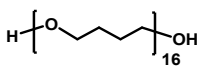


Fig. S7. Mass spectrum of peak 6-18 (polytetrahydrofuran diols) in the above Fig. S5

Table S3. Retention time, chemical structure and molecular weight of the peaks in above Fig. S5-S7

Peak number	Time (min)	Chemical structure	Molecular weight
1	2.14-2.69		198
2	11.78-12.16		256
3	14.08-14.46		286
4	14.08-14.60		314
5	17.20-17.63		374
6	17.20-17.63		306
7	18.69-19.07		378
8	19.46-19.84		450
9	19.97-20.40		522
10	20.69-20.86		594
11	21.08-21.33		666
12	21.47-21.64		738
13	21.72-21.93		810
14	21.93-22.19		882
15	22.23-22.57		954
16	22.62-22.79		1026
17	22.91-23.13		1098
18	23.21-23.51		1170

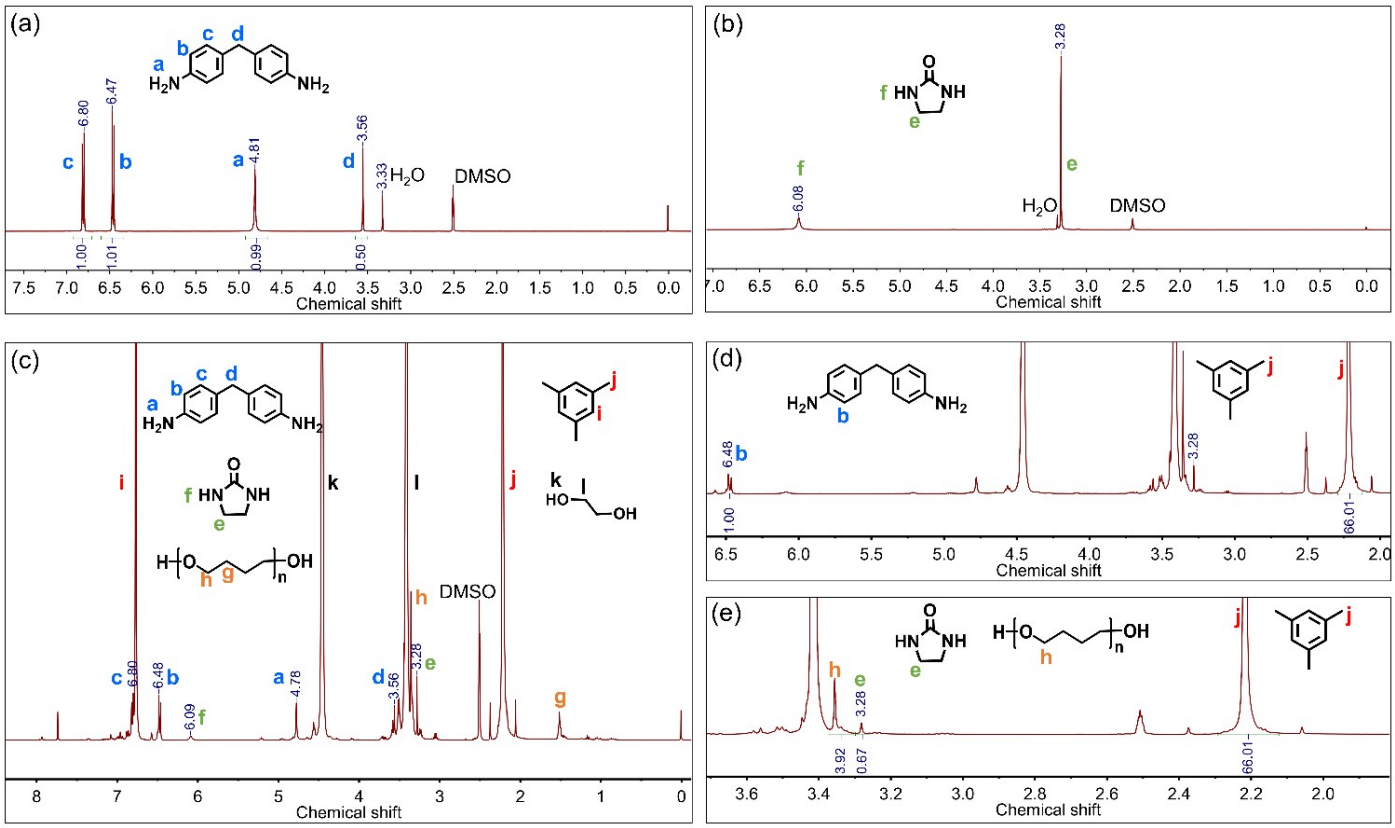


Fig. S8. ^{1}H NMR (in DMSO-d_6) of purchased 4,4'-methylenedianiline (a), 2-imidazolidinone (b) and formed glycolysis solution for spandex (c-e).

Spandex (5 g), ethylene glycol (7.5 g) and potassium carbonate (0.1 g) were reacted at 200 °C for 3 h. After glycolysis, the reaction system of spandex was cooled to room temperature and left for 3 h. It was observed that the system was divided into two layers, the upper layer was the sticky solids layer (polytetrahydrofuran diols), and the lower layer was the solution layer. Use a separating funnel to separate the two parts to obtain the upper layer of polytetrahydrofuran diols (washed with ethanol and dried, and the mass is denoted as m_s, namely 3.25 g) and the lower solution layer (the mass is denoted as m_l, namely 5 g+7.5 g-3.25 g=9.25 g). The relevant quantitative calculations of products in formed solution for spandex are as follows.

The mass of 4,4'-methylenedianiline, 2-imidazolidinone and polytetrahydrofuran diols in the solution was calculated by nuclear magnetic internal standard method. Take 17.8 mg of the solution and 17.1 mg of the internal standard mesitylene mixed for NMR testing. Take the calculation of the mass of 4,4'-methylenedianiline as an example. Since the signal intensity of hydrogen proton is proportional to the number of hydrogen proton, the ratio of the molar content of 4,4'-methylenedianiline to the molar content of mesitylene is equal to the ratio of their corresponding peak areas (Equation 1).

$$\frac{17.1\ mg \Big/ M_0 \times 9}{m_1 \Big/ M_1 \times 4} = 66.01 \qquad \text{Equation 1}$$

Where M_0 is the molar mass of mesitylene (120 g/mol), M_1 is the molar mass of 4,4'-methylenedianiline (198 g/mol), m_1 is the actual mass of 4,4'-methylenedianiline in the 17.8 mg solution. 66.01 (Figure S8d) is the ratio of the integrated areas of peak j (9 hydrogens) in mesitylene to peak b (4 hydrogens) in 4,4'-methylenedianiline. Based on the above Equation 1, m_1 can be calculated, and then the total mass of 4,4'-methylenedianiline in the solution is calculated as 0.50 g. Similarly, according to the integral area ratio, the masses of 2-imidazolidinone and polytetrahydrofuran in the solution are calculated as 0.15 g and 0.71 g, respectively.

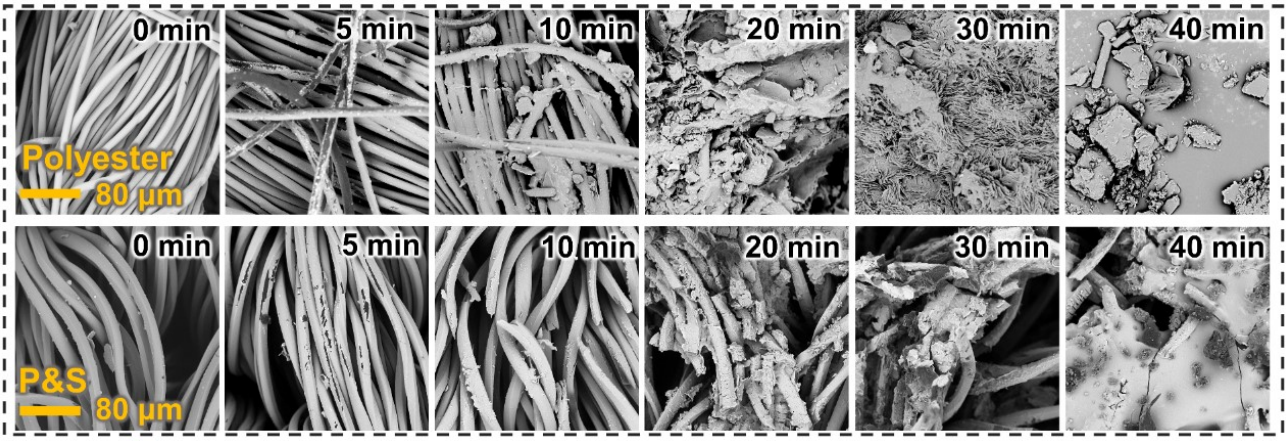


Fig. S9. SEM images of polyester fabric and polyester-spandex (P&S) blended fabric during glycolysis at different reaction time

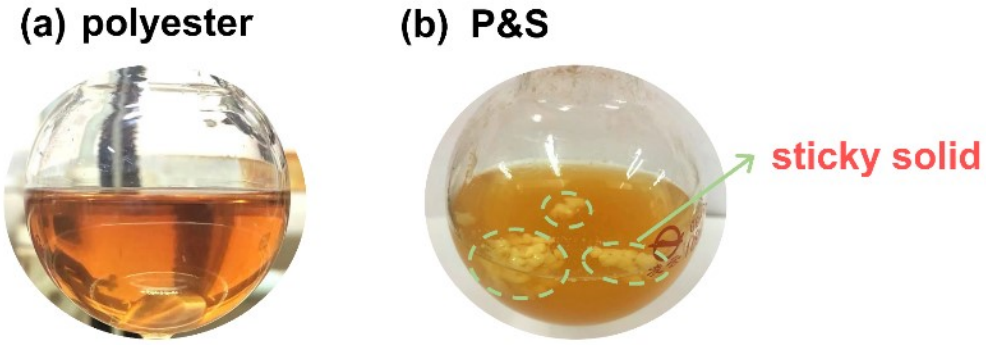


Fig. S10. Photos of polyester fabric and polyester-spandex (P&S) blended fabric after glycolysis reaction for 3h

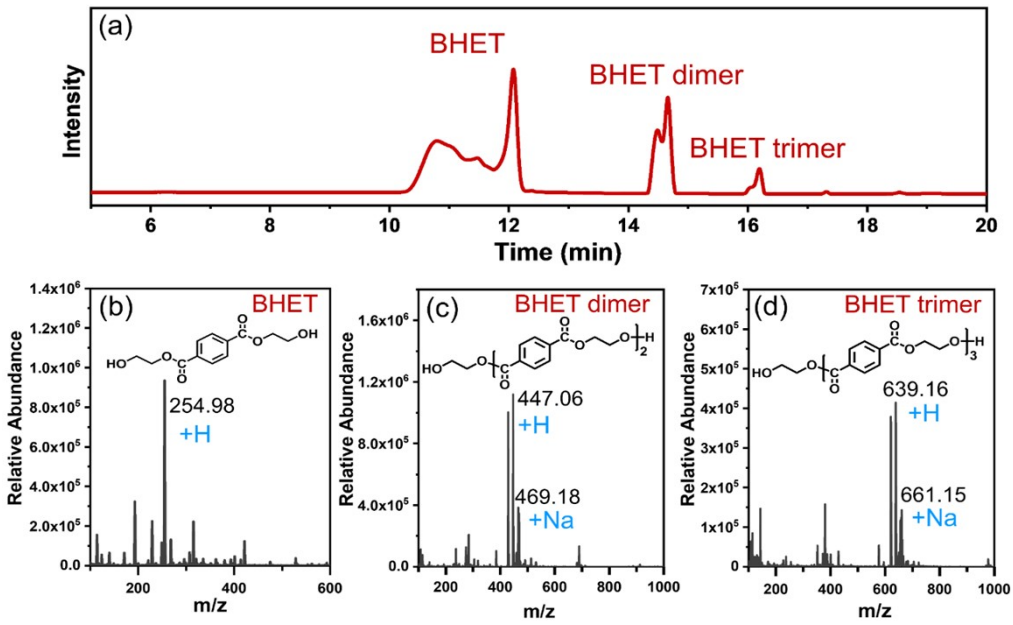
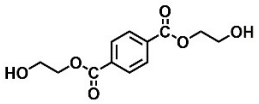
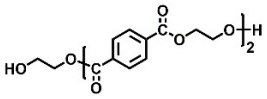
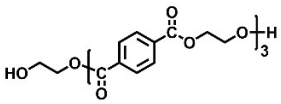


Fig. S11. (a) LC-MS chromatogram of the formed glycolysis solution for polyester fabric, (b-d) Mass spectrum of the peaks. The test conditions are the same as those in Fig. S1.

Table S4. Retention time, chemical structure and molecular weight of the peaks in above Fig. S11

Time (min)	Chemical structure	Molecular weight
10.20-12.18		254
14.31-14.78		446
15.91-16.24		638

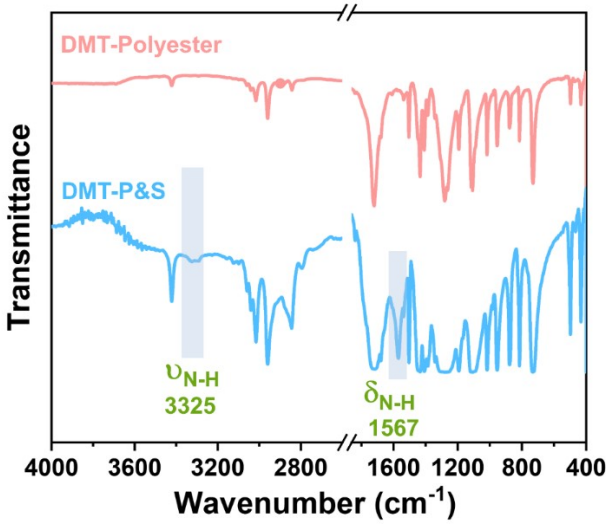


Fig. S12. FT-IR spectra of crude DMT from polyester fabric and P&S fabric

Table S5. Organic element analysis results of crude DMT come from polyester fabric and P&S fabric

Sample	C (%)	H (%)	N (%)
theoretical DMT	61.86	5.15	0
crude DMT obtained from polyester	62.08	5.13	0
crude DMT obtained from P&S	61.72	5.61	0.22

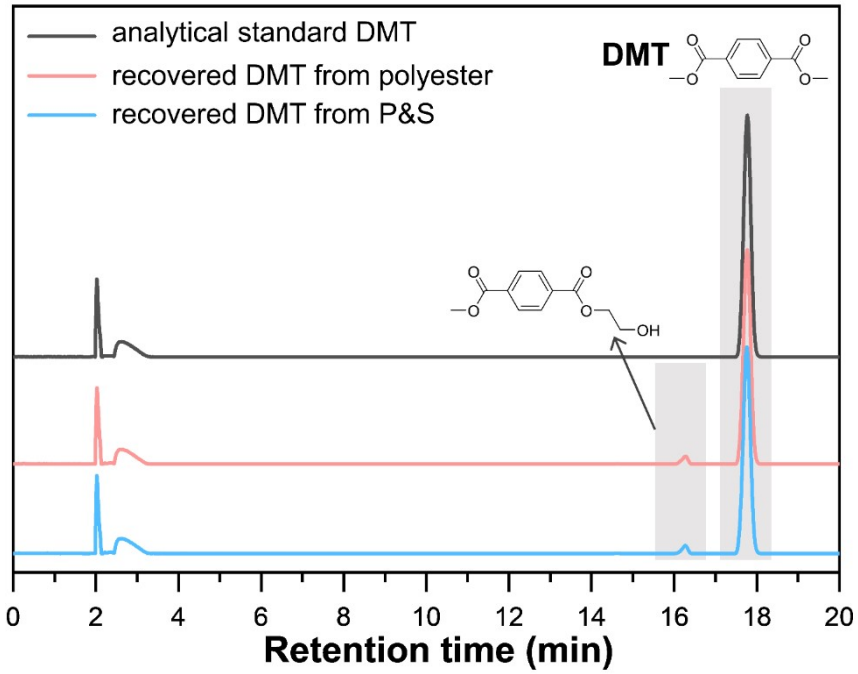


Fig. S13. HPLC chromatogram of analytical standard DMT, recovered DMT form polyester and recovered DMT from P&S. (High performance liquid chromatography (HPLC), separation was carried out on a Hypersil Gold column (150 mm × 2.1 mm, 5 um, Thermo), column temperature = 30 °C, detector temperature = 50 °C. Solvent methanol/water (gradient: The proportion of methanol in the mobile phase is 5% in 0-5 minutes, increases from 5% to 20% in 5-8 minutes, increases from 20% to 60% in 8-13 minutes, and increases from 60% in 13-18 minutes to 95%, in 18-23 min, the methanol content is kept at 95%, in 23-23.1 min, the methanol content is reduced from 95% to 5%, and in 23.1-30min, the methanol content was 5%), flow rate of 0.5 mL/min, injection volume of 10 μL, and run time of 30 min. In HPLC testing, peak area is proportional to concentration. According to the concentration and peak area of the analytical standard DMT, as well as the peak area of recovered DMT form polyester or P&S, the DMT concentration in recovered DMT form polyester or P&S is calculated.)

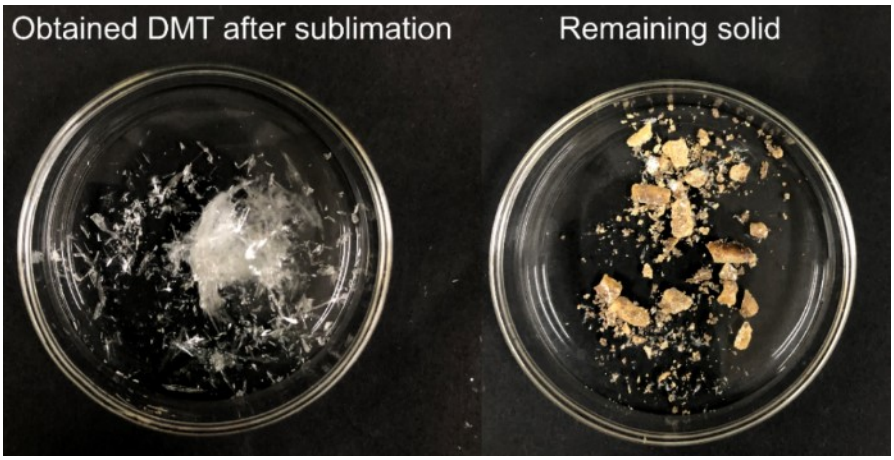


Fig. S14. For crude DMT come from P&S fabric, digital photos of obtained DMT after sublimation and remaining solid

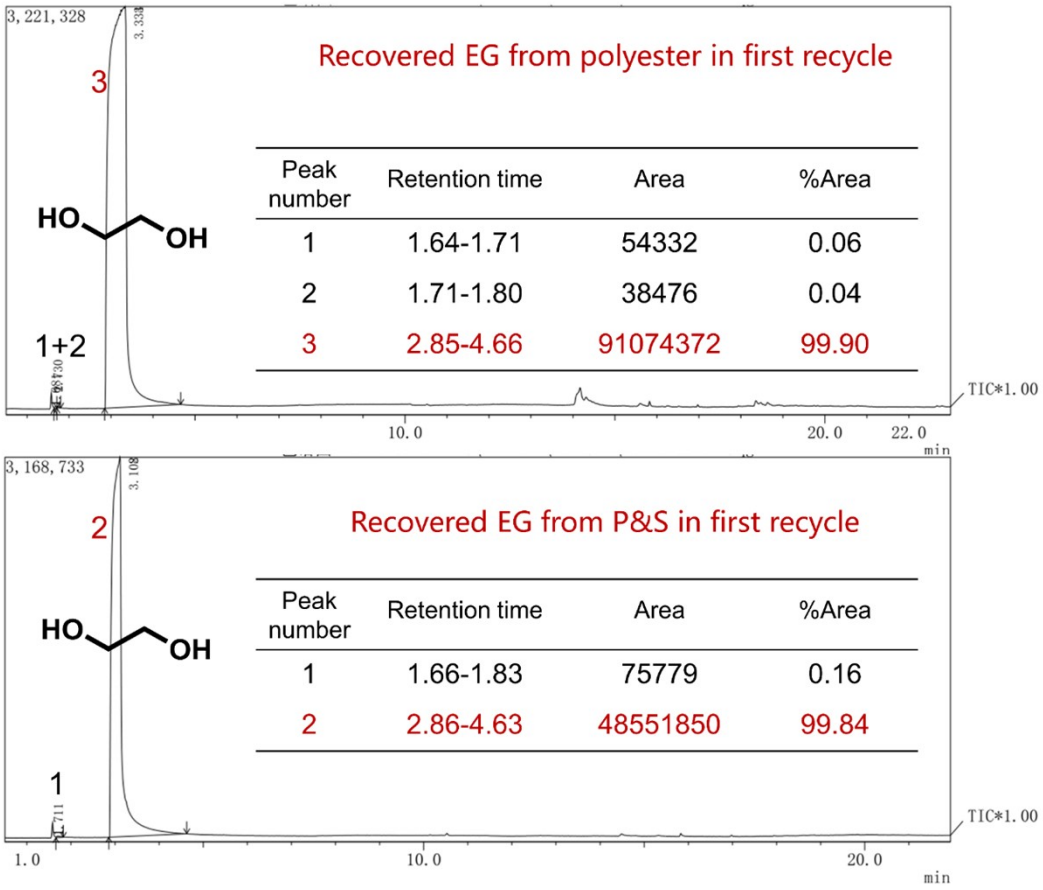


Fig. S15. GC-MS chromatogram of recovered EG form polyester and recovered EG from P&S in first recycle. Gas chromatography-mass spectrometer (GCMS-QP2010 Plus), column temperature = 50 °C, injection temperature=290 °C, after diluting the sample 100 times, injection volume of 0.2 μL.

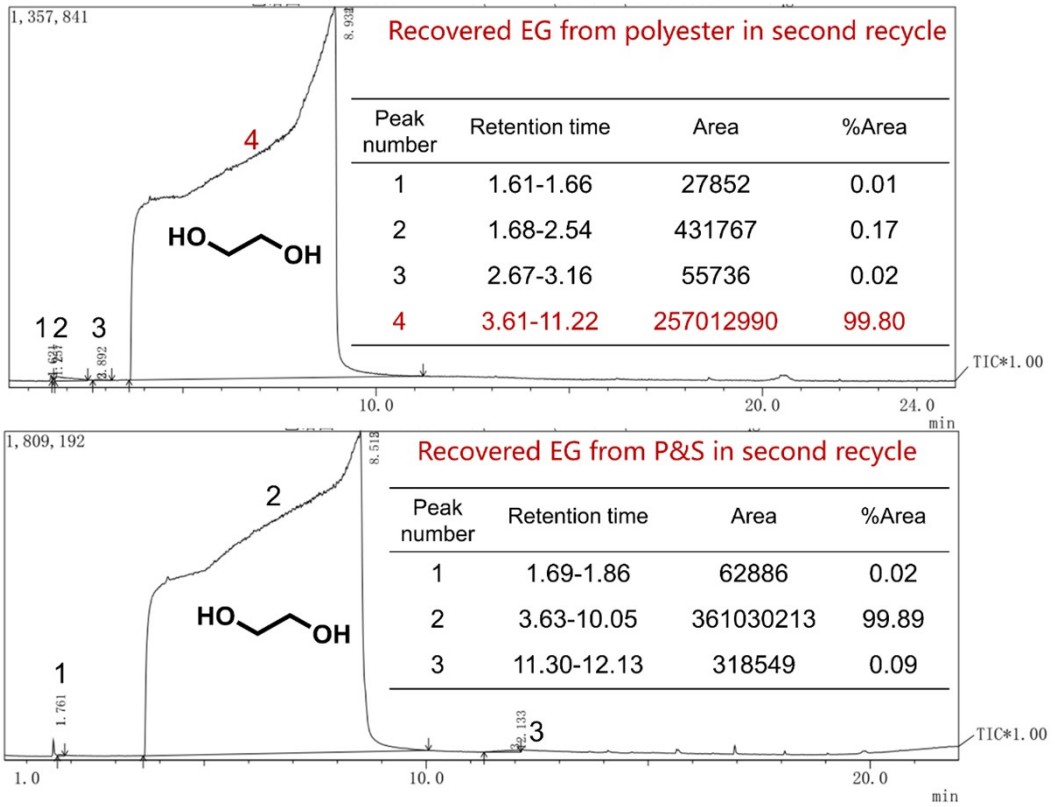


Fig. S16. GC-MS chromatogram of recovered EG form polyester and recovered EG from P&S in second recycle. The test conditions are the same as those in Fig. S15.

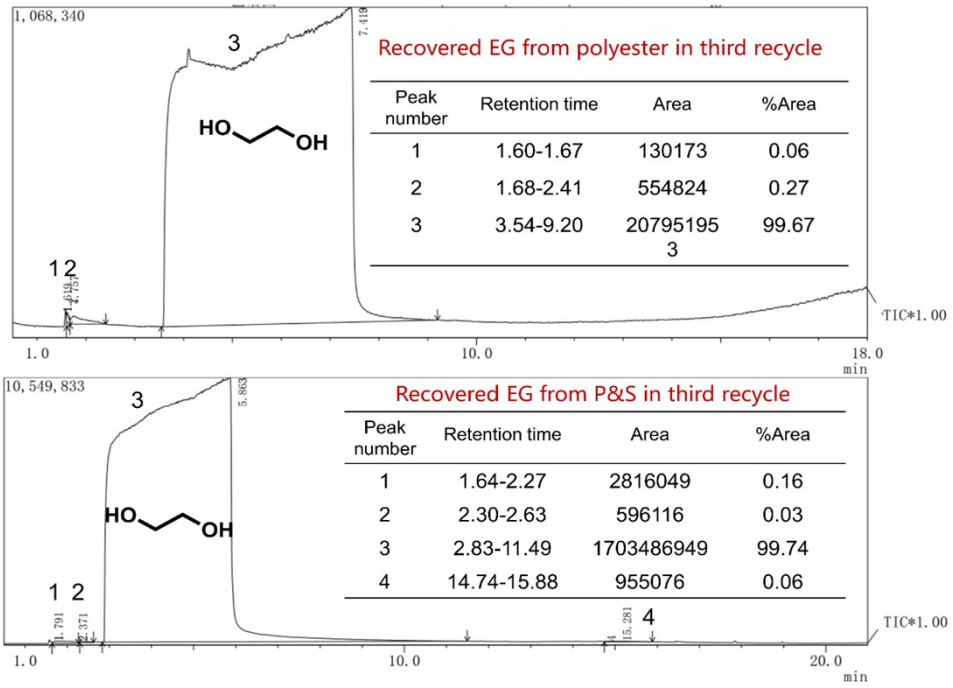


Fig. S17. GC-MS chromatogram of recovered EG form polyester and recovered EG from P&S in third recycle. The test conditions are the same as those in Fig. S15.

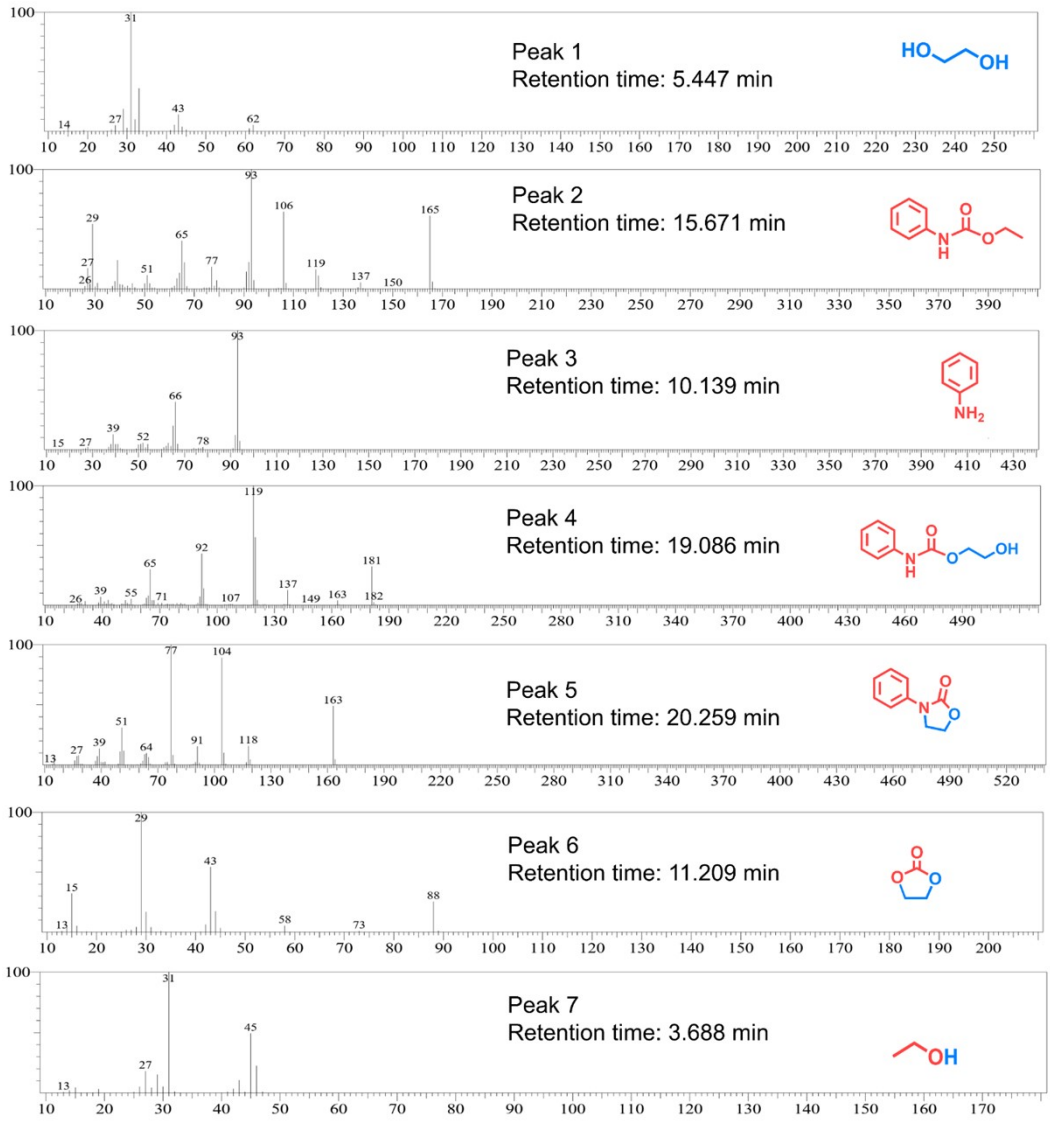


Fig. S18. Mass spectrum of peaks in Figure 5(a). The test conditions are the same as those in Figure S4.

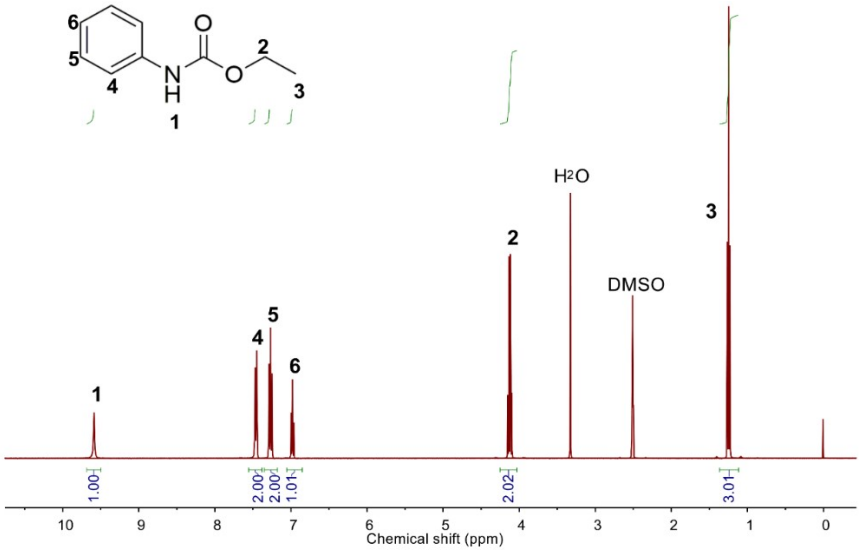


Fig. S19. ^{1}H NMR (in DMSO-d_6) spectrum of purchased phenylurethane

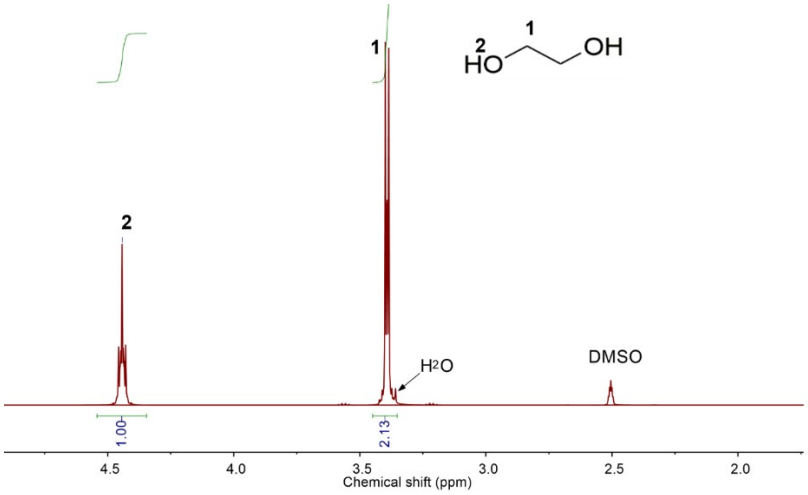


Fig. S20. ^{1}H NMR (in DMSO-d_6) spectrum of purchased ethylene glycol

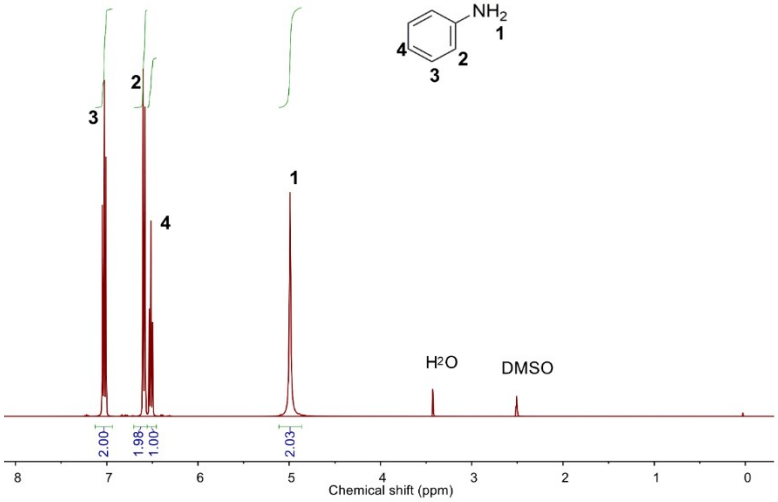


Fig. S21. ^{1}H NMR (in DMSO-d_6) spectrum of purchased aniline

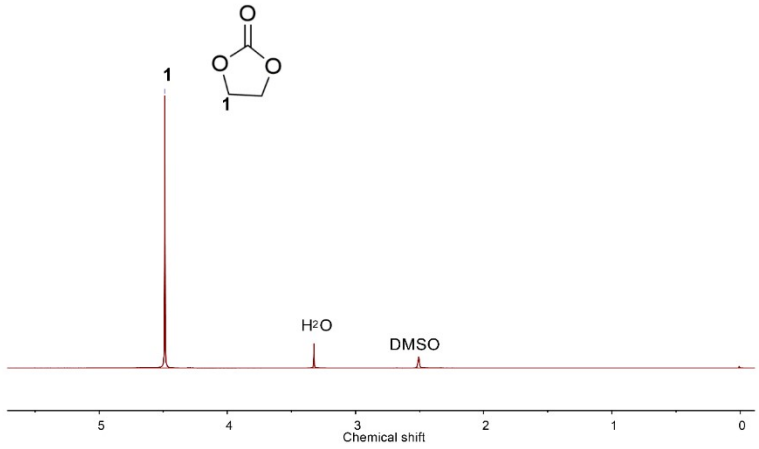


Fig. S22. ^{1}H NMR (in DMSO-d_6) spectrum of purchased ethylene carbonate

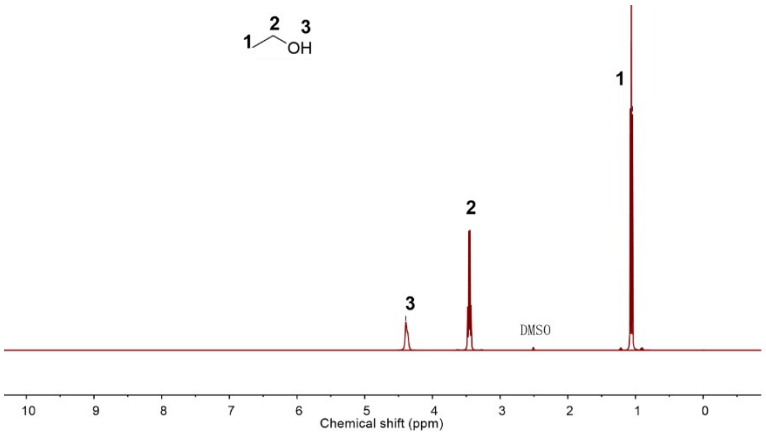


Fig. S23. ^{1}H NMR (in DMSO-d_6) spectrum of purchased ethanol

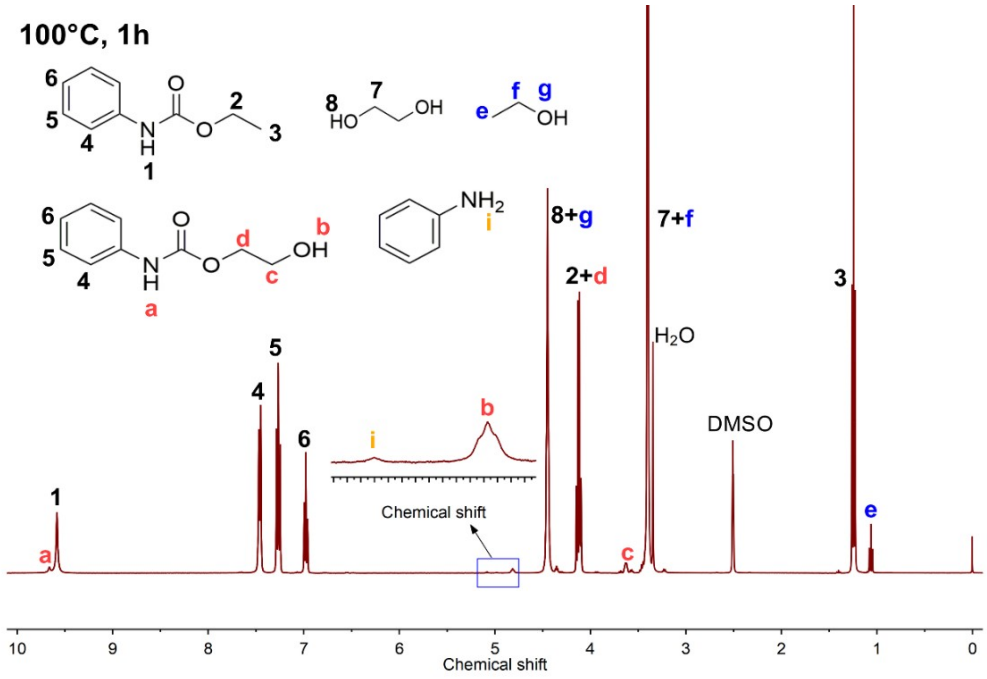


Fig. S24. ^{1}H NMR (in DMSO-d_6) spectrum of the obtained mixture after the reaction of phenylurethane and ethylene glycol at 100 °C for 1 h

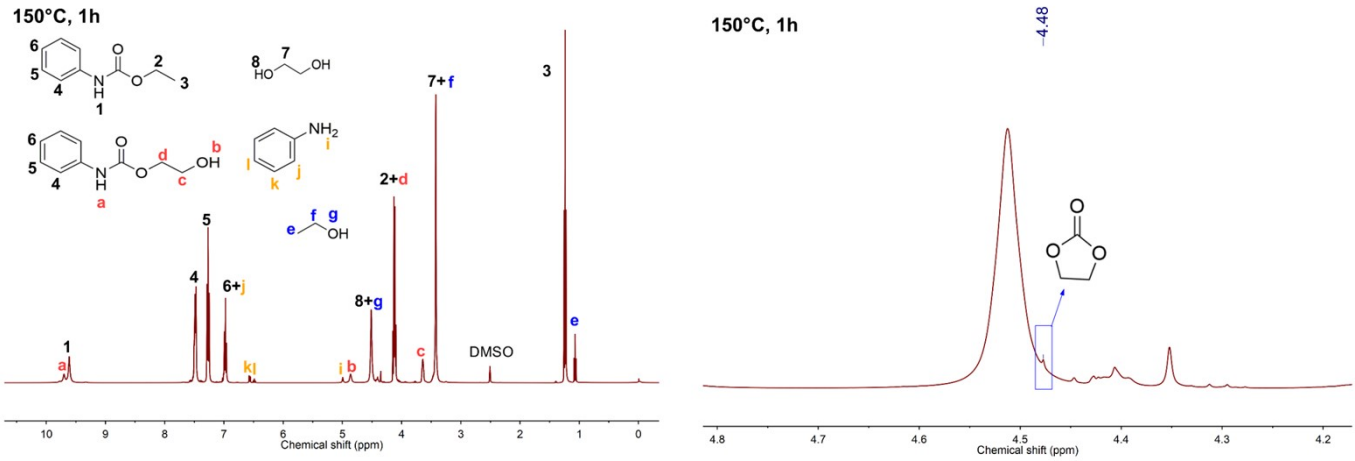


Fig. S25. ^{1}H NMR (in DMSO-d_6) spectrum of the obtained mixture after the reaction of phenylurethane and ethylene glycol at 150 °C for 1 h

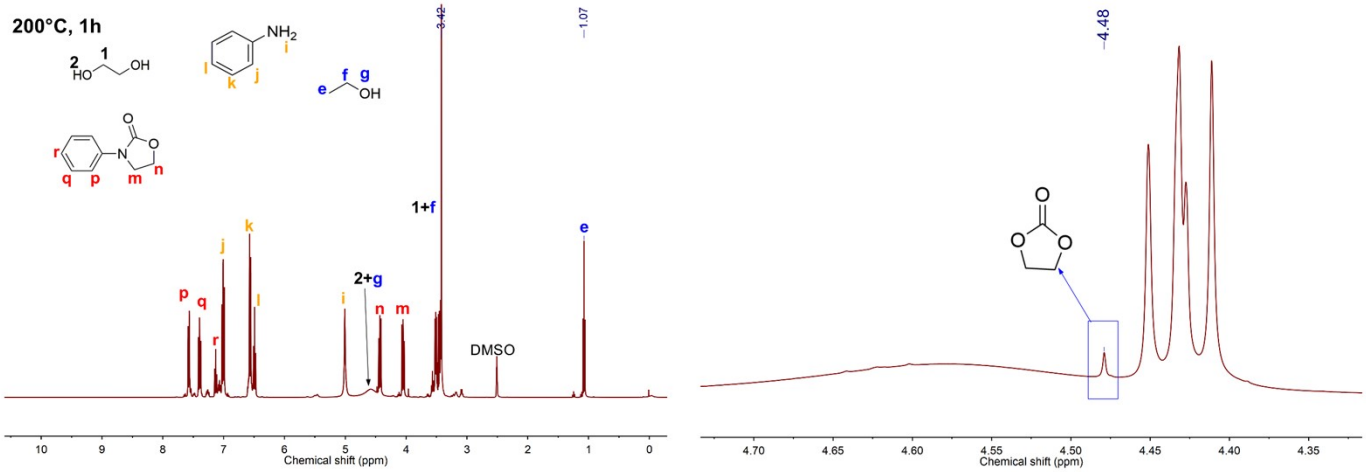


Fig. S26. ^{1}H NMR (in DMSO-d_6) spectrum of the obtained mixture after the reaction of phenylurethane and ethylene glycol at 200 °C for 1 h

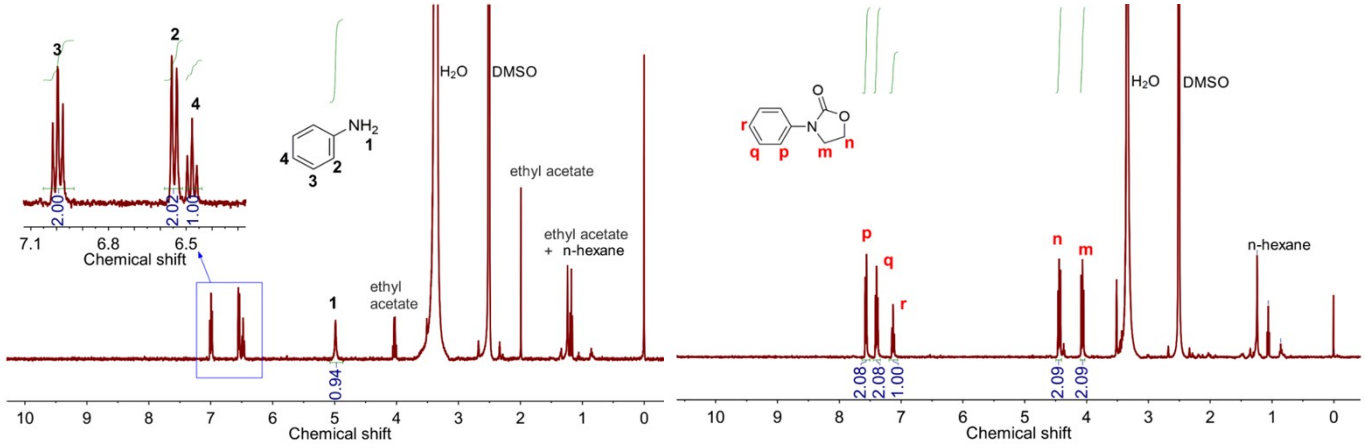


Fig. S27. ^{1}H NMR (in DMSO-d_6) spectrum of separated aniline and 3-phenyl-2-oxazolidinone from the reaction mixture (200 °C for 1 h). The separation steps are as follows. Step 1, the product was separated by thin-layer chromatography on silica gel in a developing solvent (volume ratio ethyl acetate:n-hexane=1:2). Step 2, the product adsorbed on the silica gel was scraped off and ground, and ethyl acetate was added to dissolve it. Step 3, prepare a filter device with diatomaceous earth, and wash the impurities in the diatomaceous earth with ethyl acetate. Step 4, the ethyl acetate with the product was filtered to remove the silica gel. Step 5: Spin the solution to dry to obtain the product

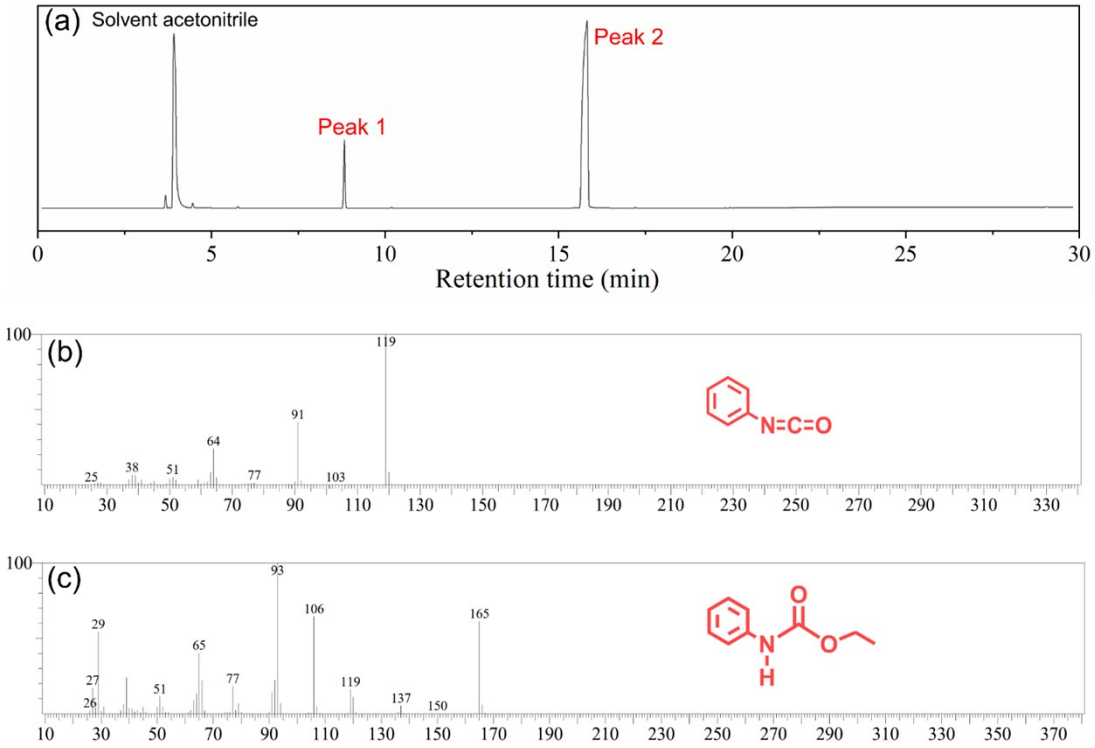


Fig. S28. (a) GC-MS chromatogram of reactant phenylurethane, (b) Mass spectrum of the peak 1, (c) Mass spectrum of the peak 2. The test conditions are the same as those in Fig. S4.

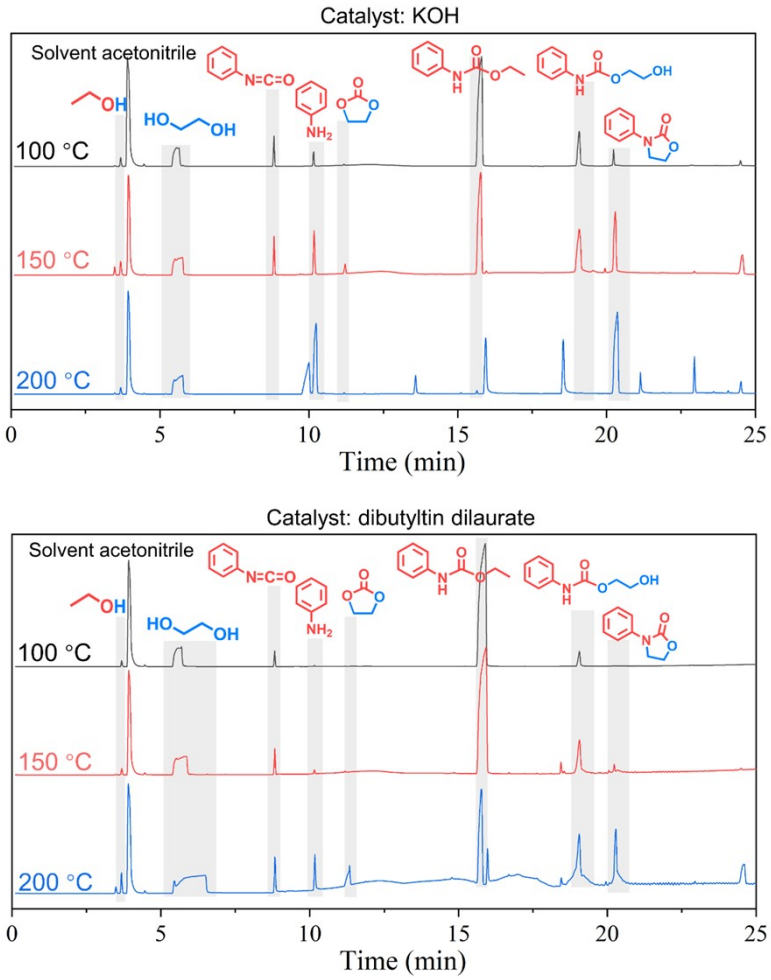


Fig. S29. (a) GC-MS of formed solutions after the reaction of phenylurethane with ethylene glycol (under different catalyst) at different temperatures for 1 h. Test conditions are the same as those in Fig. S4.

Optimised Cartesian Coordinates for Phenylurethane Glycolysis.

Reactants complex:

O	1.84183800	0.79826100	-1.51067100
H	0.87875300	1.66763200	-0.43895700
C	2.83044000	0.09347200	-1.04132600
O	2.98566300	-1.12852300	-1.45230500
O	3.64067600	0.59536200	-0.17161300
C	-5.99013400	0.16187200	-0.98399000
H	-6.88278800	0.40456500	-1.54846700
C	-5.80409600	0.67679600	0.29996600
H	-6.55232100	1.32427600	0.74299800
C	-4.65671100	0.36869800	1.02244200
H	-4.51517900	0.77237800	2.01956800
C	-3.67449400	-0.46618200	0.46987100
C	-3.86074800	-0.99289800	-0.81373100
H	-3.12117100	-1.64868300	-1.24673000
C	-5.01463000	-0.67077200	-1.52859700
H	-5.14724400	-1.08420300	-2.52223200
N	-2.55210700	-0.74920500	1.27832700
H	-2.60290700	-0.42408800	2.23591700
C	-1.36572900	-1.30787500	0.92290600
O	-0.55823500	-1.39334000	2.00048400
O	-1.05344500	-1.69559100	-0.19760400
C	0.77137300	-1.95420000	1.78941300
H	0.66084600	-2.95012000	1.35773300
H	1.30378100	-1.31268200	1.08623800
C	1.46202600	-1.99955200	3.13330400
H	0.91218700	-2.62759700	3.83858500
H	1.56757700	-0.99826400	3.55740800
H	2.46131100	-2.42499200	3.00608700
O	0.22737400	2.12949700	0.15386900
C	0.88452500	3.22249400	0.79398300
H	0.27298500	3.51447200	1.65374900
H	1.87002100	2.91937600	1.16614900
C	1.03660100	4.41466700	-0.14731800
H	0.05650100	4.70387400	-0.54298300
H	1.68330600	4.15275700	-0.98719800
O	1.66247200	5.53110100	0.50686800
H	1.07020100	5.84162800	1.20352800
K	0.46080600	-1.29158800	-2.32214000
K	5.02696200	-1.57994600	0.12932700

Transition state TS1:

O	1.88326900	0.51262900	-1.46389000
H	1.16230900	0.44594600	-0.78873200
C	3.10595400	0.73375600	-0.85654300
O	4.04187000	1.04005200	-1.63396400
O	3.17990700	0.58959400	0.39077500
C	-4.84527700	2.49596800	-1.06537900
H	-5.45307400	3.32868300	-1.39975200
C	-5.11401000	1.86080800	0.14952600
H	-5.93603400	2.19965500	0.77119700
C	-4.33239700	0.79407400	0.57956600
H	-4.54888500	0.31091700	1.52774800
C	-3.25612600	0.32386800	-0.19872900
C	-2.98934900	0.96649800	-1.42031300
H	-2.17069800	0.62415600	-2.03687500
C	-3.77815400	2.03799800	-1.83782500
H	-3.54997800	2.51827000	-2.78371100
N	-2.53532200	-0.78277100	0.26731700
H	-2.69057000	-0.95986700	1.25141400
C	-1.16670800	-1.08587400	-0.14815100
O	-0.68196900	-2.11423800	0.78900200
O	-0.99335400	-1.37737900	-1.39129200
C	-1.36988300	-3.37961700	0.74234700
H	-2.37150300	-3.27276100	1.17085500
H	-1.48299900	-3.69979600	-0.29896600
C	-0.57037600	-4.39374100	1.53926600
H	-0.44778100	-4.06877000	2.57591600
H	0.42318500	-4.55855600	1.11100400
H	-1.09595900	-5.35274400	1.54277900
O	-0.25733000	0.05917600	0.19492000
C	-0.21670100	0.53947700	1.54579300
H	-1.15171700	0.30903600	2.06344100
H	0.60461000	0.06452100	2.09149300
C	-0.02057100	2.05123900	1.51270100
H	-0.84733000	2.52353800	0.97246000
H	0.91288900	2.30340300	1.00721900
O	0.08673300	2.58861900	2.84018200
H	-0.76410600	2.47579000	3.28293200
K	1.43855900	-2.29599500	-1.17067600
K	5.74057100	1.36092300	0.38167300

Intermediate:

O	1.86552200	0.04026100	-1.39946600
H	1.14264500	0.27743600	-0.75912000
C	3.10202800	0.35145100	-0.88869800
O	4.07896300	0.03296900	-1.61423900
O	3.15757400	0.91439000	0.23505100
C	-5.48266800	0.88941200	-1.39621800
H	-6.30632000	1.27637500	-1.98483200
C	-5.51736800	0.94190200	-0.00038300
H	-6.37277700	1.37522200	0.50719100
C	-4.45974100	0.44655900	0.75389300
H	-4.49727600	0.49574500	1.83805500
C	-3.32930800	-0.12547800	0.13500900
C	-3.29934800	-0.17380600	-1.27053900
H	-2.44746000	-0.60865500	-1.77316300
C	-4.36512200	0.33031200	-2.01558200
H	-4.31550500	0.28129400	-3.09852400
N	-2.32244800	-0.64814800	0.95207200
H	-2.38010500	-0.30927200	1.90381200
C	-0.92832600	-0.84084800	0.52079300
O	-0.19258700	-1.09267900	1.75253200
O	-0.74805200	-1.69446400	-0.42689300
C	-0.30463500	-2.42371400	2.28039100
H	-1.35147800	-2.64519500	2.51648600
H	0.03257200	-3.14659600	1.53128900
C	0.55078600	-2.51230400	3.53021000
H	0.21149100	-1.80525100	4.29233200
H	1.59956600	-2.30130100	3.30343000
H	0.48836500	-3.52075200	3.94921400
O	-0.35537900	0.47722900	0.08535900
C	-0.39077700	1.58289700	0.99489300
H	-1.36655100	1.64028900	1.48859200
H	0.38300400	1.47932800	1.76177700
C	-0.15705600	2.85401900	0.18729600
H	-0.92903200	2.95794700	-0.58213300
H	0.81738100	2.81876400	-0.30234500
O	-0.13459500	4.01204300	1.03582200
H	-1.01742100	4.13014300	1.40837500
K	0.96504700	-2.36461100	-2.14439500
K	5.80777900	0.92782800	0.19720200

Transition state TS2-b:

O	2.36141000	-0.52253600	-1.76591400
H	1.52039100	-0.31824700	-1.27881000
C	3.45704300	-0.34266600	-0.95622200
O	3.27396300	0.03963900	0.22988600
O	4.56973200	-0.58484000	-1.49520600
C	-0.87988700	4.19967600	-0.44766400
H	-1.03099100	5.26859900	-0.35072200
C	-1.47023000	3.49447100	-1.49655000
H	-2.08672000	4.01314800	-2.22263300
C	-1.28540700	2.11836600	-1.61457100
H	-1.76013200	1.57547000	-2.42536200
C	-0.48974200	1.41996200	-0.69437500
C	0.13115300	2.13929300	0.33973300
H	0.79394900	1.62480400	1.02174400
C	-0.07870500	3.51313000	0.46565500
H	0.40843800	4.05118700	1.27179300
N	-0.27424800	0.02234200	-0.85371300
H	-0.70904600	-0.29202700	-1.71696200
C	-0.72477100	-0.87445800	0.25885700
O	-0.54706300	-2.16992700	-0.33965100
O	-0.16600200	-0.67208100	1.39997000
C	-0.77448700	-3.28210400	0.54096300
H	-0.09513300	-3.21616800	1.39527100
H	-1.80152900	-3.24871000	0.92067800
C	-0.53380400	-4.56037900	-0.23860500
H	0.49267500	-4.60401700	-0.61280900
H	-1.21742000	-4.64058200	-1.08828900
H	-0.69640500	-5.42423100	0.41218500
O	-2.21290000	-0.67865900	0.45642200
C	-3.10342400	-1.01897800	-0.60406700
H	-2.82770100	-0.51039600	-1.53647700
H	-3.09547900	-2.09823300	-0.78841500
C	-4.50352700	-0.58121100	-0.19128200
H	-4.52418300	0.49798300	-0.00328600
H	-4.80702800	-1.09888300	0.72068000
O	-5.47415500	-0.92971400	-1.18924300

H	-5.28799100	-0.41341100	-1.98367300
K	-1.88189100	0.84183200	2.60453800
K	5.86814900	-0.02753400	0.74807900

Products-b complex:

O	-1.98739100	-1.64557100	-0.65473000
H	-1.50275100	-0.18501100	0.59660600
C	-2.64383000	-1.26960800	-1.72320900
O	-3.92365800	-1.09580200	-1.65105100
O	-2.00765200	-1.08494700	-2.83008600
C	-2.48977000	4.47474900	0.54348100
H	-2.78626500	5.49780100	0.34367800
C	-2.27968200	4.03793600	1.85341500
H	-2.41408200	4.72505700	2.68230800
C	-1.89926000	2.72424300	2.11466000
H	-1.73950100	2.39577700	3.13698900
C	-1.71857000	1.80752900	1.06305200
C	-1.93386900	2.25148100	-0.25448900
H	-1.80478600	1.55726900	-1.07848600
C	-2.31446700	3.56747300	-0.50396000
H	-2.47768400	3.88453300	-1.52865000
N	-1.28492400	0.50805700	1.31552900
H	-1.46848200	0.17569800	2.25356600
C	3.09773000	-0.84911900	0.43883600
O	3.15186000	-1.31719800	1.67783200
O	2.45973500	-1.32605900	-0.47328900
C	2.36659900	-2.52118200	1.96391300
H	1.31883500	-2.29406600	1.76332300
H	2.70226100	-3.31004100	1.28981600
C	2.60116900	-2.87595500	3.41268400
H	2.27427200	-2.07056300	4.07448200
H	3.65642300	-3.08595300	3.60201400
H	2.02492000	-3.77290300	3.65397500
O	3.86719500	0.23362000	0.35555000
C	3.92927500	0.89396000	-0.93830300
H	4.32265900	0.19292300	-1.67698500
H	2.92691900	1.21262700	-1.22719900
C	4.85560600	2.08732700	-0.76346900
H	5.84036700	1.75516200	-0.42083000
H	4.44438000	2.77809700	-0.02610800
O	4.96183600	2.81413100	-1.99035700
H	5.46423400	2.27968700	-2.61817900
K	0.32812800	-1.87935800	-1.93810700
K	-4.19066700	-2.00963600	0.74128300

Transition state TS2-a:

O	2.89415400	-0.70002900	-1.17311800
H	1.97241800	-0.97397600	-0.96114300
C	3.47033800	-0.12852600	-0.06579700
O	2.78033300	-0.02837200	0.98504600
O	4.66122900	0.25008200	-0.21121000
C	-4.14737000	2.61116000	1.30552500
H	-4.91235500	3.33465400	1.56155700
C	-2.97985900	2.50957300	2.06845300
H	-2.83163000	3.15957700	2.92411100
C	-1.99812800	1.58196800	1.74429300
H	-1.09558300	1.51235900	2.34309200
C	-2.15234500	0.72276200	0.63650900
C	-3.32649200	0.83177100	-0.13212100
H	-3.46308600	0.20221800	-1.00110000
C	-4.30553800	1.76844500	0.20837600
H	-5.19897600	1.83542700	-0.40322800
N	-1.15873900	-0.23550000	0.39553300
H	-0.26884900	-0.00544800	0.82110900
C	-1.01284900	-0.96783100	-0.88771100
O	0.29502300	-1.66483200	-0.74624100
O	-1.99996700	-1.75758800	-1.16447700
C	0.27021100	-2.82001800	0.11378600
H	0.14684100	-2.50182400	1.15616800
H	-0.58182900	-3.44528700	-0.16651800
C	1.55811500	-3.60795200	-0.04355900
H	2.42845100	-3.02947400	0.27345600
H	1.70258600	-3.91823300	-1.08187000
H	1.50472700	-4.50743100	0.57668900
O	-0.78011600	-0.06278500	-1.99618300
C	0.00089100	1.12109600	-1.78715300
H	-0.62740500	1.91607100	-1.36734800
H	0.83206600	0.94068200	-1.10337100

C	0.53403200	1.55863900	-3.14464800
H	-0.29083000	1.65328300	-3.85890600
H	1.24140000	0.82271400	-3.52993800
O	1.25303100	2.79674000	-3.04427900
H	0.62291600	3.49171400	-2.81596600
K	-3.28176500	-2.20515400	1.00629300
K	4.78885800	1.12142900	2.28699300

Products-a complex:

O	2.81455600	-0.83962700	-0.80508900
H	2.30797300	-0.00625600	0.61097900
C	2.80695400	-2.15044200	-0.89693000
O	3.51745800	-2.84464000	-0.07397300
O	2.09043200	-2.71021500	-1.80875700
C	-5.18269500	-2.64893900	0.42319700
H	-5.78873300	-3.54638900	0.46296700
C	-5.50803500	-1.54070400	1.20721500
H	-6.37057800	-1.56899000	1.86335800
C	-4.72988600	-0.39003600	1.15522000
H	-4.98455000	0.47017400	1.76562100
C	-3.60938500	-0.32915800	0.31368900
C	-3.27797100	-1.43770600	-0.47382000
H	-2.41927300	-1.40802400	-1.12590400
C	-4.06868900	-2.58563400	-0.41089400
H	-3.80192500	-3.43814300	-1.02549400
N	-2.87984800	0.87986200	0.32663400
H	-3.23398400	1.59942800	0.94483900
C	-1.77682100	1.22326100	-0.38405900
O	2.30969100	0.45613200	1.48585400
O	-1.18329000	0.52412700	-1.19542300
C	1.13751400	0.07344100	2.22685400
H	0.24339200	0.47378700	1.73354100
H	1.04942900	-1.01922500	2.24057800
C	1.24086100	0.61194100	3.64014200
H	1.32473100	1.70266800	3.63722000
H	2.11338000	0.19856800	4.15465100
H	0.34846400	0.34056600	4.21116000
O	-1.40844400	2.48761300	-0.07475700
C	-0.25116700	3.01823700	-0.76377400
H	0.63416400	2.44538200	-0.47764500
H	-0.40533400	2.95139000	-1.84189500
C	-0.11774700	4.46992000	-0.32873400
H	0.00520800	4.53204300	0.75681700
H	-1.01054400	5.02983500	-0.61105300
O	0.98198900	5.09047100	-1.00122600
H	1.80232100	4.71346700	-0.65875500
K	0.84390300	-0.50003900	-2.53635100
K	4.70283700	-0.91181900	1.20008400