Supplementary Materials for

Selective deconstruction of mixed plastic by a tailored organocatalyst

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Supplementary Experimental Procedures

1. Materials and Methods

1.1 Materials

All reactions were performed using a heavy wall cylindrical pressure vessel. 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD) (Millipore Sigma 98%), trifluoracetic acid (TFA) (Millipore Sigma 99%), ethylene glycol (EG) (Millipore Sigma 99.8%), 7-methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (mTBD) (Millipore Sigma 98%), methyl trifluoracetate (mTFA) (Millipore Sigma 99%), dimethyl sulfoxide-d6 (DMSO-d6) (Millipore Sigma 99.9%), and methanol (Millipore Sigma 99%) were used as received without further purification. Poly (Bisphenol A Carbonate) (PC, M_w = 45,000 g/mol, , T_g = 150 °C, T_m = 267 °C, Density = 1.2 g/cm^3 at 25 °C) and polyamide (PA, Nylon 6, M_w = 35,000 g/mol, T_g = 63 °C, T_m = 229 °C, Density = 1.08 g/cm^3 at 25 °C) mol were purchased as granulate from Millipore Sigma and used as received. Laser+® W (L40A) polyethylene terephthalate (PET, M_w = 40,000 g/mol, Intrinsic Viscosity = 0.75 ± 0.02, dL/g, Crystallinity >45%, T_m = 242 °C, Bulk Density 1.350 g/m^3) were provided by DAK Americas. Thermoplastic polyurethane (PU) was synthesized according to the reported method[1] and characterized by ^{1}H NMR (Figure S72). Gel Permeation Chromatography (GPC) (Figure S73) determined the molecular weight of PU to be M_w 24600 g/mol with PDI 1.23.

The commercial consumer product was collected from different sources. The colorful PET bottles were manufactured by Cool Gear manufacturer. The hyper tough anti-fog PC safety glasses were manufactured by Honeywell Ademco. PU foam (thickness: 10 mm, bulk density: 0.08 g/cm) was purchased from Millipore Sigma. We tested the solubility of the PU foam in chloroform, methylene chloride, acetone, dimethyl formamide, methanol and water and it was insoluble in all of those solvent, which indicates that the PU foam is a thermoset (gel content 98%). NPP4100-HT nylon blend twisted rope was manufactured by Golberg G. The PET carpet which contains 30% PP backing was purchased from a local Home Depot. We used one of our used cloths which is made from 60% PET and 40% cotton. We collected the PE grocery bag manufactured by IPS Industries and PP cap from Cool Gear manufacturer.

1.2 Characterization Methods

^{1}H and ^{13}C NMR — Spectra were recorded on a Bruker AV III HD (^{1}H, 400 MHz) spectrometer with a broadband Prodigy cryoprobe. Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra were referenced to protons of the residual solvent (for ^{1}H) and deuterated solvent itself (for ^{13}C).

FTIR — FTIR measurements were performed using a Fourier Transform Infrared Spectrometer (Thermo Scientific, Nicolet iS50 FT-IR) with a diamond attenuated total reflection (ATR) accessory (64 scans).

Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry (MALDITOF-MS) — The samples were analyzed using a Bruker Autoflex Speed. The samples were prepared by dissolving Super-DHB (S-DHB) matrix at 60 mg/ml, sodium trifluoroacetate (NaTFA) salt at 5 mg/ml, and the sample at 10 mg/ml in THF:MeOH (50:50). Aliquots of the solutions are mixed in a 20:1:20 ratio (matrix:analyte:sample) and deposited 0.5 µl on the stainless steel target for analysis. The spectra were acquired by summing 3000 laser shots into the sum buffer in 1000-shot intervals. The samples were analyzed in triplicate, and the average peak area was calculated to generate the peak area vs. time plot. Four peaks were selected to track the deconstruction of the PET sample, m/z 277.110, m/z 469.252, and m/z 661.345 (Figure S28), representing the monomer through the tetramer of PET.

Gel Permeation Chromatography (GPC) — The multidetector size exclusion chromatography system used here comprises one PSS GRAM 10 µm guard column (8 × 50 mm, Polymer Standards Service-USA, Inc.), three PSS GRAM 10 µm linear columns (8 × 300 mm; 100, 1000, and 3000 Å, Polymer Standards Service-USA, Inc.), an Agilent model 1260 Infinity pump, a Rheodyne model 7725 manual injector with a 200 µL loop, and a Varian 390 LC detector system consisting of an RI detector and a two-angle light scattering detector (15° and 90°). The mobile phase is DMF with 0.1 M LiBr, at 60 °C at a rate of 1 mL/min. 1.41 mg/mL in 0.1 M LiBr is prepared and injected for GPC analysis.

Thermogravimetric Analysis (TGA) — Thermal gravimetric analysis was obtained using a TA Instruments Q50 Thermogravimetric Analyzer. Analysis was performed on ~10 mg of a given sample at a heating rate of 10 °C/min from 30 to 600 °C under a nitrogen atmosphere.

High performance liquid chromatography (HPLC) — Chromatograms of products were performed using Water Spherisorb 3 um ODS2 4.6 X 150mm column on an Advion A-2046 equipped with a UV-Vis detector, measuring at 254 nm, injected volume = 10 µL, isocratic gradient flow = 0.9 mL min−1, Acetonitrile(0.1% formic acid)/Water(0.1% formic acid) from 10% to 100% for 30 min at 40 °C.

2. Equations

2.1 Equation for conversion

Determination of polymer conversion for each polymer, where $W_{initial}$ is the initial mass of the polymer and W_{final} is a residual mass, which includes oligomer and unreacted polymer.

$$Conversion\ (\%) = \frac{W\ \text{initial} - \text{W final}}{W\ \text{initial}} \times 100$$

2.2 Equation for monomer yield

Determination of monomer yield for each polymer where *Mm* is the mmol of monomer and Mp is mmol of un-depolymerized polymer.

$$Monomer\ Yield\ (\%) = \frac{Mm}{Mp} \times 100$$

2.3 Equation for monomer yield from NMR

Monomer yields were determined from the peak intensity of the monomer by using an internal standard (at 1.88 ppm from catalyst) from ^{1}H NMR spectroscopy, where *Ix* and *Nx* refer to peak intensity and number of protons of the monomer, respectively, *Iis* and *Nis* denote peak intensity and number of proton of internal standard at 1.88 ppm respectively, and Mis is the mmol of internal standard.

$$\%\ of\ monomer = \left(\frac{\frac{Ix}{Nx}}{\frac{Iis}{Nis}} \times Mis\right) \times 100$$

3. Synthetic Procedure

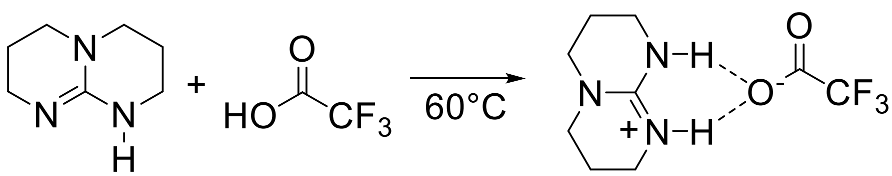
3.1 Catalyst Synthesis[2, 3]

3.1.1 General procedure for TBD:TFA synthesis — Different dual catalysts were prepared by mixing TBD and TFA at molar ratios of base to acid at 60 °C for 30 minutes and used it without further purification.

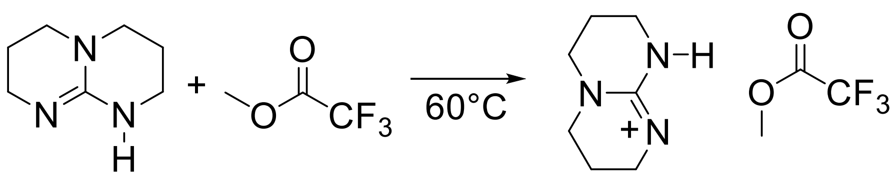
TBD: TFA (1:1): ^{1}H NMR (400 MHz, DMSO-d6) δ 8.07 (s, 2H), 3.27 (td, *J* = 6.2, 2.2 Hz, 4H), 3.18 (dq, *J* = 6.0, 2.9 Hz, 4H), 1.88 (dd, *J* = 8.6, 4.0 Hz, 4H) (Figure S16). ^{13}C NMR (101 MHz, DMSO-d6) δ 159.72, 150.83, 118.10, 46.09, 37.33, 20.20 (Figure S17).

TBD: TFA (3:1): ^{1}H NMR (400 MHz, DMSO-d6) δ 5.10 (s, 2H), 3.08 (q, *J* = 5.6 Hz, 8H), 2.02 – 1.59 (m, 4H) (Figure S74).

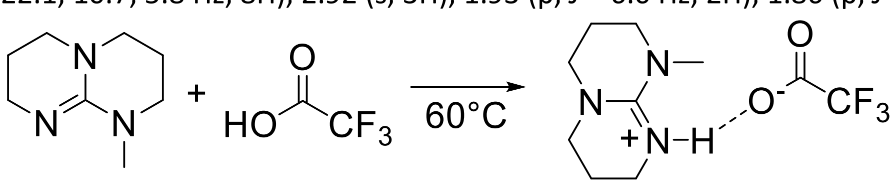
TBD: TFA (1:3): ^{1}H NMR (400 MHz, DMSO-d6) δ 15.35 (s, 1H), 7.79 (s, 2H), 3.37 – 3.21 (m, 4H), 3.17 (s, 4H), 1.85 (s, 4H) (Figure S75).



3.1.2 TBD:mTFA (1:1) synthesis — Equimolar amount of TBD and mTFA were mixed with a magnetic stir bar at 60 °C for 30 minutes and used it without further purification. ^{1}H NMR (400 MHz, DMSO-d6) δ 3.33 – 3.13 (m, 8H), 2.90 (s, 3H), 1.89 (ddp, *J* = 16.1, 11.0, 5.9 Hz, 4H) (Figure S29).

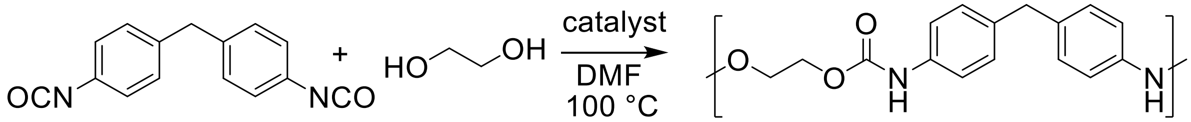


3.1.3 mTBD:TFA (1:1) synthesis — Equimolar ratio of mTBD and TFA were mixed at 60 °C for 30 minutes and used it without further purification. ^{1}H NMR (400 MHz, DMSO-d6) δ 3.27 (ddt, *J* = 22.1, 10.7, 5.8 Hz, 8H), 2.92 (s, 3H), 1.93 (p, *J* = 6.0 Hz, 2H), 1.86 (p, *J* = 5.9 Hz, 2H) (Figure S30).



3.2 Poly(urethane) Synthesis

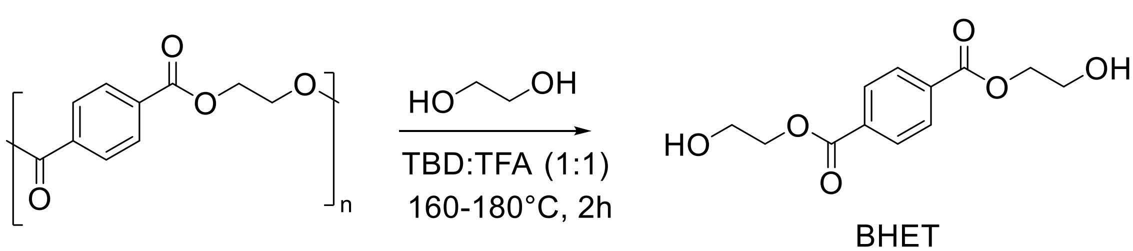
Methylene diphenyl diisocyanate (MDI) (5.3 g, 21.2 mmol), ethylene glycol (1.4 g, 21.2 mmol), dibutyltin dilaurate (5.0 mg), and 50 mL of DMF were put into a 500 mL round-bottom flask, and the reaction was heated at 80 °C in an oil bath. Then, the mixture was left to react for 12 h for complete polymerization. The final viscous solution was poured into 1 L of ethanol. The precipitate was collected and dried in a vacuum oven at 60 °C for 12 h to yield pure polyurethane with M_w 24600 g/mol, PDI 1.23 confirmed by GPC. ^{1}H NMR (400 MHz, DMSO-d6) δ 9.64 (s, 2H), 7.35 (d, *J* = 8.1 Hz, 4H), 7.09 (d, *J* = 8.1 Hz, 4H), 4.30 (s, 4H), 3.78 (s, 2H) (Figure S72).



4. Polymer Deconstruction

4.1 PET deconstruction

PET pellets (0.5 g, 2.60 mmol), EG (1.62 g, 26 mmol), and catalyst (0.035 g, 0.13 mmol) were placed in a pressure vessel with a magnetic stirrer. The deconstruction reactions were carried out at 180 °C for 2 h. When the reaction was completed, the crude product was cooled to room temperature, and a large excess of distilled water was added. The resulting solution was vigorously stirred and filtered to separate EG, catalyst, and main product from dimers, oligomers, and insolubles in water. The transparent aqueous filtrate was stored in a refrigerator at 4 °C overnight. White needle-like crystals bis(2-hydroxyethyl) terephthalate (BHET) were formed in the solution, which was then recovered by filtration before drying.
BHET — ^{1}H NMR (400 MHz, DMSO-d6) δ 8.13 (s, 4H), 4.97 (t, *J* = 5.7 Hz, 2H), 4.36 – 4.29 (m, 4H), 3.72 (q, *J* = 5.3 Hz, 4H) (Figure S26).
BHET Dimer — ^{1}H NMR (400 MHz, DMSO-d6) δ 8.15 – 8.05 (m, 8H), 4.97 (q, *J* = 5.4 Hz, 2H), 4.68 (s, 4H), 4.31 (q, *J* = 4.7 Hz, 4H), 3.71 (p, *J* = 6.4 Hz, 4H) (Figure S76).



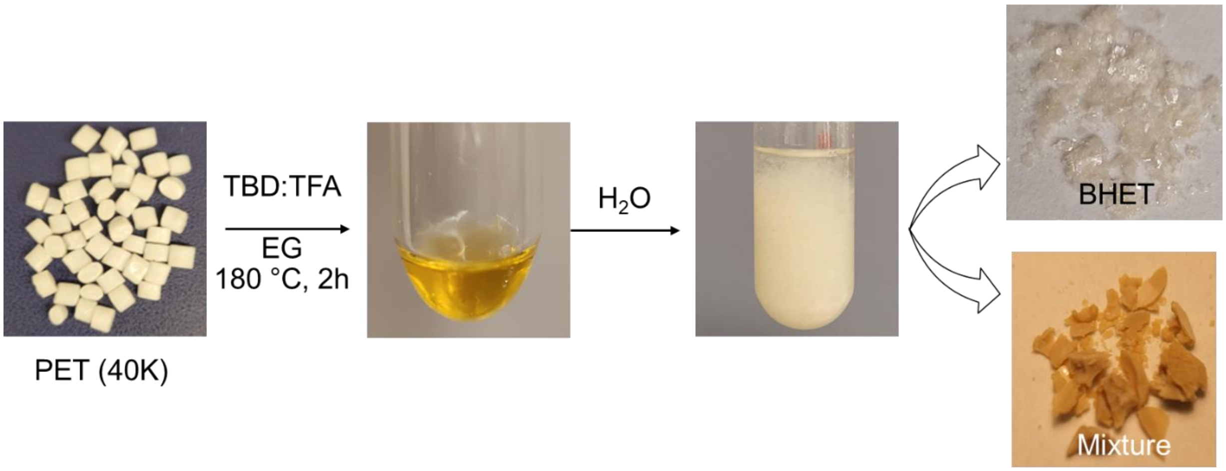


Figure S1. Deconstruction process of PET. PET (1eq.) pellets were completely deconstructed by using TBD:TFA (0.05 eq.) at 180 °C for 2 h.

4.2 Catalysis reaction optimization

PET pellets (0.5 g, 2.6 mmol, 1 eq.) were charged in a 10 mL pressure vessel equipped with a magnetic stirrer. Each depolymerization was carried out at determined EG and catalyst at a certain temperature for 2 h. The yields were obtained by ^{1}H NMR spectroscopy in DMSO-d6 using the catalyst signals as an internal standard (d =1.87 ppm, 4H) and the characteristic signals of BHET (d = 8.10 ppm, 4H) with the corresponding isolated yield.

Table S1. Optimization of the deconstruction reaction by using PET. Reaction conditions: PET (0.5 g, 1 eq.), temperature 180 °C, time 2 h, and the yield was calculated by ^{1}H NMR spectroscopy in DMSO-d6 using the catalyst signals as internal standard (d =1.87 ppm, 4H), and the characteristic signals of BHET (d = 8.10 ppm, 4H).

Entry	**PET: Catalyst:EG**	**C_{PET} (%)**	**Yield[a] (Isolated Yield) (%)**	
			BHET	**Mixture**
1	1:0.5:20	100	93 (90)	6
2	1:0.5:10	100	91 (89)	8
3	1:0.5:5	100	76 (72)	18 (15)
4	1:0.25:10	100	91 (89)	6
5	1:0.1:10	100	94 (91)	4
6	1:0.05:10	100	97 (95)	3

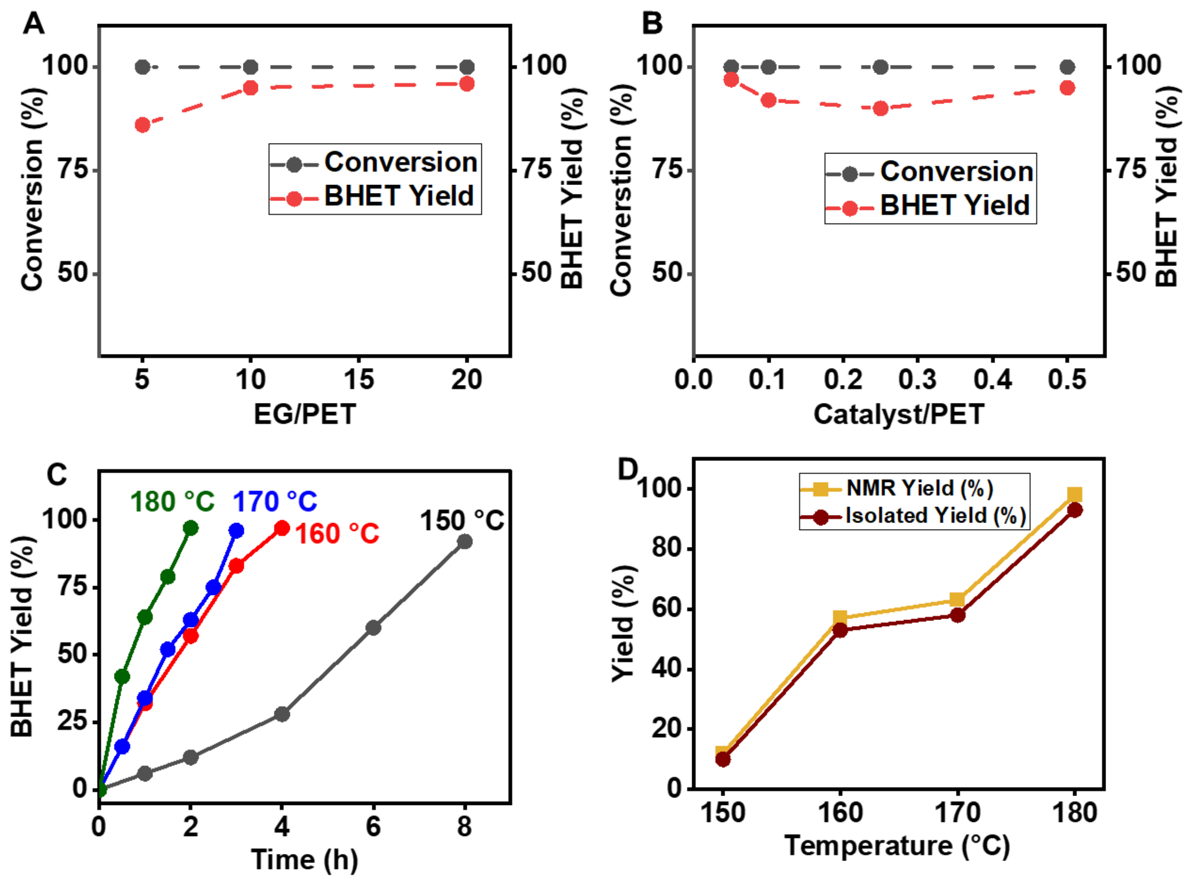
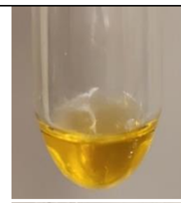


Figure S2. A) Effect of the EG amount on the conversion of PET (black line) and BHET yield (red line). Reaction conditions: PET (1 eq.), catalyst (0.05 eq.), 180 °C. (B) Effect of the catalyst amount on the conversion of PET (black line) and BHET yield (red line). Reaction conditions: PET (1 eq.), EG (10 eq.), 180 °C. (C) Effect of temperature on conversion of PET. Reactions conditions: PET (1 eq.), EG (10 eq.), catalyst (0.05 eq.). (D) Comparison of yield at different temperatures.

4.3 Catalytic activity of PET by using TBD:TFA vs TBD:MSA

In a typical experiment, 1:0.05:10 equivalents of PET pellets, catalyst and EG, respectively, were charged in a 10 mL pressure vessel equipped with a magnetic stirrer. Each deconstruction was carried out at 180 °C for 2 h. The PET conversion was calculated based on unreacted PET by using equation 2.1 (Table 2).

Table S2. Catalytic comparison between TBD:MSA (1:1) and TBD:TFA (1:1) for the deconstruction of PET at 180 °C for 2 h.

Entry	**Catalyst**	**PET:Cat:EG**	**C_{PET} (%)**	**Observation**
1	TBD:TFA (1:1)	1:0.05:10	100	
2	TBD:MSA (1:1)	1:0.05:10	60	

4.4 Catalytic activity of different PET

In a typical experiment, 1:0.05:10 equivalents of different molecular weight PET pellets, catalyst and EG, respectively, were charged in a 10 mL pressure vessel equipped with a magnetic stirrer. Each deconstruction was carried out at 180 °C for 2 h. The PET conversion was calculated based on unreacted PET by using equation 2.1(Table 3).

Table S3. Deconstruction of different molecular weights of PET polymer by using TBD:TFA as a catalyst at 180 °C for 2 h. C_{PET} = Conversion of PET polymer.

Entry	**PET (g/mol)**	**C_{PET} (%)**
1	8000	100
2	40,000	100
3	60,000	100

4.5 Large scale reaction

PET pellets (10 g, 52 mmol, 1 eq.) were charged in a 150 mL pressure vessel equipped with a magnetic stirrer. The deconstruction was carried out by using 10 eq. of EG and 0.05 eq. of catalyst at 180 °C for 4 h. The yields were obtained by ^{1}H NMR spectroscopy in DMSO-d6 using the catalyst signals as an internal standard (d =1.87 ppm, 4H) and the characteristic signals of BHET (d = 8.10 ppm, 4H) with the corresponding isolated yield.

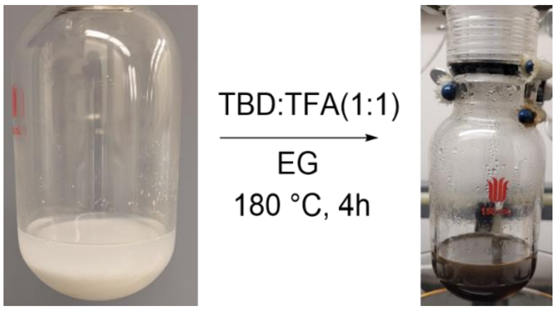


Figure S3. A complete deconstruction of PET in a large scale (10 g) using TBD:TFA as a catalyst with a ratio of PET:Cat:EG (1:0.05:10) at 180 °C for 4h.

4.6 Catalyst optimization

PET pellets (0.5 g, 2.6 mmol, 1 eq.) were charged in a 10 mL pressure vessel equipped with a magnetic stirrer. Each deconstruction reaction was carried out at determined EG and catalyst at a certain temperature for 2 h. The yields were obtained by ^{1}H NMR spectroscopy in DMSO-d6 using the catalyst signals as an internal standard (d =1.87 ppm, 4H) and the characteristic signals of BHET (d = 8.10 ppm, 4H) with the corresponding isolated yield (Figures S42 to S44).

Table S4. Optimization of the catalyst for the deconstruction of PET. Reaction conditions: PET:Cat:EG (1:0.5:20) at 180 °C for 2 h. C_{PET} = Conversion of PET polymer.

Entry	**Organocatalyst**	**Ratio**	**Melting Point (°C)**	**C_{PET} (%)**	**% Yield**	
					BHET	Other
1		1:0		60	68	31
2		1:1	157	100	96	2
3	TBD: TFA	1:3	-	20	50	46
4		3:1	82	100	55	42
5		0:1		0	0	0
7	TBD:mTFA	1:1		50	65	34
8	mTBD:TFA	1:1		32	48	46

4.7 Small-Angle Neutron Scattering (SANS)

SANS measurements were conducted using the EQ-SANS instrument at the Spallation Neutron Source of Oak Ridge National Laboratory[4, 5]. Sample-to-detector distances of 9 m, 4 m, 2.5 m, and 1.3 m were employed with minimum wavelength settings of 15 Å, 10 Å, 2.5 Å, and 1 Å, respectively, with choppers operating at 60 Hz. As a result of a combination of multiple configurations, a wide range of momentum transfers of 0.003 $Å^{-1} < q < 3$ $Å^{-1}$ was achieved, where $q=4\pi\sin(\theta)/\lambda$, 2θ is the scattering angle, and λ is the wavelength. Samples were loaded into 2 mm path length cylindrical quartz cuvettes from Hellma (Plainview, NY, USA). The original standard sample environment of the instrument was used to control the temperature to within ±1 °C by means of a water bath. Data reduction followed standard procedures[6]. The data reduction included subtraction of the appropriate solvent background. Measured SANS intensities are summarized in Figure S4A. At the very beginning of the deconstruction process, no PET, monomers, or any kinds of structural characteristics were observed, as indicated by the flat scattering curve. From the aliquots taken at 30 min, 60 min, and 90 min into the deconstruction process, strong power-law-like scattering intensities were observed. All scattering intensities from 30 min, 60 min, and 90 min were fitted with the Gunier-Porod model[7] with a Porod exponent of 4 and a dimension variable ~ 1.7, indicating the existence of large solid objects, which may be attributed to the undissolved PET. The scattering intensity was dramatically reduced in the final aliquots, which was taken 120 min into the deconstruction process. The reduced scattering intensity with a fitted dimension variable higher (1.9) than other samples suggests that the origin of the scattering intensity upturns may be different. The clear difference in the scattering intensity at the final stage from previous stages suggests that most of the PET have been deconstructed into monomers and dimers, as evidenced by other experimental results such as MALDI-TOF (Figure S28) and ^{1}H NMR. (table S4) The low-q upturn in aliquot #5 can be attributed to the phase separation of monomers and dimers due to the relatively poor hydrophilicity of dimers or bigger units. The such low-q upturn was also observed in the reference sample, where monomers and dimers were mixed in ethylene glycol. In Figure S4B, monomers in EG and dimers in EG are shown. Due to the poor hydrophilicity of dimers, dimers in EG show stronger low-q upturns indicating more aggregates or the formation of a larger structure.

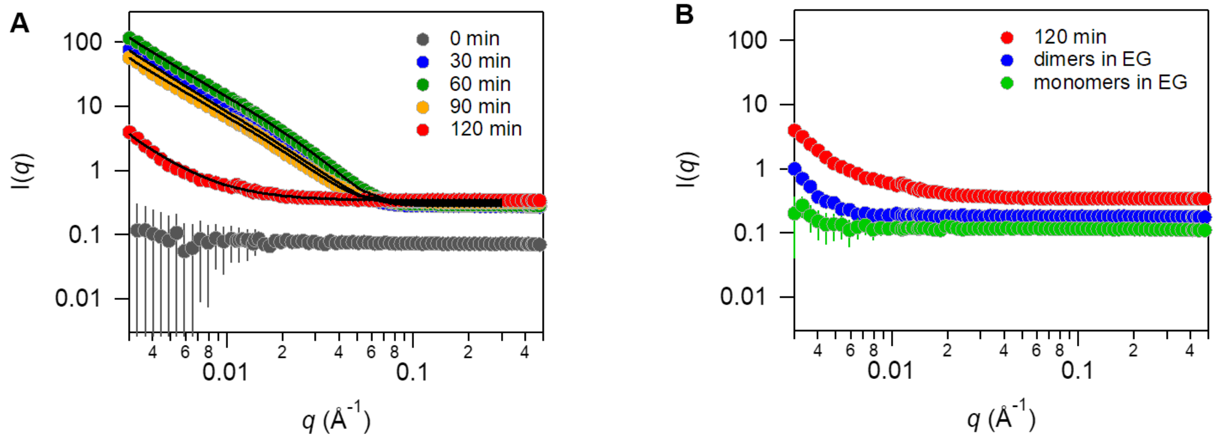


Figure S4. Measured SANS intensities. (A) At the very beginning of the deconstruction process (o min), no PET, monomers, or any kinds of structural characteristics were observed as indicated by the flat scattering curve (gray). From the aliquots taken at 30 min (blue), 60 min (green), and 90 min (yellow) strong power-law-like scattering intensities were observed due to the large size particle, which is oligomer. After 120 min, the scattering intensity was dramatically reduced (red) suggests that most of the PET have been deconstructed into small molecules like monomers and dimers. Black lines fit the Guinier-Porod model. (B) Monomers dissolved in EG show a flat scattering profile (green), while the dimers dissolved in EG show low-q upturn (blue), similar to the scattering profile of the aliquot (red) taken at 120 min into the deconstruction process.

4.8 Quantum Chemistry Calculations and Simulations of PET deconstruction

The NWChem suite of codes (version 7.0.2) was used to perform all-electron density functional theory (DFT) calculations using the hybrid meta functional m06-2x and the aug-cc-pvdz basis set. Two different continuum solvent models, the Conductor-like Screening Model (COSMO) and Solvation Model Based on Density (SDM) were used to emulate a bulk EG solvent. We used a dielectric constant of 37 D for EG for both models. The trends on interaction energies and geometries were similar, although the COSMO model tends to give smaller interaction energies than the SMD. Regarding basis set dependencies, we used both aug-cc-pvdz and cc-pvdz, with cc-pvdz giving higher interaction energies overall. We note that the diffuse basis functions of aug-cc-pvdz are likely essential for cation/anions.

First, calculations were performed on a model PET chain of eight monomers (Figure S5). This model was then used to explore interactions with TBDH+ and the TFA anion. Full geometry optimization for all cases studied/reported was performed.

Ab initio molecular dynamics (AIMD) using the same basis set and the SMD solvent model was used to study the dissociation of TBD:TFA and TBD:MSA at 180 °C. Simulations were carried out in the NVE ensemble at 180 °C using the Stochastic velocity rescaling thermostat of Bussi, Donadio, and Parrinello, J. Chem. Phys. 126, 014101 (2007) with a nuclear time step of 0.2419 fs.

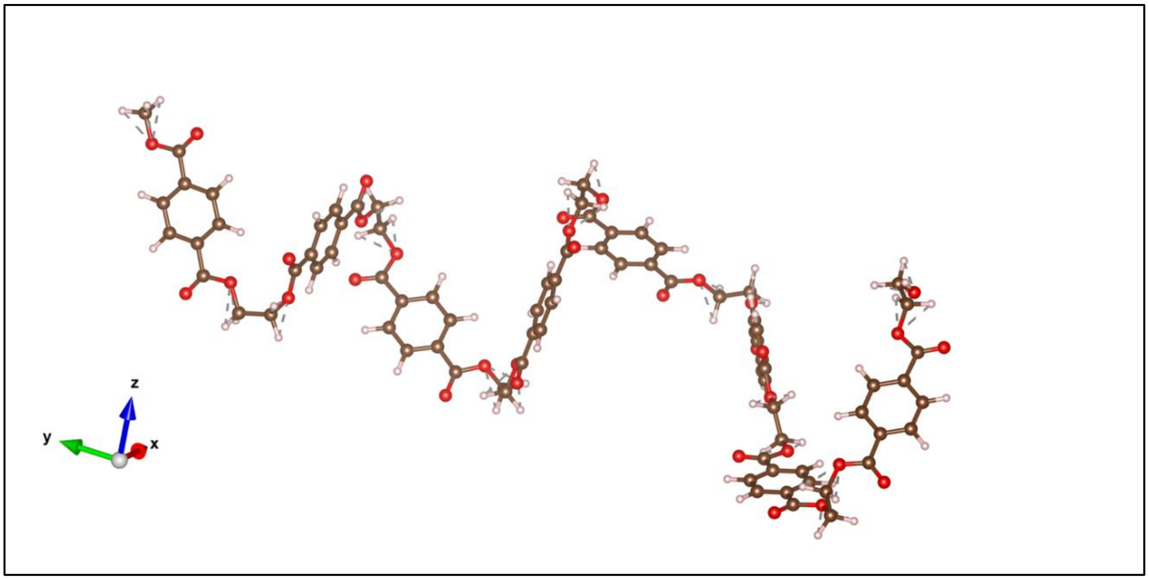


Figure S5. Optimized geometry for an 8-monomer chain of PET.

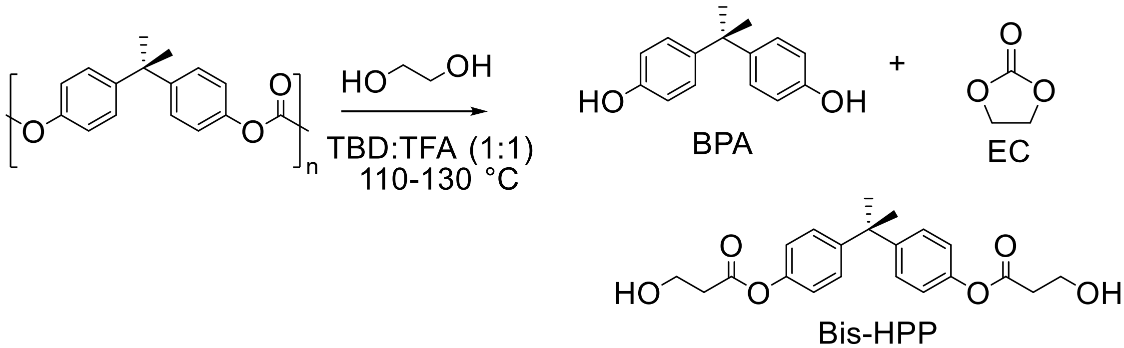
4.9 Polycarbonate (PC) deconstruction

PC pellets (0.5 g, 1.97 mmol), EG (1.22 g, 19.7 mmol], and catalyst (0.025 g, 0.10 mmol) were placed in a pressure vessel with a magnetic stirrer. The deconstruction was carried out at 130 °C for 2 h. The reaction was then cooled to room temperature before being dissolved in diethyl ether (30 mL) and water (30 mL). The organic phase was washed 3 × 20 mL with water before with $MgSO_4$ before evaporation of the solvent separated through combiflash yielding two products bisphenol A (BPA) (94%), ethylene carbonate (93%) with a small amount of bis-(hydroxypropoxy) propane (Bis-HPP) (5%) as a byproduct. The yield was calculated by using ^{1}H NMR spectroscopy in DMSO-d6 using the catalyst signals as internal standard (d =1.87 ppm, 4H), and the characteristic signals of BPA (δ 6.67 ppm), EC (δ 4.48 ppm), and Bis-HPP (δ 4.08 ppm, 2H). (Figure S6 and Table S5)

BPA—^{1}H NMR (400 MHz, DMSO-d6) δ 9.11 (s, 2H), 6.98 (d, *J* = 8.4 Hz, 4H), 6.64 (d, *J* = 8.3 Hz, 4H), 1.53 (s, 6H) (Figure S33).

EC—^{1}H NMR (400 MHz, $CDCl_3$) δ 4.48 (s, 4H) (Figure S34).

Bis-HPP—^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 4H), 7.22 – 7.15 (m, 2H), 6.90 – 6.81 (m, 2H), 4.09 (dd, *J* = 5.2, 3.9 Hz, 4H), 4.01 – 3.95 (m, 4H), 1.69 (s, 6H) (Figure S35).



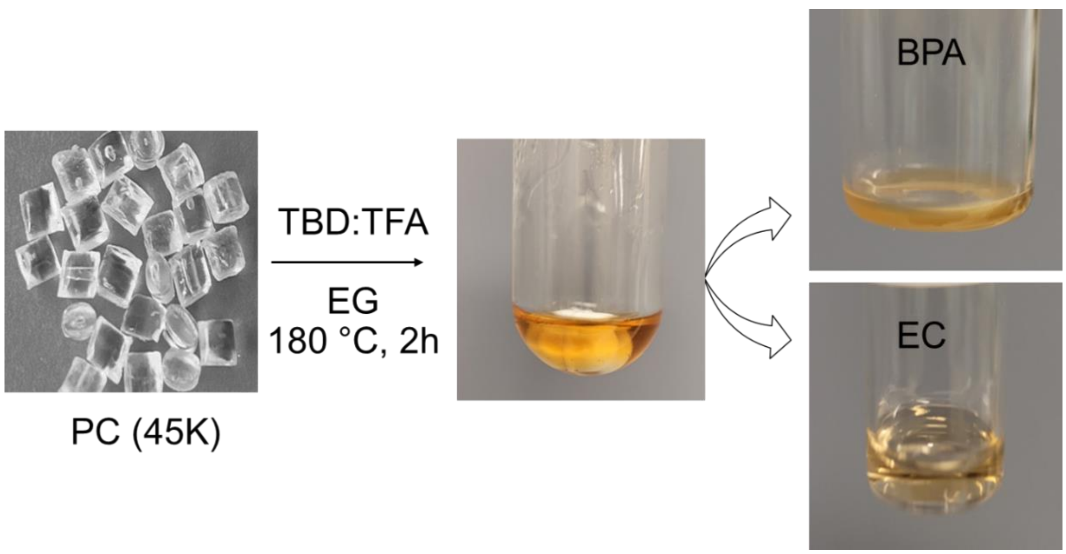
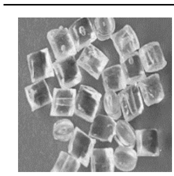


Figure S6. Deconstruction process of PC. PC (1eq.) pellets were completely deconstructed by using TBD:TFA (0.05 eq.) at 130 °C for 2 h.

Table S5. Deconstruction of PC (45,000 g/mol) using TBD:TFA as a catalyst. C_{PC} = Conversion of PC polymer.

PC pellet	**C_{PC} (%)**	**Yield (Isolated Yield) (%)**		
		BPA	**EC**	**Bis-HPP**
	100	94 (92)	93(87)	5(0)

4.10 Polyurethane deconstruction

PU pellets (0.1 g, 0.32 mmol), EG (0.20 g, 3.20 mmol) and catalyst (0.004 g, 0.016 mmol) were placed in a pressure vessel with a magnetic stirrer. The deconstruction was carried out at 150-170 °C for 2 h. After 2 h, the mixture of 1 M HCl (15 mL) and brine (5 mL) was added. The mixture was extracted with CH_2Cl_2 (4x 10 mL), and the combined organic phases were washed with brine (1x 15 mL), dried with anhydrous Na_2SO_4, filtered, and dried in vacuo to provide EG as a liquid. The acidic aqueous phase was basified with 4 M NaOH till pH reached 11-12, then extracted with CH_2Cl_2 (3x 10 mL), and the combined organic phases were dried using anhydrous Na_2SO_4, filtered, and dried in vacuo to yield methylene dianiline (MDA) (0.14 g, 80%) and bis(2-hydroxyethyl) (methylenebis(4,1-phenylene) dicarbamate (BMDC) (<17%) (Table S6). The yield was calculated by ^{1}H NMR spectroscopy in DMSO-d6 using the catalyst signals as internal standard (d =1.87 ppm, 4H), and the characteristic signals of MDA (δ 6.8 & 6.5 ppm), and BMDC (δ 7.3 & 7.1 ppm). By increasing temperature, the yield of MDA is increased and BMDC is decreased (Figure S7). ^{1}H NMR of MDA (400 MHz, DMSO-d6) δ 6.81 (dd, *J* = 7.8, 5.5 Hz, 4H), 6.47 (dd, *J* = 7.8, 5.5 Hz, 4H), 4.82 (br, 4H), 3.59 (s, 2H) (Figure S38).

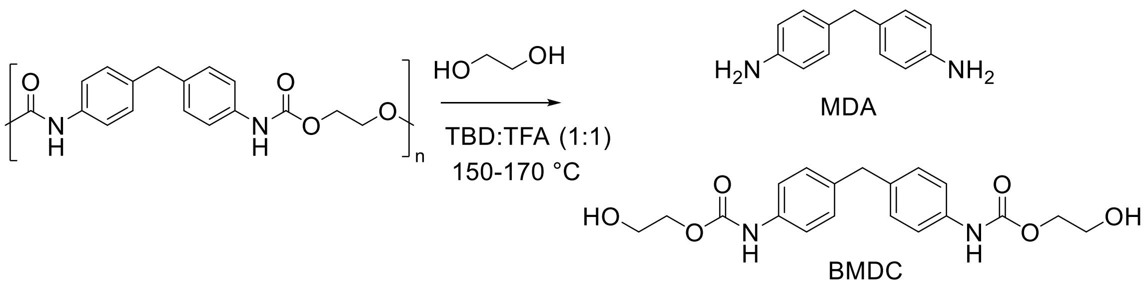


Table S6. Deconstruction of PU (24600 g/mol) using TBD:TFA as a catalyst. C_{PU} = Conversion of PU polymer.

PU pellet	**C_{PU} (%)**	**Yield (Isolated Yield) (%)**	
		MDA	**MDEA**
	100	80 (76)	17

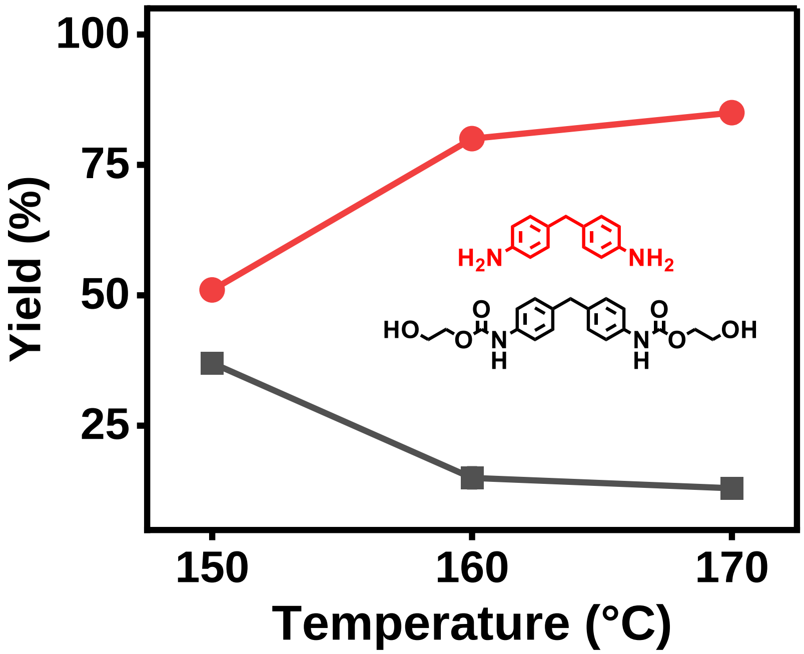


Figure S7. Effect of temperature on PU deconstruction. At low temperature (150 °C), MDA and BMDC yields equally but at 170 °C more MDA (80%) yields than BMDC (17%).

4.11 Polyamide (PA) deconstruction

Nylon-6 pellets (0.5 g, 4.4 mmol), EG (2.73 g, 44 mmol], and catalyst (0.05 g, 0.22 mmol) were placed in a pressure vessel with a magnetic stirrer. The deconstruction was carried out at 210 °C for 3h. After cooling, water was added to the reaction mixture and separated through CombiFlash® yielding caprolactam (CPL) (83%) and 2-hydroxyethyl-6-aminohexanoate (HAH) (13%) (Table S7). The yield was calculated by using ^{1}H NMR spectroscopy in DMSO-d6 using the catalyst signals as an internal standard (d =1.87 ppm, 4H), and the characteristic signals of BPA (d = 2.05 ppm, 4H). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.72 (s, 1H), 3.00 (d, *J* = 6.7 Hz, 2H), 2.03 (t, *J* = 7.4 Hz, 2H), 1.63 – 1.11 (m, 6H) (Figure S50 and S51).

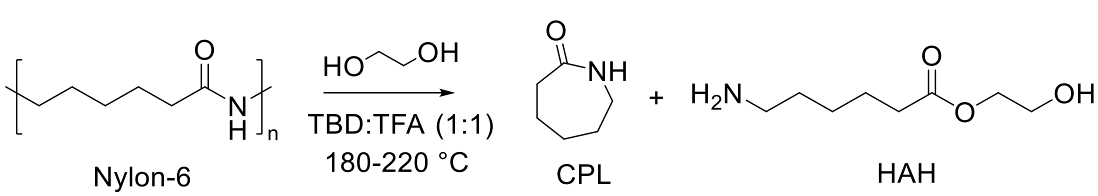


Table S7. Deconstruction of PA using TBD: TFA as a catalyst. C_{PA} = Conversion of PA polymer.

PA source	C_{PA} (%)	Yield (Isolated Yield) (%)	
		CPL	HAH
	85	85 (83)	13

4.12 Recyclability and water Susceptibility

Considering the environmental and economic viability of the proposed process, residual reactants and catalysts need to be recycled for further PET deconstruction. We studied the reusability following two processes. In the first process, after filtering the BHET crystals from the aqueous phase, the unreacted EG and catalyst were dried by vacuum evaporation at 60 °C before being stored in a vacuum oven at 60 °C overnight. Then, fresh PET flakes were added to the recycled system [EG + catalyst] using the same procedure (Figure S8A). In the second process, after the complete conversion of the PET, another batch of PET and EG was added without a catalyst to see the catalytic activity of the catalyst. In the presence of TBD:TFA, the BHET yield is observed to be constant with no loss of catalytic activity, even after 5 recycling processes (Figure S8B). Two methods yielded BHET very efficiently up to 5 cycles (Figures S54 to S57). The catalyst also performs very efficiently in the presence of up to 30% of water (Figure S10, and Figures. S58 to S61).

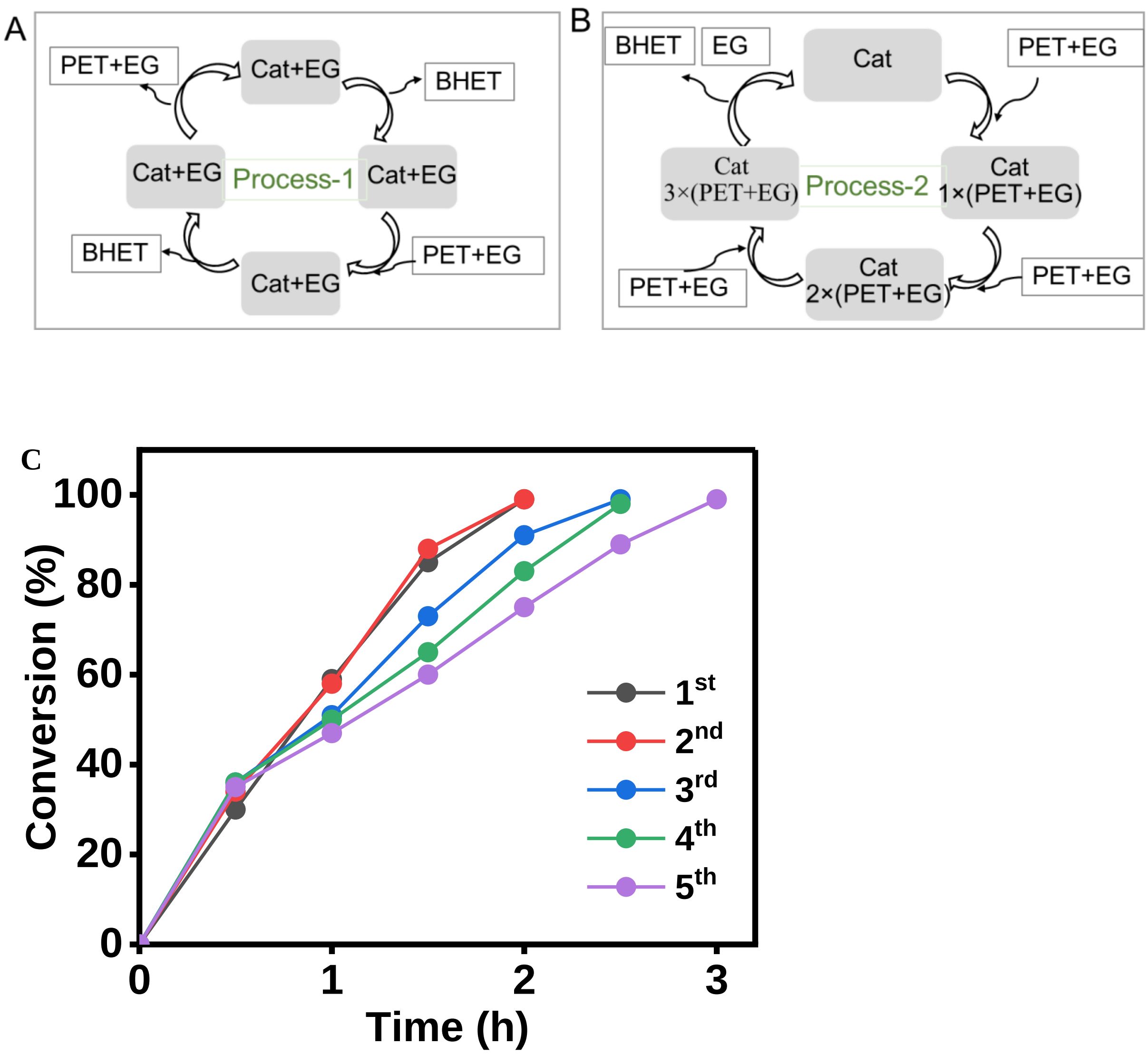


Figure S8. Recycling processes of the catalyst and EG. (A) Successive separation of the catalyst and EG after each cycle. (B) Conjugative addition of PET and EG after completion of each step. (C) (C) Assessment of catalyst stability with PET deconstruction by using TBD:TFA (1:1). Reaction conditions: PET (1 eq.), catalyst (0.05 eq.), EG (10 eq.), 180 °C at 0-3 h.

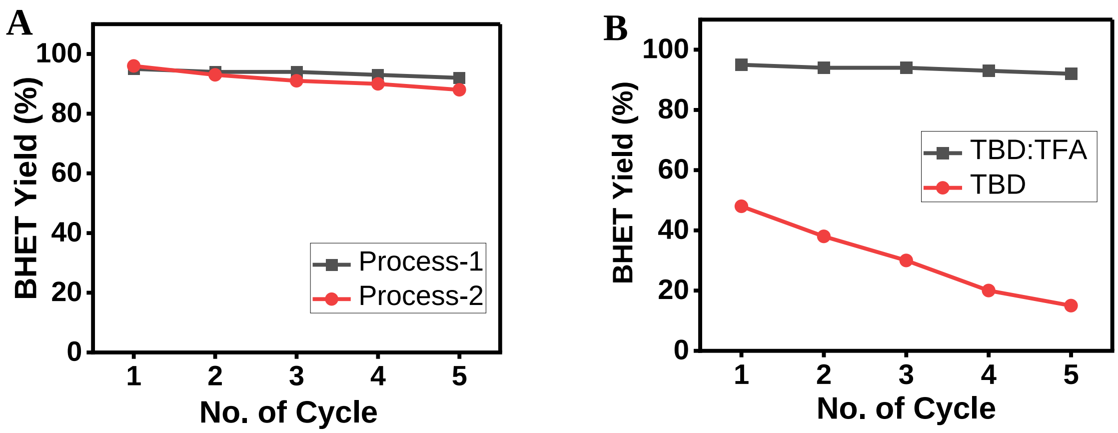


Figure S9. (A) Recycling comparison of process-1 and 2 in terms of BHET yield. (B). Recycling comparison of the catalyst TBD:TFA with TBD. Reaction conditions: PET (1 eq.), catalyst (0.05 eq.), EG (10 eq.), 180 °C at 2 h.

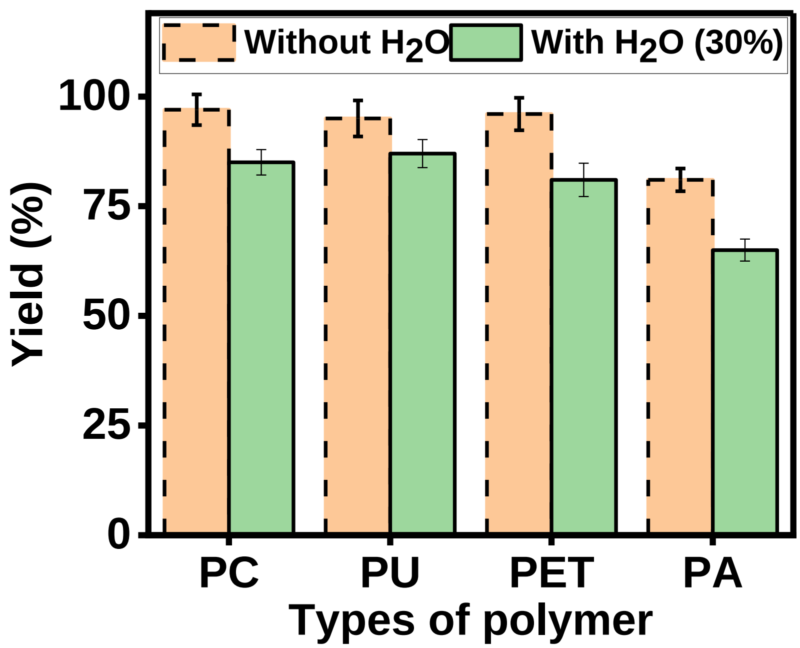


Figure S10. Effect of water (30%) on polymer deconstruction. Reaction conditions: PC/PU/PET/PA (1 eq.), ethylene glycol (10 eq.). TBD:TFA (0.05 eq.).

4.13 Mixed polymer pellets deconstruction

PC pellets (0.33 g, 1.30 mmol), PU pellets (0.41 g, 1,33 mmol), PET pellets (0.25 g, 1.3 mmol), PA pellets (0.15 g, 1.30 mmol), EG (3.17 g, 52 mmol) and TBD:TFA catalyst (0.07 g, 0.26 mmol) were charged in a 30 mL pressure vessel equipped with a magnetic stirrer. In path i, each depolymerization was carried out at a determined temperature (130 ºC, 160 ºC, 180 ºC, and 210 ºC for PC, PU, PET, and PA, respectively) for 2 h. At 130ºC only PC is fully deconstructed, whereas the rest of the polymer pellets are unreacted (Figure S11B), at 160ºC PU is deconstructed, and PET and PA are still unchanged (Figure S11C), increasing heat 180 ºC for another 2 h deconstructs PET and finally increases the temperature to 210 ºC deconstructs PA (Figure S11D). In path ii, deconstruction was carried out at 210ºC and atmospheric pressure for 3 h. The corresponding products BPA (90%), MDA(78%), BHET (88%) & CPL (75%) was purified by flash column chromatography using different chloroform: methanol mixture from 1:0 to 1:1 to 0:1 ratio as the eluent. The kinetics, conversion, and yields were determined by ^{1}H NMR spectroscopic analysis of the crude product in DMSO-d_6 using the catalyst signals as internal standard (d =1.87 ppm, 4H) correspond to the appearance of the peak at 6.99/6.44/1,53 ppm for BPA, 7.34/7.10 ppm for MDA, 8.17 ppm for BHET and 2.05 ppm for CPL (Figures S63 to S67).

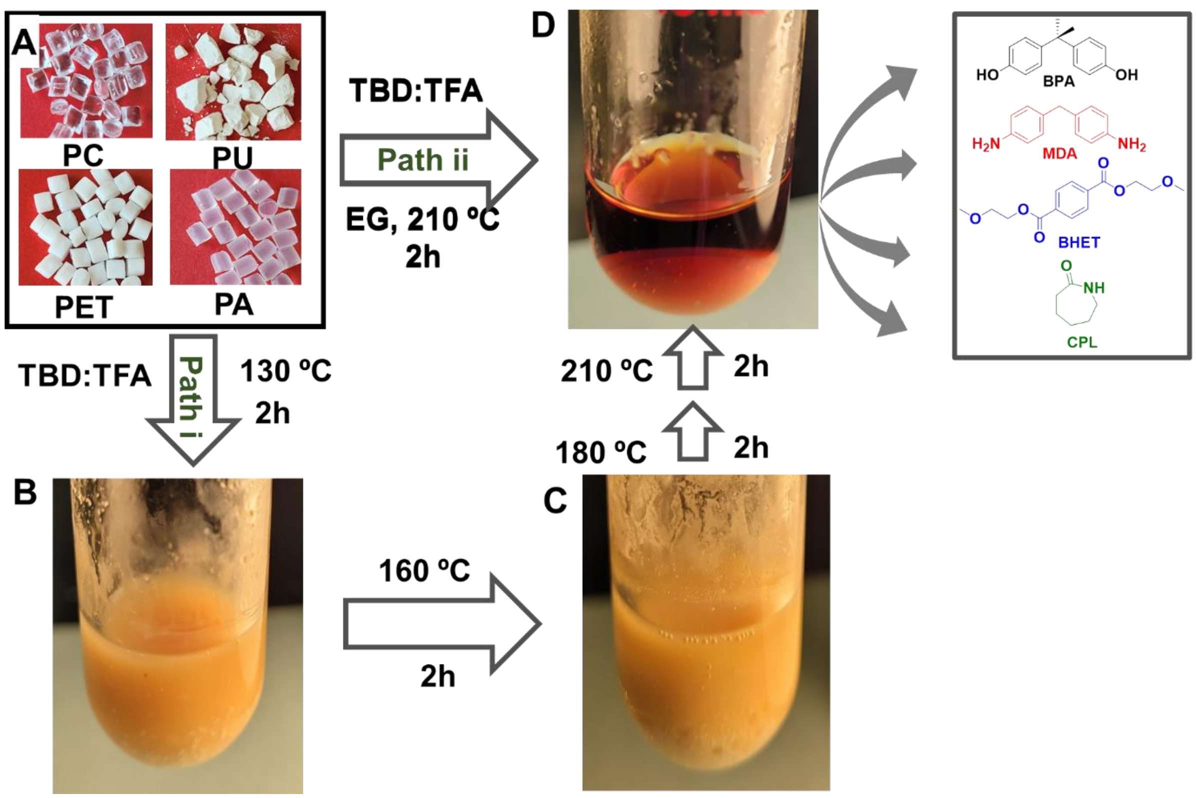


Figure S11. Selective deconstruction of the mixed polymer pellets by using TBD:TFA as a catalyst (A-D) Path-A: Deconstruction was carried out at 130°C, 160°C, 180°C and 210°C for PC, PU, PET and PA respectively. Path-B: Deconstruction was carried out at 210 °C and atmospheric pressure for 3 h.

5. Commercial Polymer Deconstruction

5.1 General procedure for the deconstruction of PC, PU, PET, and PA consumer products

Polymeric consumer product contains additives and is often produced as blends of different polymers. Therefore, the catalyst stability with these complex products was tested in selected experiments. A combination of the plastic (0.5 g), derived from corresponding polymer consumer products, TBD:TFA as catalyst (0.034 g), EG (1.61 g), and determining temperature (130 ºC, 160 ºC, 180 ºC, and 210 ºC for PC, PU, PET and PA consumer product, respectively) for 2 h, were subjected to glycolysis conditions. As depicted in Table S8, all tested consumer products are fully deconstructed. The corresponding products (BPA, MDA, BHET & CPL) was purified by either crystallization or flash column chromatography. The conversion and yields were determined by ^{1}H NMR spectroscopic analysis of the crude product in DMSO-d_6 using the catalyst signals as internal standard (d =1.87 ppm, 4H) correspond to the appearance of the peak at 6.99/6.44/1,53 ppm for BPA, 7.34/7.10 ppm for MDA, 8.17 ppm for BHET and 2.05 ppm for CPL.

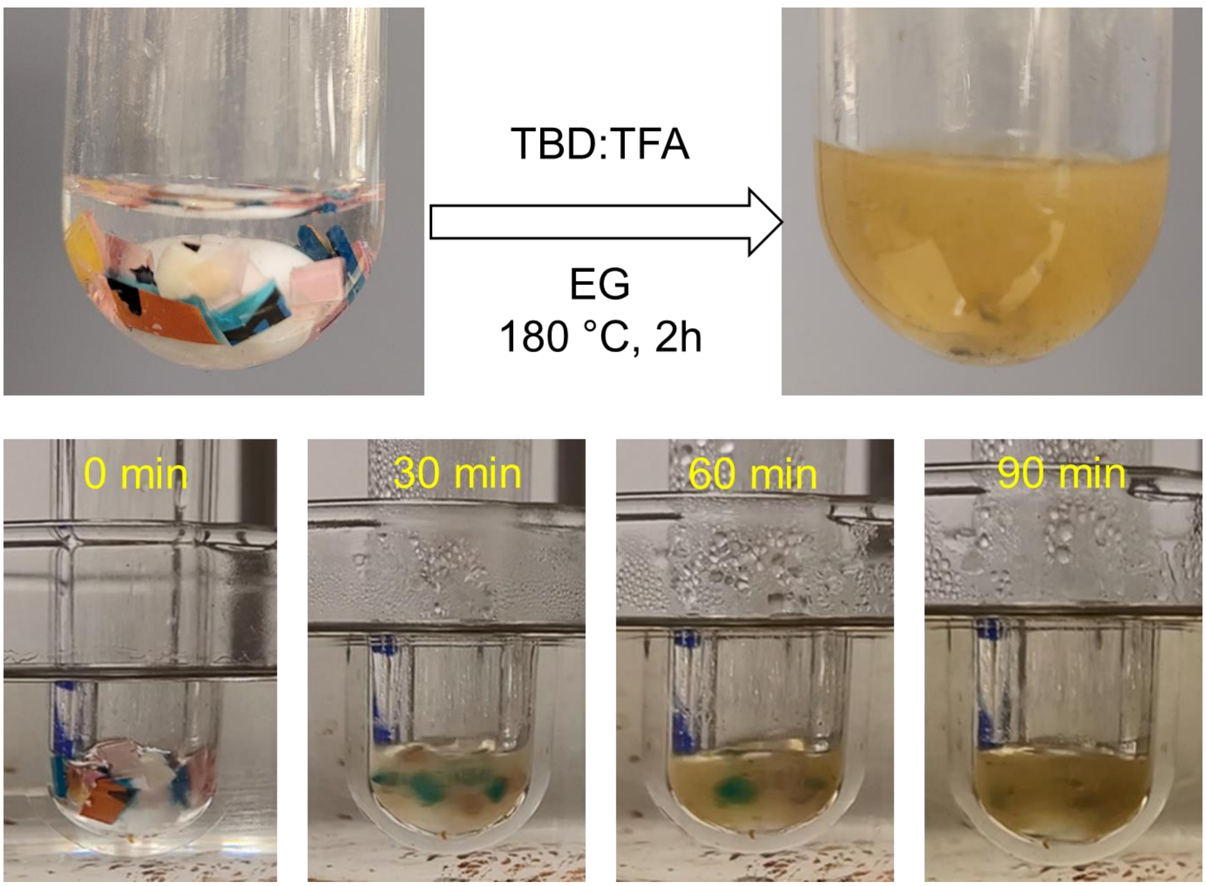
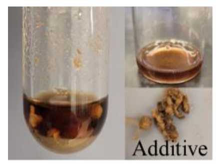
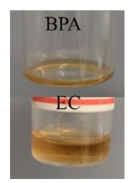
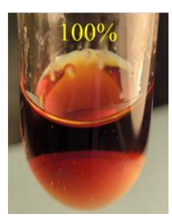
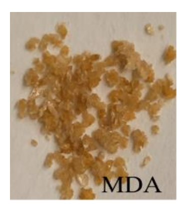


Figure S12. Deconstruction of colored PET bottle at different time intervals using TBD:TFA as a catalyst and EG as a substrate. At a certain interval, the colored fragment disappears, and the formation of a solution indicates the progression of the PET bottle deconstruction.

Table S8. Glycolysis of commercially available sources using TBD:TFA as a catalyst. Reaction condition: Plastic (1 eq.), Cat. (0.05 eq.), EG (10 eq.), time 2 h, temp (130~ 210 °C).

	Consumer Plastic		**Conversion (%)**	**Purified products**
A	PET bottle			
B	Polyester carpet			
C	Polyester cloth			
D	Safety goggles			
E	PU foam			
F	Nylon rope			

5.2 General procedure for the deconstruction of mixed plastic consumer products

In a typical experiment, commercial polymers like safety goggles (0.33 g, 1.30 mmol), foam (0.41 g, 1,33 mmol), colored bottles (0.25 g, 1.3 mmol), nylon rope (0.15 g, 1.30 mmol), ethylene glycol (3.17 g, 52 mmol) and TBD: TFA catalyst (0.07 g, 0.26 mmol) were charged in a 30 mL pressure vessel equipped with a magnetic stirrer. In path A, each deconstruction was carried out at a determined temperature (130 ºC, 160 ºC, 180 ºC, and 210 ºC for PC, PU, PET, and PA consumer products, respectively) for 2 h. In path B, deconstruction was carried out at 210 ºC and atmospheric pressure for 3 h. The corresponding monomers from respective consumer products were purified by flash column chromatography using chloroform: methanol mixture from 1:0 to 1:1 to 0:1 ratio as the eluent. The kinetics, conversion, and yields were determined by ^{1}H NMR spectroscopic analysis of the crude product in DMSO-d_6 using the catalyst signals as internal standard (d =1.87 ppm, 4H) correspond to the appearance of the peak at 6.99/6.44/1,53 ppm for BPA, 7.34/7.10 ppm for MDA, 8.17 ppm for BHET and 2.05 ppm for CPL.

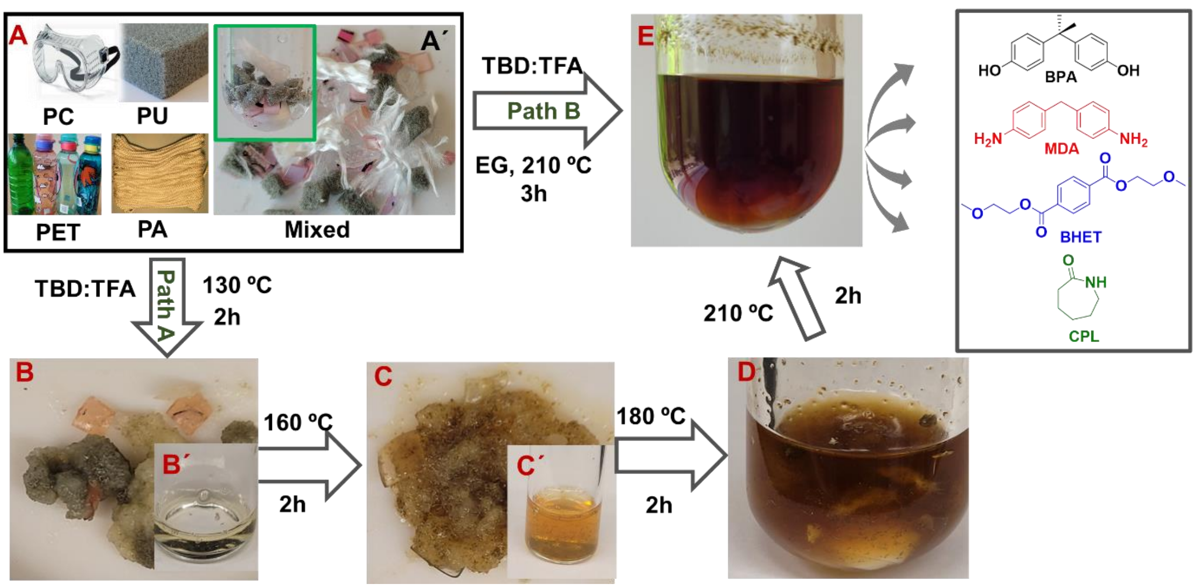


Figure S13. Selective deconstruction of mixed plastic waste by using TBD: TFA as a catalyst and EG as a substrate and solvent with consumer plastic waste of safety goggles, foam, colored bottle, and nylon rope (A) cut into small pieces and mixed manually (A´). Path-A: Deconstruction was carried out at a determined temperature. At 130ºC for 2 h, only safety goggles are fully deconstructed and separated (B´), whereas the rest of the polymer pellets are unreacted (B). At 160ºC for 2 h, foam is deconstructed and separated (C´), keeping bottles and rope intact (C). The remaining mixture then heats at 180ºC for another 2 h to deconstruct the colored bottle while keeping the nylon rope intact (D) and finally increasing the temperature to 210ºC for 2 h deconstruct nylon rope (E). Path-B: Deconstruction was carried out at high heat (210ºC) and atmospheric pressure for 3 h to deconstruct the mixed plastic at a time (D). Finally, the compound was purified by CombiFlash®. Reaction conditions: safety goggles (0.33 g, 1.30 mmol), foam (0.41 g, 1,33 mmol), colored bottles (0.25 g, 1.3 mmol), nylon rope (0.15 g, 1.30 mmol), ethylene glycol (3.17 g, 52 mmol) and TBD:TFA catalyst (0.07 g, 0.26 mmol) under atmospheric pressure.

5.3 Selective deconstruction in the presence of a mixture of various plastics

During our investigations, the impact of complex polymer mixtures on the catalytic deconstruction reaction was tested. In the presence of poly(propylene) (PP) cap, and poly(ethylene) (PE) bag, the glycolysis of PET bottle and mixed condensation polymer were conducted using TBD:TFA as catalyst under standard conditions. In these experiments, full conversion of the selected polymer was observed, and none of the described additional polymers hampered the selective deconstruction of the condensation polymer.

Deconstruction of PET bottle with cap: A combination of 0.5 g of PET bottle, EG (10 eq.), and TBD:TFA (0.05 eq.) were heated at 180 °C for 2 h. After completion, the blue color cap was fully recovered (98%) through filtration without any influence on the catalytic performance of the catalyst.

Deconstruction of PET bottle with polyethylene (PE) bag: PET water bottle (0.5 g) and PE bags (0.2 g) were depolymerized by using TBD:TFA (0.035 g) and EG (1.61 g) at 180 °C for 2 h in a glass pressure vessel. After two hours, the unreacted PE bags easily separated (99%) (Figure S14).

Deconstruction of PC, PU, PET, PA with polyethylene (PE) bag: A mixture of PC, PU, PET and PU commercial plastic (0.5 g) and PE bags (0.2 g) were depolymerized by using TBD:TFA (0.035 g) and EG (1.61 g) at 180 °C for 2 h in a glass pressure vessel. After two hours, the unreacted PE bags can easily be separated (97%) from the reaction solution.

Deconstruction of fabrics (40% polyester & 60 % cotton): Cloth (0.5 g) were deconstructed by using TBD:TFA (0.035 g) and EG (1.61 g) at 180 °C for 2 h in a glass pressure vessel. Polyester was deconstructed to make BHET monomer, whereas the unreacted cotton was fully recovered (98%).

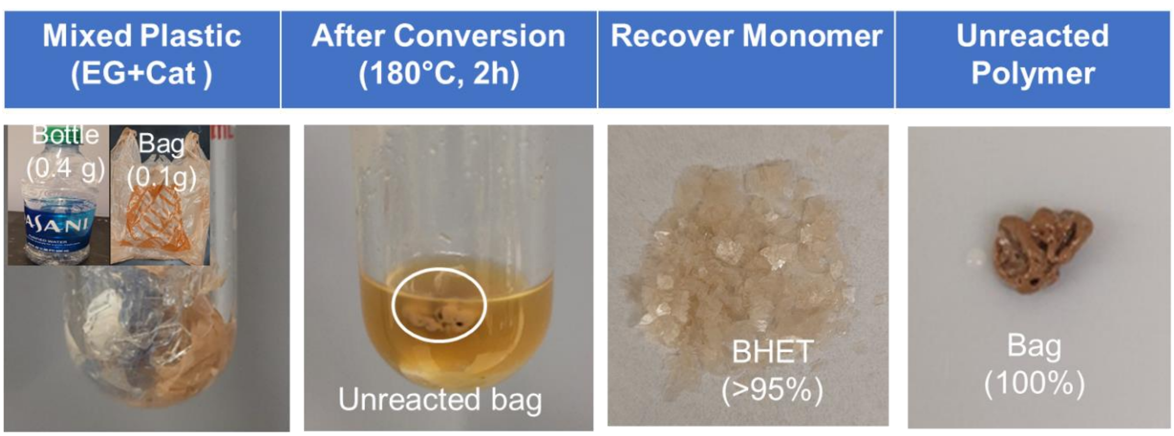


Figure S14. Deconstruction of the mixed PET bottle and PE bag produce BHET with keeping PE intact.

6. Life Cycle Assessment (LCA)

Goal and scope of the study — This study aims to estimate the environmental impact and energy consumption of polymers synthesized from materials derived from polymer deconstruction processes (PC, PU, PET, and PA) and compare them to conventional polymers. The inputs for the polymer deconstruction process in LCA modeling include targeted polymer, EG, water, and a catalyst. The amount of energy used during polymer deconstruction was also added to the model (Electricity, medium voltage, US). The data from performed preliminary LCA models for polymer deconstruction is further used to build an LCA model for polymer synthesized from deconstruction products(monomers). The compared LCA models for conventional polymers were built based on the data provided by Ecoinvent V3.0 database. The system boundary for this LCA study includes: (1) polymer deconstruction and (2) production of polymer "from recycled". The selected functional unit for this study is 1 kg of polymer.

Life cycle inventory and Impact Assessment — Polymer deconstruction results in the mixture of monomers which are further used for the synthesis of polymer "from recycled". Data for the building of the life cycle inventory (LCI) model consist of the material and energy inputs to (1) deconstruct polymer and (2) fabricate a polymer from resulting monomers obtained during polymer deconstruction ("from recycled"). Inventory of all chemicals used in LCA modeling is listed in Table 9. The inputs for polymer deconstruction modeling were based on lab-scale results. The information for synthesizing polymers "from recycled" was taken from stoichiometric calculations of materials needed for polymer synthesis. Our model assumes that the excess EG, catalyst, and water are recycled and returned to the process.

LCA method was used as a tool to estimate the environmental impacts linked with the polymer deconstruction process used in this study. LCA model was built according to the international standards ISO 14040 and ISO 14044 (ISO, 2006b, c). To conduct the LCA, the SimaPro V 9.1 software and TRACI II (U.S., 2008) method were used. The lab-scale LCA model was created for each polymer deconstruction process based on the initial experimental results to identify significant environmental contributors. We excluded the impact of recycled polymers in polymer deconstruction process considering them as waste material and credited it as 'avoided virgin polymer' to receive a negative value on the environmental impact balance, resulting in a 'positive' contribution[8]. The energy consumption was added to each LCA model based on the energy balance calculation for the lab-scale process (1 kg) (Table 12). Energy consumption of polymer deconstruction and synthesis of polymer "from recycled" was evaluated using the Cumulative Energy Demand V1.11 method. The energy footprint for each polymer was expressed in MJ/kg eq. Using of the non-renewable, fossil fuels category.

For the polymer synthesis from deconstructed monomers, LCA models were built according to the assumptions and literature data including mass and energy balances for each type of polymer.

Life cycle Inventory Data Collection — Data collected for LCA modeling was based on a combination of primary data derived from the lab experiments for material and energy balances, the literature, and assumptions when information on chemicals used in the synthesis was missing from various LCA databases. The polymer deconstruction process includes the use of a high-grade catalyst, which was fabricated in the study and can be fully recovered after use. Its life cycle production information could not be found in LCA databases. Therefore, considering the recyclability of the catalyst of 100%, it was not included in the chemical inventory list. The overall LCA input data of this study has been divided into the following parts:

- Primary data was obtained using the experimental results of the laboratory scale of each polymer deconstruction process.

- Secondary data was collected based on the literature review for the polymer synthesis from specific monomers used in the study. All of the data regarding the synthesis of this polymer was generated based on the experimental results and mass balances found in the literature.

Table S9. Inventory of all chemicals/electricity used in LCA modeling

#	Name of the component	Database	Year	Location
1.	Ethylene glycol	Eco invent 3	2010	Europe (RER)
2.	Polycarbonate	Eco invent 3	2010	Europe (RER)
3.	Polyurethane, flexible foam	Eco invent 3	2021	Europe (RER)
4.	Polyethylene terephthalate, bottle grade	Industry data 2.0	2016	Europe (RER)
5.	Polyamide(Nylon 6.6)	Industry data 2.0	2015	Europe (EU)
6.	Pentane	Eco invent 3	2010	Europe (RER)
7.	Deionized water	Eco invent 3	2018	Europe (RER)
8.	Phosgene	Eco invent 3	2014	Europe (RER)
9.	Electricity, medium voltage	Eco invent 3	2015	US

Table S10. Impact assessment of polymer deconstruction process.

Impact Category	Unit	BPA	BHET	MDA	CL
Ozone depletion	kg CFC^{-11} eq	$1.95 \cdot 10^{-8}$	$2.22 \cdot 10^{-7}$	$8.47 \cdot 10^{-9}$	$8.37 \cdot 10^{-9}$
Global warming	kg CO_2 eq	1.02	0.437	0.364	0.235
Smog	kg O_3 eq	0.038	0.0161	0.015	0.00751
Fossil fuel depletion	MJ surplus	3.19	1.72	0.752	0.44
Acidification	kg SO_2 eq	0.00307	0.00129	0.00132	0.00563
Respiratory effects	kg PM2.5 eq	0.00589	0.000297	0.000409	0.000259
Eutrophication	kg N eq	0.00036	0.000237	0.000335	0.000162
Non cancerogenics	CTUh	$5.86 \cdot 10^{-8}$	$1.86 \cdot 10^{-8}$	$1.56 \cdot 10^{-8}$	$1.35 \cdot 10^{-7}$
Cancerogenics	CTUh	$5.85 \cdot 10^{-9}$	$2.05 \cdot 10^{-9}$	$4.69 \cdot 10^{-9}$	$3.02 \cdot 10^{-9}$
Ecotoxicity	CTUe	0.306	0.155	0.195	0.173

Table S11. Impact assessment and cumulative energy demand of virgin polymers and polymers made from recycled monomers.

Impact category	Unit	PC		PU		PET		PA	
		C*	R**	C*	R**	C*	R**	C*	R**
Global warming	kg CO_2 eq/kg polymer	7.76	1.41	5.04	0.88	2.17	0.54	6.51	0.34
Fossil energy demand	MJ/kg polymer	99.75	31.97	87.64	24.57	136.42	15.34	119.91	4.96

C*-conventional; R**-from recycled

Table S12. Energy consumption for the synthesis and purification of 1 kg of polymer deconstruction

Energy Usage:	Time, h	Power, Watt	Consumption, kWh
Hot Plate	2	1000	1
Centrifuge	0.08	575	0.046
Vacuum Oven	12	600	1.2

The energy consumption for the polymer deconstruction process was estimated based on the energy balance calculation. The energy consumption of the hot plate, centrifuge, and vacuum oven was calculated based on the power specification of each piece of equipment and the amount of time it was used.

7. Spectral Data

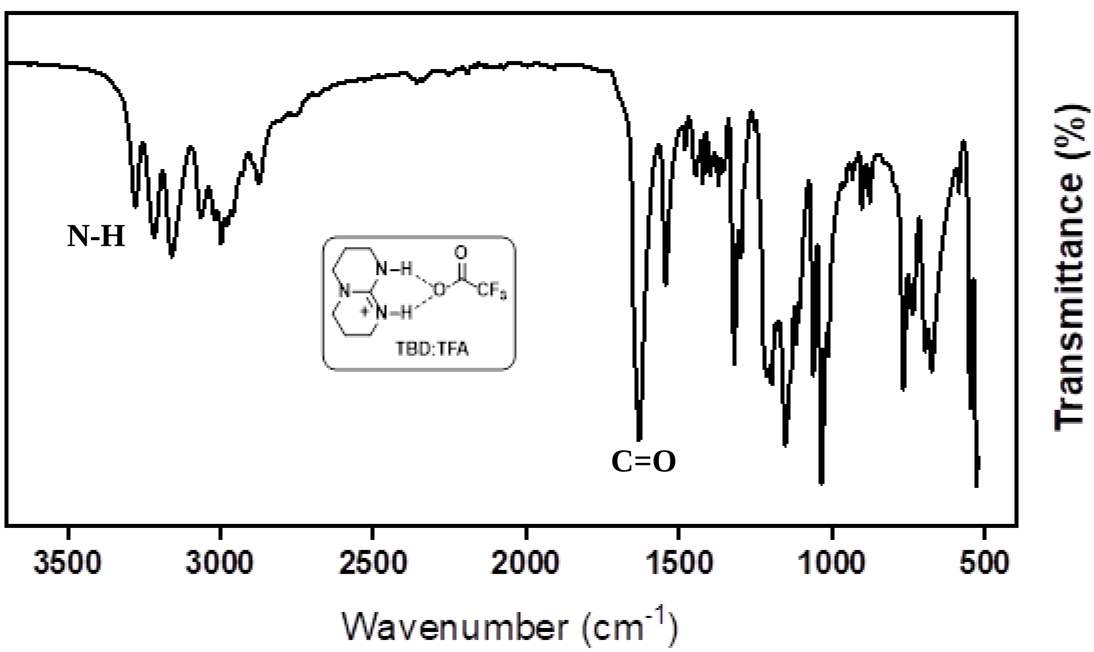


Figure S15. FTIR spectrum of TBD:TFA (1:1)**.** In the IR spectrum, the presence of ketone (C=O) and various N-H peaks as well as the disappearance of the acid peak indicate the successful formation of the TBD:TFA

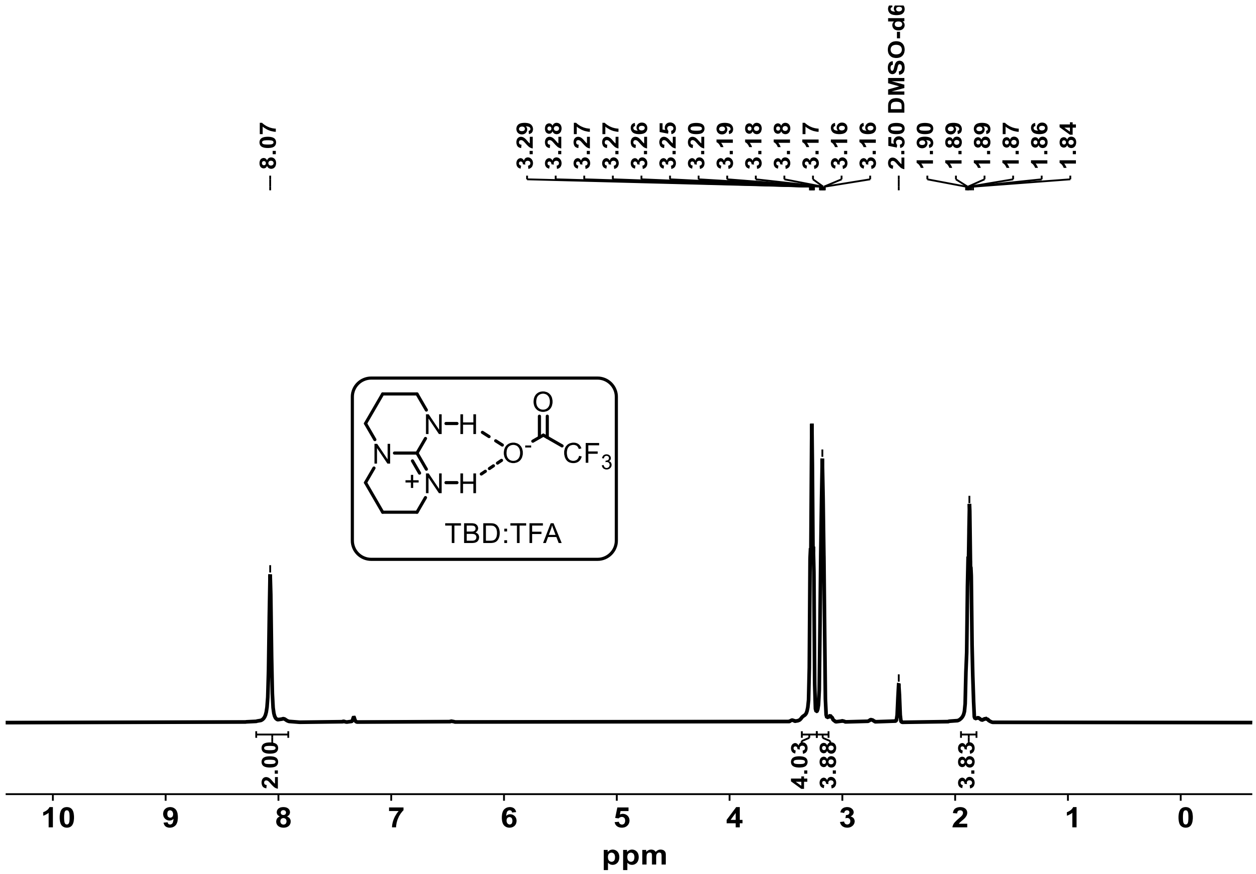


Figure S16. ^{1}H NMR spectrum of TBD : TFA (1 : 1) in DMSO-d6 (400 MHz, 298 K)

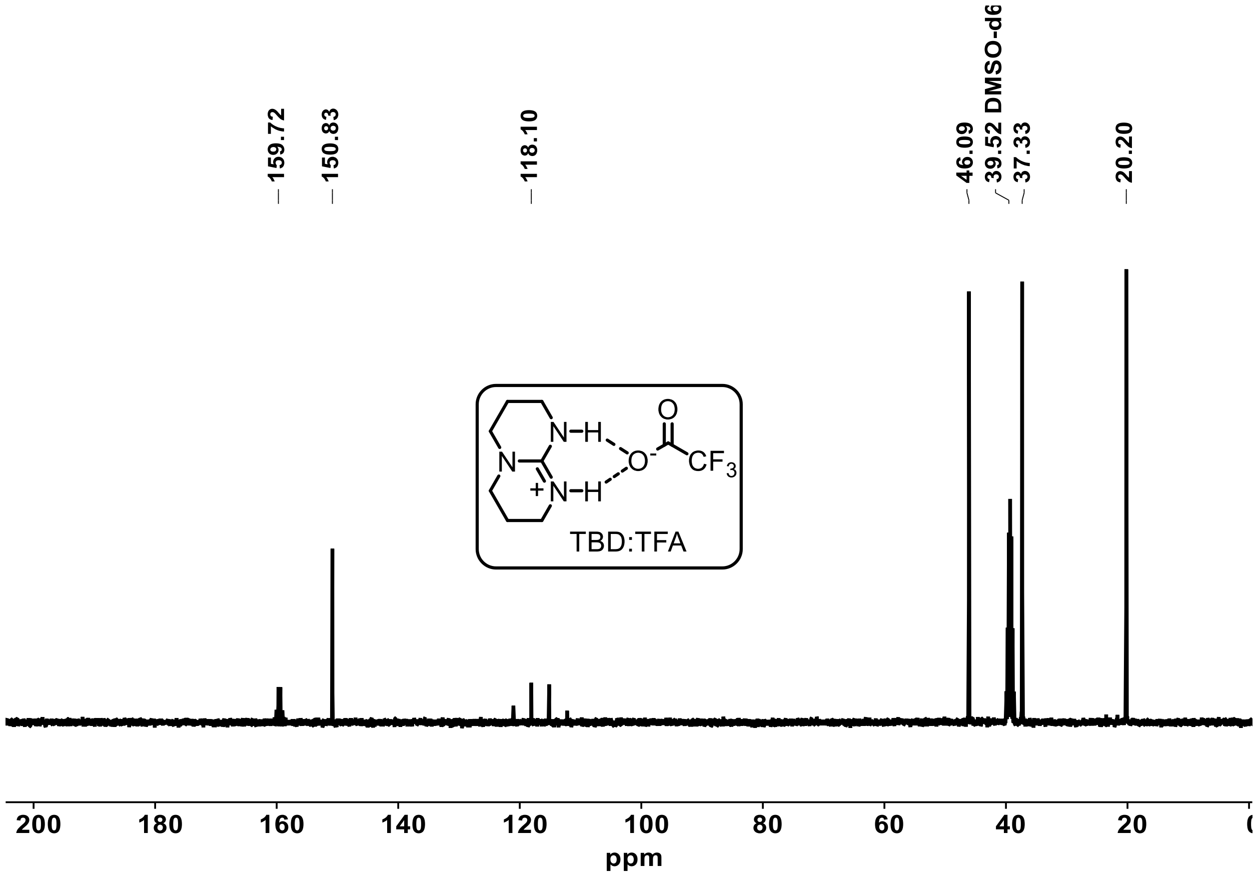


Figure S17. [13]C NMR spectrum of TBD : TFA (1 : 1) in DMSO-d6 (400 MHz, 298 K).

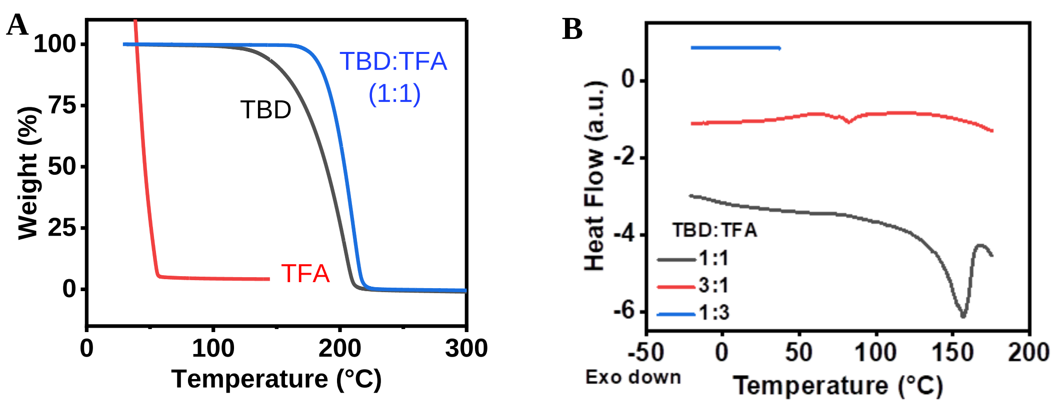


Figure S18. (A) Thermogravimetric analysis for TBD, TFA and TBD:TFA (1 : 1). (B) Dynamic Scattering Calorimetry (DSC) of different ratios (1:1, 3:1 & 1:3) of TBD:TFA.

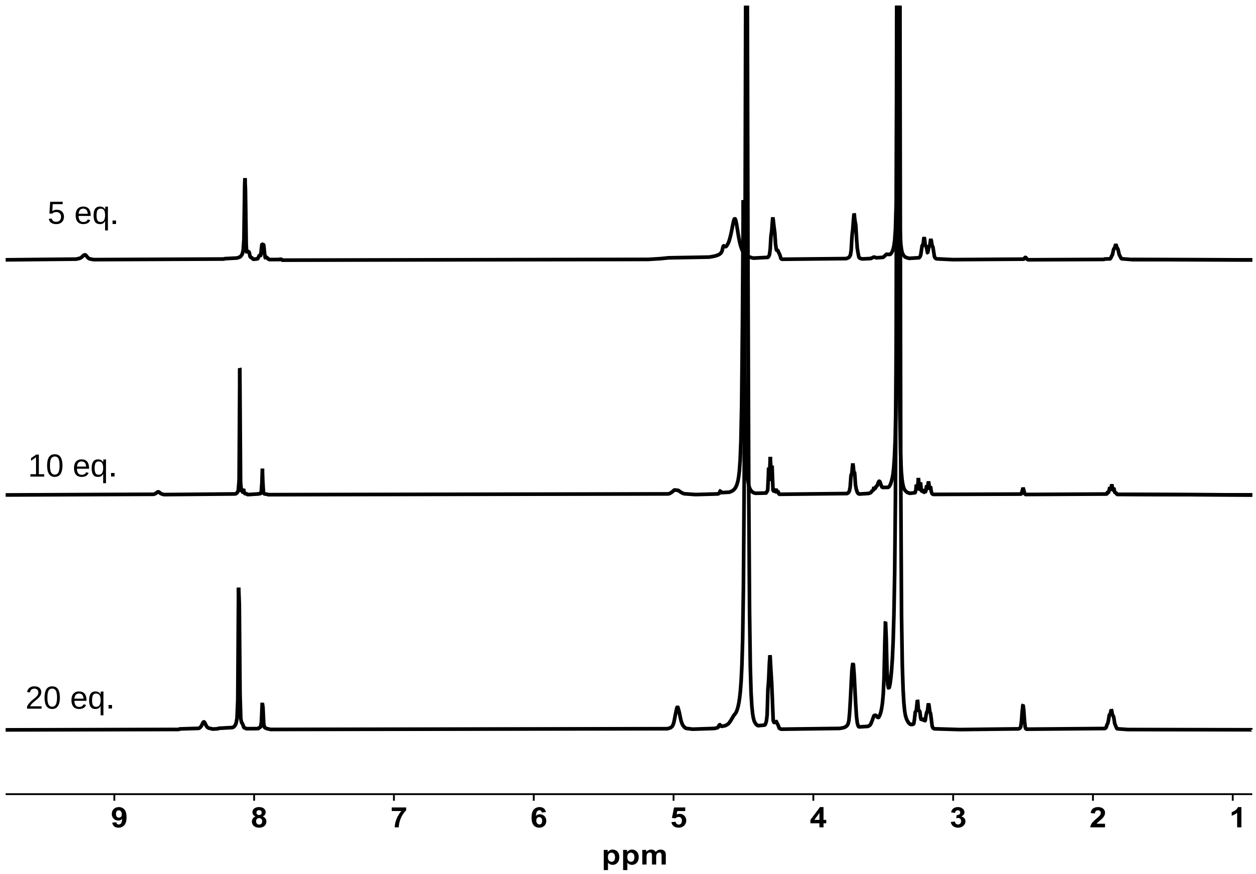


Figure S19. Stacked ^{1}H NMR spectra of the deconstructed PET (0.5 g, 2.6 mmol, 1 eq.) using the different equivalent of EG, and TBD:TFA (1:1) (0.33 g, 1.3 mmol, 0.50 eq.) as a catalyst at 180 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

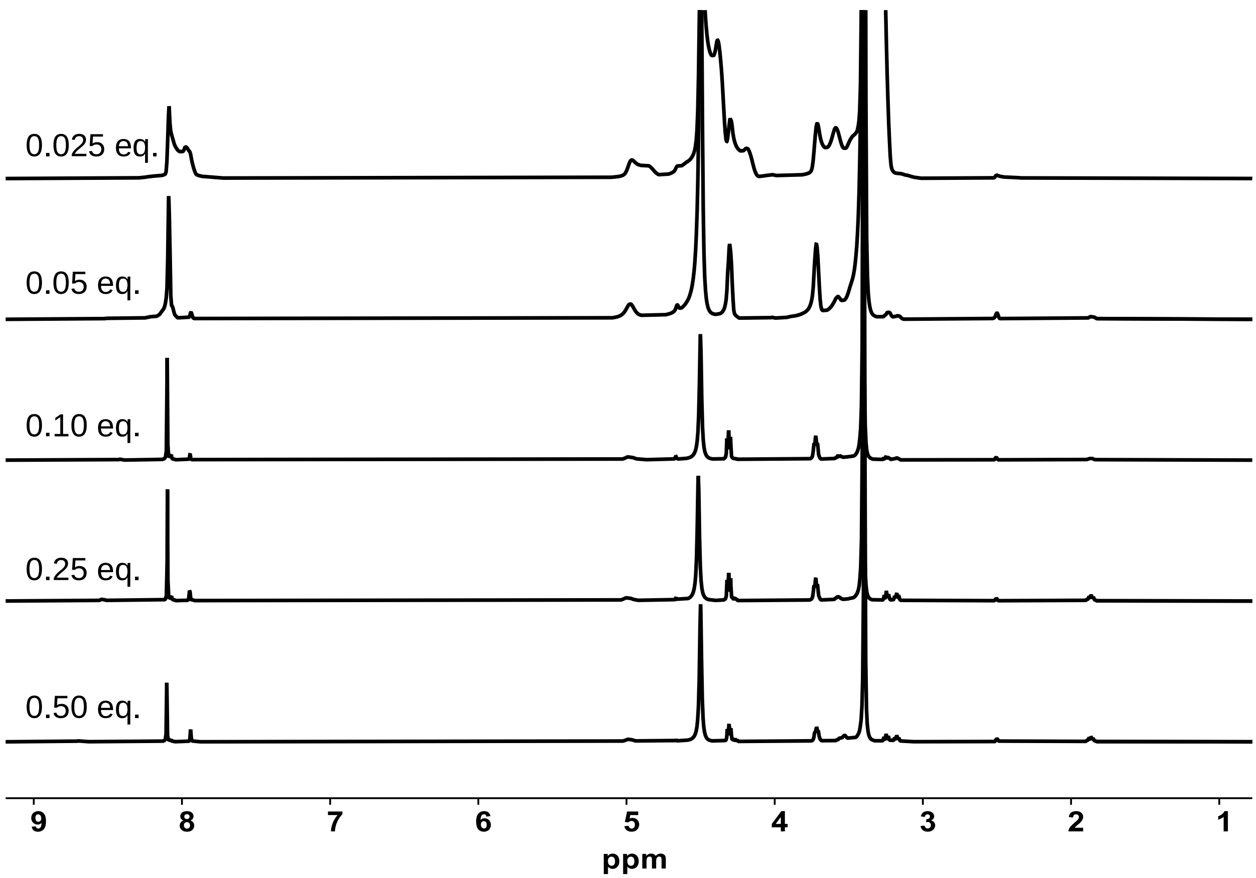


Figure S20. Stacked ^{1}H NMR spectra of the deconstruction process withed PET (0.5 g, 2.6 mmol, 1 eq.). EG (1.61 g, 26 mmol, 10 eq.) and different ratios of TBD:TFA (1:1) as a catalyst at 180 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

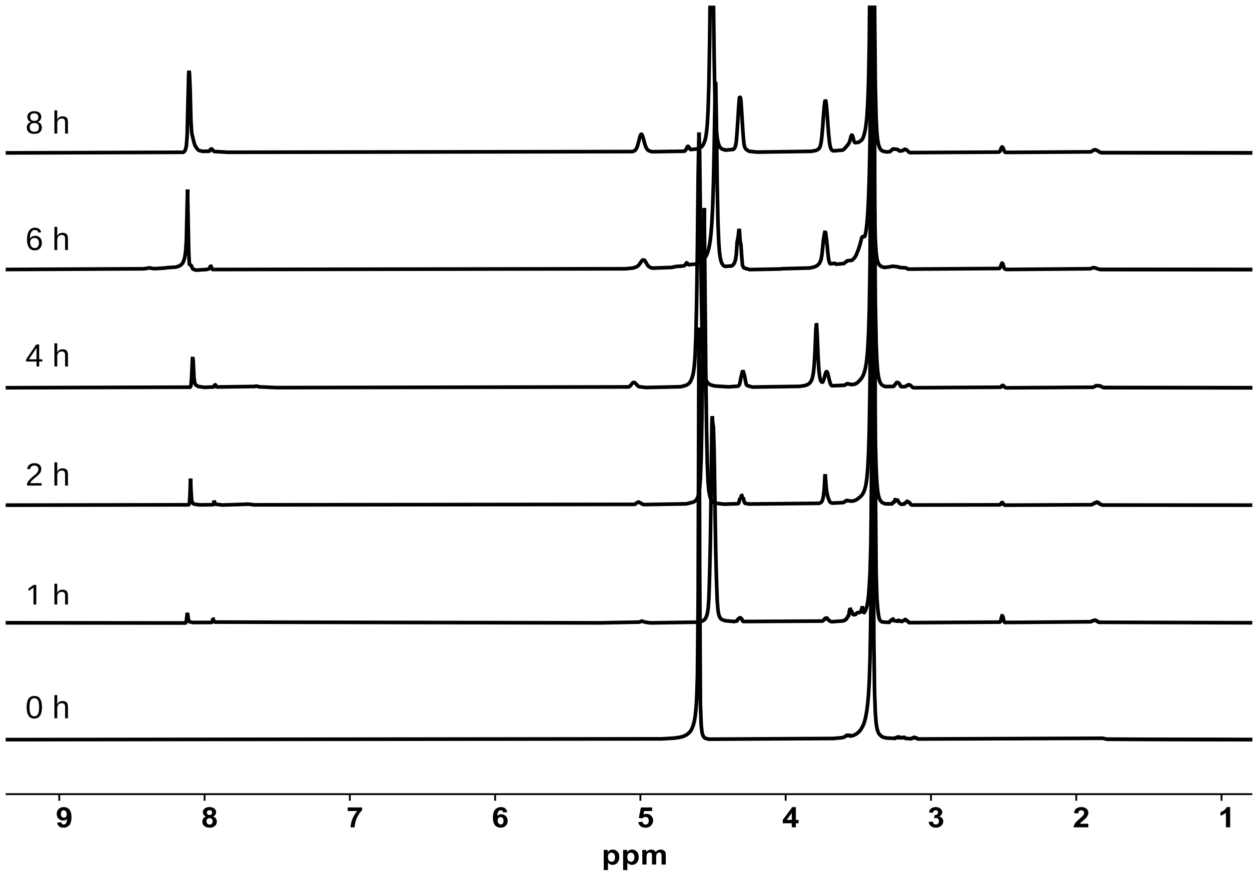


Figure S21. Stacked ^{1}H NMR spectra in the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.) using EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), at 150 ºC (DMSO-d6, 400 MHz, 298 K).

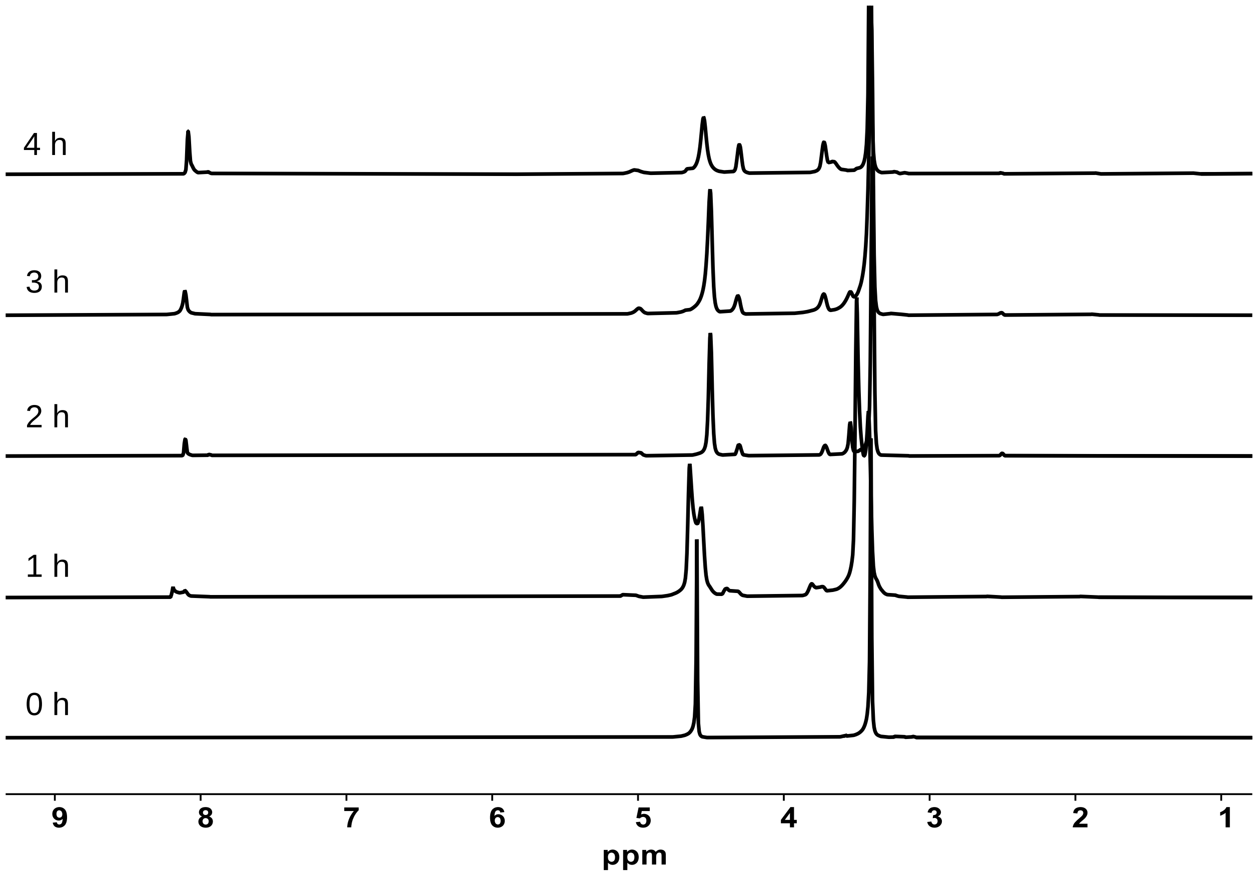


Figure S22. Stacked ^{1}H NMR spectra from the PET deconstruction (0.5 g, 2.6 mmol, 1 eq.), EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), as a catalyst at 160 ºC (DMSO-d6, 400 MHz, 298 K).

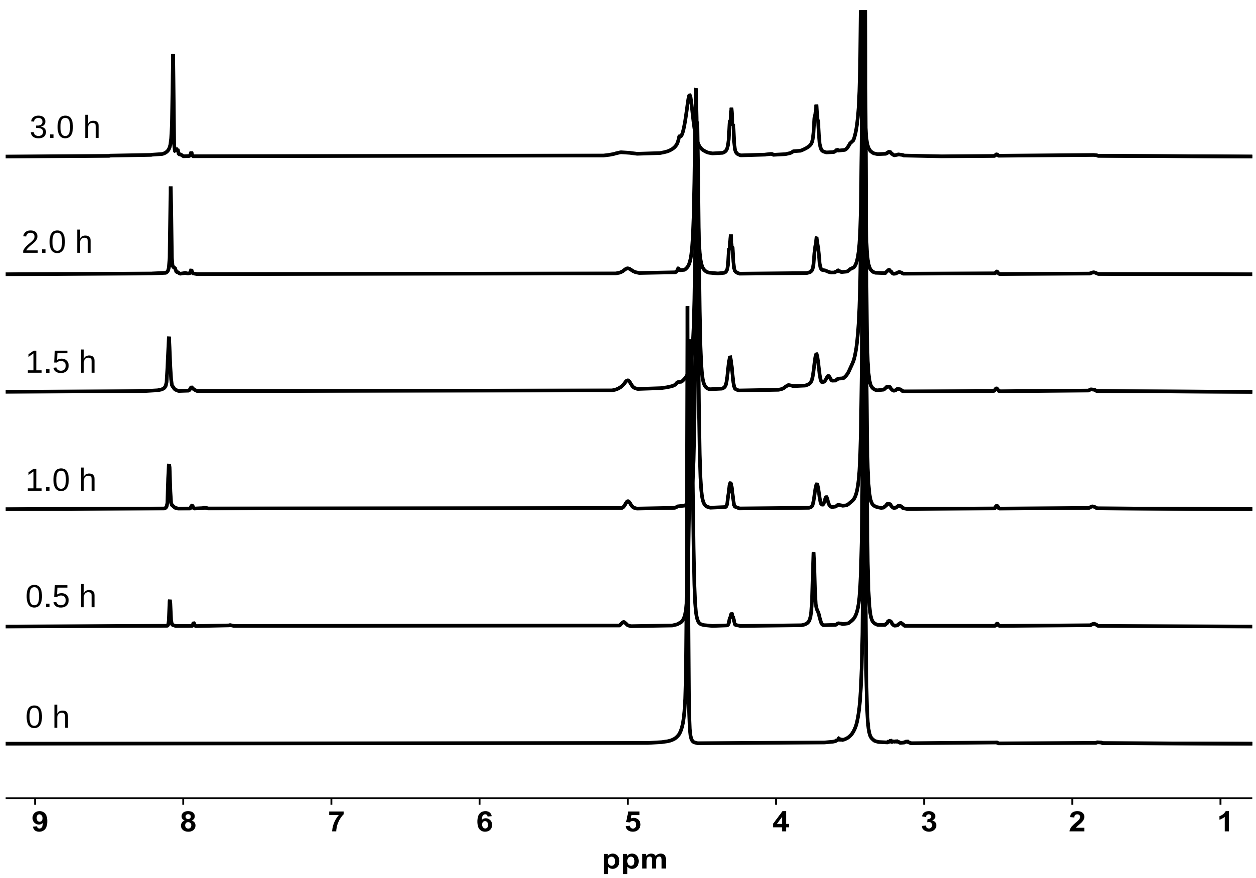


Figure S23. Stacked ^{1}H NMR spectra of the deconstructed PET (0.5 g, 2.6 mmol, 1 eq.) using EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), at 170 ºC (DMSO-d6, 400 MHz, 298 K).

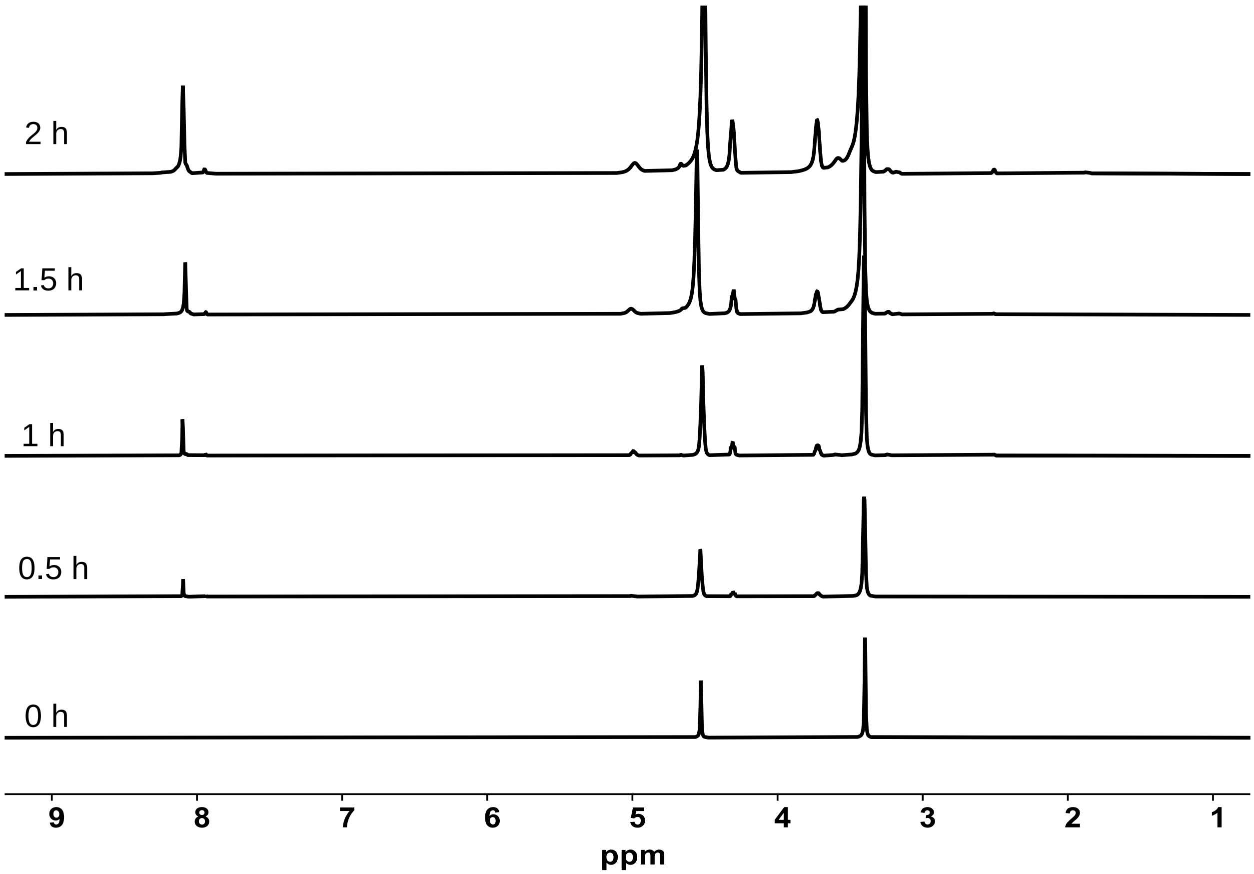


Figure S24. Stacked ^{1}H NMR spectra from the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.) using EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.) at 180 ºC (DMSO-d6, 400 MHz, 298 K).

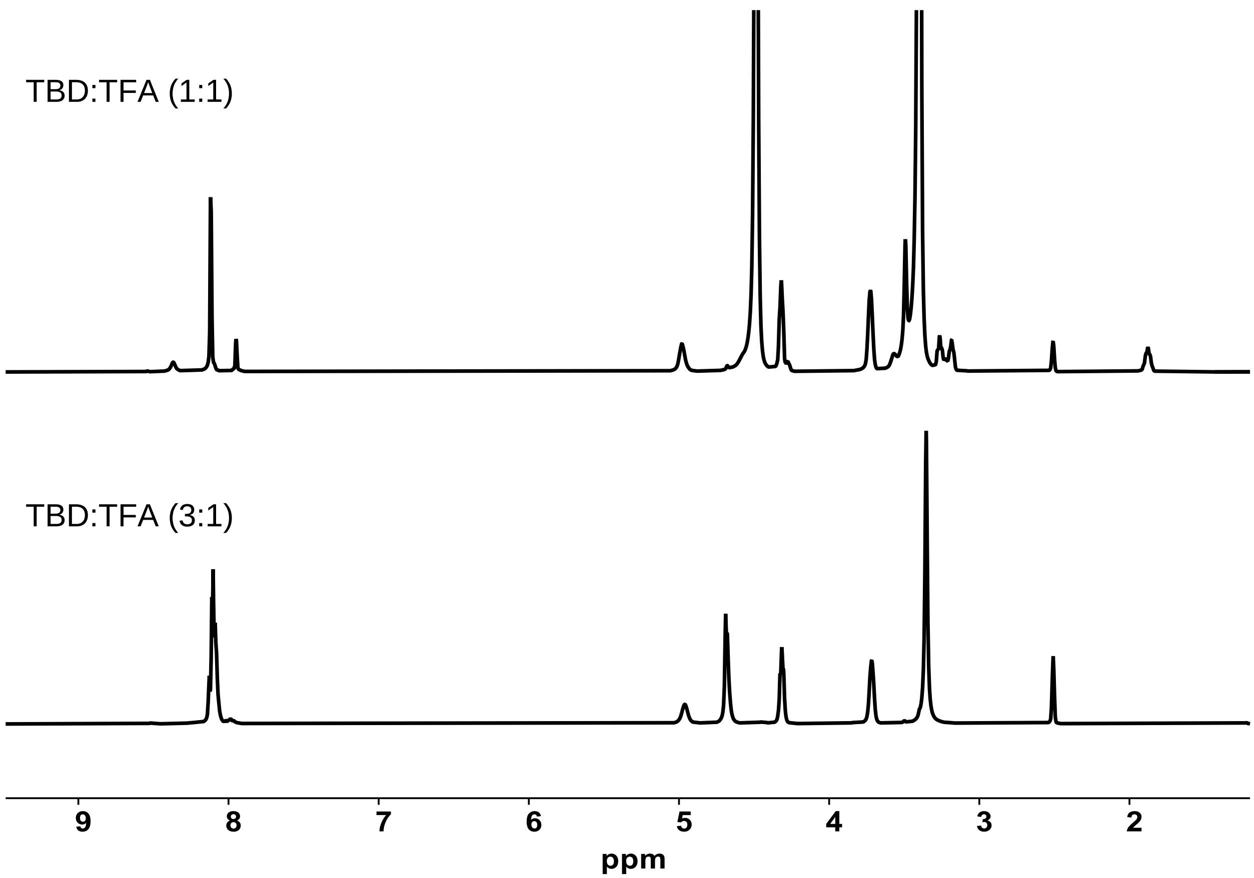


Figure S25. Stacked ^{1}H NMR spectra of the deconstruction of PET by using TBD:TFA (1:1) and TBD:TFA (3:1) (DMSO-d6, 400 MHz, 298 K).

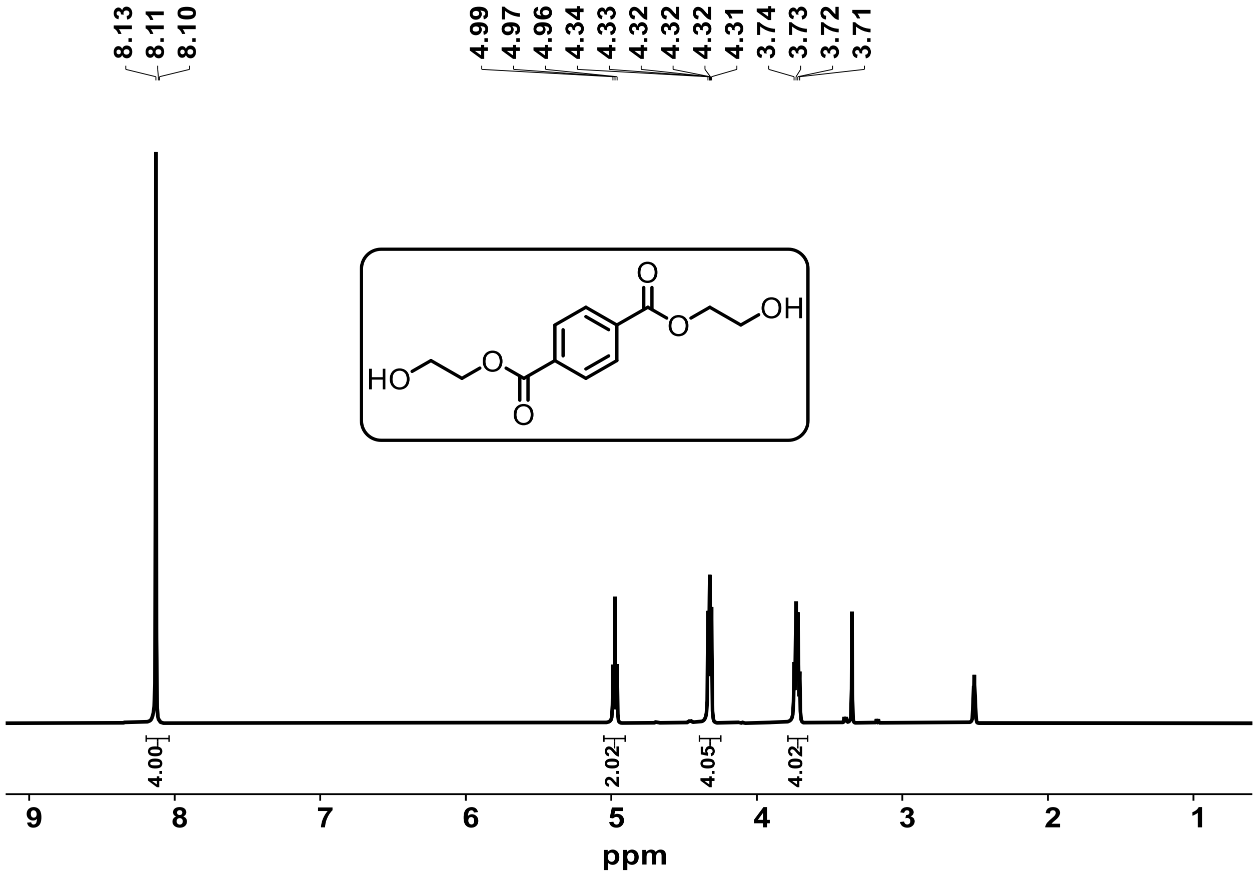


Figure S26. ^{1}H NMR spectra of the BHET (DMSO-d6, 400 MHz, 298 K).

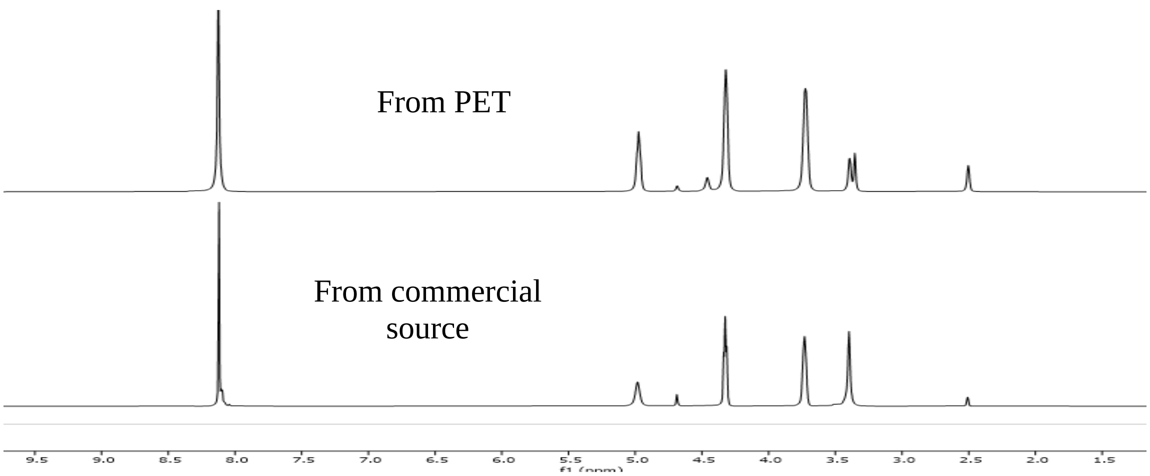


Figure S27. ^{1}H NMR comparison of BHET obtained from PET and commercial source.

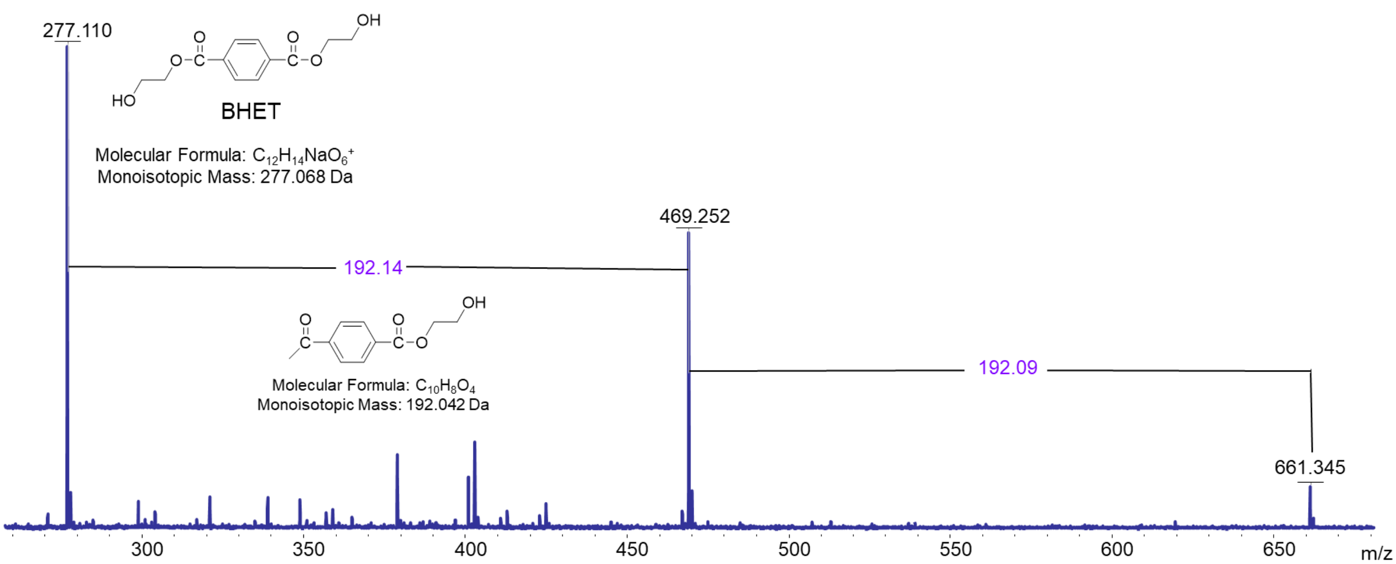


Figure S28. MALDI-TOF of the crude products from the deconstruction of PET. The peak indicates the formation of BHET with high yield, and some mixture of monomer and dimer also formed.

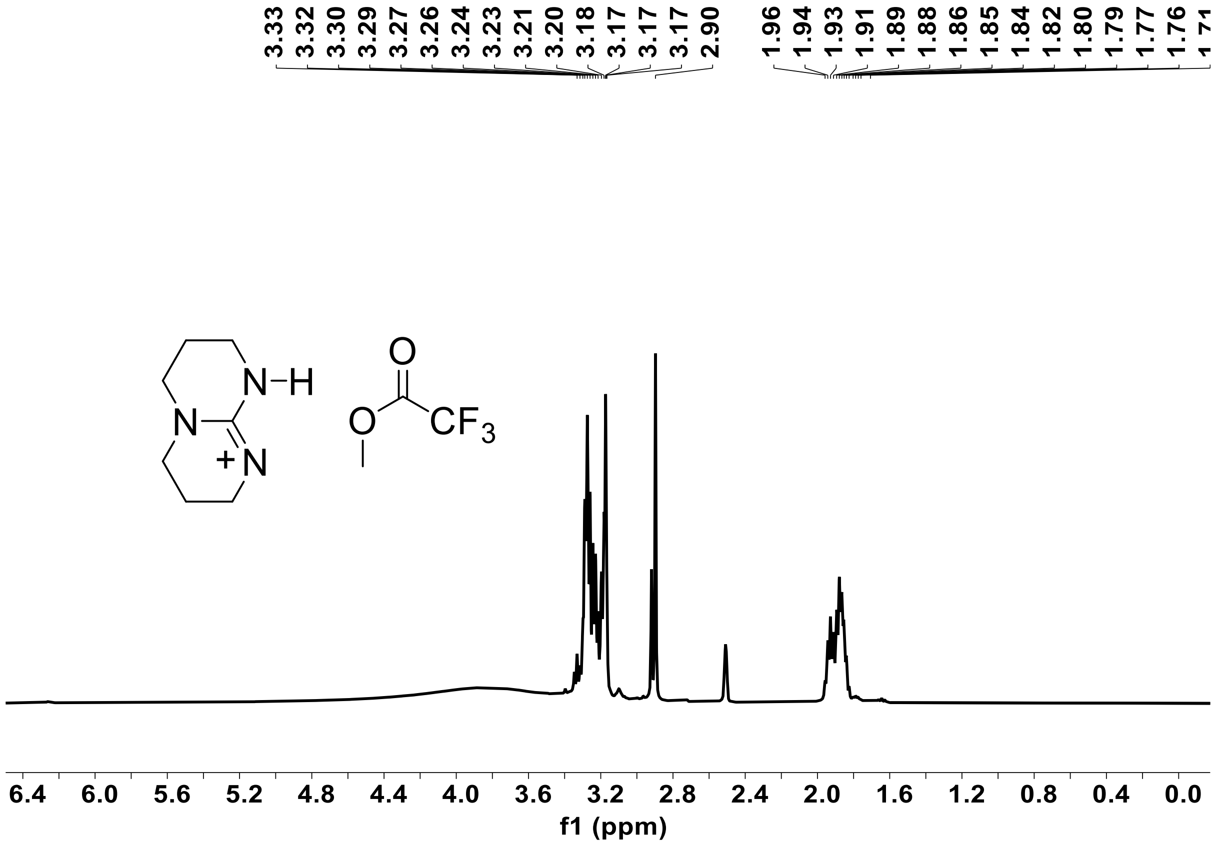


Figure S29. ^{1}H NMR spectrum of TBD:mTFA (1:1) in DMSO-d6 (400 MHz, 298 K).

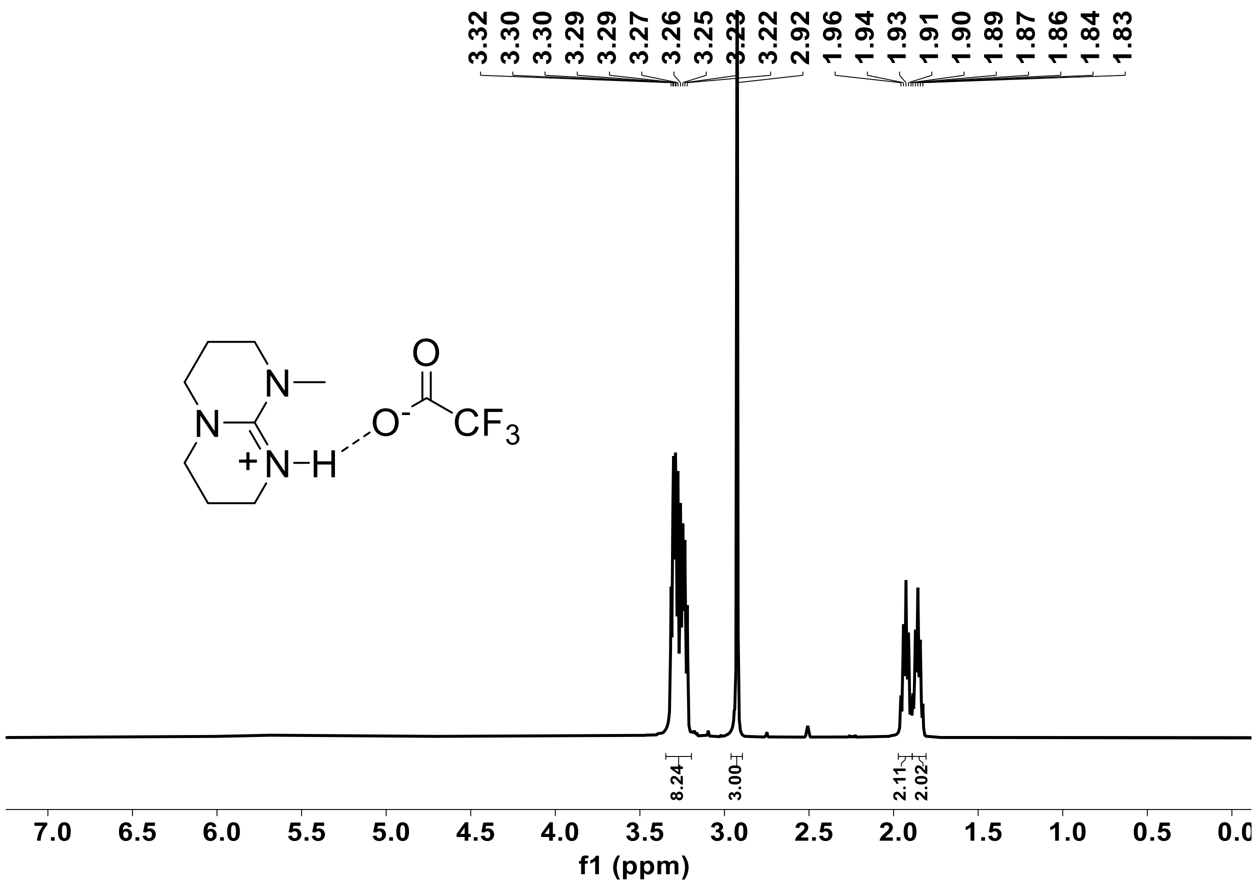


Figure S30. ^{1}H NMR spectrum of mTBD:TFA (1:1) in DMSO-d6 (400 MHz, 298 K).

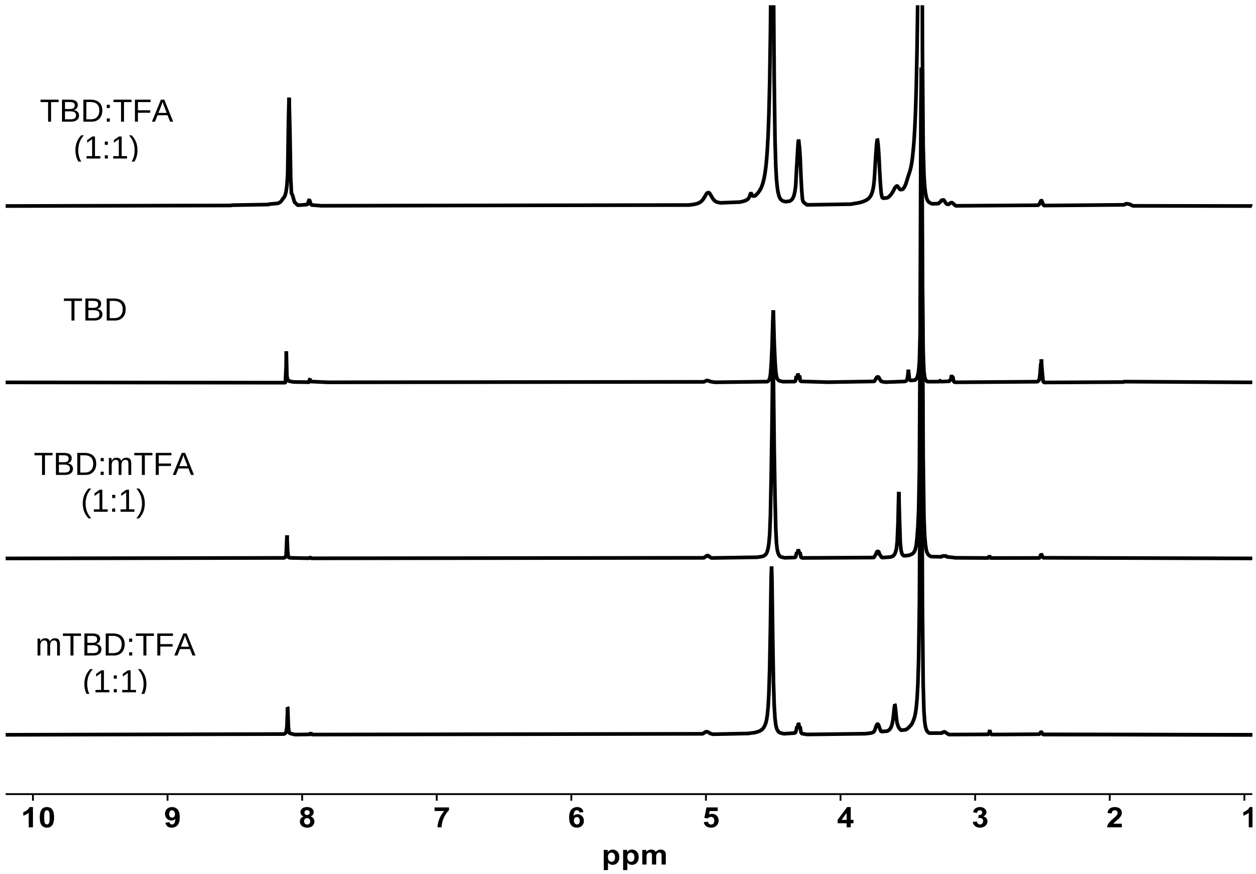


Figure S31. Stacked ^{1}H NMR spectra of the deconstructed PET (0.5 g, 2.6 mmol, 1 eq.) using EG (1.61 g, 26 mmol, 10 eq.), and 0.05 eq. of different types of catalyst at 180ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

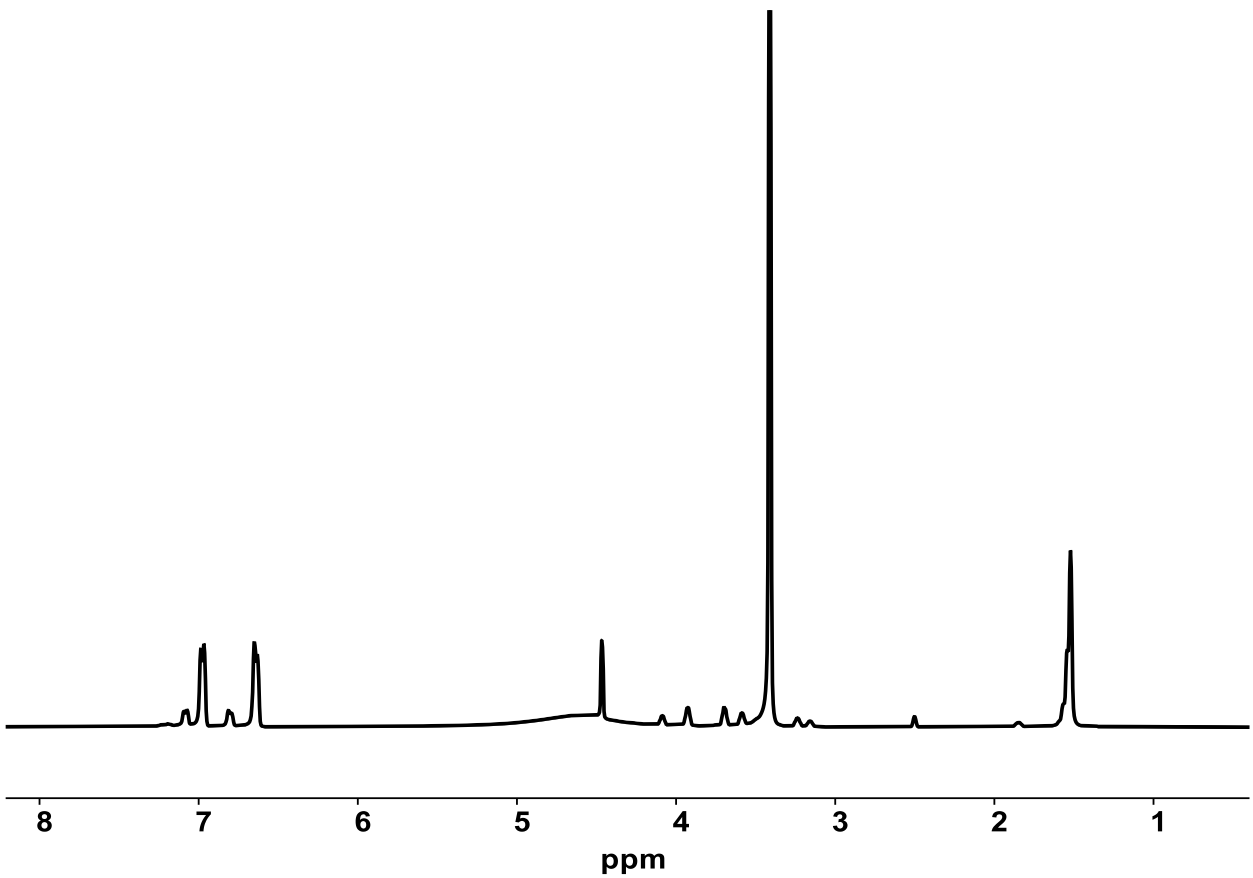


Figure S32. ^{1}H NMR spectrum of the depolymerization of PC (0.5 g, 2.0 mmol, 1 eq.) using EG (1.2 g, 20 mmol, 10 eq.), and TBD:TFA (0.025 g, 0.1 mmol, 0.05 eq.) at 130 v ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

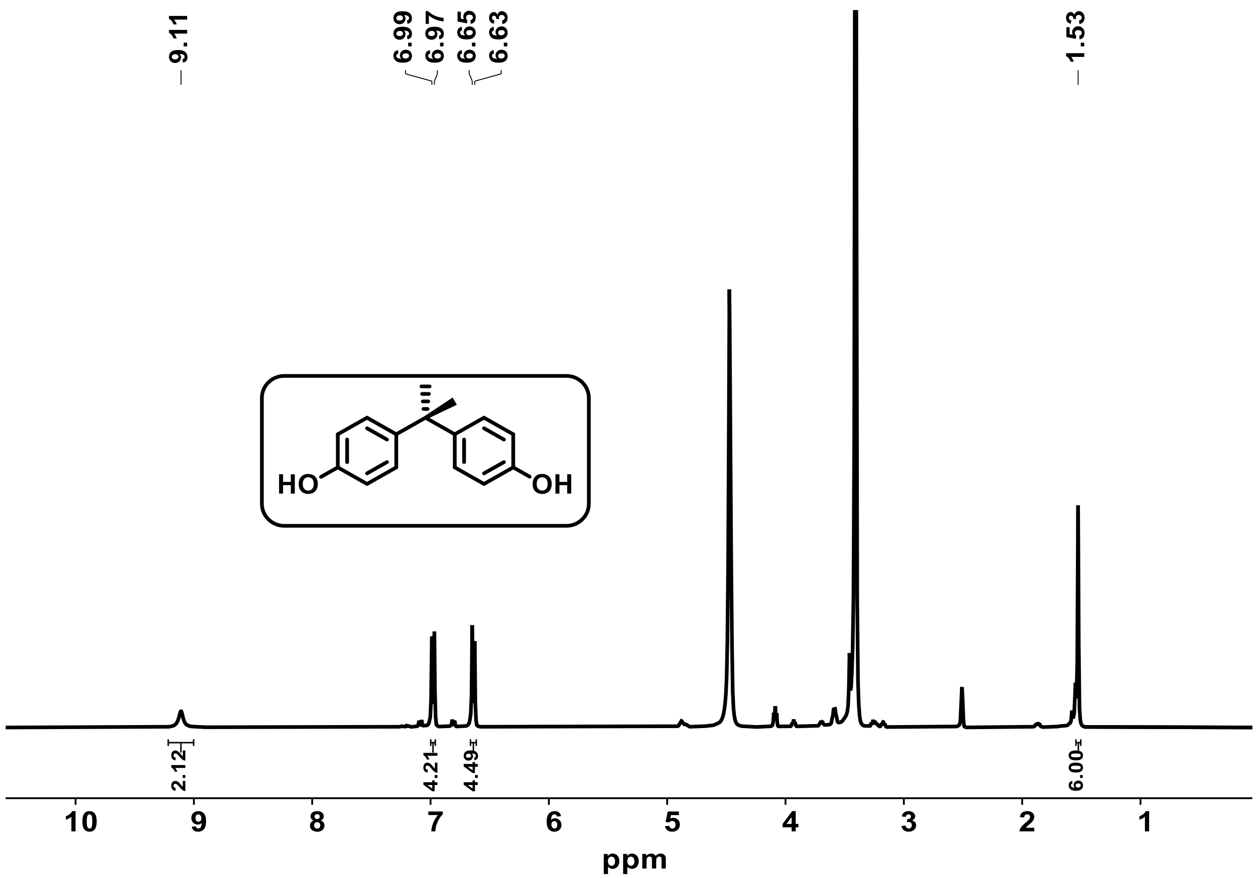


Figure S33. ^{1}H NMR spectrum BPA formed from the deconstruction of PC (0.5 g, 2.0 mmol, 1 eq.) using EG (1.2 g, 20 mmol, 10 eq.), and TBD:TFA (0.025 g, 0.1 mmol, 0.05 eq.), at 130 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

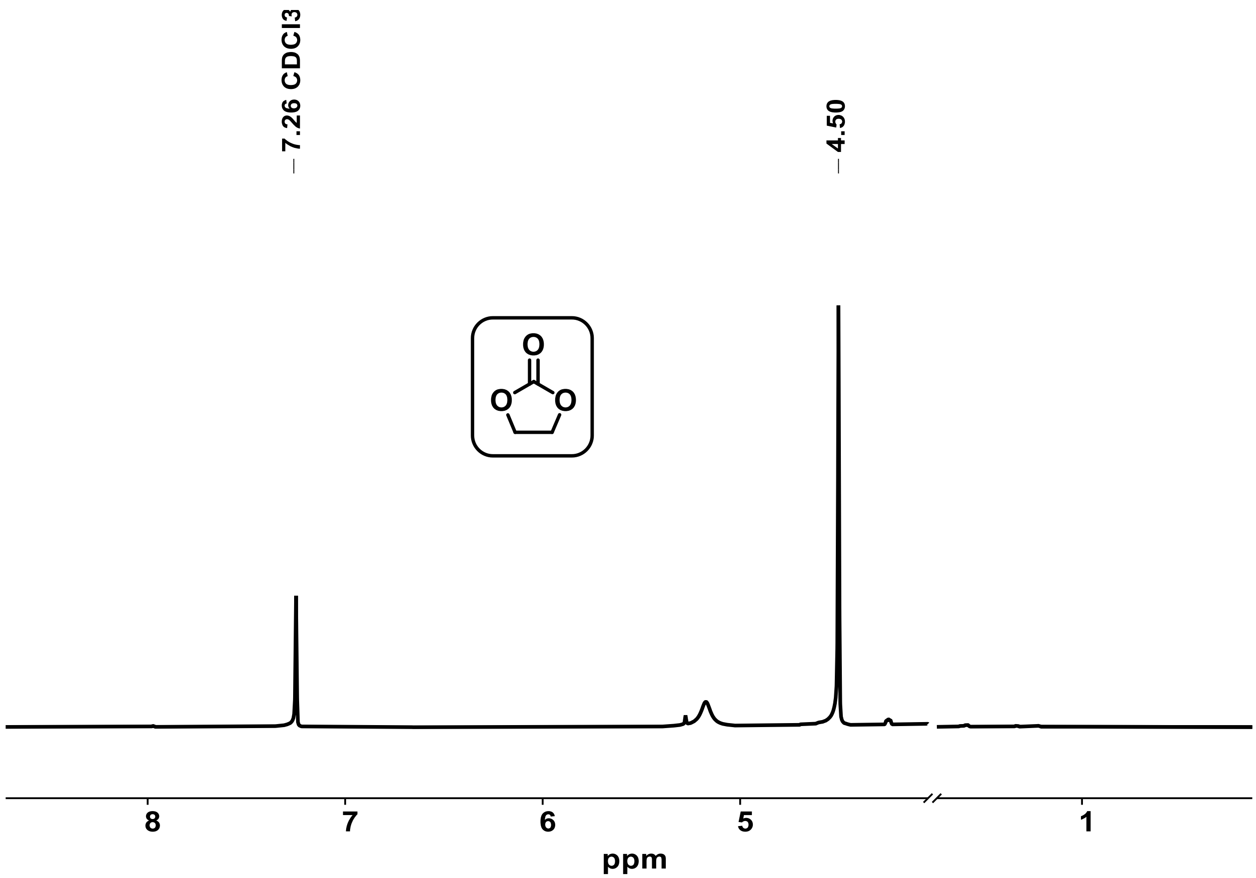


Figure S34. ^{1}H NMR spectrum EC formed from the deconstruction of PC (0.5 g, 2.0 mmol, 1 eq.), EG (1.2 g, 20 mmol, 10 eq.), and TBD:TFA (0.025 g, 0.1 mmol, 0.05 eq.), as a catalyst at 130 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

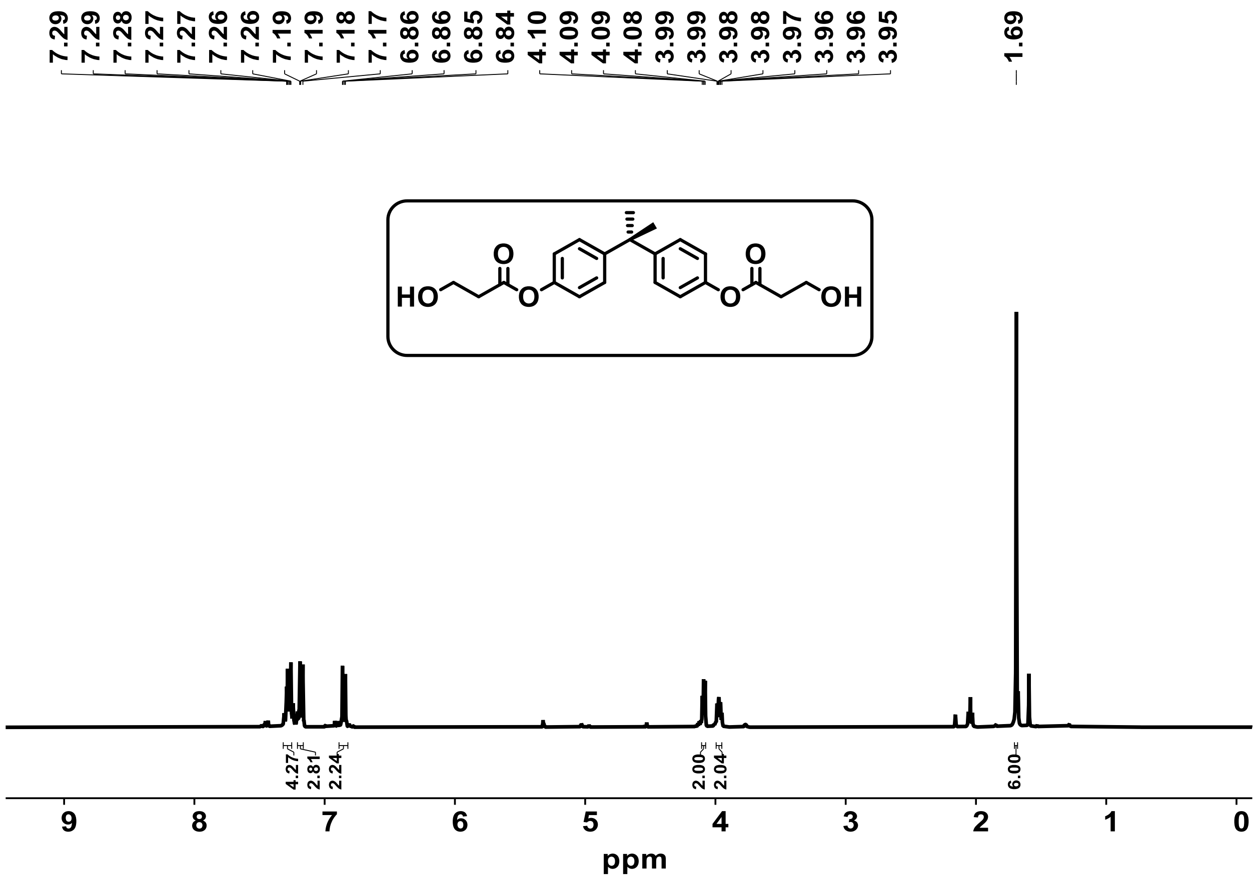


Figure S35. ^{1}H NMR spectrum Bis-HPPP formed from the deconstruction of PC (0.5 g, 2.0 mmol, 1 eq.), EG (1.2 g, 20 mmol, 10 eq.), and TBD:TFA (0.025 g, 0.1 mmol, 0.05 eq.), as a catalyst at 130 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

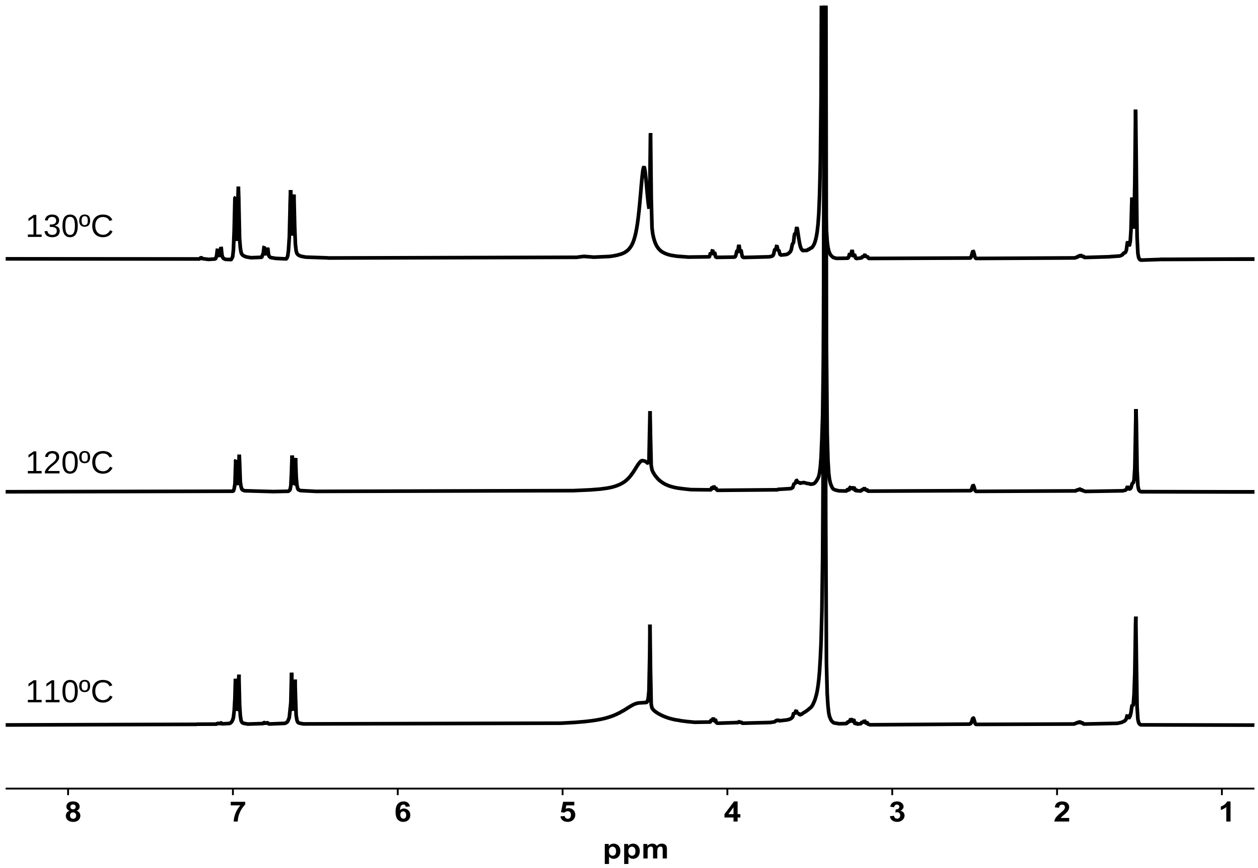


Figure S36. Stacked ^{1}H NMR spectra from the deconstruction of PC (0.5 g, 2.0 mmol, 1 eq.), EG (1.2 g, 20 mmol, 10 eq.), and TBD:TFA (0.025 g, 0.1 mmol, 0.05 eq.), as a catalyst at different temperature for 2h (DMSO-d6, 400 MHz, 298 K).

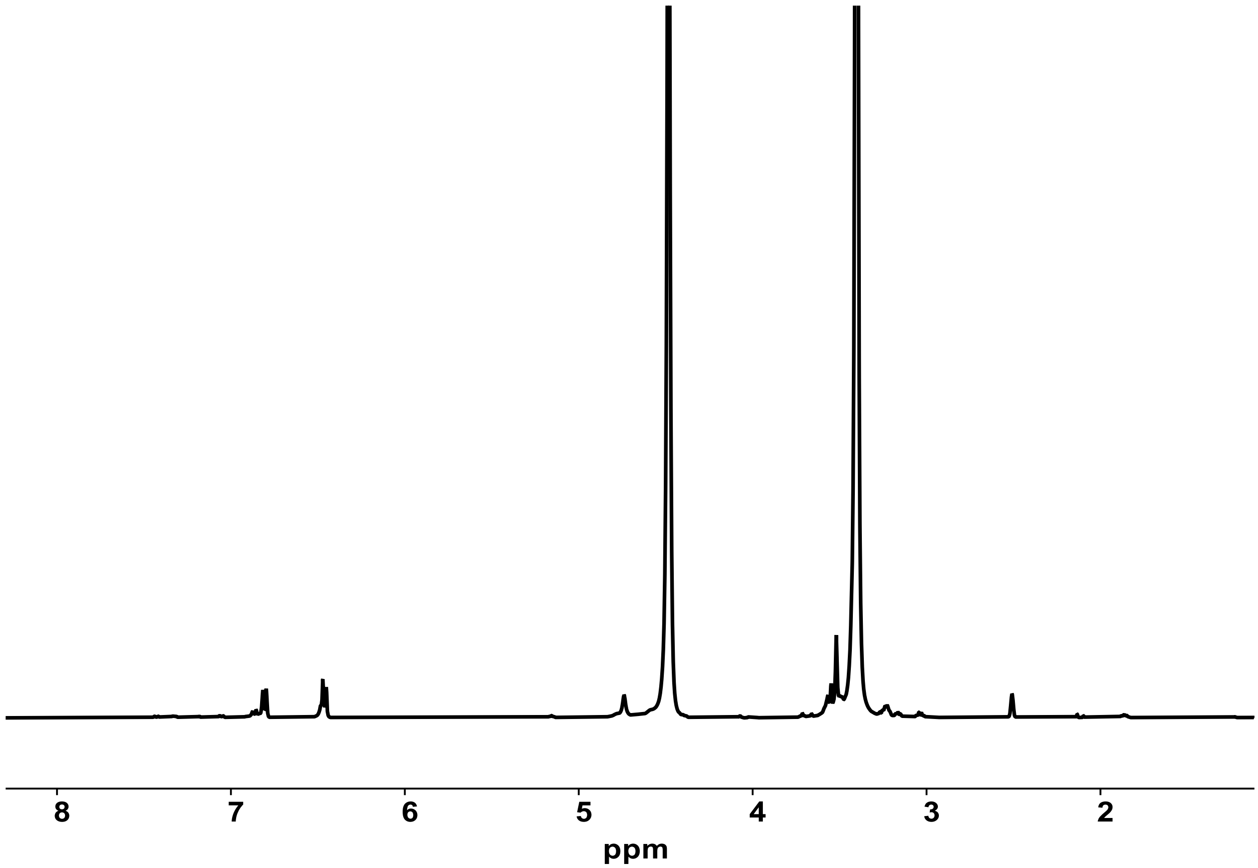


Figure S37. ^{1}H NMR spectrum from the deconstruction of PU (0.25 g, 0.8 mmol, 1 eq.), EG (0.49 g, 8.00 mmol, 10 eq.), and TBD:TFA (0.01 g, 0.04 mmol, 0.05 eq.), as a catalyst at 160 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

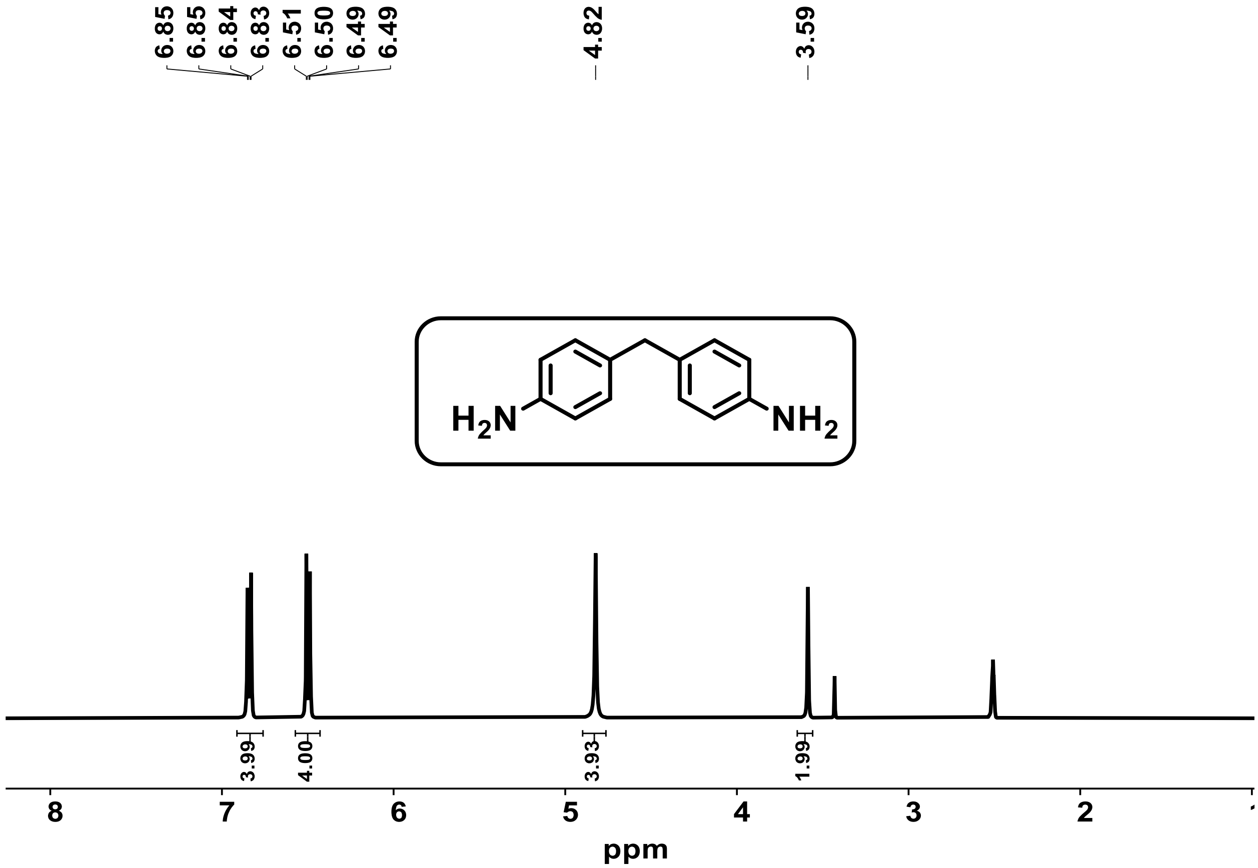


Figure S38. [1]H NMR spectrum from the deconstruction of PU (0.25 g, 0.8 mmol, 1 eq.), EG (0.49 g, 8.00 mmol, 10 eq.), and TBD:TFA (0.01 g, 0.04 mmol, 0.05 eq.), as a catalyst at 160 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

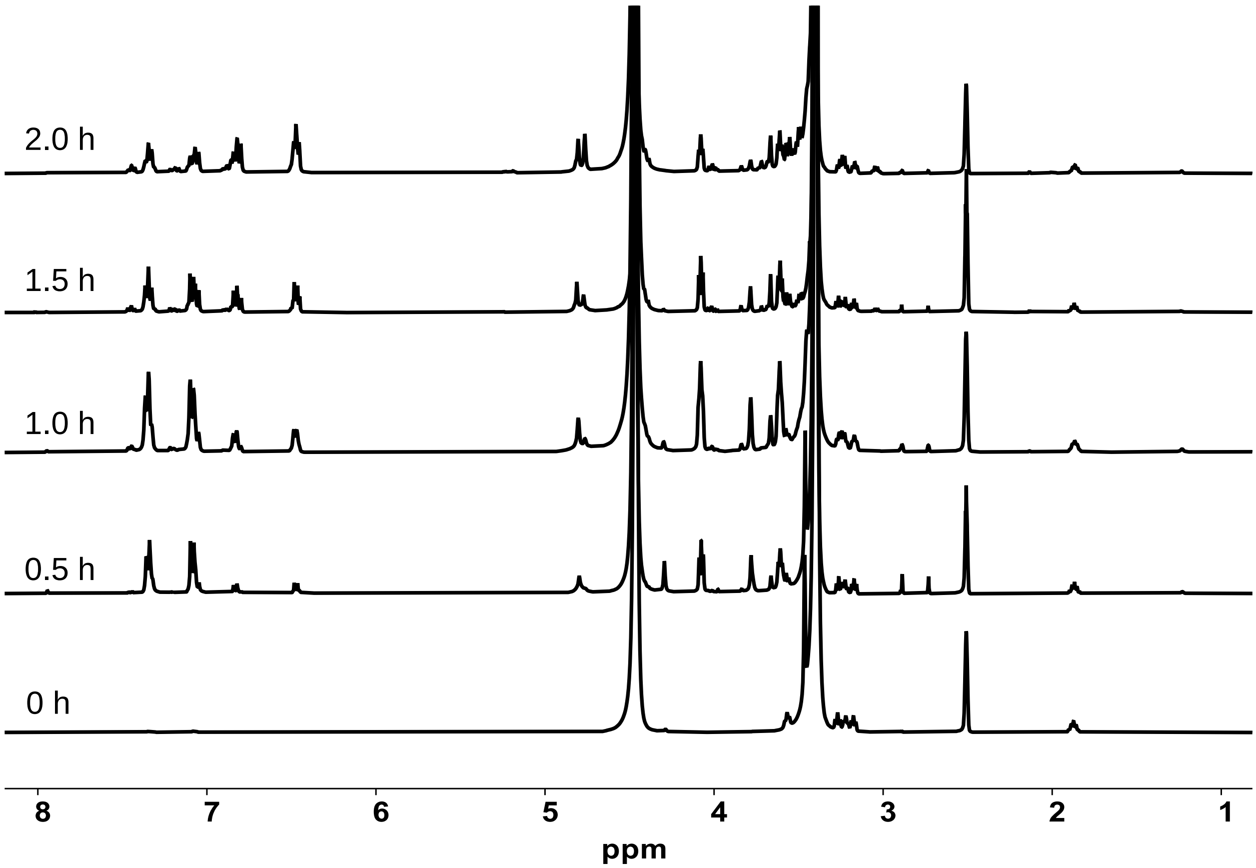


Figure S39. Stacked ^{1}H NMR spectra of the deconstructed PU (0.1 g, 0.32 mmol, 1 eq.), EG (0.2 g, 3.2 mmol, 10 eq.), and TBD:TFA (0.004 g, 0.016 mmol, 0.05 eq.), as a catalyst at 150 ºC (DMSO-d6, 400 MHz, 298 K).

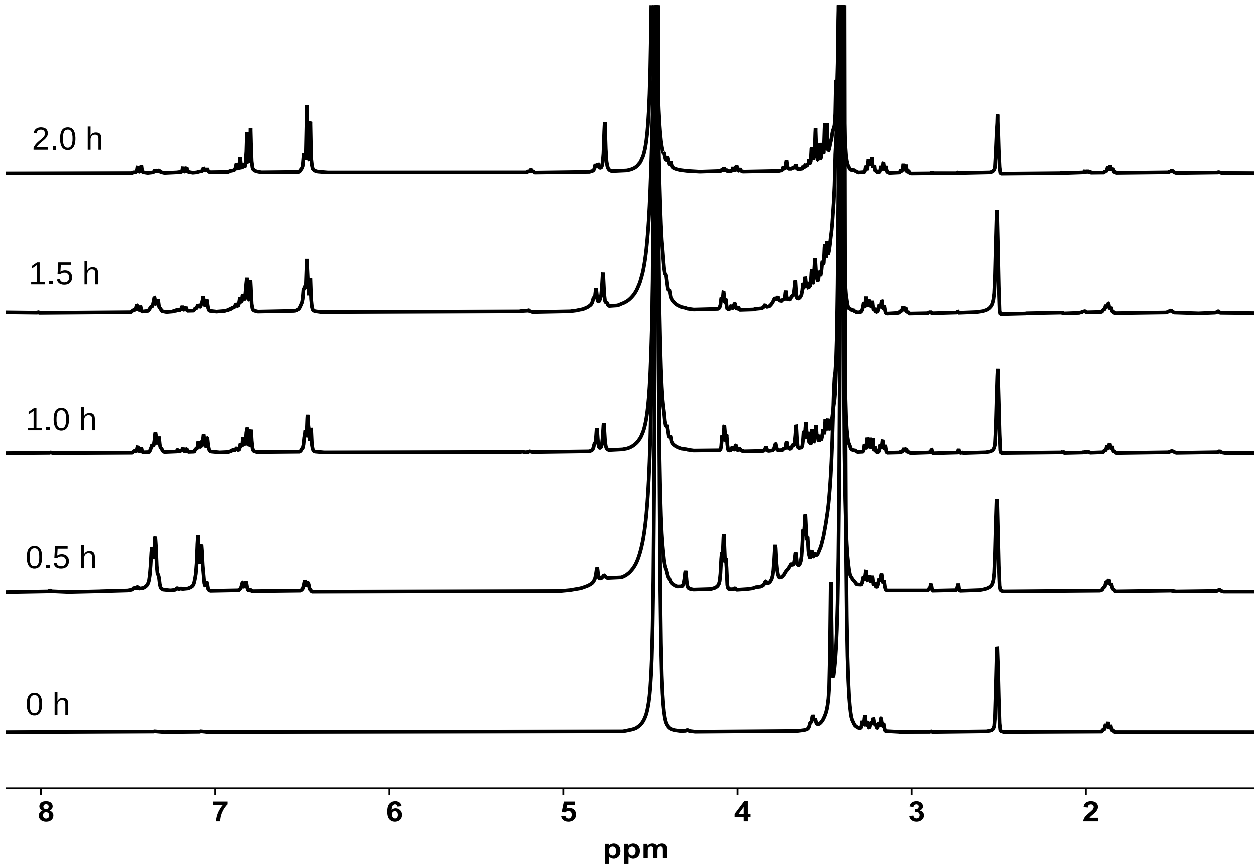


Figure S40. Stacked ^{1}H NMR spectra of the deconstructed PU (0.1 g, 0.32 mmol, 1 eq.), EG (0.2 g, 3.2 mmol, 10 eq.), and TBD:TFA (0.004 g, 0.016 mmol, 0.05 eq.), as a catalyst at 160 ºC (DMSO-d6, 400 MHz, 298 K).

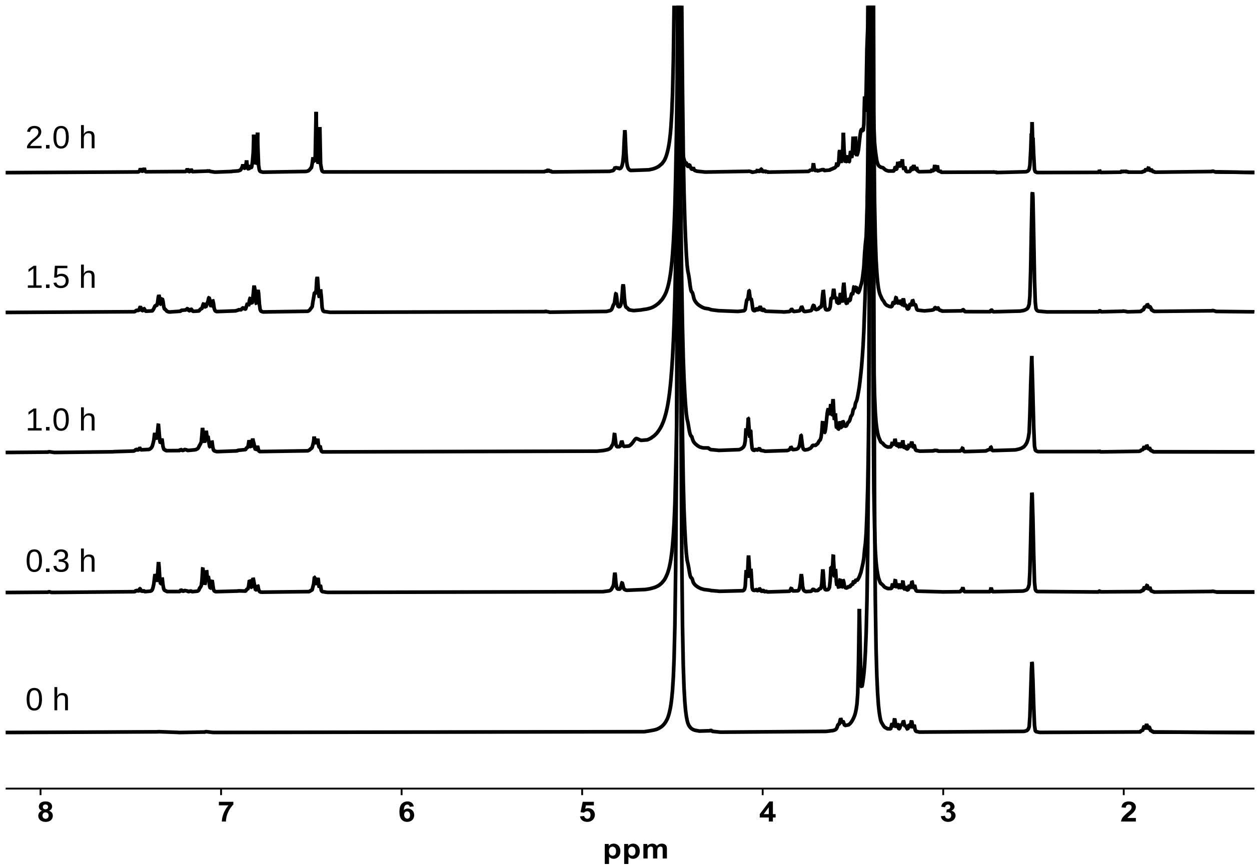


Figure S41. Stacked ^{1}H NMR spectra from the deconstruction of PU (0.1 g, 0.32 mmol, 1 eq.), EG (0.2 g, 3.2 mmol, 10 eq.), and TBD:TFA (0.004 g, 0.016 mmol, 0.05 eq.), as a catalyst at 170 ºC (DMSO-d6, 400 MHz, 298 K).

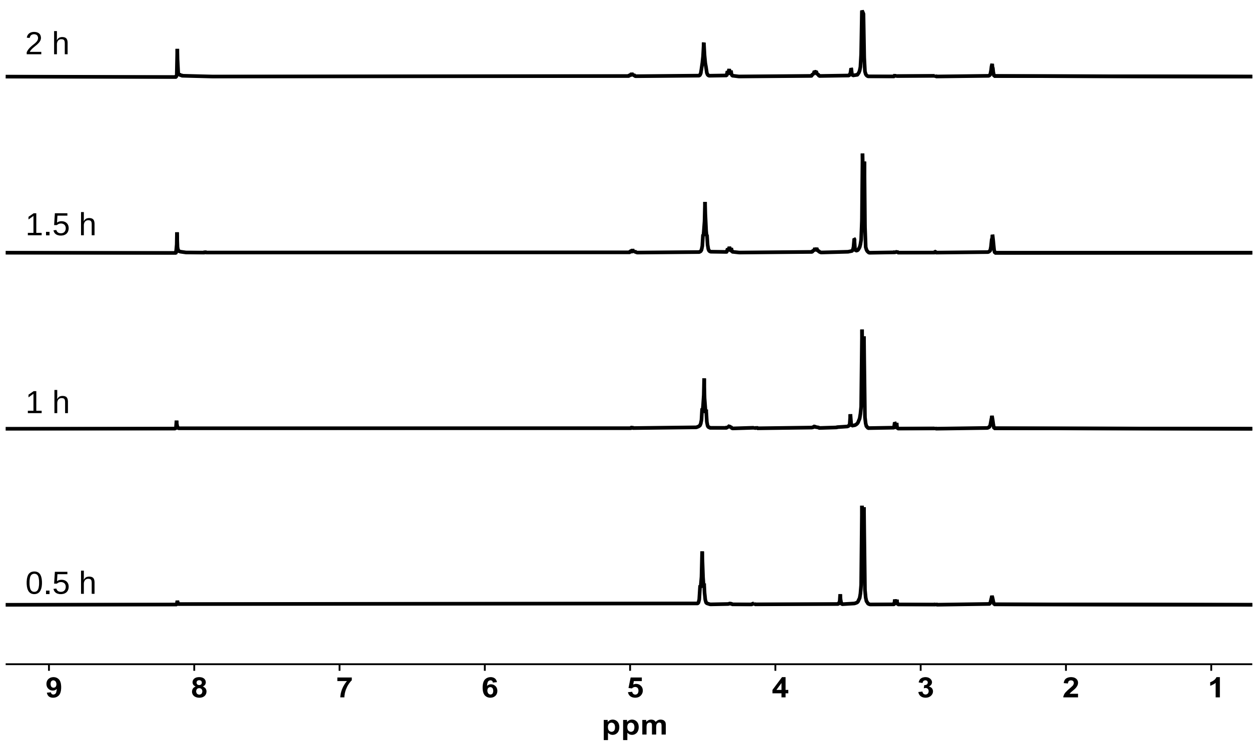


Figure S42. Stacked ^{1}H NMR spectra from the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.), EG (1.61 g, 26 mmol, 10 eq.), and mTBD:TFA (0.037 g, 0.13 mmol, 0.05 eq.), as a catalyst at 180 ºC (DMSO-d6, 400 MHz, 298 K).

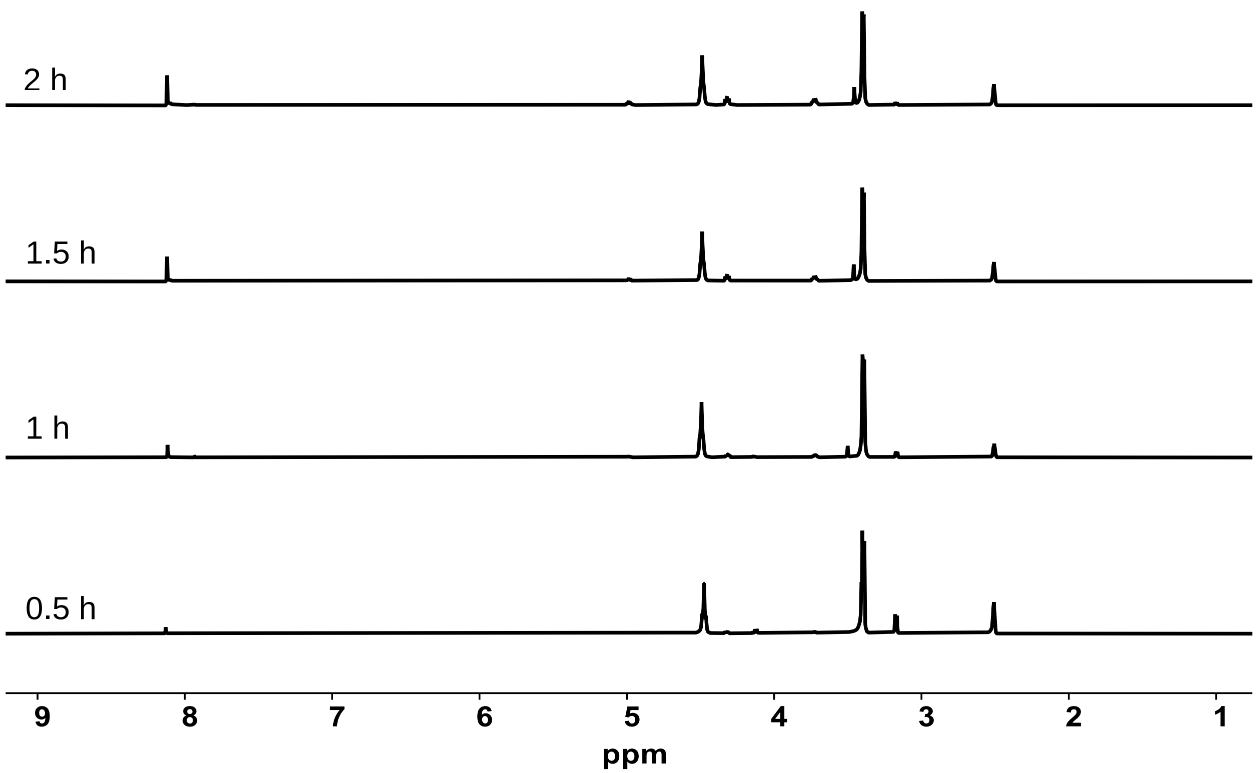


Figure S43. Stacked ^{1}H NMR spectra from the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.), EG (1.61 g, 26 mmol, 10 eq.), and TBD:mTFA (0.037 g, 0.13 mmol, 0.05 eq.), as a catalyst at 180 ºC (DMSO-d6, 400 MHz, 298 K).

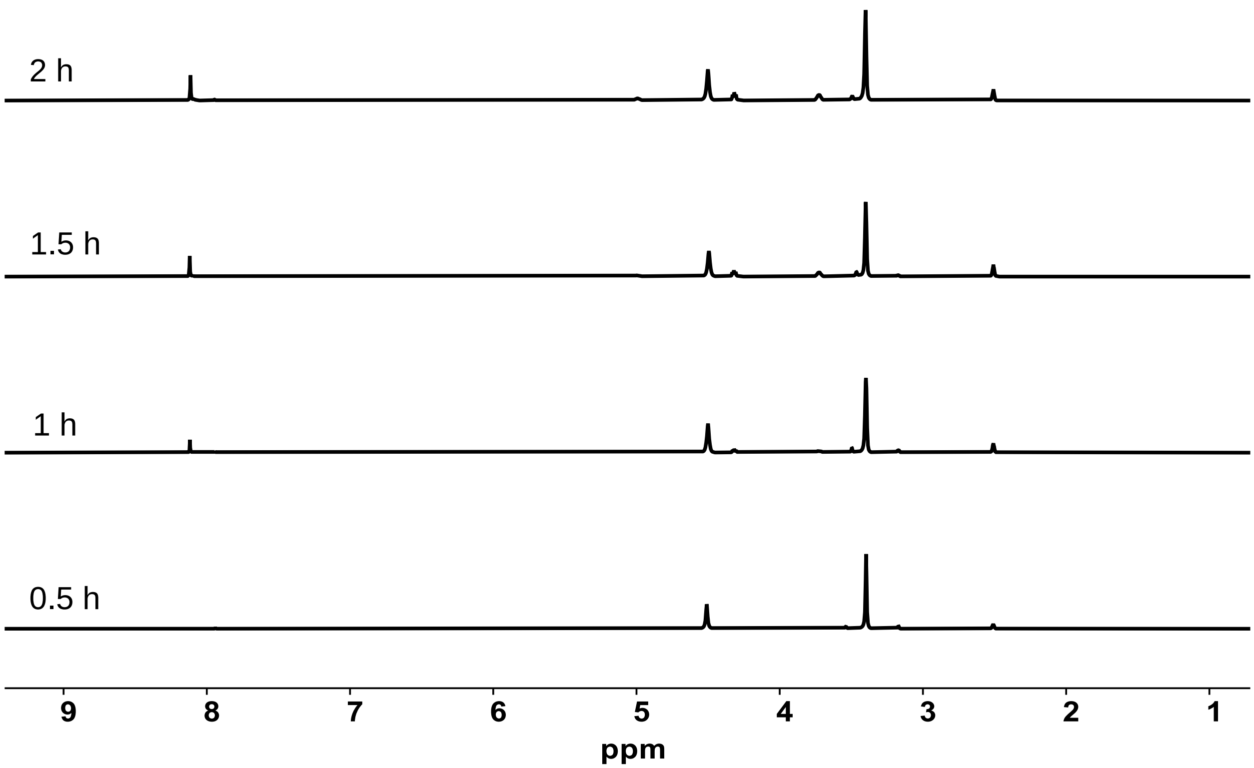


Figure S44. Stacked ^{1}H NMR spectra from the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.), EG (1.61 g, 26 mmol, 10 eq.), and TBD (0.018 g, 0.13 mmol, 0.05 eq.), as a catalyst at 180 ºC (DMSO-d6, 400 MHz, 298 K).

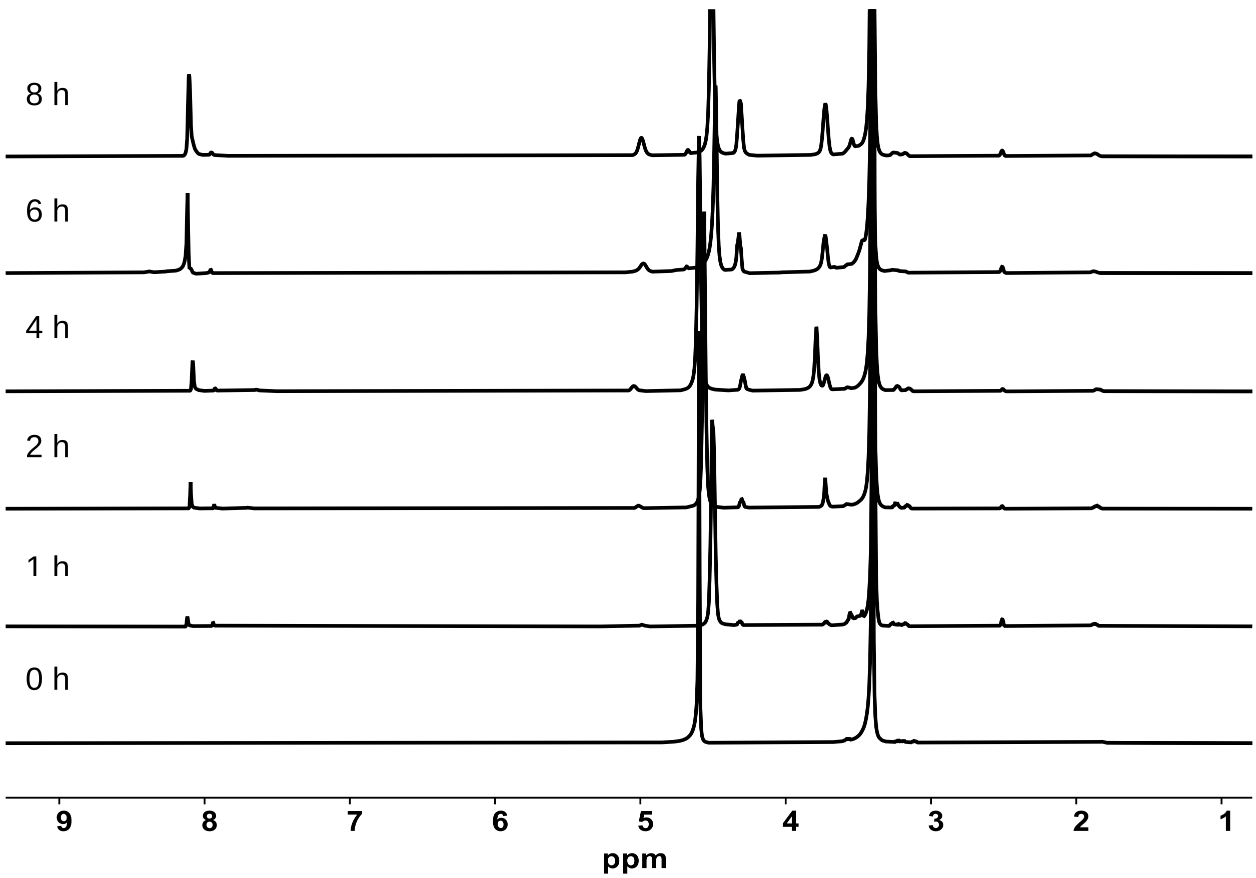


Figure S45. Stacked ^{1}H NMR spectra in the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.) using EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), at 150 ºC (DMSO-d6, 400 MHz, 298 K).

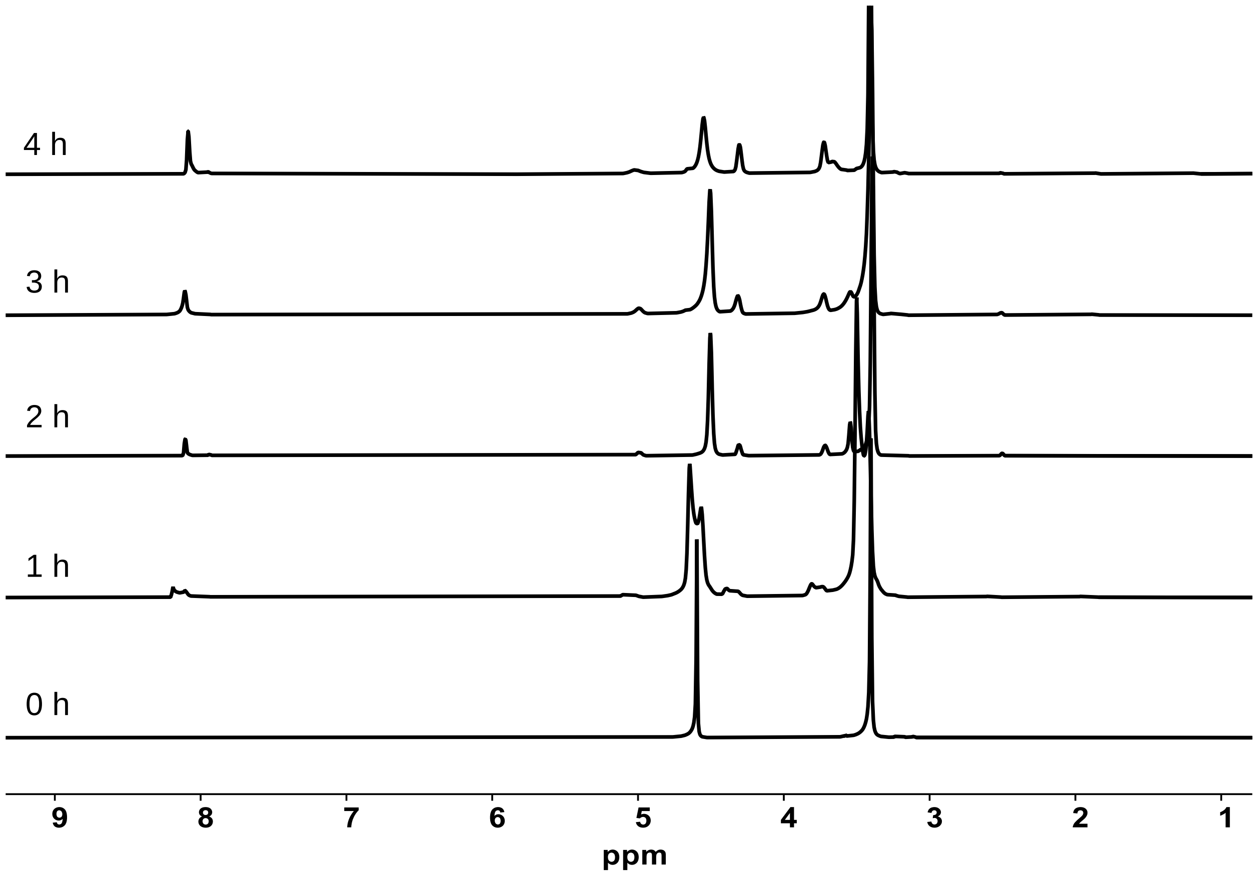


Figure S46. Stacked ^{1}H NMR spectra from the PET deconstruction (0.5 g, 2.6 mmol, 1 eq.), EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), as a catalyst at 160 ºC (DMSO-d6, 400 MHz, 298 K).

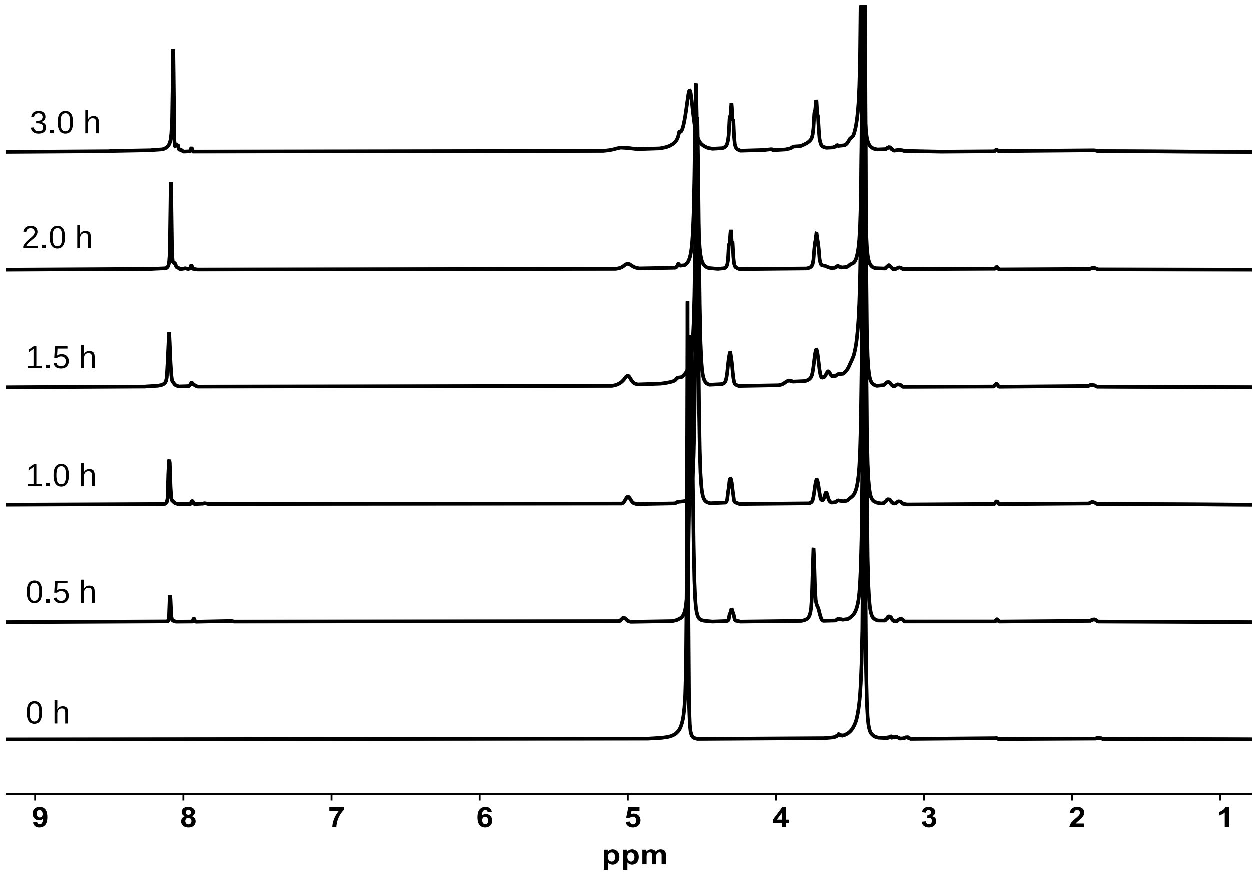


Figure S47. Stacked ^{1}H NMR spectra of the deconstructed PET (0.5 g, 2.6 mmol, 1 eq.) using EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), at 170 ºC (DMSO-d6, 400 MHz, 298 K).

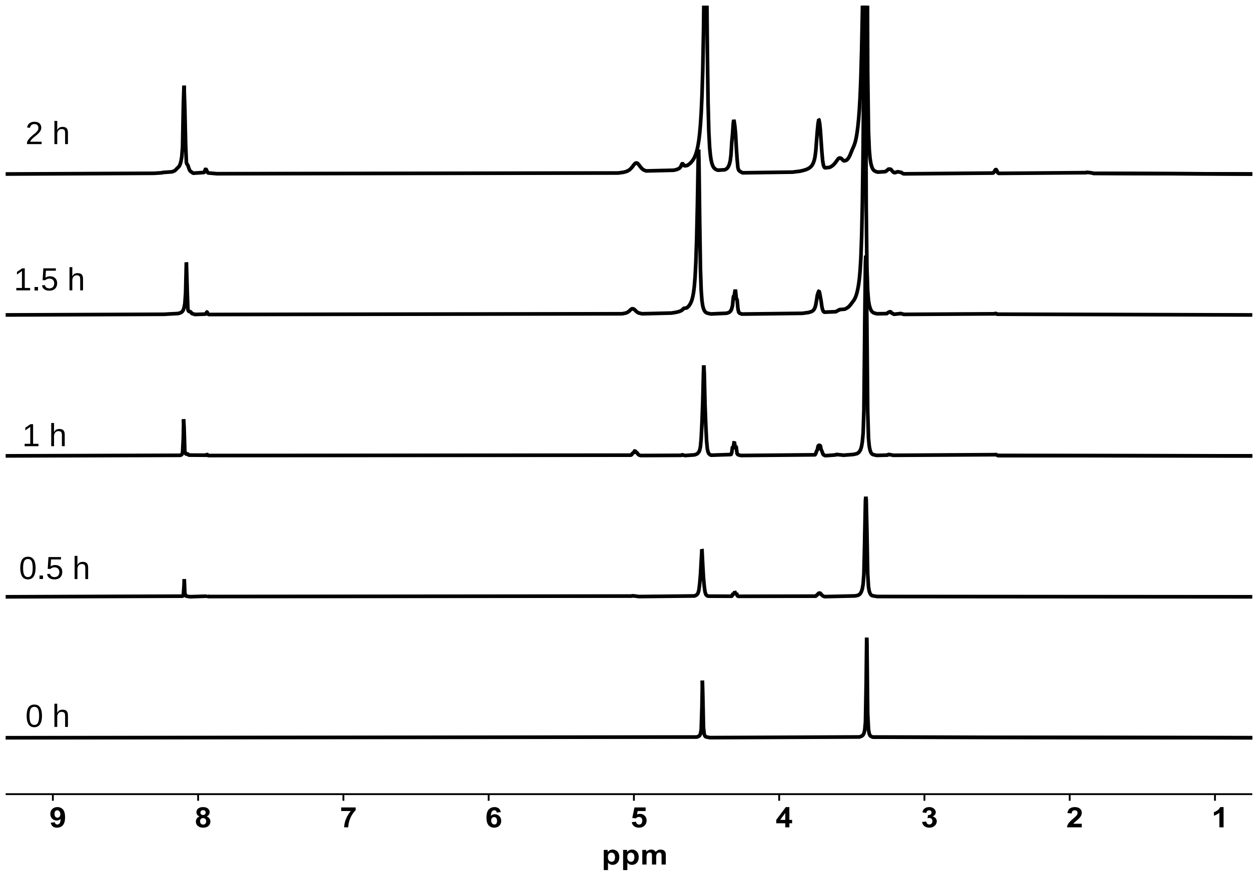


Figure S48. Stacked ^{1}H NMR spectra from the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.) using EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.) at 180 ºC (DMSO-d6, 400 MHz, 298 K).

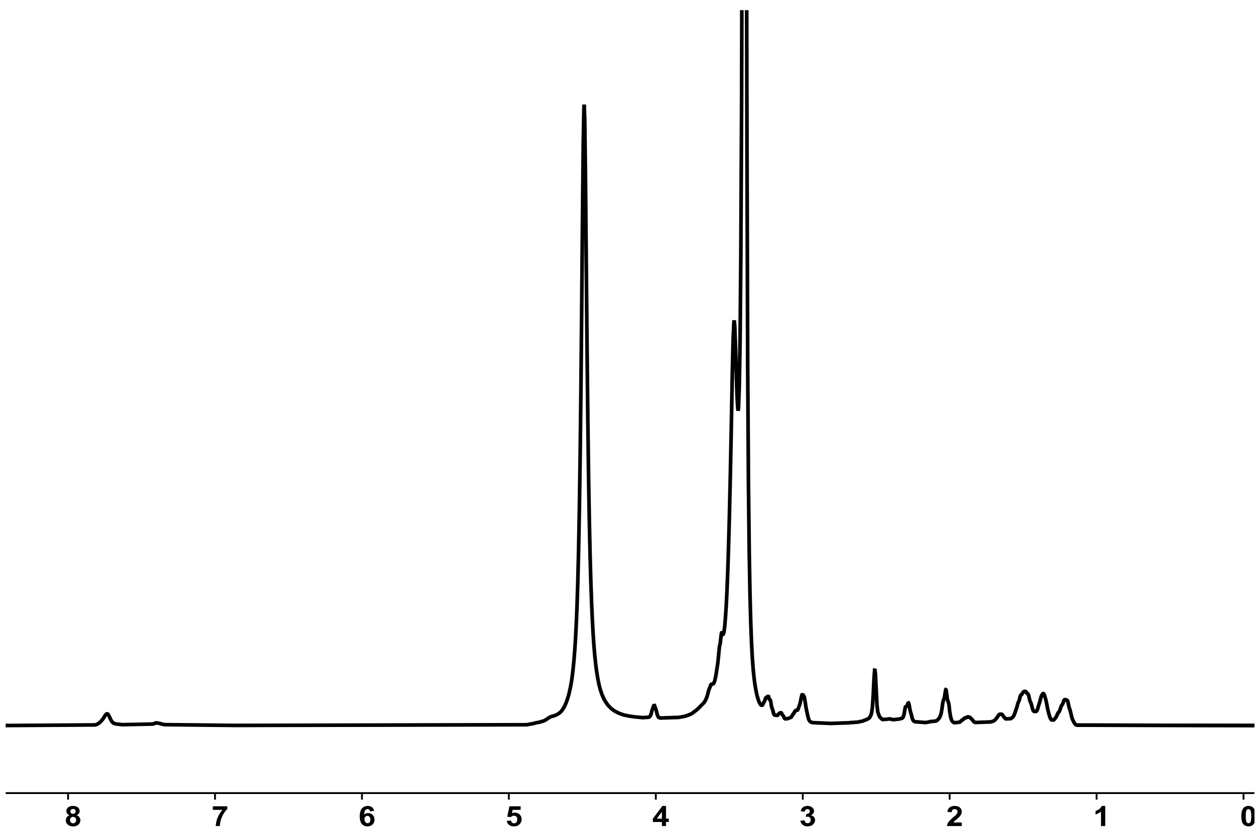


Figure S49. ^{1}H NMR spectrum of the deconstructed PA (Nylon-6) (0.5 g, 4.4 mmol, 1 eq.), EG (2.73 g, 44 mmol, 10 eq.), and TBD:TFA (0.05 g, 0.22 mmol, 0.05 eq.), as a catalyst at 210 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

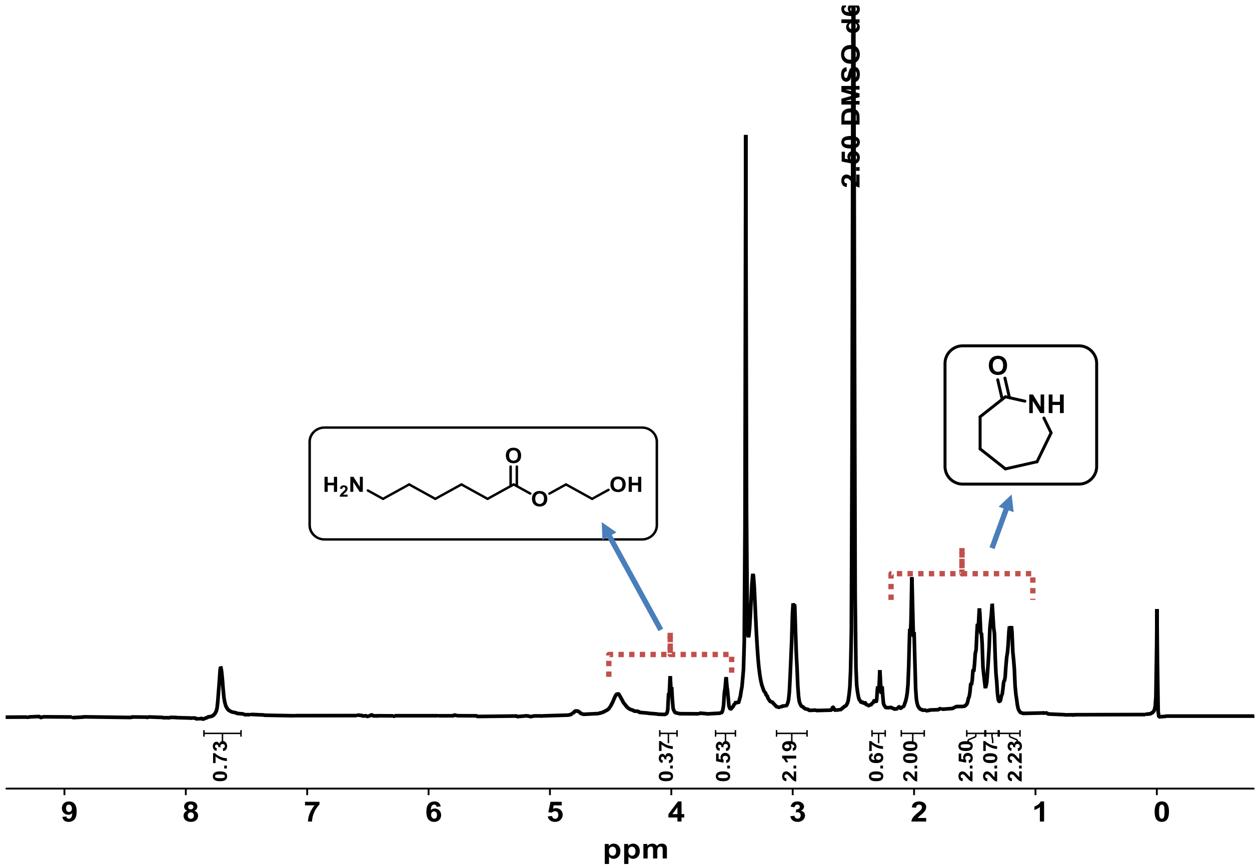


Figure S50. [1]H NMR spectrum of mixed product (after precipitation) formed by the deconstruction of PA (Nylon-6) (0.5 g, 4.4 mmol, 1 eq.), EG (2.73 g, 44 mmol, 10 eq.), and TBD:TFA (0.05 g, 0.22 mmol, 0.05 eq.), as a catalyst at 210 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

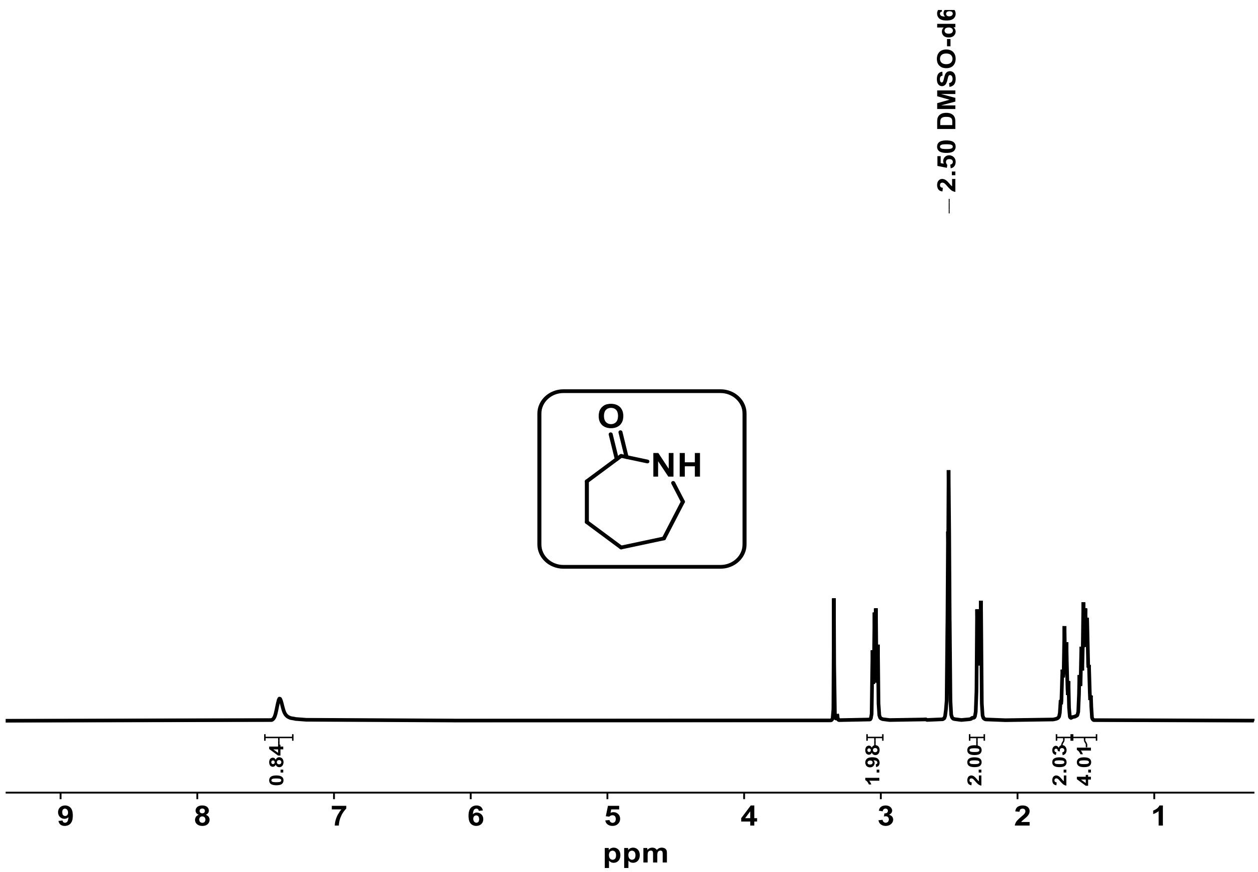


Figure S51. ^{1}H NMR spectrum of the pure CPL from Nylon-6 (DMSO-d6, 400 MHz, 298 K).

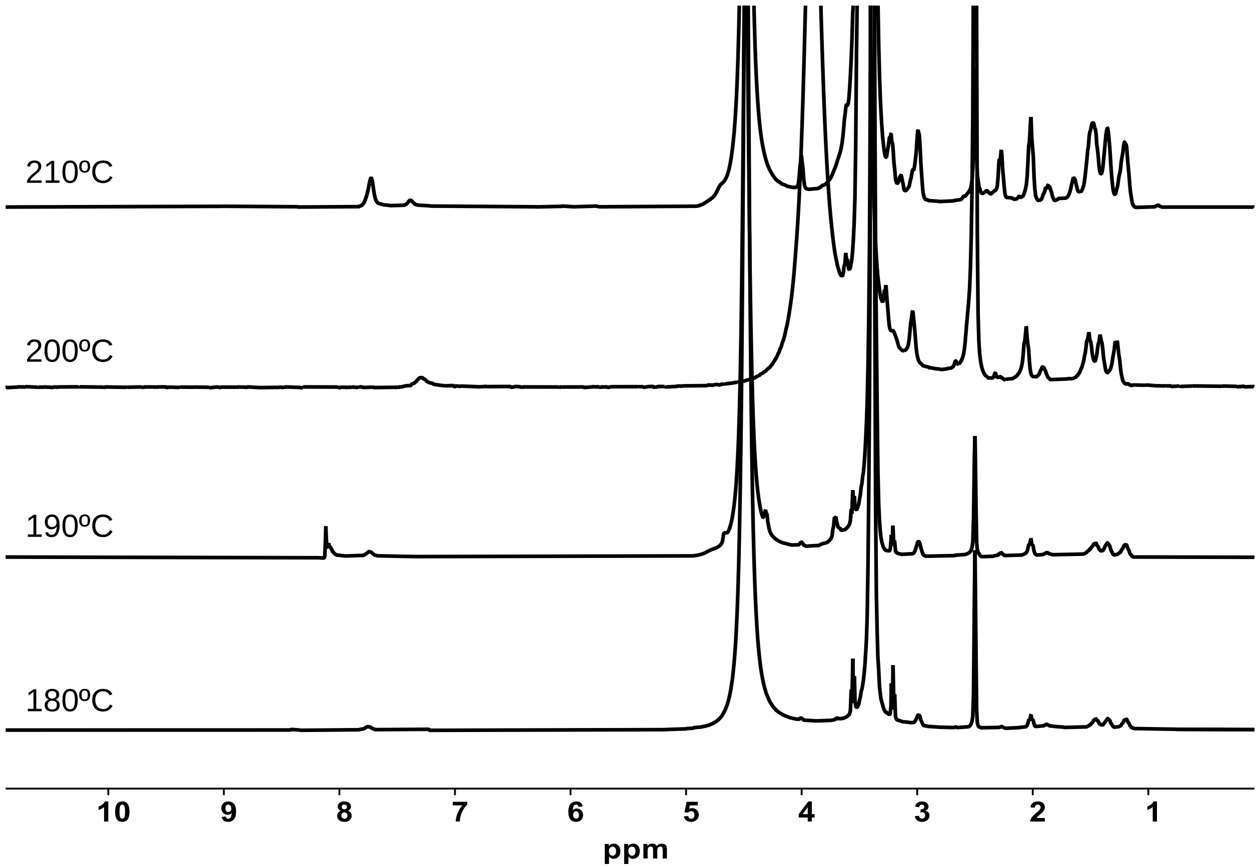


Figure S52. Stacked ^{1}H NMR spectra of the deconstruction of PA (Nylon-6) (0.5 g, 4.4 mmol, 1 eq.), with EG (2.73 g, 44 mmol, 10 eq.), and TBD:TFA (0.05 g, 0.22 mmol, 0.05 eq.), as a catalyst at different temperature for 3h (DMSO-d6, 400 MHz, 298 K).

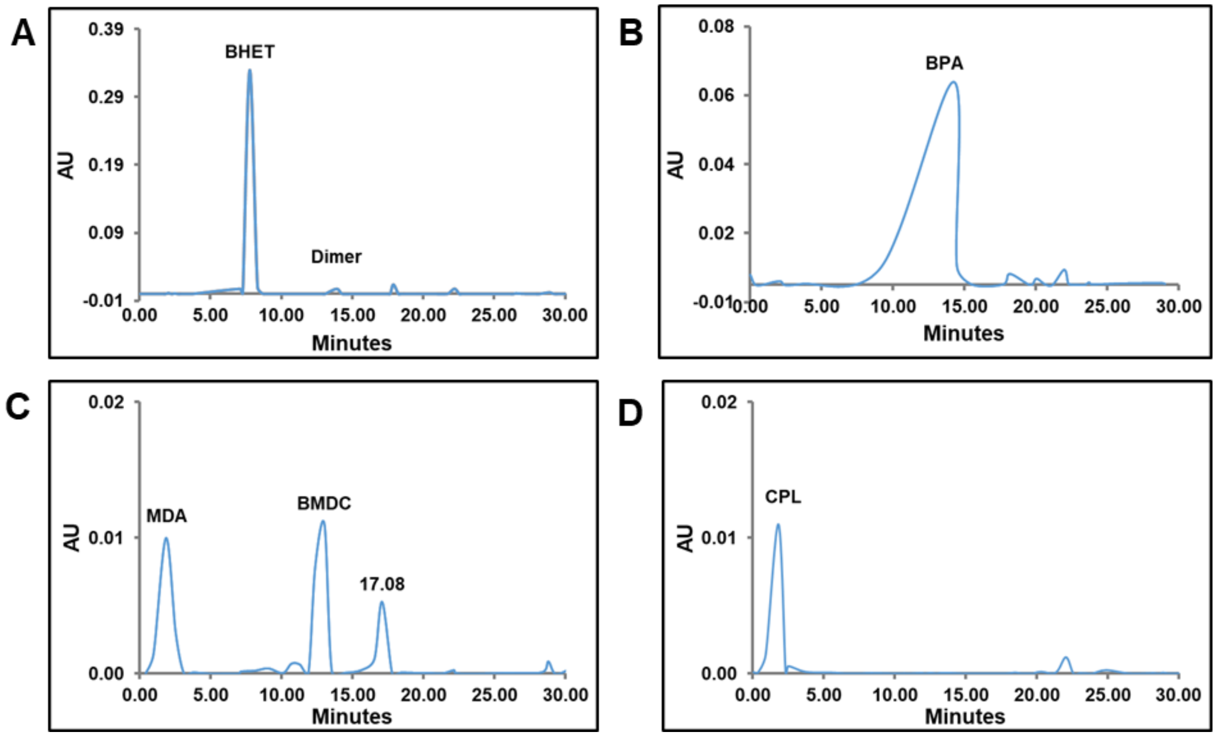


Figure S53. HPLC analysis of (A) PET, (B) PC, (D) PU and (E) PA deconstruction with TBD:TFA as a catalyst. Reaction conditions: Polymer (1 eq), catalyst (0.05 eq), EG (05 eq).

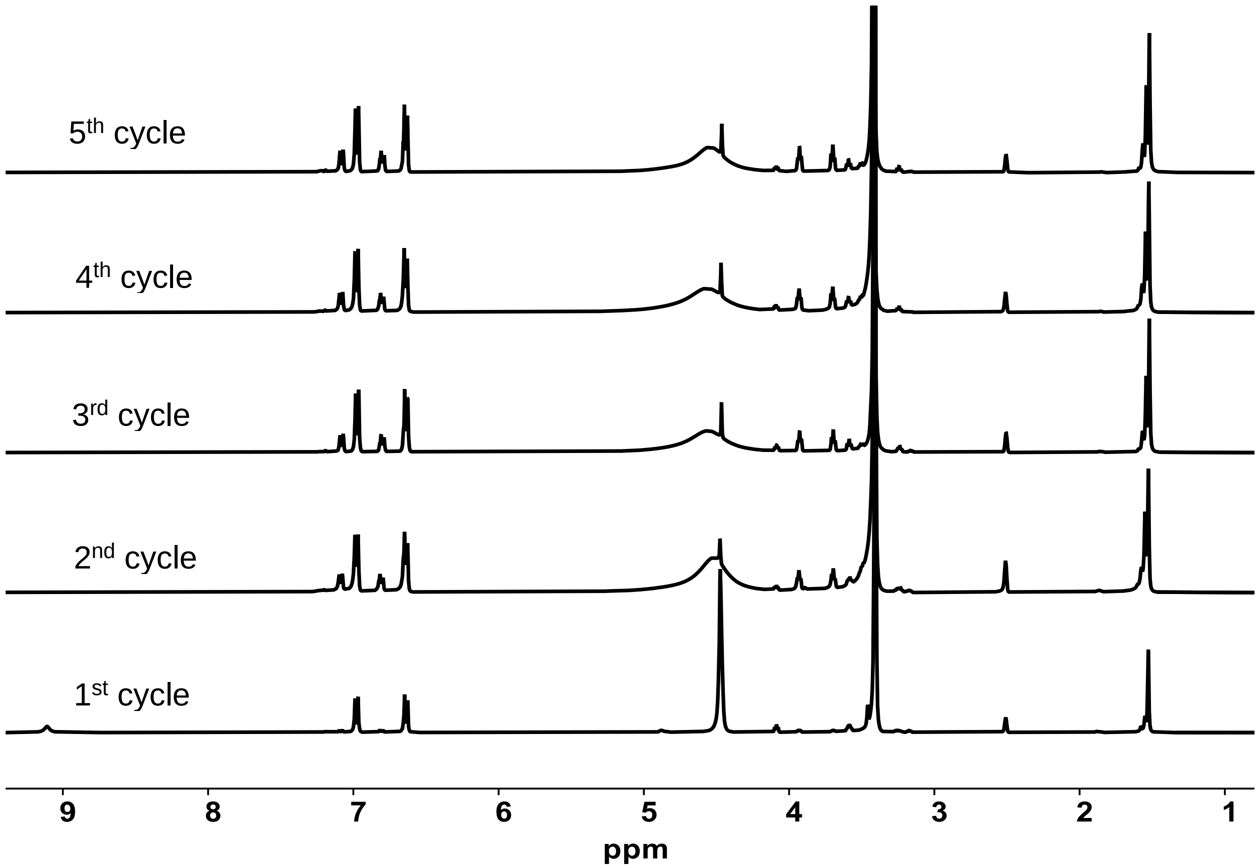


Figure S54. Stacked ^{1}H NMR spectra of the recyclability of the catalyst (TBD:TFA) for the deconstruction of PC at 130 ºC (DMSO-d6, 400 MHz, 298 K).

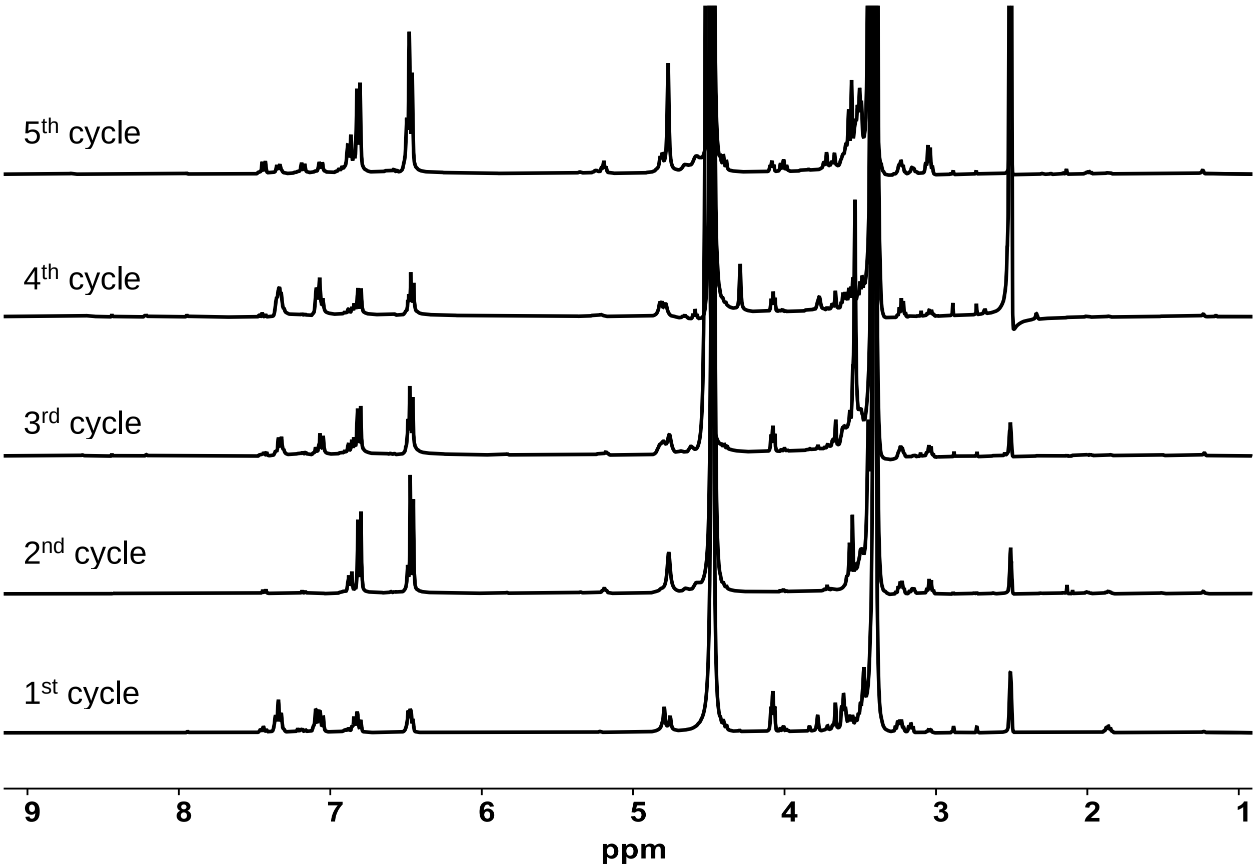


Figure S55. Stacked ^{1}H NMR spectra of the recyclability of the catalyst (TBD:TFA) for the deconstruction of PU at 160 ºC (DMSO-d6, 400 MHz, 298 K).

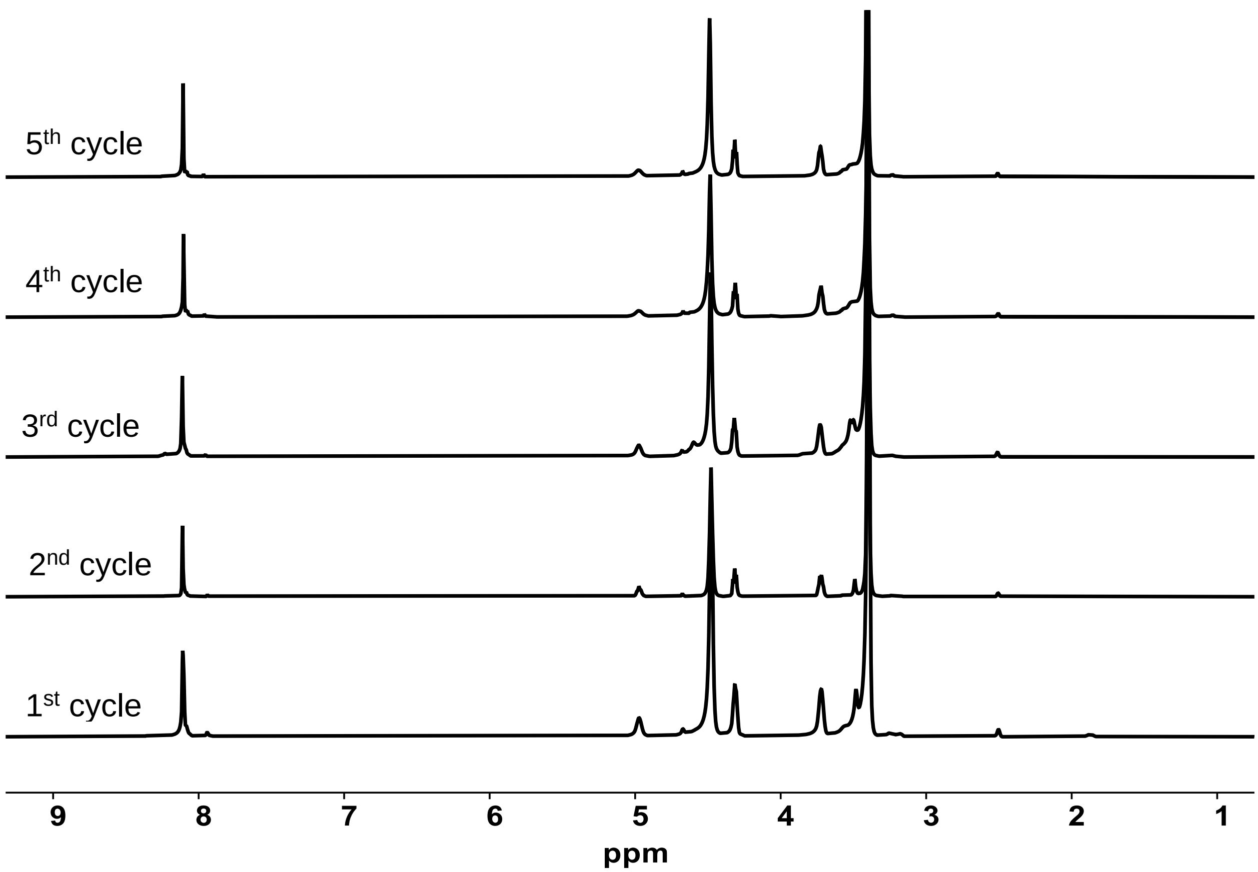


Figure S56. Stacked ^{1}H NMR spectra of the recyclability of the catalyst (TBD:TFA) for the deconstruction of PET at 180 ºC (DMSO-d6, 400 MHz, 298 K).

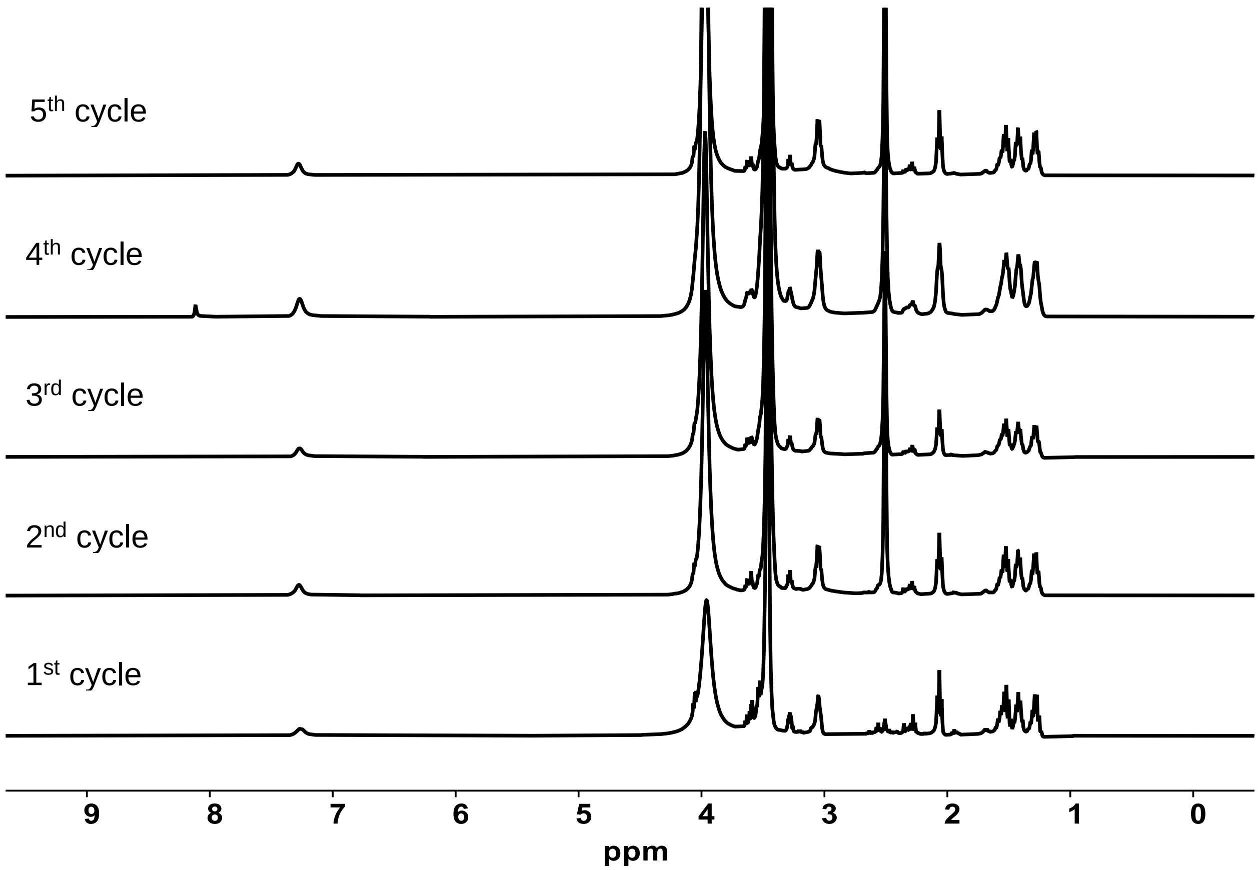


Figure S57. Stacked ^{1}H NMR spectra of the recyclability of the catalyst (TBD:TFA) for the deconstruction of PU at 130 ºC (DMSO-d6, 400 MHz, 298 K).

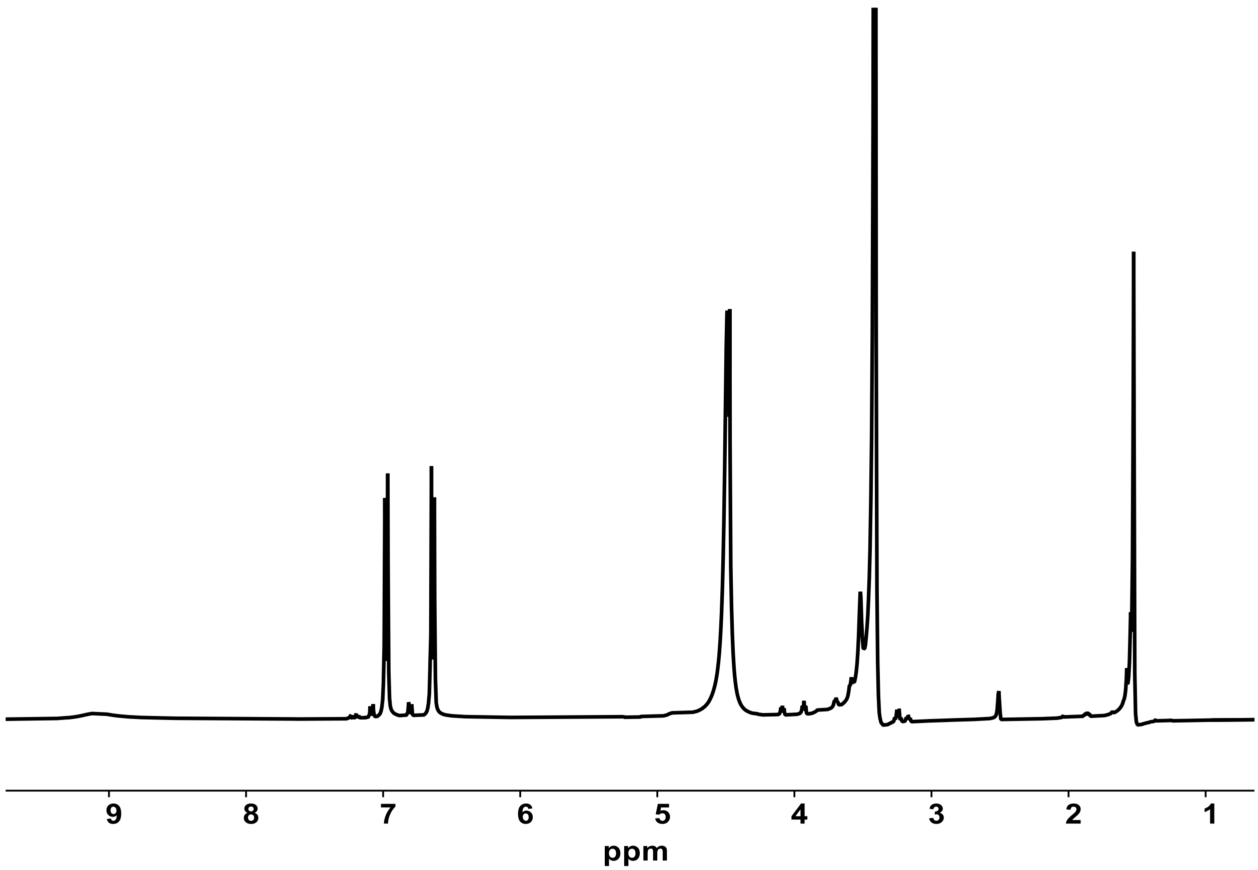


Figure S58. ^{1}H NMR spectrum of the deconstruction of PC (0.5 g, 2.0 mmol, 1 eq.), EG (1.2 g, 20 mmol, 10 eq.), and TBD:TFA (0.025 g, 0.1 mmol, 0.05 eq.), as a catalyst at 130 ºC for 2 h with 30% H_2O (DMSO-d6, 400 MHz, 298 K).

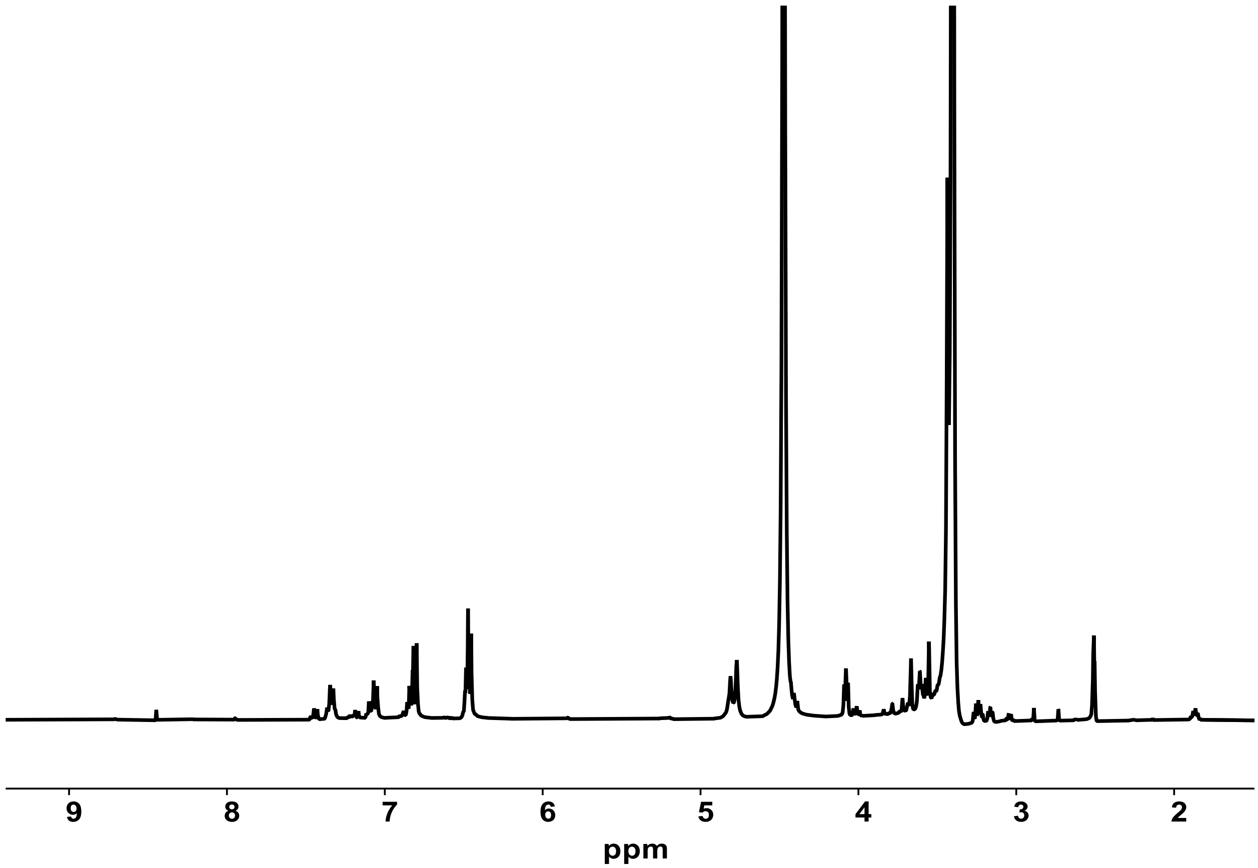


Figure S59. [1]H NMR spectrum of the deconstruction of PU (0.1 g, 0.32 mmol, 1 eq.), EG (0.2 g, 3.2 mmol, 10 eq.), and TBD:TFA (0.004 g, 0.016 mmol, 0.05 eq.), as a catalyst at 170 ºC for 2 h with 30% H_2O (DMSO-d6, 400 MHz, 298 K).

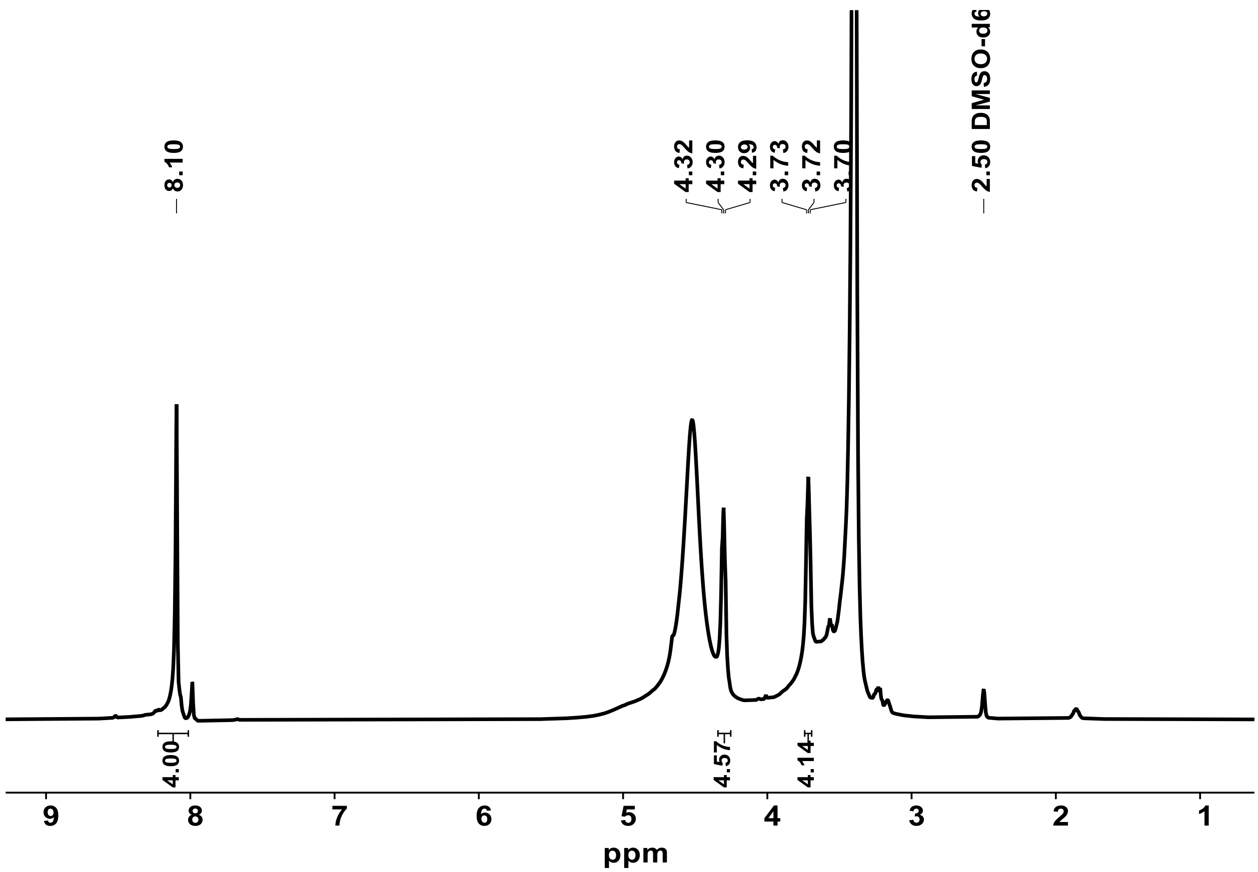


Figure S60. [1]H NMR spectrum of the deconstruction of PET (0.5 g, 2.6 mmol, 1 eq.), EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), as a catalyst at 180 ºC with 30% H_2O (DMSO-d6, 400 MHz, 298 K).

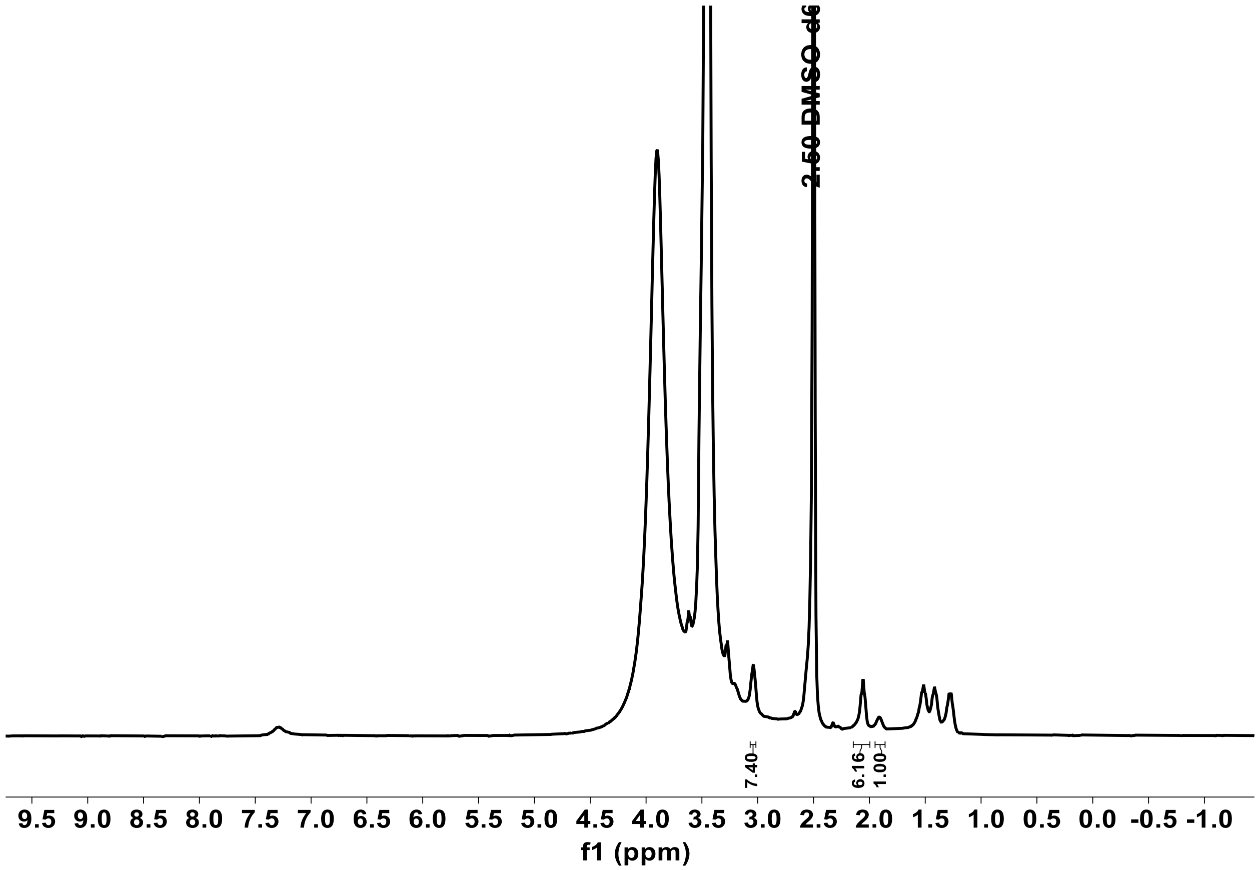


Figure S61. ^{1}H NMR spectrum of the deconstruction of PA (Nylon-6) (0.5 g, 4.4 mmol, 1 eq.), EG (2.73 g, 44 mmol, 10 eq.), and TBD:TFA (0.05 g, 0.22 mmol, 0.05 eq.), as a catalyst at 210 ºC for 2 h with 30% H_2O (DMSO-d6, 400 MHz, 298 K).

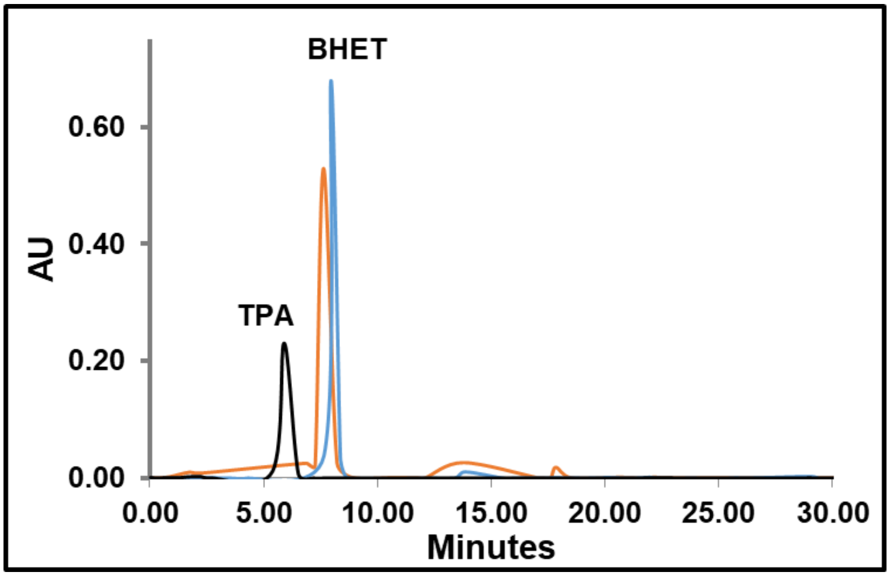


Figure S62. HPLC analysis of PET deconstruction in the presence of 30% water with TBD:TFA as a catalyst. Reaction conditions: PET (1 eq), catalyst (0.05 eq), EG (05 eq). Black: For pure Terephthalic acid (TPA), Blue: For pure BHET monomer, and Orange: Reaction of PET in 30% water.

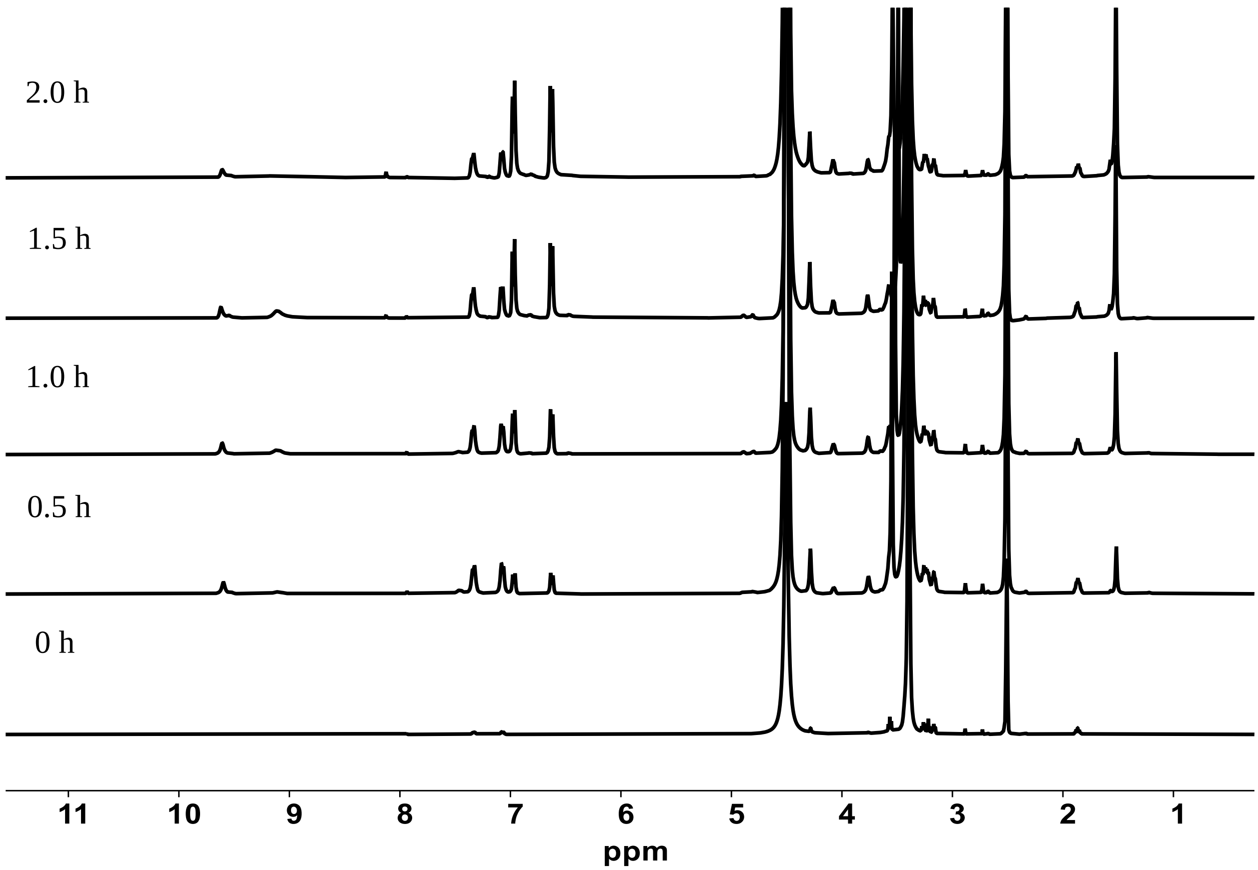


Figure S63. Stacked ^{1}H NMR spectra of the deconstruction of mixed plastic pellets PC (0.33 g, 1.3 mmol), PU (0.41 g, 1.3 mmol), PET (0.25 g, 1.3 mmol), & PA (0.15 g, 1.3 mmol), EG (3.17 g, 52 mmol, 10 eq.), and TBD:TFA (0.07 g, 0.26 mmol, 0.05 eq.), as a catalyst at 130 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

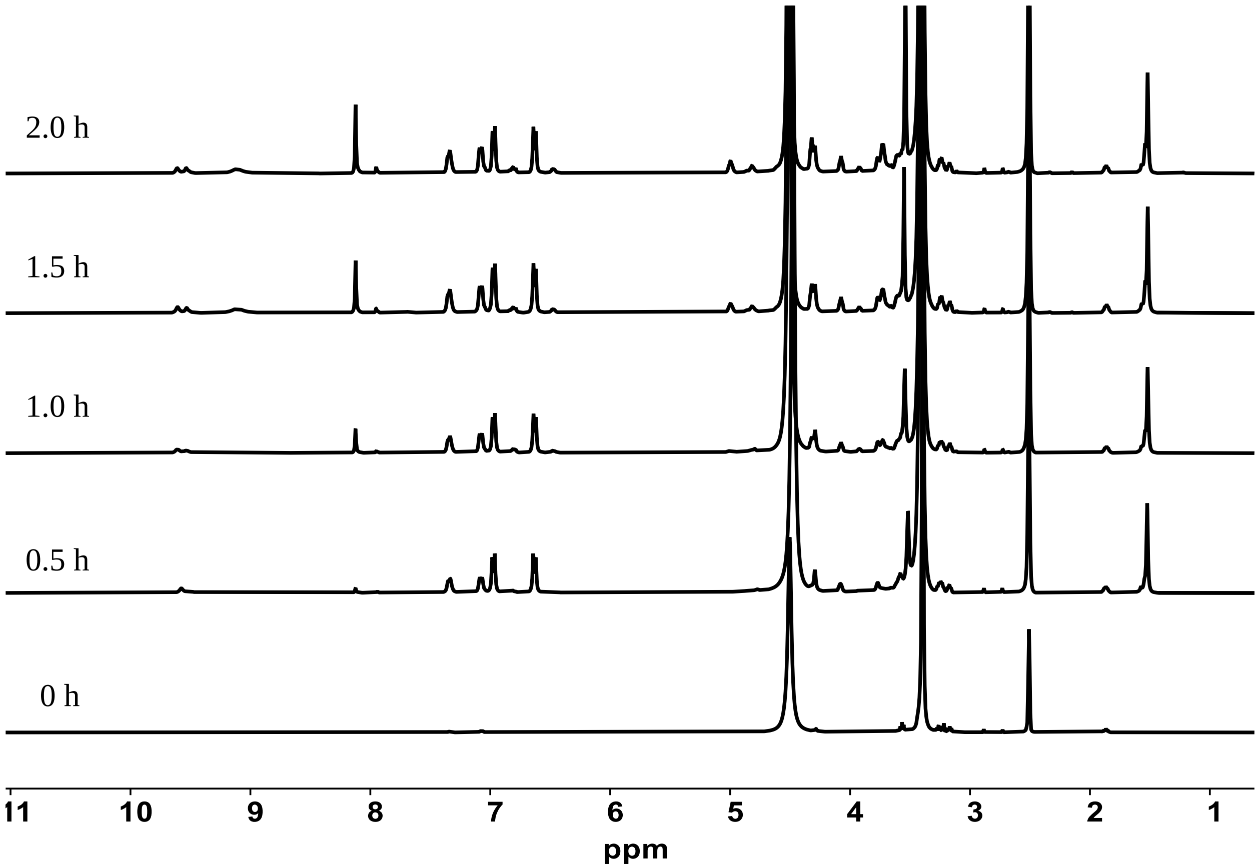


Figure S64. Stacked ^{1}H NMR spectra of the deconstruction of mixed plastic pellets PC (0.33 g, 1.3 mmol), PU (0.41 g, 1.3 mmol), PET (0.25 g, 1.3 mmol), & PA(0.15 g, 1.3 mmol), EG (3.17 g, 52 mmol, 10 eq.), and TBD:TFA (0.07 g, 0.26 mmol, 0.05 eq.), as a catalyst at 160 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

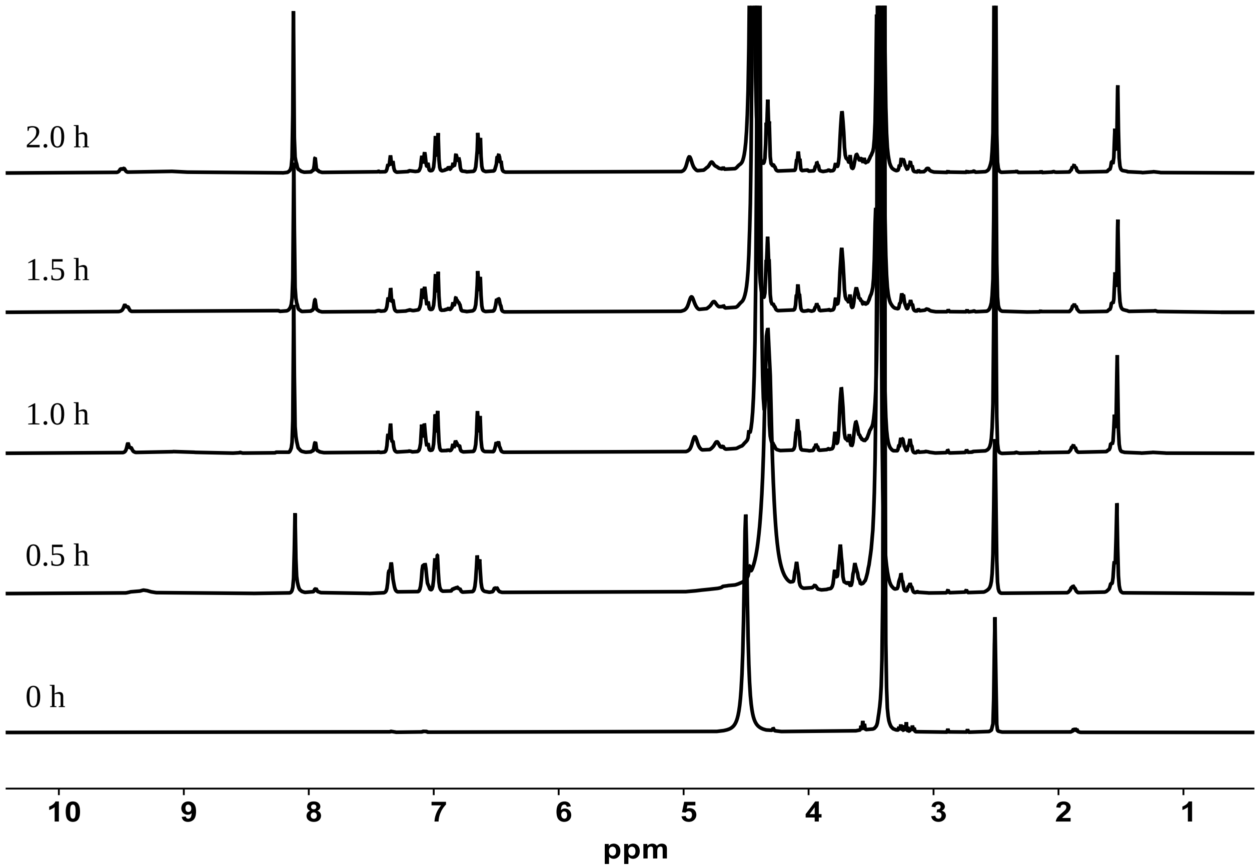


Figure S65. Stacked ^{1}H NMR spectra of the deconstruction of mixed plastic pellets PC (0.33 g, 1.3 mmol), PU (0.41 g, 1.3 mmol), PET (0.25 g, 1.3 mmol), & PA(0.15 g, 1.3 mmol), EG (3.17 g, 52 mmol, 10 eq.), and TBD:TFA (0.07 g, 0.26 mmol, 0.05 eq.), as a catalyst at 180 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

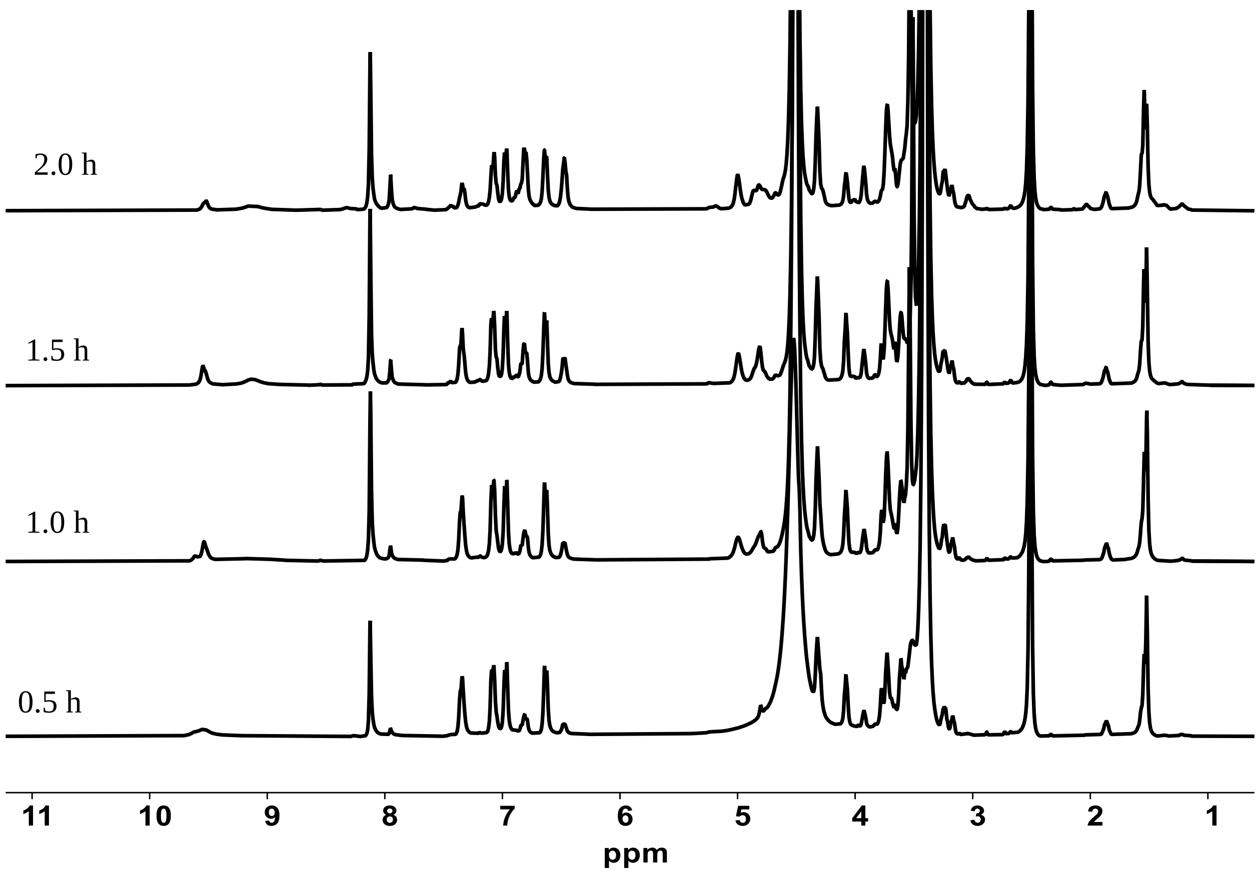


Figure S66. Stacked ^{1}H NMR spectra of the deconstruction of mixed plastic pellets PC (0.33 g, 1.3 mmol), PU (0.41 g, 1.3 mmol), PET (0.25 g, 1.3 mmol), & PA(0.15 g, 1.3 mmol), EG (3.17 g, 52 mmol, 10 eq.), and TBD:TFA (0.07 g, 0.26 mmol, 0.05 eq.), as a catalyst at 210 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

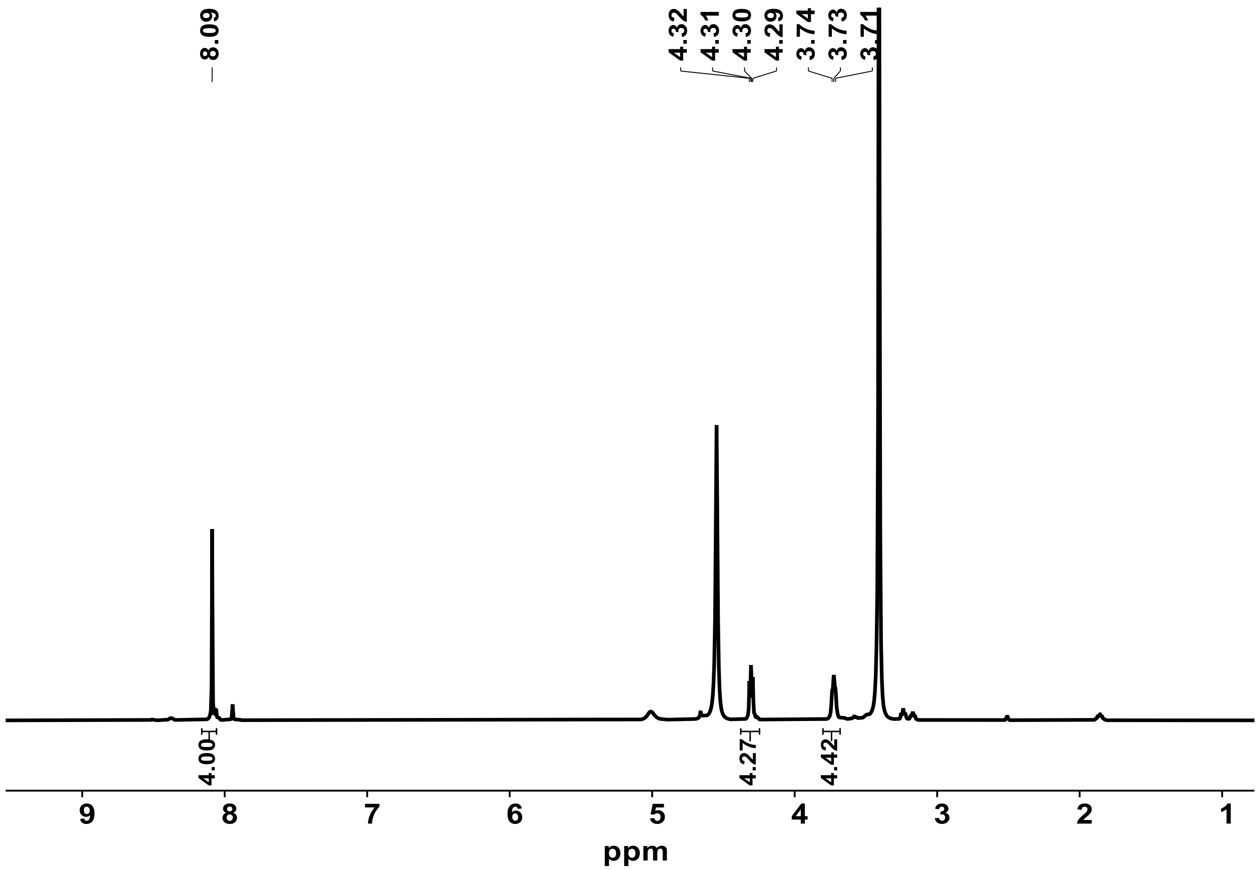


Figure S67. ^{1}H NMR spectrum of the deconstruction of commercial PET bottle (0.5 g, 2.6 mmol, 1 eq.), EG (1.61 g, 26 mmol, 10 eq.), and TBD:TFA (0.035 g, 0.13 mmol, 0.05 eq.), as a catalyst at 180 ºC (DMSO-d6, 400 MHz, 298 K).

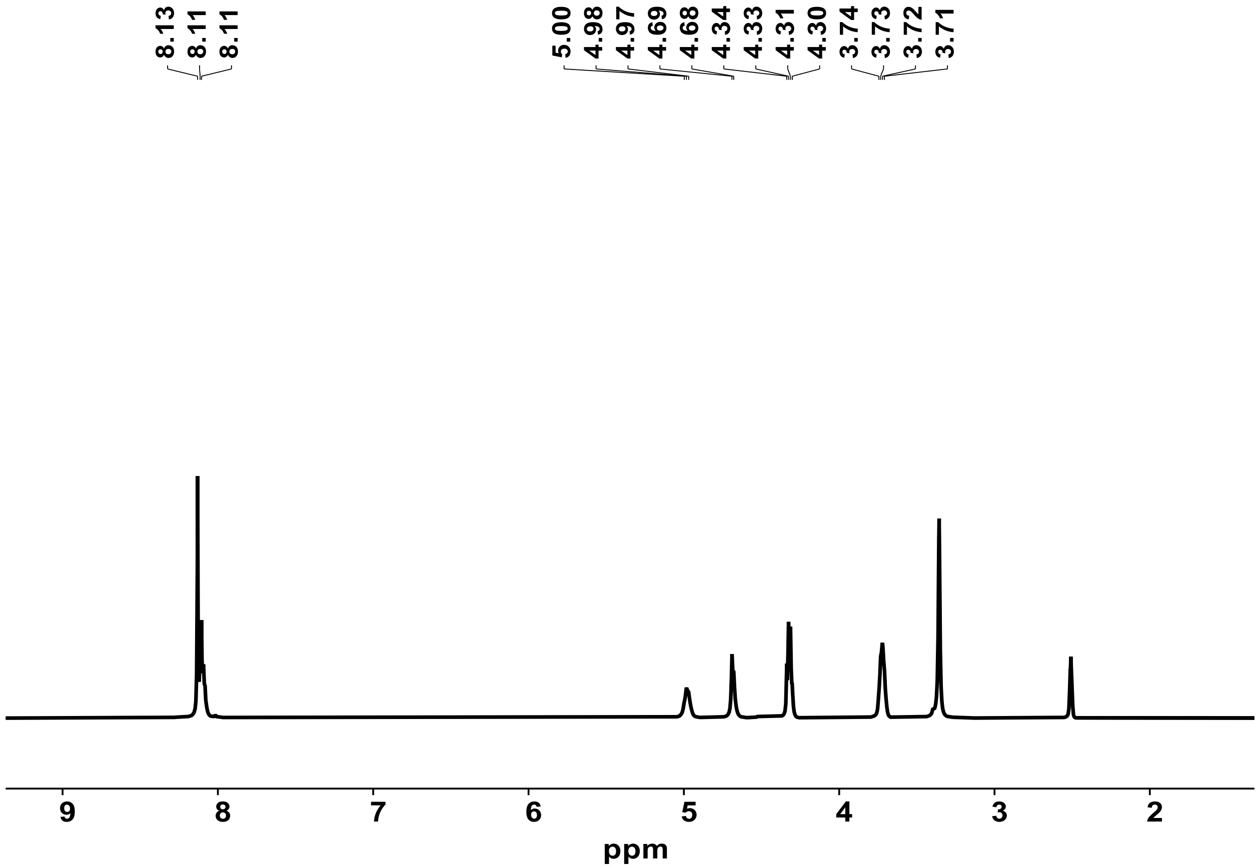


Figure S68. ^{1}H NMR spectrum of the mixture of BHET monomer and dimer from the deconstruction of carpet (0.5 g), EG (1.61 g), and TBD:TFA (0.035 g), as a catalyst at 180 ºC (DMSO-d6, 400 MHz, 298 K).

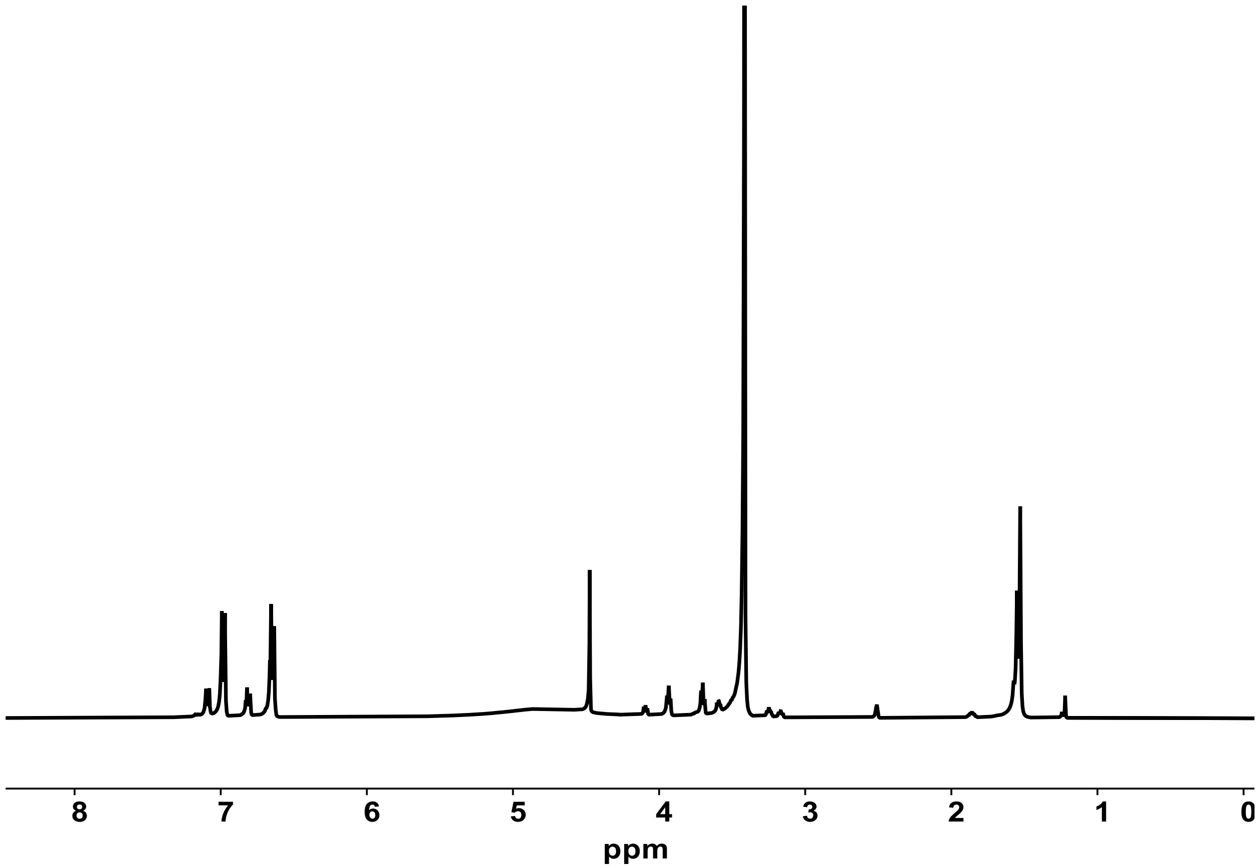


Figure S69. ^{1}H NMR spectrum of the deconstruction of commercial PC (safety goggles) (0.5 g, 2.0 mmol, 1 eq.), EG (1.2 g, 20 mmol, 10 eq.), and TBD:TFA (0.025 g, 0.1 mmol, 0.05 eq.), as a catalyst at 130 ºC for 2 h (DMSO-d6, 400 MHz, 298 K).

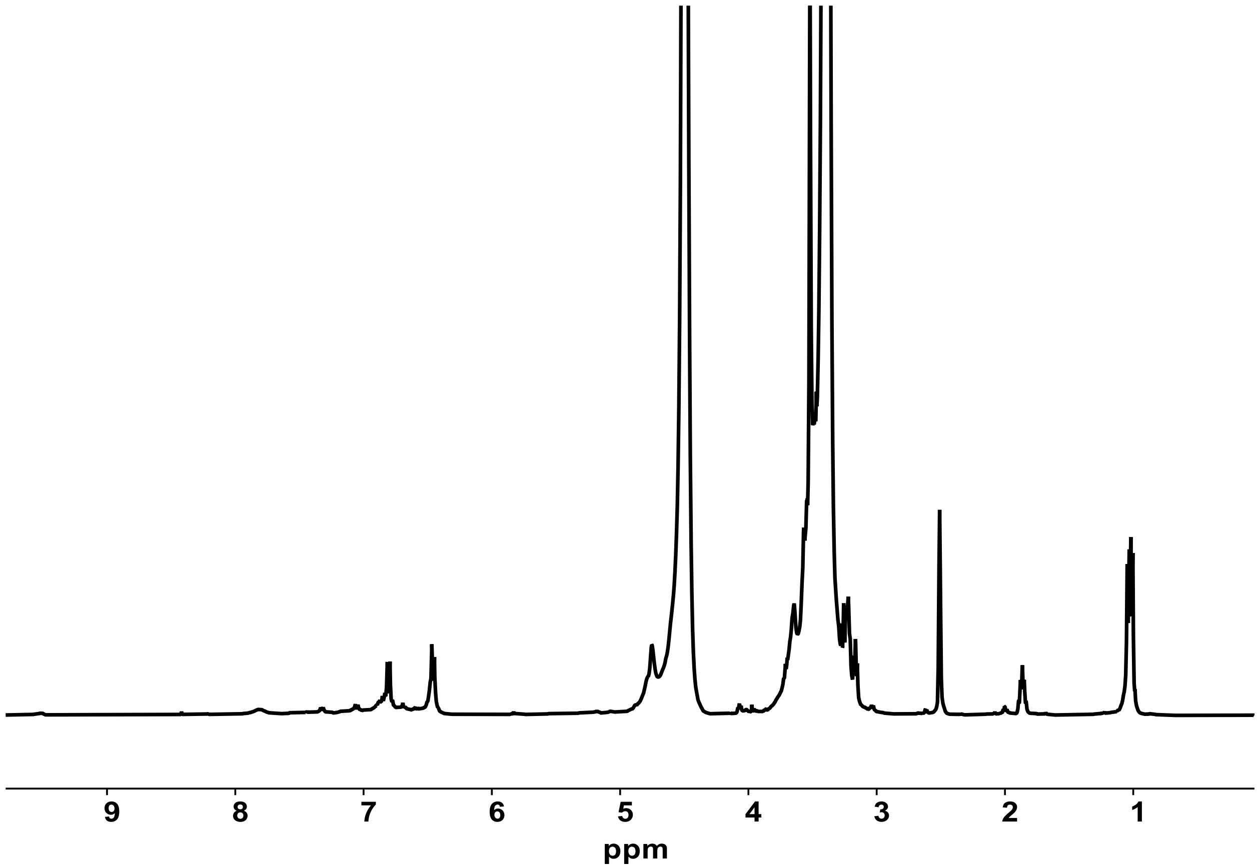
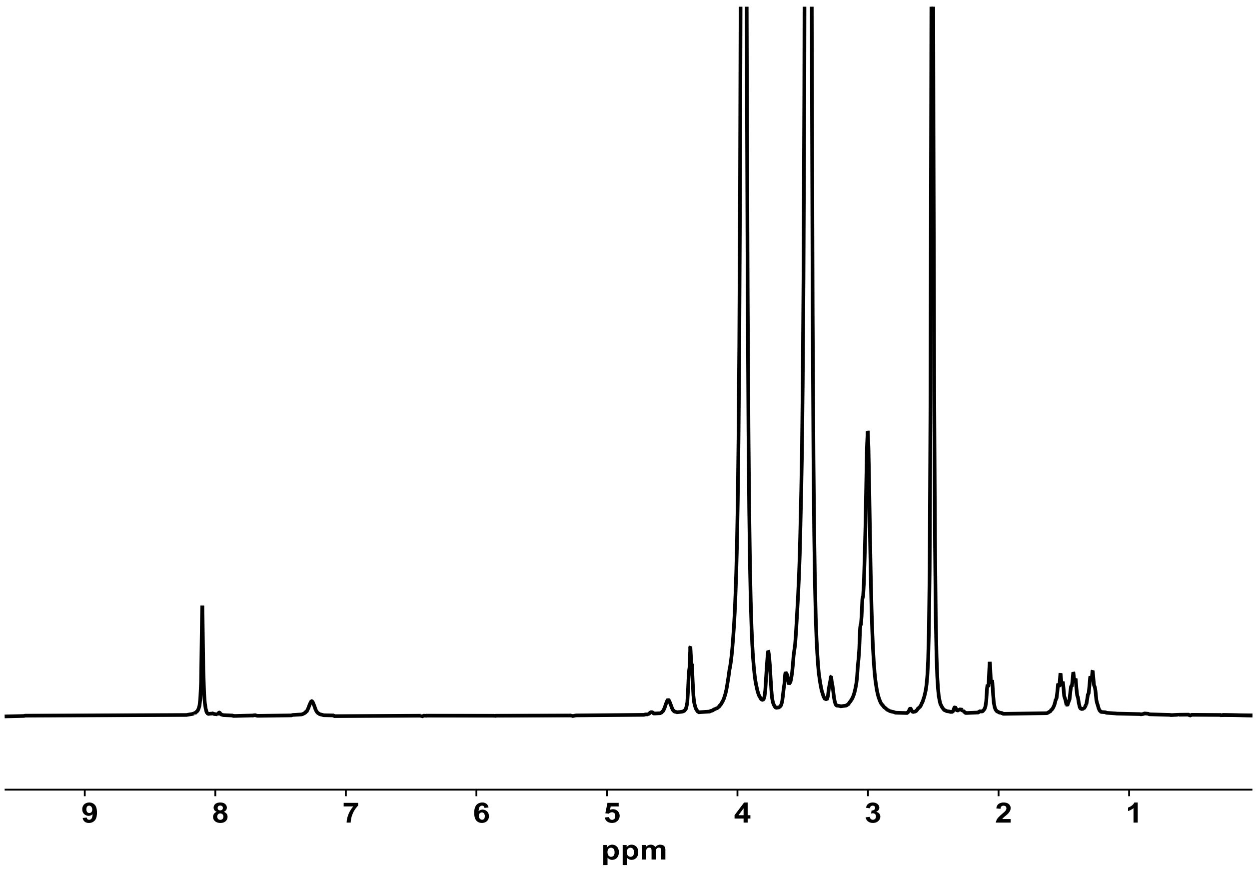


Figure S70. ^{1}H NMR spectrum of the deconstruction of commercial PU (foam) (0.1 g, 0.32 mmol, 1 eq.), EG (0.2 g, 3.2 mmol, 10 eq.), and TBD:TFA (0.004 g, 0.016 mmol, 0.05 eq.), as a catalyst at 170 ºC (DMSO-d6, 400 MHz, 298 K).



Figeure S71. ^{1}H NMR spectrum of the deconstruction of commercial PA (Nylon rope) (0.5 g, 4.4 mmol, 1 eq.), EG (2.73 g, 44 mmol, 10 eq.), and TBD:TFA (0.05 g, 0.22 mmol, 0.05 eq.), as a catalyst at 210 ºC for 3h (DMSO-d6, 400 MHz, 298 K).

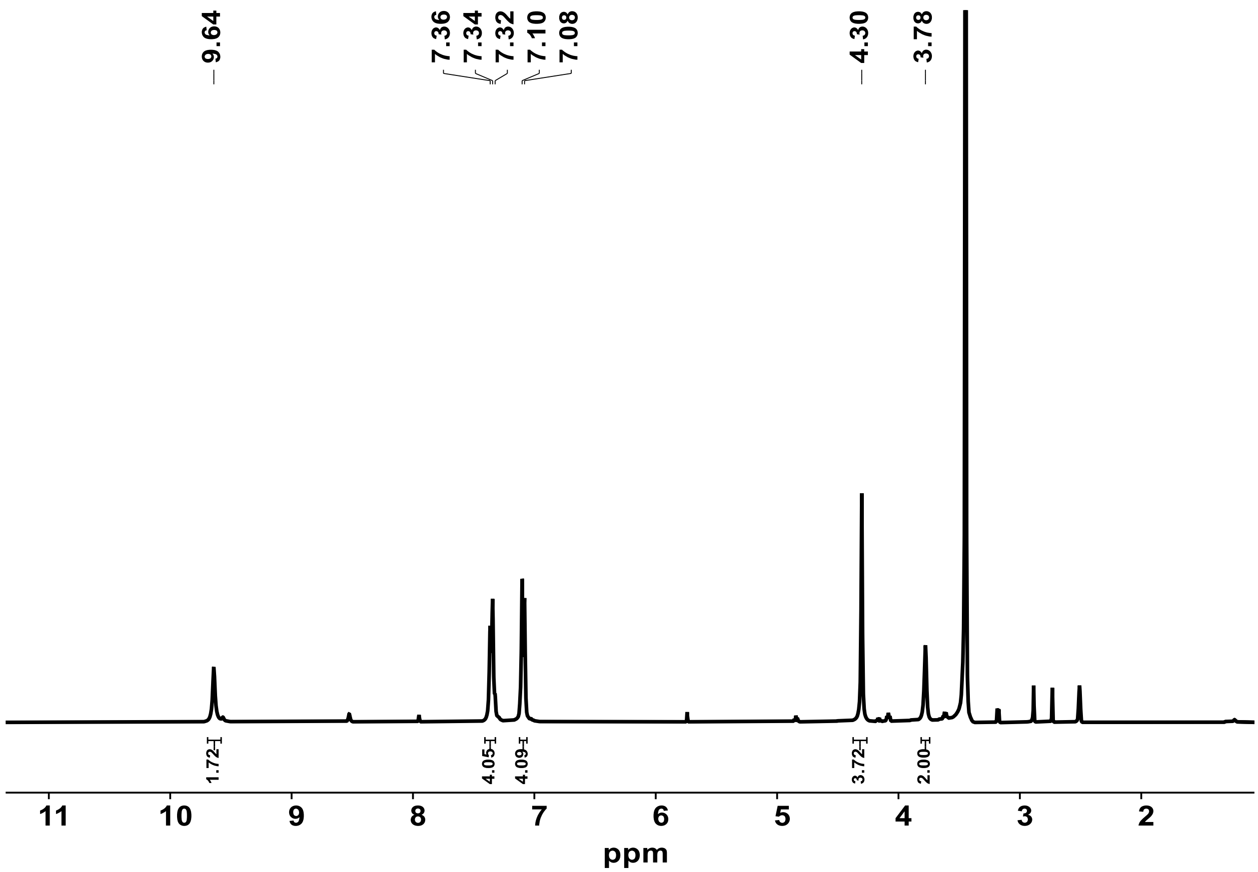


Figure S72. ^{1}H NMR spectra of the formation of PU in DMSO-d6 (400 MHz, 298 K).

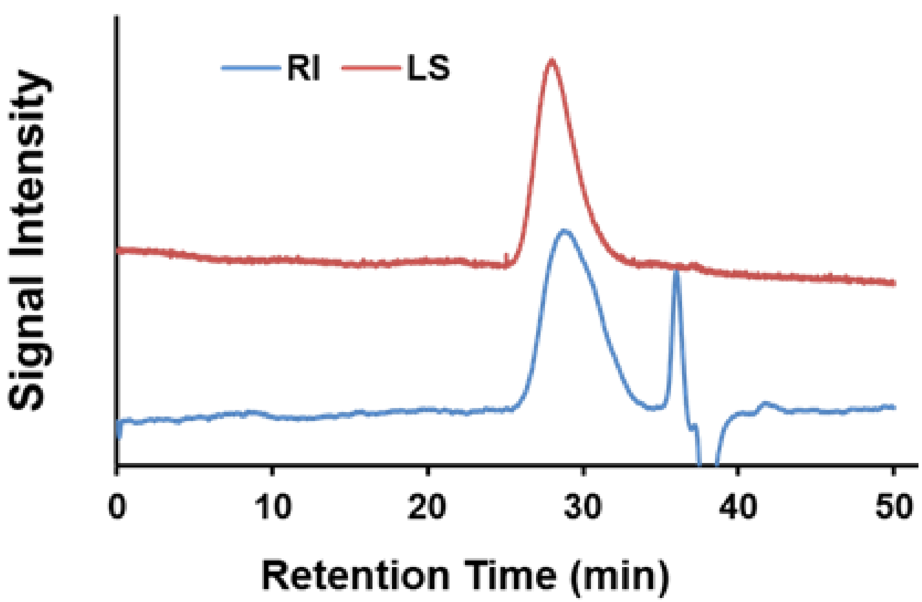


Figure S73. GPC chromatograph for the synthesized PU.

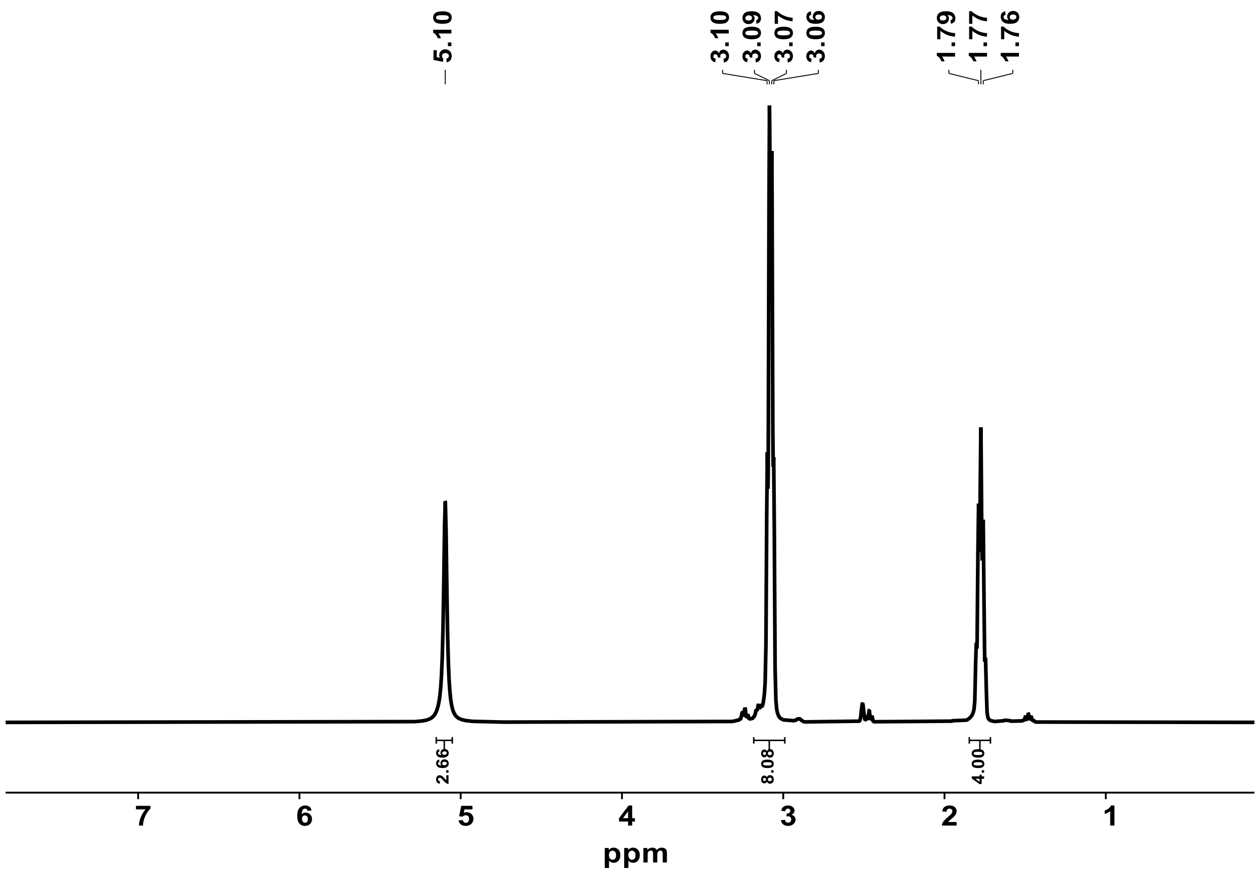


Figure S74. ^{1}H NMR spectrum of TBD:TFA (3:1) in DMSO-d6 (400 MHz, 298 K).

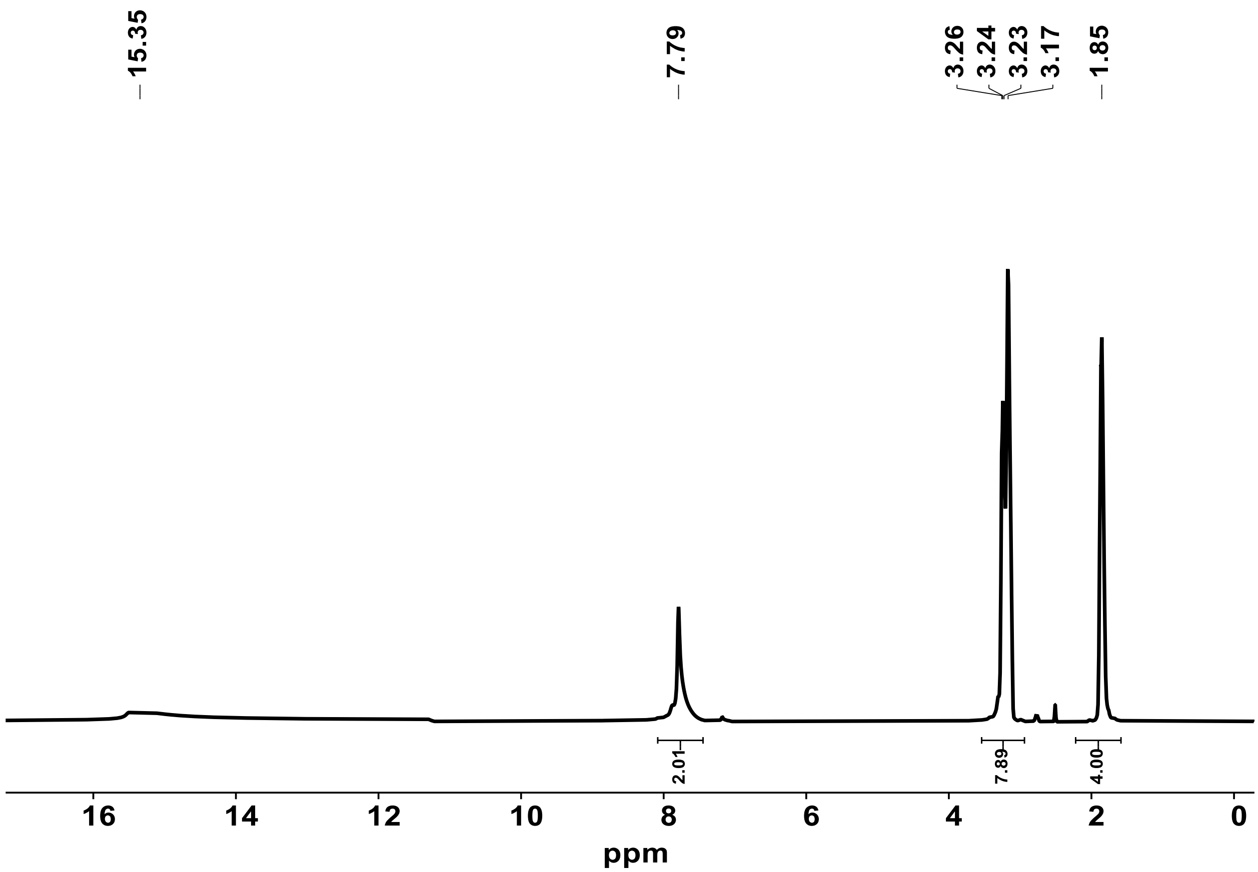


Figure S75. ^{1}H NMR spectrum of TBD:TFA (1:3) in DMSO-d6 (400 MHz, 298 K).

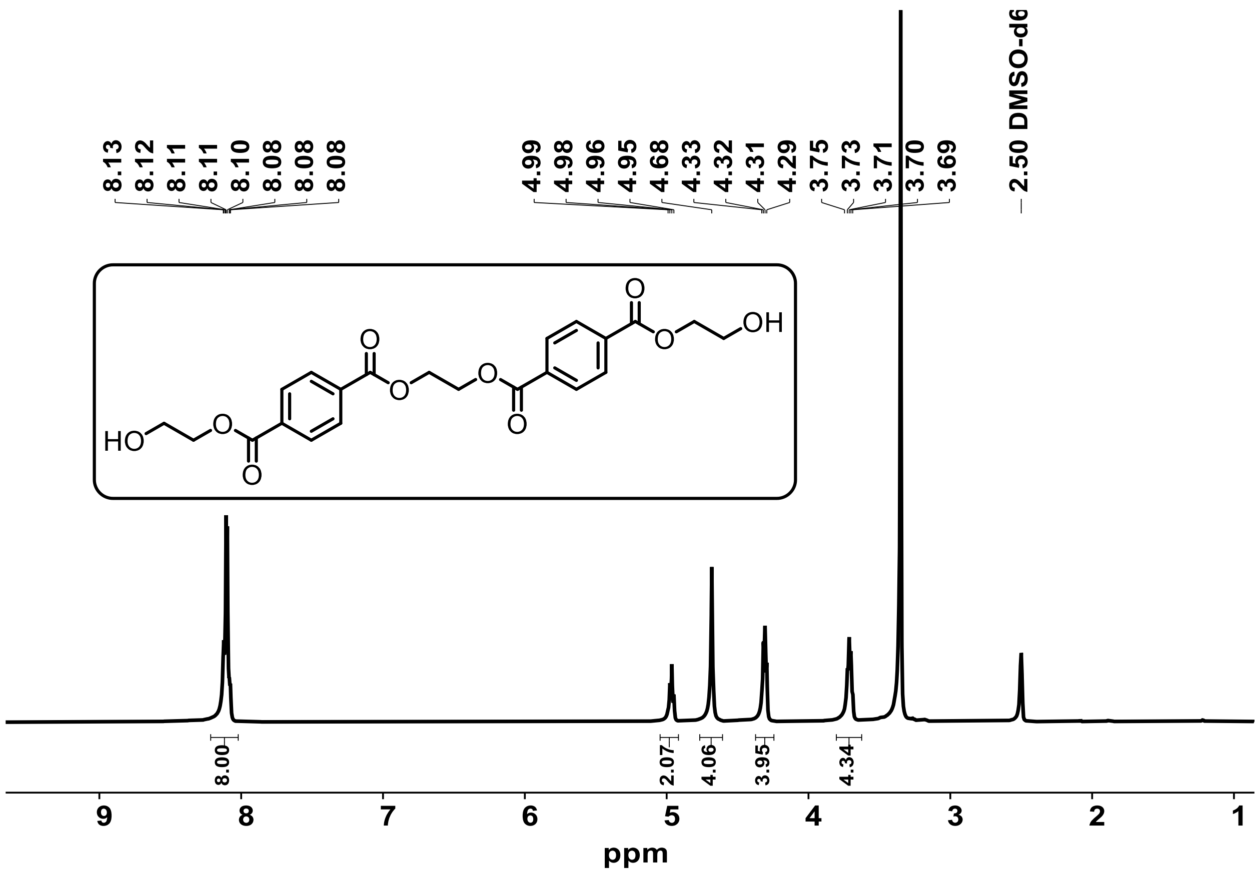


Figure S76. ^{1}H NMR spectra of the BHET dimer (DMSO-d6, 400 MHz, 298 K).

Data S1: XYZ data for TBD:MSA

Element	X	Y	Z
C	4.39750347	-6.55351235	-2.11734284
C	-4.31173590	-13.16660735	-3.61714373
C	1.11032941	1.21209990	-2.98921872
C	-2.06858996	-12.39587131	-3.17998660
C	0.36581947	0.30059390	1.10659147
O	-5.97105524	-16.73086434	-0.88696663
C	-5.82930724	-16.50400946	-3.30812100
O	-0.60166355	-1.00340221	2.86737264
O	0.62328072	0.61783295	-3.91936982
C	1.10251703	1.44705655	0.79219753
C	0.08815252	-0.07936647	2.52632801
C	-2.82976338	-17.46445324	7.22606126
O	-6.50999176	-14.04056279	-3.95617968
C	-1.44270765	-10.00073648	-3.71610462
C	-3.01254731	-13.41850665	-3.16680682
C	-4.67106854	-11.89490438	-4.07456886
C	2.90127858	5.59102994	-4.28304832
C	0.44141991	12.07508331	2.08420813
C	2.91106412	9.11488882	-1.86680250
C	-0.81384054	12.37663272	-0.08476096
C	3.45978470	7.93741654	-1.34967551
C	2.28178457	2.57976347	-4.50270296
O	3.49296940	4.54170707	-3.69792918
O	0.52929846	12.10349797	3.28594489
C	-4.46541719	13.23044956	-0.69551893
O	-5.49499405	13.43980333	-0.10338498
C	0.85814887	0.92359494	-1.55256054
C	1.86216631	1.16644077	5.36941861
O	2.44259630	5.57370990	-5.39989015
O	2.44641402	11.43104946	-1.49970389
C	2.93670564	10.40105141	-1.10736121
O	-6.11578689	18.81861868	4.32431225
C	3.45093517	6.77628947	-2.11697636
C	-5.86668409	16.86019899	0.59048518
C	2.89728851	6.79894106	-3.39975914
O	-4.35394909	13.23169360	-2.04046098
C	-5.78471185	17.65980157	-0.55503712
C	-5.87061610	19.65988722	0.79018315
C	-5.94945623	17.47007359	1.83766007
C	-5.52825267	13.55907397	-2.78608158
C	-5.54179406	15.03486844	-3.10644255
O	-5.66595394	15.71706346	-1.86234238
C	-6.07327458	21.42007094	4.56602514
C	3.47851545	1.72329476	3.73726514

C	6.82594738	0.28228130	1.52376104
O	8.44842349	0.42655486	-0.24095001
H	3.72780729	12.34385583	0.19992065
H	4.76248907	11.37112347	1.30997114
H	2.94044931	12.35287137	2.62701129
H	-5.86505258	15.77311284	0.49454122
H	-5.87197658	20.74440848	0.88772832
H	-6.01252547	16.88187330	2.75325645
H	-0.62729787	-1.45739309	0.39290479
H	-0.22147963	-0.86828252	-2.04075648
H	-5.23542271	-17.42391494	-3.34899069
H	-6.45205227	-16.41456250	-4.20917839
H	-1.05212289	-12.57092690	-2.83125655
H	-7.19442006	-15.52298866	-1.95424135
H	2.39065317	1.66891610	-5.10983798
H	-0.13145950	0.34025238	5.26513858
H	3.87626415	5.85002999	-1.73311780
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H	4.12373945	-7.26035465	-2.89842240
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H	-2.33907199	-17.45047166	8.21810277
H	-3.52459826	-16.44162761	3.22512234
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H	9.75849544	-4.16199712	-0.32872550
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H	10.09753615	-1.72127357	0.03758068
H	0.58011178	-8.91897833	-1.21253921
H	0.72579165	-8.83530429	-4.28636472
C	7.41440175	-4.63049755	-1.00029974
O	-2.51153291	-19.97007043	4.66955616
C	-2.75965603	-18.86180790	4.27277741
C	2.09818567	-6.81851403	-1.13249882
C	9.08129976	-2.13932528	-0.04298173
O	8.20672241	-1.50168530	0.87981466
C	0.68870388	-8.38136482	-2.16687664
C	0.79025182	-9.35866179	-3.32312680
C	5.67303381	-6.01142512	-2.06571827
C	6.01003199	-5.13257811	-1.02985487
C	-3.72590885	-10.87746186	-4.09619833
C	-6.72183097	-16.50251681	-2.08434686
O	-4.88221823	-15.43232347	-3.27106850
C	-2.42505008	-11.12912460	-3.65108816
C	-4.52376227	-17.07832040	1.41726812
O	-3.86952272	-18.41378710	7.16061710
C	-1.80163762	-17.85090000	6.18785134
O	-2.38729363	-17.72402348	4.88940618
O	-1.70254080	-8.90814249	-4.15232030
C	-5.36052924	-14.22764294	-3.63737403

C	2.33546036	7.97235507	-3.91061131
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C	2.34050572	9.13013099	-3.14358709
C	-0.10865767	-0.54477526	0.10132098
C	0.13008397	-0.22758121	-1.23175370
C	1.35062590	1.75650277	-0.54048315
O	3.13523505	0.93516970	4.76706912
C	0.82040413	0.29124513	4.70963953
O	0.65593408	0.78708792	3.38918416
O	-6.00759759	20.80268332	3.28211713
C	-5.78961378	19.05368357	-0.45805655
C	-5.94979985	18.86405753	1.93778396
C	-6.03434387	19.45870185	3.30601828
C	-0.80480941	12.36278535	1.31349263
C	-1.96767710	12.62927918	2.04158705
C	-3.16456028	12.92695836	-0.02819503
C	-2.00002583	12.66189550	-0.75525445
C	3.77143069	11.45758500	0.84665121
C	2.71663407	11.53766850	1.92227249
H	-4.61143069	15.34482780	-3.60508329
C	5.14360423	-0.09079275	3.21255193
O	2.90605346	2.74649204	3.43971762
C	9.07046133	-3.60525898	0.32028936
C	7.90721614	-0.21430832	0.62812259
C	6.21113505	-0.56111511	2.45248903
C	6.37630058	1.59646622	1.34380316
C	5.29945877	2.05810417	2.08849325
O	7.75105636	-4.13485850	0.20534659
C	4.68593487	1.21289851	3.02142309
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H	-5.72604458	19.64051246	-1.37468694
H	-6.42032885	13.27957082	-2.21088466
H	-5.47163866	12.97527263	-3.71326819
H	-6.38821574	15.28723208	-3.76363707
H	1.16686235	-0.75078215	4.64753986
H	1.59989975	2.22961916	5.28172586
H	1.93242146	2.63801997	-0.80616455
H	1.49406920	2.07171637	1.59561035
H	-7.48771560	-17.28264686	-2.19230244
H	3.87247569	3.61003459	-5.51420671
H	-4.07551341	13.11585218	1.90725783
H	0.10531081	12.16679668	-0.63403007
H	1.90947215	7.95087070	-4.91366121
H	1.46814941	3.18380966	-4.93142925
H	4.36574766	2.75277986	-4.00356506
C	-5.68345686	17.05869395	-1.91805520
O	-5.62242804	17.68177458	-2.94830117

O	1.47298336	11.78961364	1.27312402
O	3.60830117	10.27909397	0.05607810
C	-3.14991477	12.90954129	1.37017113
C	3.76636069	-5.26866068	-0.14672164
C	5.06161730	-4.74998499	-0.07646922
O	-0.23652312	-10.35580415	-3.24511989
O	1.91399574	-7.66014695	-2.18725534
C	-3.49950789	-18.58227756	3.00200946
C	-4.56241144	-19.47495091	1.03072726
C	-3.82320304	-17.28292746	2.60224428
C	-5.64835372	-18.01321358	-0.64274725
O	-5.94770346	-18.92584109	-1.37462117
O	1.25713873	-6.66045896	-0.29043209
C	-4.89219638	-18.17546229	0.63394960
O	8.18111822	-4.68249526	-1.93375410
C	-3.86943202	-19.67830282	2.21704983
C	3.45117727	-6.19158231	-1.14878421
H	3.00523086	-4.93389435	0.56452503
H	6.43136006	-6.26741570	-2.80575049
H	1.73518635	-9.91071082	-3.25703142
H	-0.16606118	-7.69905471	-2.28063886
H	9.34330416	-3.73353937	1.37518325
H	-1.47142001	-18.88660530	6.33814872
H	-5.69418324	-11.73022434	-4.41211311
H	-0.94377975	-17.16677017	6.21754938
H	-3.19140412	-16.44384983	7.00750867
H	-4.62830953	-18.06238643	7.64012001
H	-4.86344897	-20.30717843	0.39413723
H	-3.96844987	-9.87771455	-4.45594407
H	-3.60218896	-20.67801555	2.55991623
H	-2.75104395	-14.41300680	-2.80834415
H	5.29266825	-4.03740168	0.71905264
H	-7.00129158	21.13697264	5.08116689
H	6.86721467	2.21923859	0.59590940
H	-5.22016701	21.10854396	5.18445636
H	-6.04491027	22.49856287	4.38153108
H	4.89876136	3.06273049	1.95137713
H	6.51116634	-1.60309923	2.53807856
H	1.97273463	0.88690792	6.42540792
H	-1.91883939	12.60876269	3.13034007
H	1.91887904	10.06376761	-3.51556861
H	-2.03009925	12.67823906	-1.84339966
O	2.48258993	-1.06131884	2.61979680
O	4.19862926	-2.81904148	2.17064584
H	4.25123179	-0.42001837	0.53095701
S	2.97754161	-2.10832486	1.65878901
C	3.53438098	-1.18886661	0.21358654
H	2.65431008	-0.73255381	-0.25499111

O	1.91188746	-3.01781741	1.14990237
H	4.00331925	-1.90589877	-0.47383743

Data S2: XYZ data for TBD:TFA

Element	X	Y	Z
C	4.83800566	-7.59960197	-1.98973634
C	-3.91923179	-14.18217696	-3.59956686
C	0.15933390	2.22983969	-2.40940509
C	-1.62696290	-13.58709934	-3.14963102
C	0.33913140	1.31080252	1.74427349
O	-5.88440638	-17.14977225	-0.75686732
C	-5.69499369	-17.37677181	-3.17159584
O	-0.40653148	0.24134018	3.76690345
O	-0.71579152	1.88625003	-3.15987680
C	1.26108067	2.22374168	1.20898080
C	0.37181523	0.95186387	3.18759639
C	-2.65893349	-16.18877129	7.30405054
O	-6.16365131	-14.90650293	-3.99396335
C	-0.84470658	-11.22138179	-3.58303399
C	-2.64103479	-14.53890243	-3.16087841
C	-4.18786181	-12.87732403	-4.02252132
C	2.25582358	6.21651725	-4.29804569
C	1.08892544	12.48517735	2.10191462
C	3.07467963	9.68595045	-1.94266554
C	-0.20720081	12.84042582	-0.03255009
C	3.51585290	8.44008722	-1.48839928
C	1.19728290	3.30598302	-4.21324250
O	2.79634781	5.09553587	-3.80334249
O	1.19756325	12.44758192	3.30165810
C	-3.89072482	13.60135656	-0.56261678
O	-4.90486764	13.81979025	0.05220713
C	0.23872183	1.92108120	-0.95508861
C	2.87406756	1.78286686	5.65064004
O	1.61460604	6.26818683	-5.31931246
O	2.96429413	12.03647803	-1.53621893
C	3.34020229	10.94489289	-1.18606535
O	-5.67311275	19.50182608	4.16789908
C	3.25548266	7.29926048	-2.24122613
C	-5.37553439	17.32962646	0.56002332
C	2.55435083	7.40929441	-3.44438556
O	-3.81438024	13.56731040	-1.90928954
C	-5.31387755	18.05996975	-0.63161419
C	-5.44929703	20.13448340	0.58993503
C	-5.47440005	18.01150575	1.76790481
C	-5.01421186	13.84281552	-2.63557744

C	-5.05552569	15.29830207	-3.03369566
O	-5.16723849	16.04637810	-1.82585375
C	-5.73371535	22.10916356	4.25399668
C	4.34425236	1.98342154	3.80829691
C	7.03449146	-0.09147008	1.22028831
O	8.52844349	-0.19313032	-0.64550726
H	4.37232972	12.75870962	0.13531759
H	5.37008202	11.66425350	1.16214622
H	3.64959890	12.76404095	2.56788914
H	-5.34649297	16.23960121	0.53012192
H	-5.47910298	21.22203987	0.62115387
H	-5.52459870	17.47855096	2.71681963
H	-1.33204826	-0.02878372	1.32618244
H	-1.42466924	0.50903290	-1.03457986
H	-5.17035092	-18.33519829	-3.09925184
H	-6.28317739	-17.33130371	-4.09875674
H	-0.62511992	-13.84390627	-2.81075324
H	-7.12673944	-16.21556492	-2.04520738
H	1.01625574	2.40644023	-4.82032217
H	0.72890684	1.53724145	5.78941005
H	3.58843917	6.31931291	-1.90412772
H	4.05928140	8.37200834	-0.54802832
H	4.46791209	-8.08500181	-2.89065828
H	-4.73713803	-16.05601411	1.03481760
H	-2.16351158	-15.94418782	8.26258926
H	-3.43121893	-15.92677707	3.16760989
H	5.07662585	-0.65754779	3.94707989
H	10.02831115	-4.64715023	-0.36318897
H	8.64713534	-2.75798180	-1.32447500
H	10.03642788	-2.20019182	-0.36276470
H	1.40167386	-10.61010711	-0.98078866
H	1.33399434	-10.06667925	-4.01279301
C	7.70623463	-5.41433699	-0.93992482
O	-2.12685037	-19.04110064	5.21114598
C	-2.48374055	-18.04734637	4.63409322
C	2.90752039	-8.58985314	-0.68729710
C	9.07457355	-2.73205111	-0.31260541
O	8.18922309	-2.04574358	0.57387558
C	1.38547356	-9.94282838	-1.85313679
C	1.41629693	-10.73450888	-3.14621307
C	5.99352213	-6.82853624	-2.01850066
C	6.44789042	-6.21095725	-0.85062679
C	-3.17579630	-11.92639465	-4.00885497
C	-6.61862006	-17.18332615	-1.98476989
O	-4.66667119	-16.38291187	-3.19744810
C	-1.89631554	-12.28354300	-3.57459129
C	-4.40521283	-16.96103529	1.54035210
O	-3.57724663	-17.25068649	7.43668785

C	-1.60343063	-16.62755190	6.31517991
O	-2.21230705	-16.78909233	5.03108735
O	-1.03329593	-10.08551143	-3.93256098
C	-5.04265991	-15.16399148	-3.62786133
C	2.10563203	8.65412696	-3.89359188
O	1.22054548	2.97000373	-2.83275362
C	2.54494333	3.89434164	-4.54896738
C	2.36712006	9.79281220	-3.14395627
C	-0.62308184	0.70276861	0.93706986
C	-0.67555200	1.01158332	-0.42162808
C	1.20976552	2.52608055	-0.14330235
O	3.94328185	1.24715886	4.86188886
C	1.57464603	1.16525867	5.18990756
O	1.42619670	1.53011391	3.82823206
O	-5.63811274	21.42174225	3.00793561
C	-5.35127212	19.45618948	-0.61886018
C	-5.51062846	19.40806323	1.78316922
C	-5.61530869	20.08144724	3.11225208
C	-0.17522197	12.77937927	1.36393477
C	-1.33281121	12.99050540	2.11737115
C	-2.57066315	13.31846425	0.07640877
C	-1.41142782	13.10957521	-0.67588508
C	4.37134102	11.84827338	0.74783377
C	3.36584788	11.96413371	1.86755983
H	-4.14037260	15.59456206	-3.56688540
C	5.55916186	-0.12975553	3.12689243
O	4.01192299	3.12340809	3.60265045
C	9.27367675	-4.12261427	0.23738531
C	7.98612731	-0.74823738	0.27751538
C	6.43404965	-0.79053602	2.27048899
C	6.75478797	1.26267309	1.01675895
C	5.87697862	1.91952404	1.86791589
O	8.05723237	-4.87419392	0.24319733
C	5.28449685	1.22495368	2.92605835
H	3.28317588	11.02357400	2.43192922
H	-5.30154327	19.98752148	-1.56889879
H	-5.88490913	13.58466978	-2.01992341
H	-4.97897335	13.21129115	-3.53140967
H	-5.91809247	15.50328011	-3.68575038
H	1.59798905	0.06914972	5.28066017
H	2.85472110	2.87402334	5.54270764
H	1.91438273	3.23025363	-0.58244969
H	2.00680054	2.68708445	1.85501124
H	-7.35235787	-18.00078055	-1.95863270
H	2.60416435	4.11340105	-5.62278572
H	-3.45422925	13.42585476	2.02881515
H	0.70827412	12.67750167	-0.60250017
H	1.55636510	8.70059501	-4.83333080

H	0.38585789	4.01964146	-4.42108777
H	3.34383190	3.20661109	-4.24940795
C	-5.20747907	17.38167388	-1.95769647
O	-5.16476536	17.94579797	-3.02251023
O	2.11340011	12.26684461	1.26023890
O	4.07017335	10.71853912	-0.07361743
C	-2.53211840	13.26114455	1.47280807
C	4.58870160	-7.12512383	0.37724677
C	5.74307738	-6.35183241	0.34840871
O	0.34874619	-11.68610799	-3.15891719
O	2.56278310	-9.13299961	-1.87119497
C	-3.26278952	-18.06452614	3.35579106
C	-4.28931923	-19.38410387	1.61896892
C	-3.67927896	-16.88949831	2.72515197
C	-5.48034435	-18.34032250	-0.28180211
O	-5.72167194	-19.39155692	-0.82515716
O	2.29583054	-8.77790199	0.33167840
C	-4.70918053	-18.20875092	0.98958289
O	8.35340080	-5.27488766	-1.94938064
C	-3.56862686	-19.31153624	2.80356209
C	4.14128126	-7.75223239	-0.78777569
H	4.01315511	-7.25671303	1.29277448
H	6.56261889	-6.68956227	-2.93692093
H	2.33970063	-11.32214095	-3.20678816
H	0.49388586	-9.30196228	-1.79629177
H	9.58506056	-4.07574535	1.28747760
H	-1.15278714	-17.57765756	6.62771163
H	-5.19622198	-12.63139583	-4.35360292
H	-0.83183087	-15.85512666	6.20323430
H	-3.14422065	-15.27233698	6.92368166
H	-4.36341328	-16.91468924	7.88307370
H	-4.54105770	-20.34005848	1.16077891
H	-3.35149173	-10.89909766	-4.32670956
H	-3.22910131	-20.20696857	3.32288825
H	-2.45251255	-15.55841224	-2.82961189
H	6.10410767	-5.85374639	1.24622364
H	-6.65499402	21.82348155	4.77870589
H	7.23382772	1.77489202	0.18308073
H	-4.87578456	21.86253945	4.89343132
H	-5.74110389	23.17522096	4.00844861
H	5.63030669	2.97201281	1.73364222
H	6.65093378	-1.84892082	2.40357437
H	3.08538973	1.50448643	6.69035207
H	-1.26755597	12.93338090	3.20348043
H	2.03632782	10.77834132	-3.46977753
H	-1.45975604	13.15711068	-1.76198857
O	-3.42179173	-3.19082424	-0.48181880
F	-0.87058737	-3.89720557	-0.69701555

C	-2.64799501	-2.24857925	-0.31128494
C	-1.12483400	-2.60818179	-0.40904004
F	-0.46550465	-2.34547975	0.74946157
O	-2.82945140	-1.03608738	-0.06726307
F	-0.48683376	-1.87813280	-1.35983552

Data S3: XYZ data for step 2.

Element	X	Y	Z
C	5.89949750	-8.89563434	-1.41976889
C	-3.37347497	-14.41710743	-3.91862182
C	1.08015232	2.44687087	-2.94598448
C	-1.05700462	-14.10132363	-3.33446775
C	1.11273056	1.57645116	1.22364342
O	-5.68222107	-17.48336801	-1.53738364
C	-5.44550551	-17.46378944	-3.96148068
O	0.13069498	0.78225551	3.27109362
O	0.15403469	2.17863727	-3.66627959
C	2.26924872	2.10494277	0.63718674
C	1.09940529	1.21508819	2.66177705
C	-2.67968027	-17.82516377	6.69112558
O	-5.66286607	-14.86334133	-4.44147197
C	-0.03611346	-11.79426724	-3.47406346
C	-2.15195396	-14.94376152	-3.48974311
C	-3.50010277	-13.05412485	-4.20311541
C	3.33358180	6.18780043	-4.82203798
C	2.16035906	12.12881681	1.63820576
C	4.16243983	9.67063469	-2.50496100
C	0.79627313	12.57876478	-0.43375960
C	4.68188554	8.44155042	-2.08996081
C	2.24488773	3.32791351	-4.77136241
O	3.88590452	5.06167036	-4.33200995
O	2.29801693	11.96728326	2.82428947
C	-2.92933982	13.19228238	-0.82995549
O	-3.92311521	13.37953526	-0.17406894
C	1.11195027	2.17492015	-1.47556140
C	3.80277969	1.40461653	5.03874432
O	2.66496579	6.21359554	-5.82623484
O	3.97620557	12.01172119	-2.07639796
C	4.41205748	10.93621935	-1.74830461
O	-4.29579561	18.99307530	4.12695634
C	4.42342347	7.29447467	-2.83218788
C	-4.22996481	16.91367945	0.45139797
C	3.64569982	7.38359389	-3.98819428

O	-2.89564832	13.20042694	-2.17838844
C	-4.14433652	17.67397739	-0.71910689
C	-4.10052337	19.71368731	0.56480433
C	-4.25258574	17.56190010	1.68047339
C	-4.11473023	13.51335739	-2.85918359
C	-4.13792100	14.98180976	-3.21137794
O	-4.17382915	15.69361527	-1.97650317
C	-4.17022940	21.59154772	4.28635570
C	5.31739787	1.14813833	3.23666116
C	8.16053649	-1.37947576	1.29937659
O	9.80186522	-1.81543743	-0.38513200
H	5.36593834	12.77960478	-0.40380299
H	6.47044595	11.72454381	0.55141310
H	4.71842833	12.64470810	2.05723480
H	-4.27947633	15.82596971	0.39240457
H	-4.05008574	20.79896418	0.62896619
H	-4.31938746	17.00264121	2.61328343
H	-0.94574247	0.98462060	0.95265837
H	-0.93375238	1.51778345	-1.50292100
H	-5.00667663	-18.46549511	-4.00659671
H	-5.99621607	-17.25073608	-4.88787097
H	-0.09526504	-14.49109275	-3.00915701
H	-6.83849418	-16.34578931	-2.74122976
H	2.05219219	2.42517452	-5.36958376
H	1.65698048	1.60384612	5.22504006
H	4.81769807	6.32857240	-2.52346305
H	5.28626782	8.39238565	-1.18574183
H	5.62135344	-9.45198174	-2.31341045
H	-4.58322148	-16.68624305	0.42694460
H	-2.20219876	-17.74704113	7.68596927
H	-3.33090666	-16.88441873	2.59286125
H	6.00435328	-1.41943445	3.93545074
H	11.08387370	-6.21344208	0.70469023
H	10.00122306	-4.37116453	-0.62947982
H	11.26804054	-3.78251490	0.47314498
H	2.11713247	-11.55683862	-0.78391440
H	2.30389287	-10.87432435	-3.78595002
C	8.80257206	-6.87726506	-0.14328395
O	-2.12083833	-20.28419259	4.19079437
C	-2.46025217	-19.21197391	3.76393318
C	3.66771239	-9.48784392	-0.38828009
C	10.27765558	-4.25573462	0.42617957
O	9.32055742	-3.42812753	1.09653408
C	2.21978687	-10.85568304	-1.62380216
C	2.25174445	-11.58766750	-2.95288939
C	7.13149054	-8.25938485	-1.33067075
C	7.46680325	-7.54891684	-0.17546757
C	-2.40617407	-12.21238379	-4.04610746

C	-6.38622268	-17.34262614	-2.77627826
O	-4.33105804	-16.57130078	-3.83828061
C	-1.18474360	-12.73889058	-3.61549631
C	-4.28068031	-17.65787547	0.81272310
O	-3.59837691	-18.89181007	6.62402824
C	-1.60406119	-18.08439490	5.65761813
O	-2.18983017	-18.03072461	4.35415398
O	-0.10083441	-10.60804766	-3.67706903
C	-4.58363672	-15.27670726	-4.09497999
C	3.12285160	8.61033929	-4.40011268
O	2.21908185	3.01120640	-3.37780112
C	3.61451897	3.87094230	-5.08113824
C	3.38231331	9.75499809	-3.66069205
C	-0.04822902	1.37207311	0.47119512
C	-0.04747528	1.66605245	-0.88584414
C	2.26169110	2.41246475	-0.71785232
O	4.74879538	0.59626530	4.33185918
C	2.39379540	1.04172706	4.62828565
O	2.27573622	1.39918015	3.24915254
O	-4.15019622	20.93682331	3.01841610
C	-4.07875827	19.06892750	-0.66471431
C	-4.18879823	18.95639568	1.73682571
C	-4.21846269	19.59536283	3.08472030
C	0.86363397	12.39730083	0.95097175
C	-0.28754379	12.47250614	1.73980627
C	-1.58613278	12.90528425	-0.24223830
C	-0.43467482	12.82822627	-1.02962027
C	5.44675884	11.85203568	0.17874251
C	4.47105995	11.85696387	1.32978185
H	-3.24041862	15.27448785	-3.77645217
C	6.54376947	-1.05994060	3.06095731
O	5.06667414	2.25722087	2.83659221
C	10.29290458	-5.58445405	1.13523678
C	9.17575323	-2.20146052	0.56857175
C	7.47251039	-1.86893480	2.41314443
C	7.92302708	-0.08532976	0.82933231
C	6.98904048	0.71921834	1.46893660
O	9.03193415	-6.25432286	1.02883977
C	6.30065303	0.23189781	2.58559107
H	4.47608782	10.89305316	1.86236590
H	-4.01224341	19.62699704	-1.59823178
H	-4.96995303	13.24894825	-2.22369243
H	-4.12034341	12.90593815	-3.77234501
H	-5.02297530	15.23034491	-3.81745604
H	2.19575151	-0.03440549	4.74066799
H	4.00270128	2.46395278	4.83892810
H	3.14089258	2.83231515	-1.20327359
H	3.16130651	2.26380642	1.24408186

H	-7.16471759	-18.11386441	-2.85267479
H	3.69376682	4.07630400	-6.15574319
H	-2.43102533	12.80108364	1.72830560
H	1.70497793	12.52586674	-1.03351068
H	2.51336578	8.63383611	-5.30136145
H	1.45568004	4.05931371	-4.99269917
H	4.38669672	3.15944893	-4.77237810
C	-4.11582869	17.03289222	-2.06555299
O	-4.05264863	17.62487495	-3.11415663
O	3.18500978	12.08775411	0.76581098
O	5.19526259	10.72929887	-0.67099673
C	-1.51434057	12.73069397	1.14321698
C	5.33810735	-8.10560811	0.80645224
C	6.57319593	-7.47387808	0.89682975
O	1.09486938	-12.41698711	-3.08366630
O	3.47467068	-10.17576280	-1.52852450
C	-3.20947345	-19.03025216	2.48080261
C	-4.21543097	-20.06969955	0.55303534
C	-3.58554940	-17.76834051	2.01186083
C	-5.33910985	-18.74225571	-1.20707757
O	-5.60780398	-19.70476097	-1.88463744
O	2.85197659	-9.43341575	0.49683629
C	-4.59562050	-18.80865044	0.08554894
O	9.58766512	-6.88875790	-1.05763772
C	-3.52535018	-20.17953777	1.75263928
C	5.00324548	-8.81667210	-0.34956202
H	4.61382267	-8.06495825	1.62011940
H	7.85346607	-8.30217662	-2.14539608
H	3.10740243	-12.27184473	-2.98837702
H	1.39652386	-10.12776639	-1.59214147
H	10.45698563	-5.44987892	2.21056243
H	-1.13754388	-19.06731245	5.80726426
H	-4.46497319	-12.67776859	-4.54301381
H	-0.84075706	-17.29630113	5.69047294
H	-3.15836549	-16.85486326	6.46038946
H	-4.37072050	-18.65470468	7.15362201
H	-4.47104870	-20.94848472	-0.03776294
H	-2.46961143	-11.14567220	-4.26024524
H	-3.21910696	-21.14687104	2.14873286
H	-2.07365759	-16.00751438	-3.27374355
H	6.85907700	-6.91880589	1.78913567
H	-5.09951817	21.35704221	4.81921356
H	8.48501636	0.26475155	-0.03684075
H	-3.31920305	21.26269920	4.89614477
H	-4.10255430	22.66325737	4.07593101
H	6.77835090	1.73105780	1.12287075
H	7.67362076	-2.87995076	2.76136519
H	3.94652583	1.18510051	6.10367306

H	-0.19476725	12.32802882	2.81588465
H	2.99112690	10.72611897	-3.96059225
H	-0.50819018	12.97071958	-2.10556184
H	-4.85349692	1.47322886	1.15967555
H	-5.98847991	2.29156462	2.23146663
H	-6.30344044	-0.26233995	2.11308158
C	-5.16006465	1.58004192	2.21144334
H	-4.88456218	-2.35548409	1.67910715
C	-5.55471441	0.22686832	2.75680534
H	-3.62271982	3.05605199	2.54177713
C	-4.65715427	-2.09082275	2.72504125
C	-3.98677141	2.13067508	2.99911886
N	-4.38554362	-0.66100660	2.79938989
H	-5.56481387	-2.27099091	3.31964513
H	-2.20456288	-2.68723067	1.52987074
H	-5.98481823	0.30443401	3.77261131
C	-3.13806941	-0.17404029	2.85229313
N	-2.91183396	1.13630623	2.97386561
H	-4.26813952	2.34901842	4.04252114
H	-1.93894072	1.42750665	3.02132253
N	-2.07902328	-1.00252897	2.79597697
C	-2.20720336	-2.43781976	2.60455631
C	-3.49493831	-2.90889051	3.26026455
H	-3.66141541	-3.97323929	3.05437616
H	-1.16400003	-0.56617692	2.89503193
H	-1.33398476	-2.92012877	3.06121484
H	-3.42003057	-2.77330621	4.34989694
H	-7.13261161	1.78651959	-2.51205160
O	-7.35125535	0.89521721	-2.18839030
H	-6.70571618	3.95351139	-1.10899799
O	-7.52638840	3.41725257	-1.28686614
O	-5.18645016	4.50976043	-0.85543970
C	-8.13641648	1.17545852	-1.05211048
H	-9.18503142	1.39137238	-1.32944349
F	-2.63543764	3.49941375	0.41072405
C	-7.55342153	2.38067244	-0.34155284
F	-2.72963494	5.51563499	-0.39415611
H	-6.52919346	2.13618390	-0.01434817
C	-4.81926289	4.48449234	0.33578726
C	-3.28652076	4.70514797	0.50822062
H	-8.13051450	0.27773122	-0.40777886
H	-8.14909785	2.64634844	0.55688471
O	-5.43568142	4.26203012	1.39161285
F	-2.96452719	5.18081924	1.73302304

Data S4: XYZ data for step 3.

Element	X	Y	Z
C	5.43498023	-8.94399758	-1.67437902
C	-3.75713099	-14.69281603	-4.12948830
C	0.54251096	2.14472975	-2.96737870
C	-1.44617095	-14.32397750	-3.53826725
C	0.61869704	1.91050194	1.30632381
O	-5.95238105	-17.84945460	-1.65079879
C	-5.73651223	-17.80276495	-4.07525367
O	-0.54320078	1.47526799	3.39403886
O	-0.38307967	1.74724247	-3.63424263
C	1.77301027	2.33024479	0.63338253
C	0.57319190	1.74615613	2.81755631
C	-2.96560724	-17.97051691	6.60797241
O	-6.03220657	-15.21822415	-4.65637395
C	-0.46896685	-11.99662680	-3.66877135
C	-2.52568927	-15.18927837	-3.69301884
C	-3.90693586	-13.33484859	-4.42519162
C	2.45368003	5.97139697	-5.13375842
C	1.20683326	11.99759122	1.21446519
C	3.28866276	9.52678034	-2.91399143
C	-0.17421154	12.41001148	-0.85094290
C	3.80720827	8.30796716	-2.46872240
C	1.51811967	3.02475872	-4.90764705
O	3.06795827	4.88225258	-4.63723649
O	1.34730661	11.81746252	2.39945740
C	-3.91900041	12.84817978	-1.26923616
O	-4.94157019	12.94725654	-0.63509056
C	0.61675646	2.06438476	-1.48109160
C	3.11651936	0.99049548	5.01492850
O	1.74134083	5.95110240	-6.10921184
O	3.10021086	11.87681194	-2.51795703
C	3.52211506	10.80090713	-2.17023677
O	-5.39290026	18.76504713	3.66544804
C	3.53932395	7.14259926	-3.18123296
C	-5.33870646	16.64223093	0.00756062
C	2.76777802	7.20135844	-4.34440232
O	-3.86422763	12.91348576	-2.61618983
C	-5.24007462	17.38834003	-1.17129607
C	-5.20638351	19.44301588	0.09239786
C	-5.36794682	17.30406569	1.23100666
C	-5.07525012	13.20917081	-3.31137009
C	-5.12721978	14.67838622	-3.64495087
O	-5.22978940	15.38602614	-2.41084376
C	-5.29149013	21.37590717	3.78242301

C	4.68177105	1.01388094	3.22311053
C	7.54153054	-1.33223828	1.07327010
O	9.07203848	-1.72933896	-0.72641244
H	4.44908975	12.65932662	-0.81542564
H	5.52251176	11.60573701	0.17994526
H	3.77581545	12.53078303	1.63935960
H	-5.38554097	15.55400353	-0.05050278
H	-5.15444549	20.52913980	0.15111055
H	-5.43945467	16.76041959	2.17292403
H	-1.42447798	1.32095150	1.13965103
H	-1.41166407	1.37136966	-1.38763914
H	-5.26230802	-18.79012803	-4.10853197
H	-6.31217265	-17.62445062	-4.99288853
H	-0.48077343	-14.69231120	-3.19582546
H	-7.12323561	-16.70699026	-2.83438959
H	1.35221108	2.08599168	-5.45802155
H	0.94167388	0.84053648	5.07567927
H	3.91053215	6.17948612	-2.83766329
H	4.39356636	8.27983509	-1.55185170
H	5.15832032	-9.51355936	-2.56097413
H	-4.93452837	-17.02997495	0.32452727
H	-2.44892296	-17.81158082	7.57332161
H	-3.62677645	-17.17193022	2.46508716
H	5.54686625	-1.50400006	3.83235327
H	10.56008485	-6.08901901	0.37737116
H	9.38904458	-4.27485221	-0.95532568
H	10.67130606	-3.66128024	0.11055562
H	1.68546272	-11.65898306	-0.96270958
H	1.86304598	-11.06704371	-3.97594598
C	8.31386726	-6.86745941	-0.42654548
O	-2.15322130	-20.48088561	4.00332675
C	-2.62422779	-19.44119983	3.61613637
C	3.21011530	-9.54968645	-0.63688090
C	9.68557202	-4.15219066	0.09399210
O	8.73338019	-3.34956634	0.79448417
C	1.78465784	-10.97977765	-1.82137481
C	1.81441869	-11.75637478	-3.12320606
C	6.66146787	-8.29394271	-1.59667493
C	6.99750926	-7.57432218	-0.44637249
C	-2.82972896	-12.47007800	-4.26846928
C	-6.66467300	-17.70111696	-2.88246492
O	-4.65684889	-16.86665591	-3.98396966
C	-1.59962468	-12.96367975	-3.82200983
C	-4.58218726	-17.98838280	0.70442750
O	-3.85760971	-19.05894996	6.64516768
C	-1.92065430	-18.27193467	5.56470073
O	-2.53605751	-18.26690880	4.27203797
O	-0.54688308	-10.81488390	-3.90004089

C	-4.94010546	-15.59139847	-4.30032965
C	2.26153483	8.42323163	-4.79683625
O	1.60589114	2.77631529	-3.50475285
C	2.82152362	3.65279551	-5.32581451
C	2.52337065	9.58500027	-4.08246312
C	-0.52509057	1.58862093	0.58363998
C	-0.52999320	1.64082039	-0.80471394
C	1.76318966	2.41918862	-0.75622128
O	4.18044857	0.36013824	4.28825261
C	1.79386887	0.49995412	4.46415287
O	1.65412901	0.90563735	3.12180230
O	-5.27239393	20.69533331	2.52970793
C	-5.17687419	18.78389599	-1.13130006
C	-5.30097083	18.69869420	1.27286958
C	-5.32877369	19.35506261	2.61365816
C	-0.10221742	12.22898105	0.53370555
C	-1.26020236	12.24493227	1.31685703
C	-2.57198072	12.62191866	-0.66966175
C	-1.41451315	12.60337936	-1.45242946
C	4.51086118	11.73665850	-0.22630607
C	3.51590026	11.75009058	0.90716402
H	-4.21602217	14.99529917	-4.17252501
C	6.03435620	-1.10376623	2.94439899
O	4.38275995	2.13609621	2.89275563
C	9.75471844	-5.47921262	0.80614588
C	8.51796051	-2.12644841	0.26871872
C	6.95431775	-1.86107591	2.22601357
C	7.20995202	-0.04497075	0.63803953
C	6.27475278	0.70218839	1.34450053
O	8.51435122	-6.19103044	0.71941022
C	5.68647408	0.17390091	2.49622299
H	3.49564944	10.78290381	1.42785854
H	-5.09980241	19.32890464	-2.07250770
H	-5.93372160	12.91384275	-2.69712315
H	-5.04841573	12.62006185	-4.23815472
H	-5.99189415	14.90552505	-4.28559824
H	1.80925972	-0.60397654	4.49110304
H	3.20963948	2.08236479	4.94313988
H	2.64583408	2.75291802	-1.30189167
H	2.65694901	2.61129163	1.20896429
H	-7.43625762	-18.47794537	-2.96449728
H	2.81795866	3.82541731	-6.41011422
H	-3.41965934	12.46149478	1.29365099
H	0.74095080	12.39440179	-1.44363300
H	1.64840942	8.42995789	-5.69724245
H	0.67307972	3.69573907	-5.12061296
H	3.66161880	3.00438917	-5.04169685
C	-5.18265669	16.72710342	-2.50787276

O	-5.09913217	17.31005452	-3.56170844
O	2.23414252	12.01674894	0.34481303
O	4.28390266	10.60787581	-1.07349582
C	-2.49595031	12.44408590	0.71521068
C	4.87774203	-8.14797002	0.54917449
C	6.11091941	-7.51061420	0.63321144
O	0.66127273	-12.59465232	-3.23845466
O	3.03625805	-10.28895854	-1.75150393
C	-3.41693950	-19.30998614	2.35292366
C	-4.44184921	-20.39940889	0.45902777
C	-3.86867911	-18.06823921	1.89633840
C	-5.62129829	-19.10685002	-1.30018123
O	-5.91615982	-20.07569374	-1.95843938
O	2.38069523	-9.46348821	0.23462508
C	-4.86689881	-19.15359806	-0.01355021
O	9.11261851	-6.90092840	-1.33139344
C	-3.70205598	-20.47506873	1.63409485
C	4.53996913	-8.86706448	-0.60290340
H	4.16167694	-8.10756557	1.37049568
H	7.37837433	-8.32487891	-2.41734467
H	2.67447180	-12.43485830	-3.14130609
H	0.95464738	-10.26179587	-1.80593417
H	9.91603107	-5.32749432	1.88075125
H	-1.47238309	-19.25488589	5.75027844
H	-4.88001444	-12.98207379	-4.76722776
H	-1.14496146	-17.49400885	5.56035957
H	-3.47620078	-17.02600653	6.33988242
H	-4.57948675	-18.84135393	7.24406298
H	-4.68511202	-21.28728312	-0.12560158
H	-2.91433896	-11.40507504	-4.48404595
H	-3.32735325	-21.42404003	2.01895902
H	-2.43139659	-16.25057682	-3.47014188
H	6.39450314	-6.94314514	1.51945101
H	-6.21133397	21.14165099	4.33315754
H	7.68183742	0.33808073	-0.26893219
H	-4.43028577	21.07746114	4.39393572
H	-5.24437625	22.44305512	3.54231664
H	5.97507619	1.70085562	1.02602470
H	7.22414637	-2.86713785	2.54312257
H	3.24692723	0.65396300	6.05390914
H	-1.16665831	12.09690284	2.39292371
H	2.14704186	10.55520542	-4.40645631
H	-1.49565865	12.74063161	-2.52918357
H	-5.22139532	1.41584688	1.24948204
H	-6.26482747	2.18093424	2.47636344
H	-6.67548980	-0.32068192	2.17819534
C	-5.44724757	1.46674270	2.32625957
H	-5.17845973	-2.40175941	1.36066757

C	-5.86997582	0.08873123	2.80596158
H	-3.77353673	2.81808680	2.67814197
C	-5.06323178	-2.24575713	2.44706006
C	-4.21475961	1.90668734	3.10524840
N	-4.74825693	-0.84569771	2.72108197
H	-6.03726988	-2.45398276	2.91263356
H	-2.56527336	-2.89060313	1.41271873
H	-6.24526386	0.12456088	3.84292108
C	-3.47809338	-0.41004666	2.85773977
N	-3.18946836	0.86859213	3.06955053
H	-4.49490032	2.12645031	4.14756112
H	-2.17731172	1.14898389	3.16833589
N	-2.45477561	-1.28137169	2.78849695
C	-2.63408744	-2.69930369	2.49619992
C	-3.99119035	-3.16115163	3.00846322
H	-4.18971168	-4.19365496	2.69408017
H	-1.52951197	-0.86135624	2.82951266
H	-1.82421539	-3.25652188	2.98402871
H	-4.01566284	-3.12301449	4.10815155
O	1.14990978	3.24440256	3.30260651
O	0.99200449	5.98392503	4.10336307
H	1.48152368	6.78254143	4.33037605
C	0.68678959	3.67050719	4.56614761
H	2.49102578	4.77392608	4.93505813
C	1.39971443	4.94802712	4.96903058
H	-0.40074702	3.84937562	4.54049426
H	0.90232700	2.90896499	5.33183041
H	1.13265480	5.17011844	6.02428499
F	1.53144657	6.07182466	-0.61088981
F	1.22461508	7.44332478	1.02151920
C	1.24592145	6.14033343	0.69967048
O	-1.05337545	5.95088340	0.35234445
F	2.26390962	5.57664414	1.35497149
C	-0.12362520	5.49826341	0.99181348
O	-0.21266379	4.55758417	1.86826113
H	0.59963026	4.10084555	2.45295220

Data S5: XYZ data for step 4.

Element	X	Y	Z
C	5.20688979	-8.79245423	-1.82335689
C	-4.00477123	-14.60009791	-4.06099762
C	-0.04426530	2.41946849	-2.98297542
C	-1.68875469	-14.20753538	-3.50318485
C	0.00488562	2.10941327	1.28337203
O	-6.11484268	-17.78220923	-1.54021741
C	-5.95821285	-17.72382348	-3.96778063
O	-0.97154917	1.40356682	3.39910374
O	-0.94447666	1.99340827	-3.66074946
C	0.99607768	2.86687942	0.65025912
C	-0.03266915	1.98937252	2.78961626
C	-2.97446556	-17.86671816	6.66704480
O	-6.28432628	-15.14346432	-4.54980485
C	-0.72958599	-11.87167166	-3.65881063
C	-2.76501969	-15.08266114	-3.63601591
C	-4.17286158	-13.24209073	-4.34979832
C	2.08146819	6.04518724	-5.15134896
C	0.86523563	12.16042848	1.21536507
C	2.89442816	9.60559597	-2.93236489
C	-0.55439285	12.52497884	-0.83715394
C	3.36303214	8.38112890	-2.44922543
C	1.06052323	3.16425768	-4.91523655
O	2.67560706	4.95826601	-4.62968591
O	1.02690018	12.06036020	2.40262865
C	-4.31759664	12.91014206	-1.19669607
O	-5.32240538	12.99822542	-0.54102482
C	0.00031750	2.33602142	-1.48893389
C	3.09024516	1.30615673	4.51084224
O	1.39011805	6.01858199	-6.13849475
O	2.69573336	11.95570425	-2.54712604
C	3.13741616	10.88925533	-2.20465143
O	-5.80107785	18.84273668	3.76204985
C	3.10387083	7.21235341	-3.16190060
C	-5.76438243	16.71596741	0.11319439
C	2.39509113	7.27622903	-4.36464111
O	-4.27964001	12.98717340	-2.54359809
C	-5.68227747	17.45819008	-1.06835268
C	-5.63312663	19.51689184	0.19145461
C	-5.78129245	17.38195754	1.33613939
C	-5.51009732	13.27764323	-3.21242365
C	-5.57531754	14.74708853	-3.54286977
O	-5.66784221	15.45307270	-2.30610848
C	-5.65950506	21.45695070	3.88043859

C	4.34942229	0.60595603	2.63869317
C	7.68875773	-1.34427368	0.94518180
O	9.33239831	-1.69280348	-0.75752368
H	4.07327827	12.75034771	-0.86901342
H	5.15581819	11.69376790	0.11885200
H	3.42574340	12.64799161	1.59247886
H	-5.80995476	15.62862250	0.05562696
H	-5.57959711	20.60238840	0.24892080
H	-5.84093873	16.83984124	2.27906090
H	-1.72621618	0.85104083	1.05116864
H	-1.74035209	1.08373285	-1.46842270
H	-5.47448485	-18.70561731	-4.01181448
H	-6.55279362	-17.55041453	-4.87462115
H	-0.71552011	-14.56604967	-3.17687071
H	-7.32429609	-16.64911132	-2.69389250
H	0.89753008	2.19356964	-5.40957010
H	0.99225246	0.91664917	4.90316393
H	3.46185610	6.25438631	-2.79102400
H	3.91656963	8.33955382	-1.51393417
H	4.89202318	-9.36085257	-2.69543149
H	-5.09979068	-16.97402275	0.43424712
H	-2.42816646	-17.69572683	7.61296986
H	-3.76567760	-17.12026806	2.55921110
H	5.71188167	-1.49229468	3.71174441
H	10.48841405	-6.19511653	0.09152654
H	9.41103509	-4.24661528	-1.12094962
H	10.77132818	-3.77073740	-0.08772260
H	1.48401653	-11.51264112	-0.98322769
H	1.59464060	-10.93708214	-4.00780169
C	8.17374078	-6.78866414	-0.65899154
O	-2.19209436	-20.40946113	4.02596326
C	-2.70873498	-19.38578198	3.67219314
C	3.03500532	-9.42558346	-0.69496830
C	9.75567055	-4.19147821	-0.08023491
O	8.88312929	-3.35468997	0.67976260
C	1.55969857	-10.84149666	-1.85151365
C	1.56340026	-11.62006778	-3.15174713
C	6.44570021	-8.15911282	-1.78419547
C	6.82504896	-7.43829060	-0.64816556
C	-3.09827753	-12.36796109	-4.21568844
C	-6.85921115	-17.63697793	-2.75411016
O	-4.88275769	-16.77874851	-3.89827358
C	-1.85507250	-12.85072410	-3.79250191
C	-4.71916489	-17.92821934	0.79381239
O	-3.87338538	-18.95127045	6.75681483
C	-1.96603843	-18.20876515	5.60126454
O	-2.61868191	-18.20898309	4.32510104
O	-0.81404623	-10.69866741	-3.90745300

C	-5.18989394	-15.50476921	-4.20157657
C	1.91485419	8.50084894	-4.84156295
O	1.05096482	3.00188294	-3.49532175
C	2.41101300	3.71882648	-5.29169442
C	2.17096693	9.66618534	-4.12839228
C	-0.97312946	1.44506855	0.53617449
C	-0.98078533	1.56882716	-0.85339920
C	0.99969280	2.96515812	-0.73900158
O	4.23886544	0.63029983	3.96245445
C	1.78012321	0.59024925	4.20582491
O	1.30274321	0.81991811	2.89601061
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C	-5.61847906	18.85448837	-1.03253142
C	-5.71410309	18.77698962	1.37482021
C	-5.72964478	19.43546991	2.71797444
C	-0.45806078	12.35412386	0.54620526
C	-1.60490578	12.35082202	1.34749809
C	-2.95460743	12.69963446	-0.62128598
C	-1.80838786	12.69756358	-1.42039003
C	4.14161978	11.83191503	-0.27472870
C	3.16602150	11.85711594	0.87417529
H	-4.67388026	15.07193859	-4.08121693
C	6.14306801	-1.12758583	2.78157427
O	3.50155259	0.99432264	1.85262809
C	9.74478152	-5.54813269	0.57379014
C	8.72979665	-2.10528418	0.19571428
C	7.16928777	-1.82429999	2.14908901
C	7.20444046	-0.16197563	0.37293942
C	6.13943454	0.50257464	0.96735148
O	8.45354887	-6.16989720	0.50064991
C	5.60370748	-0.00348682	2.15098436
H	3.16114204	10.89405949	1.40374656
H	-5.55396000	19.39809386	-1.97471999
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H	-5.49317913	12.69497849	-4.14119213
H	-6.45146949	14.96955580	-4.16963512
H	1.92691057	-0.49704505	4.33286044
H	3.09151762	2.34354452	4.13276035
H	1.77577784	3.55696837	-1.22203961
H	1.79951600	3.36017131	1.20894538
H	-7.62695370	-18.41567543	-2.82604999
H	2.45293948	3.85386692	-6.37900219
H	-3.76862800	12.52730439	1.35563398
H	0.35191416	12.52054450	-1.44172127
H	1.34584663	8.51143906	-5.77034816
H	0.25473590	3.84550134	-5.22360424
H	3.20813603	3.04929325	-4.94815294
C	-5.64348247	16.79474812	-2.40609533

O	-5.58966850	17.37660874	-3.45699817
O	1.87038065	12.10238918	0.32429668
O	3.89152986	10.69580603	-1.10622014
C	-2.85449166	12.52304989	0.76259811
C	4.74483570	-8.02000219	0.42887702
C	5.97874117	-7.37398415	0.46279352
O	0.40783711	-12.46207700	-3.23612788
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C	-3.50385855	-19.24799920	2.40903095
C	-4.53633080	-20.33245036	0.51438365
C	-3.99619747	-18.01242773	1.98123490
C	-5.76566129	-19.04065705	-1.21238841
O	-6.05978989	-20.00599333	-1.86962530
O	2.24493160	-9.35982526	0.20839470
C	-4.98479534	-19.08715829	0.05999718
O	8.92767075	-6.82278279	-1.59637740
C	-3.76943245	-20.40798731	1.67338983
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H	7.13436246	-8.19729947	-2.62803925
H	2.42154910	-12.30078496	-3.18394817
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H	-1.52452222	-19.19340073	5.78657832
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H	-4.79418513	21.15387026	4.48589979
H	-5.60798715	22.52084249	3.63377656
H	5.70025793	1.41373205	0.55805958
H	7.57401891	-2.74082329	2.57193128
H	3.27510955	1.28587944	5.59134863
H	-1.48999038	12.21110244	2.42265633
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H	-5.63214558	1.62770618	1.37339994
H	-6.76918106	2.27883411	2.58485761
H	-6.96089499	-0.23747392	2.26601608
C	-5.88720379	1.64118711	2.44227086
H	-5.21065633	-2.16002931	1.41951094

C	-6.20056393	0.22698104	2.90571332
H	-4.34455298	3.12631743	2.81883155
C	-5.17281615	-2.02742424	2.51389565
C	-4.71805818	2.18866731	3.24701178
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H	-6.14155148	-2.33743950	2.92132071
H	-2.54523977	-2.42668162	1.61004839
H	-6.58715974	0.23446688	3.93815018
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N	-2.68439175	-0.84233195	2.99708842
C	-2.70503587	-2.26423179	2.68771824
C	-4.04460952	-2.85263126	3.11030680
H	-4.12587448	-3.88889895	2.75712497
H	-1.80125209	-0.31823982	3.09688627
H	-1.87876313	-2.74314445	3.22450492
H	-4.12911270	-2.85082828	4.20651131
O	0.55484331	3.07061515	3.37472020
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H	0.77331410	5.57962032	3.11487354
C	0.00871865	3.54987006	4.60397402
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H	0.12993244	2.81545529	5.41146950
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O	3.68685753	4.75159153	0.61053681
C	4.58598446	4.26900471	1.31110758
F	6.27602622	4.62459979	-0.38640091
O	4.55331962	3.45873287	2.25712150
C	6.01999746	4.78084079	0.93137241
F	6.17841541	6.09531446	1.19518686
F	6.99892821	4.13353026	1.58843575

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