Supplementary Information (SI) for Green Chemistry.

Supporting information

Hydrogenation-Induced Selective Degradation of PET Wastes

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1. General information

All reagents and chemicals were of analytical grade and used as received without any further purification. Detailed description of the reagents and chemicals is shown below: commercial 10 wt.% Pd on carbon (wetted with ca. 55% water) was purchased from Leyan, 10 wt.% Pt/C was purchased from Energy Chemical, 5 wt.% Ru/C was purchased from Meryer. Polyethylene terephthalate (PET, supplied by Macklin Inc.), polybutylene terephthalate (PBT, supplied by Klamar), poly (butyleneadipate-co-terephthalate (PBAT, supplied by Macklin Inc.), polyethylene naphthalate (PEN, supplied by Dongguan Zhongyou New Material Co.) were used as received. Internal standards 1,3,5-trimethoxybenzene and maleic acid were purchased from Bide Pharmatech Ltd. 1,4-Dioxane was purchased from Energy Chemical. Trifluoroacetic acid was purchased from Meryer. Waste PET materials were collected from daily life and used without further purification or after simply washing with water. All reactions were carried out using Wattcas autoclave (WP-MASR-500A). ^{1}H and ^{13}C NMR data were recorded with Bruker Advance III (400 MHz) spectrometer with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. The chemical shifts (δ) were given in parts per million relative to DMSO-d6 (2.50 ppm for ^{1}H and 39.50 ppm for ^{13}C) or D_2O (4.79 ppm for ^{1}H). Gas chromatography (GC) analyses were obtained on SHIMADZU GC-2014C equipped with an HK-5 30 m x 0.25 mm ID x 0.25 μm capillary column (SHIMADZU) and an FID detector. The following GC oven temperature programs were used: 50°C hold for 2 min, ramp 50 °C/min to 100°C and hold for 0.5 min, ramp 15 °C/min to 200 °C and hold for 2 min, ramp 50 °C/min to a final temperature of 280°C, and hold for 2 min. Nitrogen was used as a carrier gas, with a constant column flow of 1.4 mL/min. The injector temperature was held at 300°C. All GC-yields were obtained by establishing response factors of authentic samples from commercial sources. Gas chromatography-mass (GC-MS) analyses were obtained on SHIMADZU GC-MS-2010 equipped with a Rtx-5MS 30 m x 0.25 mm x 0.25 μm capillary column (SHIMADZU). The following GC oven temperature programs were used: 50°C hold for 3 min, ramp 25 °C/min to 150°C and hold for 1 min, ramp 25 °C/min to a final temperature of 280°C and hold for 6 min. Helium was used as a carrier gas, with a constant column flow of 1 mL/min. The injector temperature was held at 250°C.

2. General procedure for the hydrothermal degradation of PET

2.1 The hydrothermal degradation of PET under various conditions

To an oven dried quartz tube, commercial PET (180 mg, 0.94 mmol of the single repeat unit or 360 mg, 1.88 mmol of the single repeat unit), the catalyst (0 - 0.75 mol%), and solvent (1.5 - 4.5 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5 MPa) three times and finally charged with H_2 (1.2 - 3 MPa) or N_2 (3 MPa). The reactor was heated to 160-180°C and kept stirring at 500 rpm for 20 h. After completion of the reaction, ethyl acetate was added for extraction, leading to an aqueous phase and an organic phase. Maleic acid (150 mg), used as an internal standard, was added to the aqueous phase. 0.1 mL of the aqueous solution was taken out and mixed with D_2O (0.5 mL) for ^1H NMR analysis, measuring the NMR yield of ethylene glycol (EG). Meanwhile, the organic phase was concentrated by rotary evaporation and then eluted with petroleum ether, affording the solid residue and the eluent, respectively. After adding 1,3,5-trimethoxybenzene (15 mg) as the internal standard, the mixed eluent was analyzed by gas chromatography (GC) to afford the GC yield of 4-methyl-1-cyclohexanecarboxylic acid, while the solid residue was dissolved in DMSO-d6 and analyzed by ^1H NMR spectroscopy to afford the NMR yield of 1,4-cyclohexanedicarboxylic acid (1,4-CHDA). Note that the catalytic amount of catalyst and yields of products are based on the single repeat unit of PET.

2.2 Standard procedure for hydrothermal degradation of PET wastes

To an oven dried quartz tube, commercial PET or PET waste (180 mg, 0.94 mmol of the single repeat unit), Pd/C (5 mg), and H_2O (3 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5

MPa) three times and finally charged with H_2 (1.2 MPa). The reactor was heated to 180°C and kept stirring at 500 rpm for 20 h. After completion of the reaction, ethyl acetate was added for extraction, leading to an aqueous phase and an organic phase. Maleic acid (150 mg), used as an internal standard, was added to the aqueous phase. 0.1 mL of the aqueous solution was taken out and mixed with D_2O (0.5 mL) for ^{1}H NMR analysis, measuring the NMR yield of ethylene glycol (EG). The organic phase was concentrated by rotary evaporation to obtain the mixture of 1,4-cyclohexanedicarboxylic acid (1,4-CHDA) and 4-methyl-1-cyclohexanecarboxylic acid. Then, petroleum ether (boiling range: 30-60°C) was added to dissolve 4-methyl-1-cyclohexanecarboxylic acid. Finally, pure 1,4-CHDA was obtained as white solid by filtration and washed with petroleum ether (3 x 6 mL). Meanwhile, 1,3,5-trimethoxybenzene (15 mg), as the internal standard, was added to the combined petroleum ether phase containing 4-methyl-1-cyclohexanecarboxylic acid, and 1.5 mL of the liquid was taken out for gas chromatography (GC) yield analysis. Note that the catalytic amount of catalyst and yields of products are based on the single repeat unit of PET (0.94 mmol).

2.3 The hydrothermal degradation of 20-Gram-Scale PET

To an oven dried quartz tube, PET (20 g, 104 mmol of the single repeat unit), Pd/C (828.1 mg), and H_2O (90 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5 MPa) three times and finally charged with H_2 (3 MPa). The reactor was heated to 180°Cand kept stirring at 500 rpm for 30 h. Note that the catalytic amount of catalyst and yields of products are based on the single repeat unit of PET (104 mmol).

2.4 The product isolation procedure

After completion of the reaction, ethyl acetate was added for extraction, separating the reaction mixture into aqueous phase and organic phase. The aqueous phase was concentrated by rotary evaporation to obtain the pure EG. The organic phase was concentrated by rotary evaporation to obtain the mixture of 1,4-

cyclohexanedicarboxylic acid (1,4-CHDA) and 4-methyl-1-cyclohexanecarboxylic acid. Then, petroleum ether (boiling range: 30-60°C) was added to dissolve 4-methyl-1-cyclohexanecarboxylic acid. Finally, pure 1,4-CHDA was obtained as white solid by filtration and washed with petroleum ether (3 x 20 mL).

2.5 The hydrothermal degradation of PBT, PBAT and PEN

To an oven dried quartz tube, PBT (207 mg, 0.94 mmol of the single repeat unit) [or PBAT (404 mg, 0.94 mmol of TPA unit and 0.99 mmol of adipic acid unit), or PEN (227 mg, 0.94 mmol of the single repeat unit)], Pd/C (5 mg), and H_2O (3 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5 MPa) three times and finally charged with H_2 (1.2 or 3 MPa). The reactor was heated to 180°C and kept stirring at 500 rpm for 20 h. After extraction with ethyl acetate, an aqueous phase and an organic phase were obtained. Maleic acid (150 mg), as an internal standard, was added to the aqueous phase. 0.1 mL of the aqueous solution was taken out and mixed with D_2O (0.5 mL) for ^{1}H NMR analysis, measuring the NMR yield of the corresponding diol product. Meanwhile, the organic phase was concentrated by rotary evaporation and then eluted with petroleum ether, affording the solid residue and the eluent, respectively. After adding 1,3,5-trimethoxybenzene (15 mg) as the internal standard, the solid residue was dissolved in DMSO-d6 and analyzed by ^{1}H NMR spectroscopy to afford the NMR yield of the corresponding diacid products. Note that the catalytic amount of catalyst and yields of products are based on the single repeat unit of each polymer (0.94 mmol).

2.6 Procedures for catalyst cycling experiment

To an oven dried quartz tube, commercial PET (1 g, 5.21 mmol of the single repeat unit), Pd/C (41.4 mg), and H_2O (6 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5 MPa) three times and finally charged with H_2 (3 MPa). The reactor was heated to 180°C and kept stirring at 500 rpm for 20 h. After completion of the reaction, ethyl acetate was added, then the solid catalyst and the liquid were separated by centrifugation. The obtained solid catalyst was washed with ethanol and dried overnight. The collected catalyst was directly used in the next cycle of experiment under the same reaction conditions. Note: the yields of products were analyzed following the procedure in section 2.2, the catalytic amount of catalyst and yields of products are based on the single repeat unit of PET (5.21 mmol).

3. Mechanistic investigation

3.1 Time course experiment

To an oven dried quartz tube, commercial PET (180 mg, 0.94 mmol of the single repeat unit) or PECHD (184 mg, 0.94 mmol of the single repeat unit), Pd/C (5 mg), and H_2O (3 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5 MPa) three times and finally charged with H_2 or N_2 (1.2 MPa). The reactor was heated to 180°C and kept stirring at 500 rpm for 3 h, 6 h, 9 h, 12 h, 15 h, or 20 h. After completion of the reaction, the mixture was concentrated by rotary evaporation. Subsequently, 1,3,5-trimethoxybenzene (15 mg) was added as the internal standard. After dissolving in 1 mL of DMSO-d6, the solution was analyzed by ^1H NMR spectroscopy to afford the NMR yield of 1,4-cyclohexanedicarboxylic acid (1,4-CHDA) or terephthalic acid (TPA). Note that the catalytic amount of catalyst and yields of products are based on the single repeat unit of each polymer (0.94 mmol).

3.2 Characterizations

3.2.1 The preparation procedure of partial hydrogenated PET and PECHD

To an oven dried quartz tube, commercial PET (180 mg, 0.94 mmol of the single repeat unit), Pd/C (5 mg), and 1,4-dioxane (3 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5 MPa) three times and finally charged with H_2 (1.2 MPa). The reactor was heated to 180°C and kept stirring at 500 rpm for 3 h to get partial hydrogenated PET. Alternatively, for the synthesis of PECHD, the same procedure was followed, but with the following modifications: Pd/C (20 mg) was used instead, and the auto-clave was charged with H_2 at 3 MPa. The reactor was heated to 180°C and kept stirring at 500 rpm for 20 h to get PECHD. Then pure partial hydrogenated PET or PECHD was directly obtained by removing the reaction solvent and the catalyst solid.

3.2.2 X-ray Diffraction (XRD) analysis of PET and hydrogenated PET

XRD measurements were done at room temperature on a Rigaku Miniflex600 X-ray diffractometer with a Cu−Kα X-ray source (λ = 1.5406 Å), equipped with a position-sensitive detector in the angular range of $10° \leq 2\theta \leq 80°$ with the step size 0.02° and a scan rate of 1deg/min calibrated against corundum standards.

3.2.3 Differential scanning calorimetry (DSC) analysis of PET and hydrogenated PET

DSC analysis was performed on DSC3 (Mettler-Toledo) to determine the thermodynamic properties of polyesters. All the samples were heated from -40°C to 280°C at 10°C/min under N_2 atmosphere.

3.2.4 Thermogravimetric analysis (TGA) analysis of PET and hydrogenated PET

All the samples were tested by TGA2 (Mettler-Toledo) under N_2 atmosphere and heated from 30°C to 600°C at 10 C/min.

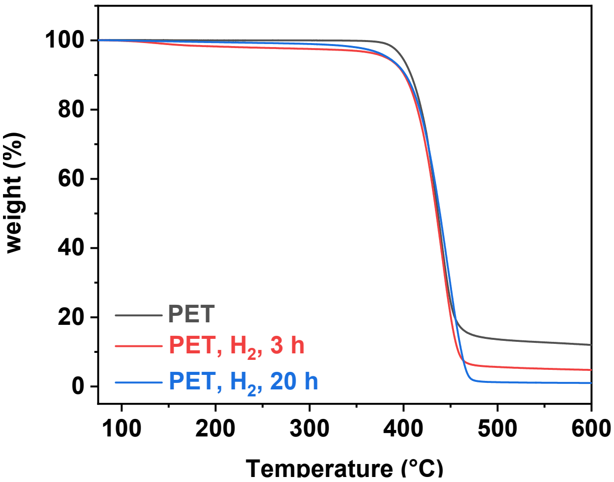


Figure S1. TGA curves of PET, partial hydrogenated PET, and PECHD

3.2.5 The preparation procedure of recovered polymers for SEM, GPC, FT-IR and ^{1}H NMR analysis

To an oven dried quartz tube, commercial PET (180 mg, 0.94 mmol of the single repeat unit), Pd/C (5 mg), and H_2O (3 mL) were added. Then, the tube was placed in a 500 mL of auto-clave, and the auto-clave was charged and purged with N_2 (0.5 MPa) three times and finally charged with H_2 (1.2 MPa). The reactor was heated to 180°C and kept stirring at 500 rpm for 3 h or 6 h or 9 h. After the completion of the reaction, the aqueous reaction phase was extracted with ethyl acetate for three time. Then, the remaining aqueous solution was filtered to collect the recovered polymers, which was then dried overnight at 60 °C and analyzed by SEM, GPC, FTIR and ^{1}H NMR.

3.2.6 Scanning electron microscope (SEM) analysis of original PET and recovered polymers

SEM images of original PET and recovered polymer after 3 h or 6 h reaction were acquired using a JSM-7610E microscope (Japan), with samples sputter-coated with gold.

3.2.7 Gel permeation chromatography (GPC) analysis of original PET and recovered polymers

GPC analysis of original PET and recovered polymer after 3 h, 6 h, or 9 h reaction were conducted using an Agilent infinity 1260II. Hexafluoroisopropanol (HFIP) was used as the mobile phase at flow rate of 1 mL/min. Samples were prepared by dissolving 2 mg polyester in 1 ml mobile phase and filtering the solution with a 0.2 µm nylon syringe filter before injection into the GPC.

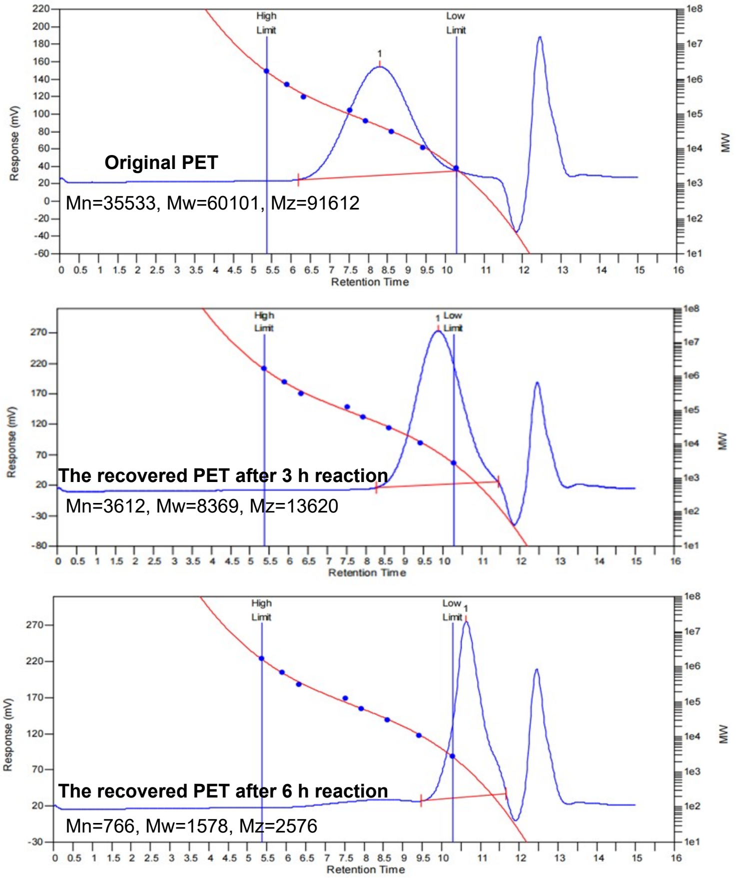


Figure S2. GPC results of PET and recovered polymer after 3 h and 6 h reaction

3.2.8 Fourier Transform infrared spectroscopy (FT-IR) analysis of original PET and recovered polymers

FT-IR spectra of original PET and recovered polymer after 3 h, 6 h, or 9 h reaction were collected by Nicolet 5700. All sample physically mixed with KBr and the mixed powder was pressed into a transparent sheet and tested by the spectrometer.

3.2.9 ^{1}H NMR spectra of original PET and recovered polymers

The original PET sample and the recovered polymers after 3 h reaction, 6 h reaction, or 9 h reaction were each dissolved in 1 mL of 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP). Subsequently, 0.1 mL of each solution was taken out and mixed with $CDCl_3$ (0.5 mL) for ^{1}H NMR. ^{1}H NMR data were recorded with Bruker Advance III (400 MHz) spectrometer with tetramethylsilane as an internal standard.

3.3 Density Functional Theory (DFT) Studies

3.3.1 Computational methods

All density functional theory (DFT) calculations were performed using the Gaussian 16 software package[1]. Geometry was optimized using the 6-311G (d,p)[2][3] functional with M062X[4] for all atoms. Vibrational frequencies were calculated for the stationary points to confirm if the optimized structure is a local minimum on the respective potential energy surface. The CHelpG charges[5] were obtained by performing single-point calculations on the optimized structures with the 6-311G (d,p) functional with the basis set of M062X for all atoms. Solvation energy corrections were calculated in methanol solvent with the SMD continuum solvation model[6] based on the gas phase optimized geometries. Fukui functions[7][8][9][10] were calculated in the following way: The neutral cyclohexane and phenyl ester derivatives (with N electrons) were subjected to geometry optimization, and total local atomic electron populations were determined by the electron populations analysis. The electron populations of the corresponding anionic ester derivatives (N+1 electrons) were calculated without geometry re-optimization. Fukui electrophilicity indices were calculated for each atom by subtracting the atomic electron population in the neutral ester derivatives from the population in the anionic ester derivatives.

3.3.2 Calculation of Fukui indices

Nucleophilicity Fukui functions $f^-(r)$ were obtained from the total atomic charge values ρ_N of the neutral species and the total atomic charge values ρ_{N-1} of the cationic species following equation 1; Electrophilicity Fukui functions $f^+(r)$ were obtained from the total atomic charge values ρ_{N+1} of the neutral species and the total atomic charge values ρ_N of the cationic species following equation 2:

$$(1)\ Nucleophilicity\ Fukui\ functions: \quad f^-(r) = \rho_N(r) - \rho_{N-1}(r) \approx \rho^{HOMO}(r)$$

$$(2)\ Electrophilicity\ Fukui\ functions: \quad f^+(r) = \rho_{N+1}(r) - \rho_N(r) \approx \rho^{LOMO}(r)$$

Furthermore, the condensed version of the Fukui function could be used for the quantitative evaluation of the possibility that an atom could act as a reactive site. The definition of condensed Fukui function for an atom, say A, can be written as

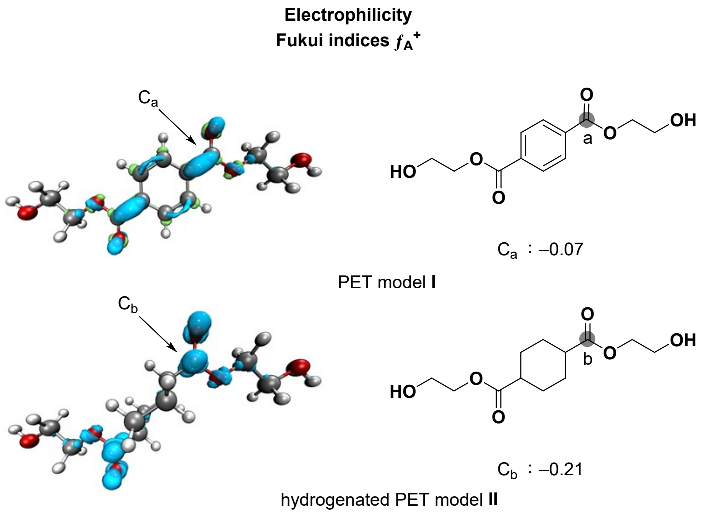
$$f_A^+ = p_{N+1}^A - p_N^A$$

where p^A is the electron population number of atom A. Since the atomic charge is defined as $q^A = Z^A - p^A$, where Z is the charge of atomic nuclear, the f_A^+ can be expressed as the difference of atomic charges in two states (note that the two Z terms are canceled), equation 3. By analogous treatments, one can easily formulate other types of condensed Fukui function f_A^-, equation 4.

$$(3)\ \mathit{Electrophilicity\ Fukui\ Indices}:\quad f_A^+ = q_N^A - q_{N+1}^A$$

$$(4)\ \mathit{Nucleophilicity\ Fukui\ Indices}:\quad f_A^- = q_{N-1}^A - q_N^A$$

Fukui functions were used to explain the difference of reaction rate between reactant PET model **I** and hydrogenated PET model **II** in the reductive hydrolysis. As shown in Figure S3, the Electrophilicity Fukui indices of Ca in 1a and Cb in 1b are -0.07 and -0.21, respectively, which indicates that the Cb has higher electrophilicity than the Ca. Therefore, the reductive hydrolysis prefers to occur at the C_b of hydrogenated PET model **II**. The computational results have verified the experimental observations. The isosurface of the Fukui function shown below was plotted by condensing it to atomic value via population analysis using the software Multiwfn[11] and VMD[12].



Atom	Neutral charge	Anionic charge	f_A^+
C_a	**0.87**	**0.80**	**-0.07**
C_b	**0.91**	**0.70**	**-0.21**

Figure S3. The calculated electrophilicity Fukui indices of carbonyl carbons in PET model **I** and hydrogenated PET model **II**.

3.3.3 Cartesian coordinates (Å) and energies of optimized structures

1a

6-311G(d,p) SCF energy: -916.94496068 a.u.

6-311G(d,p) enthalpy: -916.669783 a.u.

6-311G(d,p) free energy: -916.738290 a.u.

6-311G(d,p) SCF energy in solution: -916.96984662 a.u.

6-311G(d,p) enthalpy in solution: -916.694669 a.u.

6-311G(d,p) free energy in solution: -916.763176 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.030391	-0.942305	-0.000096
C	-0.290878	-1.362122	-0.000092
C	-1.319468	-0.421926	-0.000169

C	-1.030368	0.942309	-0.000192
C	0.290901	1.362131	-0.000176
C	1.319489	0.421940	-0.000143
H	1.839426	-1.660360	-0.000017
H	-0.548704	-2.413817	-0.000044
H	-1.839378	1.660393	-0.000187
H	0.548746	2.413824	-0.000217
C	-2.722435	-0.935119	-0.000165
O	-3.014733	-2.099593	-0.000187
O	-3.629045	0.052497	-0.000154
C	-4.997313	-0.367585	-0.000075
H	-5.201578	-0.972190	-0.885255
H	-5.201366	-0.972588	0.884881
C	-5.834703	0.891137	0.000318
H	-5.593968	1.484812	-0.889381
H	-5.593619	1.484461	0.890158
O	-7.179430	0.458815	0.000499
H	-7.749200	1.229592	0.000448
C	2.722444	0.935142	-0.000143
O	3.014737	2.099615	-0.000095
O	3.629045	-0.052495	-0.000167
C	4.997304	0.367582	-0.000009
H	5.201624	0.972210	-0.885165
H	5.201322	0.972549	0.884978
C	5.834671	-0.891154	0.000332
H	5.593697	-1.484452	0.890218
H	5.593803	-1.484840	-0.889326
O	7.179405	-0.458856	0.000307

H	7.749154	-1.229648	0.000933

1b

6-311G(d,p) SCF energy: -920.55851705 a.u.

6-311G(d,p) enthalpy: -920.211572 a.u.

6-311G(d,p) free energy: -920.284913 a.u.

6-311G(d,p) SCF energy in solution: -920.58709473 a.u.

6-311G(d,p) enthalpy in solution: -920.240150 a.u.

6-311G(d,p) free energy in solution: -920.313491 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.749656	0.149034	-1.261496
C	-1.148871	0.929821	-0.000068
C	-0.749663	0.148972	1.261323
C	0.749649	-0.149023	1.261321
C	1.148866	-0.929816	-0.000103
C	0.749654	-0.148977	-1.261500
H	-1.018143	0.720194	2.153920
H	-0.641175	1.898700	-0.000045
H	-1.316051	-0.787079	-1.290913
H	-1.018119	0.720307	-2.154064
H	1.316035	0.787096	1.290727
H	1.018122	-0.720286	2.153893
H	0.641170	-1.898695	-0.000122
H	1.316049	0.787137	-1.290877
H	1.018119	-0.720215	-2.154090
H	-1.316050	-0.787148	1.290684

C	-2.625422	1.248139	-0.000078
O	-3.372558	0.127124	0.000006
O	-3.102206	2.348626	-0.000081
C	-4.789031	0.326118	0.000049
H	-5.087595	0.891074	-0.884650
H	-5.087529	0.891153	0.884721
C	-5.418185	-1.048523	0.000135
H	-5.086625	-1.597110	-0.889340
H	-5.086547	-1.597035	0.889627
O	-6.815155	-0.836303	0.000188
H	-7.253652	-1.688619	0.000221
C	2.625420	-1.248135	-0.000112
O	3.372561	-0.127122	-0.000008
O	3.102204	-2.348622	-0.000106
C	4.789035	-0.326120	0.000051
H	5.087606	-0.891081	-0.884642
H	5.087522	-0.891152	0.884728
C	5.418194	1.048519	0.000138
H	5.086656	1.597098	-0.889350
H	5.086537	1.597040	0.889618
O	6.815163	0.836294	0.000227
H	7.253663	1.688608	0.000178

4. GC-MS chromatogram of 2a

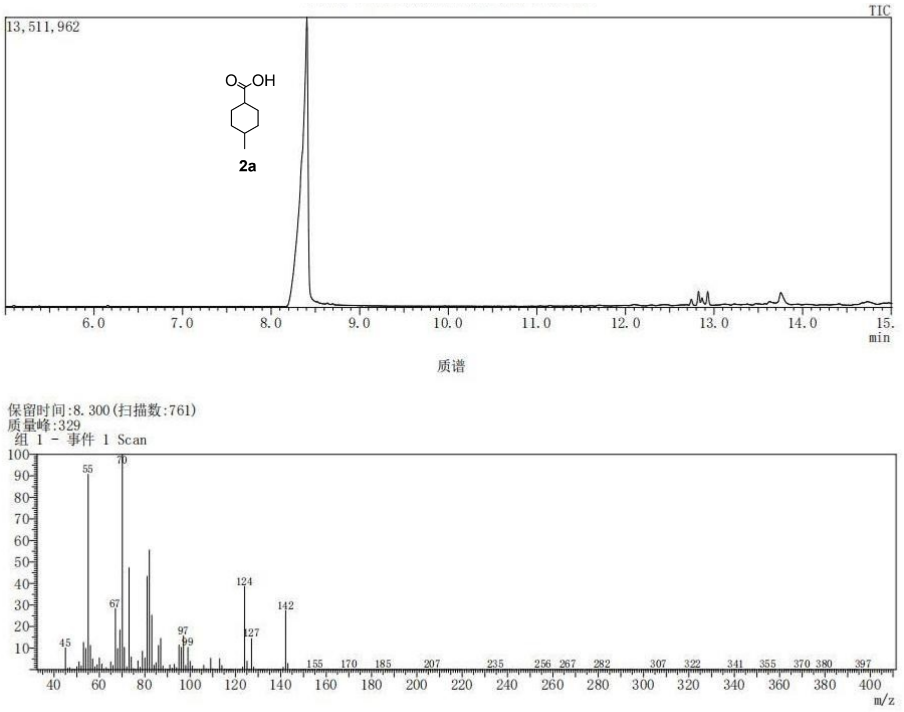
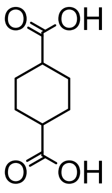


Figure S4. GC-MS chromatogram of **2a**

5. NMR data of the products



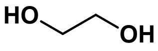
1a

trans/cis=4/5

1,4-Cyclohexanedicarboxylic acid (1a)[13]

^{1}H NMR (400 MHz, DMSO-d6) δ 12.06 (br., trans+cis, 3.6H), 2.37 (s, cis, 2H), 2.15(s, trans, 1.6H), 1.95-1.84 (m, trans, 3.2H), 1.76-1.65 (m, cis, 4H), 1.64-1.51 (m, cis, 4H), 1.39-1.25 (m, trans, 3.2H).

^{13}C NMR (100 MHz, DMSO-d6) δ 176.46, 176.15, 41.73, 27.74, 25.63.

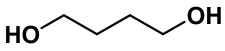


1b

Ethylene glycol (1b)[14]

^{1}H NMR (400 MHz, DMSO-d6) δ 4.52 (br., 2H), 3.39 (s, 4H).

^{13}C NMR (100 MHz, DMSO-d6) δ 63.02.

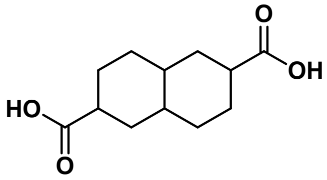


2b

Butane-1,4-diol (2b)[14]

^{1}H NMR (400 MHz, D_2O) δ 3.76-3.54 (m, 4H), 1.71-1.47 (m, 4H).

^{13}C NMR (100 MHz, D_2O) δ 61.51, 28.83.



3a

Decahydronaphthalene-2,6-dicarboxylic acid (3a)

^{1}H NMR (400 MHz, DMSO-d6), δ12.05 (br., 2H), 2.36-2.10 (m, 2H), 1.89-0.75 (m, 14H).

^{13}C NMR (100 MHz, DMSO-d6) δ 176.83, 43.02, 33.67, 30.58, 27.71, 23.09.

HRMS (ESI) for $C_{12}H_{17}O_4$ $[M-H]^-$: calculated 225.1121, found 225.1128.

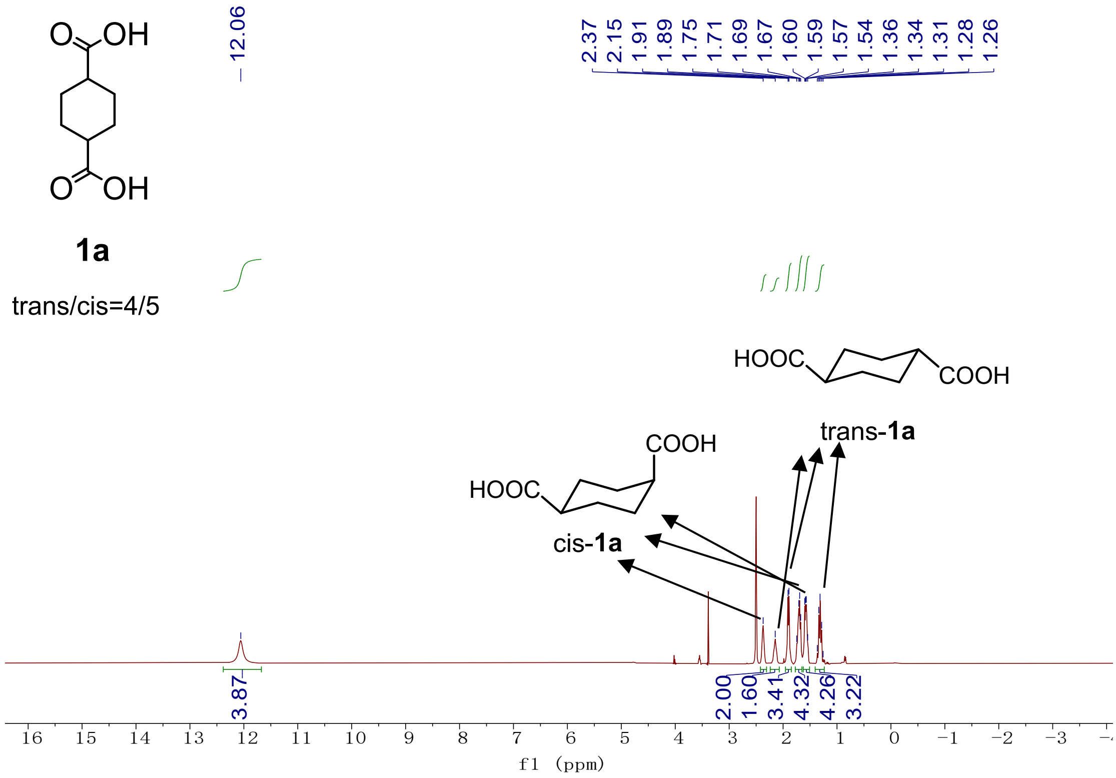


Figure S5. ^{1}H NMR of compound **1a**

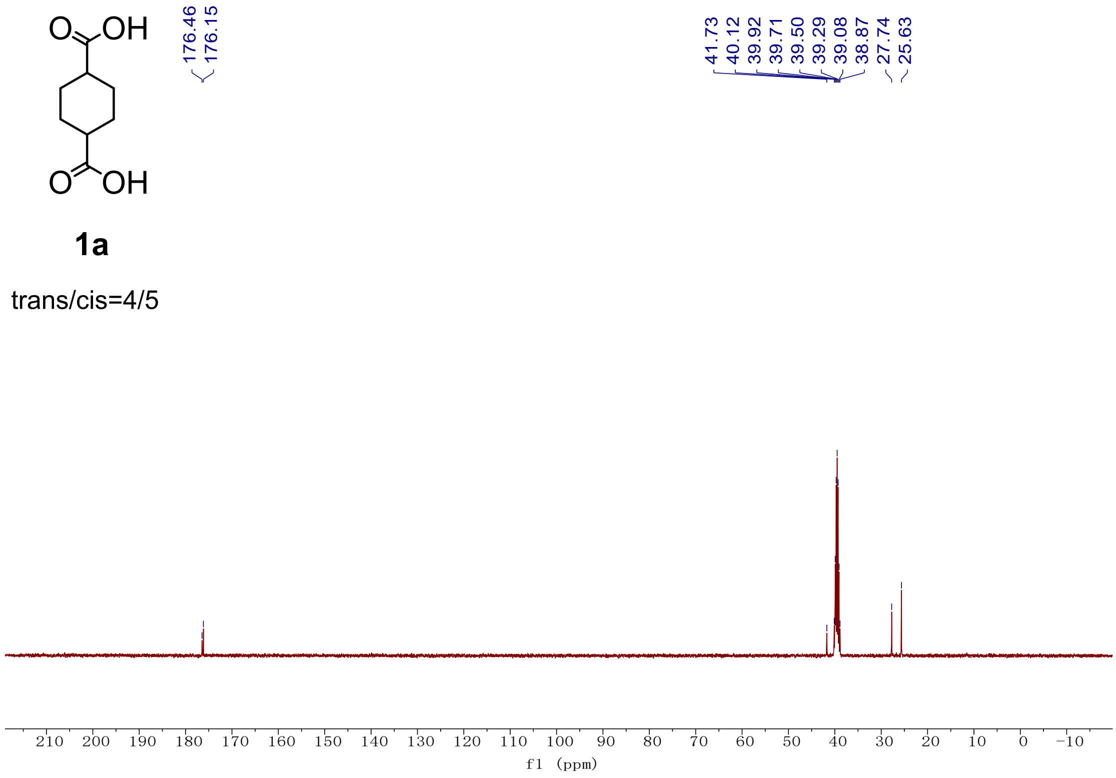


Figure S6. ^{13}C NMR of compound **1a**

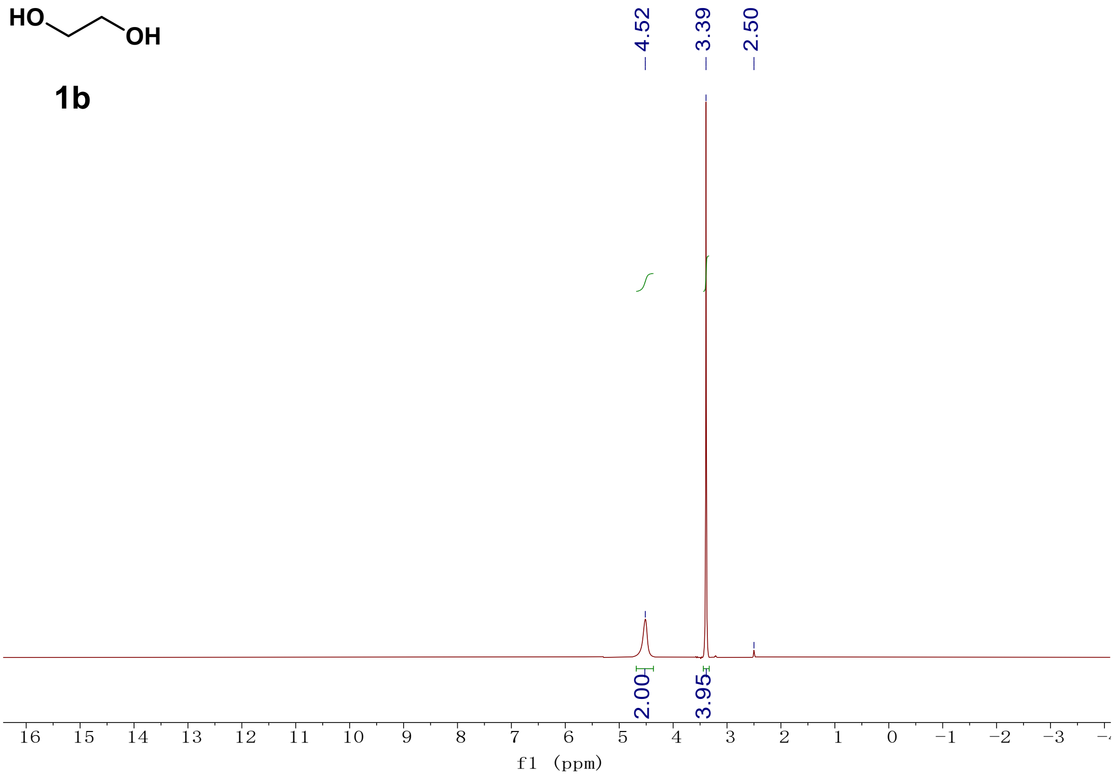


Figure S7. ^{1}H NMR of compound **1b**

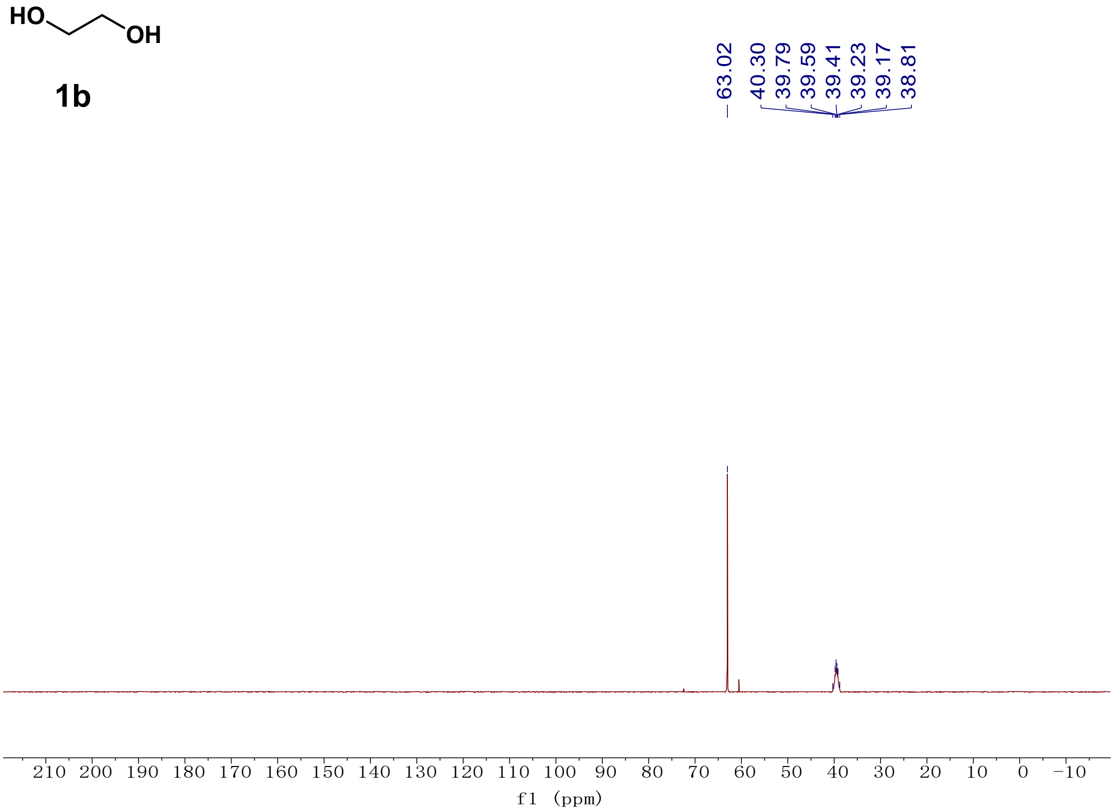


Figure S8. ^{13}C NMR of compound **1b**

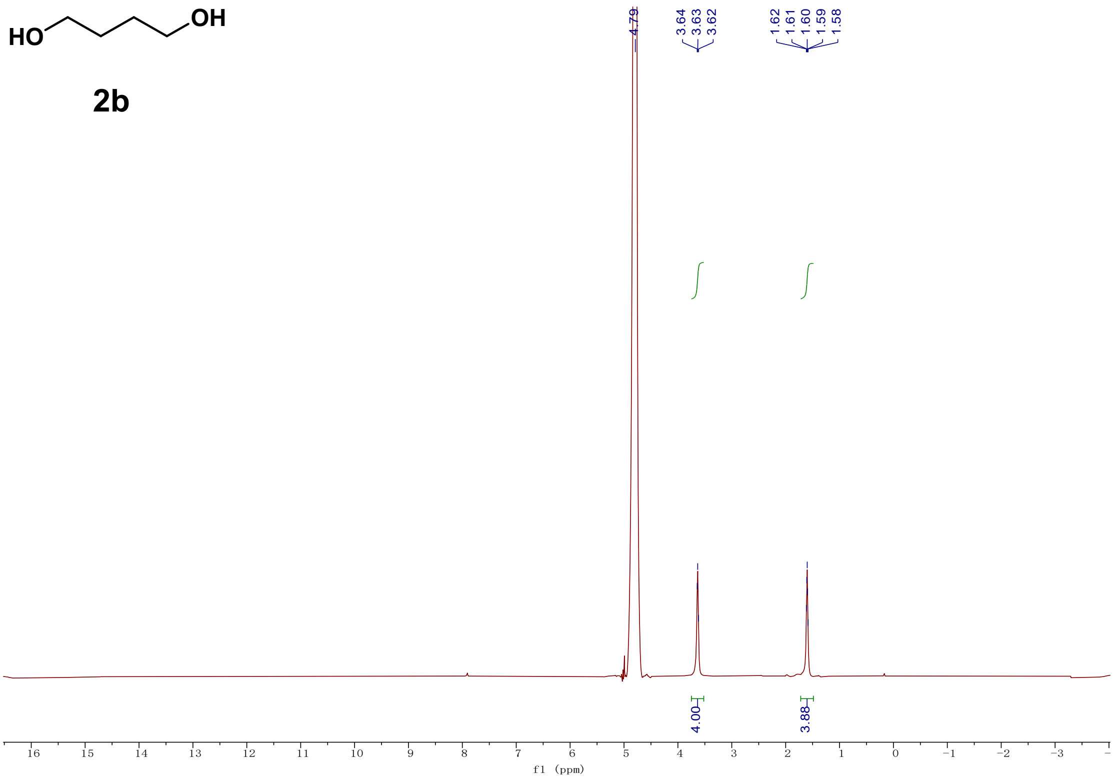


Figure S9. ^{1}H NMR of compound **2b**

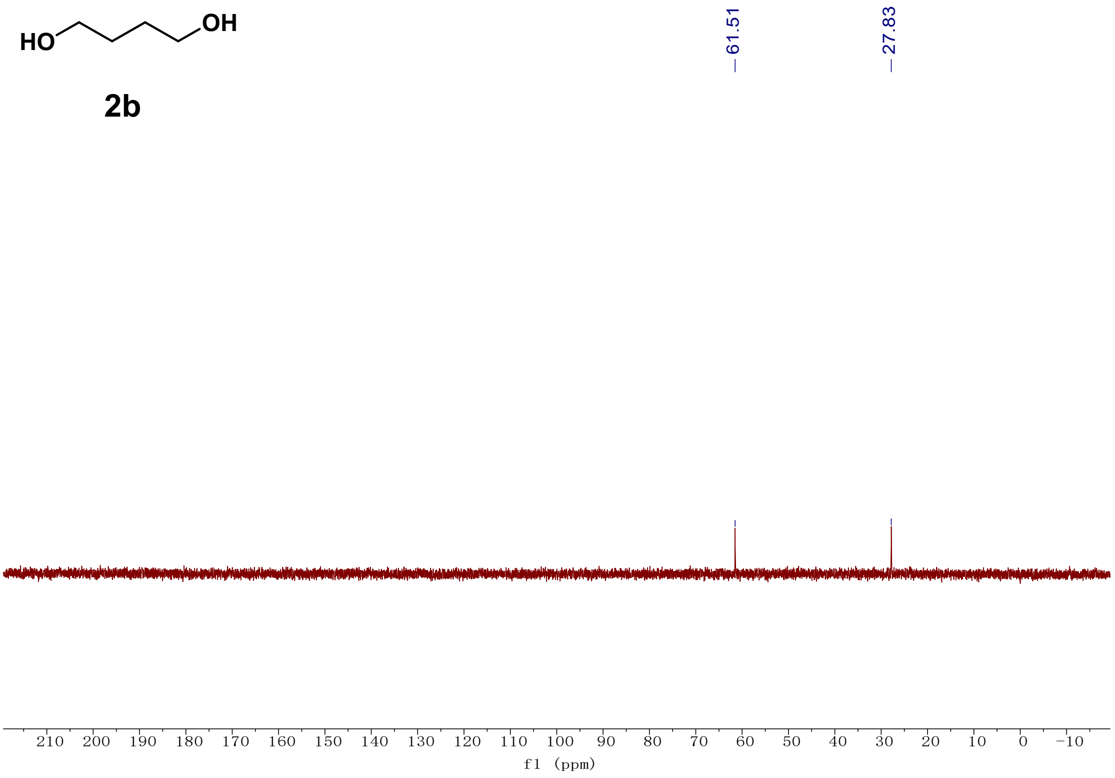


Figure S10. ^{13}C NMR of compound **2b**

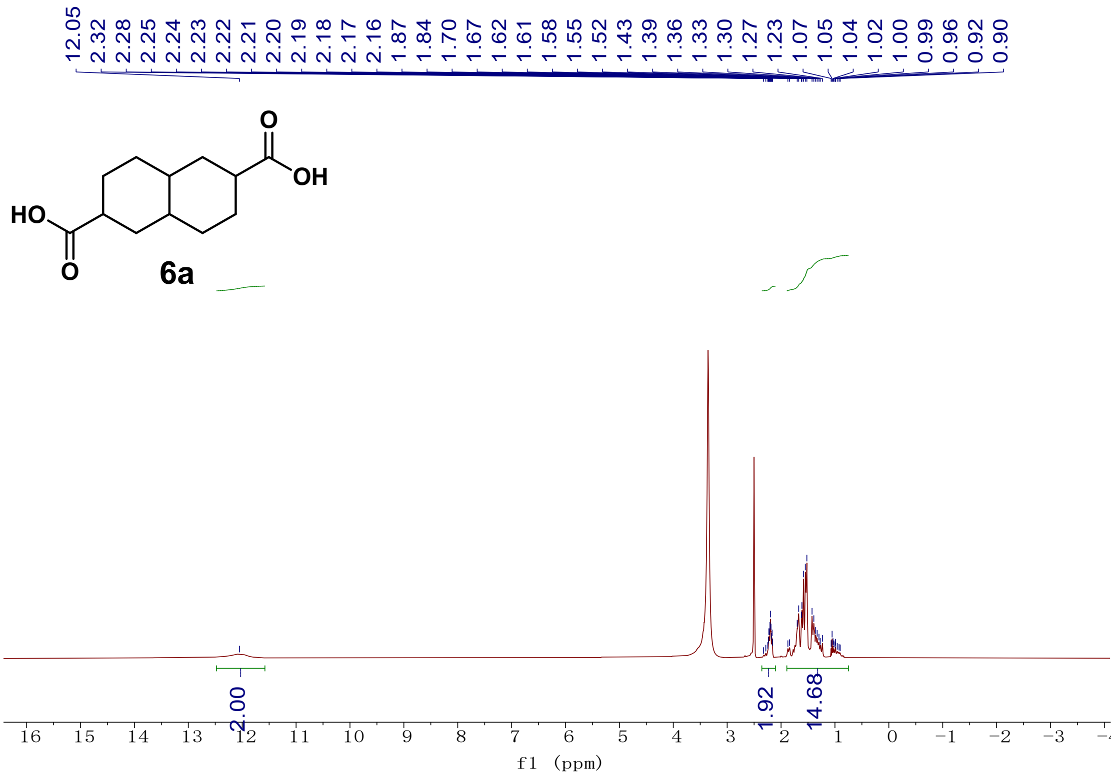


Figure S11. ^{1}H NMR of compound **6a**

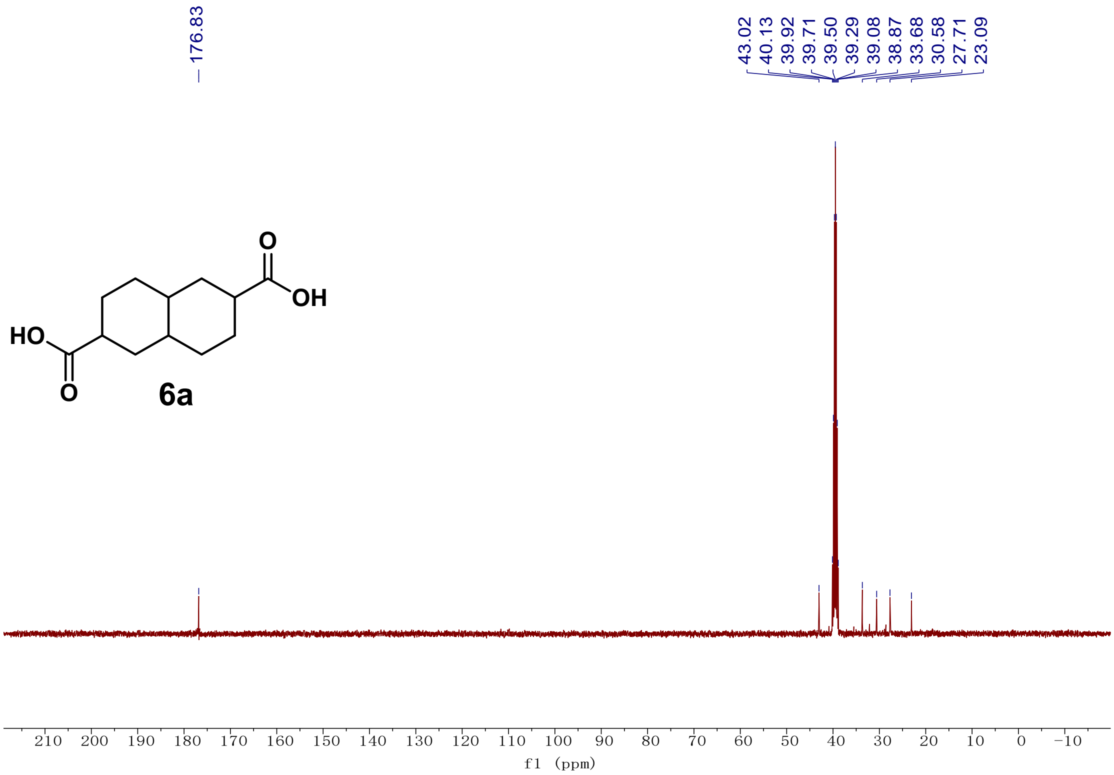


Figure S12. ^{13}C NMR of compound **6a**

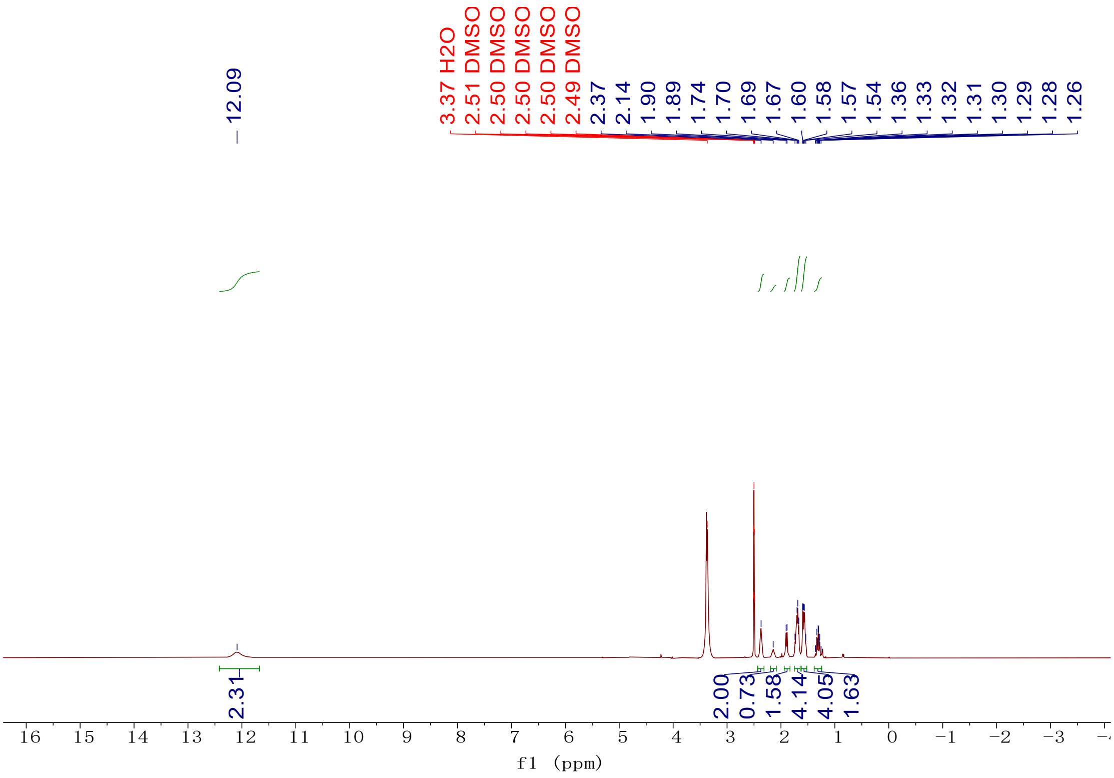


Figure S13. ^{1}H NMR of 1,4-CHDA from commercial PET pellets

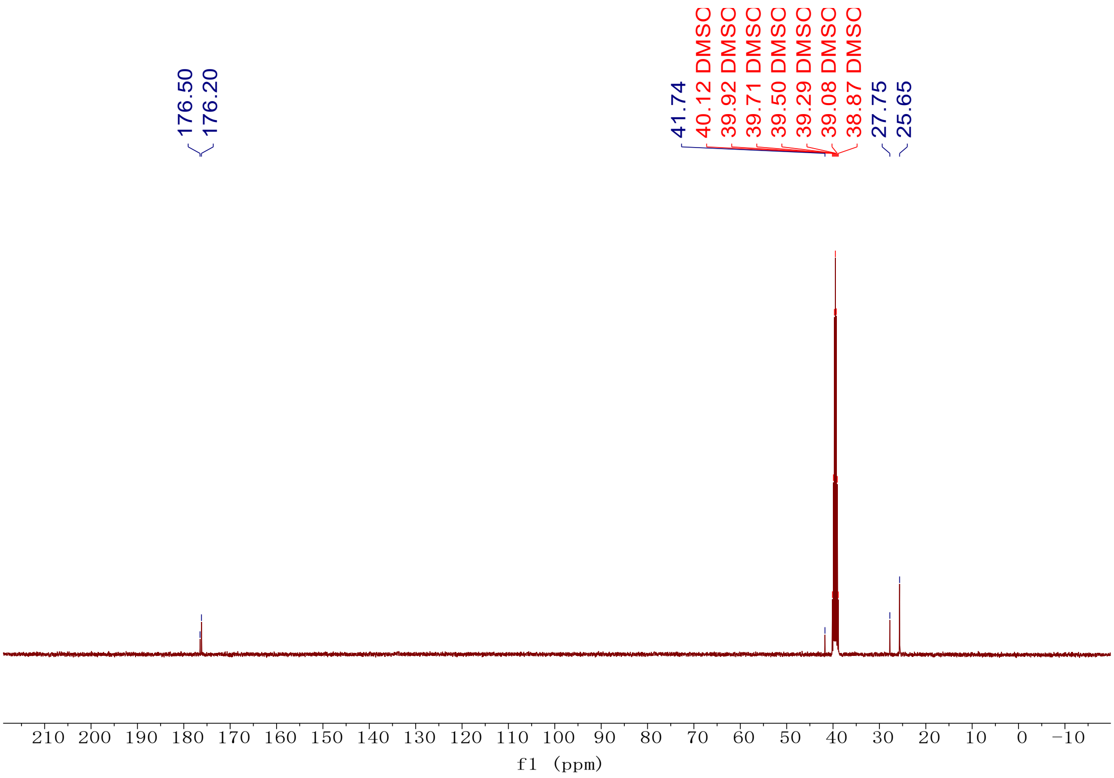


Figure S14. ^{13}C NMR of 1,4-CHDA from commercial PET pellets

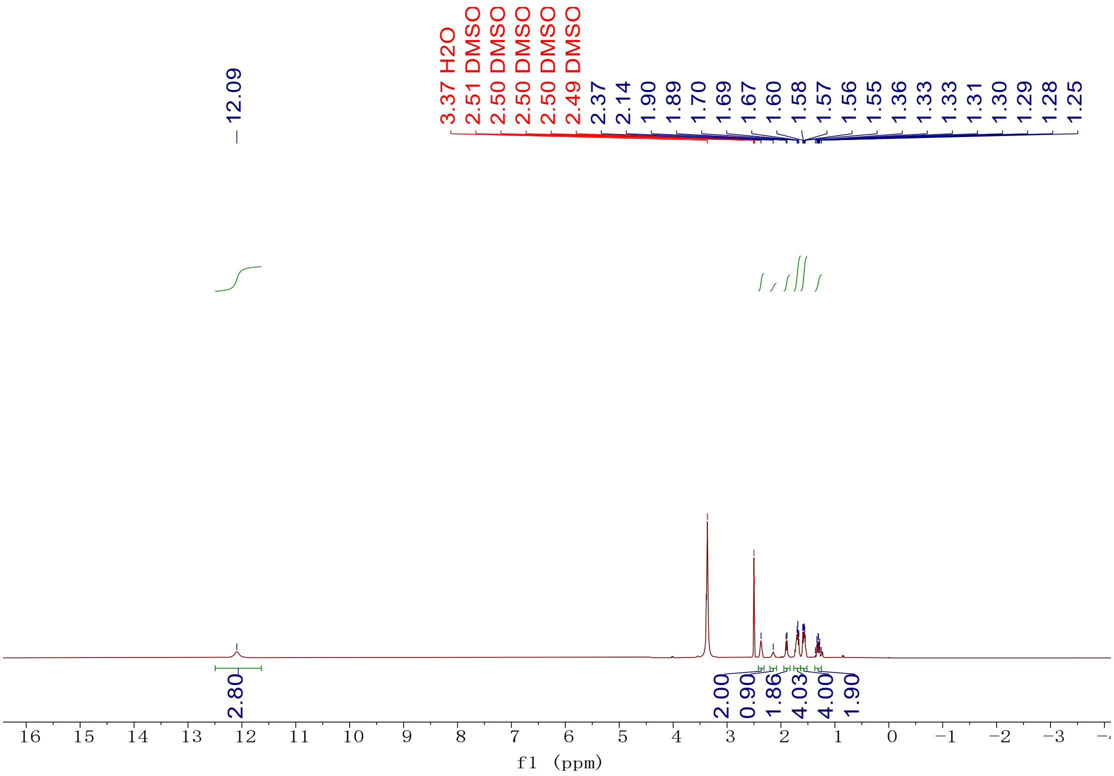


Figure S15. ^{1}H NMR of 1,4-CHDA from food container

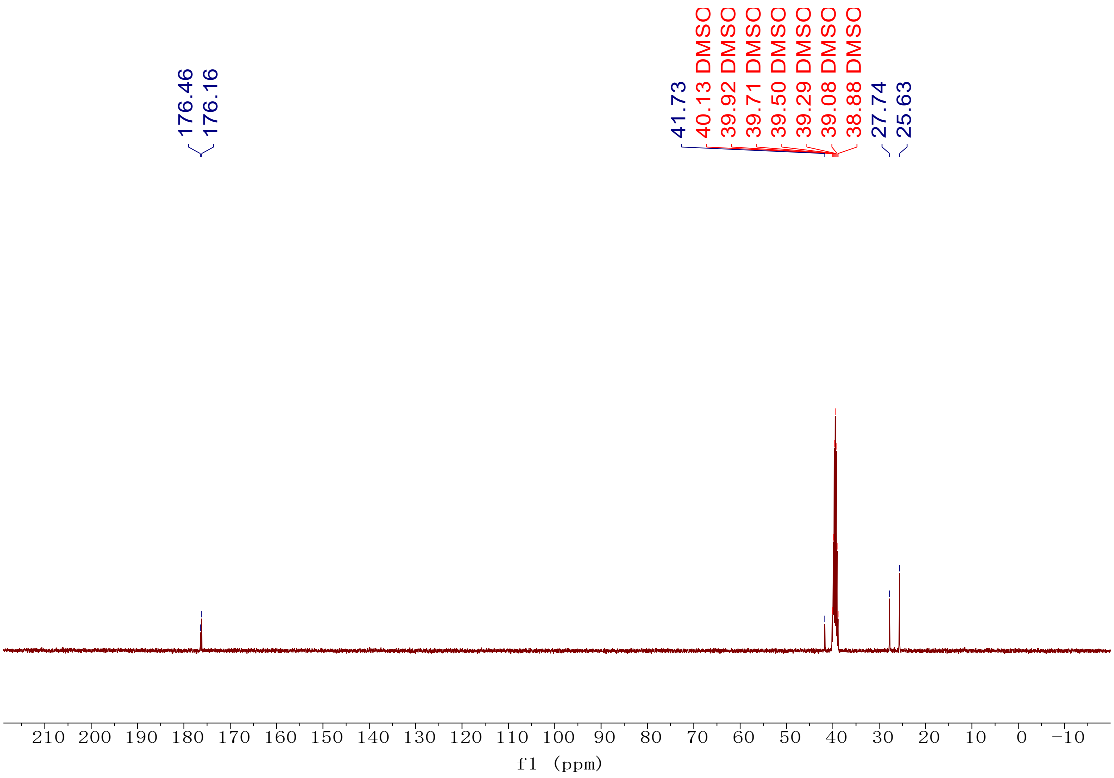


Figure S16.^{13}C NMR of 1,4-CHDA from food container

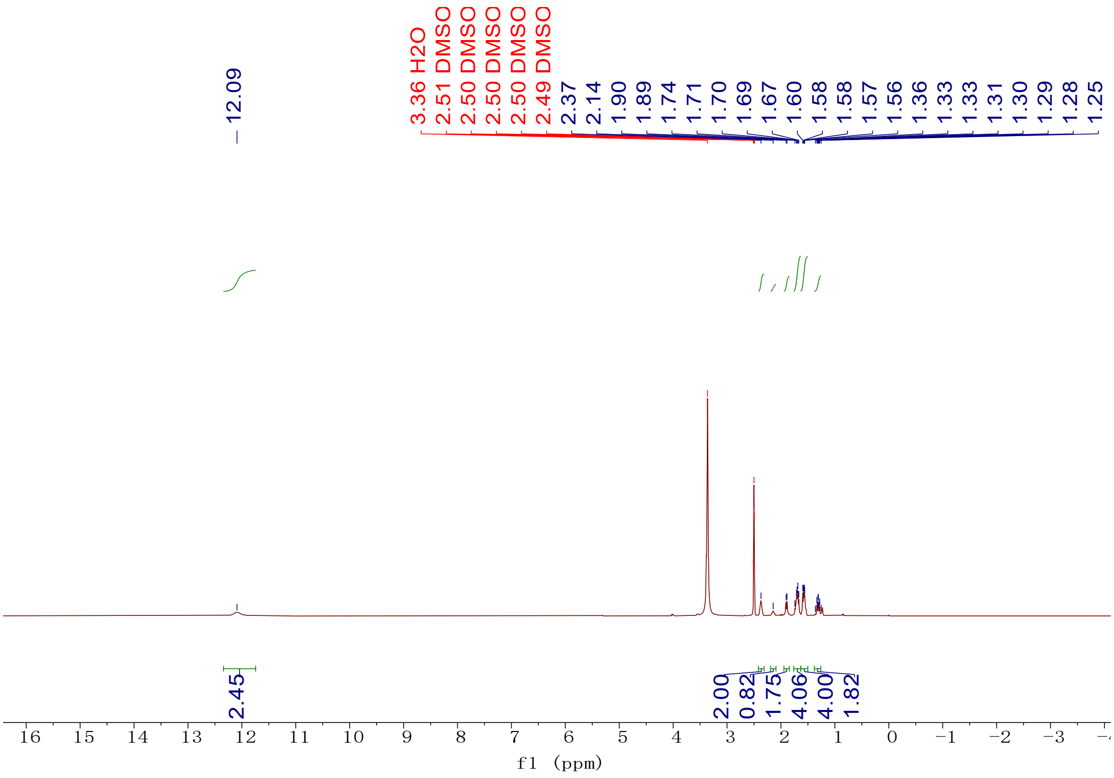


Figure S17. ^{1}H NMR of 1,4-CHDA from food tray

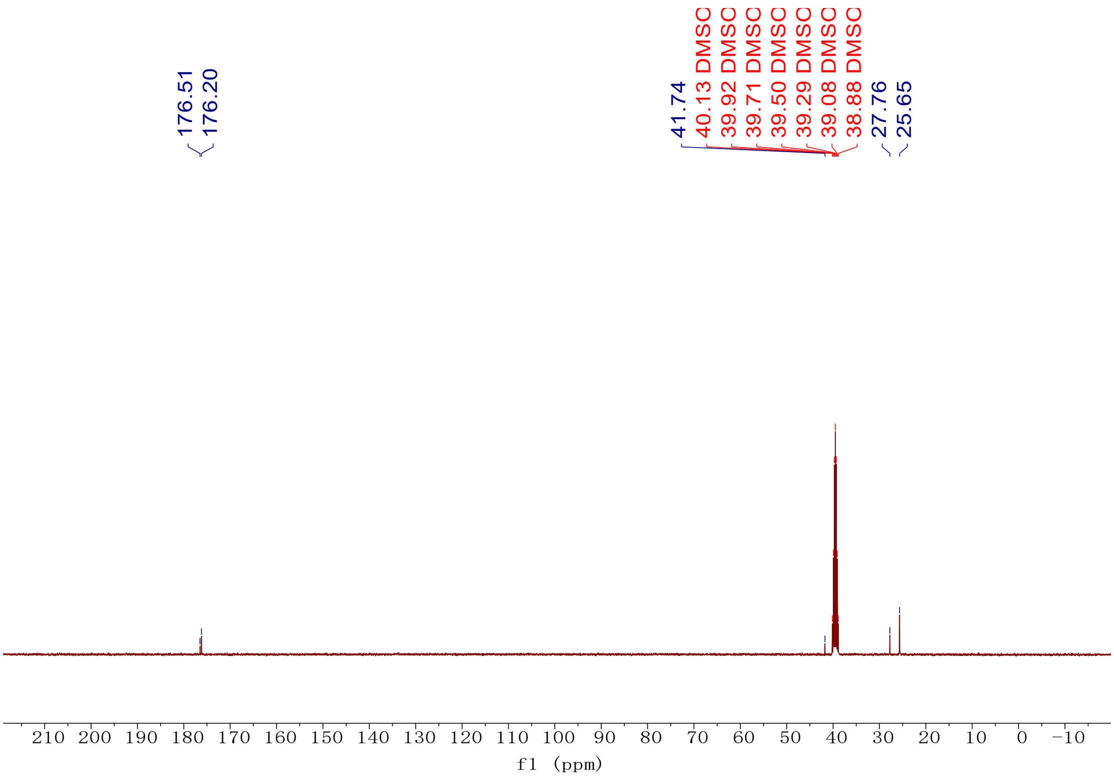


Figure S18. ^{13}C NMR of 1,4-CHDA from food tray

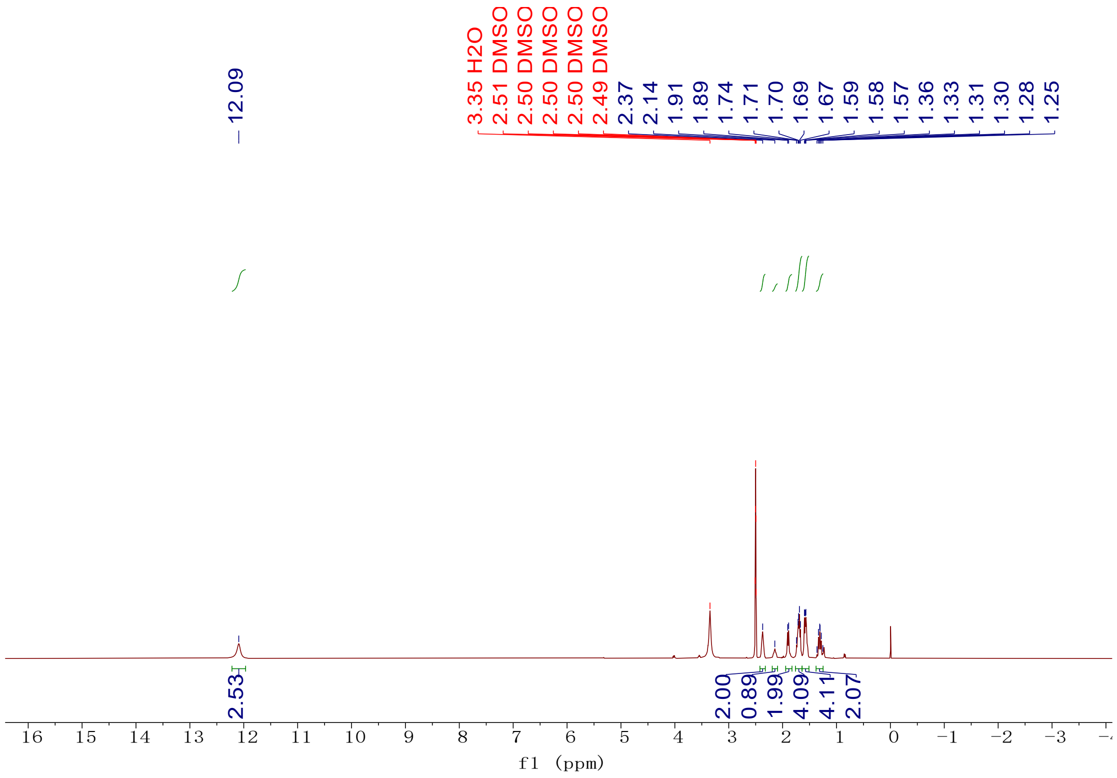


Figure S19. ^{1}H NMR of 1,4-CHDA from colorless water bottle

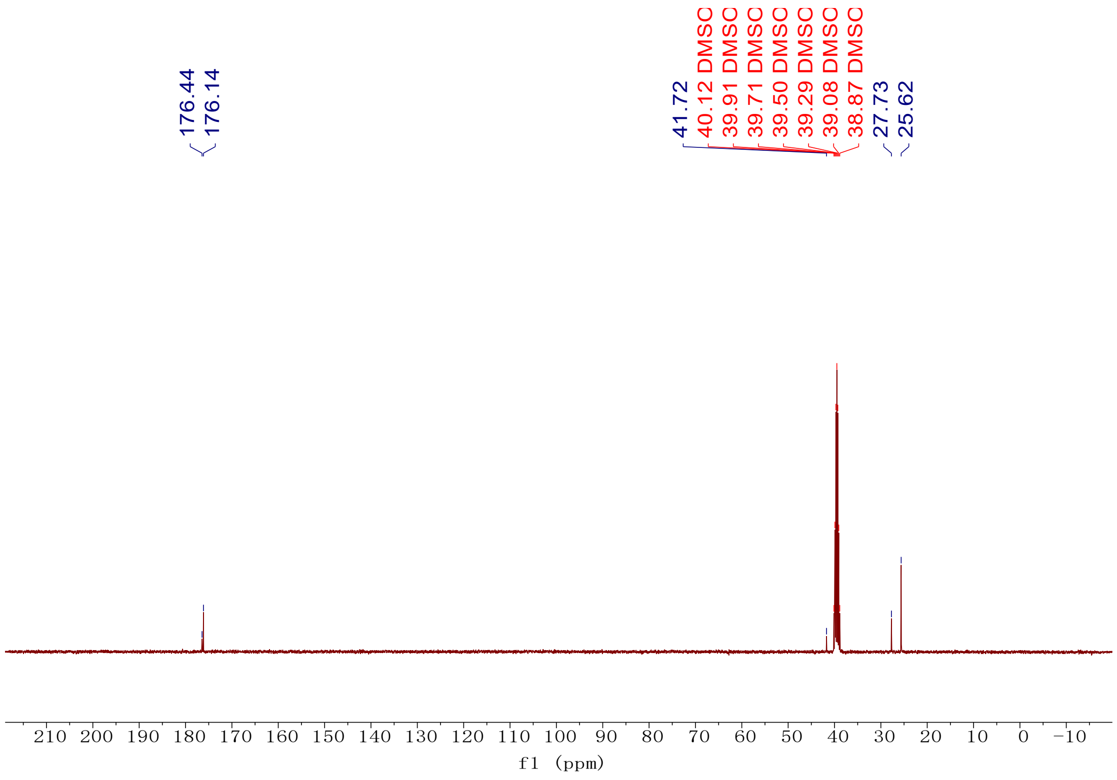


Figure S20. ^{13}C NMR of 1,4-CHDA from colorless water bottle

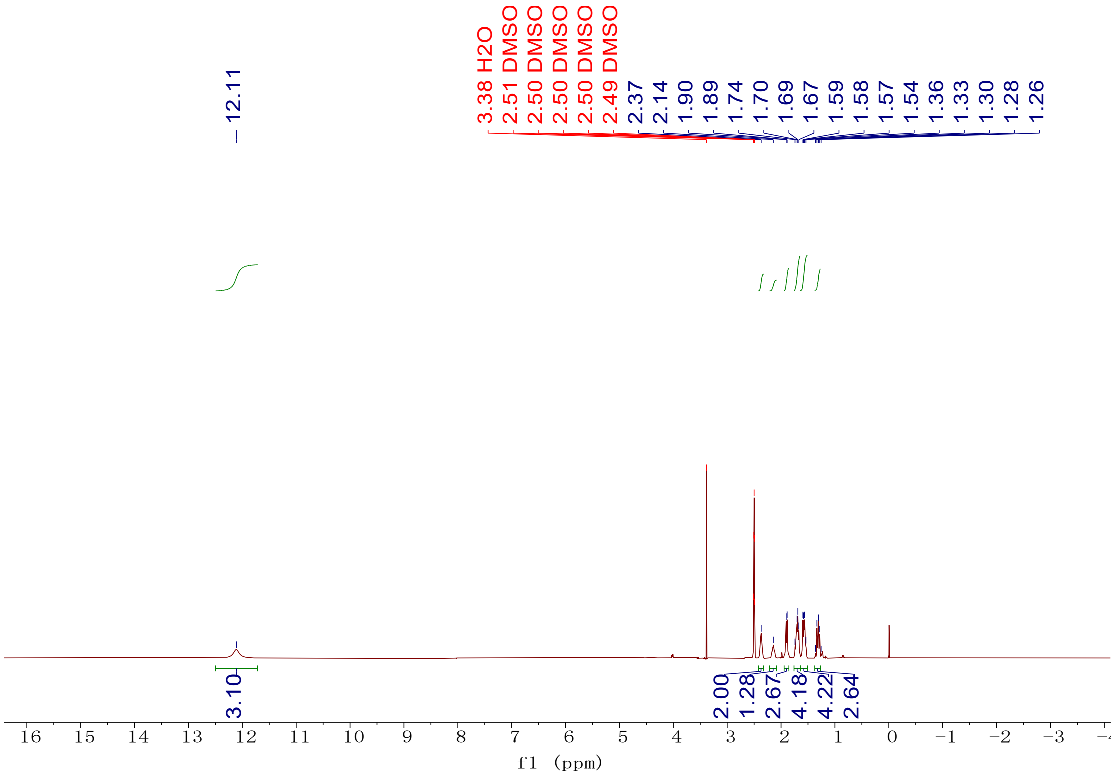


Figure S21. ^{1}H NMR of 1,4-CHDA from green water bottle

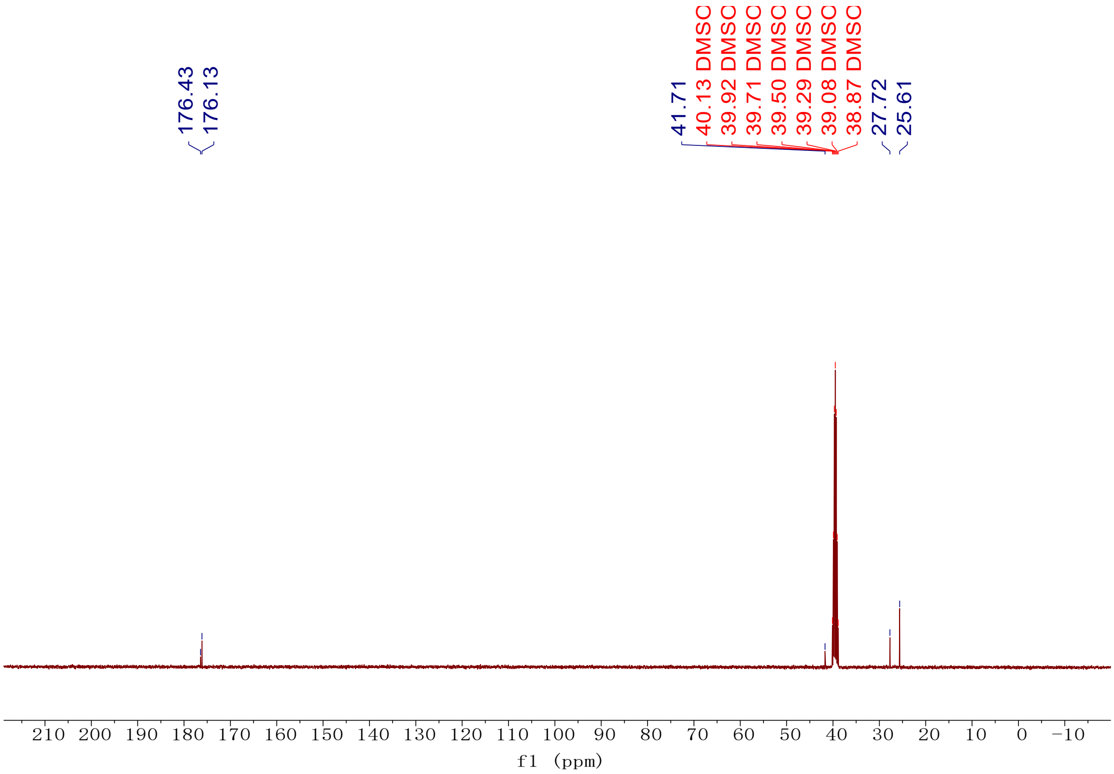


Figure S22. ^{13}C NMR of 1,4-CHDA from green water bottle

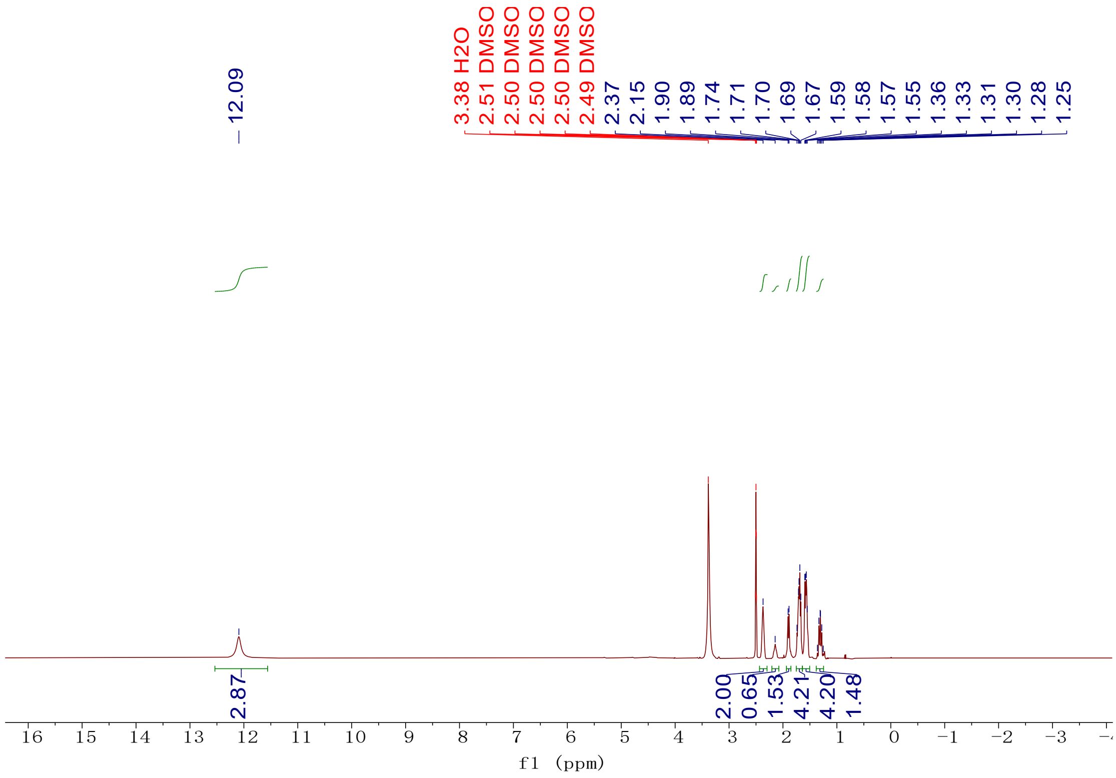


Figure S23.^{1}H NMR of 1,4-CHDA from tape

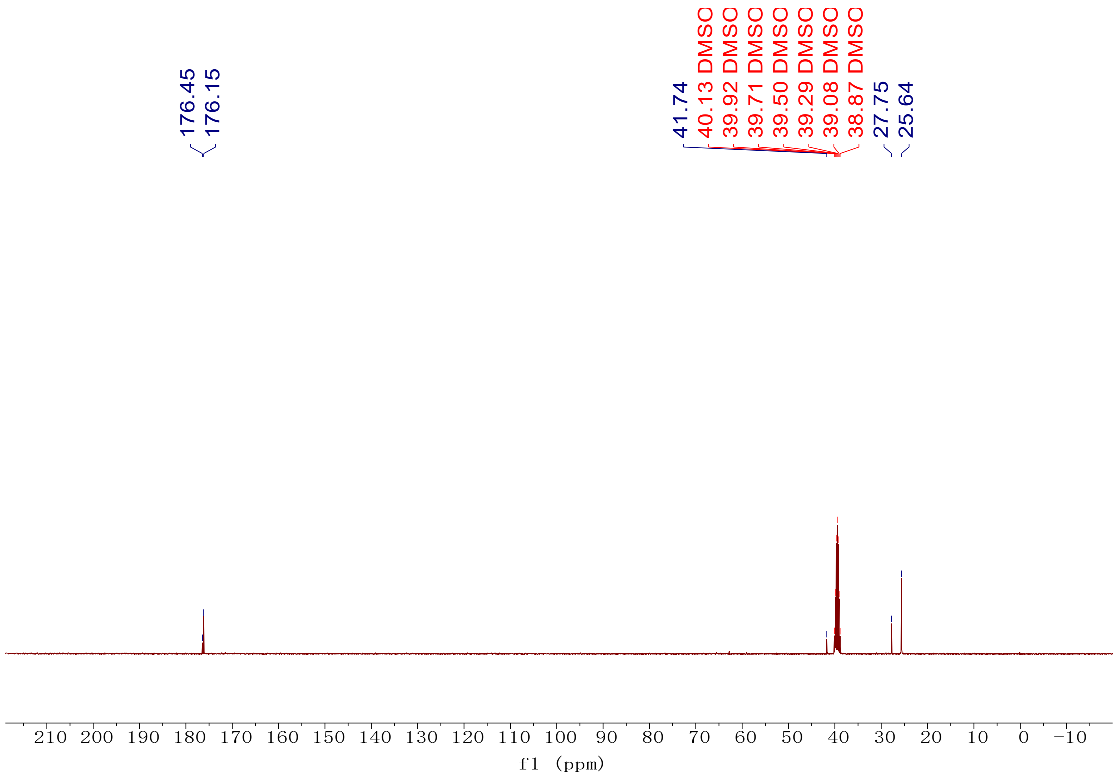


Figure S24. ^{13}C NMR of 1,4-CHDA from tape

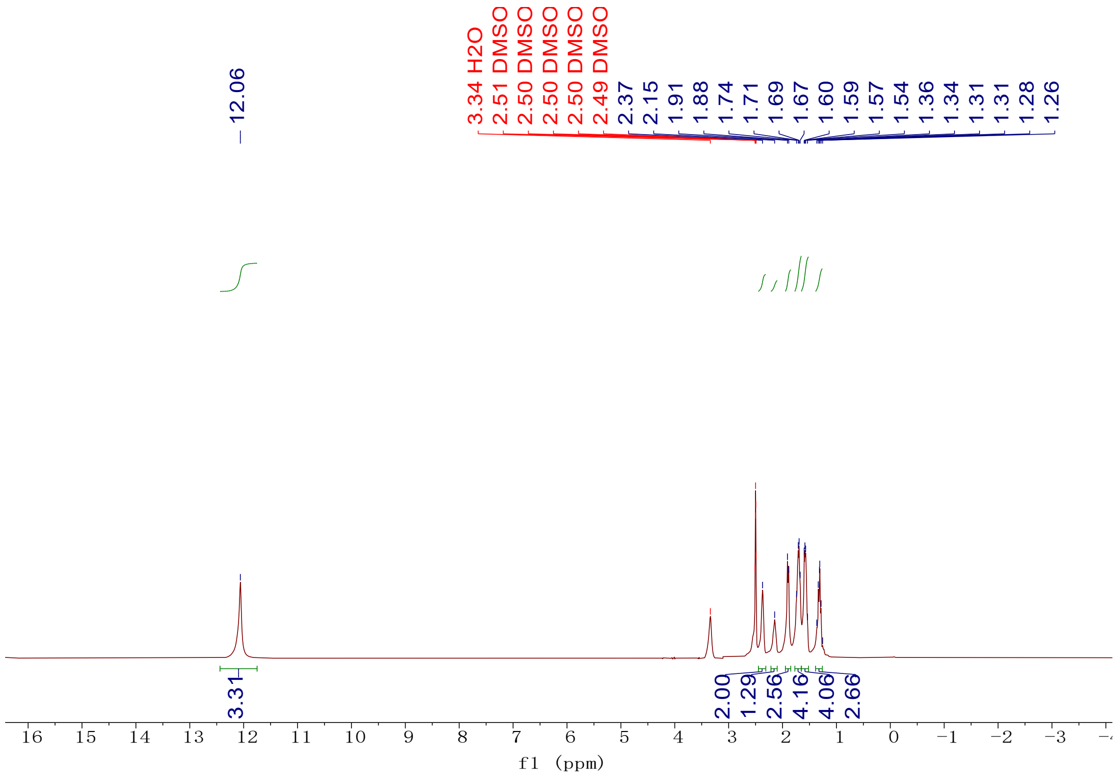


Figure S25. ^{1}H NMR of 1,4-CHDA from strapping band

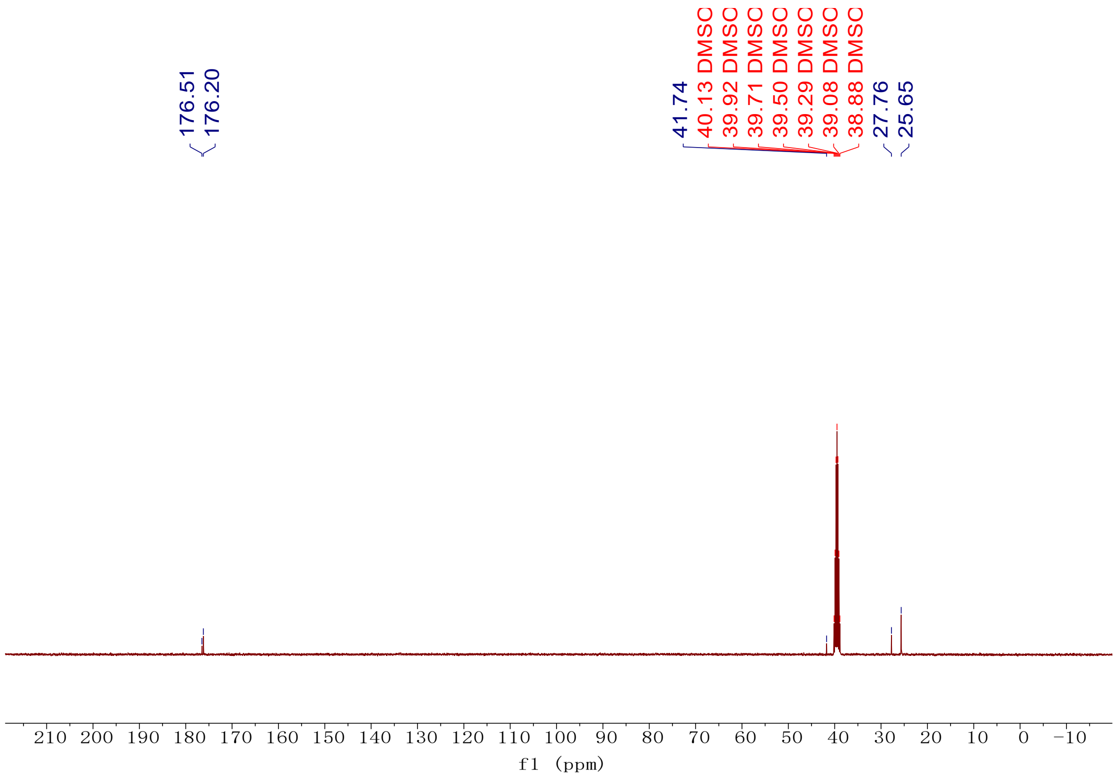


Figure S26.^{13}C NMR of 1,4-CHDA from strapping band

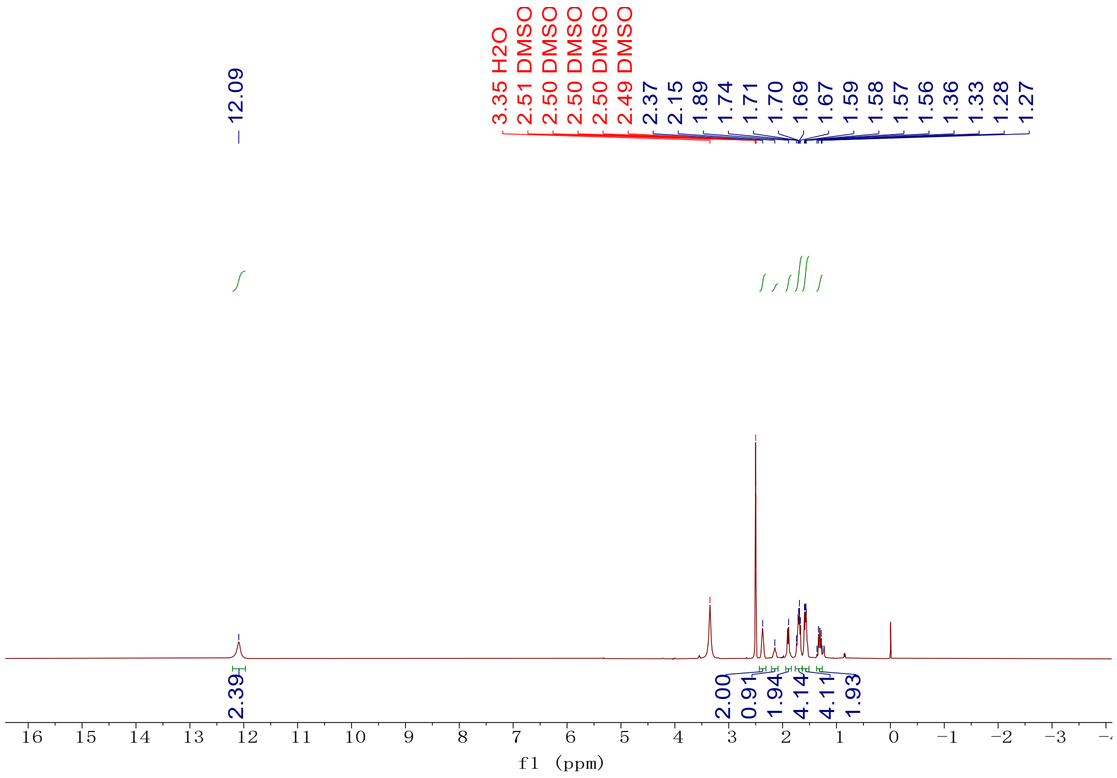


Figure S27. ^{1}H NMR of 1,4-CHDA from sticker

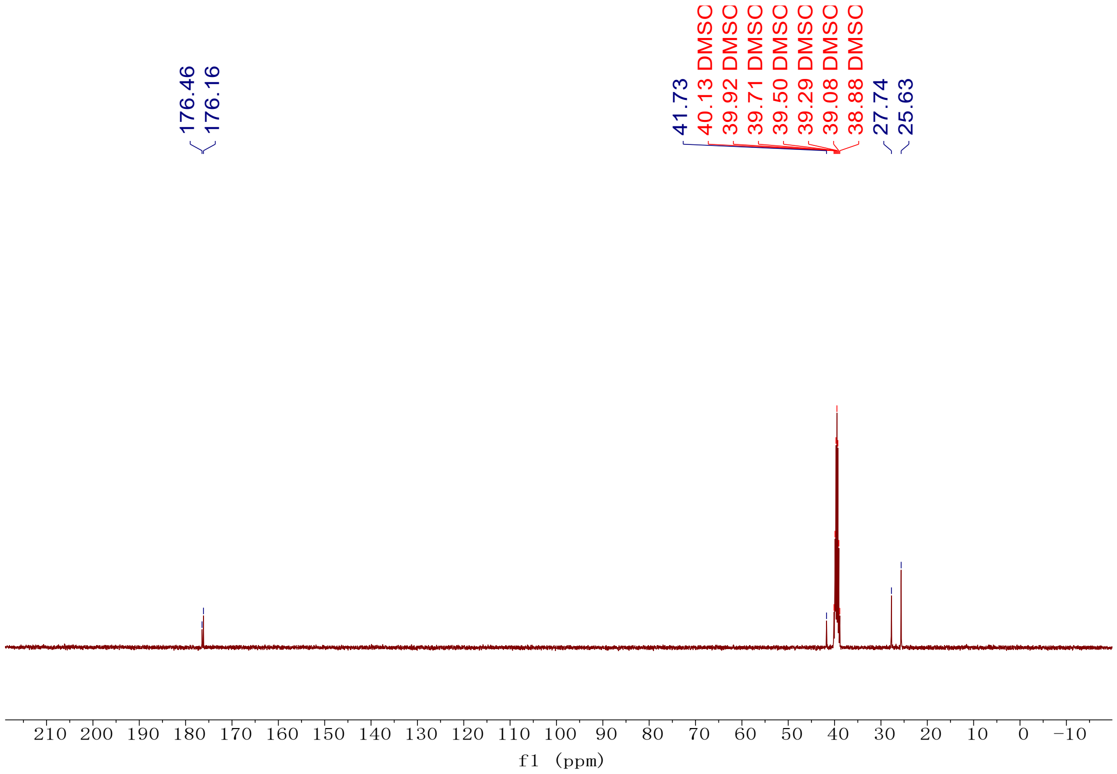


Figure S28. ^{13}C NMR of 1,4-CHDA from sticker

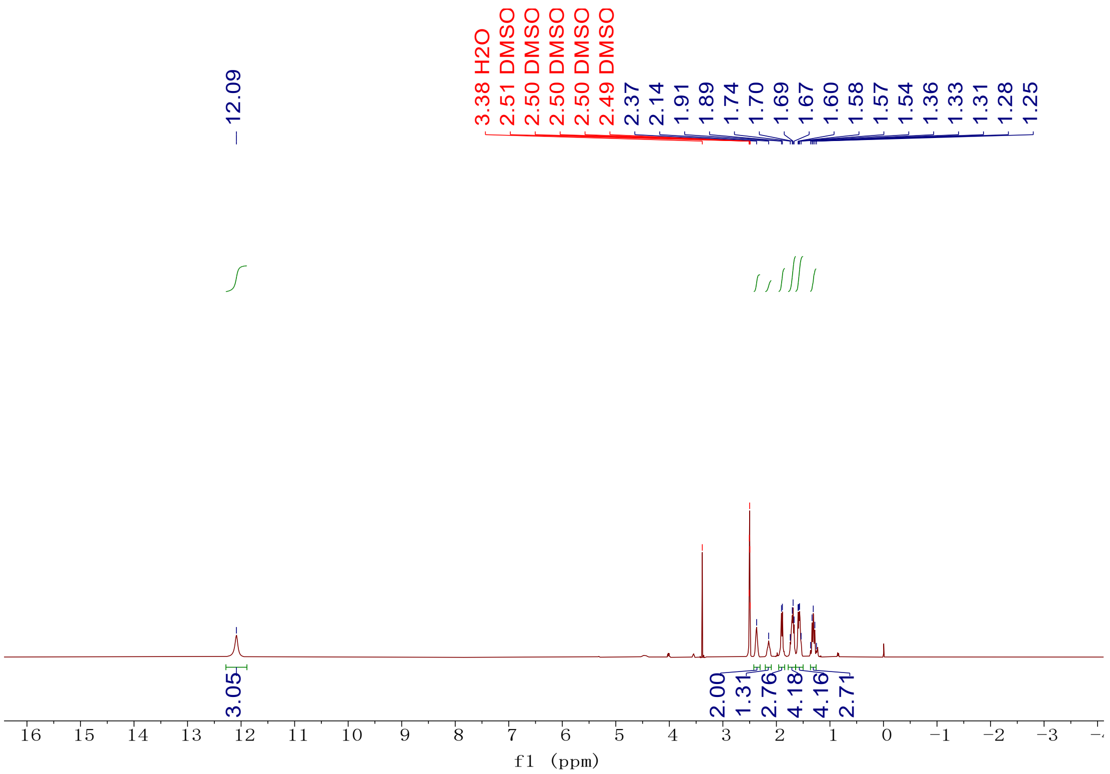


Figure S29. ^{1}H NMR of 1,4-CHDA from PET sheet

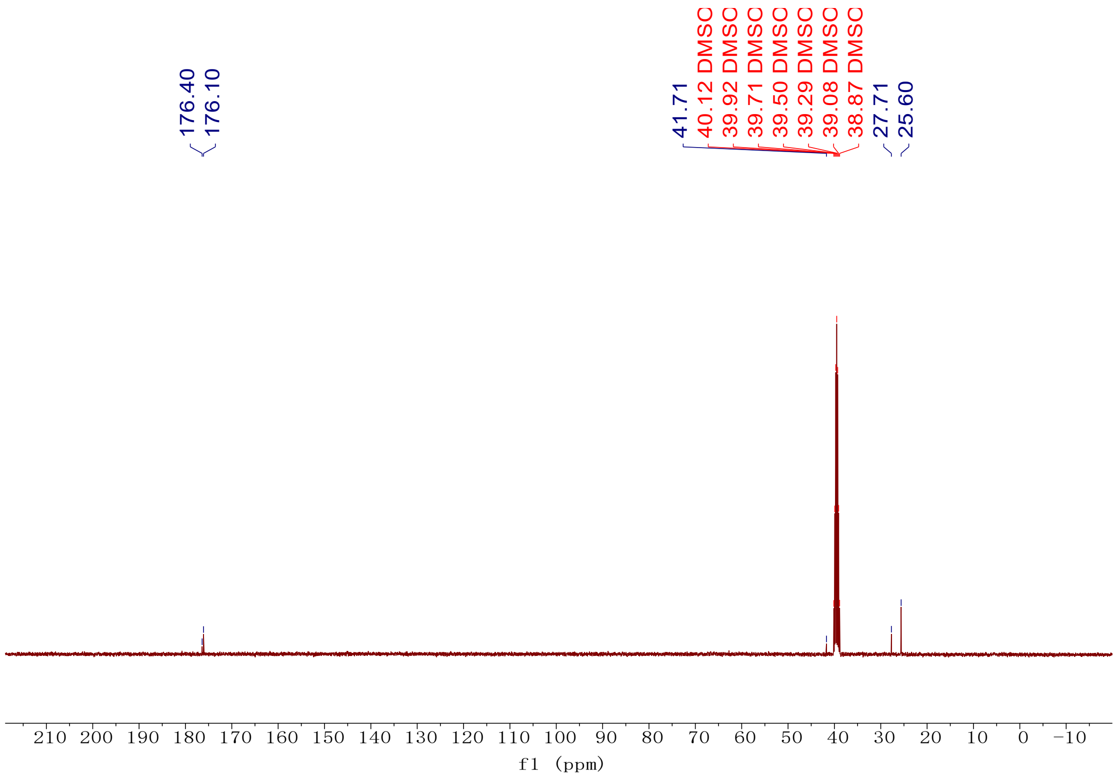


Figure S30. ^{13}C NMR of 1,4-CHDA from PET sheet

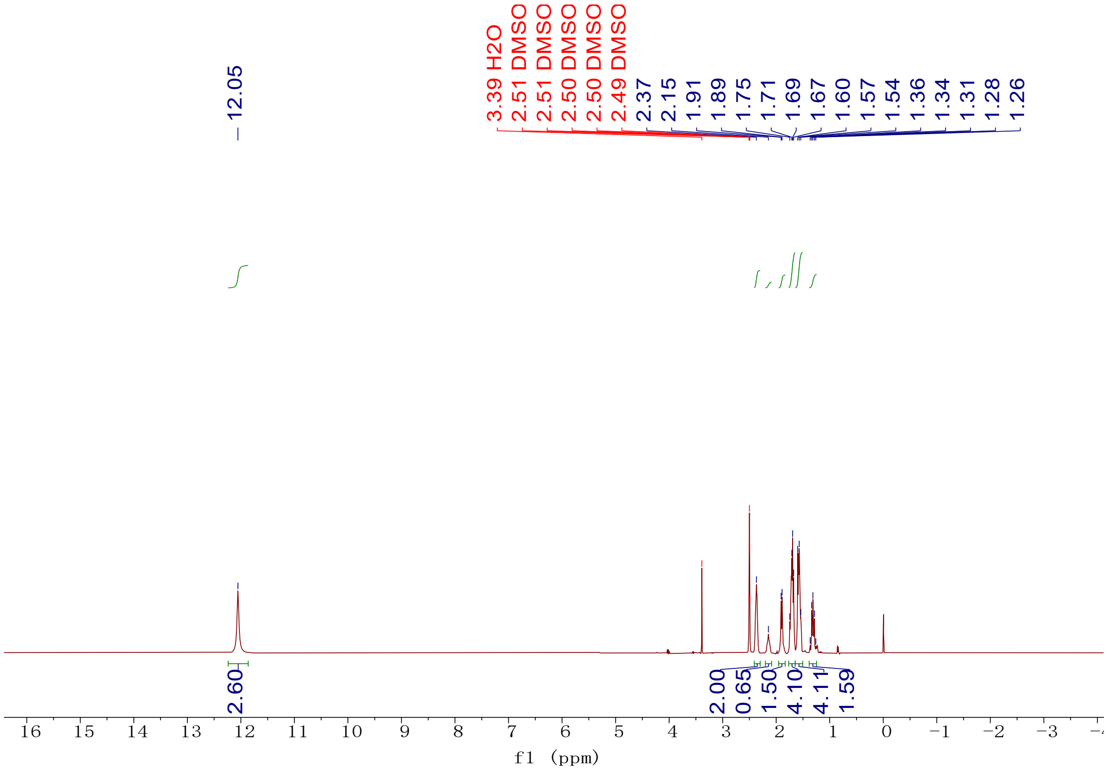


Figure S31. ^{1}H NMR of 1,4-CHDA from PET fabric

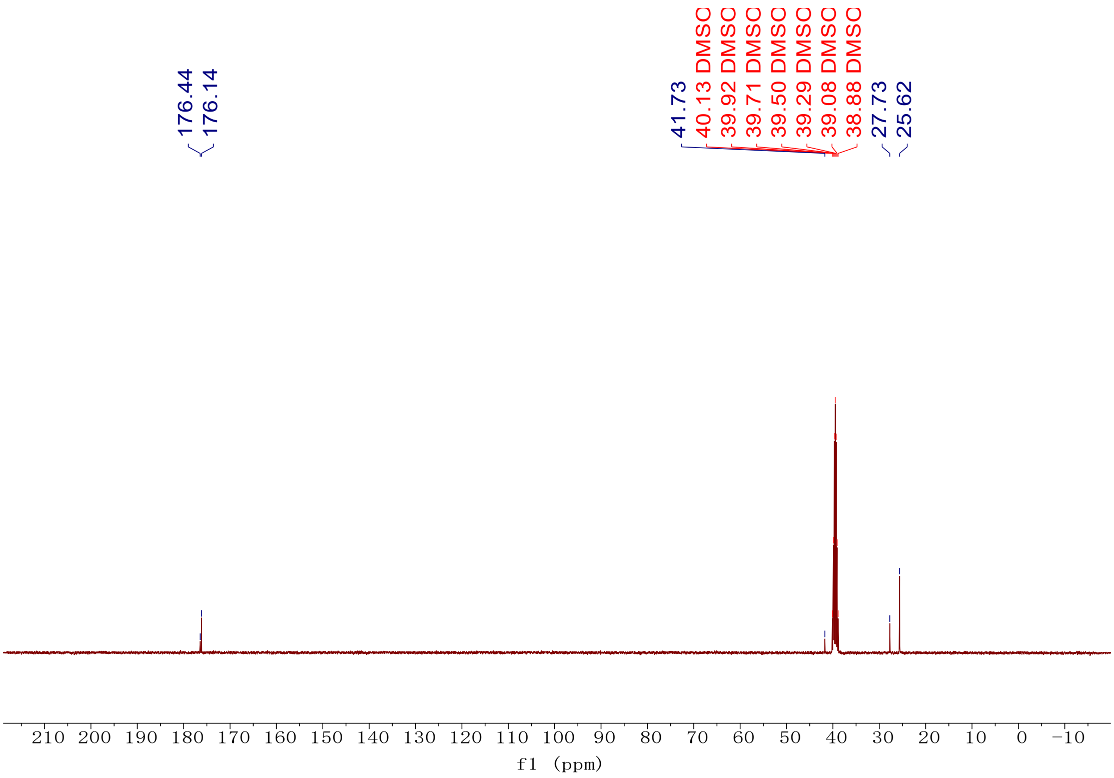


Figure S32. ^{13}C NMR of 1,4-CHDA from PET fabric

6. References

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