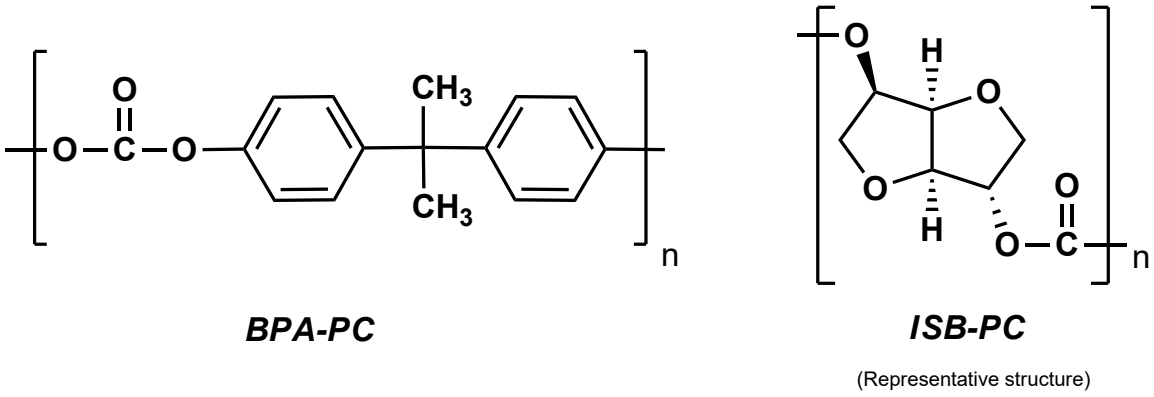
Supporting Information

This document contains supplement figures and tables referenced in the manuscript.

Contents:

S1. Comparison of PC structures



BPA-PC ***ISB-PC***

(Representative structure)

Figure S1. Chemical structures of the commercial polycarbonates used for comparison: (left) petrochemical-based polycarbonate (BPA-PC) and (right) representative bio-based polycarbonate (ISB-PC). The ISB-PC structure is shown as a representative repeat unit because the exact comonomer composition of the commercial grade is proprietary.

S2. Green Metrics Calculation for Solvent-Free Synthesis of ISB-Based Polycarbonate

Detailed green chemistry metrics (E-factor, PMI, Atom Economy) based on experimental values and theoretical analysis.

To evaluate the environmental efficiency of the solvent-free melt polycondensation process used to synthesize EO-functionalized isosorbide-based polycarbonate (ISB-PC), standard green chemistry metrics were calculated using the following formulas:

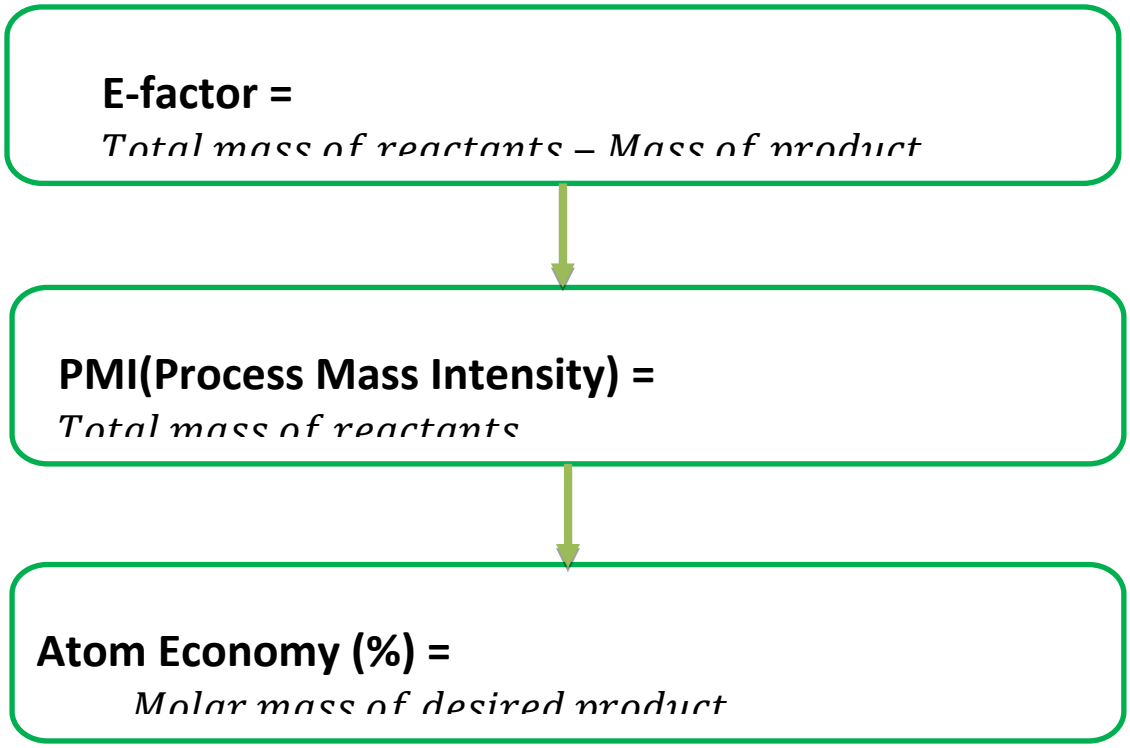


Figure S2. Calculation workflow for green metrics.

The calculation was based on the following experimental data:

Parameter	Value
Total mass of reactants	567.96 g
Mass of product (ISB-PC)	286.79 g
Estimated molar mass of ISB-PC repeating unit	~364 g/mol

Main byproduct	Phenol (94.11 g/mol)

Results of the calculations:

• E-factor = (567.96 – 286.79) / 286.79 = 0.98

• PMI = 567.96 / 286.79 = 1.98

• Atom Economy = 286.79 / (286.79 + approx. 281.38 phenol) × 100 ≈ 50.5%

These values indicate that the synthetic process is resource-efficient, produces minimal waste, and aligns with green chemistry principles, with phenol as the only stoichiometric byproduct.

S3. NMR Spectra

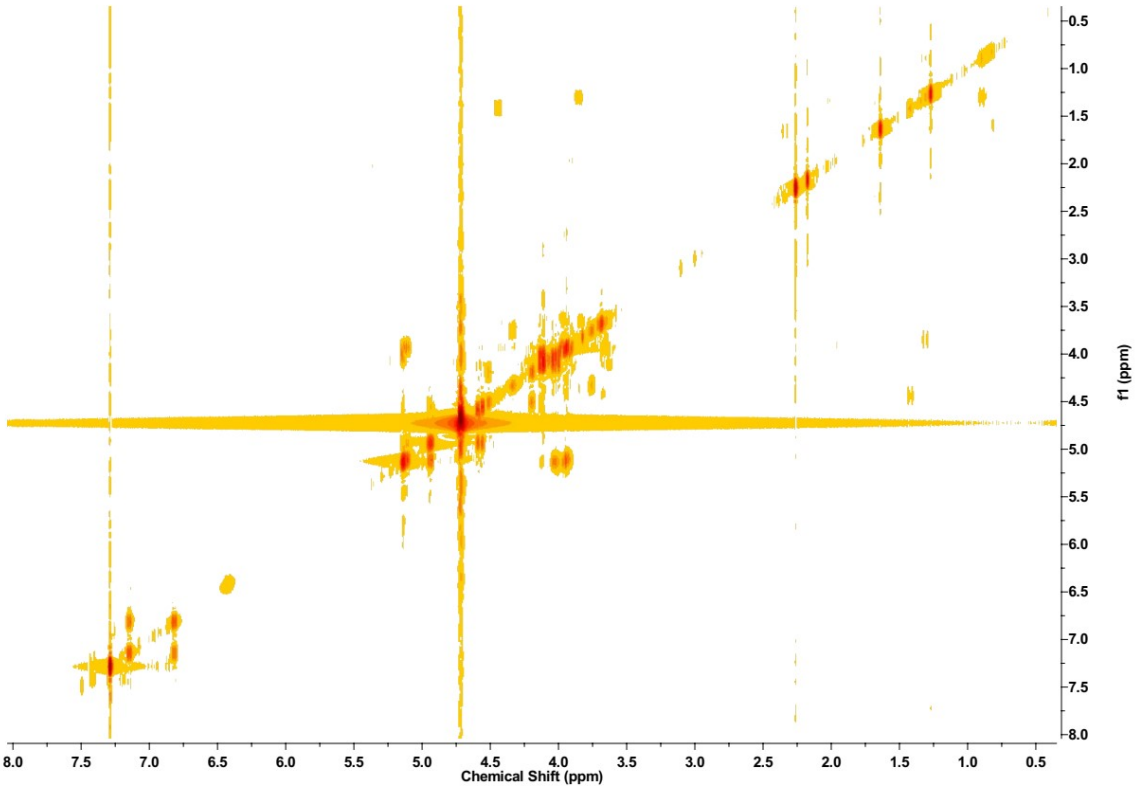


Figure S3-1. Full 2D ^{1}H–^{1}H COSY spectrum of ISB-PC ($CDCl_3$, 500 MHz), showing the complete spectral map used for analysis. The enlarged region of interest is provided in Figure S3-3. A weak cross-peak is observed within the overlapping EO methylene region (4.2–4.6 ppm); however, no sequence-specific correlations (including b_1/b_1') are assigned due to peak overlap and limited signal resolution.

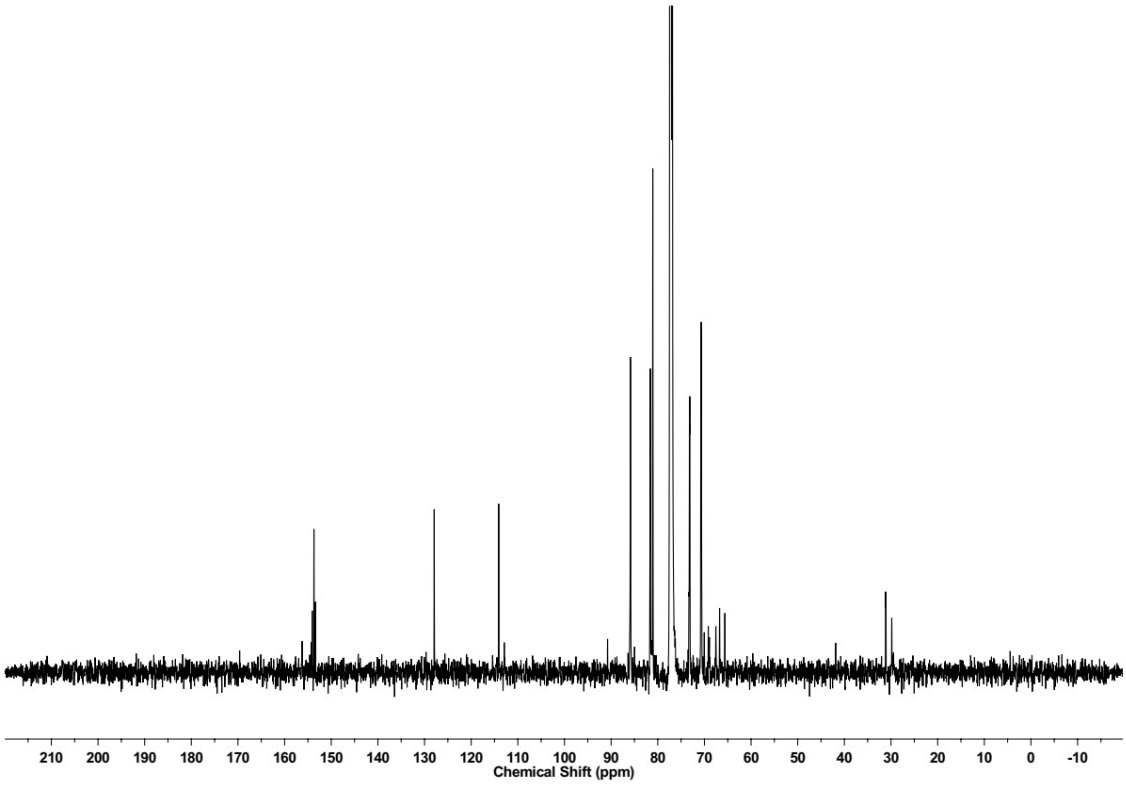


Figure S3-2. Full ^{13}C NMR spectrum of ISB-PC in $CDCl_3$ (100 MHz, ~35 mg/mL, re-acquired under reviewer's recommended conditions). The expanded carbonate region (δ 156–151 ppm) is presented in the main text (Figure 1D), where three distinct peaks at δ 154.08, 153.71, and 153.38 ppm are clearly resolved with markedly improved signal-to-noise ratio, confirming the carbonate sequence assignments.

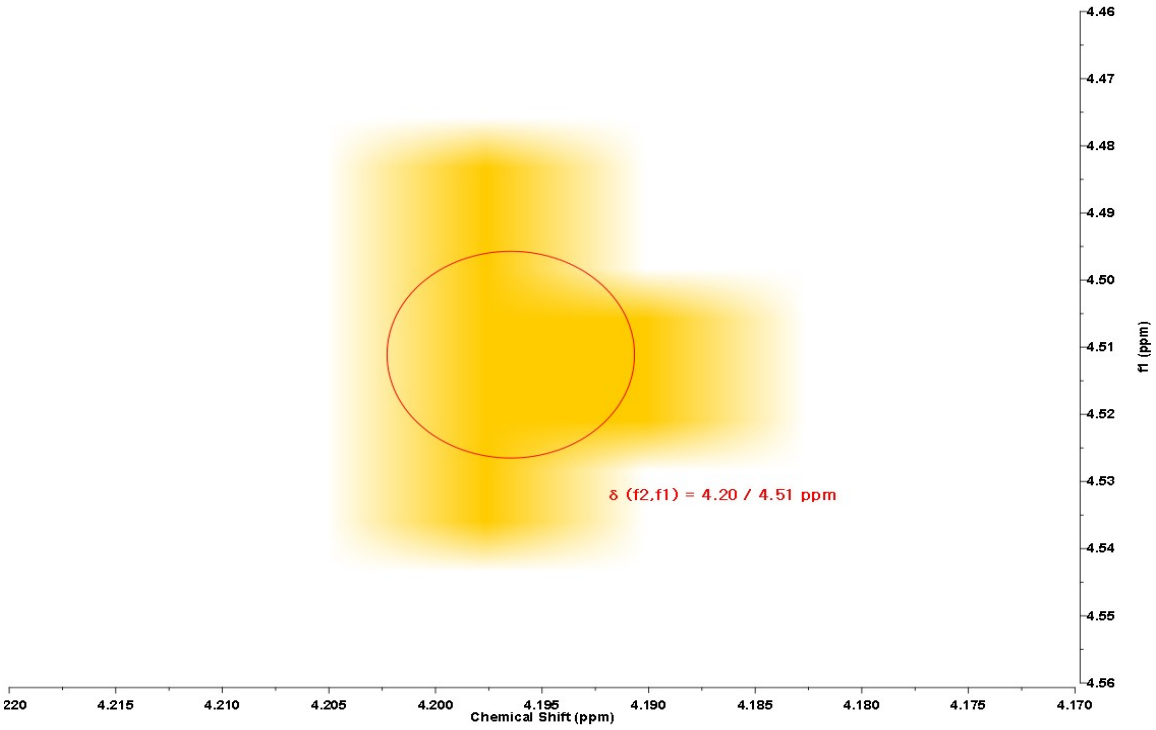


Figure S3-3. Enlarged 2D ^{1}H–^{1}H COSY spectrum highlighting the weak cross-peak within the EO methylene region (4.2–4.6 ppm). Due to spectral overlap and limited resolution, this feature is not assigned to any sequence-specific proton correlation.

Table S1. Excerpt from TopSpin audit trail confirming re-acquisition and processing of the ^{13}C NMR spectrum at high concentration (~35 mg/mL in $CDCl_3$).

Note: All NMR measurements (^{1}H, COSY, and ^{13}C) were performed at 298 K using a Bruker AVANCE 500 MHz spectrometer. The COSY spectrum was acquired at 35 mg mL^{-1} with extended acquisition time and an enlarged ROI to enhance cross-peak visibility, while the ^{13}C spectrum was re-acquired at high concentration with extended acquisition time to improve signal-to-noise ratio.

No.	Date & Time (KST)	User	Process	Notes
1	2025-08-12 05:50:06	nmrsu	Acquisition	^{13}C NMR acquisition started (Bruker AVANCE 500 MHz, CAB AV4 BASIC).
2	2025-08-12 06:44:05	nmrsu	Acquisition	Acquisition completed, new dataset created (UUID: 32ccbeca…).
3	2025-08-12 15:43:36	nmrsu	Processing	Raw data processing initiated (LB = 1, SI = 32K).
4	2025-08-12 15:43:37	nmrsu	Processing	Peak picking (apk), baseline correction (abs), phase adjustment.
5	2025-08-13 08:58:30–34	nmrsu	Processing	Final processing: apbk, ht, apk, abs (baseline correction repeated).