Electronic Supplementary Material (ESI) for RSC Advances.

Role of *cis*-1,4-Cyclohexanedicarboxylic Acid in the Regulation of Structure and Properties of Poly(butylene adipate-*co*-butylene 1,4-cyclohexanedicarboxylate) Copolymer

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Sequence distribution analysis for PBAC-50

The sequence distribution of PBAC-50 is determined by analysis of ^{13}C NMR spectra of the sample which is showed in Figure S1. All peaks with different chemical shifts can be assigned to carbons accordingly in the final product. Special attention is paid to the peaks locate at region I in the range of 173.0 to 175.5ppm. These peaks are carbons of carbonyl group in both butylene adipate unit and butylene 1,4-cyclohexanedicarboxylate unit. Further analysis revealed that these peaks are not perfect single peak but contain shoulders resulting from different sequences. The chemical structure of all possible sequences are showed in Figure S2. All peaks for carbonyl group in the range of 173.0 to 175.5ppm were curve fitted and resolved into two components as showed in Figure S3. The peak fitting results are collected in Table S1. As a result, the sequence distribution of PBAC-50 copolymer can be calculated from the integration of the resolved peaks in Table S1 according to equations (S1) to (S5)[1].

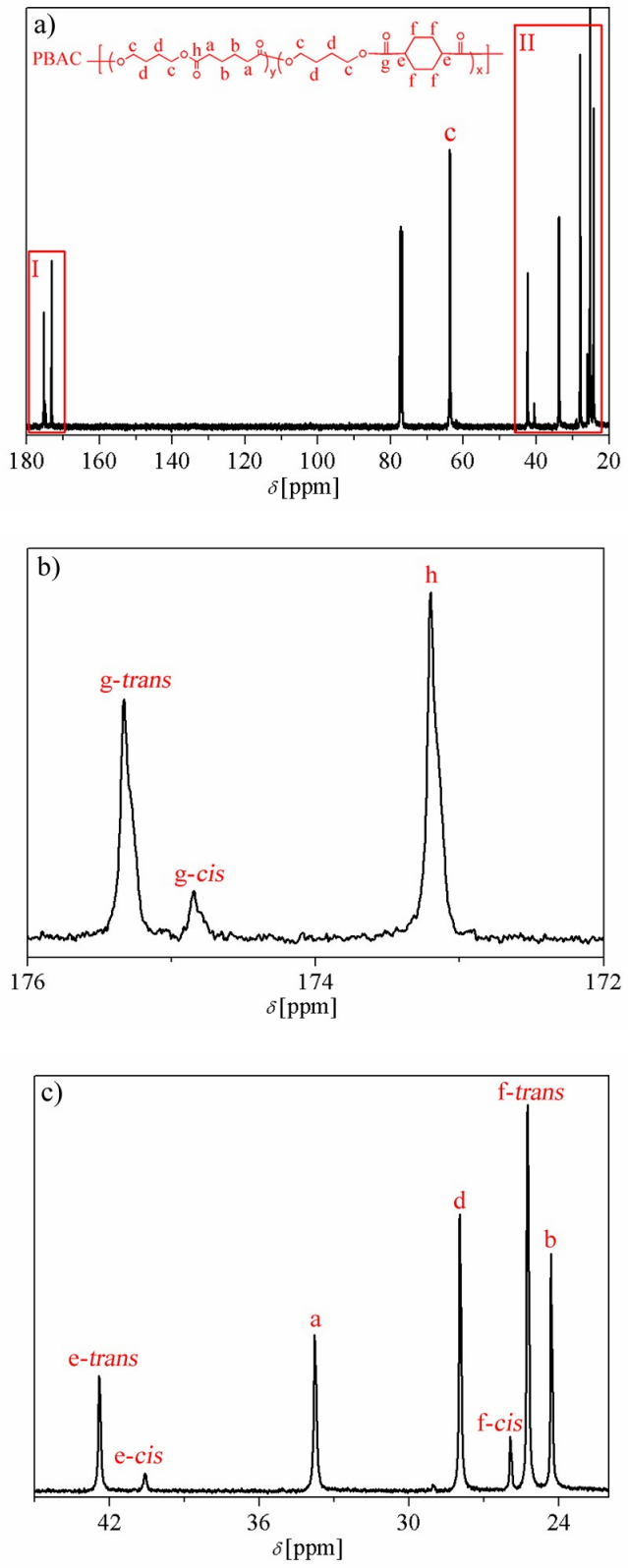


Figure S1 ^{13}C NMR (400MHz, $CDCl_3$) spectra of PBAC-50 copolymer, a) full spectra, b) region I and c) region II.

In the first place, the composition of PBAC-50, namely the amount of PBC and

PBA in the copolymer is calculated by using equation (S1). The calculated PBC amount is 46%, which is very close to the one from ^{1}H NMR analysis. Secondly, the amount of *trans*-CHDA can be calculated from equation (S2), which is 84%. This result is also in great agreement with that from ^{1}H NMR analysis. More importantly, the number-average lengths of PBC ($L_{n,PBC}$) and PBA ($L_{n,PBA}$) units are calculated according to equation (S3) and (S4), which are 2.24 and 1.62 respectively. And the degree of randomness (R) is then obtained according to equation (S5), which is 1.06.

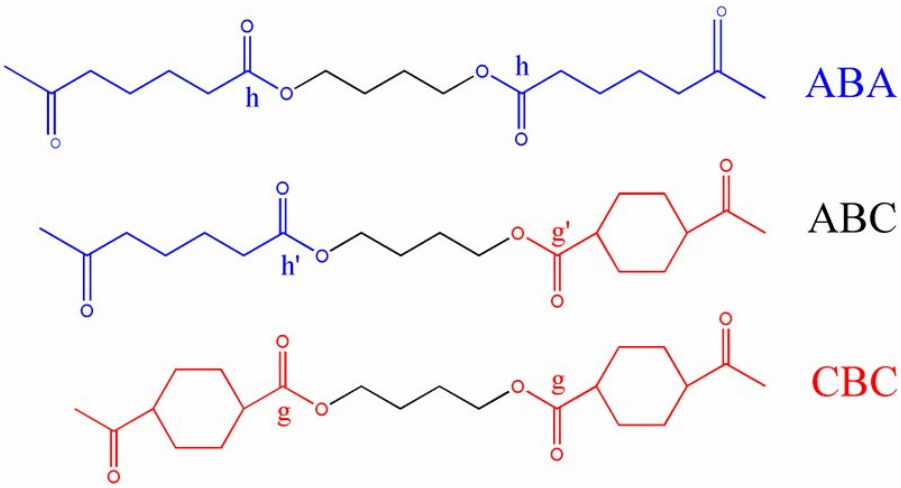
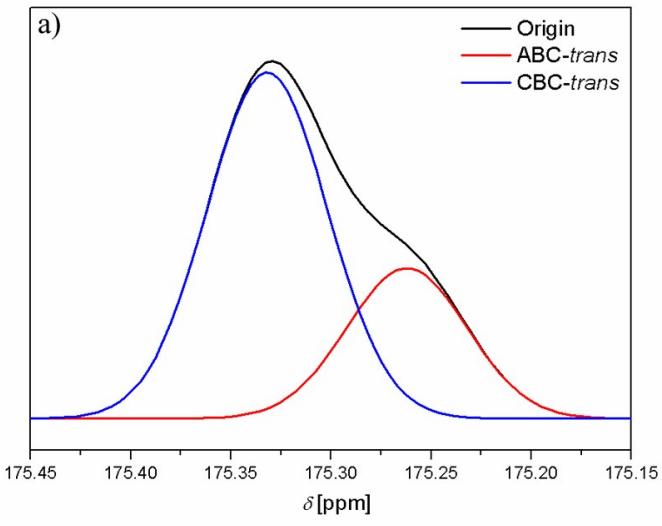


Figure S2 Chemical structure of ABA, ABC and CBC units in PBAC copolymers



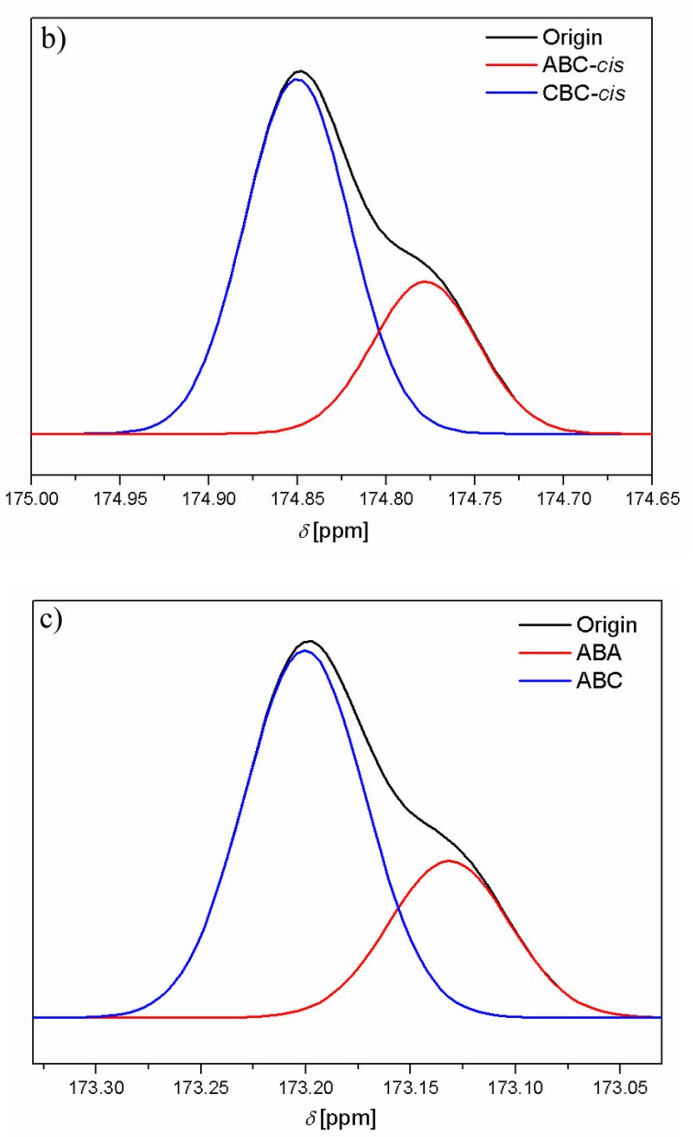


Figure S3 Peak fitting for chemical shifts of carbons of a) g-*trans*, b) g-*cis* and c) h.

Table S1 Peak fitting results for PBAC-50 copolymer

Peak	h	h'	g-*trans*	g-*cis*	g'-*trans*	g'-*cis*
δ (ppm)	173.13	173.20	175.33	174.85	175.26	174.78
Sequence	ABA	ABC	CBC	CBC	ABC	ABC
Integration	0.35	0.83	0.59	0.11	0.26	0.04

$$\text{PBC } mol\% = \frac{I_{\text{g - trans}} + I_{\text{g - cis}} + I_{\text{g'-trans}} + I_{\text{g'-cis}}}{I_{\text{h}} + I_{\text{h'}} + I_{\text{g - trans}} + I_{\text{g - cis}} + I_{\text{g'-trans}} + I_{\text{g'-cis}}} \times 100\% \quad \text{(S1)}$$

$$trans\text{-CHDA } mol\% = \frac{I_{\text{g - trans}} + I_{\text{g'-trans}}}{I_{\text{g - trans}} + I_{\text{g - cis}} + I_{\text{g'-trans}} + I_{\text{g'-cis}}} \times 100\% \quad \text{(S2)}$$

$$L_{\text{n, PBC}} = 1 + \frac{2(I_{\text{g - trans}} + I_{\text{g - cis}})}{I_{\text{h'}} + I_{\text{g'-trans}} + I_{\text{g'-cis}}} \quad \text{(S3)}$$

$$L_{\text{n, PBA}} = 1 + \frac{2I_{\text{h}}}{I_{\text{h'}} + I_{\text{g'-trans}} + I_{\text{g'-cis}}} \quad \text{(S4)}$$

$$R = \frac{1}{L_{\text{n, PBC}}} + \frac{1}{L_{\text{n, PBA}}} \quad \text{(S5)}$$

Table S2 Calculated composition and sequence distribution of PBAC-50 copolymer

Sample	PBC (mol%)	PBA (mol%)	*trans*-CHDA (mol%)	$L_{\text{n,PBC}}$	$L_{\text{n,PBA}}$	R
PBAC-50	46	54	84	2.24	1.62	1.06

References

(1) Wu, B.; Xu, Y.; Bu, Z.; Wu, L.; Li, B.-G.; Dubois, P. *Polymer.* **2014**, *55*, 3648–3655.