Supplementary Information (SI) for Polymer Chemistry. This journal is © The Royal Society of Chemistry 2025

**Supporting Information** 

Achieving very high performance polybenzoxazines from natural

renewable isoliquiritigenin: Design, preparation and property

investigation

Xie Lin and Kan Zhang\*

Institute of Polymer Materials, School of Materials Science and Engineering, Jiangsu University,

Zhenjiang 212013, China.

\*: To whom correspondence should be addressed:

Kan Zhang: zhangkan@ujs.edu.cn

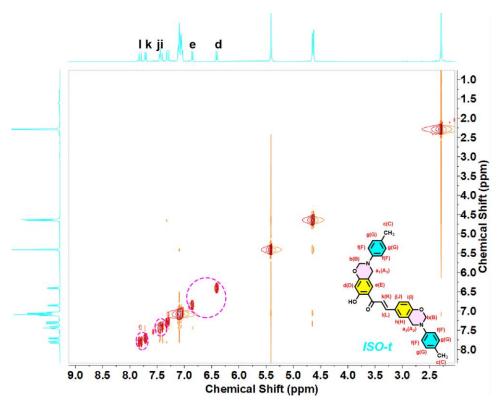


Figure S1. 2D <sup>1</sup>H-<sup>1</sup>H NOESY NMR spectrum of ISO-t in CDCl<sub>3</sub>.

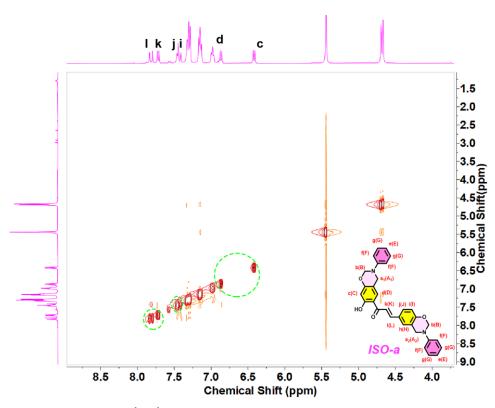


Figure S2. 2D  $^{1}\text{H-}^{1}\text{H}$  NOESY NMR spectrum of ISO-a in CDCl<sub>3</sub>.

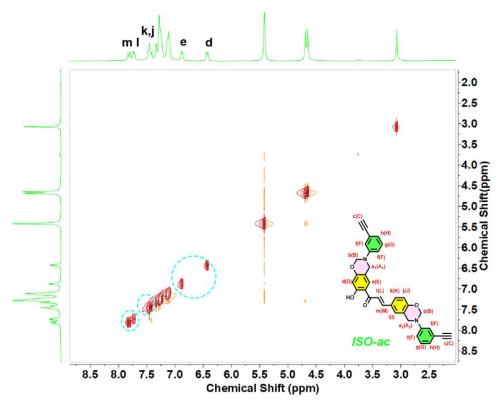


Figure S3. 2D <sup>1</sup>H-<sup>1</sup>H NOESY NMR spectrum of ISO-ac in CDCl<sub>3</sub>.

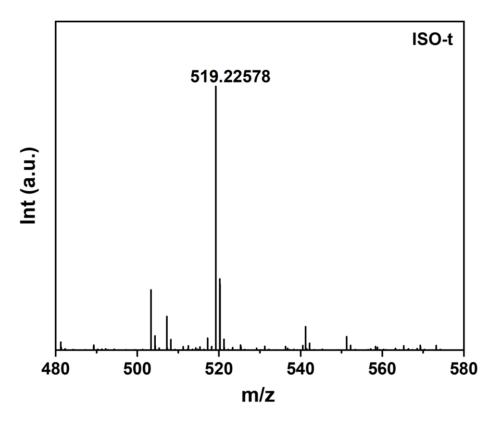


Figure S4. HR-MS spectrum of ISO-t.

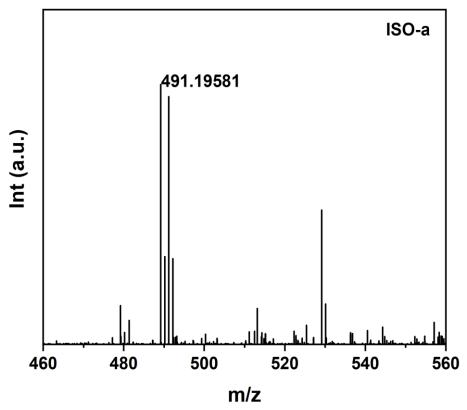


Figure S5. HR-MS spectrum of ISO-a.

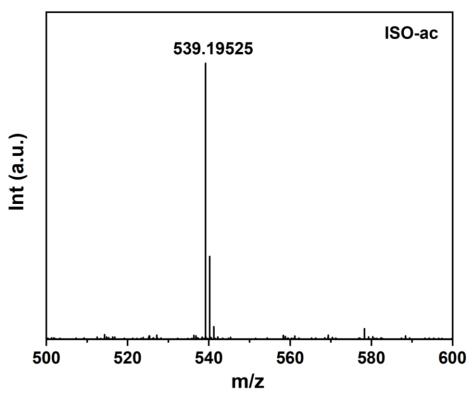


Figure S6. HR-MS spectrum of ISO-ac.



Figure S7. Sample images of Dynamic mechanical analysis.

## Swelling tests and calculation of the crosslinking density

The swelling percentage was calculated from the mass changes using the following equation (S1):

Swelling(%) = 
$$\frac{W_2 - W_1}{W_1} \times 100$$
 equation (S1)

 $W_1$  and  $W_2$  are the weight (g) of the initial sample and the weight of the sample after immersion, respectively. Then, using the Flory–Rehner equation [Equations (S2)–(S4)] and the results of the swelling test, the cross-linking density can be calculated.

$$M_C = \frac{-\rho_P V_S V_r^{1/3}}{\ln(1 - V_r) + V_r + \chi V_r^2}$$
 equation (S2)  

$$V_r = \frac{1}{1 + Q_m}$$
 equation (S3)  

$$V_c = \frac{1}{2M_C}$$
 equation (S4)

where  $M_C$  is the molecular weight between the crosslinking nodes,  $\rho_P$  is the density of the polybenzoxazines ( $V_S$  is the molar volume of the solvent ( $V_S$  toluene

=106.8 cm<sup>3</sup> /mol),  $\chi$  is the interaction coefficient between the polybenzoxazines-solvent, which we took the hypothesis that  $\chi$  approximated to 0.5,  $V_r$  is the volume fraction of the polymer in the swollen specimen,  $Q_m$  is the increased weight of polybenzoxazines in toluene, and  $V_c$  is the cross-link density.