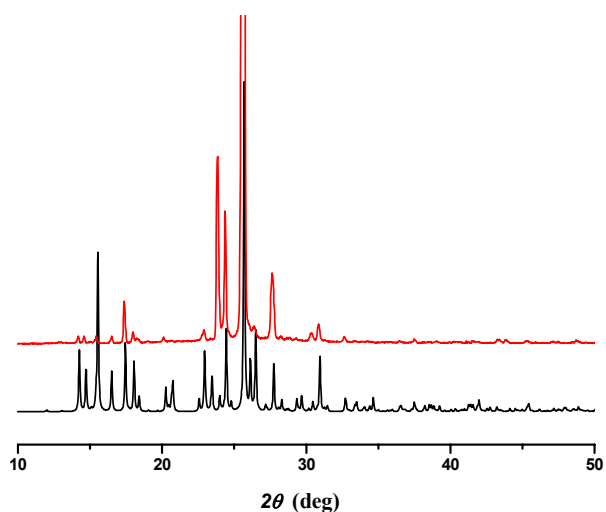


*Electronic Supplementary Information (ESI)*

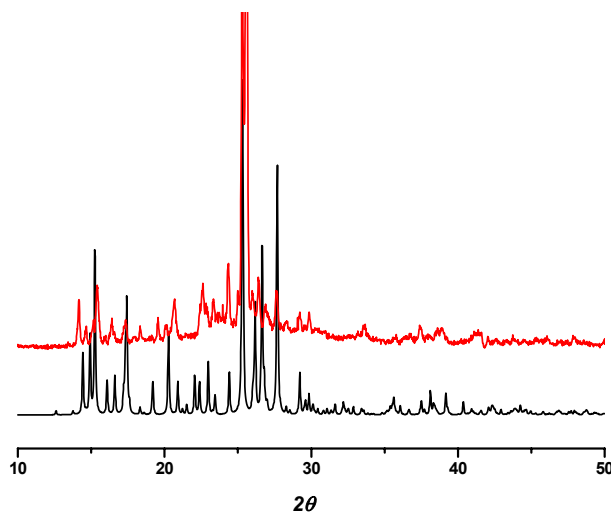
**Co-crystallization of a versatile building block**

**4-amino-3,5-bis(4-pyridyl)-1,2,4-triazole with R-isophthalic acids (R = -H, -NH<sub>2</sub>, -SO<sub>3</sub>H, and -COOH): Polymorphism and substituent effect on structural diversity**

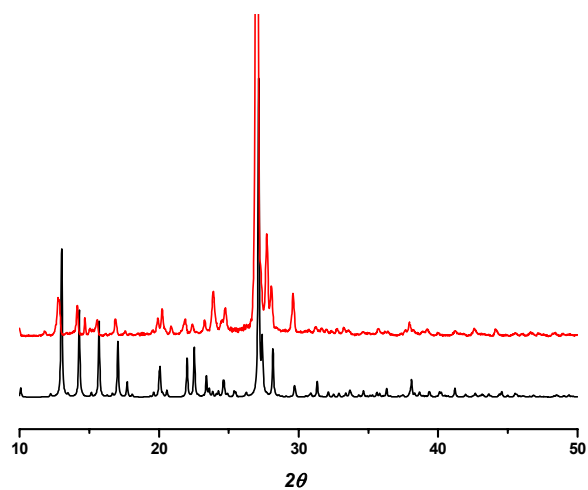
**Miao Du,\* Xiu-Juan Jiang, Xue Tan, Zhi-Hui Zhang, and Hua Cai**



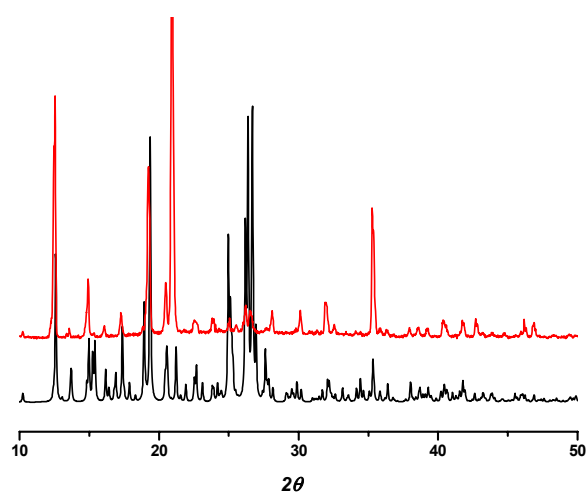
**(a)**



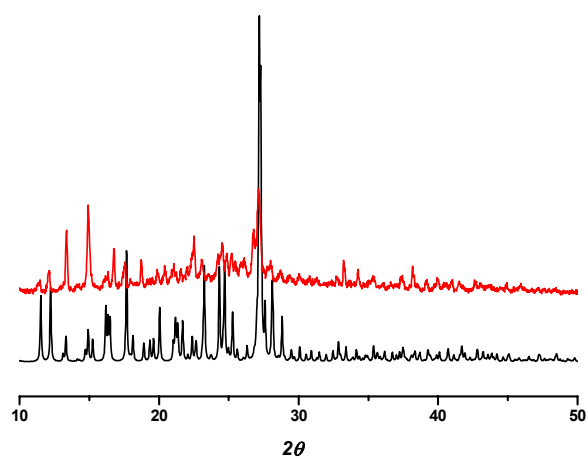
**(b)**



(c)

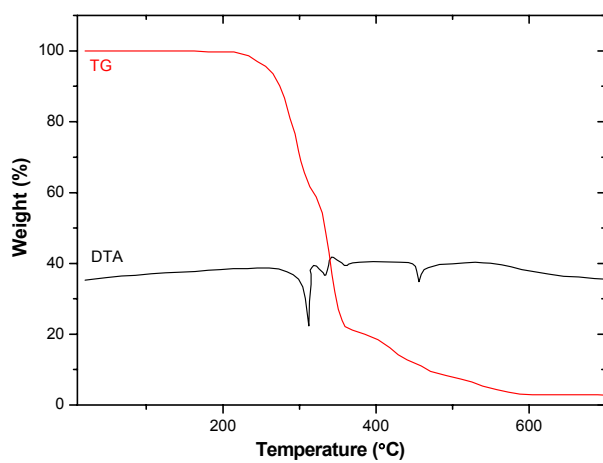


(d)

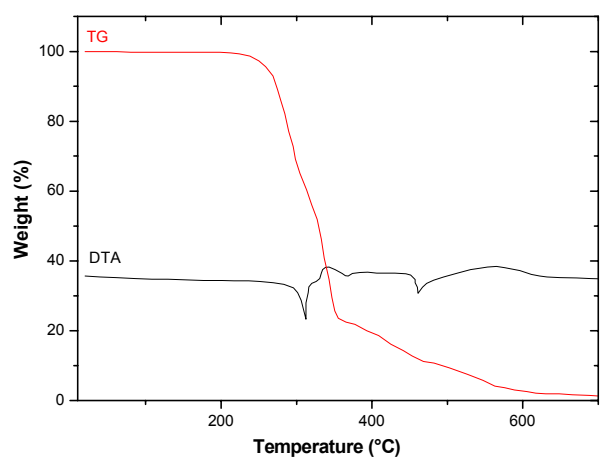


(e)

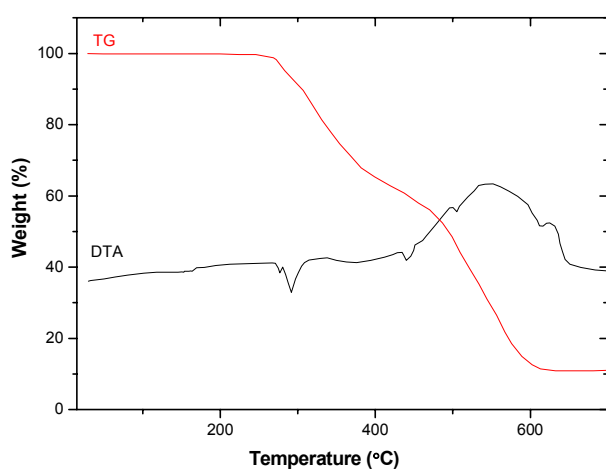
Fig. S1 Experimental (red) and calculated (black) PXR D patterns for 1–5 (from *a* to *e*).



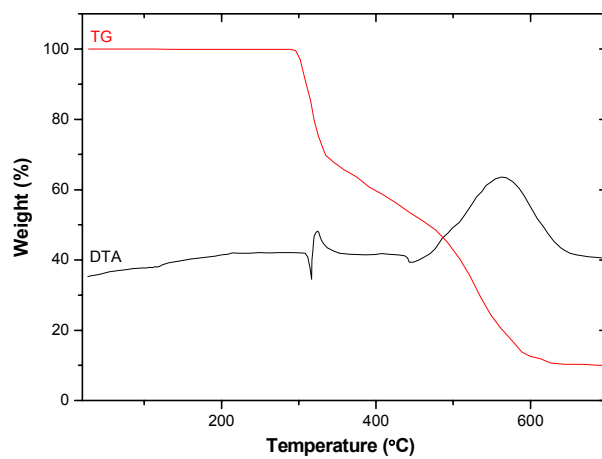
(a)



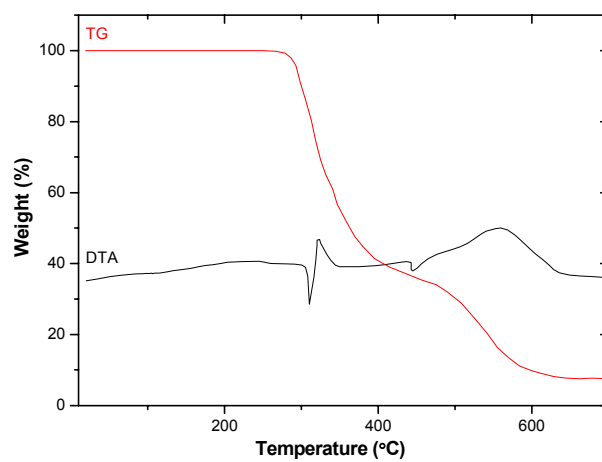
(b)



(c)



(d)



(e)

Fig. S2 TG-DTA curves for compounds 1–5 (from *a* to *e*).

**Table S1. List of the co-crystallizing products of 4-bpt with various R-H<sub>2</sub>ip under different synthetic routes**

product	Route I	Route II	Route III
4-bpt + H <sub>2</sub> ip	<b>1</b>	<b>1</b>	<b>1</b>
4-bpt + H <sub>2</sub> ip + Cd(NO <sub>3</sub> ) <sub>2</sub> or Pb(NO <sub>3</sub> ) <sub>2</sub>	—	—	<b>2</b>
4-bpt + NH <sub>2</sub> -H <sub>2</sub> ip	<b>3</b>	<b>3</b>	unknown species A
4-bpt + SO <sub>3</sub> H-H <sub>2</sub> ip	<b>4</b>	<b>4</b>	<b>4</b>
4-bpt + CO <sub>2</sub> H-H <sub>2</sub> ip	unknown species B	unknown species B	<b>5</b>