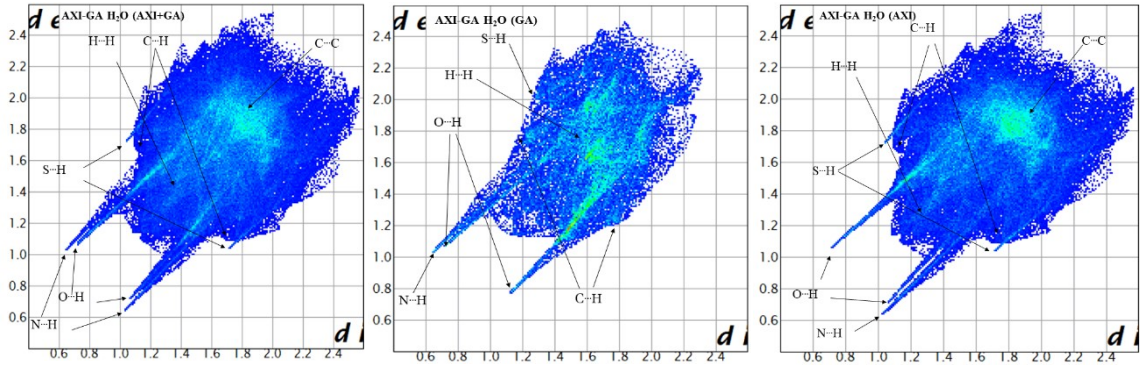
Supplementary data for

Two anhydrous forms and one monohydrate of a cocrystal of axitinib and glutaric acid: characterization, property evaluation and phase transition study

Bo-Ying Ren[a], Xia-Lin Dai[b], Jia-Mei Chen*[b], Tong-Bu Lu[a]

(a)


AXI-GA H2O (AXI+GA)
H···H
C···H
C···C
S···H
O···H
N···H
AXI-GA H2O (GA)
S···H
H···H
O···H
N···H
C···H
AXI-GA H2O (AXI)
C···H
C···C
H···H
S···H
O···H
N···H

(b)

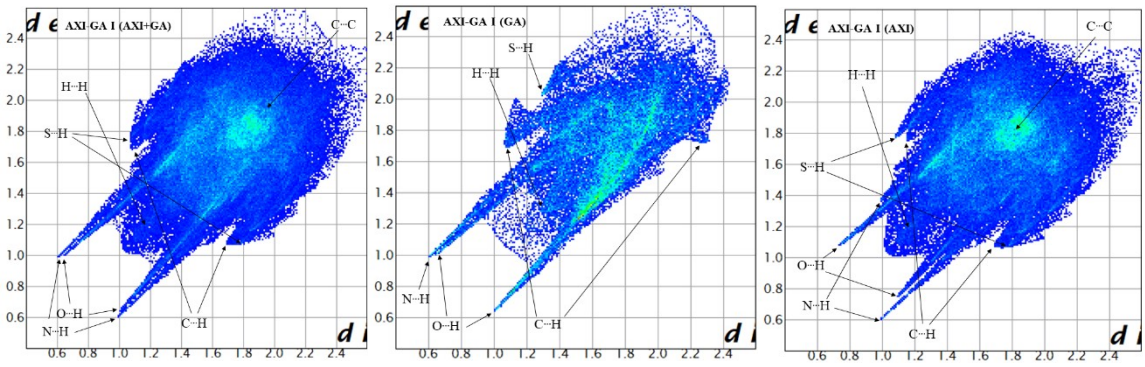

AXI-GA I (AXI+GA)
C···C
H···H
S···H
O···H
N···H
C···H
AXI-GA I (GA)
S···H
H···H
N···H
O···H
C···H
AXI-GA I (AXI)
C···C
H···H
S···H
O···H
N···H
C···H

Figure S1. 2D fingerprint plots of the Hirshfeld surfaces of (a) **AXI-GA·H_2O** (b) **AXI-GA I**.

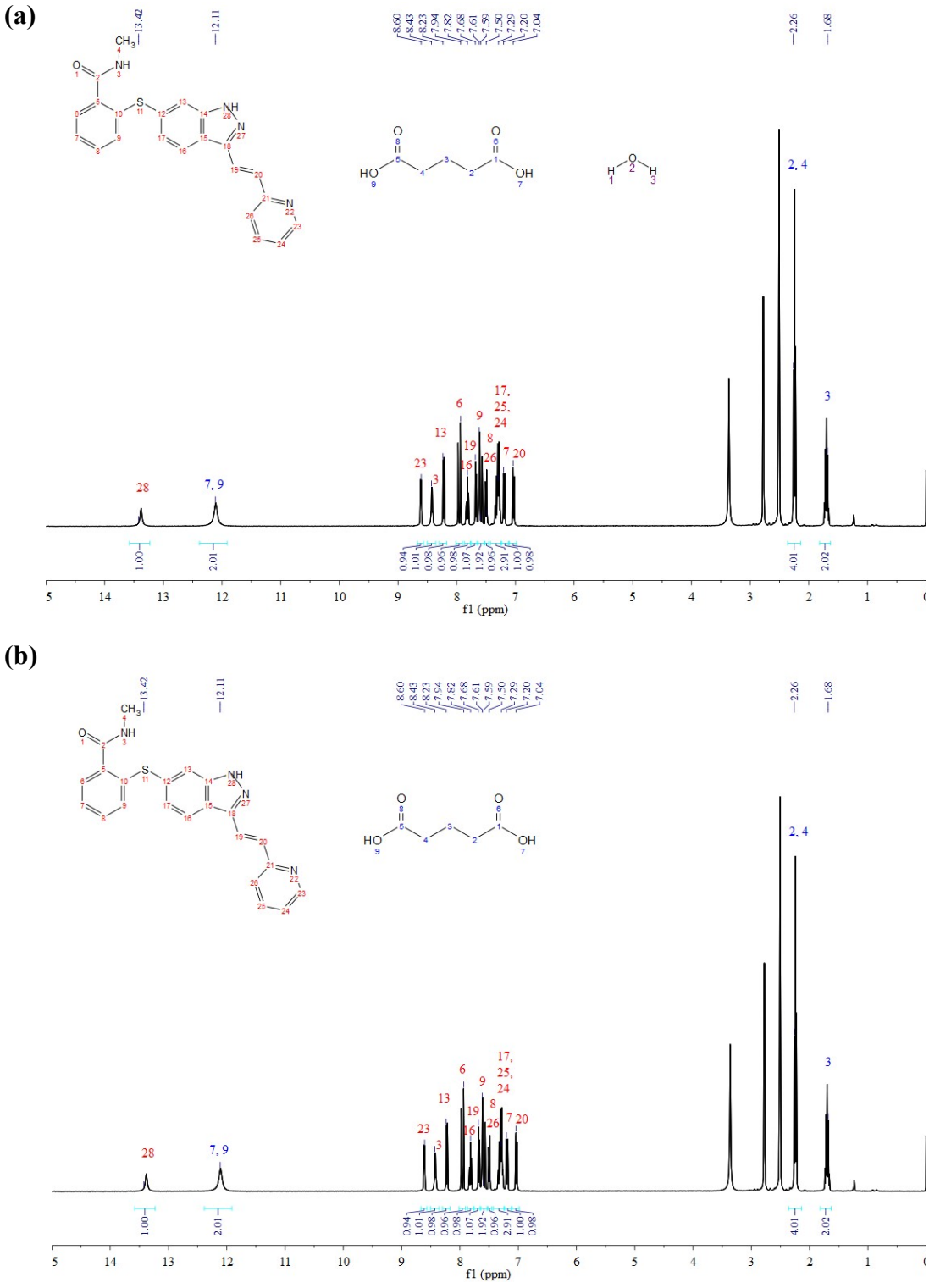


Figure S2. [1]H NMR spectra of (a) **AXI-GA·H_2O** and (b) **AXI-GA I.**

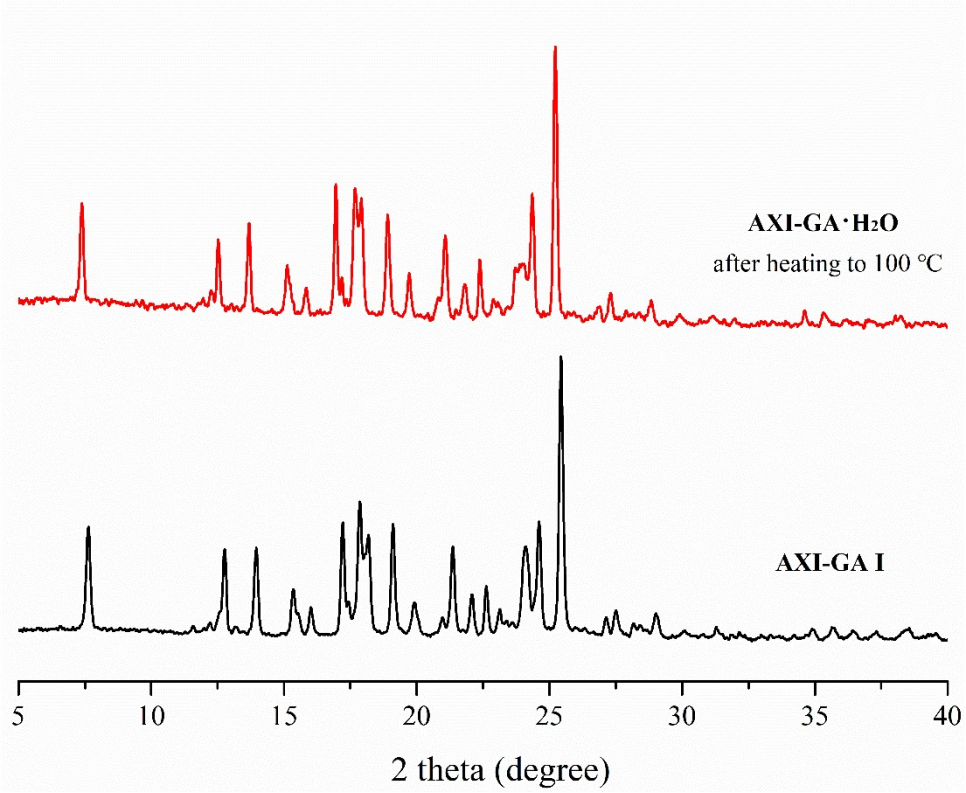


Figure S3. PXRD patterns of **AXI-GA·H_2O** after heating to 100 °C.

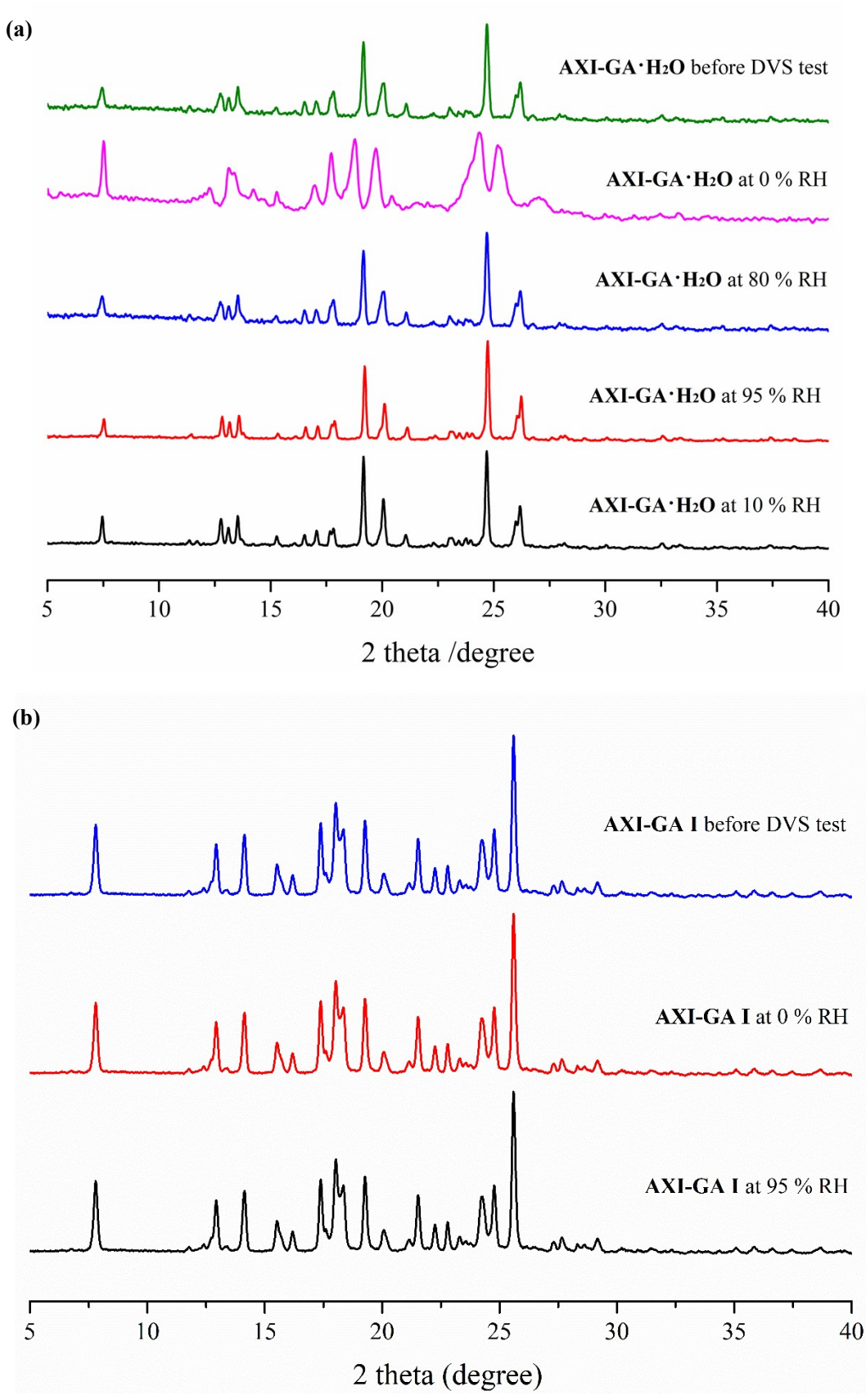
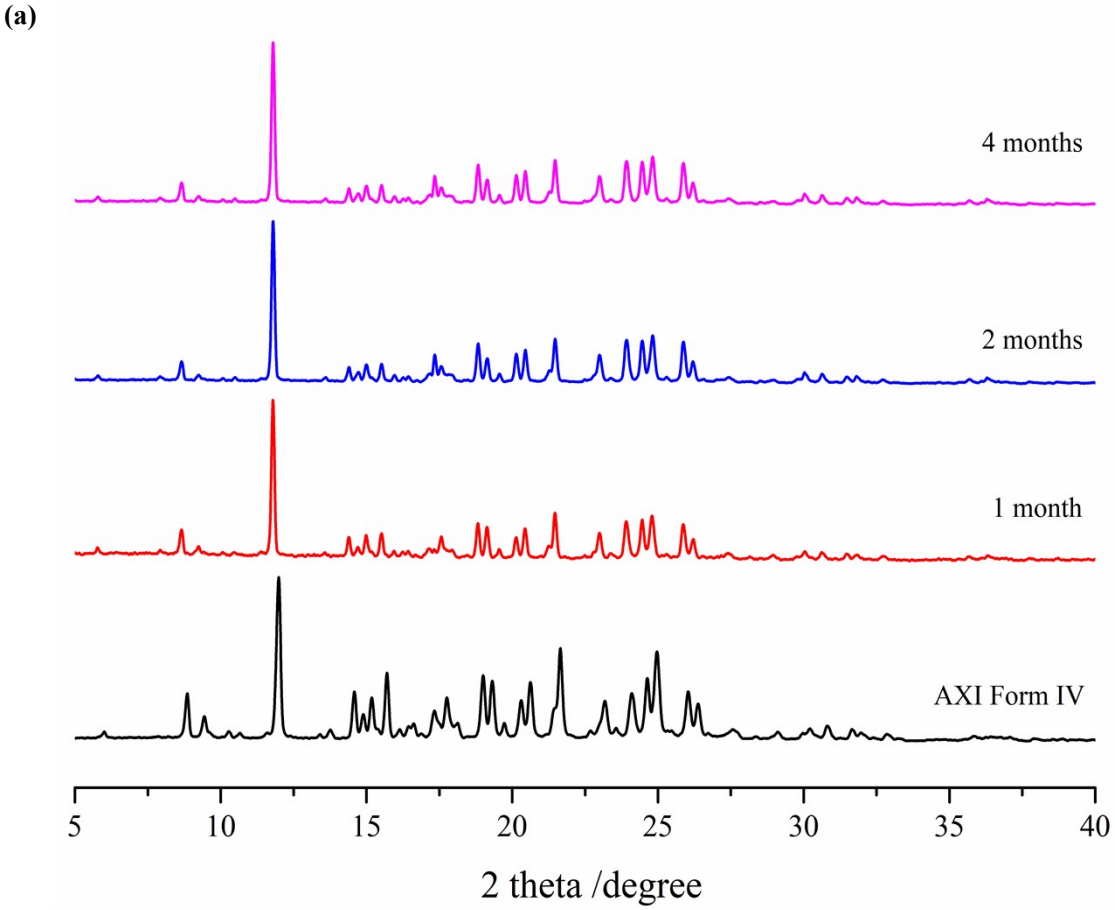
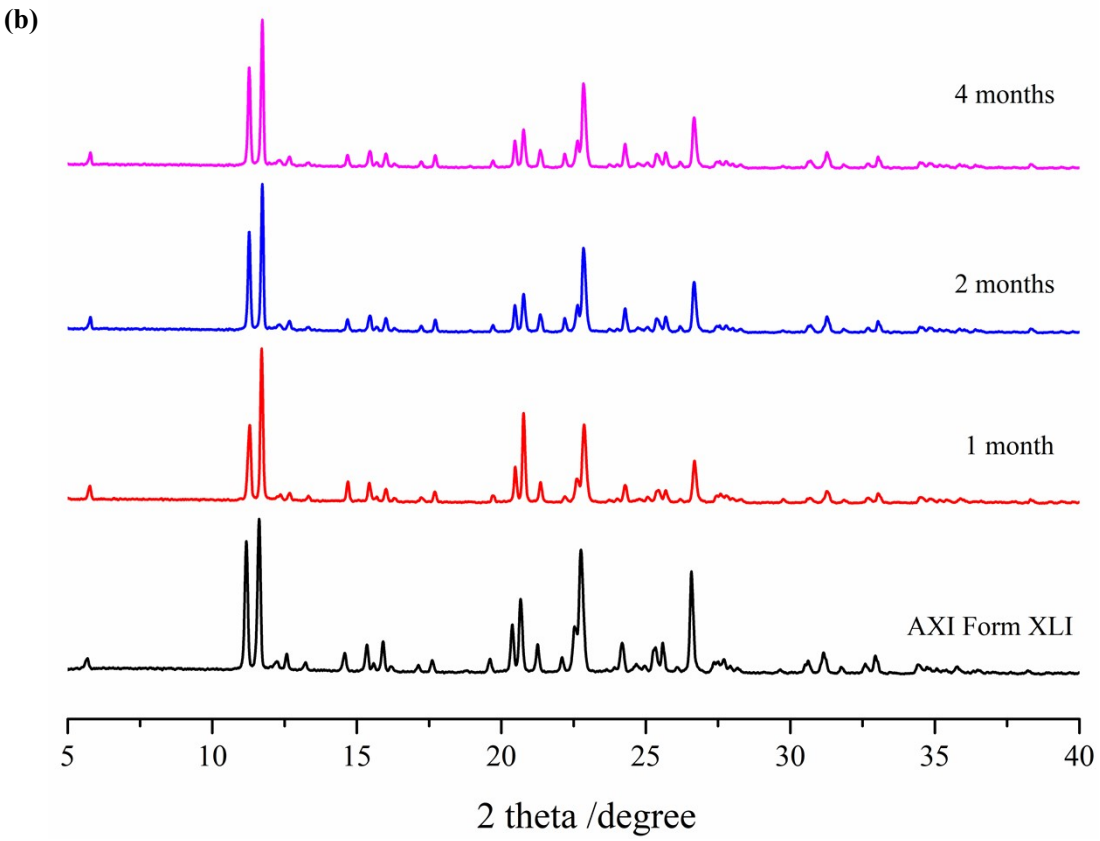
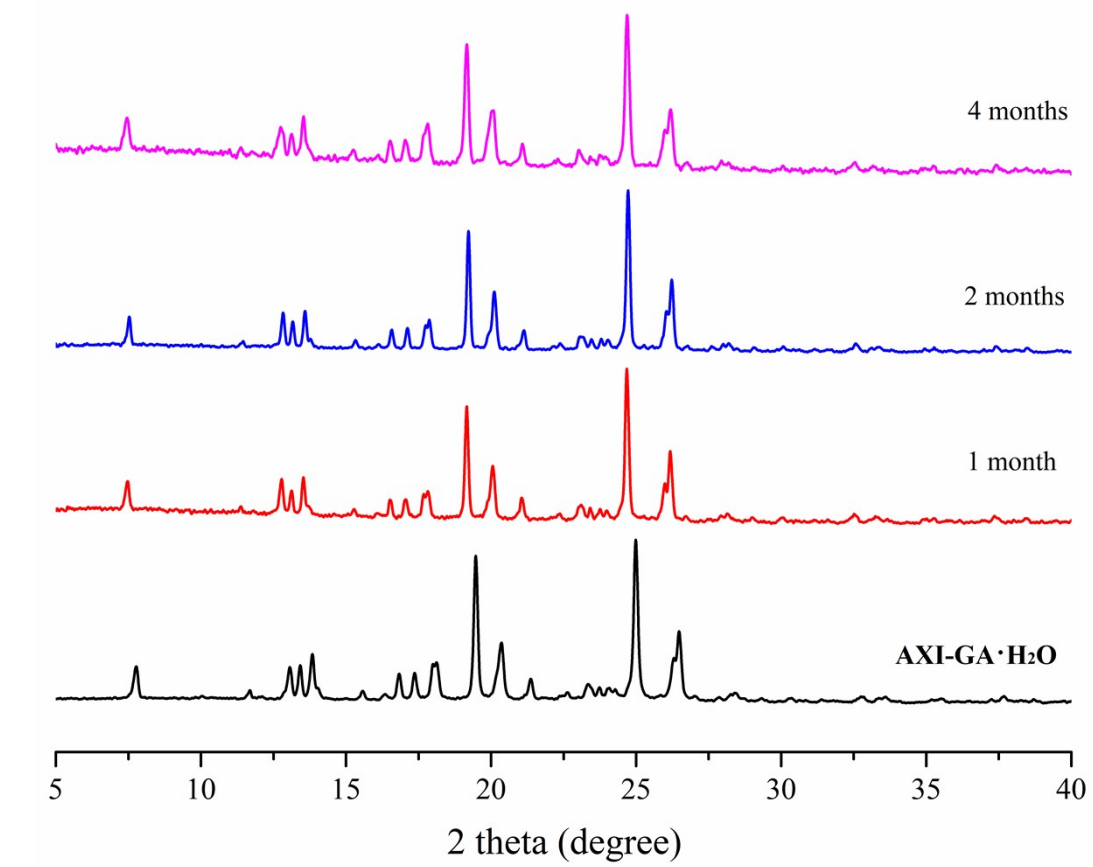


Figure S4. PXRD patterns of (a) **AXI-GA·H_2O** and (b) **AXI-GA I** involving in DVS test. A phase change from **AXI-GA·H_2O** to a metastable form (referring to **AXI-GA II)** was observed at 0% RH, which converted back to **AXI-GA·H_2O** at 80% RH.

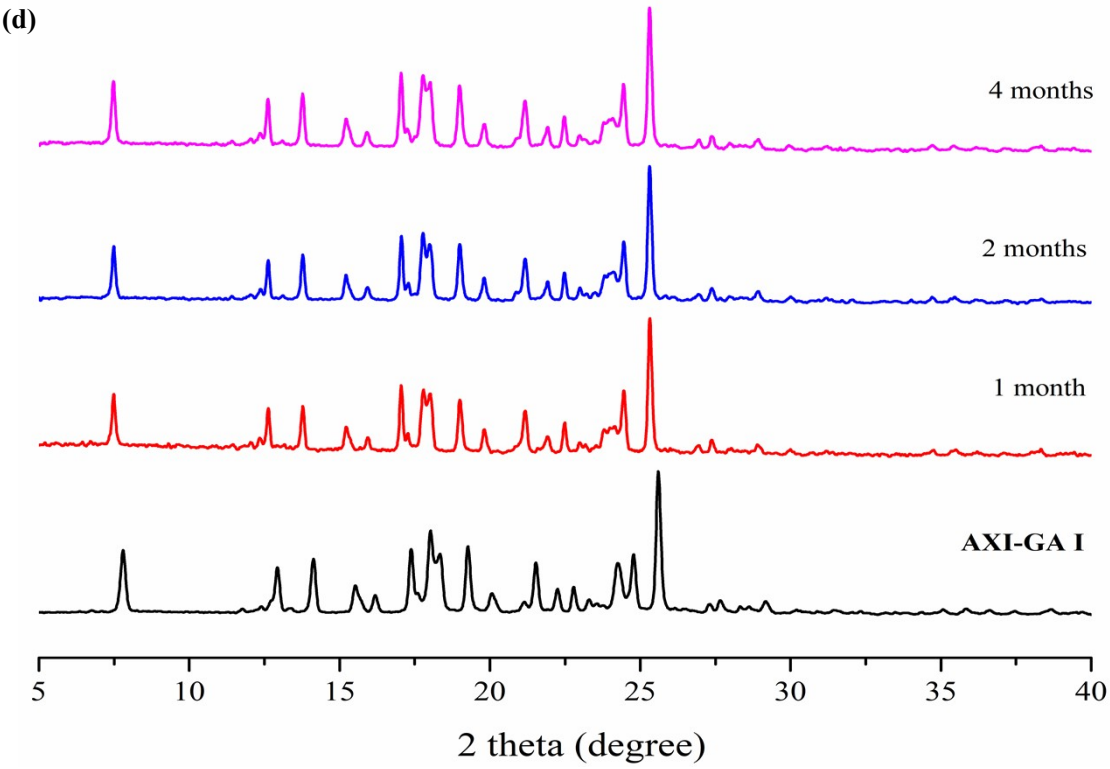

(a)
4 months
2 months
1 month
AXI Form IV
5
10
15
20
25
30
35
40
2 theta /degree


(b)
4 months
2 months
1 month
AXI Form XLI
5
10
15
20
25
30
35
40
2 theta /degree

(c)


4 months
2 months
1 month
AXI-GA·H2O
5
10
15
20
25
30
35
40
2 theta (degree)

(d)


4 months
2 months
1 month
AXI-GA I
5
10
15
20
25
30
35
40
2 theta (degree)

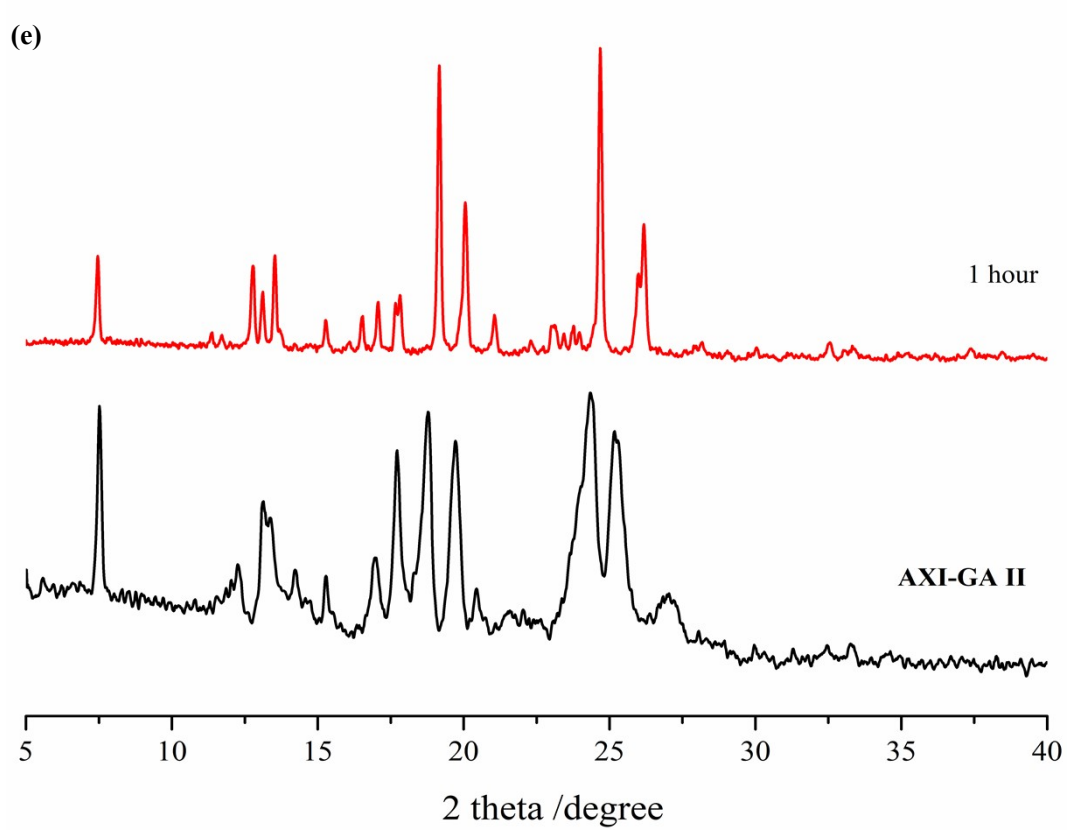


Figure S5. PXRD patterns of (a) **AXI Form IV**, (b) **AXI Form XLI**, (c) **AXI-GA·H_2O**, (d) **AXI-GA I** and (e) **AXI-GA II** under 40 °C/75% RH accelerated conditions.

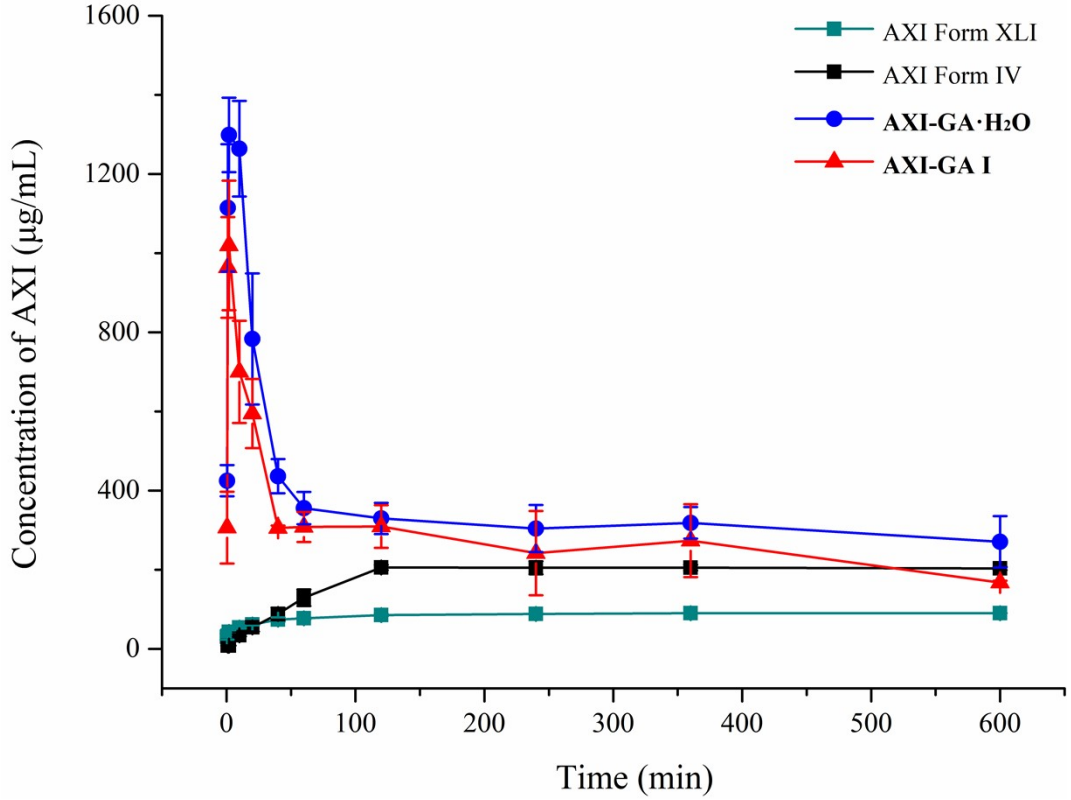


Figure S6. Powder dissolution profiles for **AXI-GA·H_2O**, **AXI-GA I** and **AXI** within 10 h.

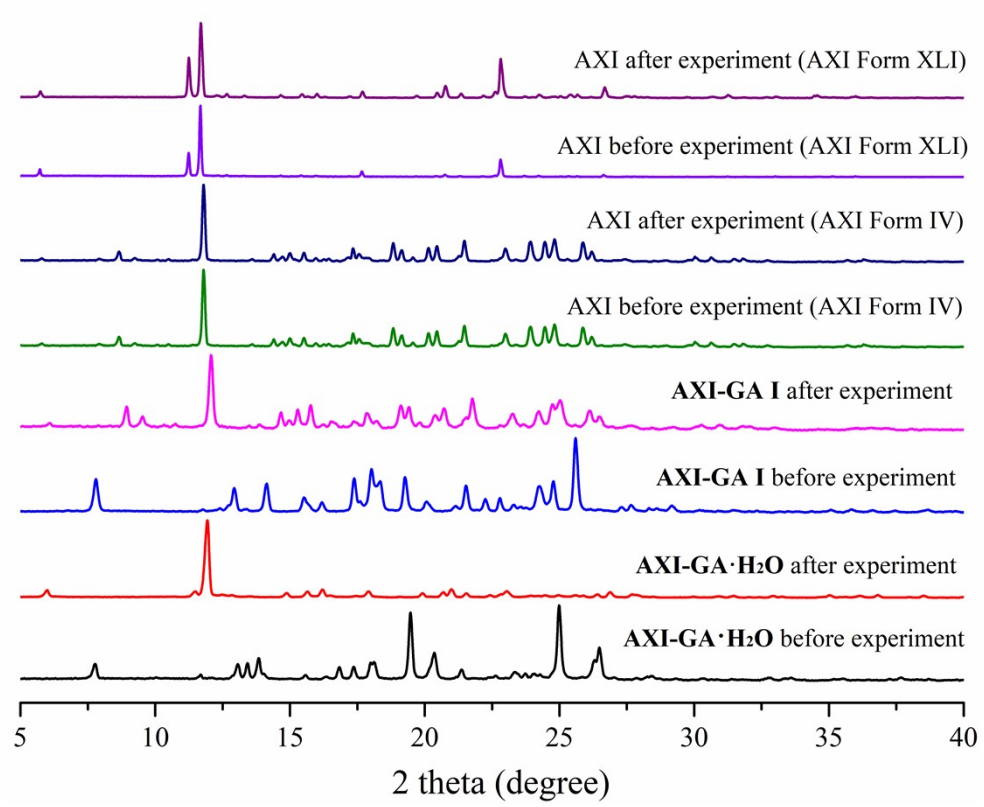


Figure S7. PXRD patterns of the residual solids of **AXI-GA·H_2O**, **AXI-GA I**, **AXI Form IV** and **XLI** after powder dissolution experiments.

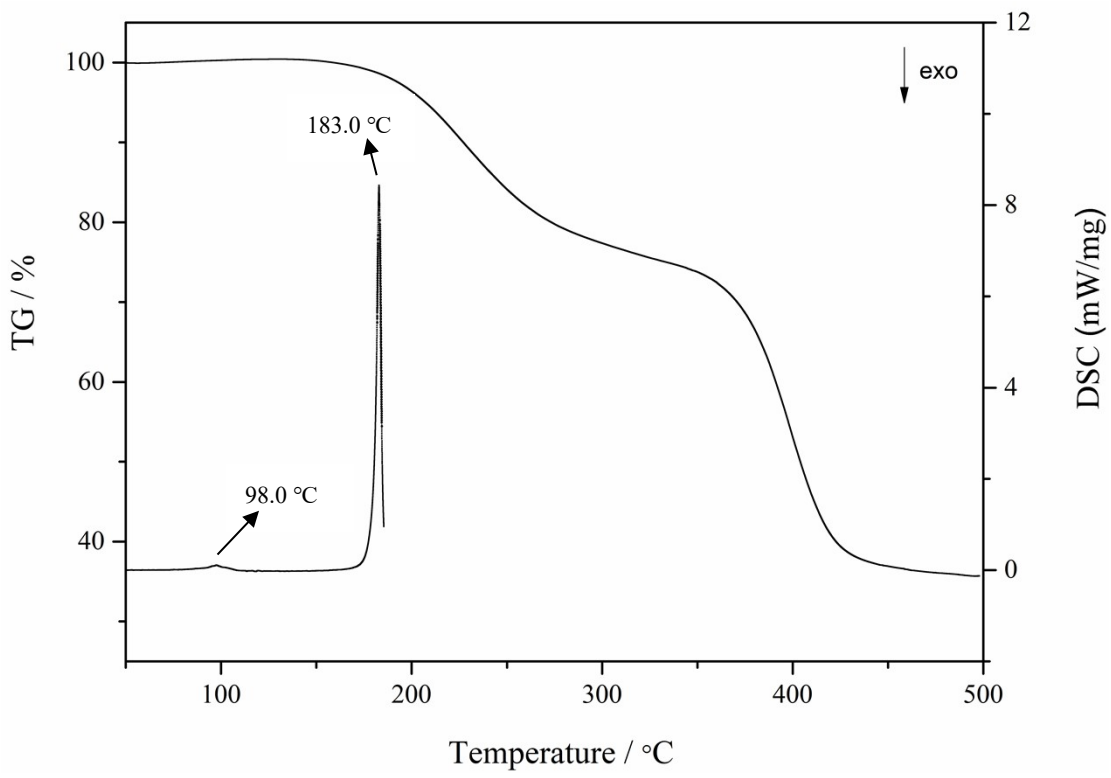


Figure S8. TG-DSC curves of **AXI-GA II**.

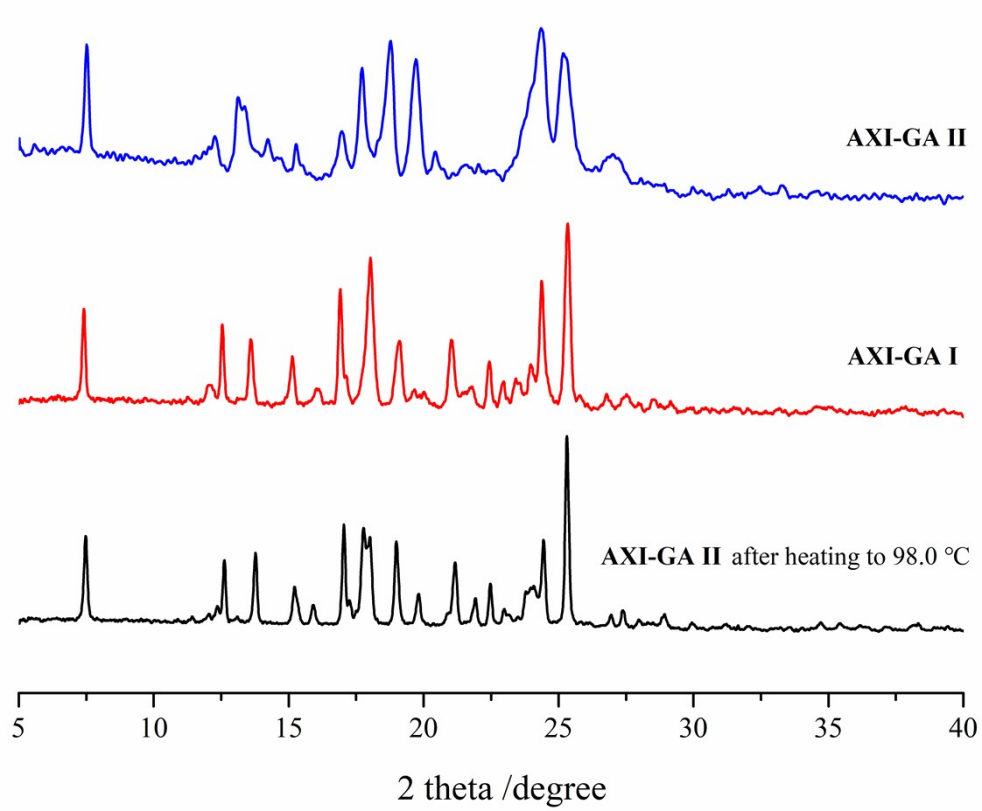


Figure S9. PXRD patterns of **AXI-GA II** and its powder sample heating after 98.0 °C.

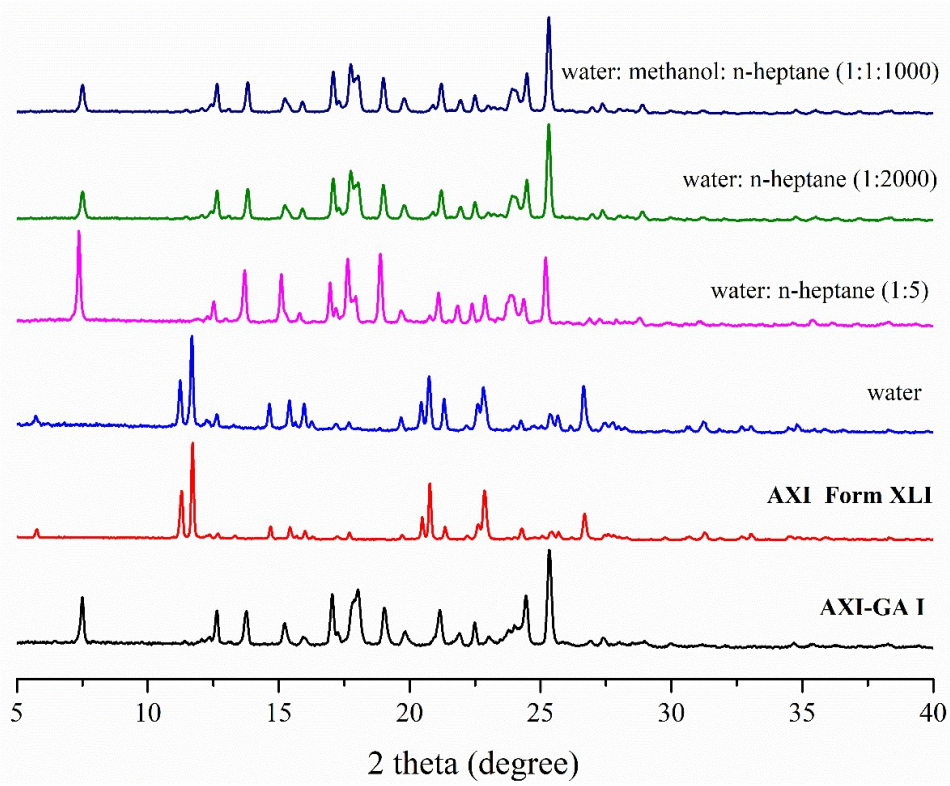


Figure S10. PXRD patterns of the residual solids of powdered 1:1 mixture of **AXI-GA·H_2O** and **AXI-GA I** after slurry in various solvents.