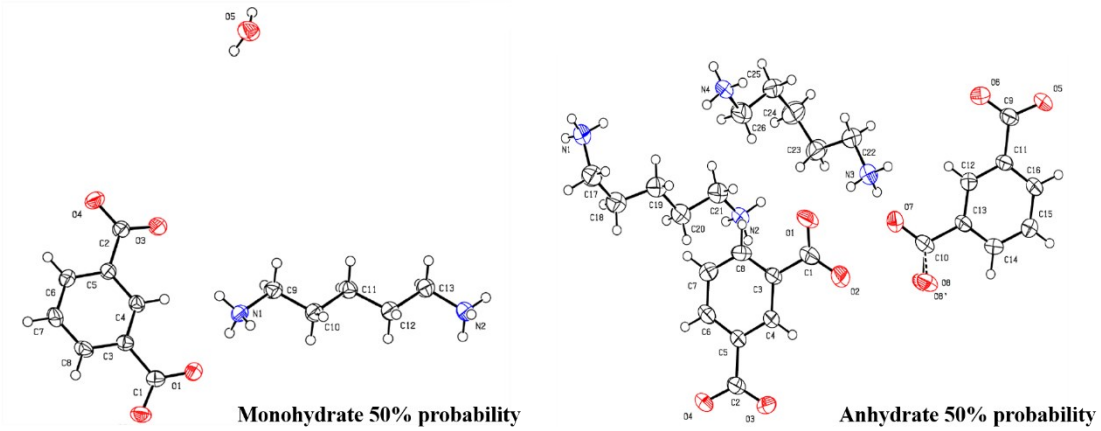
Electronic Supplementary Material (ESI) for RSC Advances.

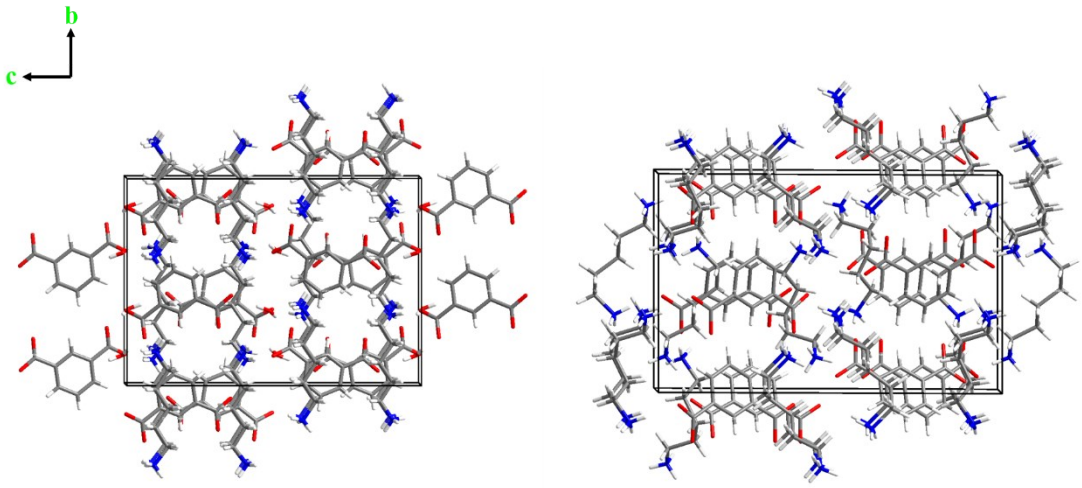
Supporting information

Figure S1 The asymmetric unit diagrams of the PDA-IPA crystal forms, showing the atom-numbering schemes. Displacement ellipsoids are drawn at the 50% probability level.



(a) (b)

Figure S2 Packing diagrams of the PDA-IPA monohydrate (a) and anhydrate (b).



(a) (b)

Table S1 Hydrogen bonds data of the PDA-IPA two crystal forms.

Monohydrate				
D—H···A	D(D-H) / Å	d(H···A) / Å	d(D···A)/ Å	D—H···A
N1—H1A···O1	0.8900	2.0400	2.911(2)	167.00
N1—H1B···O3	0.8900	1.7800	2.637(2)	159.00
N1—H1C···O2	0.8900	1.9800	2.849(2)	163.00
N2—H2A···O2	0.8900	1.9000	2.781(2)	171.00
N2—H2B···O4	0.8900	1.9300	2.779(2)	160.00
N2—H2C···O5	0.8900	1.9600	2.814(2)	161.00
O5—H5C···O1	0.8500	2.0300	2.870(2)	170.00
O5—H5D···O4	0.8500	1.9200	2.757(2)	170.00
C7—H7···O1	0.9300	2.5200	3.258(2)	136.00

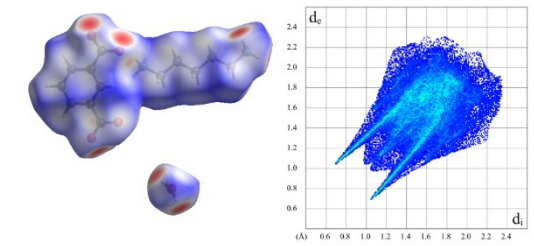
Anhydrate				
D—H···A	D(D-H) / Å	d(H···A) / Å	d(D···A)/ Å	D—H···A
N1—H1A···O8	0.8900	1.9100	2.792(3)	169.00
N1—H1B···O2	0.8900	1.9400	2.809(3)	167.00
N1—H1C···O6	0.8900	1.9100	2.793(3)	174.00
N2—H2A···O5	0.8900	1.9200	2.790(3)	166.00
N2—H2B···O5	0.8900	1.8900	2.755(3)	162.00
N2—H2C···O7	0.8900	1.9700	2.851(3)	171.00
N3—H3A···O1	0.8900	1.9500	2.823(3)	165.00
N3—H3B···O3	0.8900	1.8700	2.754(3)	175.00
N3—H3C···O7	0.8900	1.9100	2.787(3)	170.00
N4—H4A···O2	0.8900	1.9000	2.785(3)	177.00
N4—H4B···O4	0.8900	1.9200	2.791(3)	167.00
N4—H4C···O4	0.8900	1.9400	2.808(3)	165.00
C4—H4···O3	0.9300	2.5100	2.816(3)	100.00
C19—H19B···O8	0.9700	2.3400	3.250(4)	156.00
C22—H22B···O1	0.9700	2.5200	3.255(4)	133.00

Table S2 Torsion angles (°) data of the PDA-IPA two crystal forms.

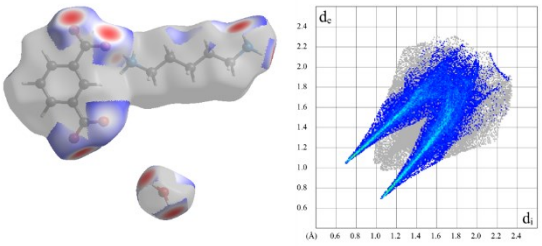
Monohydrate		**Anhydrate**	
O1-C1-C3-C4	8.8(3)	O1-C1-C3-C4	-161.4(3)
O1-C1-C3-C8	-173.09(18)	O1-C1-C3-C8	17.8(4)
O2-C1-C3-C4	-170.06(18)	O2-C1-C3-C4	-19.2(4)
O2-C1-C3-C8	8.1(3)	O2-C1-C3-C8	-161.6(3)
O3-C2-C5-C4	4.4(3)	O3-C2-C5-C4	-9.1(4)
O3-C2-C5-C6	-174.43(19)	O3-C2-C5-C6	173.5(3)
O4-C2-C5-C4	4.0(3)	O4-C2-C5-C4	170.4(3)
C1-C3-C4-C5	177.56(17)	O4-C2-C5-C6	-7.1(4)
C8-C3-C4-C5	-0.6(3)	C1-C3-C4-C5	179.5(3)
C1-C3-C8-C7	-177.74(18)	C8-C3-C4-C5	0.3(4)
C4-C3-C8-C7	0.4(3)	C1-C3-C8-C7	179.5(3)
C3-C4-C5-C2	-178.37(17)	C4-C3-C8-C7	-1.3(4)
C3-C4-C5-C6	0.5(3)	C3-C4-C5-C2	-176.4(3)
C2-C5-C6-C7	178.62(19)	C3-C4-C5-C6	1.2(4)
C4-C5-C6-C7	-0.2(3)	C2-C5-C6-C7	175.7(3)
C5-C6-C7-C8	0.1(3)	C4-C5-C6-C7	-1.8(4)
C6-C7-C8-C3	-0.2(3)	C5-C6-C7-C8	1.0(4)
N1-C9-C10-C11	178.13(17)	C6-C7-C8-C3	0.6(4)
C9-C10-C11-C12	174.65(18)	O5-C9-C11-C12	174.1(3)
C10-C11-C12-C13	-176.08(18)	O5-C9-C11-C16	-9.0(4)
C11-C12-C13-N2	-178.68(17)	O6-C9-C11-C12	-7.0(4)
Anhydrate (continued)			
O6-C9-C11-C16		170.0(3)	
O7-C10-C13-C12		17.4(4)	
O7-C10-C13-C14		-159.8(3)	
O8-C10-C13-C12		-167.4(3)	
O8-C10-C13-C14		15.5(4)	
C9-C11-C12-C13		177.5(3)	

C16-C11-C12-C13	0.5(4)
C9-C11-C16-C15	-176.7(3)
C12-C11-C16-C15	0.4(4)
C11-C12-C13-C10	-178.0(3)
C11-C12-C13-C14	-0.8(4)
C10-C13-C14-C15	177.6(3)
C12-C13-C14-C15	0.3(4)
C13-C14-C15-C16	0.5(4)
C14-C15-C16-C11	-0.8(4)
N1-C17-C18-C19	69.3(4)
C17-C18-C19-C20	-179.6(3)
C18-C19-C20-C21	168.3(3)
C19-C20-C21-N2	-174.3(3)
N3-C22-C23-C24	168.9(2)
C22-C23-C24-C25	-68.8(4)
C23-C24-C25-C26	-66.1(4)
C24-C25-C26-N4	175.3(2)

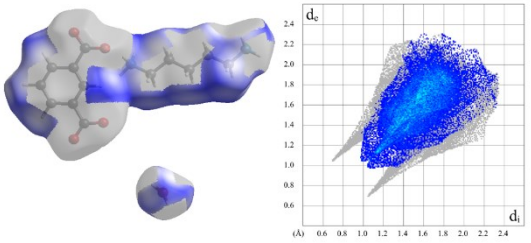
Figure S3 Hirshfeld surface and its corresponding fingerprint plots of the monohydrate.



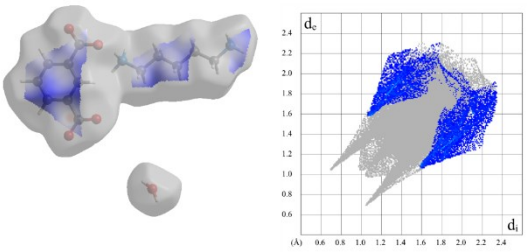
(a) All···All



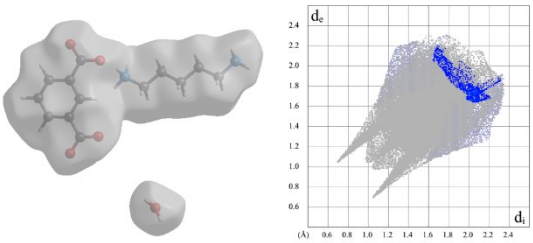
(b) H···O/O···H (41.3%)



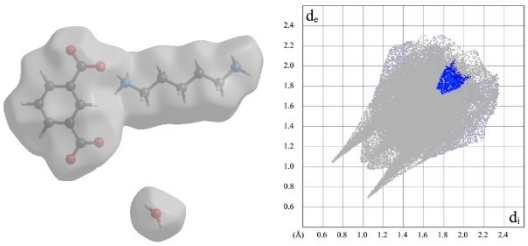
(c) H···H (42.8%)



(d) H···C/C···H (12.6%)



(e) O···C/C···O (1.7%)



(f) C···C (1.5%)

Figure S4 Hirshfeld surface and its corresponding fingerprint plots of the anhydrous form.

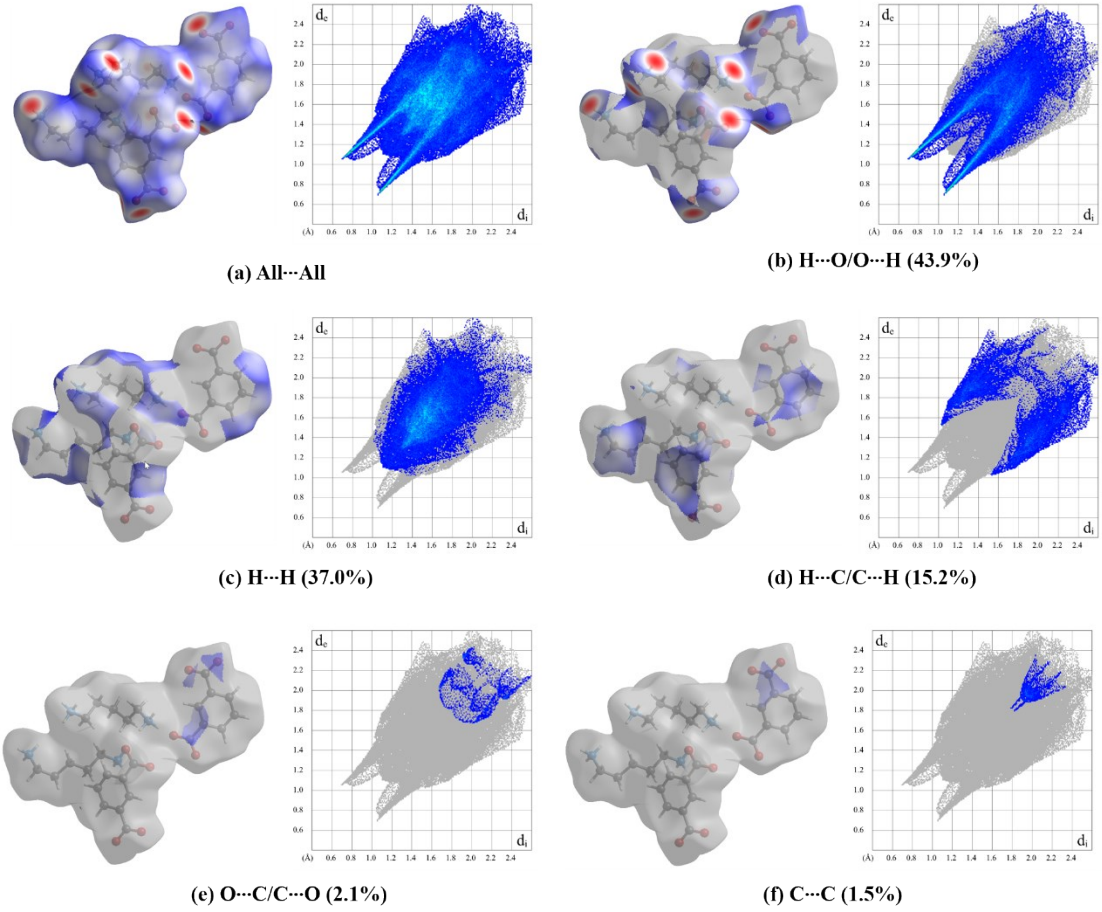


Figure S5 The distance of hydrogen-bond contacts of the monohydrate in Figure 7.

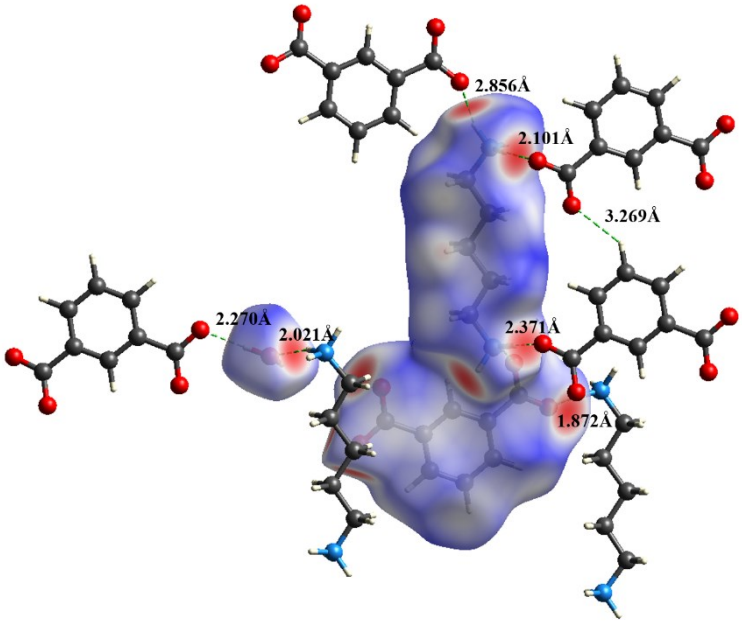


Figure S6 The distance of hydrogen-bond contacts of the anhydrous form in Figure 7.

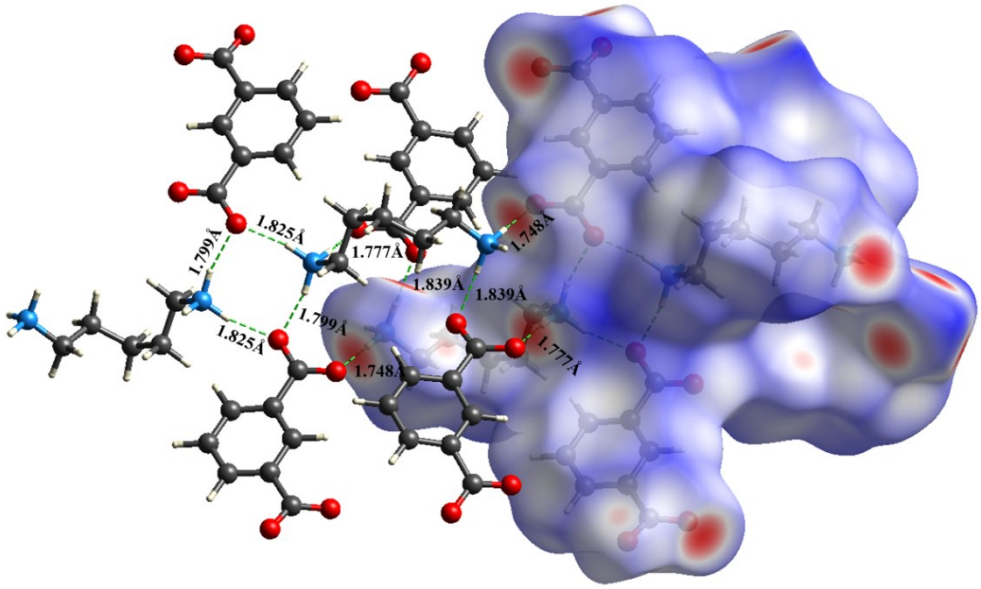


Figure S7 PXRD diagram of the monohydrate of PDA-IPA after dehydration.

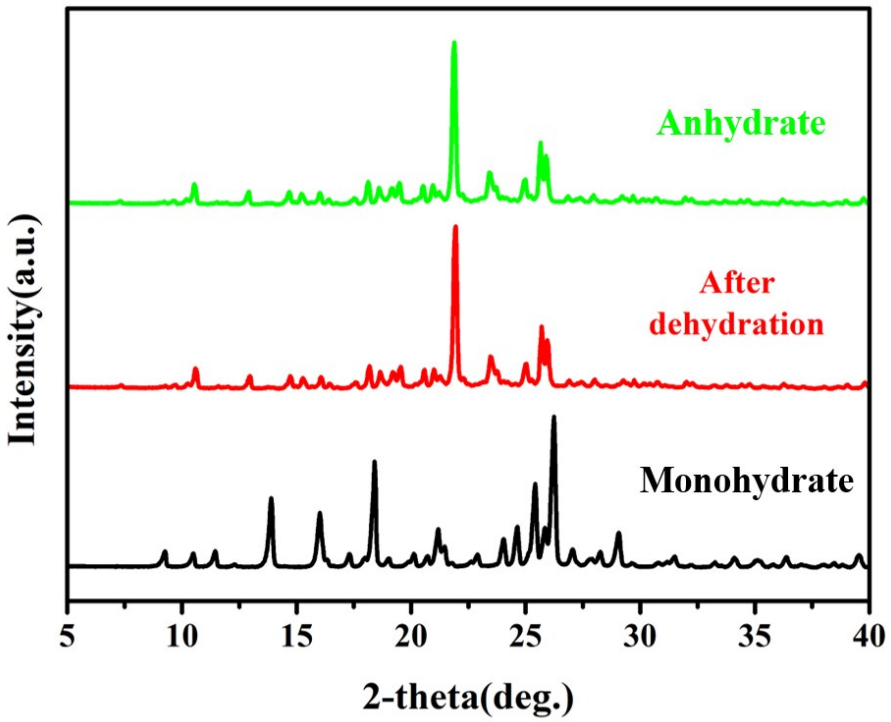
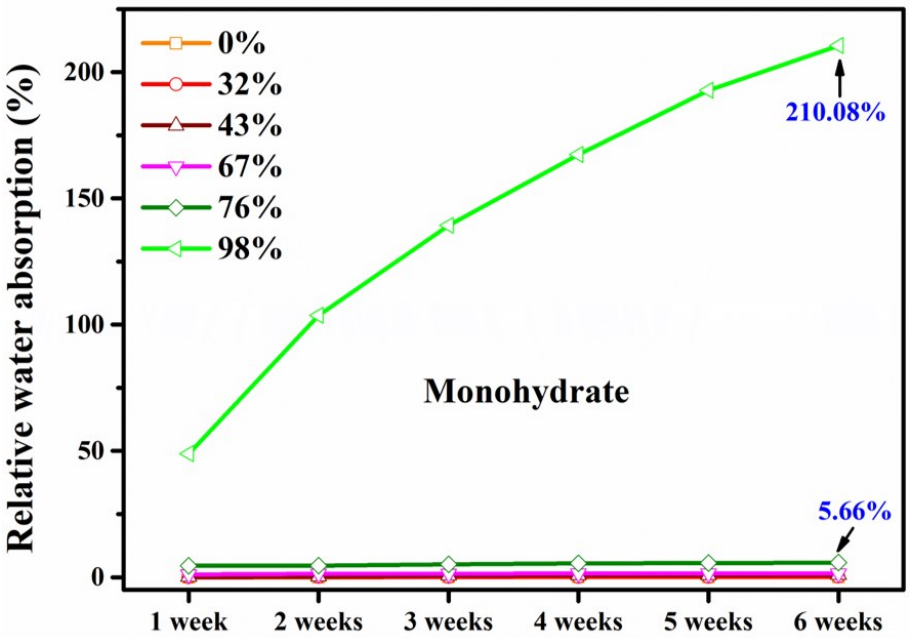
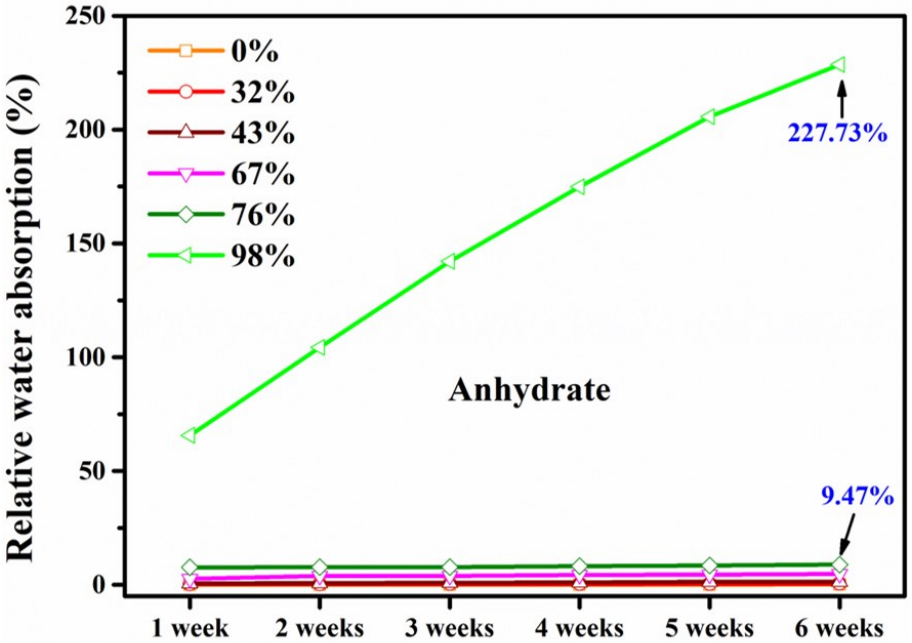


Figure S8 Hygroscopicity of two PDA-IPA crystal forms under the surrounding conditions with different relative humidity.



(a)



(b)

Figure S9 PXRD diagram of PDA-IPA under different water activity at 25℃.

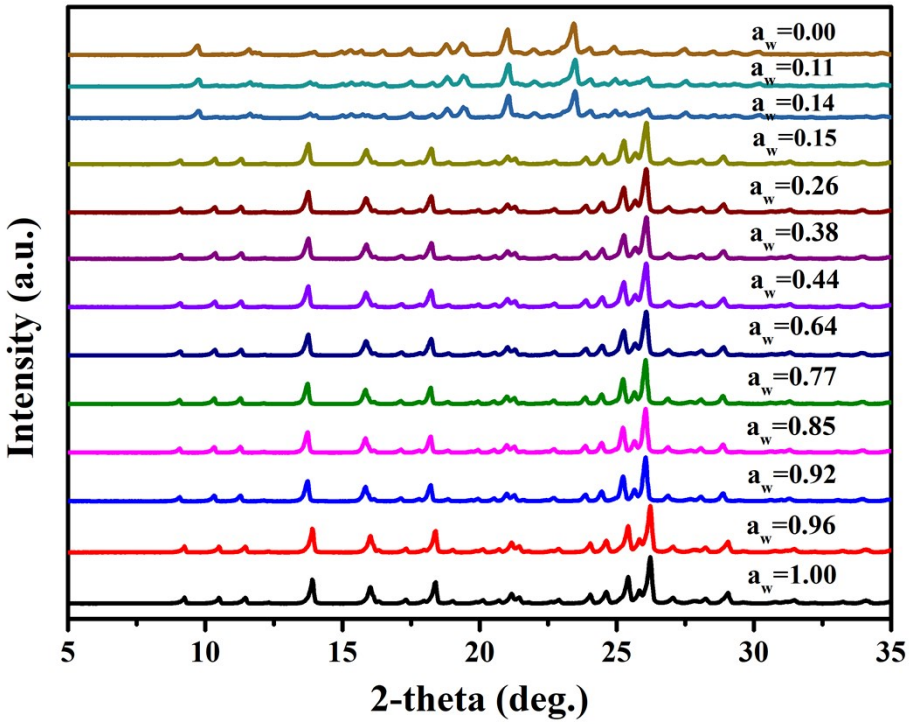


Figure S10 The critical water activities of the two forms of PDA-IPA at 25℃.