Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supporting Information

A peculiar dehydration and solid-solid phase transition of the active pharmaceutical ingredient AZD9898 based on in situ single crystal-to-single crystal transformations

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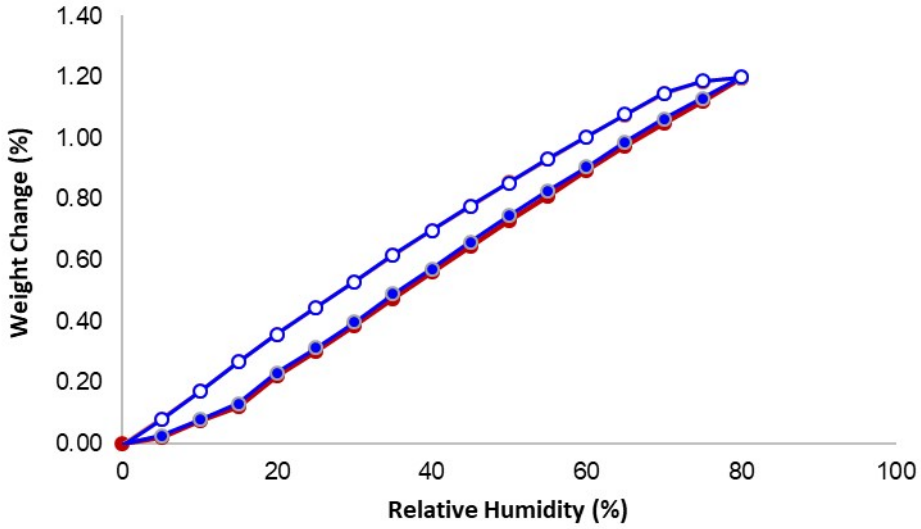

Fig. S1 DVS chart of AZD9898 Form A hydrate. Red and blue lines indicate the first and second cycle, respectively. Close and open symbols represent sorption and desorption, respectively. Top and bottom dashed blacklines show theoretical mass where Form A and B exist.

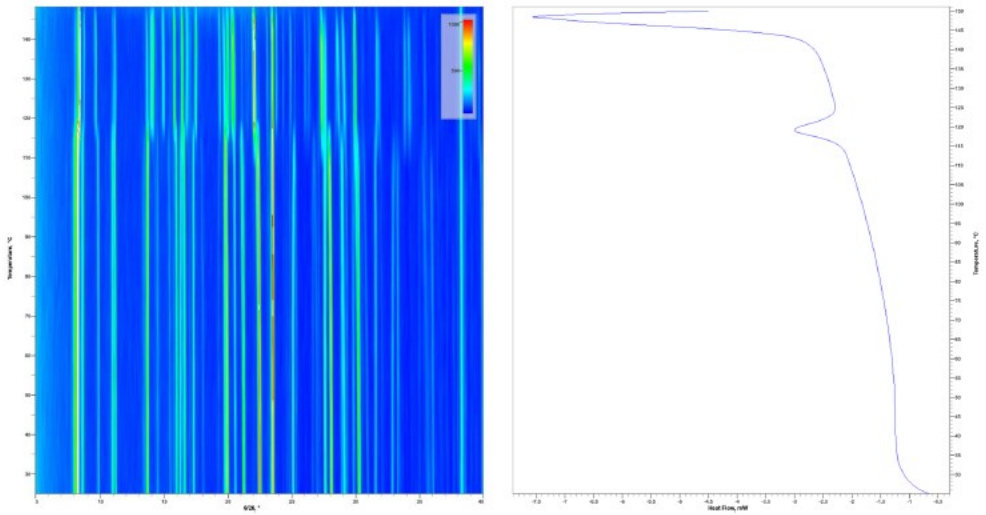

Fig. S2 XRD (left) and DSC (right) of AZD9898 Form B.

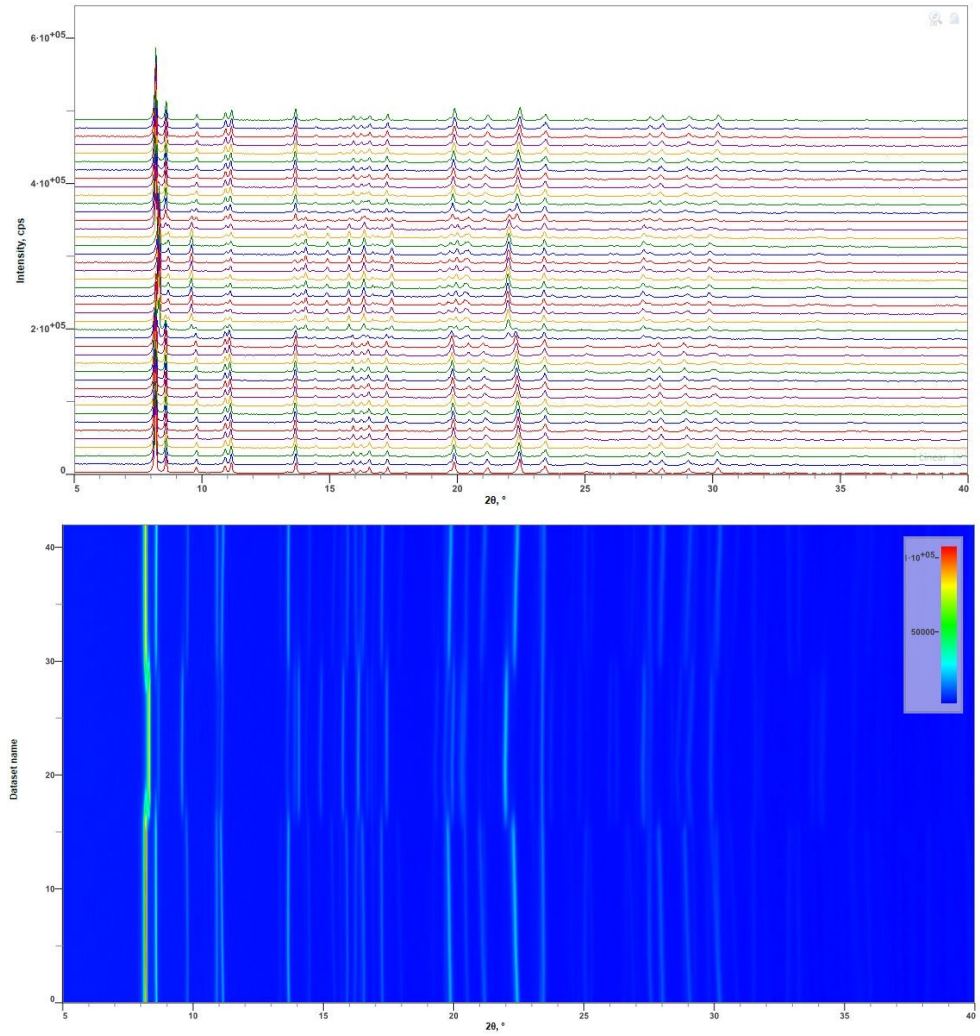

Fig. S3 XRD profiles from RT → 140 °C → RT showing reversible transformation between AZD9898 Form B and C.

Table S1 Hydrogen bond for AZD9898 Form A

H Bond	D - H (Å)	H...A (Å)	D...A (Å)	D - H...A (◦)
O103 -H...N203[1]	0.82(4)	2.03(4)	2.833(4)	166(5)
O203-H...N103[2]	0.86(5)	1.89(4)	2.712(4)	160(5)
C107-H...O202[3]	0.99	2.52	3.359(5)	142
C115-H...O1W[4]	0.98	2.32	2.877(11)	116
C101-H...O201[3]	0.95	2.58	3.302(5)	132
C101-H...O202[3]	0.95	2.54	3.411(5)	153
C114-H...F201[5]	0.95	2.54	3.414(4)	153
C201-H...O101[6]	0.95	2.60	3.350(5)	136
C214-H...F101[7]	0.95	2.49	3.366(4)	153
C217-H...F103	1.00	2.46	3.074(4)	119

[1] 1+x,y,1+z; [2] -1+x,y,-1+z; [3] 1+x,y,z; [4] x,y,-1+z; [5] x,-1+y,z; [6] -1+x,y,z; and [7] x,1+y,z

Table S2 Hydrogen bond for AZD9898 Form B

H Bond	D - H (Å)	H...A (Å)	D...A (Å)	D - H...A (◦)
O103-H...N203[1]	0.86(6)	2.00(6)	2.858(6)	175.5(17)
O203-H...N103[2]	0.86(6)	1.90(5)	2.730(5)	161(5)
C107-H...O202[3]	0.97	2.56	3.382(6)	142
C101-H...O202[3]	0.93	2.51	3.373(6)	155
C214-H...F101[4]	0.93	2.55	3.418(6)	156
C217-H...F103	0.98	2.53	3.136(6)	120

[1] 1+x,y,1+z; [2] -1+x,y,-1+z; [3] 1+x,y,z; and [4] x,1+y,z

Table S3 Hydrogen bond for AZD9898 Form C

H Bond	D - H (Å)	H...A (Å)	D...A (Å)	D - H...A (◦)
O103-H...O202[1]	0.82	2.02	2.687(10)	138
O203-H...N103[2]	0.82	2.01	2.803(8)	163
C209-H...O204[3]	0.96	2.58	3.467(15)	154

[1] 1+x,1+y,1+z; [2] -1+x,y,-1+z; and [3] x,y,1+z