Electronic Supplementary Information (ESI)

Structural and computational insights into the enhanced solubility of dipfluzine by complexation: salt and salt-cocrystal

Wei Guo,[a,b] Shuang Du,[a] Yulong Lin,[a] Bo Lu,[c] Caiqin Yang,[a] Jing Wang,*[a] and Yanli Zeng*[c]

[a] School of Pharmacy, Hebei Medical University, Shijiazhuang 050017, People's Republic of China.
[b] Biological post-doctoral mobile research center, Hebei Medical University, Shijiazhuang 050017, People's Republic of China.
[c] College of Chemistry and Material Science, Hebei Normal University, Shijiazhuang 050024, People's Republic of China.

* Corresponding author. Tel: (86)-311-86265622; Fax: (86)-311-86265622; e-mail: jingwang@home.ipe.ac.cn (J. Wang), yanlizeng@hebtu.edu.cn (Y.L. Zeng)

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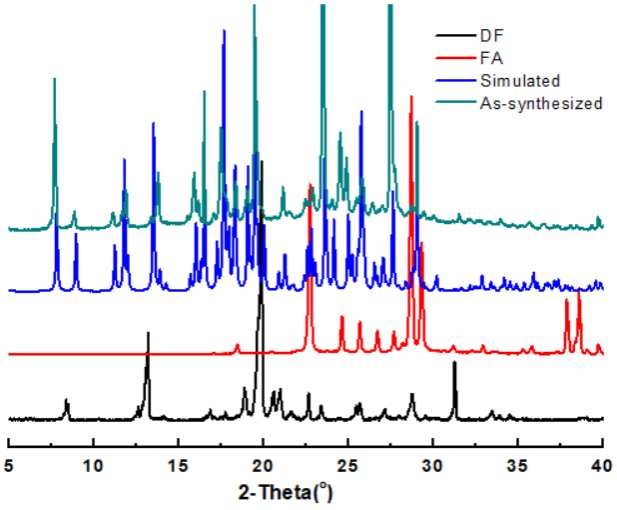


Fig. S1 Powder X-ray diffraction patterns of salt **1** and corresponding reactants.

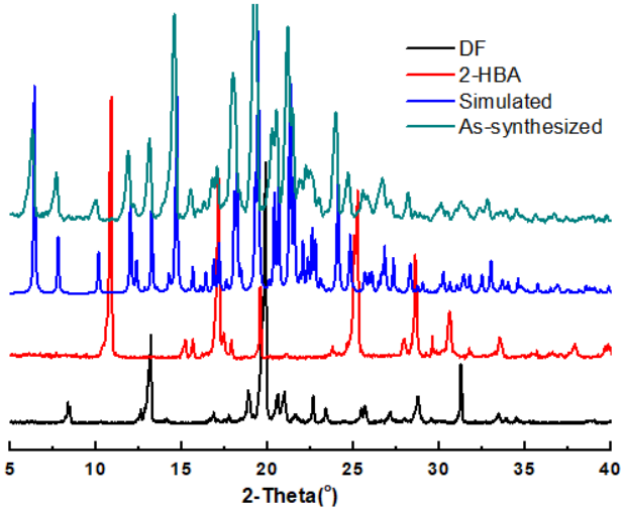


Fig. S2 Powder X-ray diffraction patterns of salt **2** and corresponding reactants.

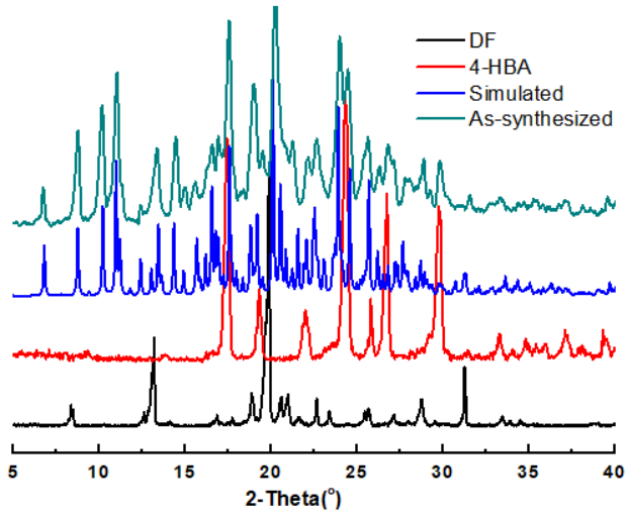


Fig. S3 Powder X-ray diffraction patterns of salt-cocrystal **3** and corresponding reactants.

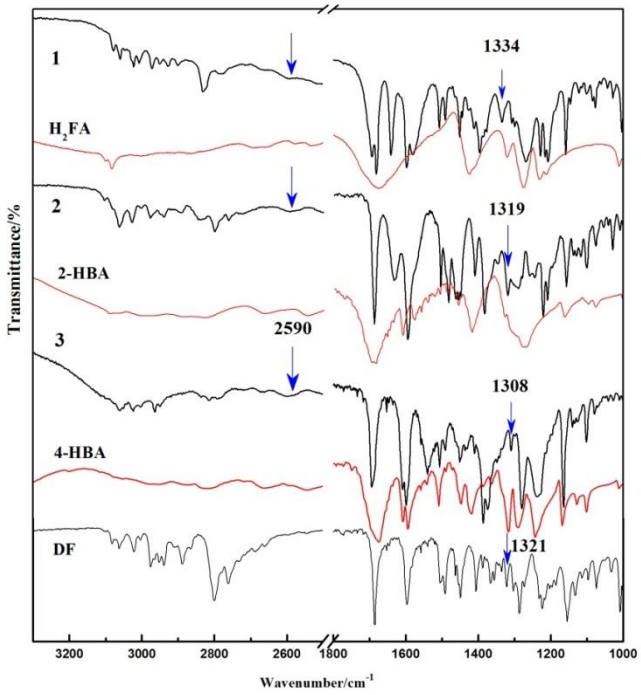


Fig. S4. FT-IR spectra of pure DF, complexes **1**–**3** and carboxylate acid coformers.

Table S1 Possible hydrogen-bonding geometries in the crystal structures of **1–3**.

Crystal forms	D–H···A	D···A(Å)	H···A(Å)	D–H···A (°)	Symmetry codes
1	N2–H2A···O2	3.2311	2.43	149	
	N2–H2A···O3	2.7094	1.89	152	
	O5–H5···O2	2.5284	1.73	169	*x*, –*y* + 1/2, *z* – 1/2
	C15–H15B···O3	3.3074	2.35	168	*x*, –*y* + 3/2, *z* + 1/2
	C17–H17B···O4	3.1274	2.42	129	*x*, *y* + 1, *z*
	C24–H24···O1	3.4289	2.56	155	–*x*, *y* – 1/2, –*z* + 3/2
2	N2–H2A···O3	2.735(8)	1.87	161	–*x* + 1, –*y* + 1, –*z*
	O4–H4···O3	2.507(12)	1.77	150	
	C9–H9B···O2	3.174(6)	2.40	136	–*x* + 1, –*y* + 1, –*z*
	C10–H10A···O2	3.142(5)	2.23	157	
3	N1–H1'···O10	2.6729	1.86	151	*x*, *y* – 1, *z* + 1
	O3–H3···O10	2.6207	1.85	155	*x*, *y*, *z* + 1
	N3–H3'···O4	2.7712	1.89	171	
	O6–H6···O5	2.5340	1.75	160	
	O8–H8···O11	2.6035	2.07	121	–*x* + 1, *y* – 1/2, –*z* + 1
	O9–H9···O4	2.6118	1.77	168	
	C6–H6A···O7	3.2918	2.38	165	*x*, *y* – 1, *z*
	C11–H11A···N5	3.0465	2.49	116	*x*, *y*, *z* + 1
	C14–H14B···O5	3.4540	2.55	156	
	C35–H35B···O7	3.1762	2.21	176	–*x* + 1, *y* – 1/2, –*z* + 1
	C40–H40A···O9	3.3024	2.59	130	
	C41–H41A···N5	3.4930	2.58	157	
	C41–H41B···O11	3.4411	2.50	165	*x*, *y* – 1, *z*
	C57–H57···O9	3.4481	2.57	159	

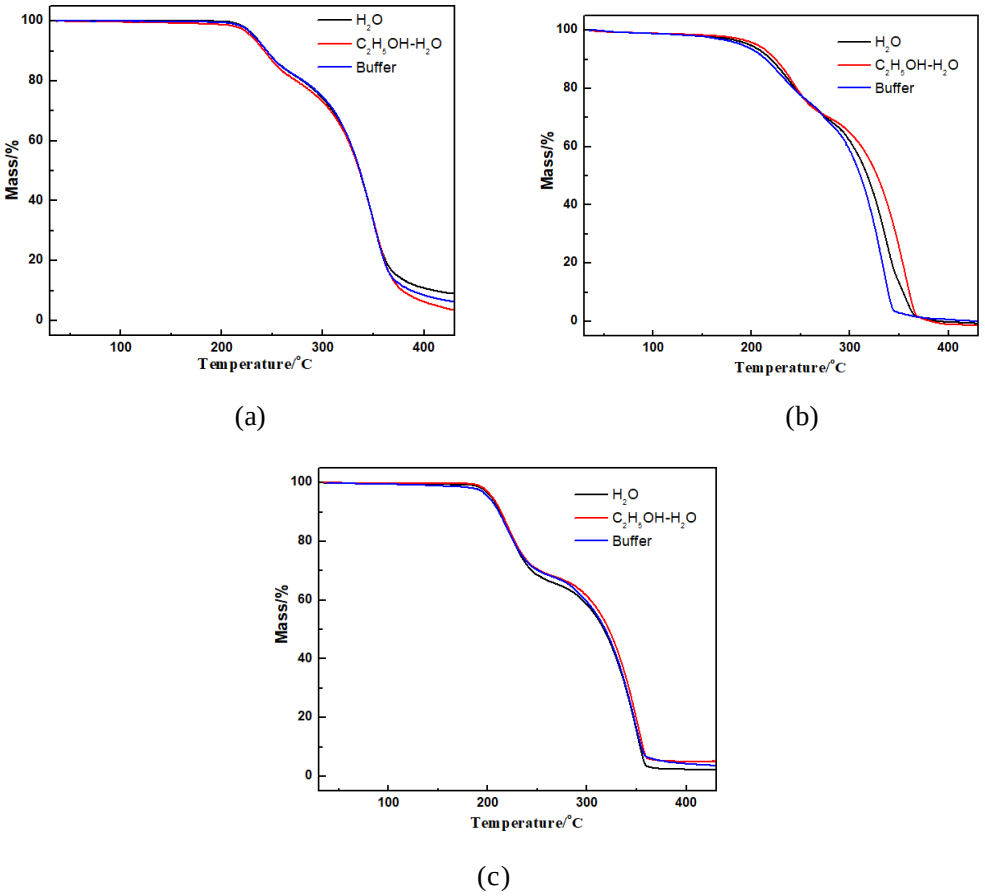
Table S2 The data calculated from TGA traces of DF and complexes **1**–**3**.

Sample	Temperature range of weight lose (°C)	Theoretical losing weight[a] (%)	Experimental losing weight (%)	Melting enthalpy (J/g)
DF	255–425	100	99.6	108.1
1	203–246	21.8	21.5	112.4
2	163–235	24.9	24.6	59.47
3	181–235	33.2	33.1	101.3

[a] Theoretical losing weight is the theoretical weight percent of coformer in each complex.

Table S3 The pH values of suspensions at equilibrium for complexes **1**–**3**.

Sample \ Medium	Pure water	Ethanol solution (30%)	Acetate buffer
1	4.26	4.45	4.54
2	5.01	5.16	4.56
3	4.58	4.98	4.56



(a) (b)

(c)

Fig. S5 TG traces for **1**–**3** (a)–(c) after the dissolution experiment in different solvent systems.