

Electronic Supplementary Information

**Suppressed hydration in metoclopramide hydrochloride by salt
cocrystallisation**

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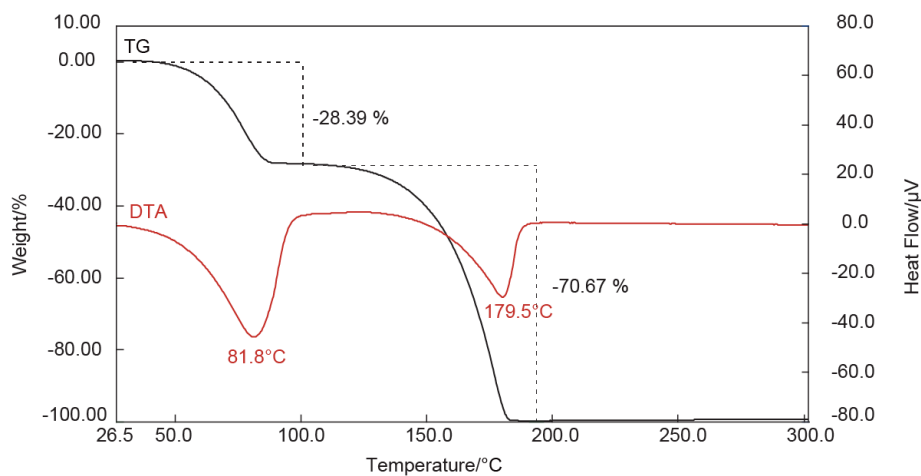


Fig. S1 TG-DTA thermogram of OXA dihydrate used in this study. TG and DTA curves are indicated by black and red lines, respectively.

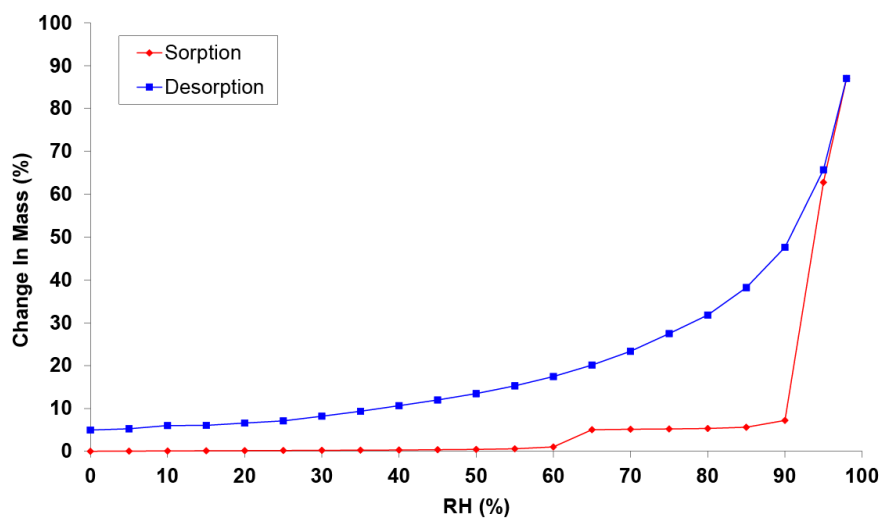


Fig. S2 Dynamic vapor sorption (DVS) measurement results of MCPHCl-Anh at 0–100% RH. The measurement was conducted at 25°C.

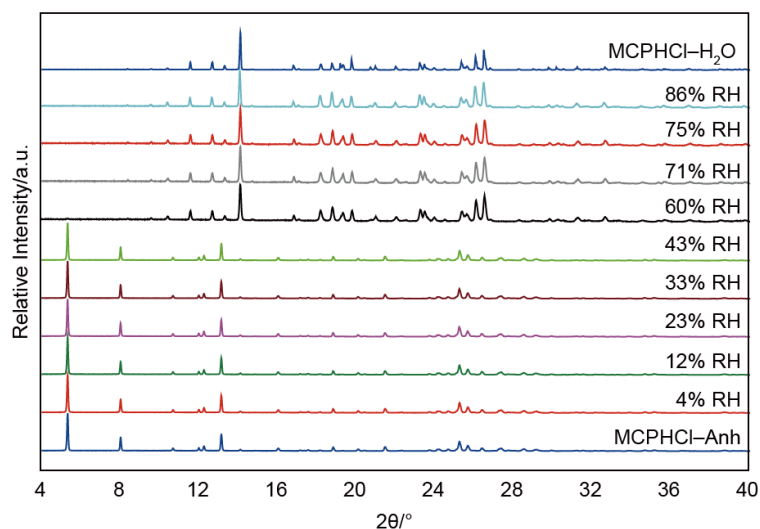


Fig. S3 PXR D pattern of MCPHCl-Anh after 2 days exposure in humidity-controlled environment at ambient temperature. Experimental PXR D pattern of MCPHCl-Anh and MCPHCl-H₂O are included as reference.

Table S1 Hydrogen bond parameters in MCPHCl-H₂O

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	D-H...A (°)
N(1)-H(1B)...Cl(1)	0.841(19)	2.684(18)	3.0078(15)	104.5(14)
N(1)-H(1B)...O(3) ¹	0.841(19)	2.146(19)	2.9606(18)	163.2(17)
N(1)-H(1A)...Cl(2) ²	0.865(19)	2.394(19)	3.2460(15)	168.6(16)
N(2)-H(2)...O(1)	0.848(17)	2.075(16)	2.7103(15)	131.3(14)
N(3)-H(3)...Cl(2)	0.924(17)	2.176(18)	3.0785(12)	165.1(14)
O(3)-H(3B)...O(2)	0.79(2)	1.99(2)	2.7622(16)	170(2)
O(3)-H(3C)...Cl(2) ³	0.86(2)	2.35(2)	3.1989(14)	169(2)
C(3)-H(3A)...O(2)	0.95	2.40	2.7465(17)	100.8
C(9)-H(9A)...O(2)	0.99	2.33	2.7588(17)	104.9
C(13)-H(13B)...O(2)	0.99	2.38	3.3307(18)	161.7

$$^1 -x + 1/2, y - 1/2, -z + 1/2$$

$$^2 -x + 1, -y, -z + 1$$

$$^3 -x, -y, -z + 1$$

Table S2 Hydrogen bond parameters in MCPHCl-Anh

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	D-H...A (°)
N(1)-H(1B)...Cl(1)	0.88	2.58	2.993(4)	109.7
N(1)-H(1A)...O(2) ¹	0.88	2.03	2.893(5)	166.1
N(2)-H(2)...O(1)	0.88	1.91	2.622(5)	136.5
C(3)-H(3A)...O(2)	0.95	2.43	2.768(6)	100.4
C(9)-H(9A)...O(2)	0.99	2.40	2.782(6)	102.1
N(3)-H(3)...Cl(2)	1.00	2.13	3.127(5)	174.1
C(9)-H(9B)...Cl(2)	0.99	2.82	3.478(5)	124.5
C(13)-H(13B)...Cl(2) ²	0.99	2.81	3.770(7)	164.6

$$^1 x - 1/2, -y + 3/2, -z + 1$$

$$^2 -x + 1, y - 1/2, -z + 1/2$$