

# Crystal structure elucidations of ondansetron salts and considerations of the dehydration behaviors

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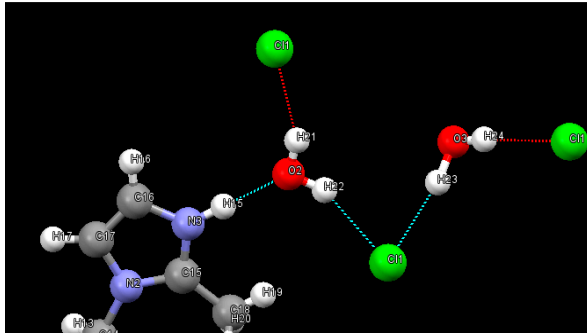
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The lists of interactions were shown in Table S1.

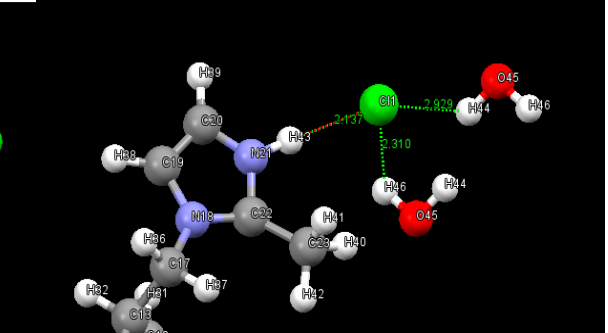
Table S1. The list of interactions observed in each crystal structure.

crystal form	number	Atom 1	Atom 2	length (Å)
HCl dihydrate	1	H15	O2	1.744
	2	Cl1	H22	2.266
	3	Cl1	H21	2.350
	4	Cl1	H23	2.199
	5	Cl1	H24	2.382
HCl hemihydrate	1	H43	Cl1	2.137
	2	H44	Cl1	2.929
	3	H46	Cl1	2.310
HCl anhydrate	1	H42	Cl43	2.000
HBr dihydrate	1	Br23	H24A	2.390
	2	Br23	H24B	2.441
	3	Br23	H25A	2.495
	4	Br23	H25B	2.534
	5	H2	O24	1.785
HBr anhydrate A	1	Br	H15	2.228
HBr anhydrate B	1	H42	Br43	2.086
HI dihydrate	1	I23	H24A	2.692
	2	I23	H25B	2.653
	3	O1	H24B	1.919
	4	H2	O25	1.811
	5	O24	H25A	1.866
HI anhydrate	1	I23	H2	2.908

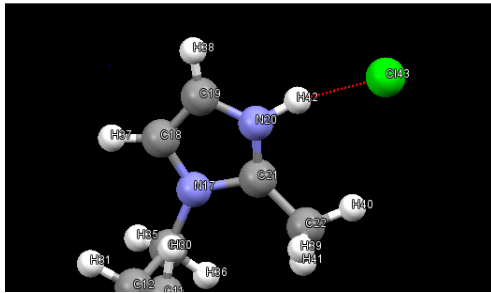
(A)



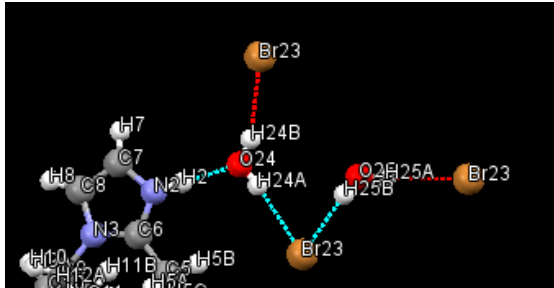
(B)



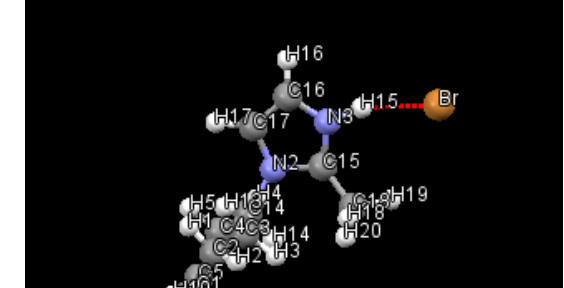
(C)



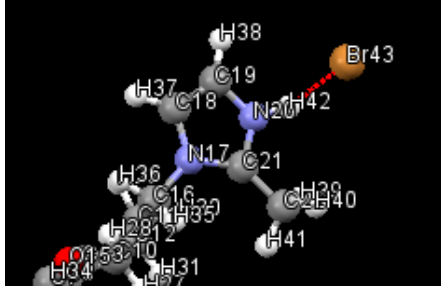
(D)



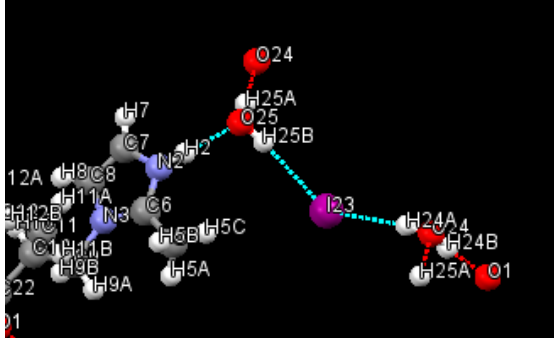
(E)



(F)



(G)



(H)

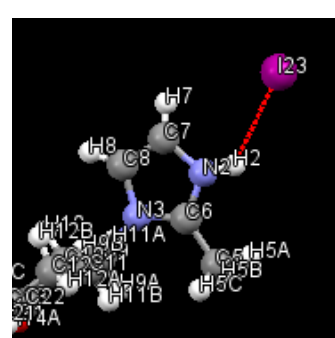


Figure S1. Numbering of atoms for each crystal form, (A) HCl dihydrate, (B) HCl hemihydrate, (C) HCl anhydrate, (D) HBr dihydrate, (E) HBr anhydrate A, (F) HBr anhydrate B, (G) HI dihydrate, and (H) HI anhydrate.

PXRD patterns of ondansetron salts were shown in Figure S2.

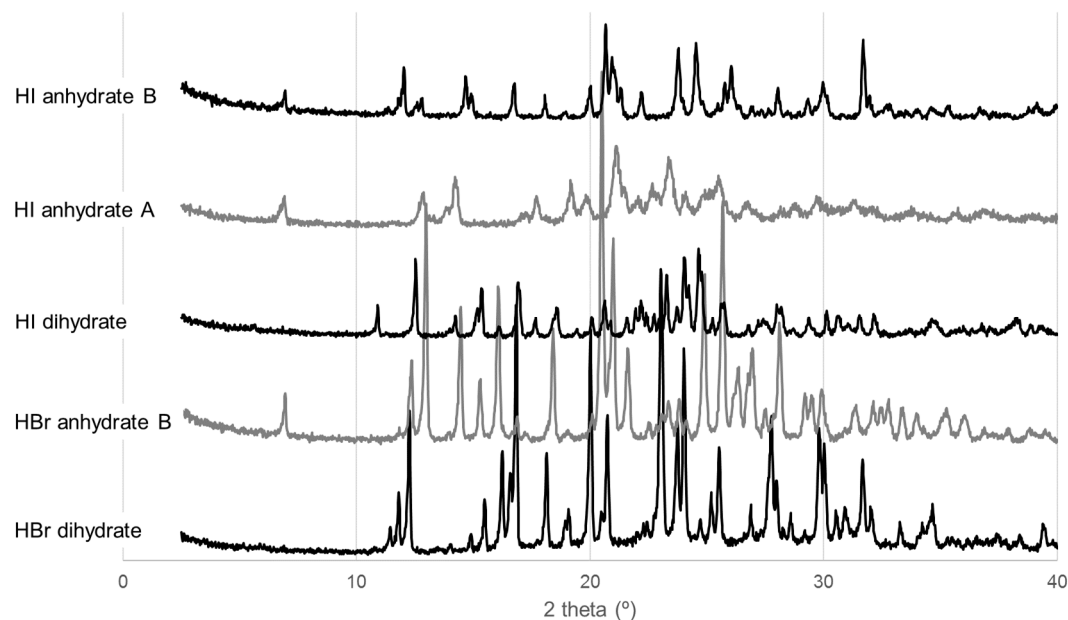


Figure S2. PXRD patterns of ondansetron salts.

DSC curves of ondansetron salts were shown in Figure S3.

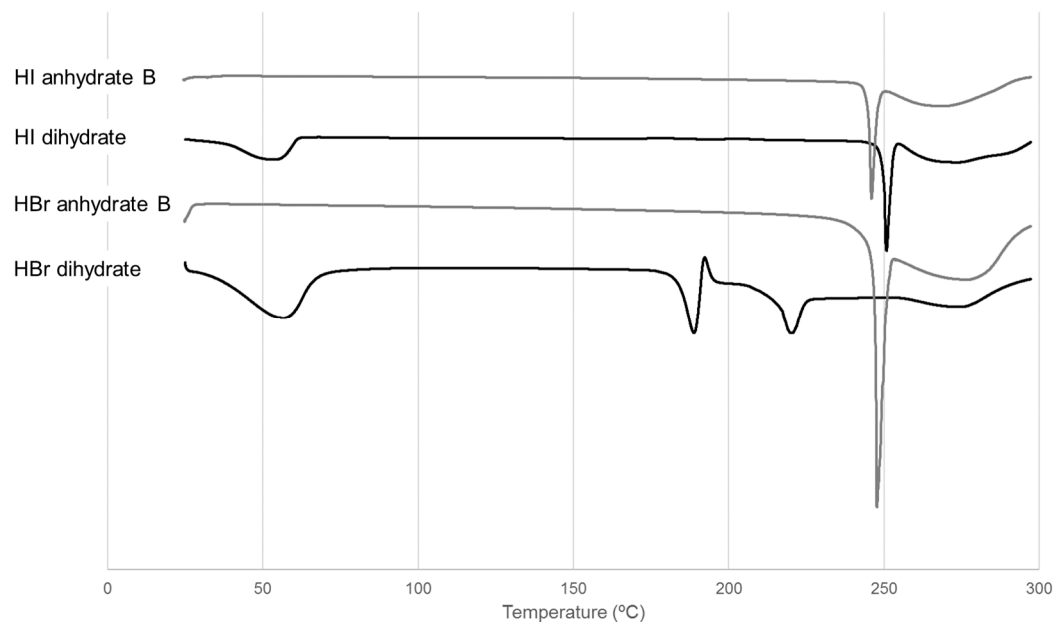


Figure S3. DSC curves of ondansetron salts

TGA curves of ondansetron salts were shown in Figure S4.

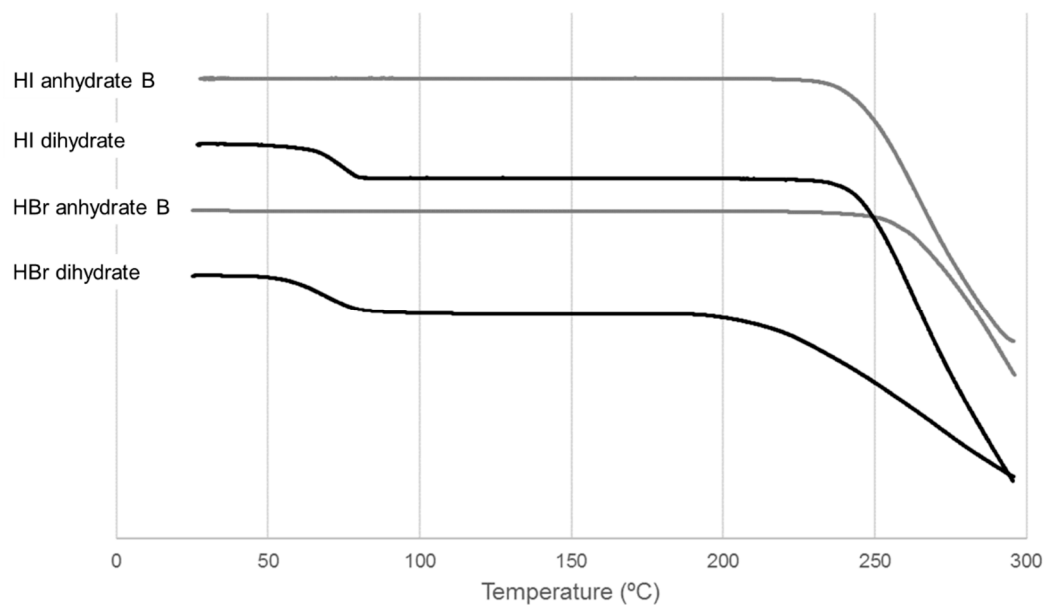


Figure S4. TGA curves of ondansetron salts.

An experiment of XRD with heating of HBr dihydrate was conducted at SPring-8 BL19B2. Results were shown in Figure S5.

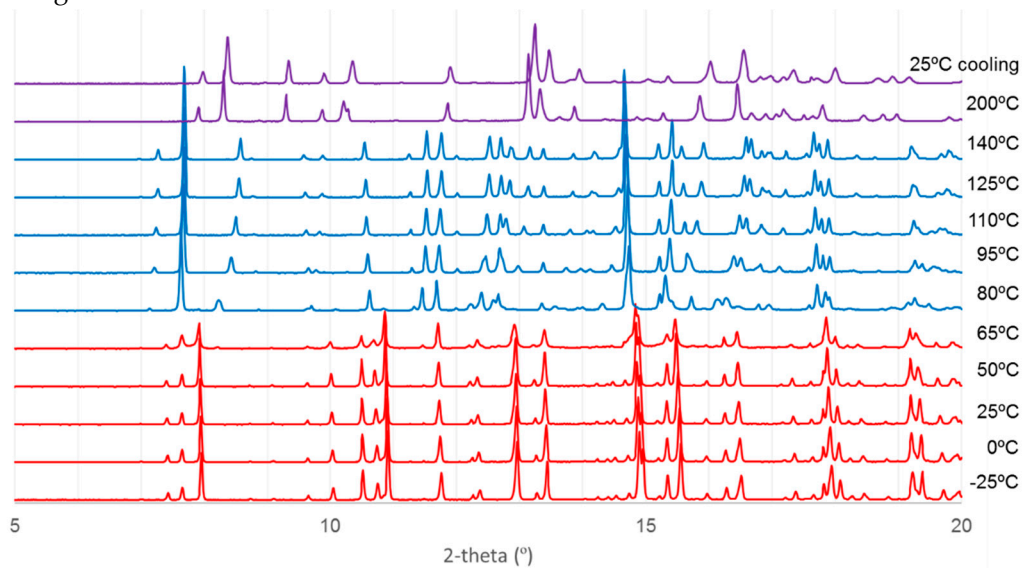


Figure S5. XRD with heating measurement of HBr dihydrate at SPring-8 BL19B2. Red patterns indicated the dihydrate, blue patterns indicated the anhydrate A, and purple patterns indicated the anhydrate B.

For deeper understanding the crystal transition profile of a dihydrate with heating, an experiment of XRD with heating of HI dihydrate was conducted at SPring-8 BL19B2. Results were shown in Figure S6.

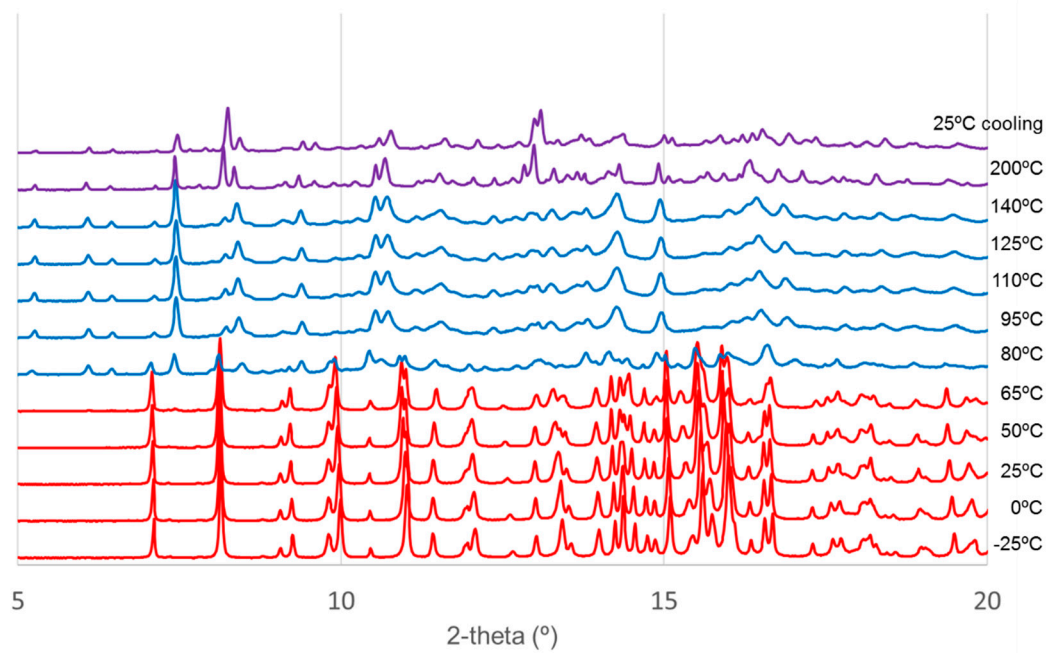


Figure S6. XRD with heating measurement of HI dihydrate at SPring-8 BL19B2. Red patterns indicated the dihydrate, blue patterns indicated the anhydrate A, and purple patterns indicated the anhydrate B.