Polymorphs and hydrates of Etoricoxib, a selective COX-2 inhibitor

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Electronic Supplementary Information

Contents

1. ORTEP Diagrams of hemihydrate polymorphs

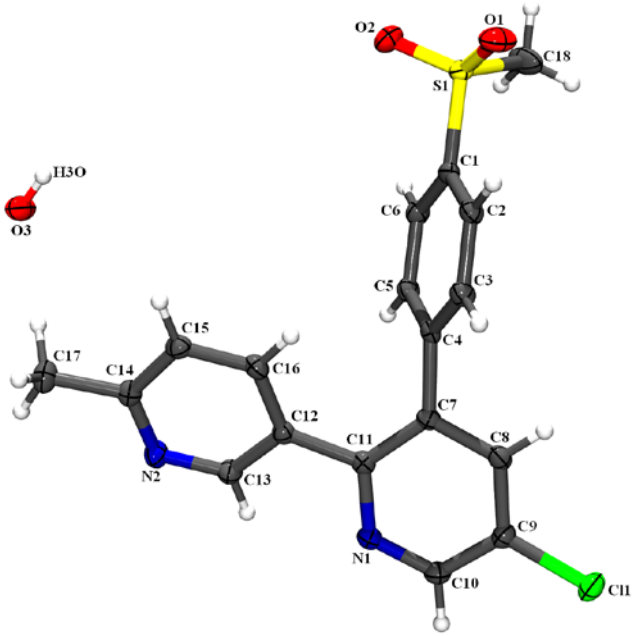


Fig. S1.1 Thermal ellipsoid diagram of hemihydrate **I** at 50% probability

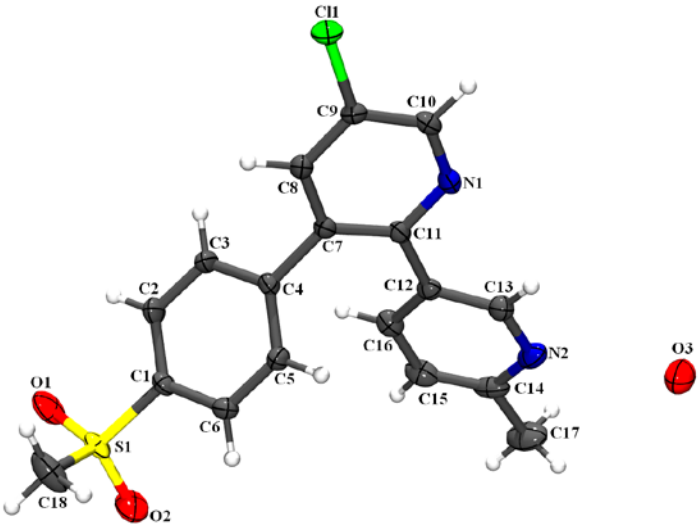


Fig. S1.2 Thermal ellipsoid diagram of hemihydrate **II** at 50% probability

2. Comparison of PXRD patters reported in patents with simulated patterns generated from single crystal structures

Form IV

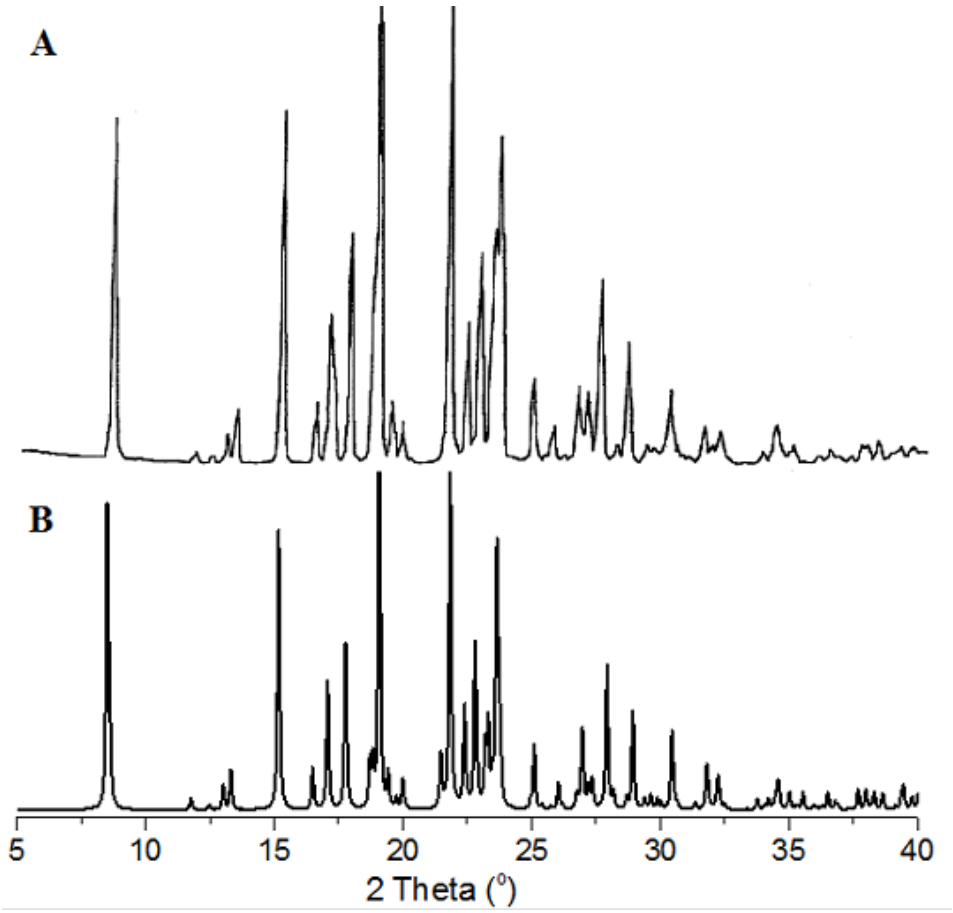


Fig. S2.1. PXRD patterns of form IV; patent (A) and that generated from the single crystal structure (B)

Hemihydrate I

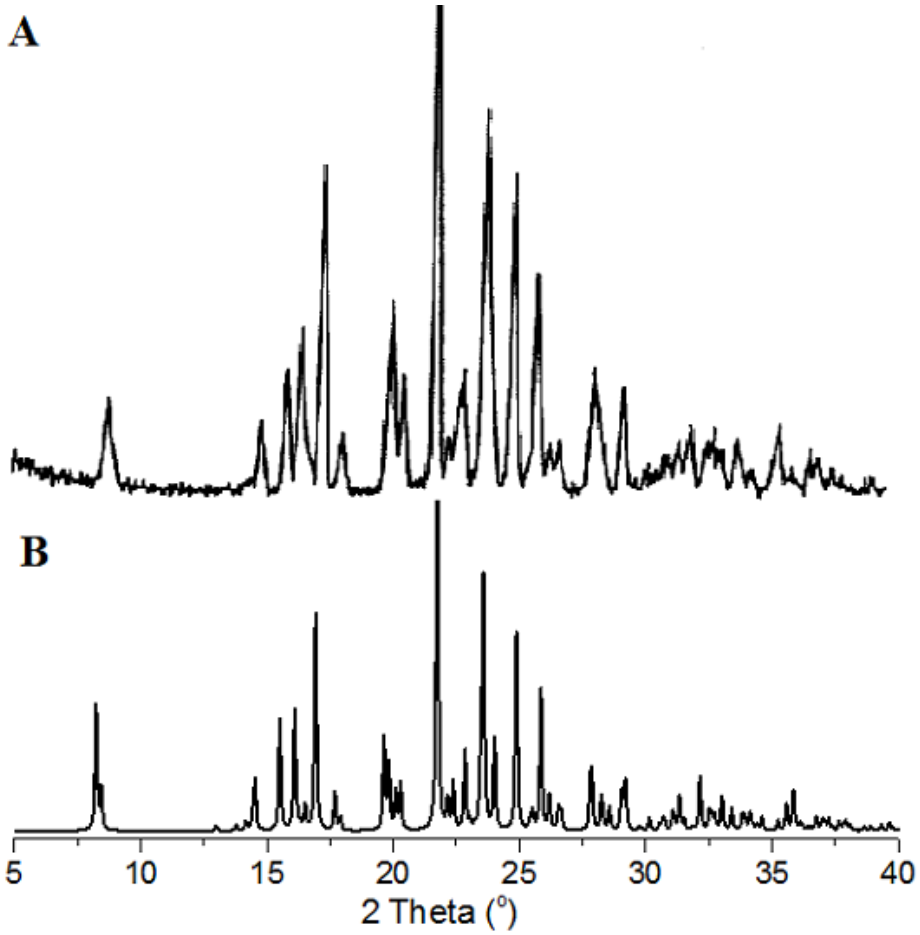


Fig. S2.2. PXRD patterns of Hemihydrate I; patent (A) and that generated from the single crystal structure (B)

Hemihydrate II

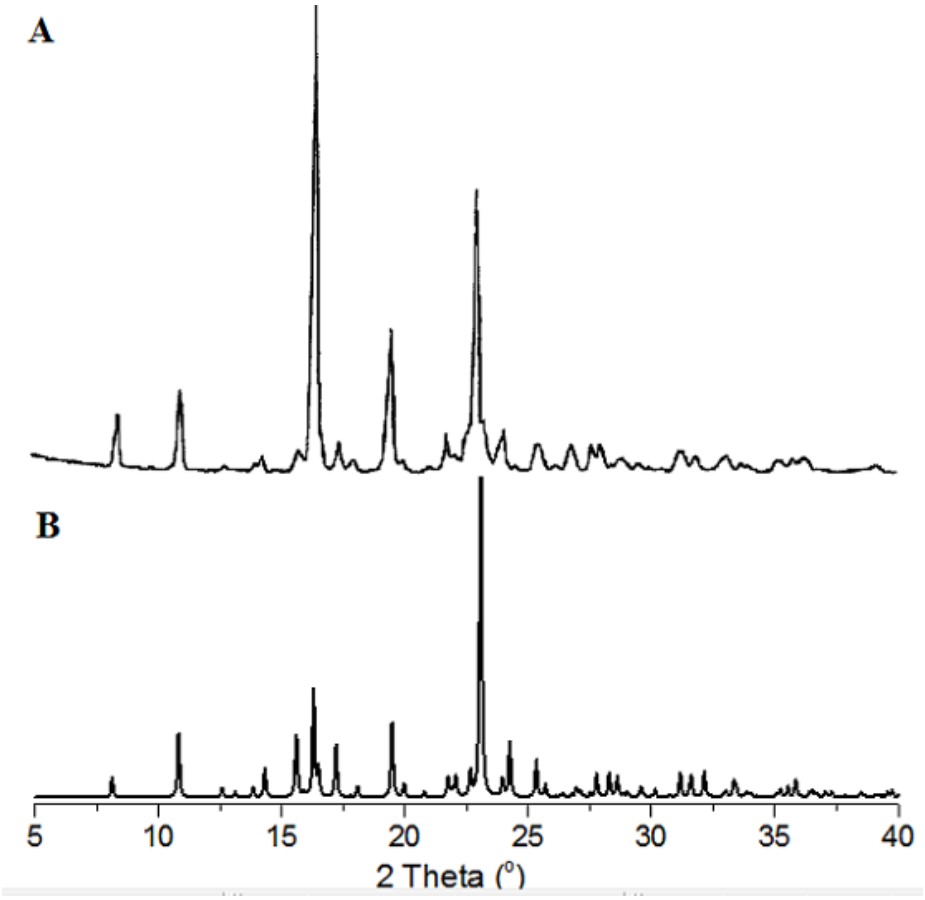
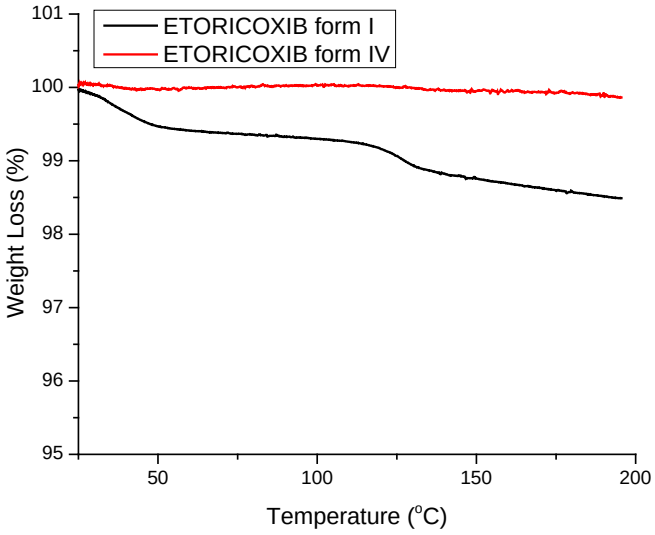


Fig. S2.3. (A) PXRD patterns of Form III in patent and (B) simulated PXRD pattern for hemihydrate II generated from the single crystal structure.

3. TGA plots for Form I and form IV



4. Hydrogen Bonding Table with normalized H-atom Positions[†]

	D–H···A	Symmetry code	D–H	H···A	D–H···A
Form I	C2–H2···O1	.	1.09	2.43	103
	C5–H5···N1	x, -1+y, z	1.09	2.55	156
	C8–H8···O4	.	1.09	2.26	165
	C10–H10···O2	1/2-x, -1+y, -1/2+z	1.09	2.28	162
	C13–H13···Cl2	1/2-x, -1+y, -1/2+z	1.09	2.74	137
	C17–H17B···O3	-1/2+x, 1-y, z	1.09	2.58	140
	C18–H18B···O1	x, -1+y, z	1.09	2.59	125
	C21–H21···N4	x, 1+y, z	1.09	2.54	156
	C24–H24···O4	.	1.09	2.47	102
	C26–H26···O1	.	1.09	2.30	168
	C28–H28···O3	1-x, 1-y, 1/2+z	1.09	2.36	139
	C35–H35B···O2	1/2+x, 1-y, z	1.09	2.40	162
	C36–H36C···N3	1-x, 1-y,-1/2+z	1.09	2.44	143
Form IV	C1–H1···N1	3-x, 1-y, 2-z	1.09	2.54	132
	C3–H3···O1	1-x, 2-y, 2-z	1.09	2.51	136
	C7–H7···O1	1+x, y, z	1.09	2.23	169
	C10–H10···O1	.	1.09	2.52	101
	C12–H12C···O2	1-x, 2-y, 1-z	1.09	2.54	120
Hemihydrate 1	O3–H3O···N2	x, 3/2-y, 1/2+z	0.99	1.89	177
	C2–H2···O1	.	1.09	2.48	102
	C3–H3···O1	x, 3/2-y, -1/2+z	1.09	2.48	152
	C5–H5···O1	1-x, 1-y, 1-z	1.09	2.60	133
	C10–H10···O2	x, y, -1+z	1.09	2.45	160
	C17–H17C···O3	.	1.09	2.50	166
	C18–H18A···O3	1-x, 1-y, 1-z	1.09	2.39	134
Hemihydrate 2	C2–H2···O1		1.09	2.49	101
	C10–H10···O2	x, y, 1+z	1.09	2.39	172
	C17–H17C···O3	x, 1/2-y, -1/2+z	1.09	2.47	143

[†] F. H. Allen, O. Kennard, D. G. Watson, L. Brammer, A. G. Orpen, R. Taylor, *J. Chem. Soc. Perkin Trans. 2*, 1987, S1.

5. Distance range observed in aromatic sufone and aromatic C–H interactions in CSD analysis

To search for aromatic sulfones RSO_2R' (R= Ar, R'=Me) for sulfone to aromatic C–H interactions, the following restrictions were applied: Only organics, no errors, not disordered,

not polymeric, no ions, 3D coordinates determined. The S=O···H–C distance was restricted to less than the sum of the van der Waals radii.

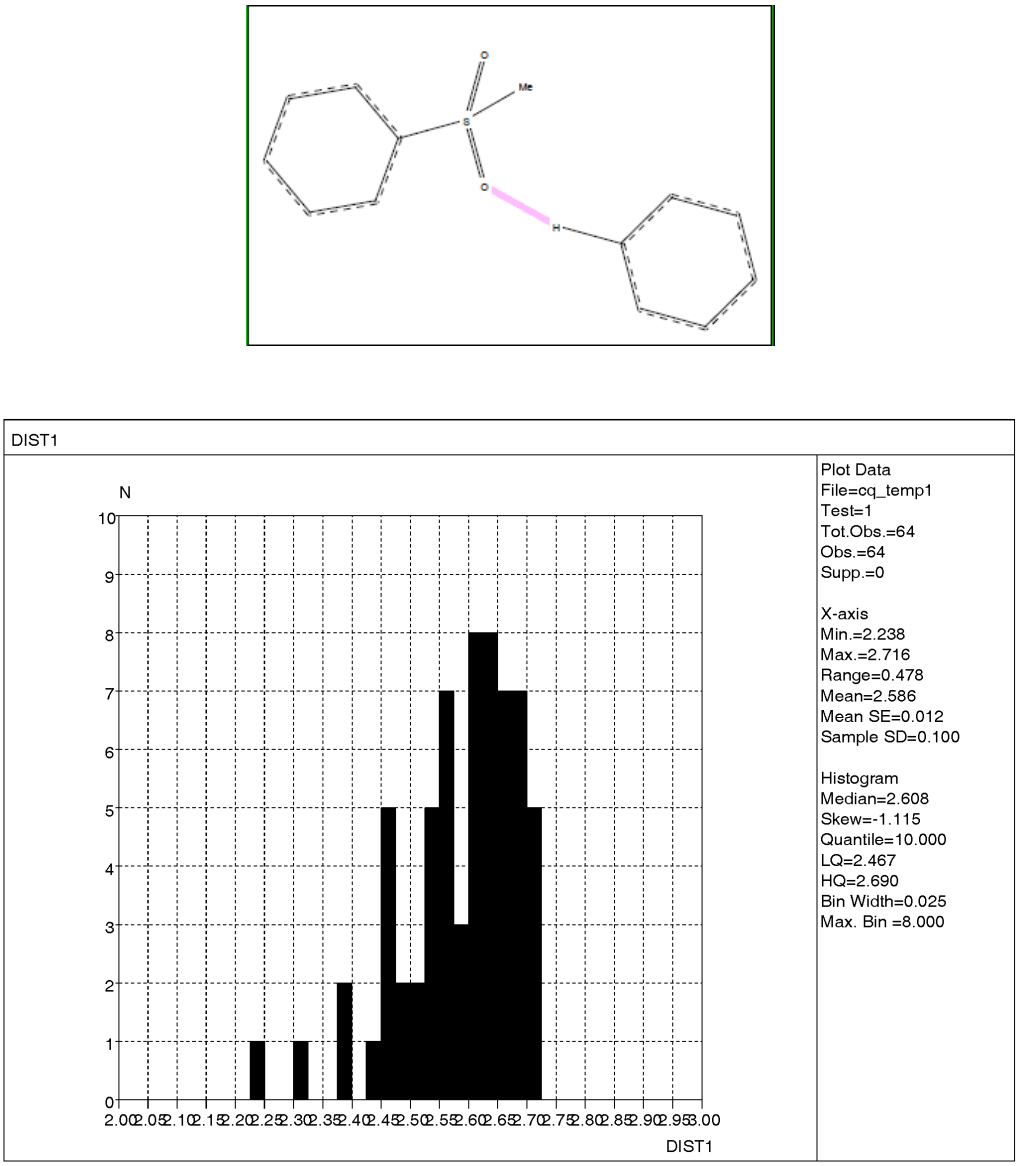


Fig. S5.1 Distribution of S=O···H–C distances as observed in aromatic sulfone (R= Ar, R'=Me) to aromatic C–H interaction.

6. Difference map for locating water hydrogen atoms in hemihydrate II