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Supporting information for article:

A new crystal form of the NSAID dexketoprofen

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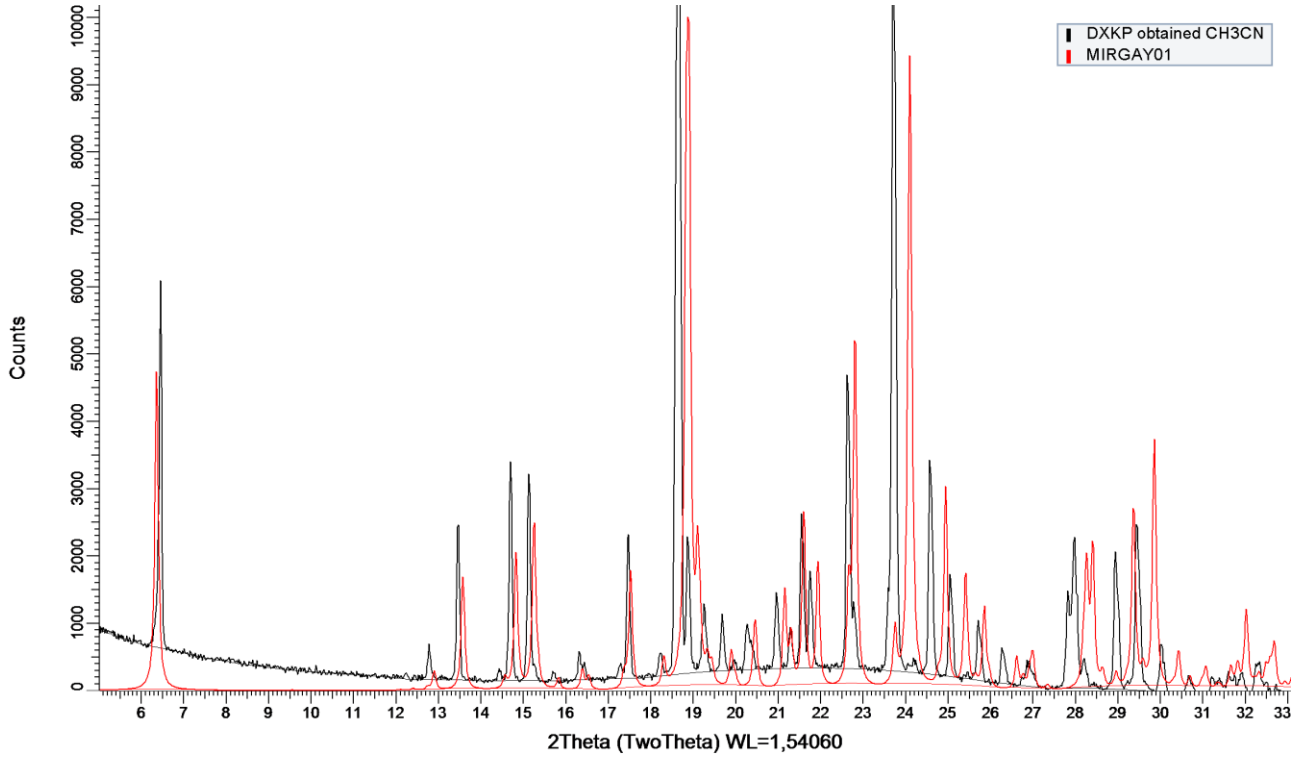

Figure S1. Superimposition of the XRPD pattern (collected at 300K) of the DXKP sample recrystallised from CH_3CN with the theoretical one of **DXKP-α** (MIRGAY01). Data for MIRGAY01 were collected at 100K this explains the peaks shift observed in the figure.

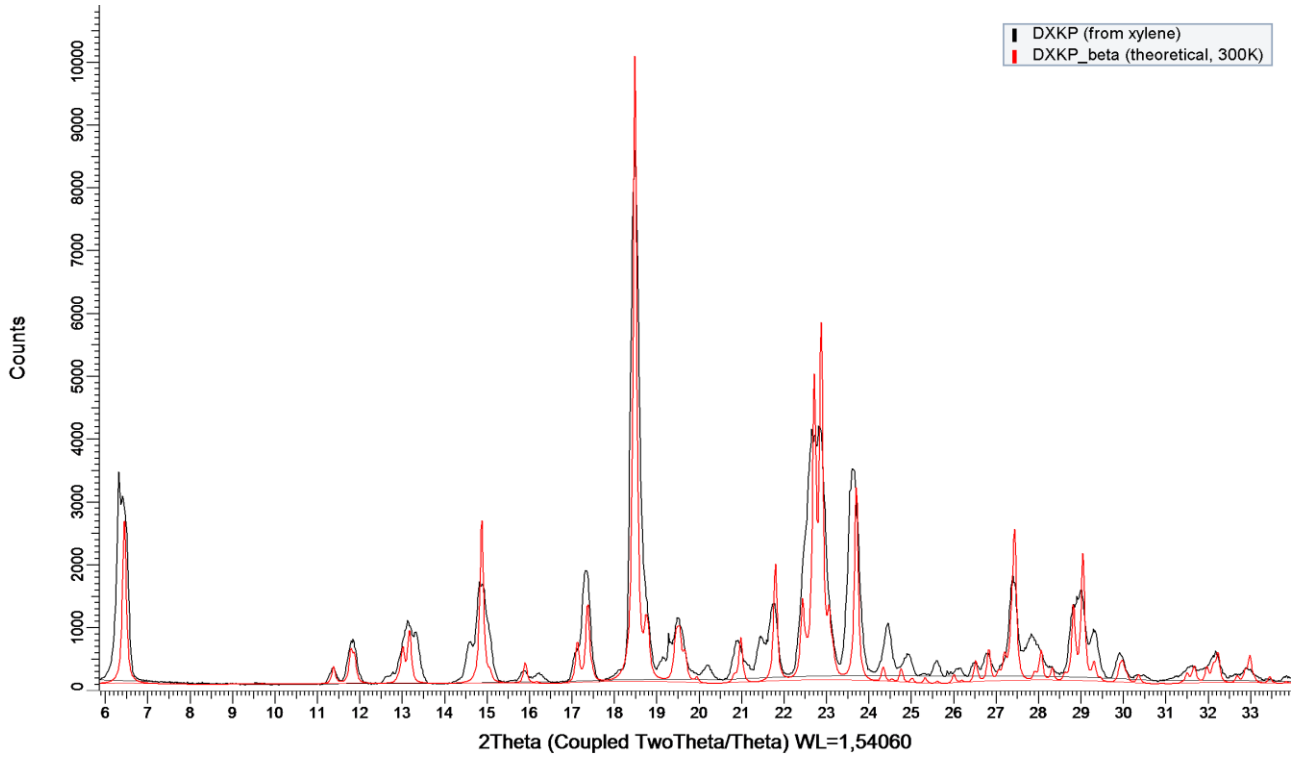

Figure S2. Superimposition of the XRPD pattern (collected at 300K) of the DXKP sample recrystallised from xylene with the theoretical one of **DXKP-β** (obtained by single crystal data collected at 300K).

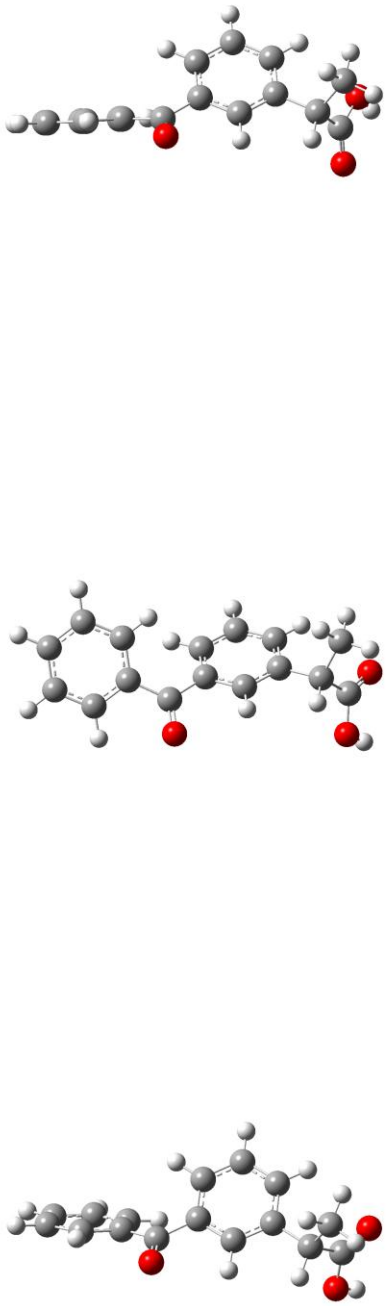

Figure S3. The three conformational isomers found in the solid state structures optimised with the B3LYP functional (top: DXKP-βA; middle: DXKP-βB; bottom: DXKP-αA).

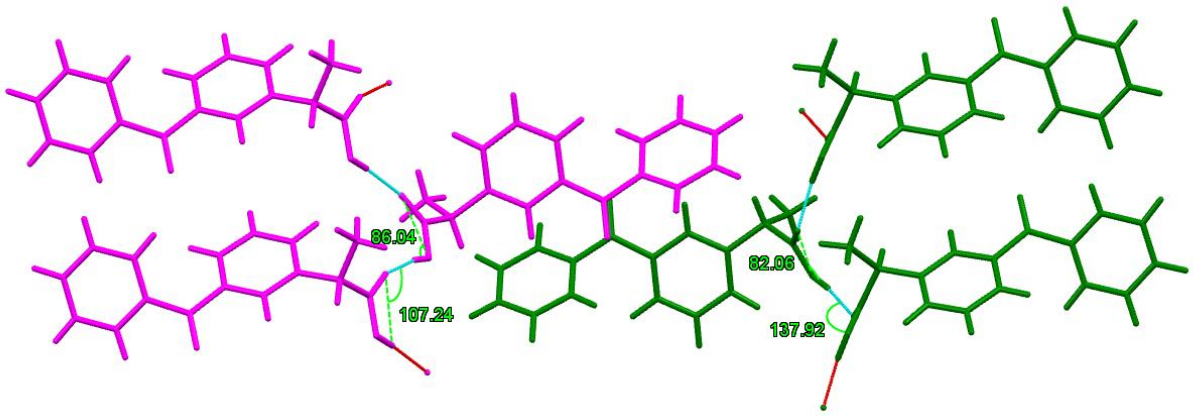

Figure S4. Catemer motifs described by the dexketoprofen molecules, together with the characterising geometrical parameters: SS-S catemer for the DXKP-βB molecules (magenta); SA-S catemer for the DXKP-βA molecules (green).

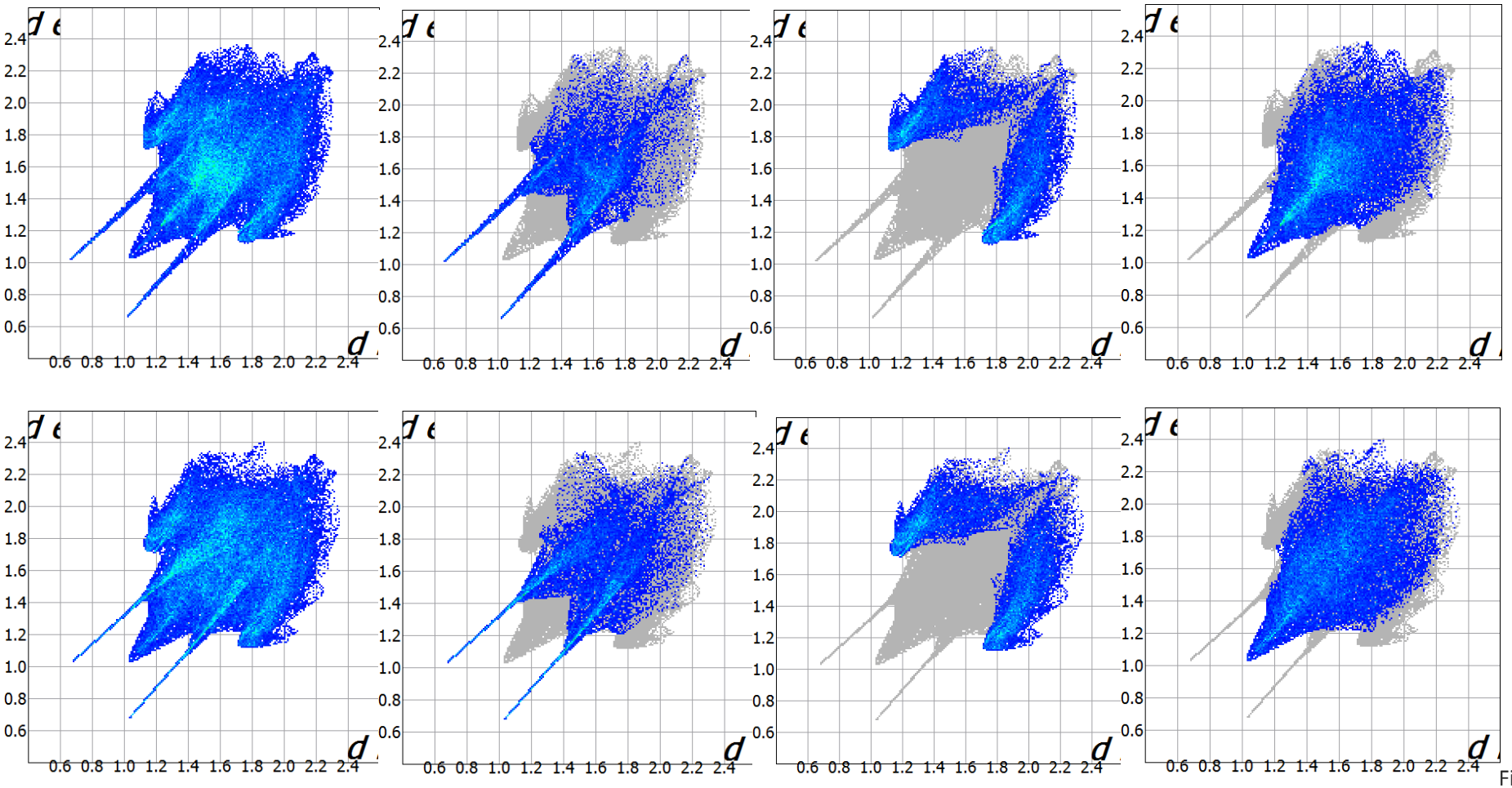

Figure S5. Fingerprint plots of the dexketoprofen independent molecules full (left), broken down into contributions from O…H, C…H and H…C (from left to right). Top: DXKP-βA; bottom: DXKP-βB

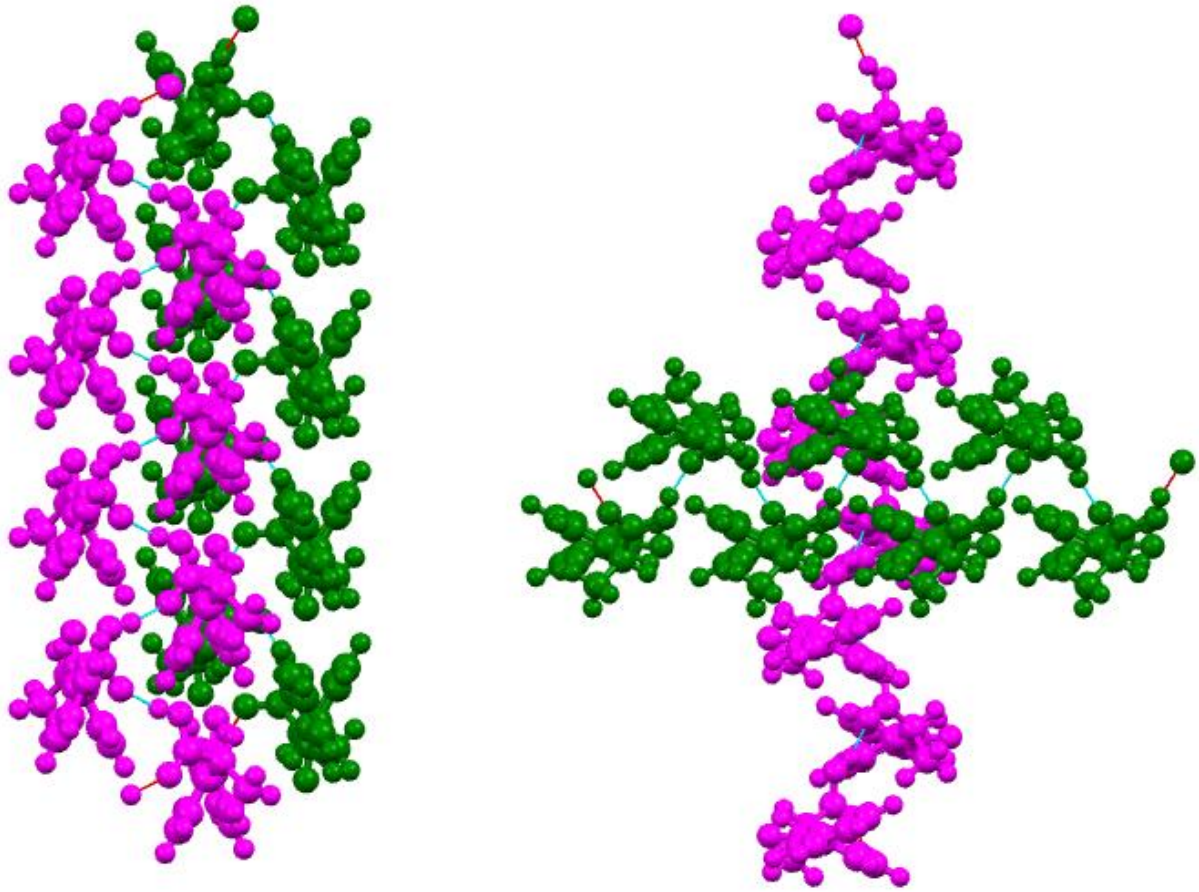

Figure S6. Crystal packing viewed along the *c* axis direction of **DXKP-β** (left) and **DXKP-α** (right).

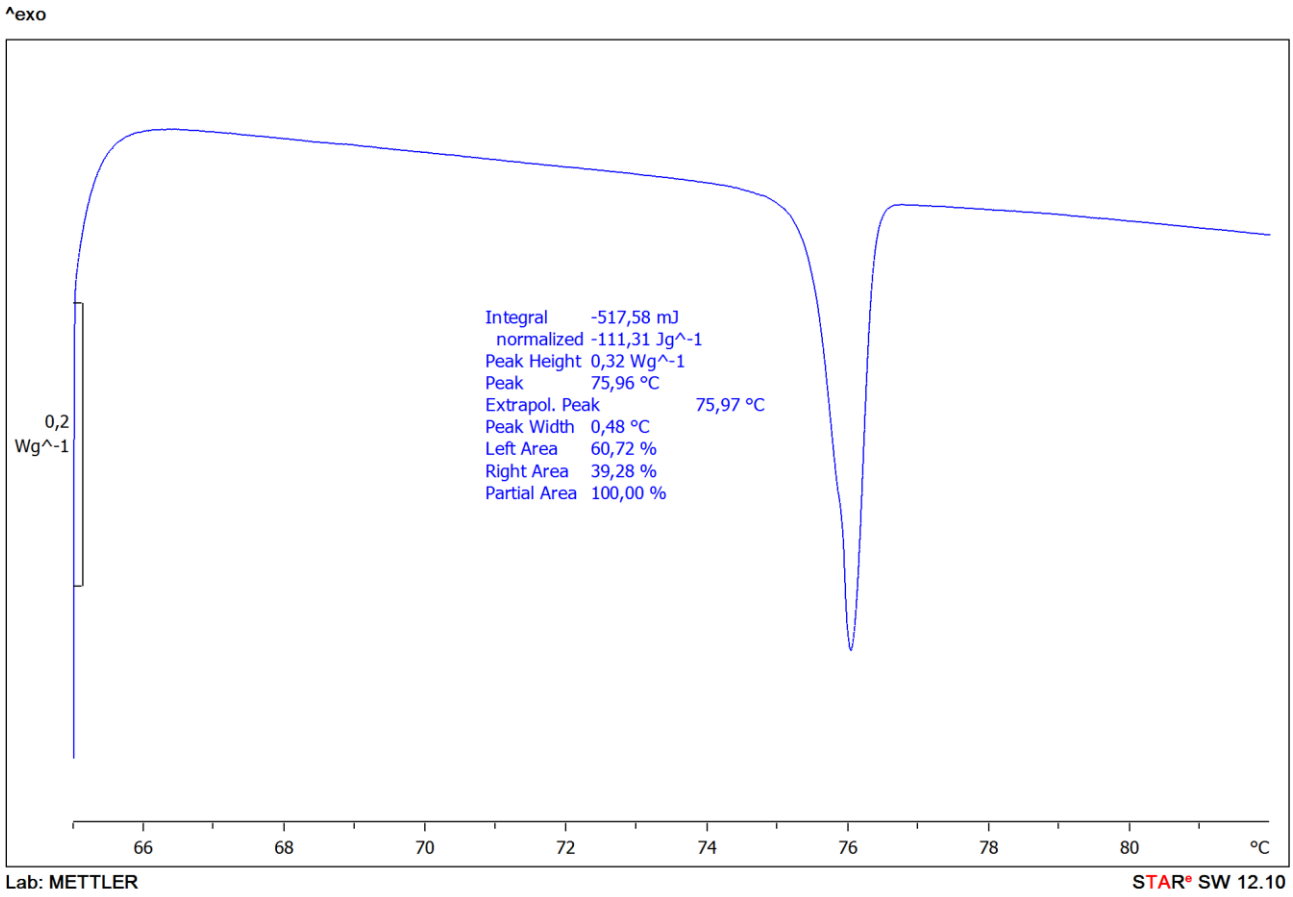

Figure S7. Experimental DSC curve of **DXKP_α** during the heating step. The experiment was performed at a 0.10 K/min rate.

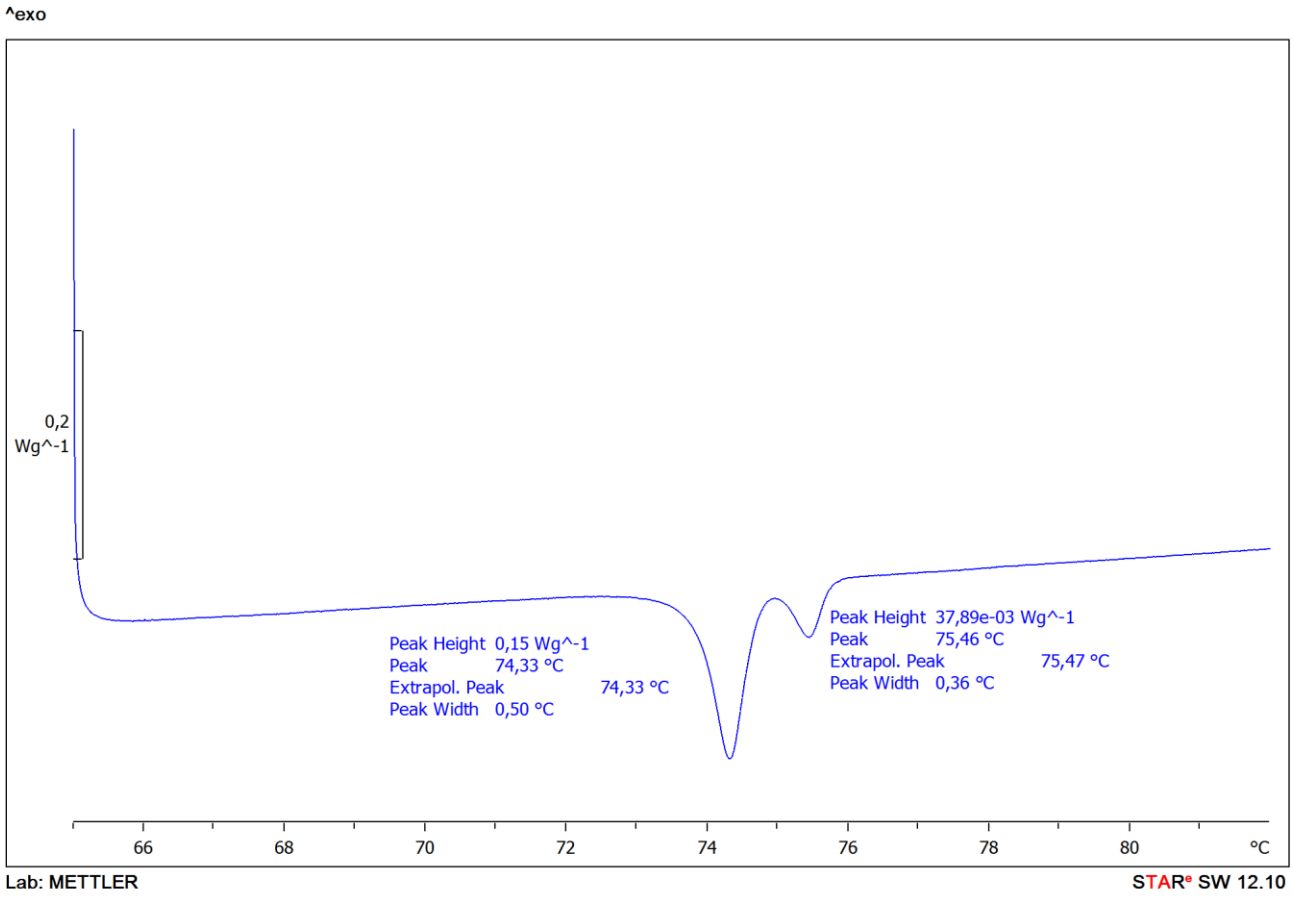

Figure S8. Experimental DSC curves of DXKP α and β mixture, obtained from xylene, during the heating step. The experiment was performed at 0.10 K/min rate.

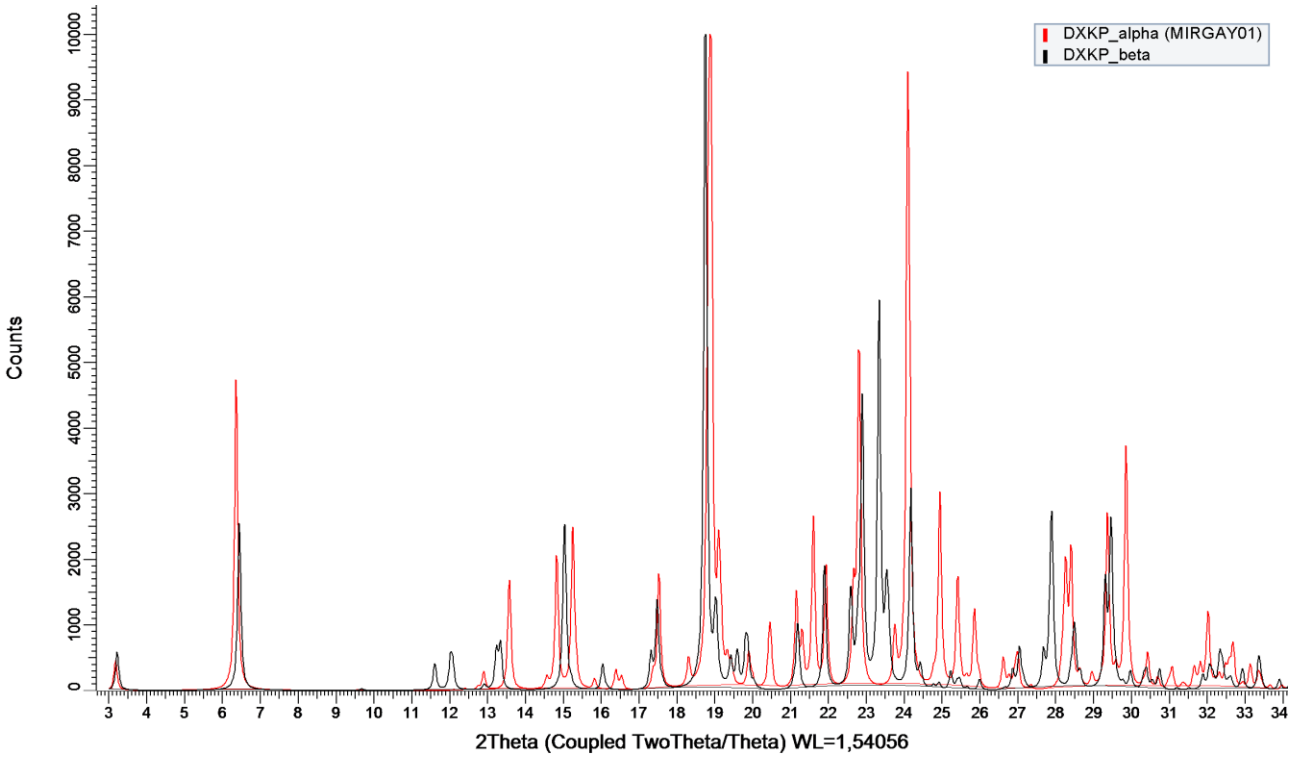

Figure S9. Superimposition of the theoretical patterns of **DXKP-α** (MIRGAY01) and **DXKP-β**.

	DXKP-β		**DXKP-α (MIRGAY01)**		**KEMRUP01**
	A	B	Mol. A	Mol. B	(S)- enantiomer
O1-C10-C8-C9	124.6(2)	-46.9(3)	-26.6	-40.5	-47.7
C2-C3-C7-O3	21.4(3)	-20.1(3)	22.1	-22.7	-20.2
C12-C11-C7-O3	32.5(3)	-31.4(3)	26.8	-26.7	-31.5
C1/C6 – C11/C16	54.78(6)	52.54(5)	51.4	50.4	51.9

Table S1. Dihedral angles and angles between the mean aromatic planes defining the conformation of the ketoprofen molecule as found in the solid state structure of **DXKP-β**, **DXKP-α** and **KEMRUP01**.

T(K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)
300	7.7688(5)	6.0959(3)	27.386(1)	90.801(5)	1296.8(1)
320	7.797(5)	6.122(4)	27.39(2)	90.75(5)	1307(1)
340	7.806(7)	6.110(6)	27.41(3)	90.39(8)	1307(2)

Table S2. Cell parameters of **DXKP-β** determined, by means of single-crystal X-ray diffraction, at 300, 320 and 340 K.