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Supporting Information

Impact of the Structural Binding Energies on Dissolution Rates for Single Faceted-Crystals

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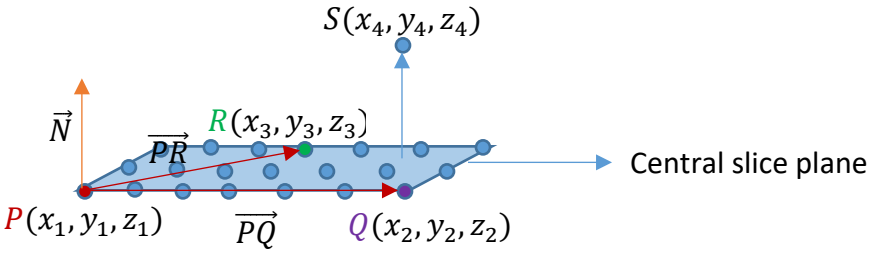


Figure S1: Schematic of the perpendicular projected distance calculations of molecules from the plane on which reference molecule is located

Calculation of Perpendicular Projections

A plane is defined in the central slice in such a way that all of the molecules of the central slice fall on the plane as shown in Figure. Since all of the molecules in the plane are coplanar, any three molecular positions P, Q and R can be used to define two vectors $\overrightarrow{PQ}$ and $\overrightarrow{PR}$ which are coplanar and lie parallel to the plane. The cross product of the vectors $\overrightarrow{PQ}$ and $\overrightarrow{PR}$ ($\overrightarrow{PQ}$ X $\overrightarrow{PR}$) generates a vector $\vec{N}$ (a, b, c) which is normal to the plane of vectors $\overrightarrow{PQ}$ and $\overrightarrow{PR}$. Coordinates of any of the points P, Q or R can be used along with the normal vector $\vec{N}$ to calculate the equation of the plane for the central slice as shown in equations S.1 and S.2. Any molecule $S(x_4, y_4, z_4)$ which does not lie on this plane, can have infinite distances from the central slice plane, but the shortest distance from the plane will be the one which is a normal projection to the plane. The shortest distance between the plane (based on cross-product $\overrightarrow{PQ}$ X $\overrightarrow{PR}$ and point P) and the given molecule $S(x_4, y_4, z_4)$ can be calculated as given in equation S.3. The distances of other molecules outside of this plane to this plane can be calculated in the same way as normal projections to the plane.

$$Central\ slice\ plane = a(x - x_1) + b(y - y_1) + c(z - z_1) = 0 \qquad (S.1)$$

$$Central\ slice\ plane = ax + by + cz = d \qquad (S.2)$$

$$Shortest\ distance\ between\ S\ and\ slice\ plane = \frac{|ax_4 + by_4 + cz_4 - d|}{\sqrt{a^2 + b^2 + c^2}} \qquad (S.3)$$

Table S1: Interaction energies arranged in descending order inside the ibuprofen crystal structure for face (011)

Slice	X	Y	Z	VDW +	VDW -	Total VDW	Electro static	H bond +	H bond -	Total H Bond	Total Energy
0	10.2466	15.9957	5.08908	-2.136	2.475	0.339	-1.274	-58.752	52.196	-6.556	-7.491
1	1.8022	12.0527	10.7915	-4.53	1.86	-2.669	-0.172	0	0	0	-2.841
-1	3.54766	12.0527	0.204459	-4.53	1.86	-2.669	-0.172	0	0	0	-2.841
1	1.8022	4.16672	10.7915	-3.798	1.111	-2.687	-0.005	0	0	0	-2.691
-1	3.54766	4.16672	0.204459	-3.798	1.111	-2.687	-0.005	0	0	0	-2.691
0	10.2466	8.10972	5.08908	-3.521	1.981	-1.541	-0.143	0	0	0	-1.684
0	-4.42039	8.10972	5.08908	-2.106	0.478	-1.627	-0.007	0	0	0	-1.635
0	2.67493	15.5483	5.498	-1.593	0.338	-1.255	0.054	0	0	0	-1.202
0	2.67493	-0.22372	5.498	-1.593	0.338	-1.255	0.054	0	0	0	-1.202
1	-5.29313	11.6053	10.3826	-1.46	0.583	-0.877	0.005	0	0	0	-0.872
1	-5.29313	3.71928	10.3826	-1.46	0.583	-0.877	0.005	0	0	0	-0.872

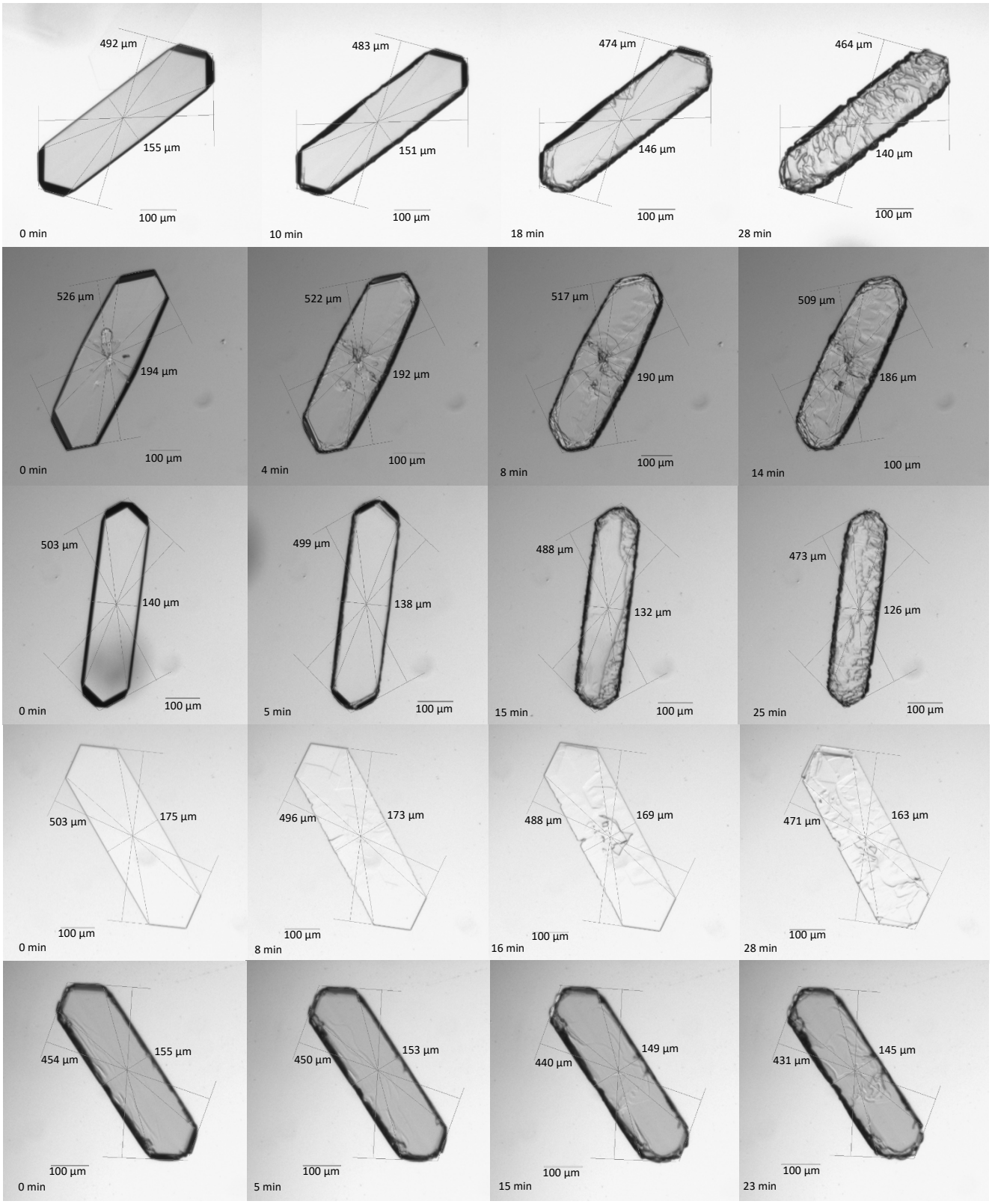


Figure S2: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -1.36%

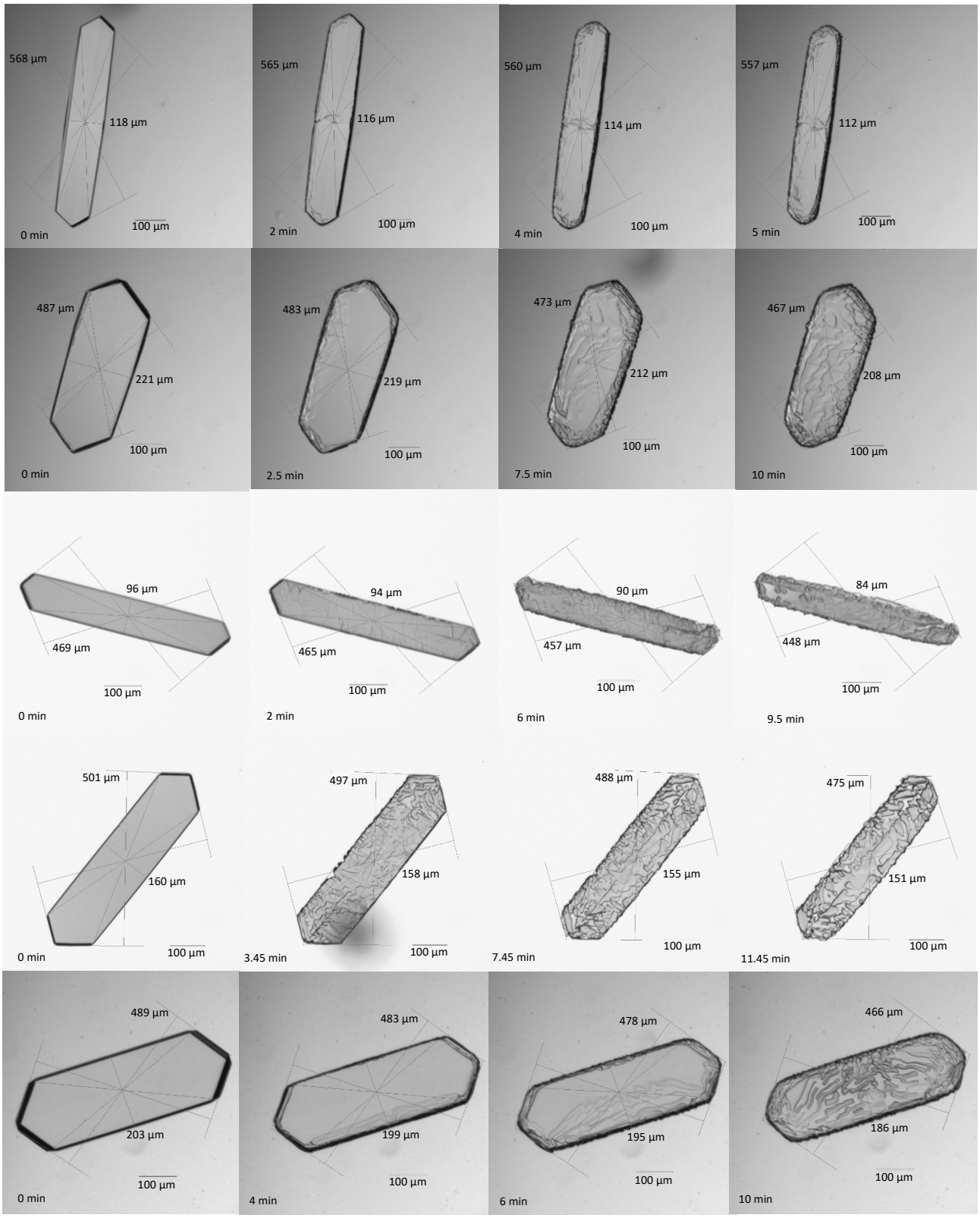


Figure S3: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -3.24%

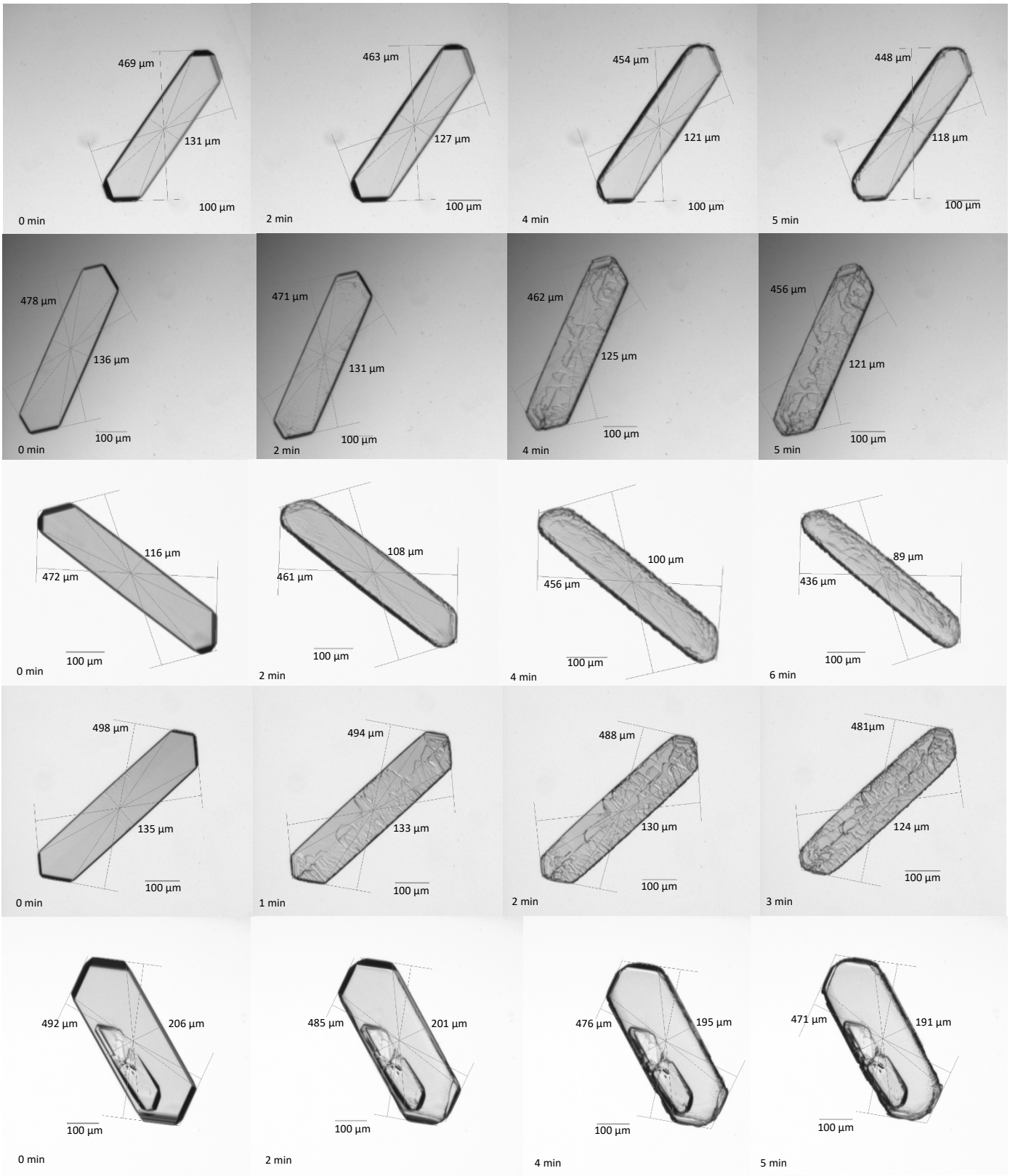


Figure S4: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -5.09%

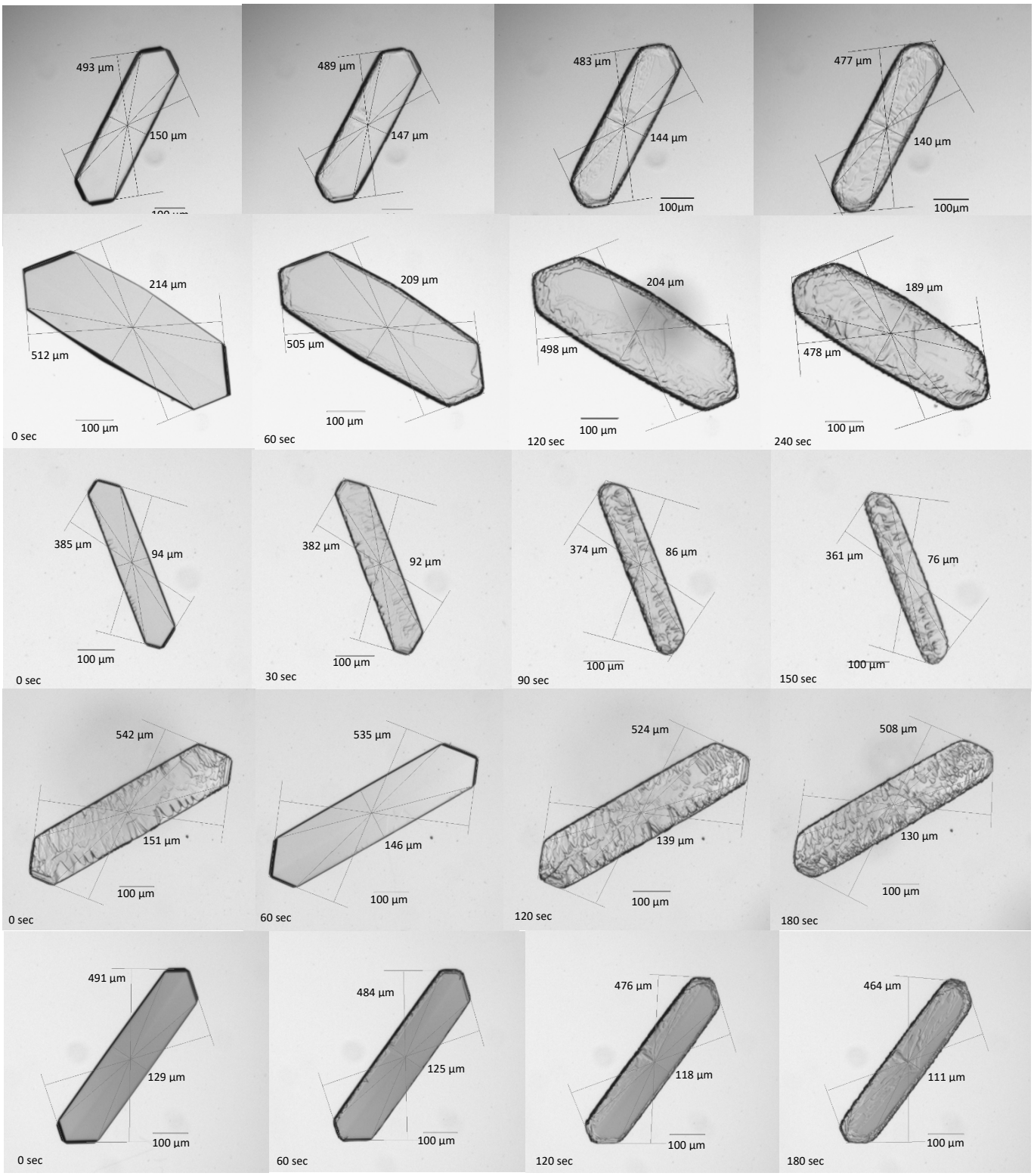


Figure S5: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -6.9%

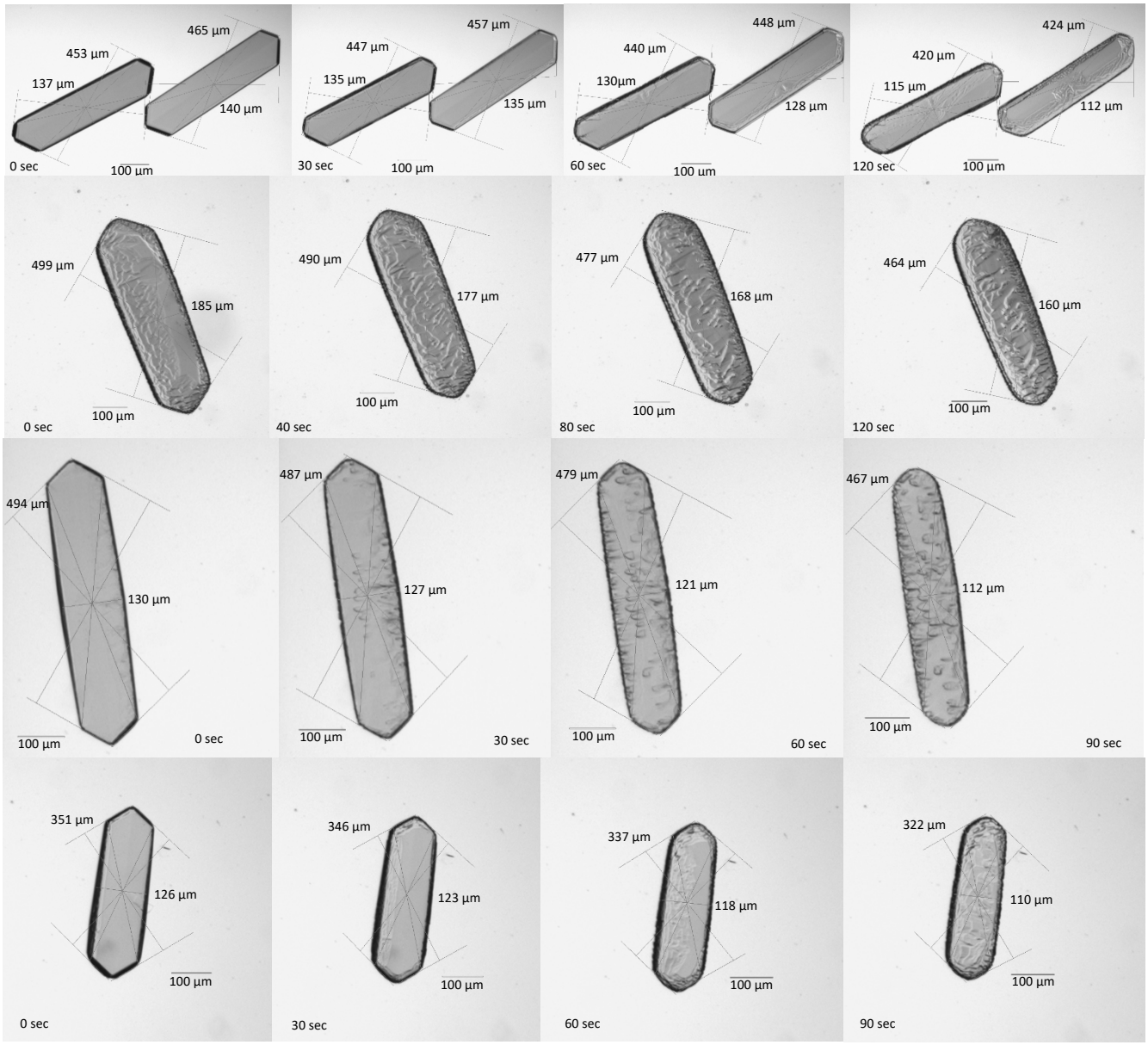


Figure S6: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -8.66%

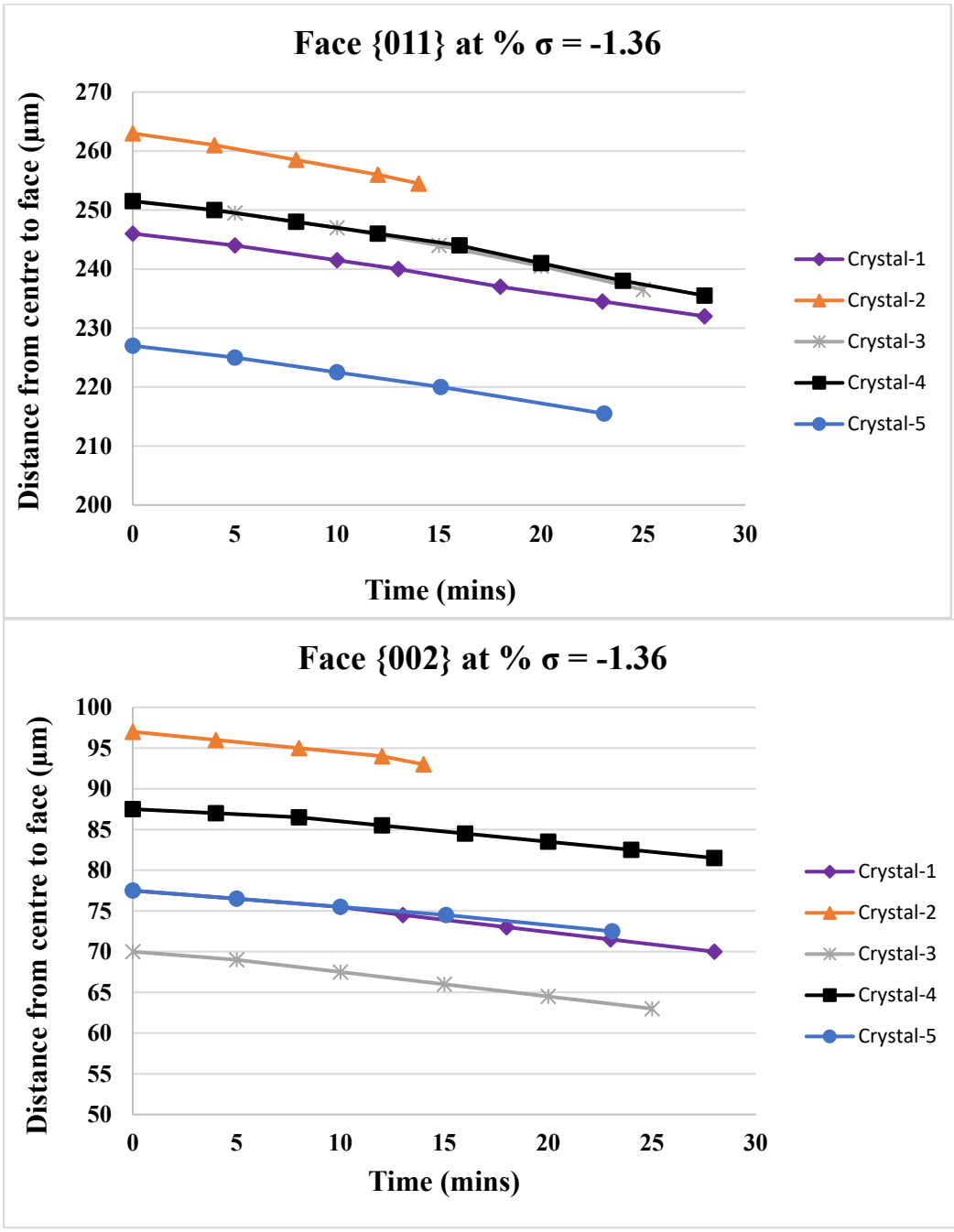
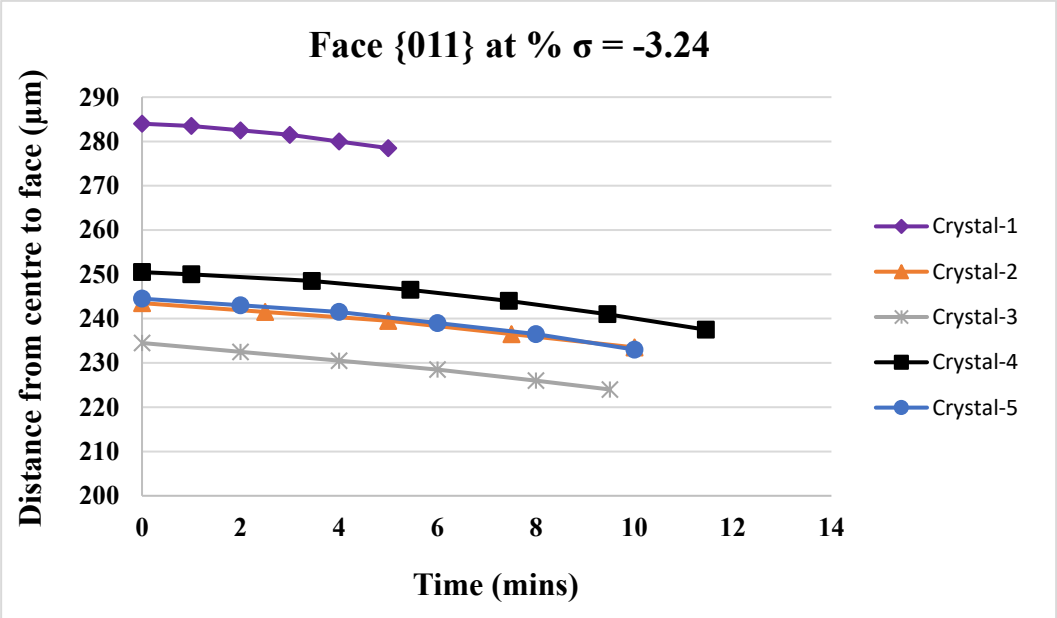


Figure S7: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -1.36%

Table S2: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -1.36%

Crystal	Face {011}		Face {002}	
	Equation	R^2 Value	Equation	R^2 Value
Crystal-1	y = -0.5116x + 246.37	0.9977	y = -0.2734x + 77.86	0.9919
Crystal-2	y = -0.6082x + 263.22	0.9967	y = -0.2744x + 97.085	0.9878
Crystal-3	y = -0.6x + 252.33	0.9854	y = -0.2857x + 70.238	0.9967
Crystal-4	y = -0.5804x + 252.38	0.9884	y = -0.2217x + 87.917	0.9871
Crystal-5	y = -0.5006x + 227.32	0.9964	y = -0.2147x + 77.583	0.9965



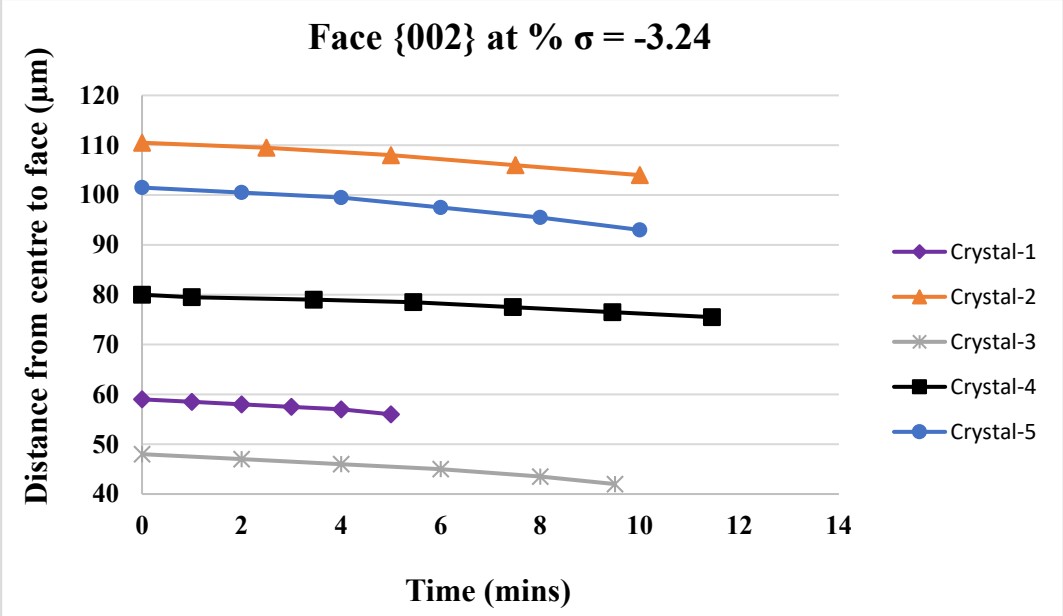


Figure S8: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -3.24%

Table S3: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -3.24%

Crystal	Face {011}		Face {002}	
	Equation	R^2 Value	Equation	R^2 Value
Crystal-1	y = -1.1143x + 284.45	0.9729	y = -0.5714x + 59.095	0.9796
Crystal-2	y = -x + 243.9	0.9889	y = -0.66x + 110.9	0.9829
Crystal-3	y = -1.0939x + 234.71	0.9962	y = -0.6115x + 48.257	0.9802
Crystal-4	y = -1.1166x + 251.53	0.9633	y = -0.3797x + 80.146	0.9738
Crystal-5	y = -1.1357x + 245.26	0.9739	y = -0.85x + 102.17	0.9687

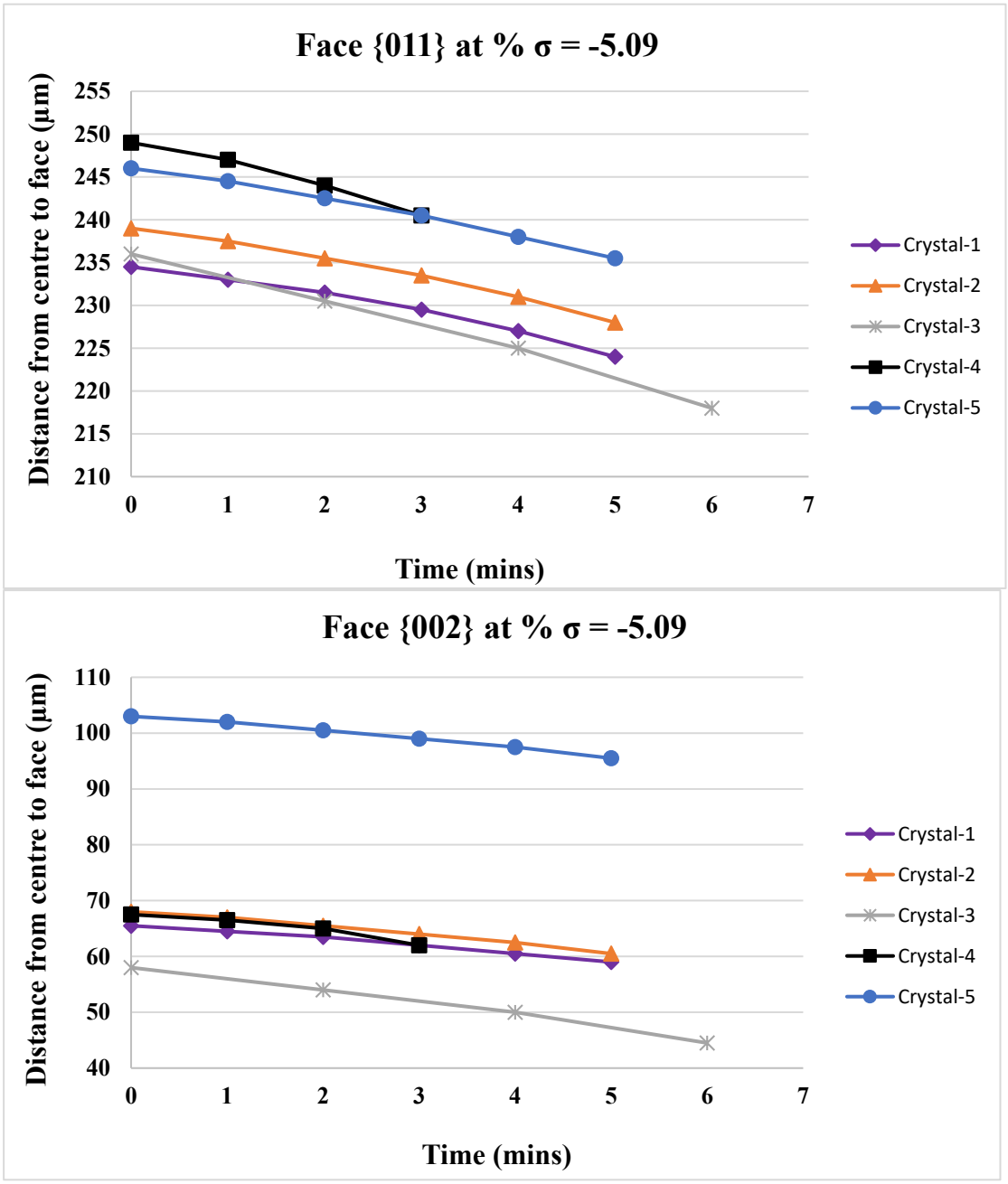


Figure S9: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -5.09%

Table S4: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -5.09%

Crystal	Face {011}		Face {002}	
	Equation	R^2 Value	Equation	R^2 Value
Crystal-1	y = -2.0714x + 235.1	0.9789	y = -1.3143x + 65.786	0.9911
Crystal-2	y = -2.1857x + 239.55	0.987	y = -1.5x + 68.333	0.9916
Crystal-3	y = -2.975x + 236.3	0.9962	y = -2.225x + 58.3	0.9932
Crystal-4	y = -2.85x + 249.4	0.986	y = -1.8x + 67.95	0.9391
Crystal-5	y = -2.1143x + 246.45	0.9923	y = -1.5x + 103.33	0.9916

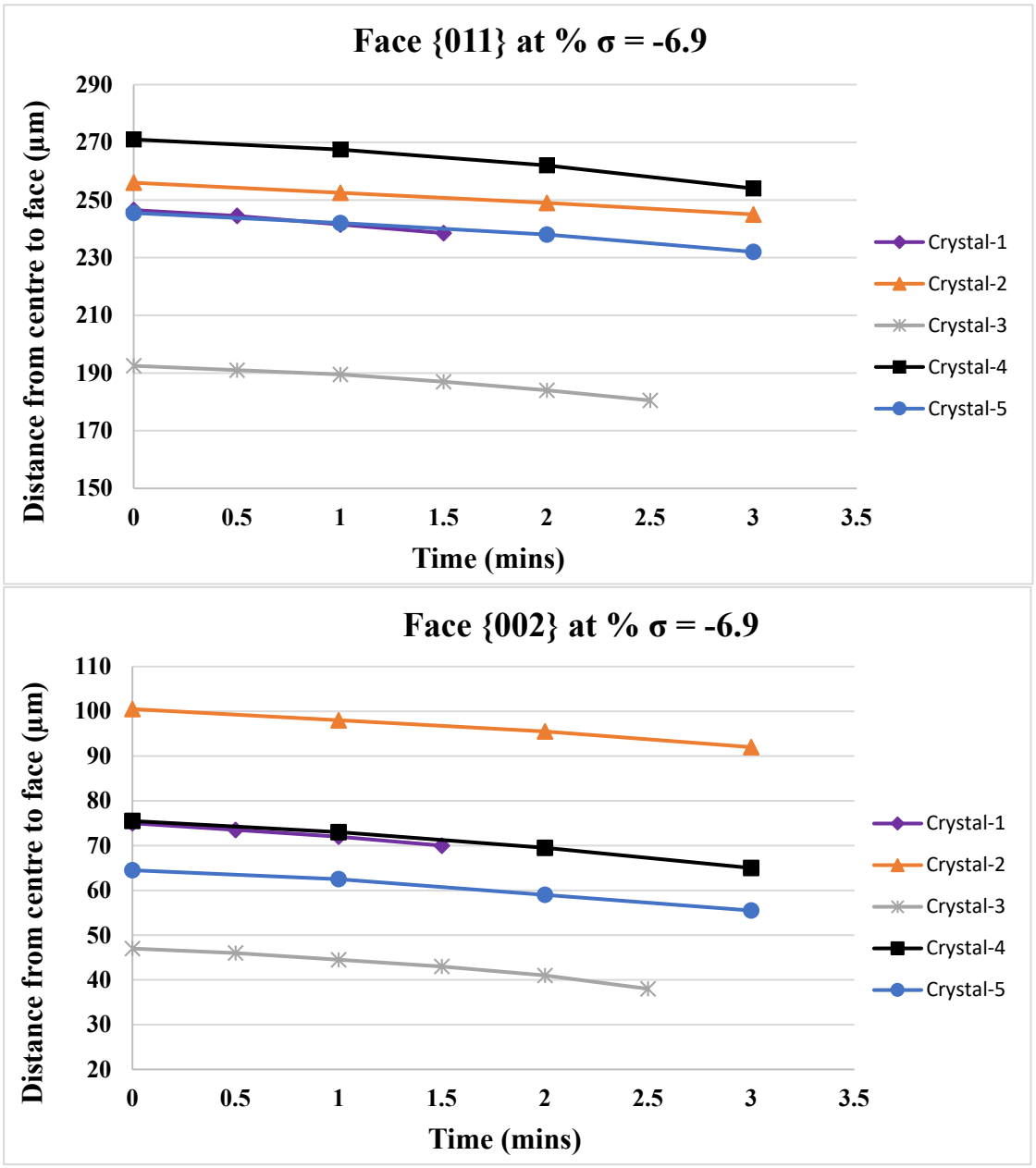
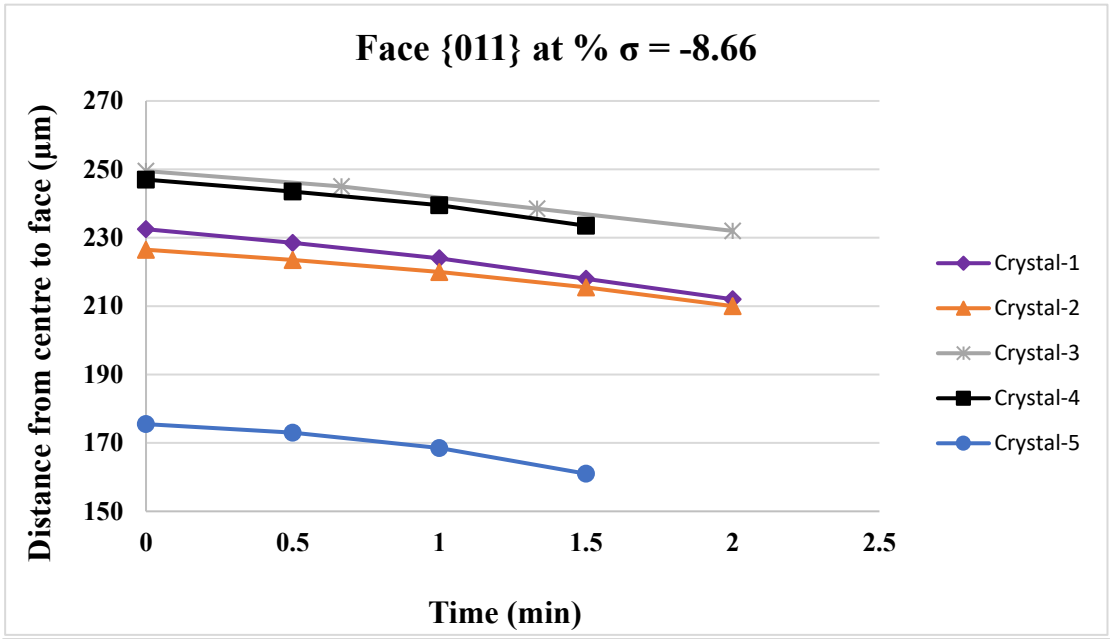


Figure S10: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -6.9%

Table S5: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -6.9%

Crystal	Face {011}		Face {002}	
	Equation	R^2 Value	Equation	R^2 Value
Crystal-1	y = -5.4x + 246.8	0.9918	y = -3.3x + 75.1	0.9945
Crystal-2	y = -3.65x + 256.1	0.9989	y = -2.8x + 100.7	0.9924
Crystal-3	y = -4.7714x + 193.38	0.9698	y = -3.5143x + 47.643	0.967
Crystal-4	y = -5.65x + 272.1	0.9692	y = -3.5x + 76	0.9839
Crystal-5	y = -4.45x + 246.05	0.9834	y = -3.05x + 64.95	0.9857



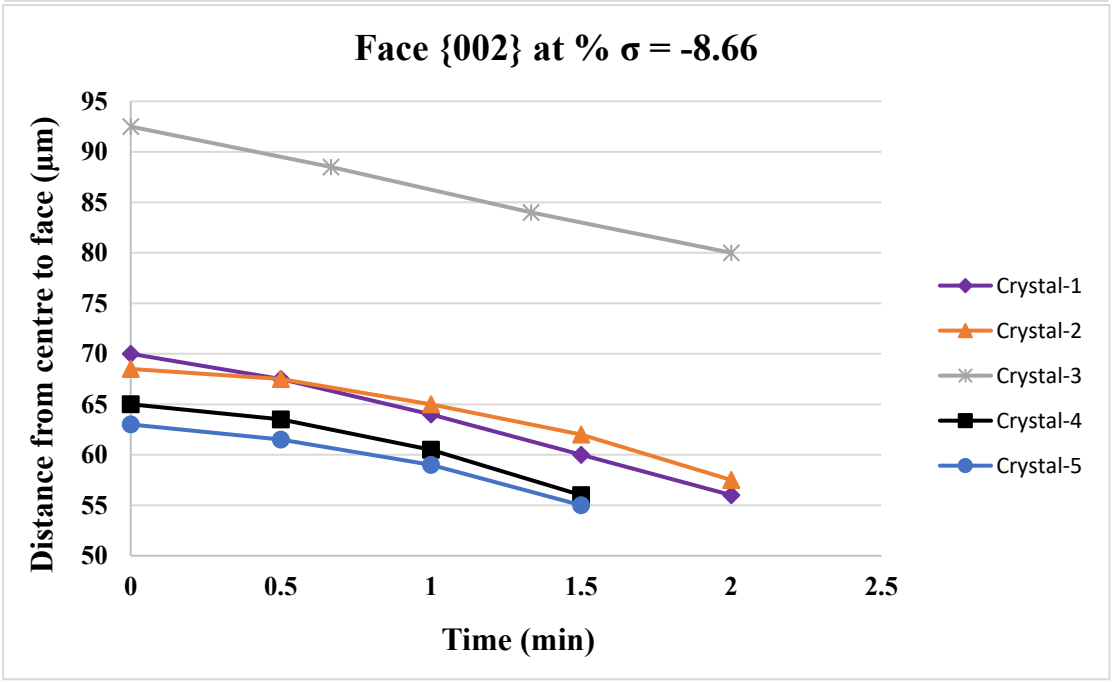


Figure S11: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -8.66%

Table S6: Data from Ibuprofen dissolution in 95% v/v Ethanol: Water solution σ = -8.66%

Crystal	Face {011}		Face {002}	
	Equation	R^2 Value	Equation	R^2 Value
Crystal-1	y = -10.3x + 233.3	0.9915	y = -7.1x + 70.6	0.9923
Crystal-2	y = -8.2x + 227.3	0.9848	y = -5.5x + 69.6	0.9489
Crystal-3	y = -8.85x + 250.1	0.9932	y = -6.3x + 92.55	0.9994
Crystal-4	y = -8.9x + 247.55	0.9834	y = -6x + 65.75	0.9524
Crystal-5	y = -9.6x + 176.7	0.9481	y = -5.3x + 63.6	0.9571

Table S7: Dissolution fluxes from faces (011) and (002) of ibuprofen crystals in 95% ethanol as a function of % undersaturation.

% Undersaturation	Face (011)		Face (002)	
	Average ($\mu mol/s.m^2$)	Std. Dev ($\mu mol/s.m^2$)	Average ($\mu mol/s.m^2$)	Std. Dev ($\mu mol/s.m^2$)
1.36	45.51	4.18	21.40	2.51
3.24	91.20	4.18	58.31	6.68
5.09	203.88	20.05	140.08	20.05
6.89	407.76	41.76	274.61	13.36
8.67	764.40	10.86	499.37	21.72