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Supporting information for article:

Hydrogen-bonded structures and interaction energies in two forms of the SGLT-2 inhibitor sotagliflozin

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supporting information

Hydrogen-bonded structures and interaction energies in two forms of the SGLT-2-inhibitor sotagliflozin

Thomas Gelbrich,* Verena Adamer, Marijan Stefinovic, Andrea Thaler and Ulrich J. Griesser

Powder X-ray diffraction

X-ray powder diffraction patterns were obtained with a PANalytical X'Pert PRO diffractometer equipped with a theta/theta coupled goniometer in transmission geometry, Cu-K$\alpha_{1,2}$ radiation (λ = 1.5419 Å) with a focusing mirror and a solid state PIXcel detector. The patterns were recorded at a tube voltage of 45 kV and a tube current of 40 mA, applying a stepsize of 2θ = 0.013° with 40 s per step (255 channels) in the angular range of 2° ≤ 2θ ≤ 40° at ambient conditions.

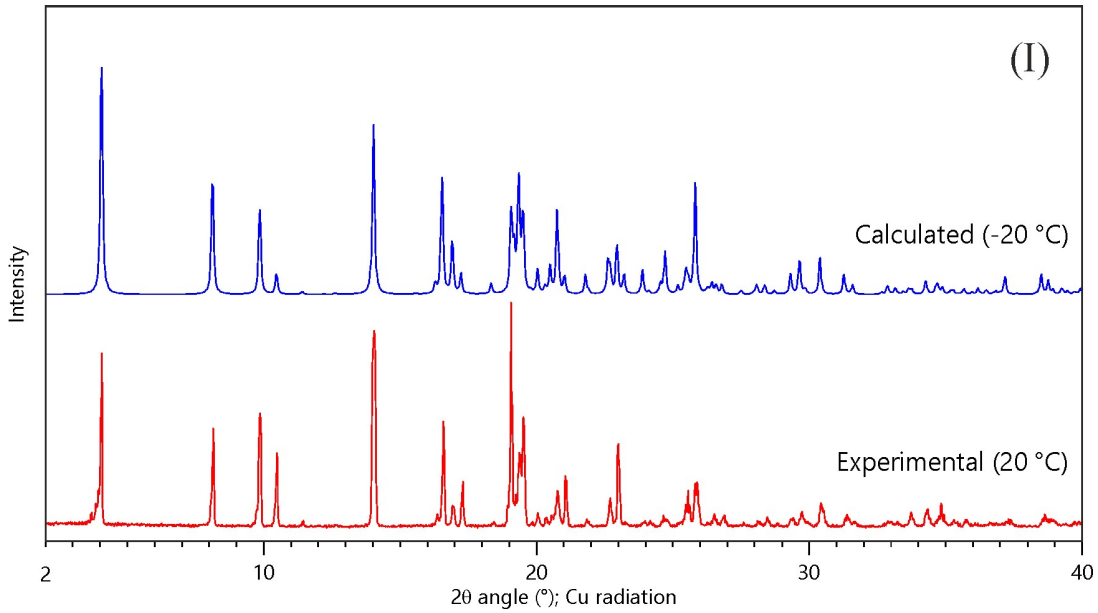

Figure S1. Comparison of experimental and calculated PXRD patterns for (I).

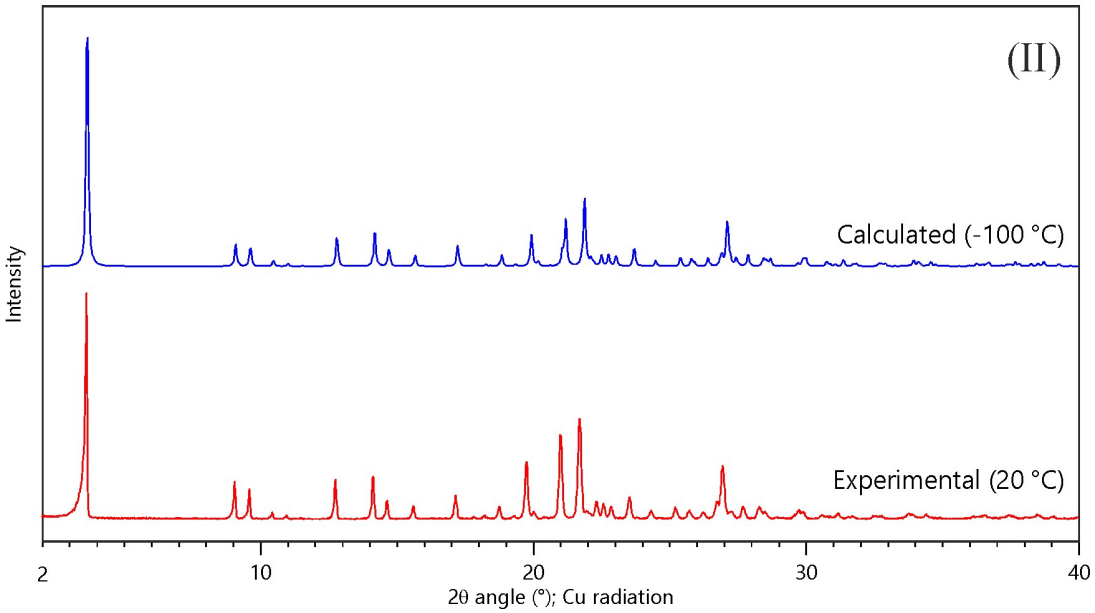

Figure S2. Comparison of experimental and calculated PXRD patterns for (II).

PIXEL calculations

Table S1. Total Pixel energies (E_T) for pairwise interactions (kJ mol^{-1}) in (I), separated into contributions from coloumbic (E_C), polarization (E_P), dispersion (E_D) and repulsion (E_R) terms. The total Pixel energy of the crystal is -236.5 kJ mol^{-1}.

Symmetry operation	E_C	E_P	E_D	E_R	E_T	Hydrogen bond(s)
x-1, y, z	-26.4	-9.6	-62.0	33.8	-64.2	-
-x+2, y+0.5, -z+1.5	-83.5	-34.0	-25.9	90.6	-52.5	O9—H9···O10^{i}, O10—H10···O11^{i}
-x+1, y-0.5, -z+1.5	-44.0	-19.9	-30.1	59.2	-34.8	O11—H11···O9^{ii}
x-0.5, -y+0.5, -z+1	-5.2	-3.5	-31.5	16.6	-23.6	-
x-0.5, -y+1.5, -z+1	-5.0	-2.3	-28.7	12.4	-23.6	-
x, y-1, z	-14.8	-5.2	-23.8	21.2	-22.5	-

Table S2. Total Pixel energies (E_T) for pairwise interactions (kJ mol^{-1}) in (II), separated into contributions from Coloumb (E_C), polarization (E_P), dispersion (E_D) and repulsion (E_R) terms. The total Pixel energy of the crystal is -150.9 kJ mol^{-1}.

Symmetry operation	E_C	E_P	E_D	E_R	E_T	Hydrogen bond
Interactions sotagliflozin - sotagliflozin						
x-1, y, z	-28.4	-14.8	-104.9	65.6	-82.5	-
-x+1, y-0.5, -z+0.5	-35.3	-17.3	-22.8	48.0	-27.4	O9—H9···O10^{i}
-x, y+0.5, -z+0.5	-29.2	-9.1	-12.7	25.4	-25.5	O11—H11···O9^{ii}
x, y-1, z	-6.2	-3.7	-23.9	15.3	-18.4	-
x-0.5, -y+0.5, -z+1	-6.2	-2.6	-18.4	11.5	-15.6	-
Interaction sotagliflozin – water [a]						
x, y, z	-76.7	-35.7	-12.1	95.0	-29.5	O10—H10···O1*W*
Interactions water – sotagliflozin [b]						
-x, y+0.5, -z+0.5	-28.6	-27.6	-14.1	48.9	-21.4	O1*W*—H1*W*···S7^{ii}
-x, y-0.5, -z+0.5	-48.4	-21.2	-13.2	62.2	-20.6	O1*W*—H2*W*···O11^{iii}

[a] "Symmetry operation" generates the water molecule for this interaction. [b] "Symmetry operation" generates the sotagliflozin molecule for this interaction.