Electronic Supporting Information (ESI)

Solvatomorphism of Moxidectin

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1. Table of Contents

2. Additional Information on X-Ray Diffraction

Variable-temperature X-ray powder diffraction (VT-XRPD) of amorphous moxidectin

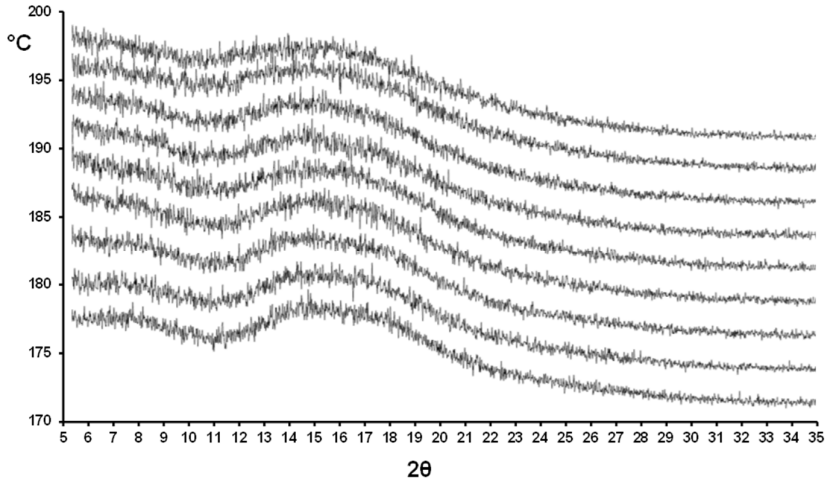

Figure S1. Variable-temperature X-ray powder diffraction (VT-XRPD) of amorphous moxidectin. Collection of diffractograms for of the amorphous form heated from 170 °C to 200 °C over the course of 5 hrs. This experiment demonstrates that no conversion of the amorphous to the crystalline form ("Form I", Table 1) is taking place[1].

Details on hydrogen bonding in known moxidectin form

Table S1. Distances [Å] and type for strong and weak hydrogen bonds observed in form I and in the solvatomorphs discussed in this work.

Solvatomorph	N°	Interaction type O–H···O	O(–H)···O Distance	Type	N°	Interaction type C–H···O	C(–H)···O Distance
Form I*	1	O4–H**···O1	2.74(1)	*Intra*mol. HB	1	C20–H18···O3	3.55(2)
					2	C36–H47···O5	3.46(2)
Moxi·2EtOH	1	O4–H53···O2'	2.760(2)	*Inter*mol. HB	1	C13–H10···O1	3.377(3)
	2	O2–H52···O10	2.700(3)	*Inter*mol. HB			
	3	O10–H65···O9	2.719(5)	*Inter*mol. HB			
	4	O9–H59···O4	2.782(4)	*Inter*mol. HB			
Moxi·2*i*PrOH	1	O4–H53···O2'	2.704(2)	*Inter*mol. HB	1	C13–H10···O1	3.429(3)
	2	O2–H52···O10	2.748(8)	*Inter*mol. HB			
	3	O10–H65···O9	2.784(8)	*Inter*mol. HB			
	4	O9–H59···O4	2.853(4)	*Inter*mol. HB			
Moxi·1.5MeNO$_2$	1	O4–H53···O1	2.763(5)	*Intra*mol. HB	1	C3–H2···O9	3.404(5)
	2	O2–H52···O3'	2.869(4)	*Inter*mol. HB	2	C20–H18···O9	3.495(5)
		O2'–H52'···O3	2.869(4)	*Inter*mol. HB	3	C20–H19···O10	3.254(6)
					4	C22–H21···O13	3.58(1)
					5	C29–H28···O14	3.54(2)
					6	C35–H44···O1	3.408(6)

***Moxidectin form I**, CSD reference code GETBOW[2]. **Sites for OH Hydrogen atoms were not assigned in the published structure[2].

3. Additional Information on Quantum Chemical Calculations

Structural parameters of the calculated solvatomorph of *n*-butanol (Moxi·2*n*BuOH)

The following lines contain the file content (text format) of the calculated structures in the *.cif format. The file can also be also found as supplementary material of this article.

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#END

4. Literature

[1] US2013143956-A1, WO2013082373-A1, **2013**.

[2] N. E. Beddall, P. D. Howes, M. V.J. Ramsay, S. M. Roberts, A. M.Z. Slawin, D. R. Sutherland, E. P. Tiley, D. J. Williams, *Tetrahedron Lett.* **1988**, *29*, 2595.