Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Insights into the opening of DNA-like double-stranded helices in lamivudine duplex IV and the first polymorph of the drug

*Cameron Capeletti da Silva and Felipe Terra Martins**

Instituto de Química, Universidade Federal de Goiás, Campus Samambaia, CP 131, 74001-970, Goiânia, GO, Brazil
***E-mail**: felipe@ufg.br

Content:

Table S1. Crystal data and refinement parameters of the lamivudine crystal structures reported in this work

solid phases		duplex IV	lamivudine hydrogen L-tartrate monohydrate	lamivudine form IV
structural formula		$2(C_8H_{12}N_3O_3S)$, $2(C_8H_{11}N_3O_3S)$, $(C_4H_4O_6)$, (CH_4O), (H_2O)[a]	$(C_8H_{12}N_3O_3S)$, $(C_4H_4O_6)$, (H_2O)	$(C_8H_{11}N_3O_3S)$
formula weight (g / mol)		1115.16	397.36	229.26
crystal system		hexagonal	monoclinic	triclinic
space group		$P6_122$	$P2_1$	$P1$
unit cell dimensions	*a* (Å)	14.486(7)	5.136(8)	6.944(3)
	b (Å)	14.486(7)	21.574(4)	7.313(4)
	c (Å)	40.741(2)	7.672(13)	10.575(5)
	α (deg)	90	90	95.32(2)
	β (deg)	90	98.937(5)	102.21(2)
	γ (deg)	120	90	106.87(2)
V (Å^3)		7404.3(9)	839.8(2)	495.4(4)
Z		6	2	2
d (g.cm^{-3})		1.501	1.571	1.537
absorption coeff. (mm^{-1})		0.281	0.254	0.318
absortpion correc.		multi-scan	multi-scan	multi-scan
		T_{min}/T_{max} 0.769	T_{min}/T_{max} = 0.819	T_{min}/T_{max} = 0.920
θ-range for data collection (deg.)		1.62-25.74	2.69-25.35	2.00-25.39
index ranges		-12 to 17	-6 to 5	-8 to 8
		-17 to 7	-25 to 25	-7 to 8
		-49 to 48	-9 to 8	-12 to 12
data collected		32524	4688	4870
unique reflections		4718	2959	2922
symmetry factor (R_{int})		0.0466	0.0454	0.0219
completeness to θ_{max} (%)		99.7	98.3	99.4

F(000)		3504	416	240
parameters refined		388	236	272
GOF on F^2		1.044	0.986	1.043
R_1 (all)		0.040 (0.0467)	0.0628 (0.1107)	0.0304 (0.0313)
wR_2 (all)		0.0998 (0.1046)	0.1643 (0.2282)	0.0842 (0.0850)
largest diff. peak/ hole ($e/Å^3$)		0.304/ -0.288	0.521/ -0537	0.334/ -0.185
Absolute structure	Flack parameter	0.02(9)	0.2(2)	-0.02(7)
	Friedel pairs	1876	1404	1112
CCDC deposit no.		1483546	1483547	1483545

[a] Water hydrogens of lamivudine duplex IV were not located in the refinement because a symmetry imposition has forced the water oxygen to lie on a special position of constrained 50% occupancy near to the lamivudine hydroxymethylene branch in the minor 30% occupancy sites.

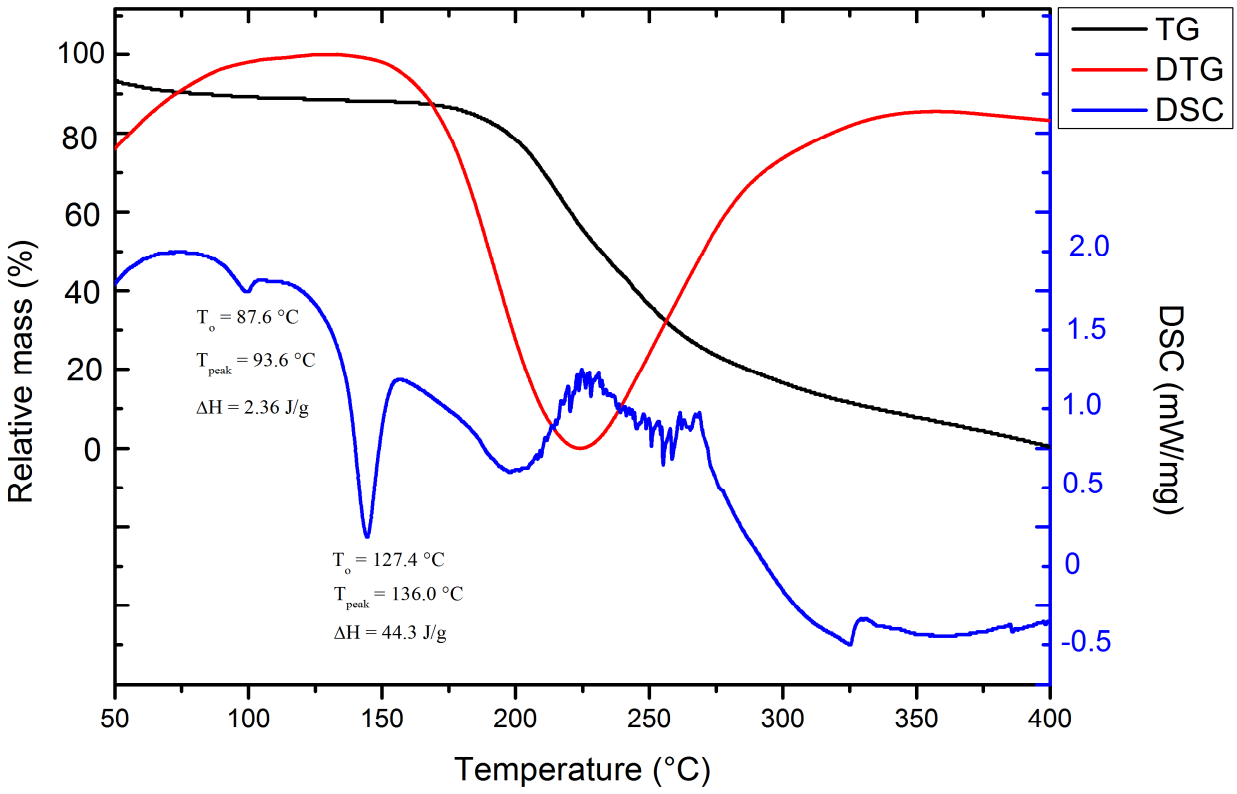

Figure S1. TG curve (black line), its derivative (red line) and DSC curve (blue line) of lamivudine duplex IV.