Synthon transferability probed with IR spectroscopy: cytosine salts as models for salts of lamivudine

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Table S1: Hydrogen bond metrics for the co-crystal and the salts

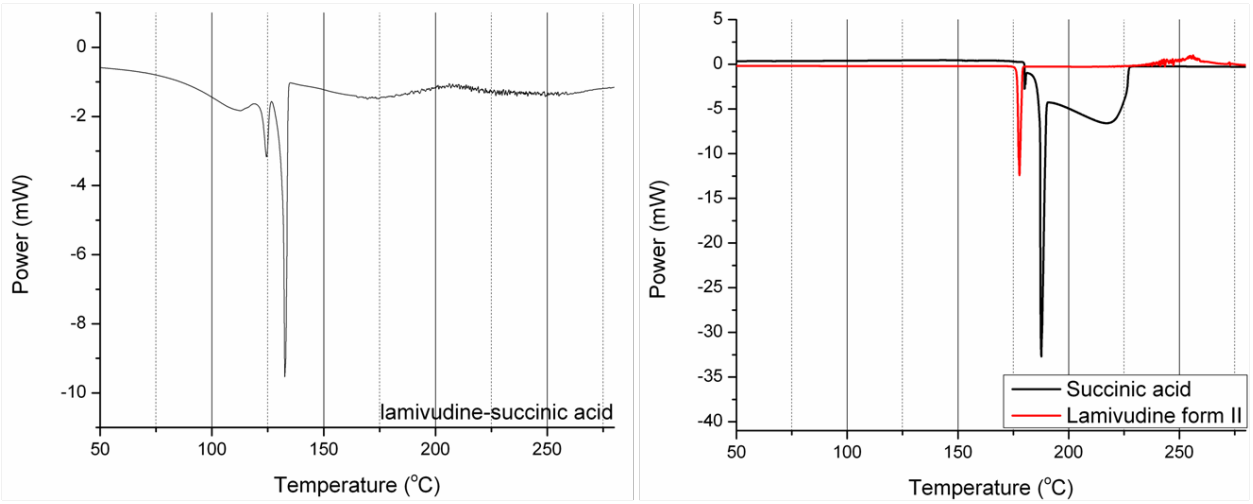
Salt/co-crystal	D-H···A	Symmetry code	D-H	H···A	D-H···A
Lamivudine-oxalate	O_{34}-H_{34}···O_4	-x+1, y-1/2, -z+1/2	0.820	2.025	2.772
	N_7-H_3···O_2	x, y-1, z	0.748	2.364	2.814
	N_7-H_3···O_4	x, y-1, z	0.748	2.536	3.268
	N_{11}-H_2···O_1	x-1/2, -y+1/2, -z	0.851	2.008	2.852
	N_8-H_{14}···O_4	x+1, y-1, z	0.785	2.117	2.867
	O_{100}-H_{23}···O_2		0.616	2.231	2.846
	N_{10}-H_{75}···O_1	x+1/2, -y+1/2, -z	0.894	2.222	3.070
	N_{10}-H_{75}···O_3	x+1/2, -y+1/2, -z	0.894	2.250	2.774
	N_{10}-H_{45}···O_2	x-1/2,-y+1/2, -z	0.905	1.951	2.831
Lamivudine- pimelic acid	N_4-H_2···O_7	-x-1, y-1/2, -z+1	0.936	2.082	3.001
	N_4-H_1···O_1	x, y, z+1	0.946	2.044	2.928
	O_9-H_{12}···O_7	-x,y-1/2,-z	0.785	2.079	2.836
	O_{10}-H_{11}···O_6	x-1, y, z+1	0.875	1.930	2.762
	N_3-H_9···O_2	x, y, z-1	0.863	2.154	2.968
	N_3-H_8···O_6		0.878	2.058	2.918
	O_8-H_{8A}···N_5	-x-1, y+1/2, -z+1	0.840	1.789	2.624

Note: The hydrogen bond metrics for lamivudine oxalate monohydrate and cytosine tribromoacetate have not been given here because the hydrogen atoms could not be located from the difference Fourier map.

Table S2. First pK_a values of the dicarboxylic acids

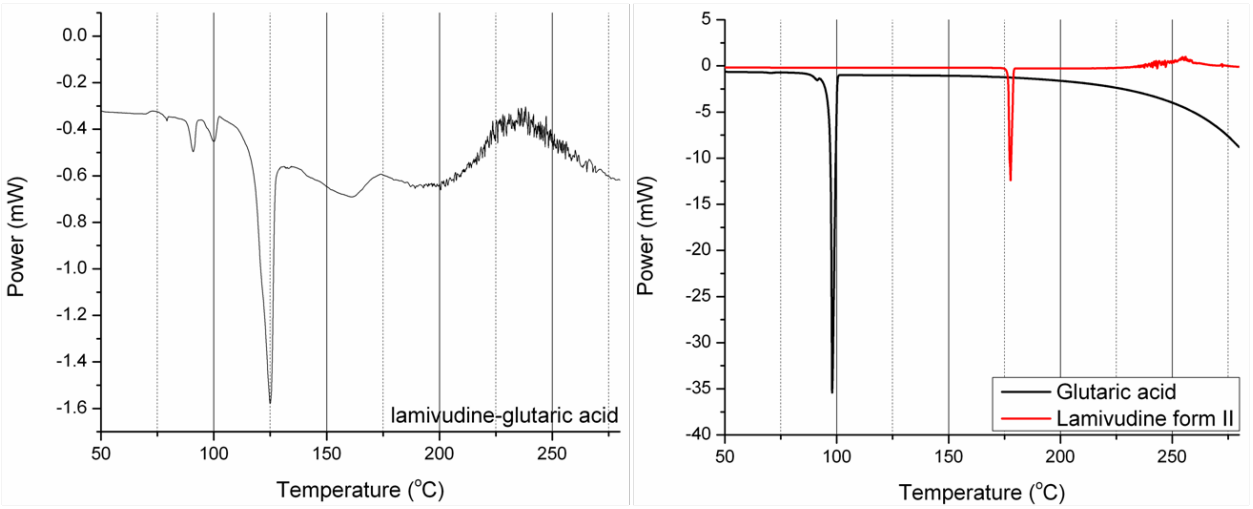
Dicarboxylic acid	**pK_{a1}**
Oxalic	1.25
Malonic	2.83
Succinic	4.20
Glutaric	4.31
Adipic	4.43
Pimelic	4.48

DSC curves



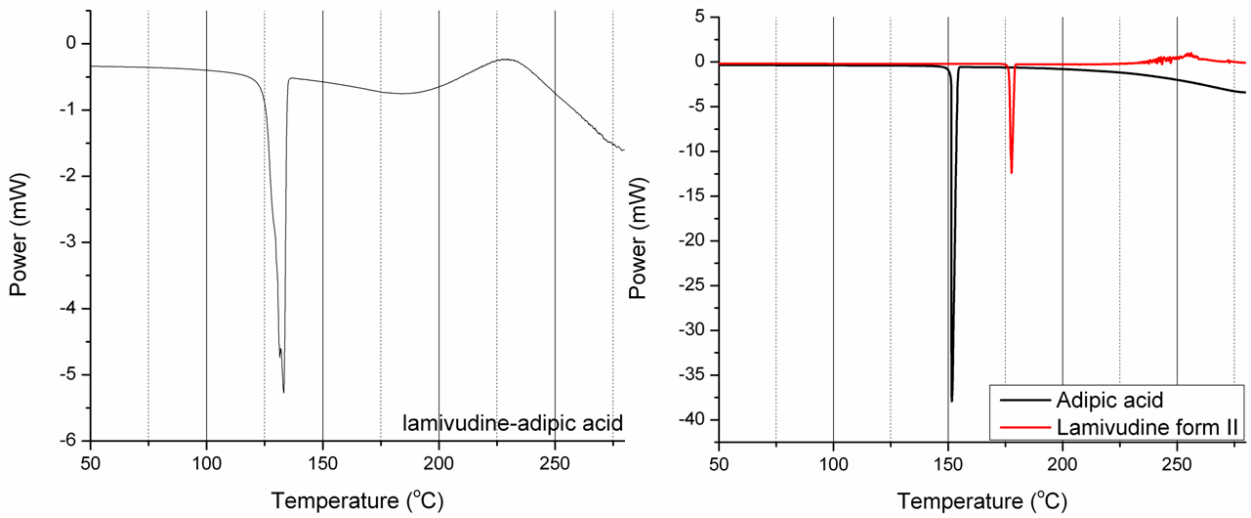
(a) **(b)**

Figure S1. (a) DSC curve of lamivudine-succinic acid and (b) superposed DSC curves of lamivudine form 2 and succinic acid. The three curves have not been superposed because of the difference in the Y scale.



(a) **(b)**

Figure S2. (a) DSC curve of lamivudine-glutaric acid and (b) superposed DSC curves of lamivudine form 2 and glutaric acid. The three curves have not been superposed because of the difference in the Y scale.



(a) **(b)**

Figure S3. (a) DSC curve of lamivudine-adipic acid and (b) superposed DSC curves of lamivudine form 2 and adipic acid. The three curves have not been superposed because of the difference in the Y scale.

PXRD patterns

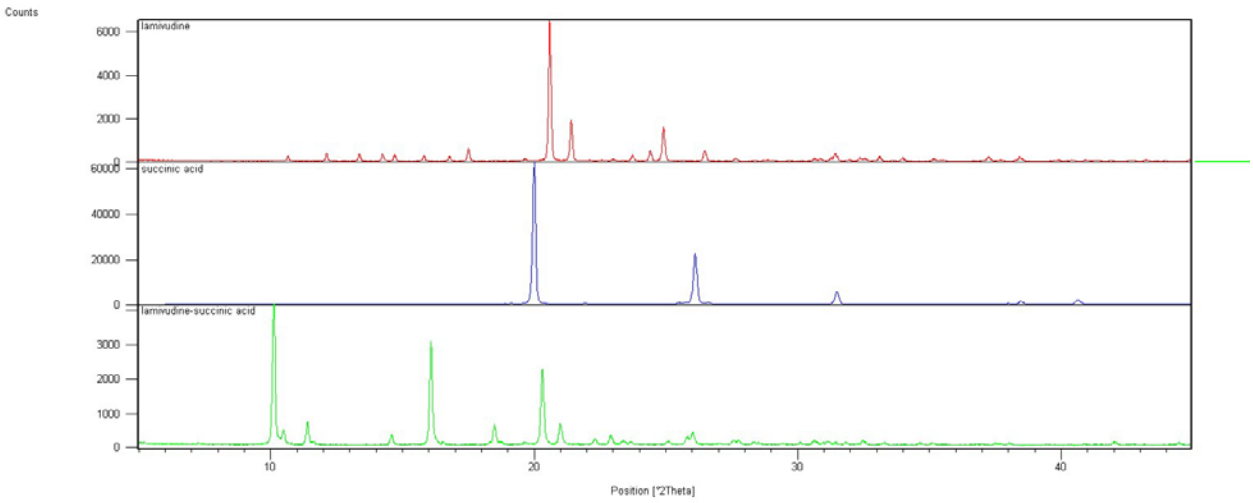


Figure S4. Comparison of the PXRD patterns of pure lamivudine, pure succinic acid and the lamivudine-succinic acid co-crystal.

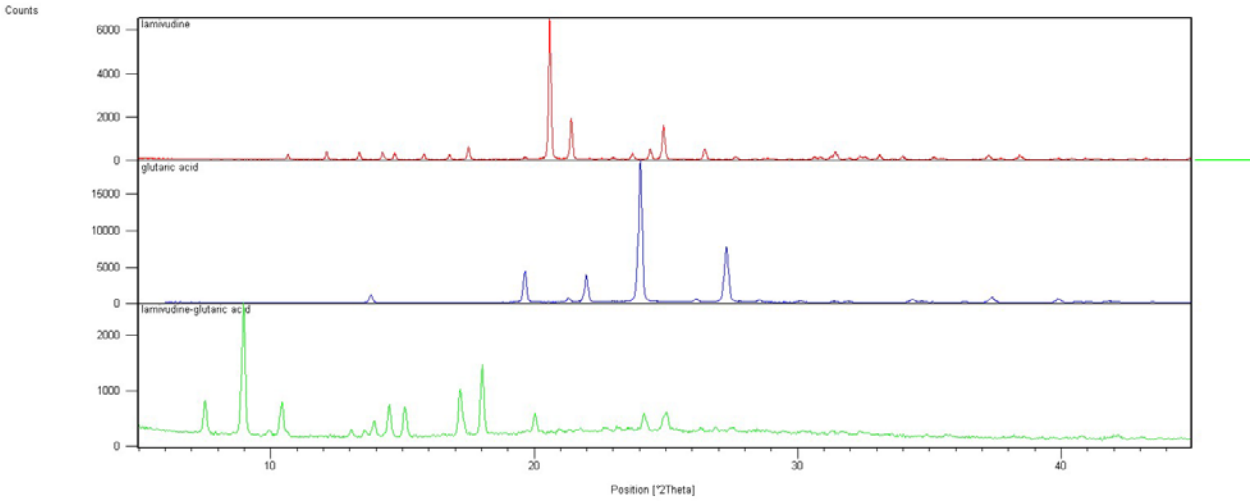


Figure S5. Comparison of the PXRD patterns of pure lamivudine, pure glutaric acid and the lamivudine-glutaric acid co-crystal.

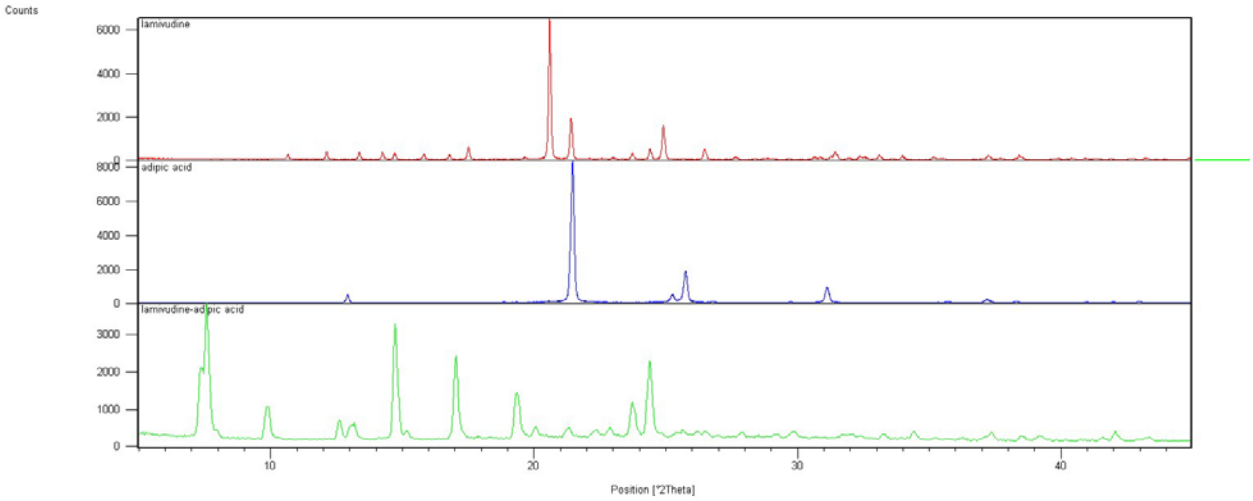


Figure S6. Comparison of the PXRD patterns of pure lamivudine, pure adipic acid and the lamivudine-adipic acid co-crystal

ORTEP diagrams

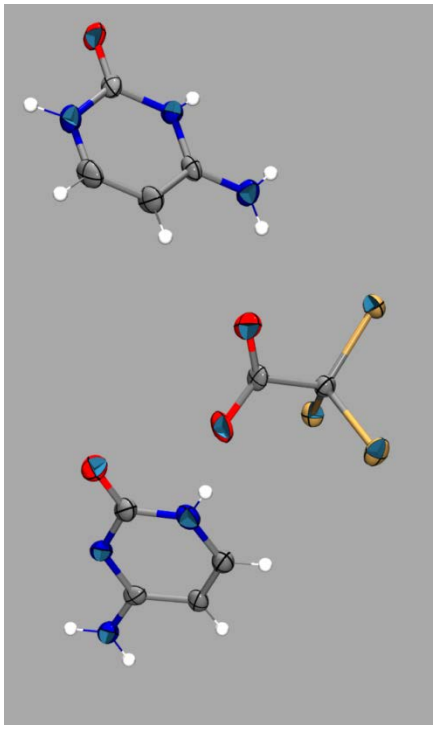


Figure S7. ORTEP diagram of cytosine tribromoacetate

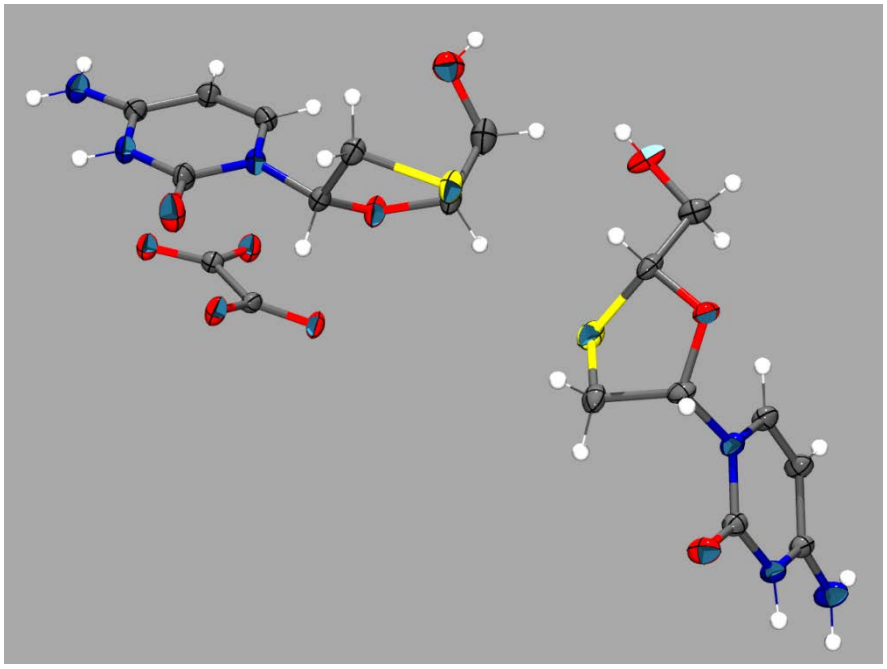


Figure S8. ORTEP diagram of lamivudine oxalate

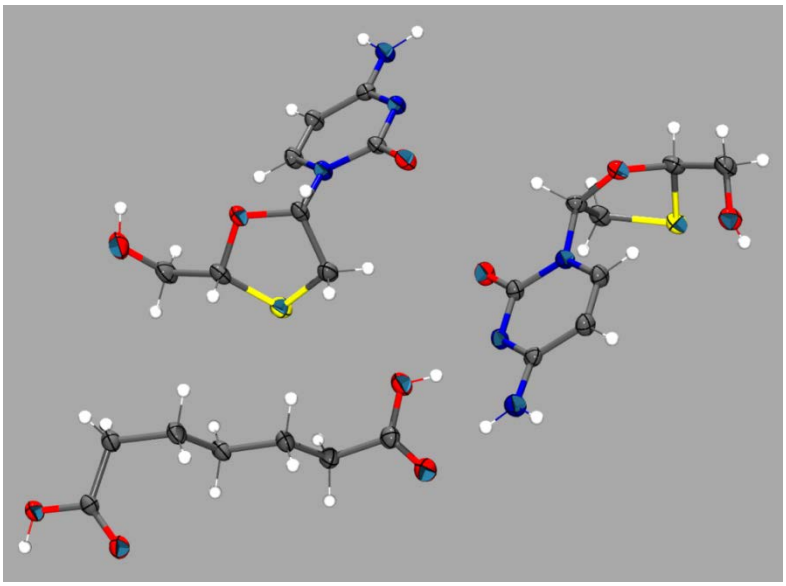


Figure S9. ORTEP diagram of lamivudine-pimelic acid co-crystal

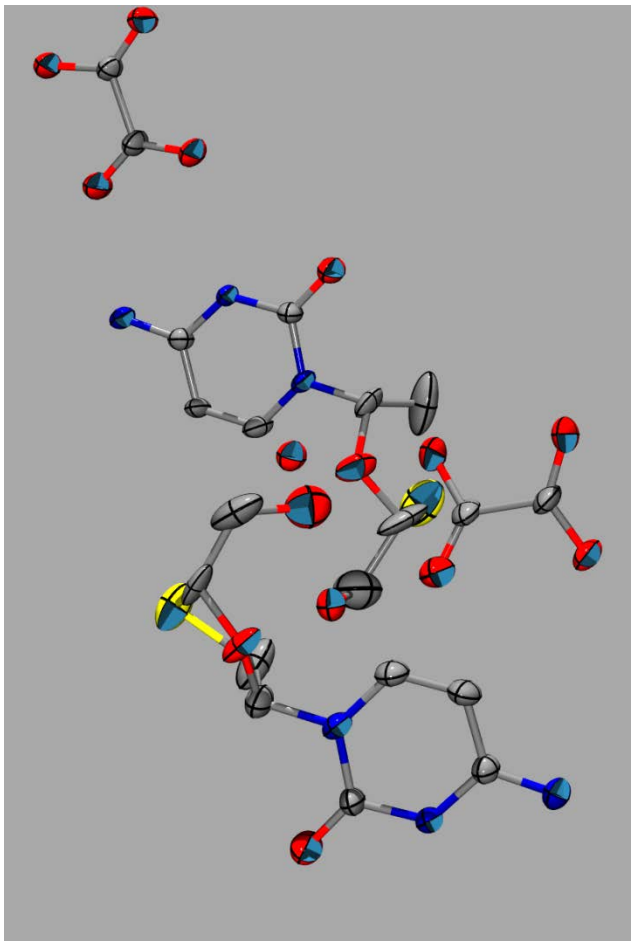


Figure S10. ORTEP diagram of lamivudine oxalate monohydrate