

New Cocrystals of Ezetimibe with L-proline and Imidazole

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Fig. S1 ORTEP of asymmetric unit in the crystal lattice of ezetimibe, EZT

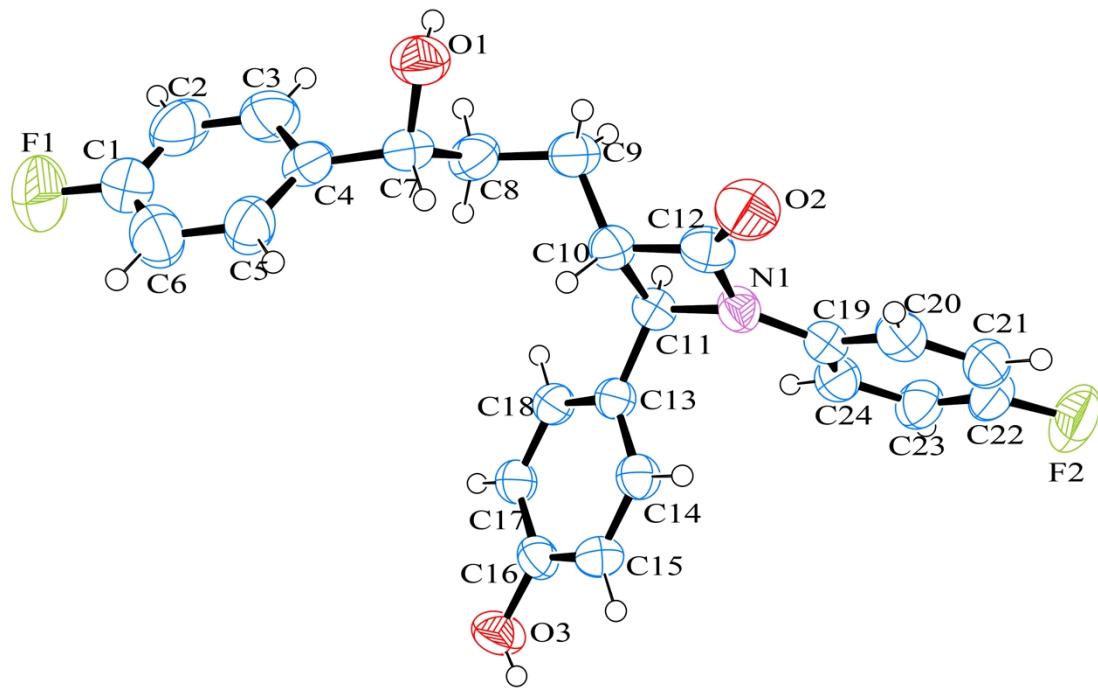


Fig. S2 Asymmetric unit of EZT-IMI cocrystal

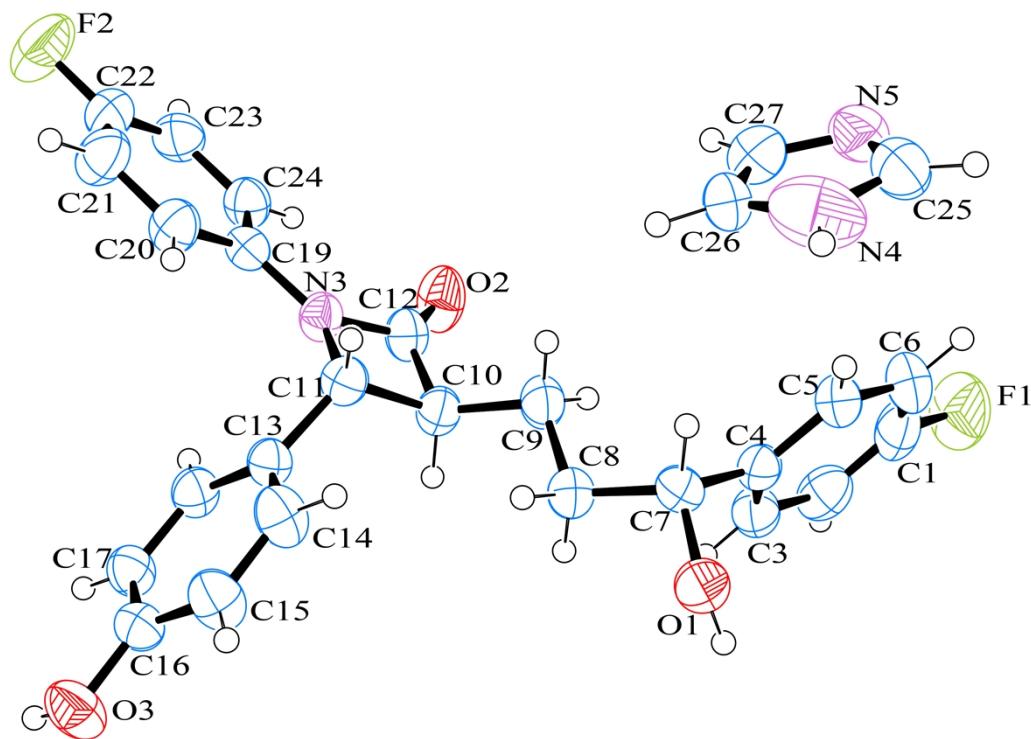


Fig. S3 ORTEP diagram of the EZT-FOR. Thermal ellipsoids are drawn at the 50 % probability level.

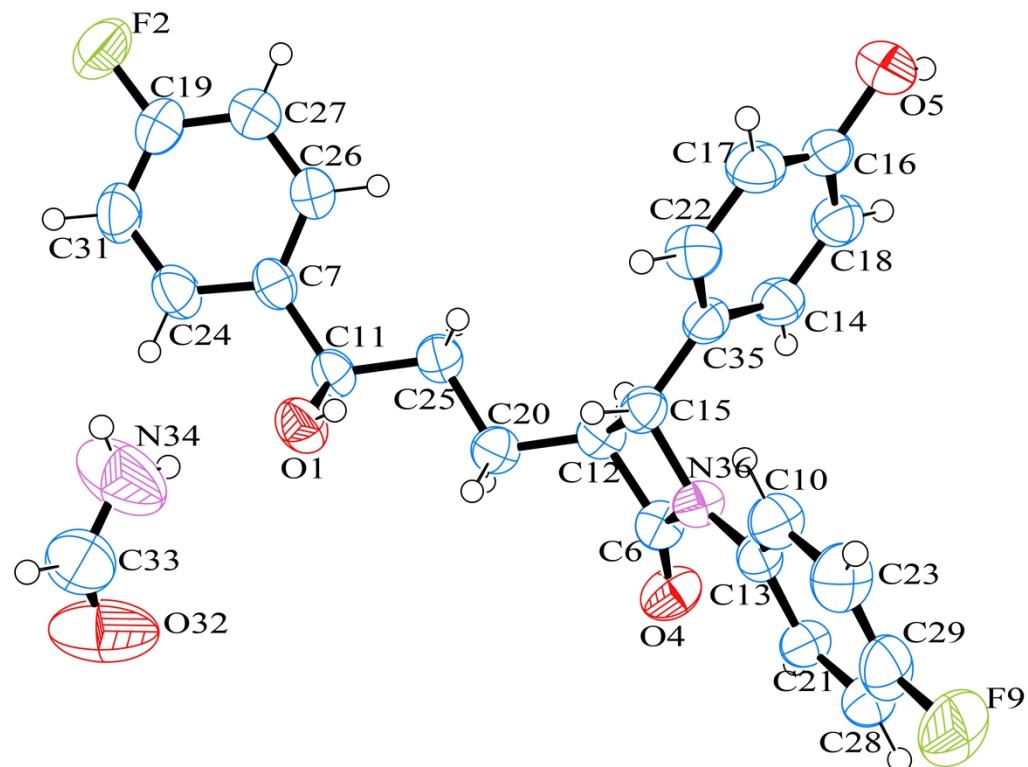


Fig. S4 TGA plot for (a) EZT-PRO and (b) EZT-IMI cocrystals

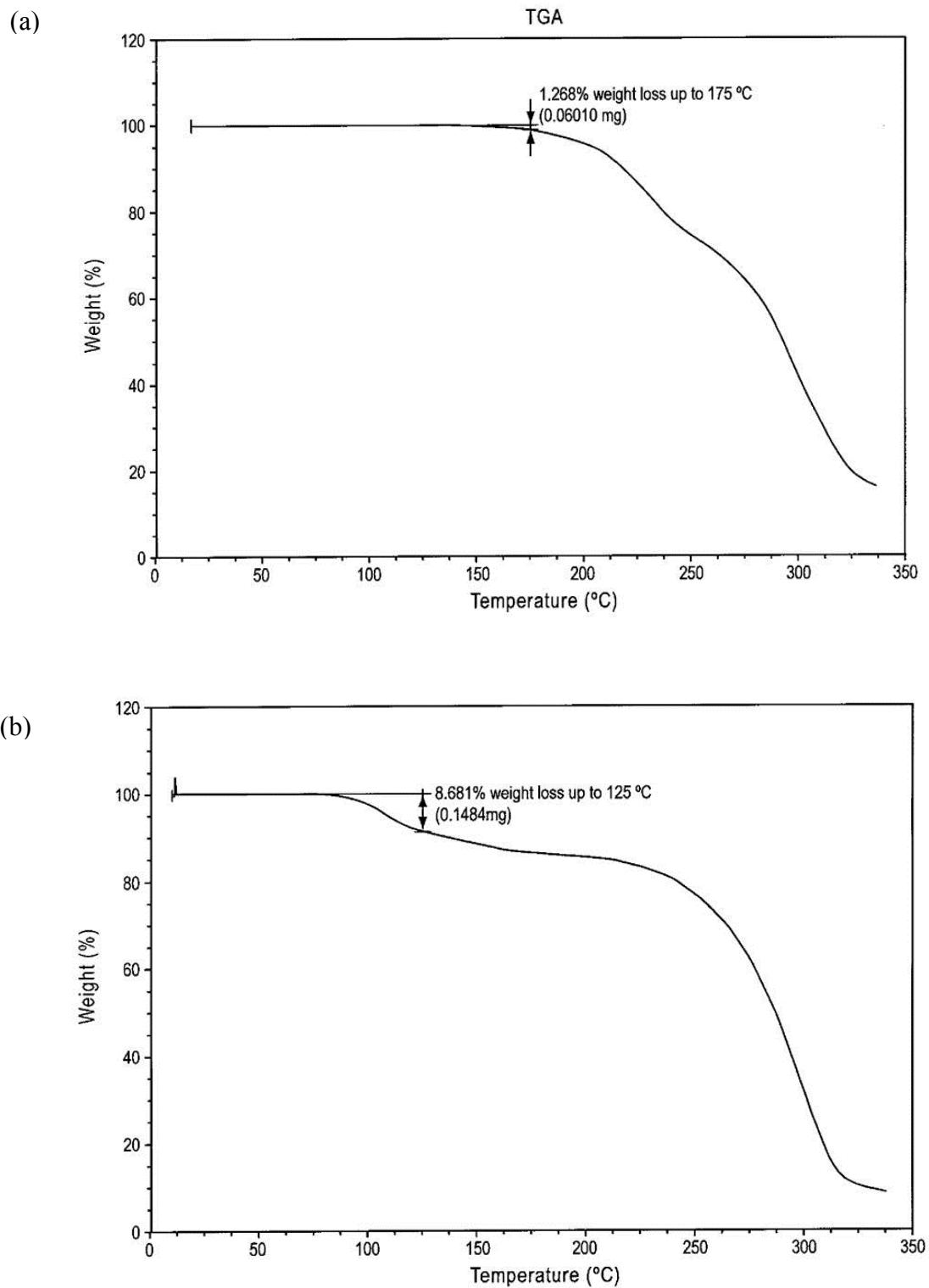
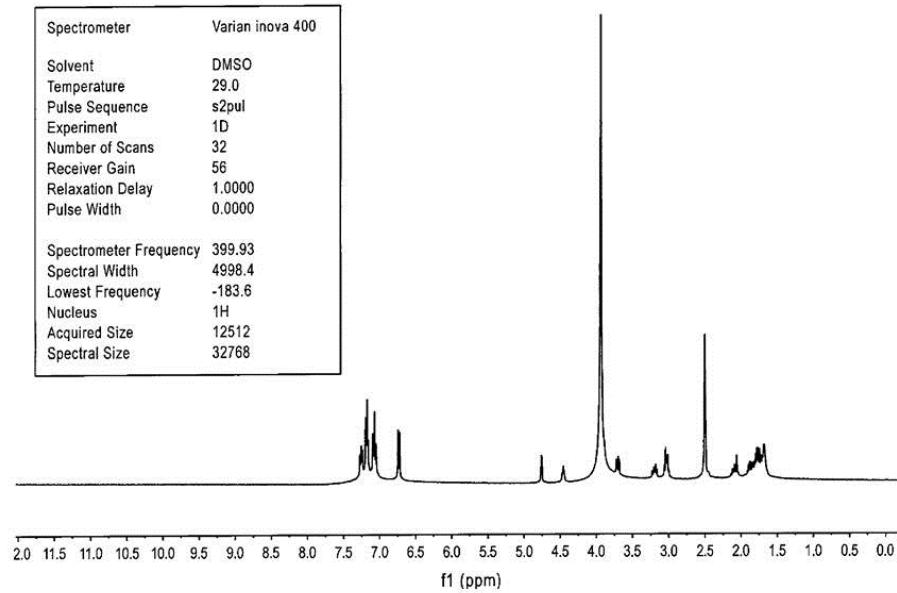


Fig. S5 ^1H -NMR plot for (a) EZT-PRO and (b) EZT-IMI cocrystals

(a)

Spectrometer	Varian inova 400
Solvent	DMSO
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	32
Receiver Gain	56
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	399.93
Spectral Width	4998.4
Lowest Frequency	-183.6
Nucleus	^1H
Acquired Size	12512
Spectral Size	32768



(b)

Spectrometer	Varian inova 400
Solvent	DMSO
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	32
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5032
Spectrometer Frequency	399.93
Spectral Width	4998.4
Lowest Frequency	-184.4
Nucleus	^1H
Acquired Size	12512
Spectral Size	32768

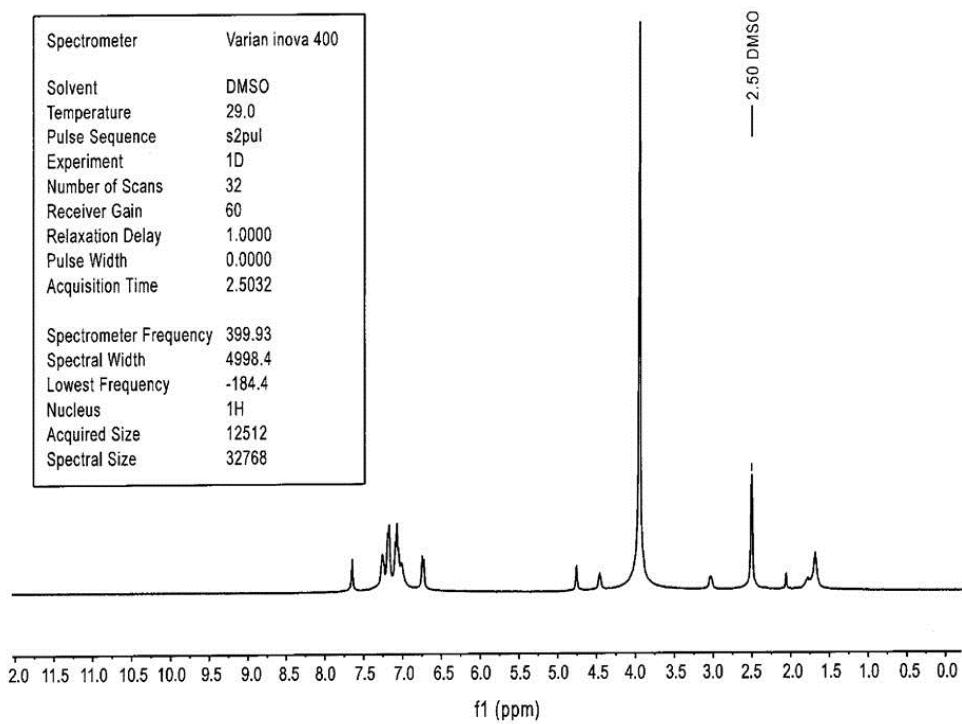


Fig. S6 XRPD of EZT-PRO before RH experiment (bottom) and after 31 days at 40 °C 75%RH (top).

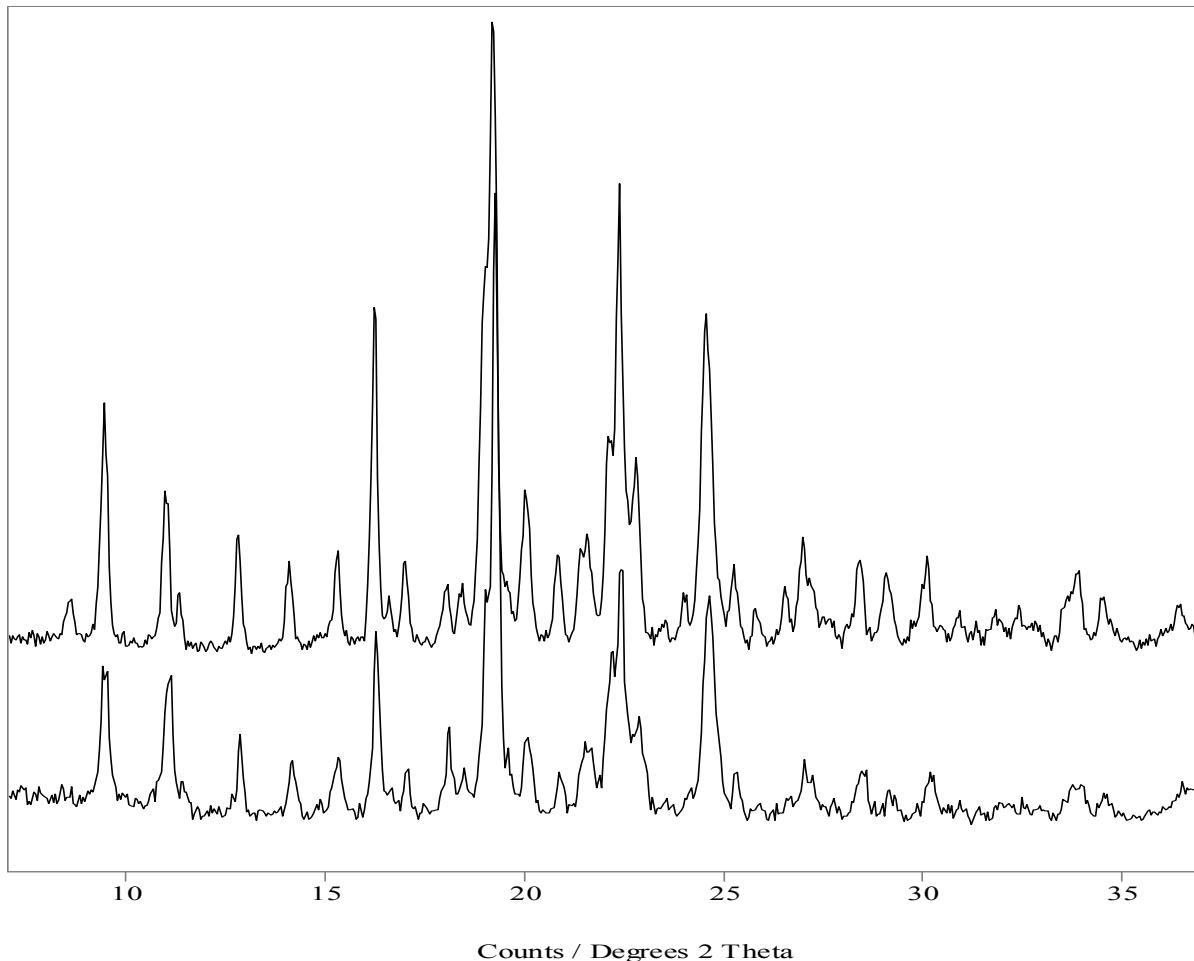


Table S1. Characteristics (distances/ \AA and angles/ $^{\circ}$) of hydrogen bonds in the molecular compounds^{\$}.

EZT			
(D-H$\ddot{\text{A}}$)	(H$\ddot{\text{A}}$)	(D$\ddot{\text{A}}$)	(D-H$\ddot{\text{A}}$)
O(1)–H(1O) $\ddot{\text{O}}$ O(2)	2.04	2.7425	143
O(3)–H(31) $\ddot{\text{O}}$ O(1)	2.01	2.7752	155
C(20)–H(20) $\ddot{\text{O}}$ O(2) (Intra)	2.57	3.1390	120
EZT-IMI			
O(1)–H(5O) $\ddot{\text{O}}$ N(5)	1.81	2.7219	169
O(3)–H(31A) $\ddot{\text{O}}$ O(1)	1.85	2.6383	160
C(8)–H(8B) $\ddot{\text{O}}$ O(3)	2.56	3.4213	150
C(10)–H(10) $\ddot{\text{O}}$ O(3)	2.45	3.3448	155
C(26)–H(26A) $\ddot{\text{O}}$ O(2)	2.03	2.9588	173
C(27)–H(27) $\ddot{\text{O}}$ F(2)	2.37	3.1902	147
C(24)–H(24) $\ddot{\text{O}}$ O(2) (Intra)	2.49	3.0909	122
EZT-FOR			
N(34)–H(34A) $\ddot{\text{O}}$ O(1)	2.11	2.9366	162
O(5)–H(51) $\ddot{\text{O}}$ O(32)	1.88	2.6989	176
O(1)–H(111) $\ddot{\text{O}}$ O(4)	1.94	2.7552	174
C(23)–H(23) $\ddot{\text{O}}$ F(2)	2.54	3.3633	148
C(33)–H(33) $\ddot{\text{O}}$ O(4)	2.59	3.4579	156
C(21)–H(21) $\ddot{\text{O}}$ O(4) (Intra)	2.49	3.0930	123

^{\$}The first column represents the atom label for the hydrogen bonds and the three numbers correspond to the distances of H $\ddot{\text{A}}$, D $\ddot{\text{A}}$ and angle of D–H $\ddot{\text{A}}$ for each interaction.