SUPPORTING INFORMATION:

Molecular interaction transferring among solvent and solute modulates the formation of Linezolid crystals

Table S1 Crystallographic Data of Linezolid Polymorphs[a]

Crystal Data	Form II	Form IV
CCDC no.	648432	648433
Space group	P212121	P1
a/b/c (Å)	6.536/9.949/24.807	6.596/10.989/12.920
α/β/γ (°)	90/90/90	69.32/88.18/74.17
Z	4	2
Volume (Å^3)	1613.116	840.744

[a] Detailed crystallographic information is taken from the Cambridge Crystal Database Center.

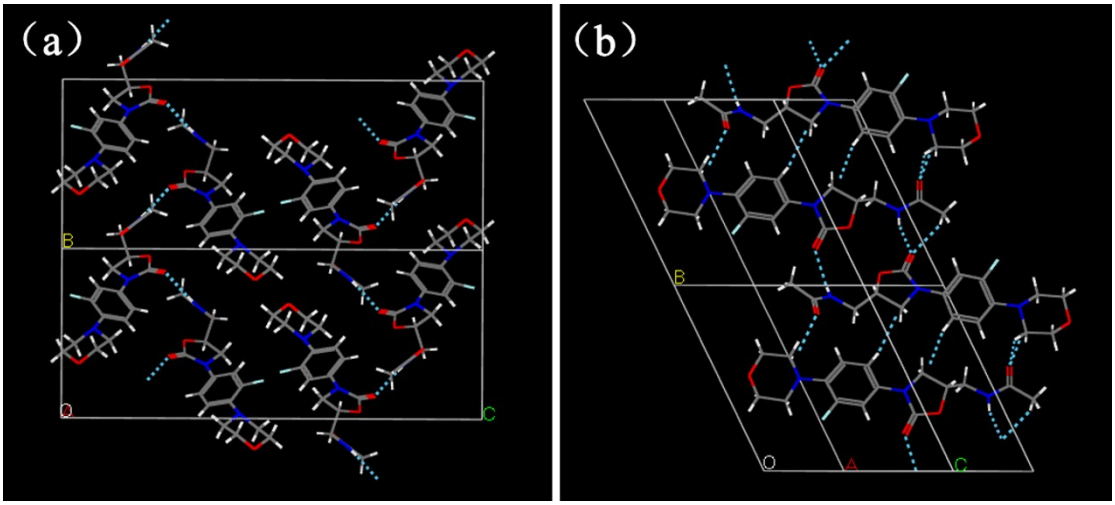

Fig. S1 The unit cell structure of Linezolid (a) Form II and (b) Form IV. (The blue dashed lines represent hydrogen bondings.)

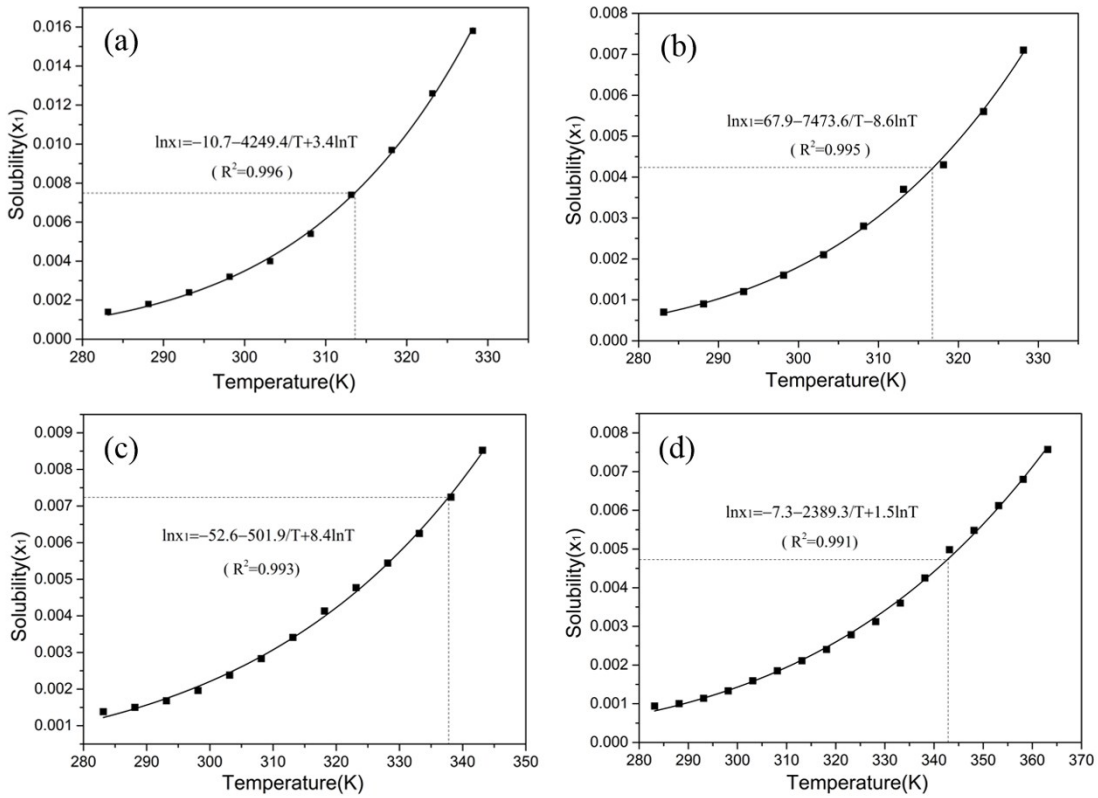

Fig. S2 The measured solubility of Linezolid in the solvent of (a) methanol; (b) ethanol; (c) ethyl acetate; (d) butyl acetate, together with the correlated curves (solid lines) via the modified Apelblat equation.

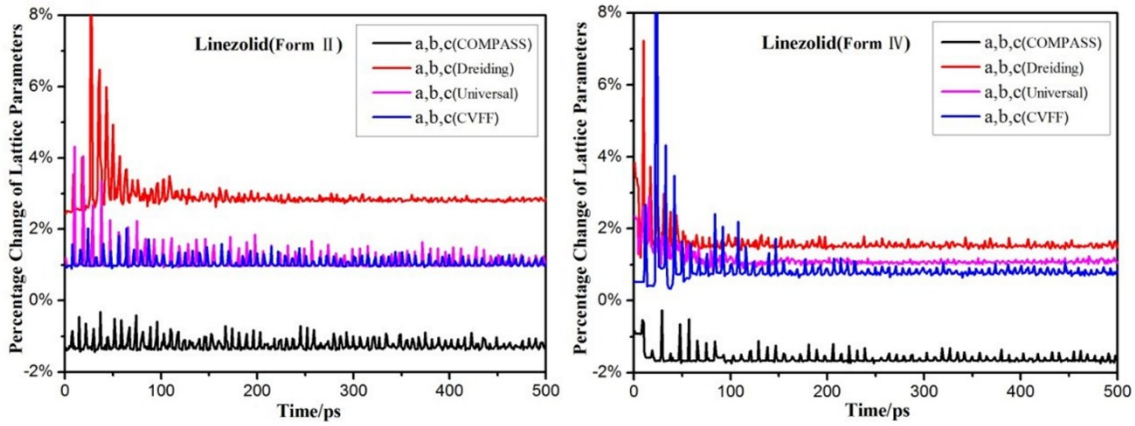

Fig. S3 The percentage changes of lattice parameters of Linezolid Form II and Form IV calculated under different force fields.

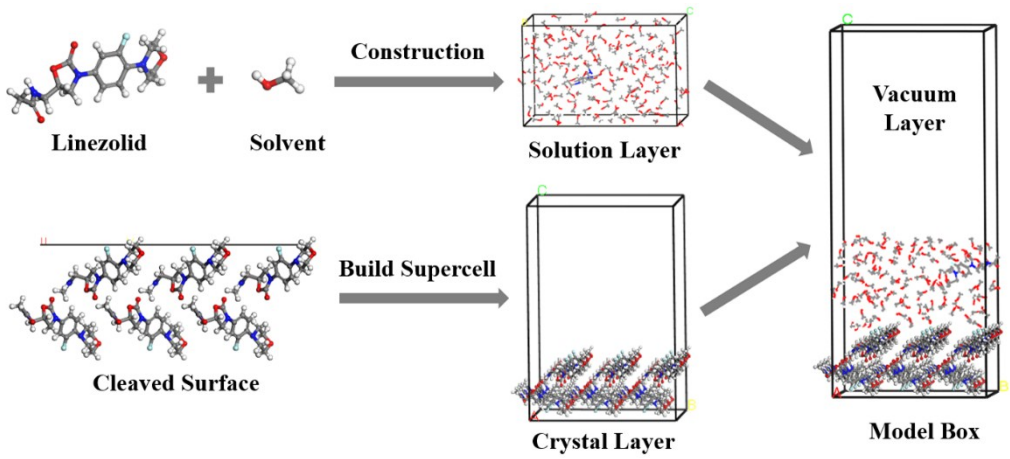

Fig. S4 The schematic of Linezolid crystal face-solution interfacial model.

The crystal face-solution interfacial model is comprised of a crystal layer that is constructed by cleaving the corresponding crystal face with a depth of 2 $\times d_{hkl}$, a solution layer established according to the solubility of Linezolid in the individual solvent, as well as a vacuum layer with the height of 50 Å to eliminate the effect of the boundary.

MD simulation was run in the NVT ensemble for 50 ps with a time step of 1 fs and the temperature was maintained at 283 K using the Nose thermostat. The electrostatic interactions were calculated by Ewald methods, with a calculation accuracy of 0.001 kcal/mol. The van der Waals forces were calculated by Atom based methods, and the cutoff distance is 12.5 Å.

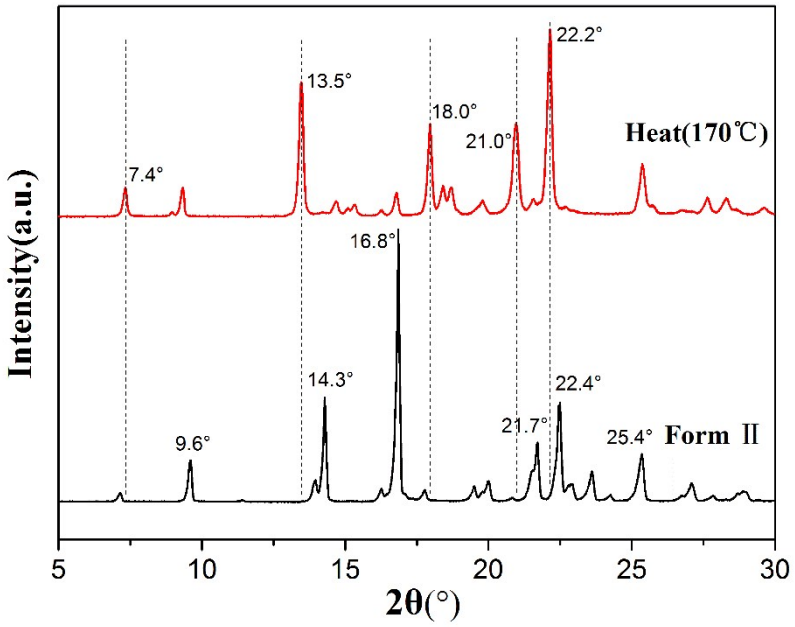

Fig. S5 PXRD patterns of Linezolid (Form II) and after heating to 170 °C.

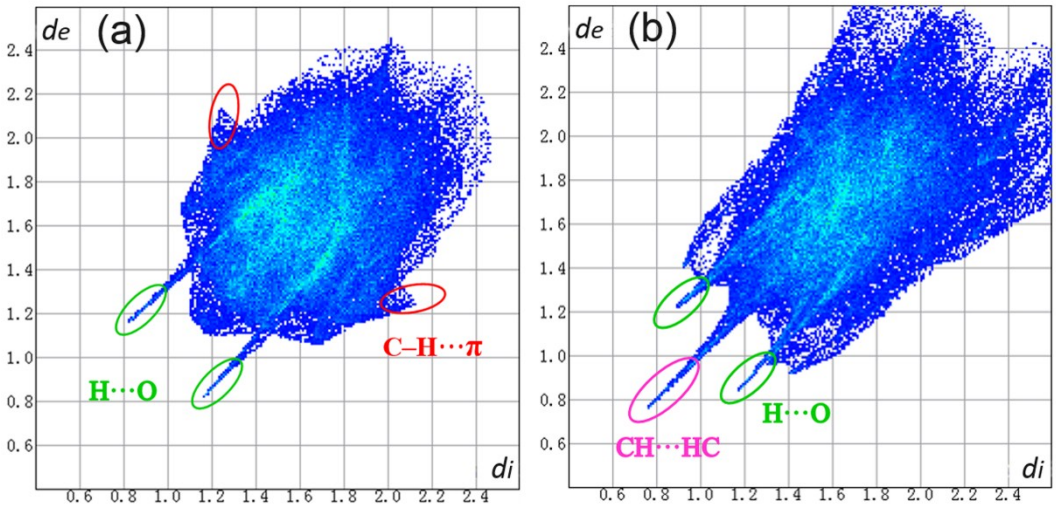

Fig. S6 Fingerprint plots for Linezolid (a) Form II and (b) Form IV.

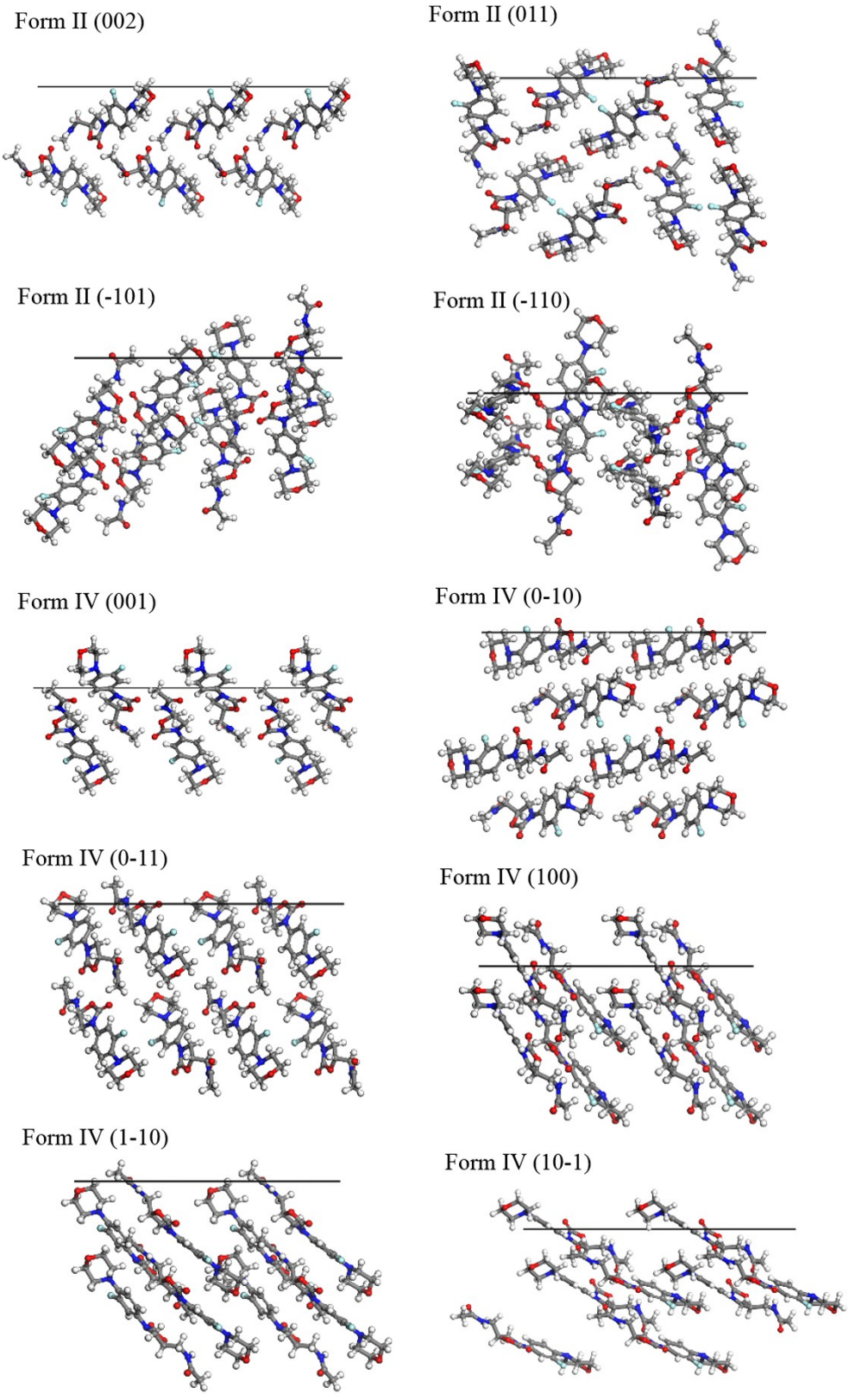

Fig. S7 Surface conformation of the morphological important faces of Linezolid polymorphs.