**Table S1** The PXRD peak positions of solid forms of deferasirox.

| Solid forms | 2$\theta$ values |
|---|---|
| DFX | 6.6°, 10.1°, 10.6°, 13.2°, 14.1°, 15.4°, 16.6°, 23.2°,25.7°, 26.2° |
| DFX-$H_2O$ | 10.0°, 10.5°, 11.9°, 13.4°, 15.6°, 19.2°, 22.6°, 24.8°, 25.8°, 26.7°, 27.8°; |
| DFX-DMF | 5.3°, 9.9°, 10.6°, 16.0°, 16.6°, 17.6°, 20.6°, 22.5°, 24.0°, 24.4°, 33.6°. |
| DFX-INA | 4.9°, 9.6°, 10.7°, 13.7°, 15.5°, 24.4°, 25.4°, 26.0°, 26.8°, 28.1°. |
| DFX-2INA | 4.8°, 11.2°, 16.5°, 22.9°, 23.4°, 24.1°, 25.1°, 25.9°, 26.8°, 27.6°. |

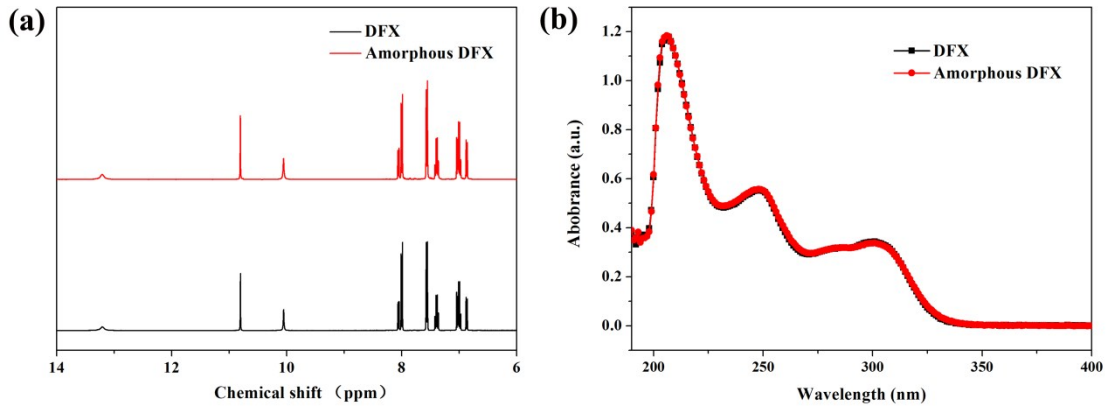


**Fig. S1** (a) The $^1$H NMR spectra of amorphous DFX and commercial DFX; (b) the UV–Vis absorption spectra of amorphous DFX and commercial DFX.

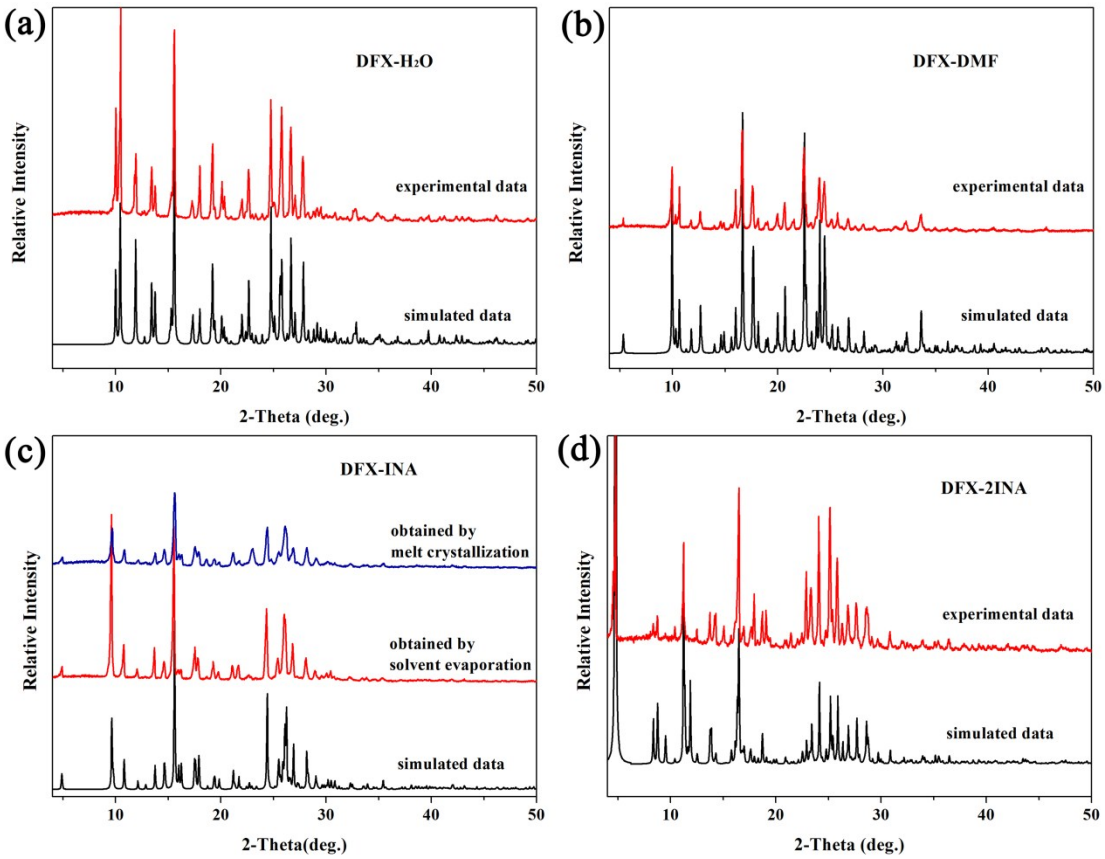


**Fig. S2** The PXRD patterns of (a) DFX-$H_2O$, (b) DFX-DMF, (c) DFX-INA and (d) DFX-2INA matched with the corresponding simulated patterns.

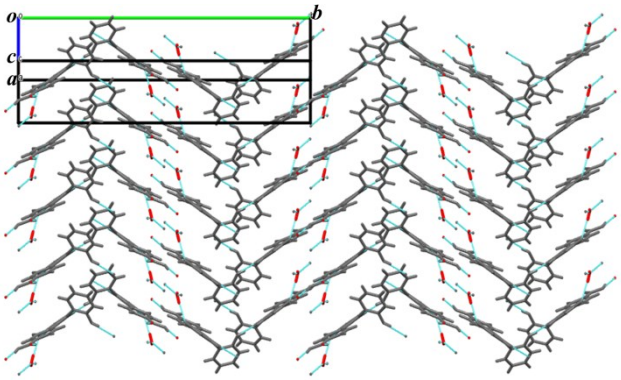


**Fig. S3** Packing diagram of DFX-$H_2O$ (DFX and $H_2O$ molecules are expressed in gray and red color, respectively).

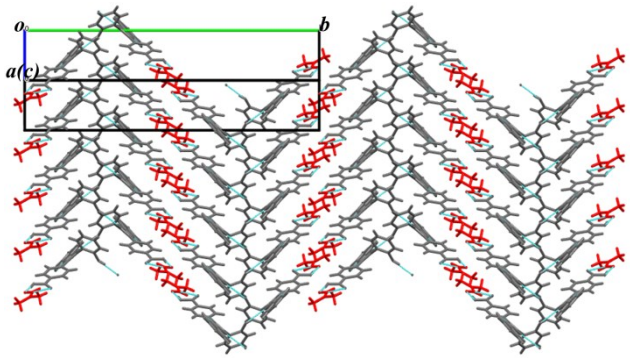


**Fig. S4** Packing diagram of DFX-DMF (DFX and DMF molecules are expressed in gray and red color, respectively).

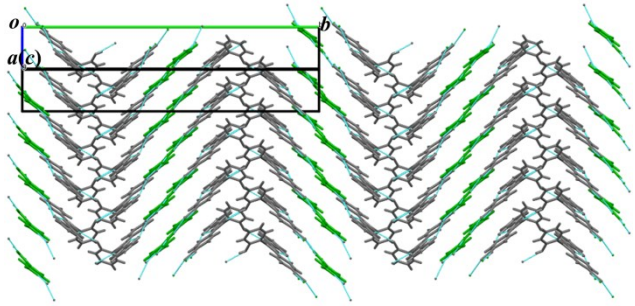


**Fig. S5** Packing diagram of DFX-INA (DFX and INA molecules are expressed in gray and green color, respectively).

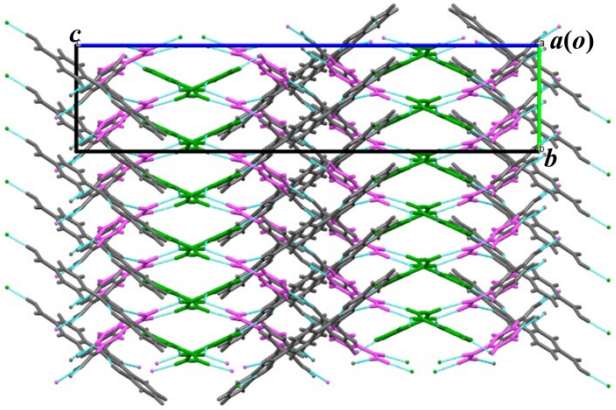


**Fig. S6** Packing diagram of DFX-2INA (DFX, I-INA, and II-INA molecules are expressed in gray, green, and pink color, respectively).

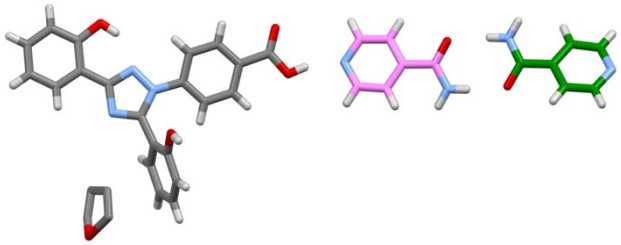

**Fig. S7** The single crystal structure of DFX-2INA without eliminating the THF carbon skeleton.

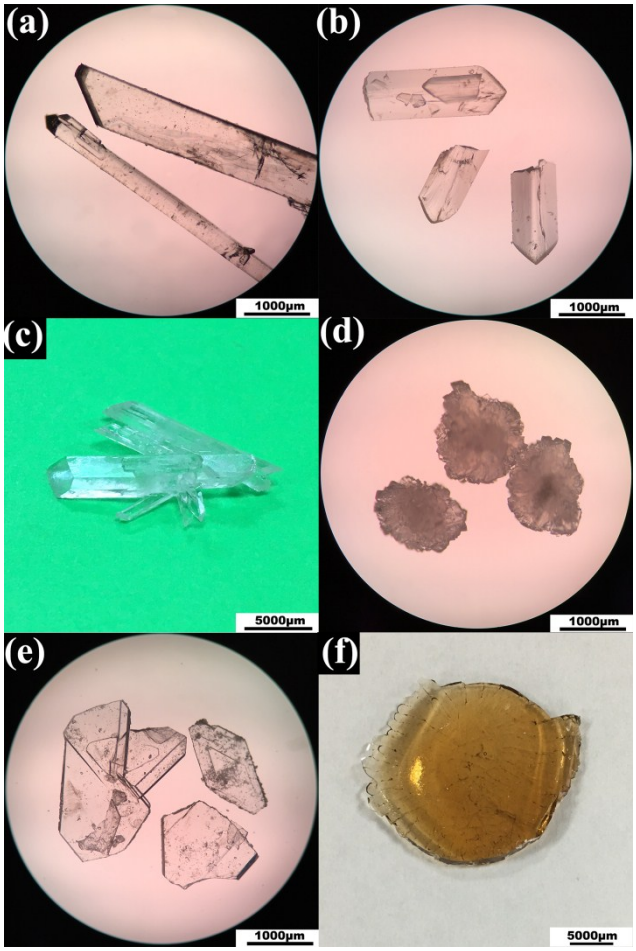


**Fig. S8** Morphological images of (a) commercial DFX crystallized from methanol, (b) DFX-$H_2O$, (c) DFX-DMF, (d) DFX-INA, (e) DFX-2INA, and (f) amorphous DFX obtained by melt quenching.

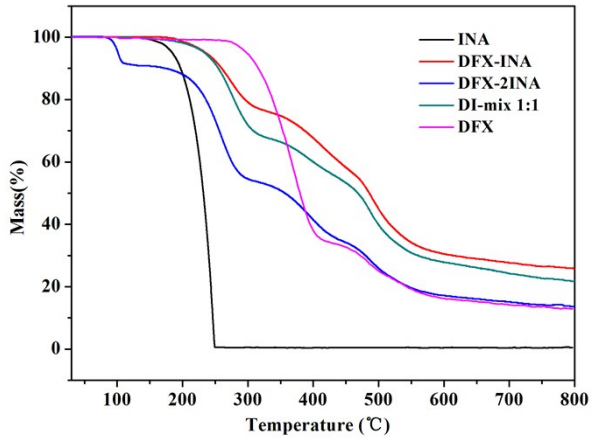


**Fig. S9** TGA curves of DFX, INA DFX-INA, DFX-2INA and DI-mix 1:1.

**Table S2** The cumulative drug release percentages of the three DFX solid forms

| Time point / min | cumulative drug release percentage / % | | | | | |
|---|---|---|---|---|---|---|
| | DFX in PBS | DFX in H2O | Amorphous DFX in PBS | Amorphous DFX in H2O | DFX-INA in PBS | DFX-INA in H2O |
| 0 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 2 | 2.43 | -- | 7.39 | -- | 11.60 | -- |
| 5 | 7.43 | -- | 23.31 | -- | 32.76 | -- |
| 10 | 16.01 | 2.01 | 45.70 | 1.88 | 51.50 | 0.70 |
| 20 | 25.22 | 3.93 | 62.96 | 3.80 | 63.35 | 1.38 |
| 30 | 32.80 | 5.17 | 69.53 | 5.18 | 67.32 | 2.07 |
| 40 | 38.54 | 5.87 | 73.78 | 6.40 | 70.59 | 2.80 |
| 60 | 46.09 | 6.43 | 76.62 | 8.42 | 73.40 | 3.96 |
| 120 | 60.16 | 6.79 | 82.89 | 12.53 | 79.62 | 6.64 |
| 180 | 68.36 | 7.23 | 83.26 | 15.56 | 83.09 | 8.50 |
| 240 | 74.00 | 7.70 | 87.61 | 16.94 | 84.56 | 9.56 |