SUPPLEMENTARY INFORMATION

The impact of chemical structure on the formation of the medium-range order and dynamical properties of selected antifungal APIs

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Density Functional Theory (DFT) calculations

The density functional theory was used for geometry optimization and determination of dipole moments. The calculations were performed using the B3LYP/6-311G(d,p) functional combined with the aug-cc-pVDZ basis set, within the Gaussian03 software package. The geometry of the optimized lowest-energy conformation for terconazole (TER) and ketoconazole (KET) is shown in Fig. S1 a and b, respectively.

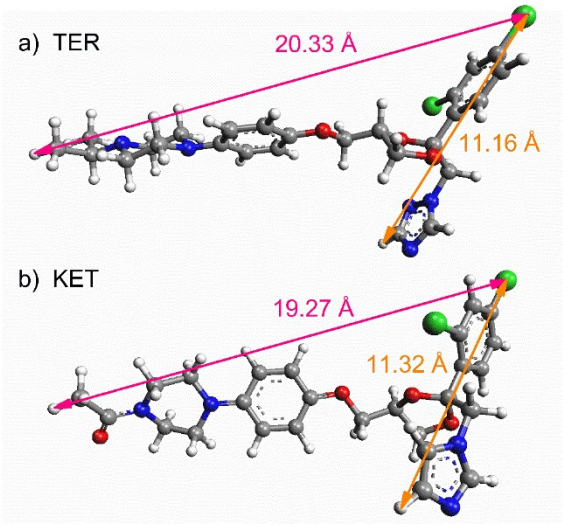

Fig. S1. Optimized geometry of (a) TER and (b) KET molecules.

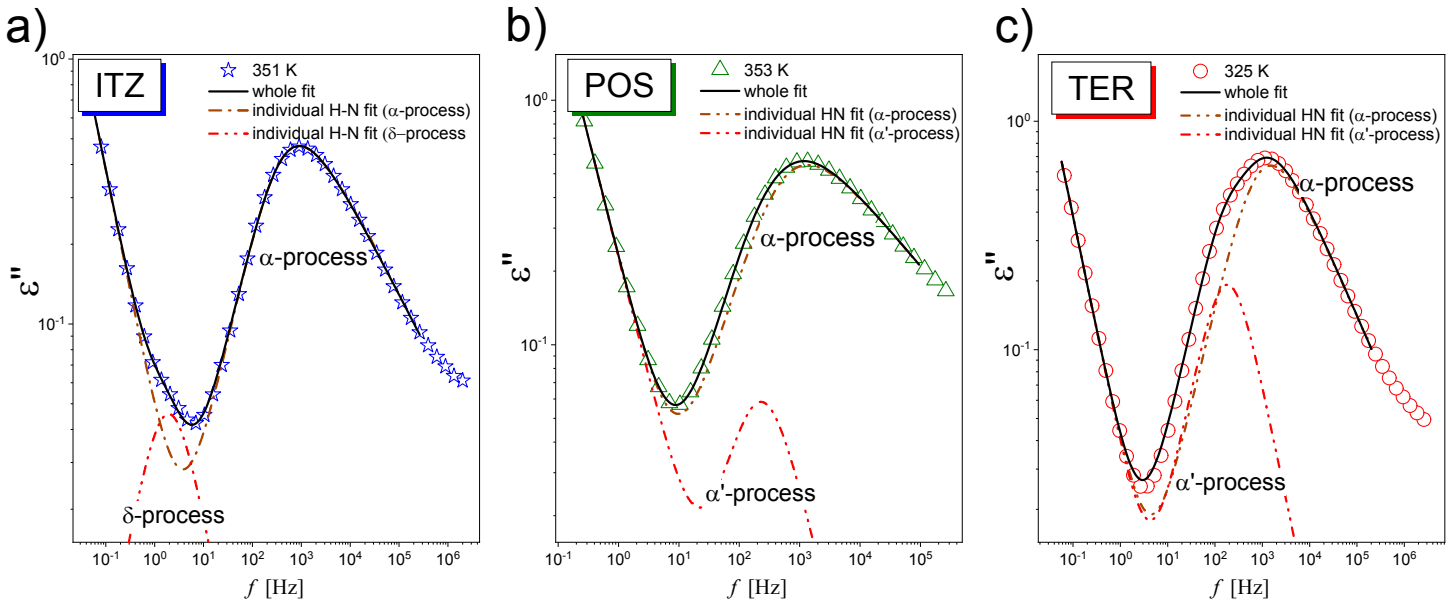

Fig. S2. Dielectric spectra of ITZ (a), POS (b), and (TER) measured at ambient pressure and indicated temperatures, together with the fits constructed from the superposition of two Havriliak-Negami (HN) functions with the additional conductivity term- Eq. (1) (black solid lines). In addition, the individual HN fits describing the δ/α'- and α-relaxation processes (red and brown dash-dotted lines, respectively) are presented.

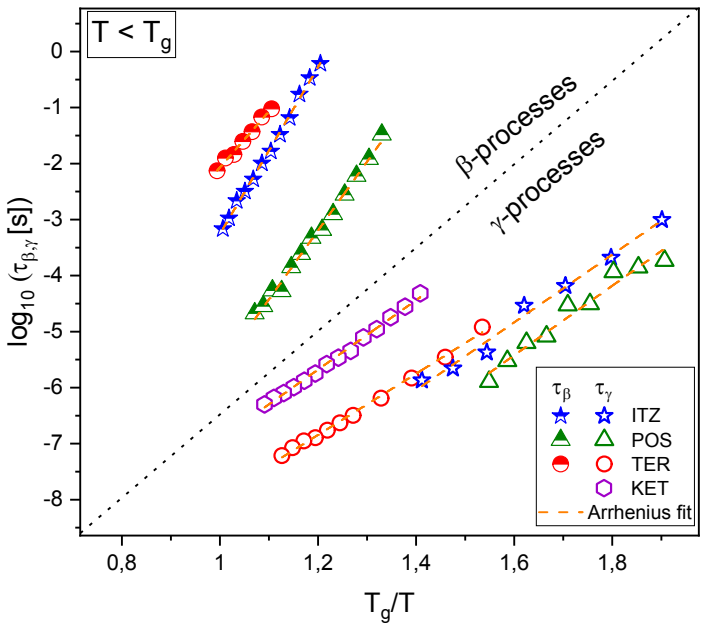

Fig. S3. Temperature dependences of the secondary β- (half-filled symbols) and γ-relaxation times (open symbols). Data for ITZ, POS and KET were taken from Ref. 1.

The values of τ_β and τ_γ for TER were determined from the analyses of dielectric spectra shown in Fig. 4c (main manuscript) with the use of superposition of two HN functions (Eq. 1). The same fitting procedure was applied in the case of ITZ and POS.[1] In the case of KET, one HN function was used to fit the data measured below the T_g.[1]

The temperature dependences of τ_β and τ_γ for TER (as for other APIs[1]) were analyzed with the use of Arrhenius equation:

$$\tau_x = \tau_\infty^x exp\left(\frac{E_x}{RT}\right) \qquad x = \beta, \gamma \tag{S1}$$

where R is a gas constant.

REFERENCES

[1] D. Heczko, E. Kamińska, K. Jurkiewicz, M. Tarnacka, K. Merkel, K. Kamiński and M. Paluch, *Mol. Liq.,* 2020, **307**, 112959.