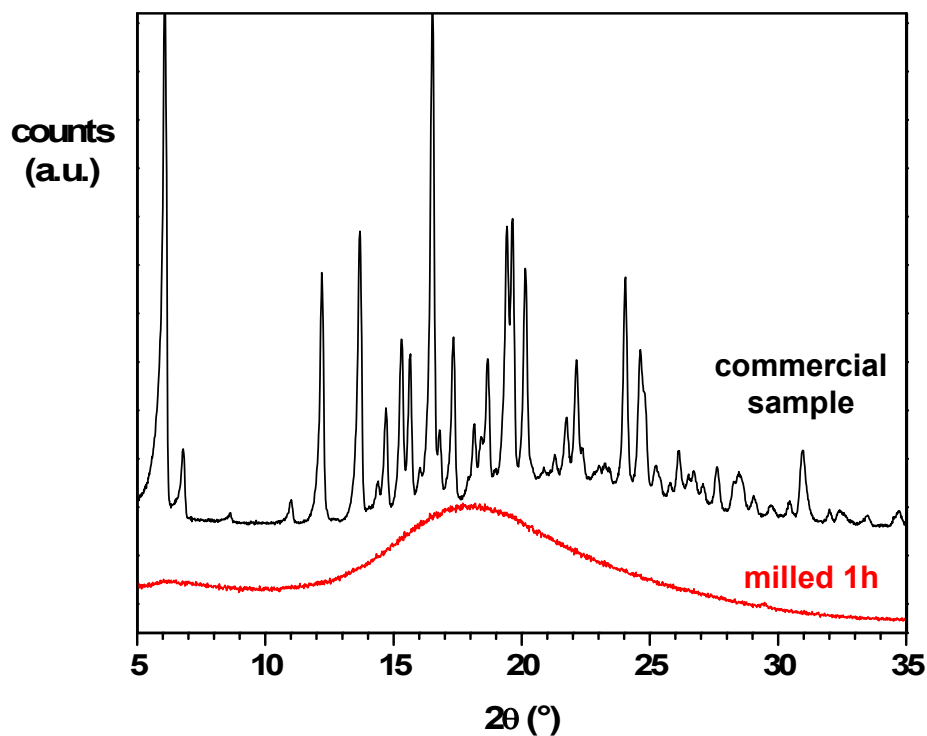# Supporting information

Figure S1: X-rays diffraction pattern of Terfenadine recorded before and after milling. The powder X-ray diffraction experiments were performed with an XPERT PRO MPD diffractometer ($\lambda_{Cu\,K\alpha}$ = 1.540 Å) equipped with an X'celerator detector. Samples were placed into Lindemann glass capillaries (Ø = 0.7 mm).
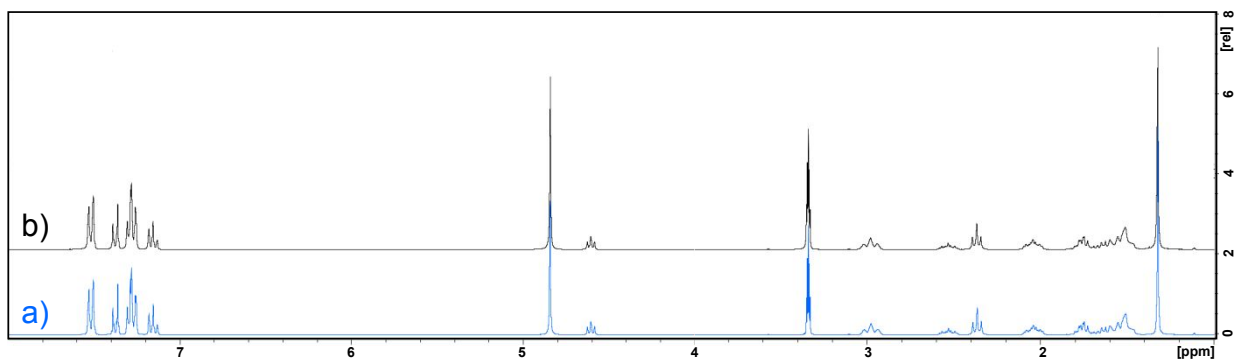
Figure S2: ^1H NMR of Terfenadine dissolved in deuterated methanol: a) commercial product; b)
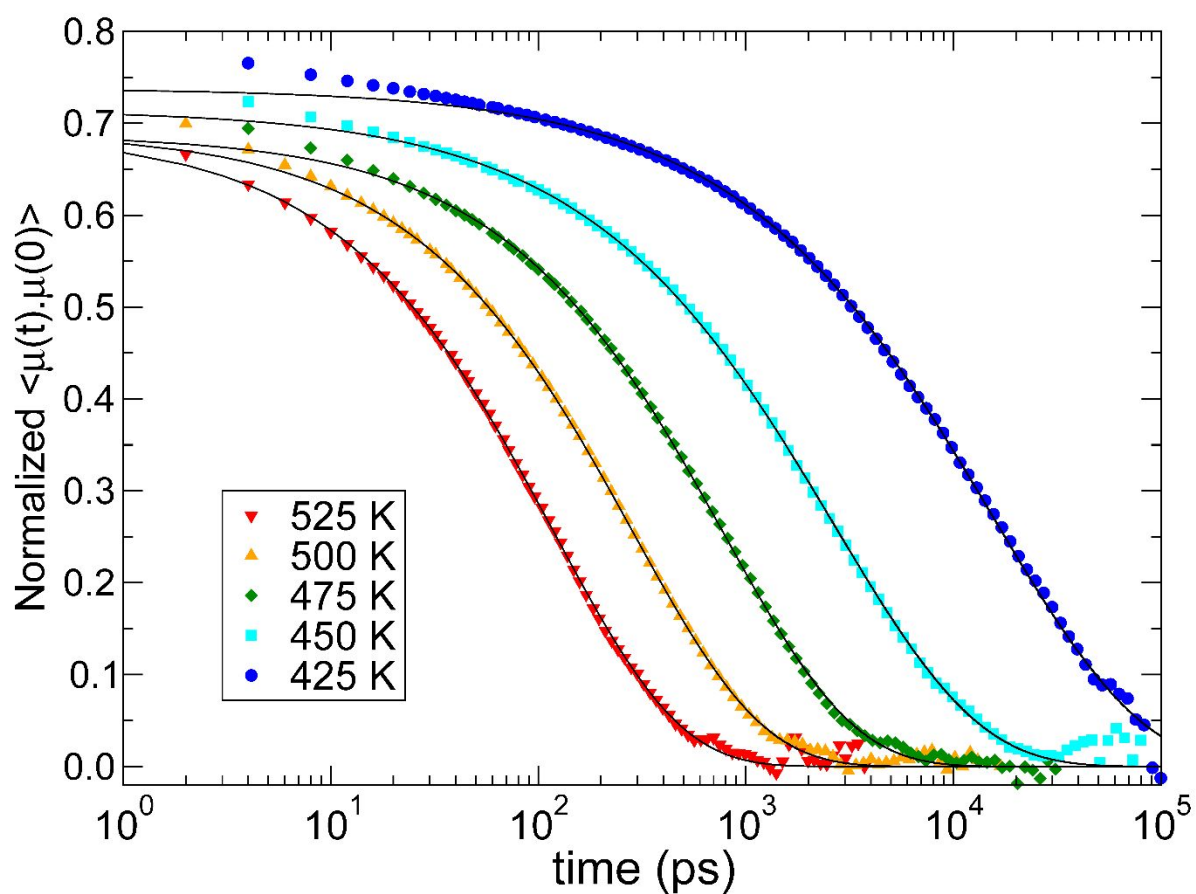
after a 4 hours milling

Figure S3: Dipole-dipole time-dependent self-correlation function of Terfenadine in the liquid

state obtained from MD simulations at different temperatures. The dependence at long times are

fitted by the expression: $\Phi_\mu(t) = A_\mu \exp\left[-\left(t/\tau_\mu^{(MD)}\right)^{\beta_\mu^{(MD)}}\right]$, *where A_μ is the amplitude of the*

$\Phi_\mu(t)$ *function,* $\tau_\mu^{(MD)}$ *is the characteristic time associated with the long time decay and* $\beta_\mu^{(MD)}$

is a parameter describing the non-exponentiality of the decay. These fits are represented as solid

lines.