

Supporting Information

Effects of nucleation on solvate and polymorph control - evaporative crystallization of taltirelin -

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Fig. SI1 shows chemical structure of taltirelin.¹¹⁻¹⁶

The XRD pattern of the α -form, β -form and γ -form polymorph was collected over the 2θ range of 3° to 40° and is shown in Fig. SI2. The PXRD patterns of the α - and β -forms have been previously reported in the literature.¹²⁻¹⁷ In this figure, characteristic XRD peaks of the γ -form were observed at 8.0° , 11.1° , 15.1° , 15.7° , 16.5° , 18.3° , 18.6° , 19.2° , 20.7° , 22.1° , 22.4° , 23.2° , 23.6° , 23.9° , 24.4° , 26.0° , 26.9° , 27.7° , 28.6° , 29.1° , 29.6° , 30.1° , 31.2° , 31.6° , 32.3° , 36.4° , and 39.2° (2θ).

The differences in the Raman spectra of the α -form and β -form have been presented in previous studies.⁴⁻¹⁷ For comparison with the α - and β -forms, the spectrum of the γ -form is shown in Fig. SI3. Distinct peak differences are clearly observed at certain positions in the Raman spectra of the three polymorphs, particularly in the $800-900\text{ cm}^{-1}$, $1200-1400\text{ cm}^{-1}$, and $1500-1700\text{ cm}^{-1}$

Fig. SI4 shows the crystal form of the taltirelin polymorph γ -form. The γ -form exhibits a prismatic shape similar to the α -form but has a smaller aspect ratio compared to the α -form.¹¹⁻¹⁷

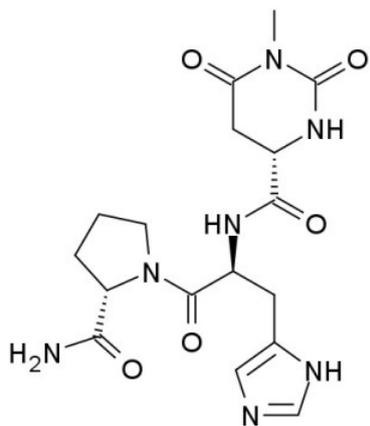


Fig. S11. Chemical structure of taltirelin

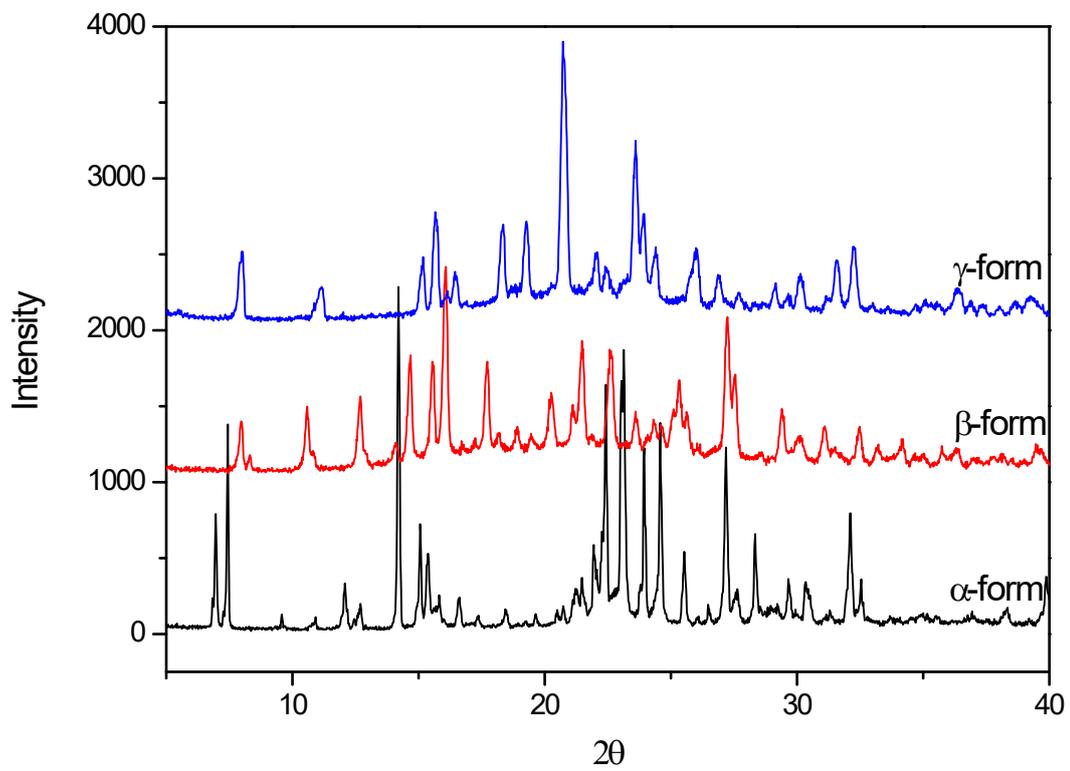


Fig. S12. XRD patterns of polymorphic forms of TTL

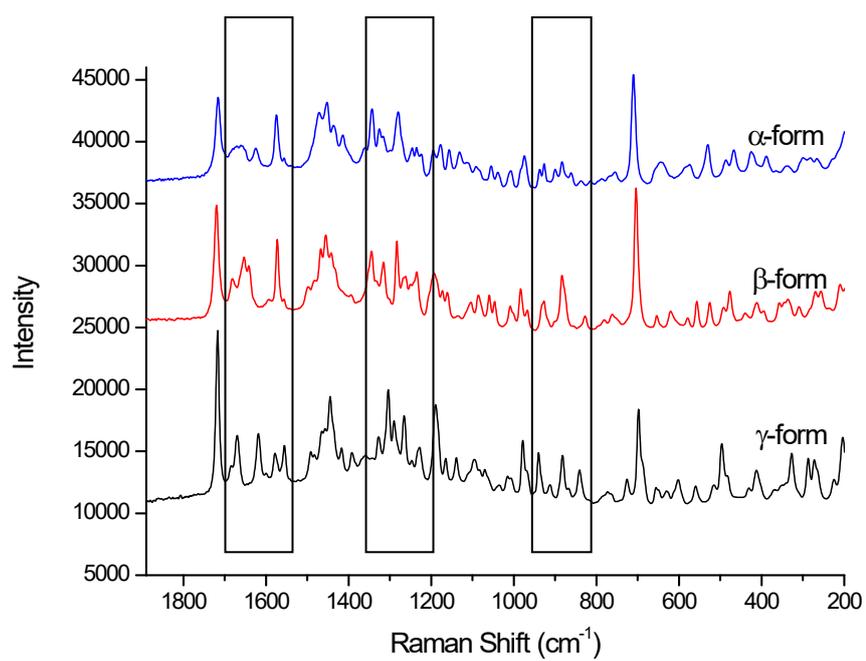
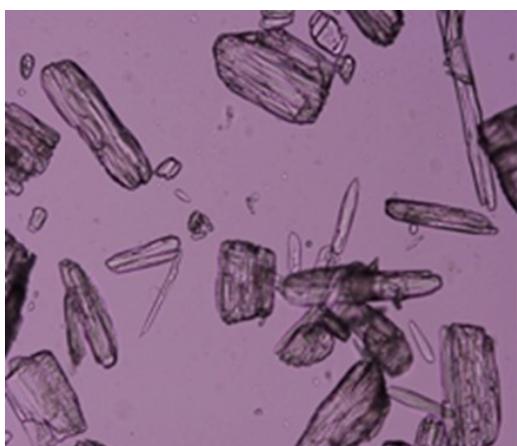


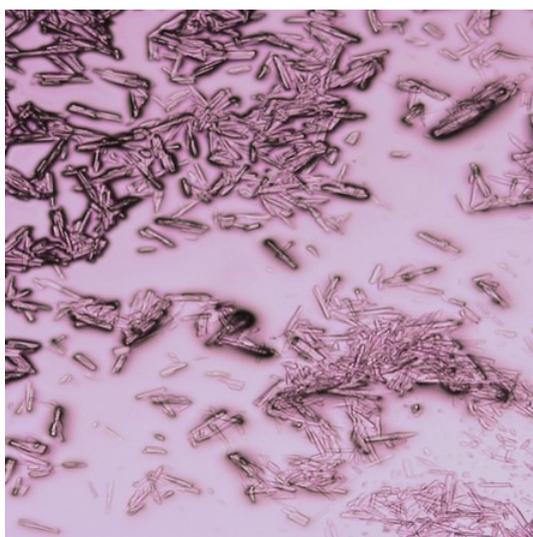
Fig. SI3. Raman spectroscopy of 3 forms of TTL



α -form



β -form



γ -form

Fig. S14. Microscopic photos of the taltirelin polymorphs