Supplementary Information

Molecular design of mechanofluorochromic dyes and their solid-state fluorescence properties

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Fig. S1 (a) Excitation and (b) fluorescence spectra of 1a before and after grinding, and after heating the ground solid at 150 °C.

Fig. S2 (a) Excitation and (b) fluorescence spectra of 1b before and after grinding, and after heating the ground solid at 150 °C.
Fig. S3 (a) Excitation and (b) fluorescence spectra of 1c before and after grinding, and after heating the ground solid at 150 °C.

Fig. S4 (a) Excitation and (b) fluorescence spectra of 1d before and after grinding, and after heating the ground solid at 150 °C.
**Fig. S5** (a) Excitation and (b) fluorescence spectra of 2a before and after grinding, and after heating the ground solid at 180 °C.

**Fig. S6** (a) Excitation and (b) fluorescence spectra of 3a before and after grinding.
Fig. S7 (a) Excitation and (b) fluorescence spectra of 4a before and after grinding, and after heating the ground solid at 160 °C.

Fig. S8 (a) Excitation and (b) fluorescence spectra of 5a before and after grinding, and after heating the ground solid at 150 °C.
**Fig. S9** (a) Excitation and (b) fluorescence spectra of 3b before and after grinding, and after heating the ground solid at 230 °C.

**Fig. S10** (a) Excitation and (b) fluorescence spectra of i1b before and after grinding, and after heating the ground solid at 200 °C.
**Fig. S11** (a) Excitation and (b) fluorescence spectra of **i4a** before and after grinding, and after heating the ground solid at 150 ºC.

**Fig. S12** (a) Excitation and (b) fluorescence spectra of **i5a** before and after grinding, and after heating the ground solid at 150 ºC.
**Fig. S13** (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 1a before and after grinding, and after heating the ground solid.

**Fig. S14** (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 1b before and after grinding, and after heating the ground solid.
**Fig. S15** (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 1c before and after grinding, and after heating the ground solid.

**Fig. S16** (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 1d before and after grinding, and after heating the ground solid.
Fig. S17 (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 2a before and after grinding, and after heating the ground solid.

Fig. S18 (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 3a before and after grinding, and after heating the ground solid.
Fig. S19 (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 4a before and after grinding, and after heating the ground solid.

Fig. S20 (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 5a before and after grinding, and after heating the ground solid.
**Fig. S21** (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of 3b before and after grinding, and after heating the ground solid.

**Fig. S22** (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of i1b before and after grinding, and after heating the ground solid.
Fig. S23 (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of i4a before and after grinding, and after heating the ground solid.

Fig. S24 (a) XRD patterns and (b) DSC curves (scan rate: 10 °C min⁻¹) of i5a before and after grinding, and after heating the ground solid.