Supplementary Information

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

Yousuke Ooyama and Yutaka Harima

Department of Applied Chemistry, Graduate School of Engineering, Hiroshima University, Higashi-Hiroshima, 739-8527, Japan.
Fax: +81 824 24 5494; Tel: +81 824 24 6534; E-mail: harima@mls.ias.hiroshima-u.ac.jp

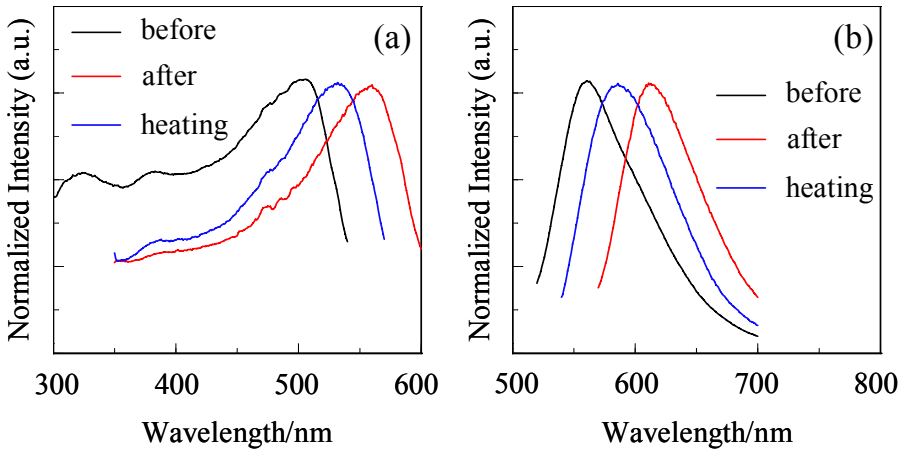

Fig. S1 (a) Excitation and (b) fluorescence spectra of **1a** before and after grinding, and after heating the ground solid at 150 ºC.

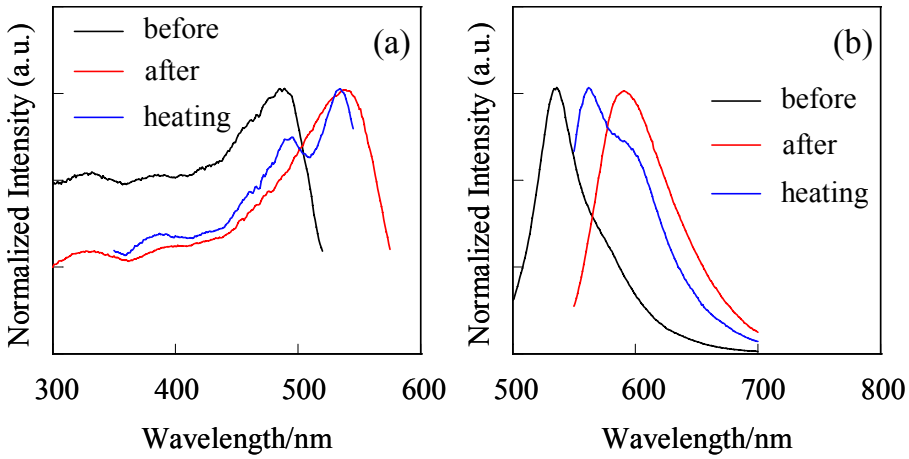

Fig. S2 (a) Excitation and (b) fluorescence spectra of **1b** before and after grinding, and after heating the ground solid at 150 ºC.

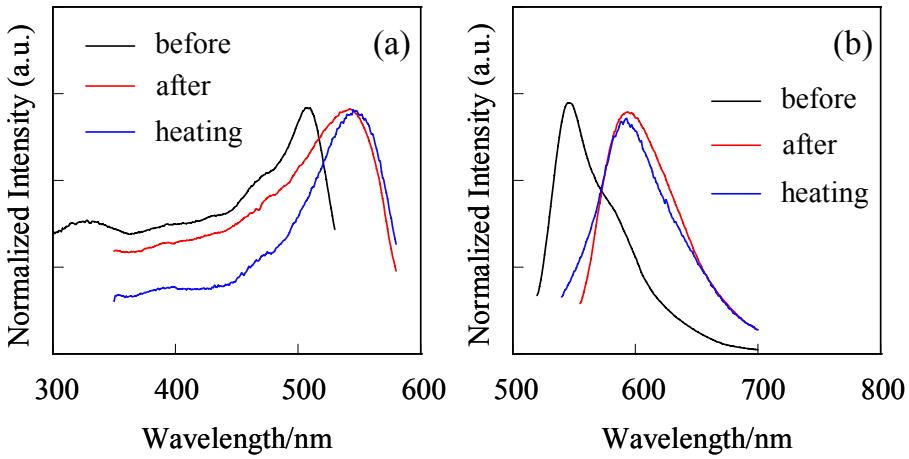

Fig. S3 (a) Excitation and (b) fluorescence spectra of **1c** before and after grinding, and after heating the ground solid at 150 ºC.

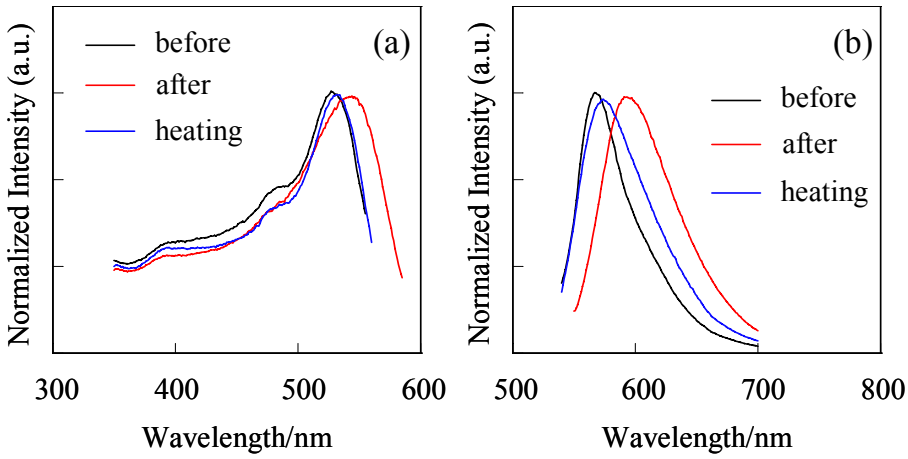

Fig. S4 (a) Excitation and (b) fluorescence spectra of **1d** before and after grinding, and after heating the ground solid at 150 ºC.

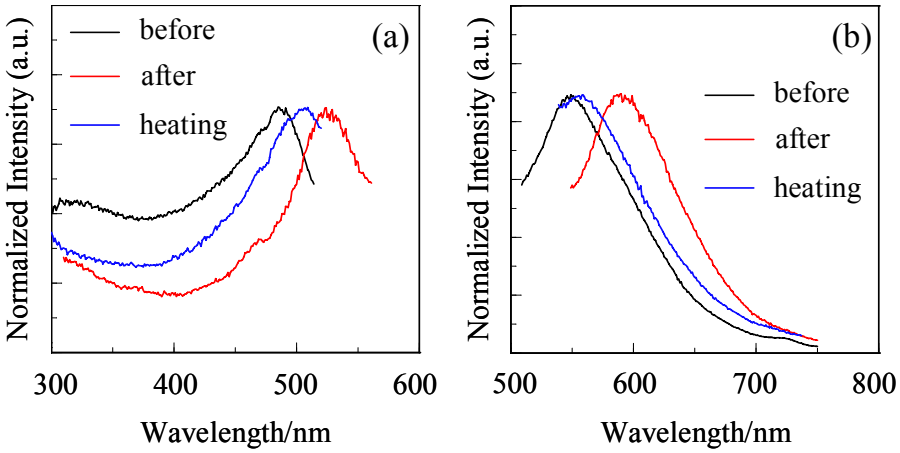

Fig. S5 (a) Excitation and (b) fluorescence spectra of **2a** before and after grinding, and after heating the ground solid at 180 ºC.

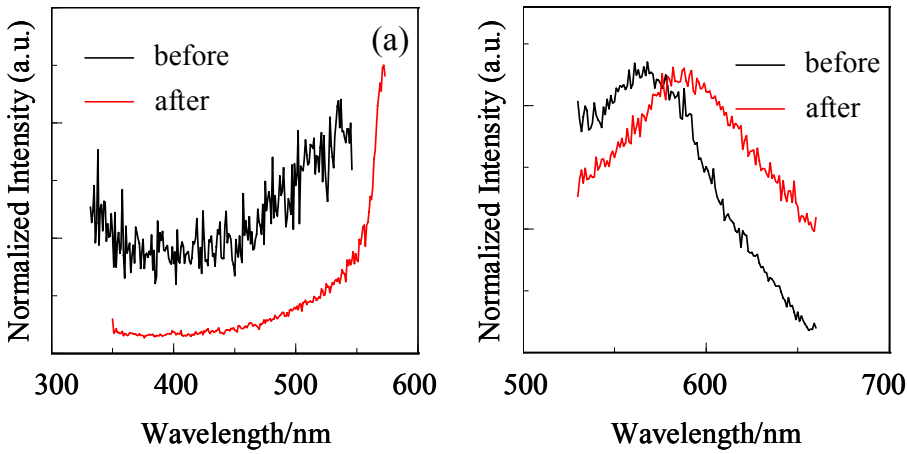

Fig. S6 (a) Excitation and (b) fluorescence spectra of **3a** before and after grinding.

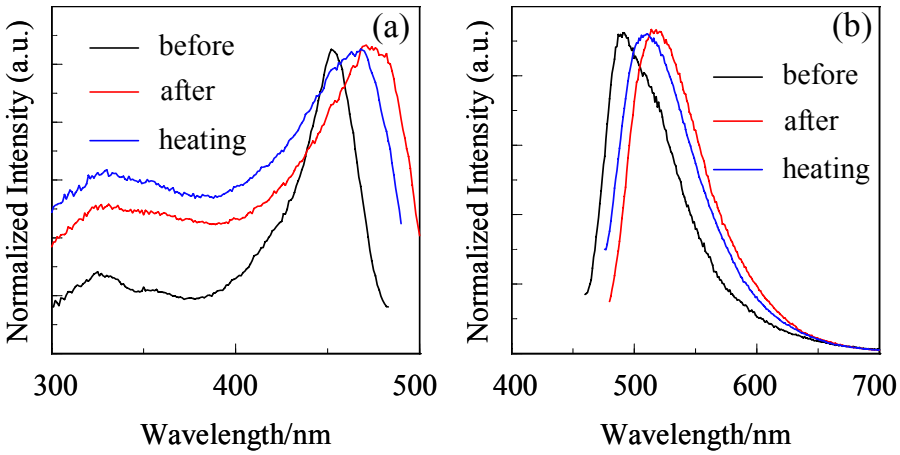

Fig. S7 (a) Excitation and (b) fluorescence spectra of **4a** before and after grinding, and after heating the ground solid at 160 ºC.

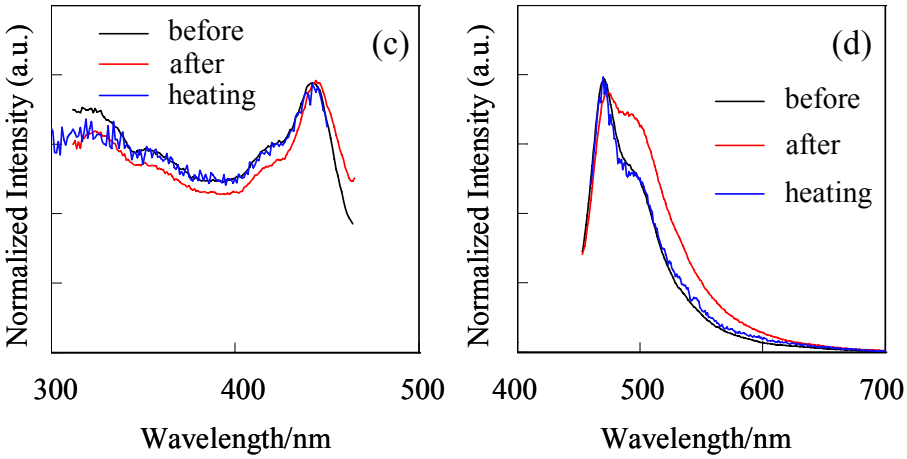

Fig. S8 (a) Excitation and (b) fluorescence spectra of **5a** before and after grinding, and after heating the ground solid at 150 ºC.

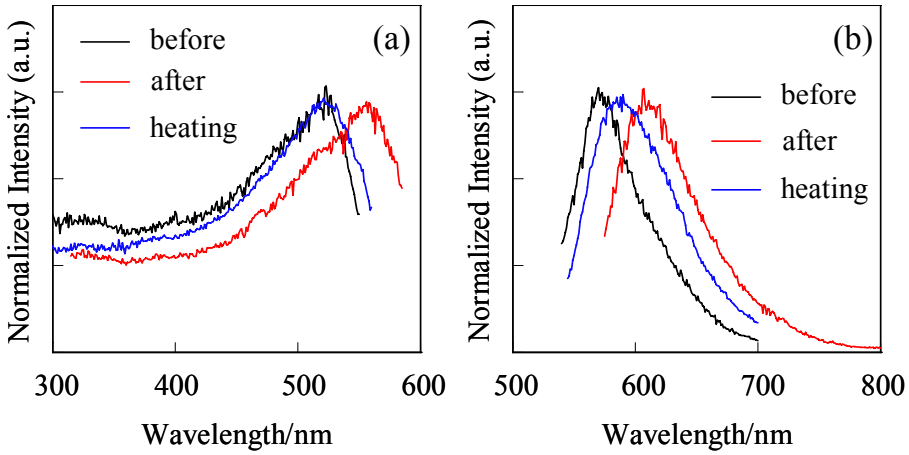

Fig. S9 (a) Excitation and (b) fluorescence spectra of **3b** before and after grinding, and after heating the ground solid at 230 ºC.

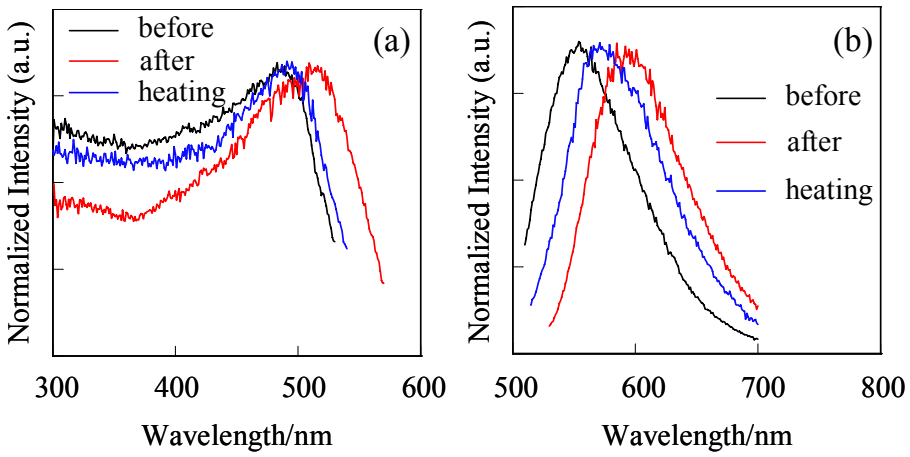

Fig. S10 (a) Excitation and (b) fluorescence spectra of **i1b** before and after grinding, and after heating the ground solid at 200 ºC.

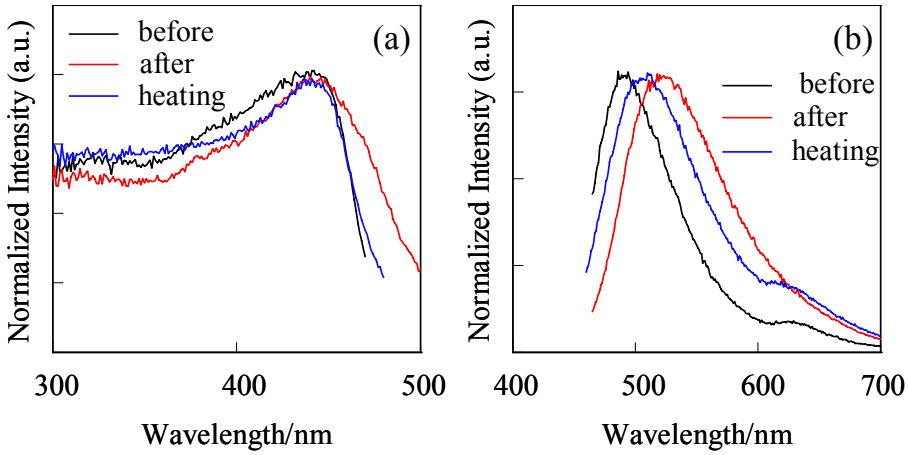

Fig. S11 (a) Excitation and (b) fluorescence spectra of **i4a** before and after grinding, and after heating the ground solid at 150 ºC.

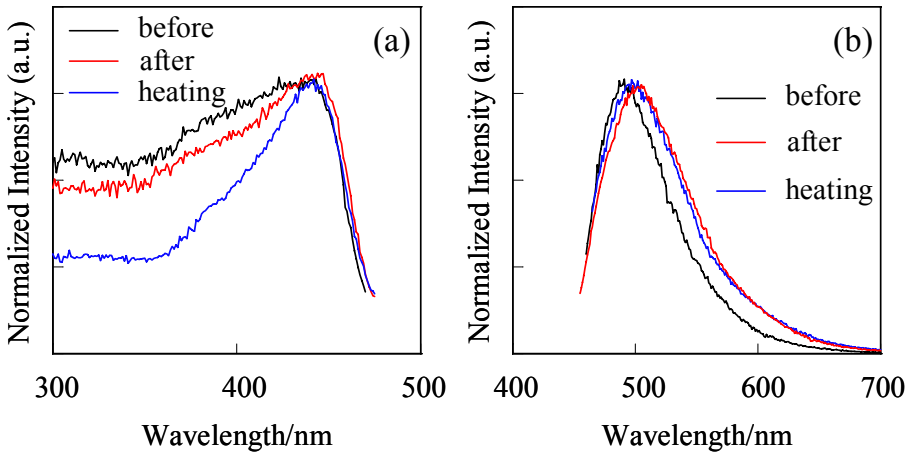

Fig. S12 (a) Excitation and (b) fluorescence spectra of **i5a** before and after grinding, and after heating the ground solid at 150 ºC.

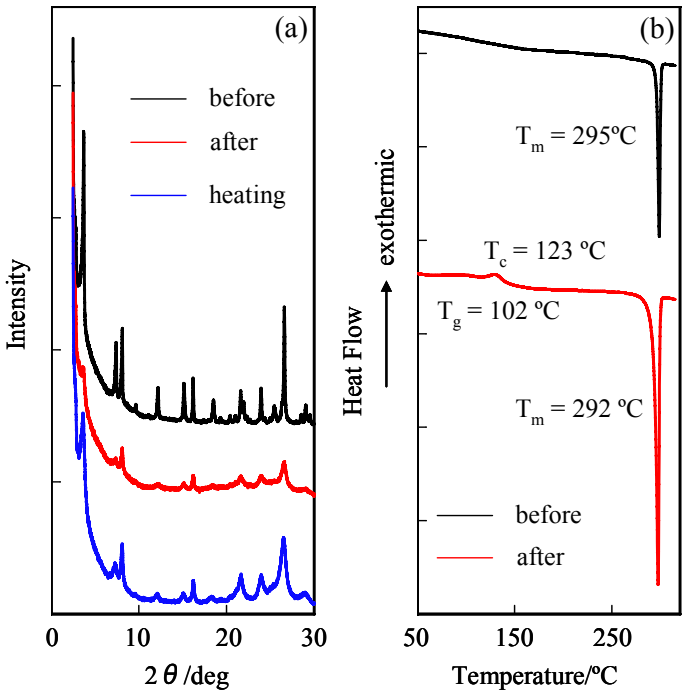

Fig. S13 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **1a** before and after grinding, and after heating the ground solid.

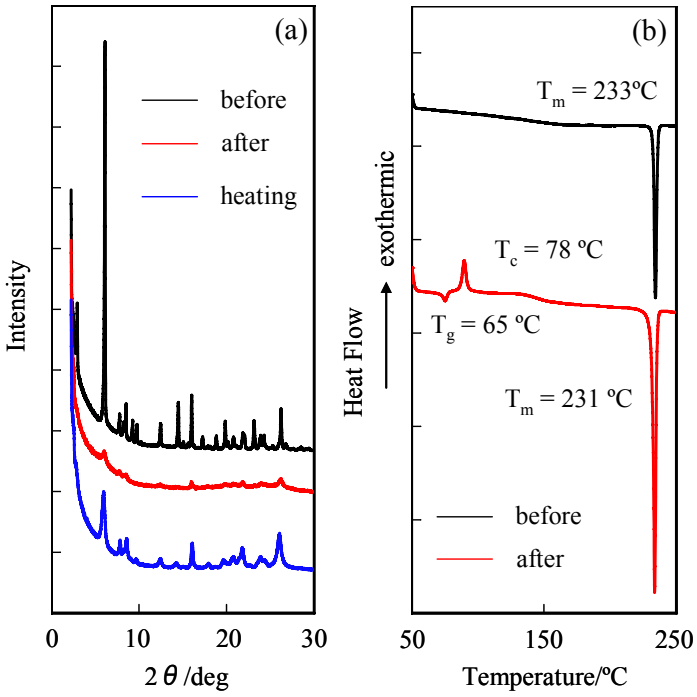

Fig. S14 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **1b** before and after grinding, and after heating the ground solid.

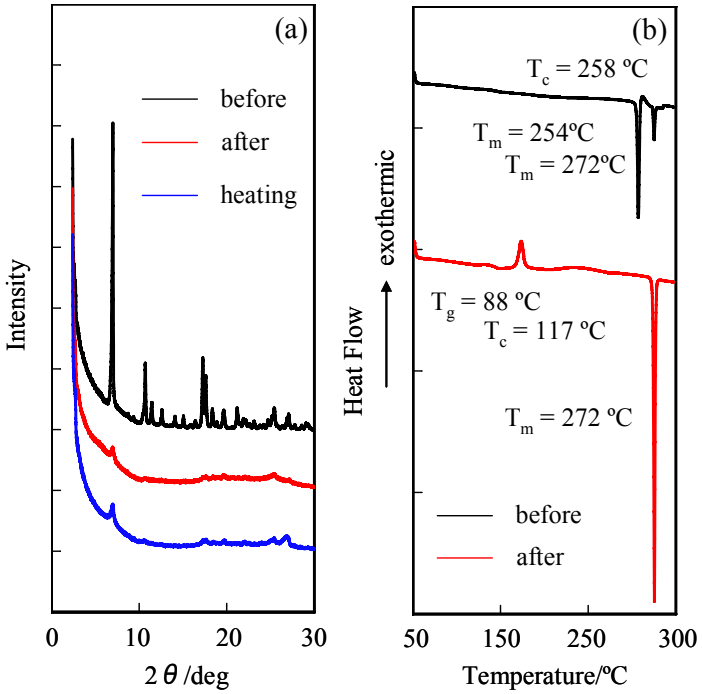

Fig. S15 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **1c** before and after grinding, and after heating the ground solid.

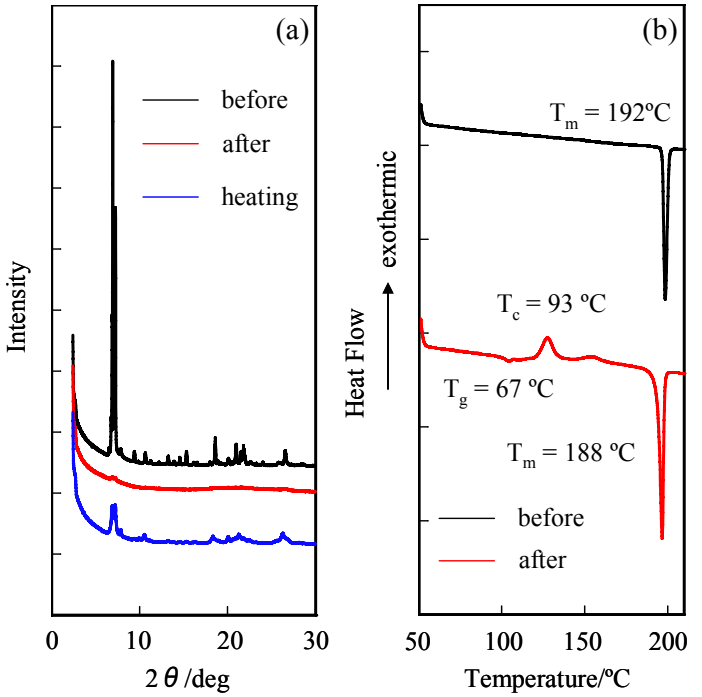

Fig. S16 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **1d** before and after grinding, and after heating the ground solid.

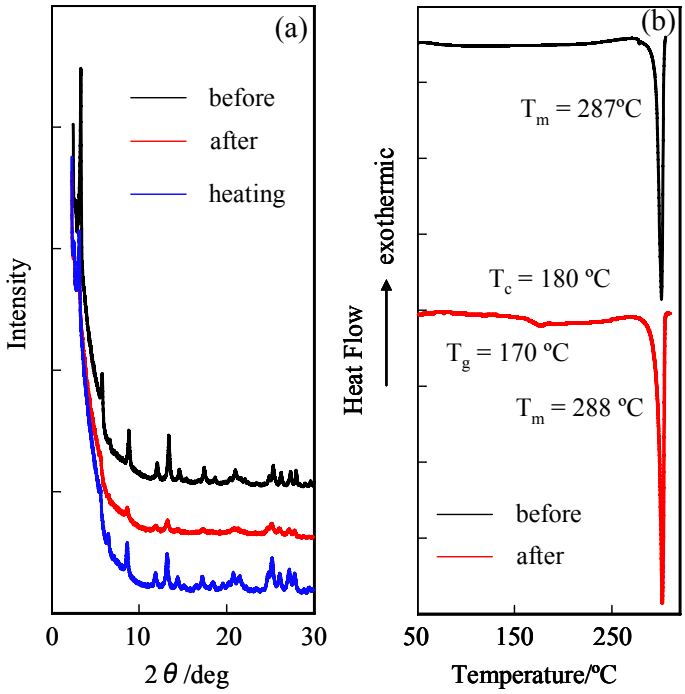

Fig. S17 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **2a** before and after grinding, and after heating the ground solid.

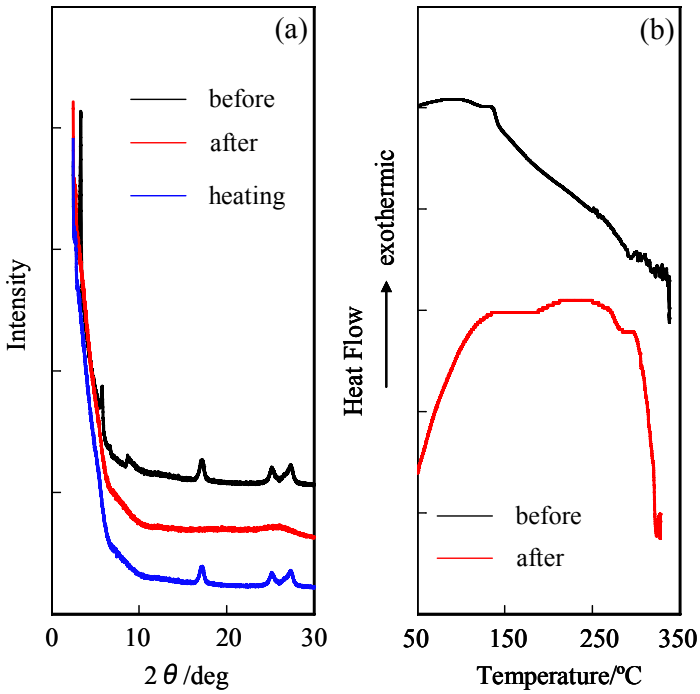

Fig. S18 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **3a** before and after grinding, and after heating the ground solid.

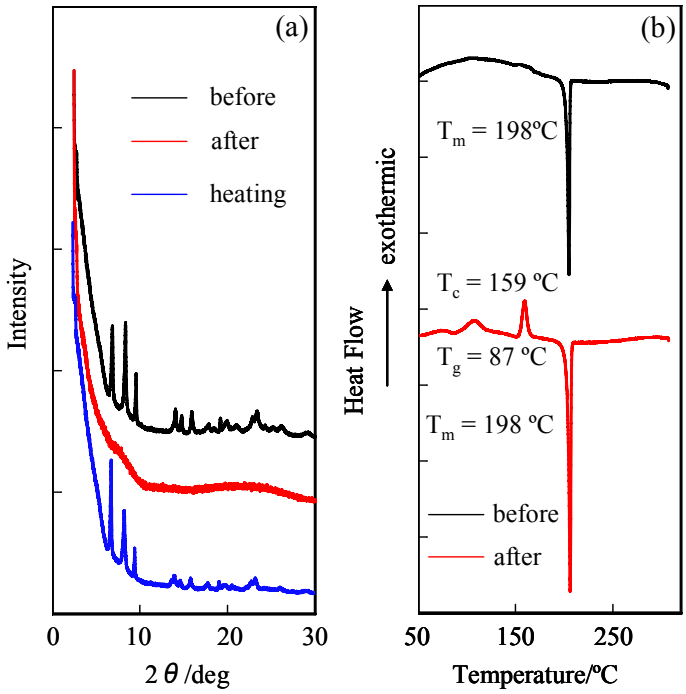

Fig. S19 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **4a** before and after grinding, and after heating the ground solid.

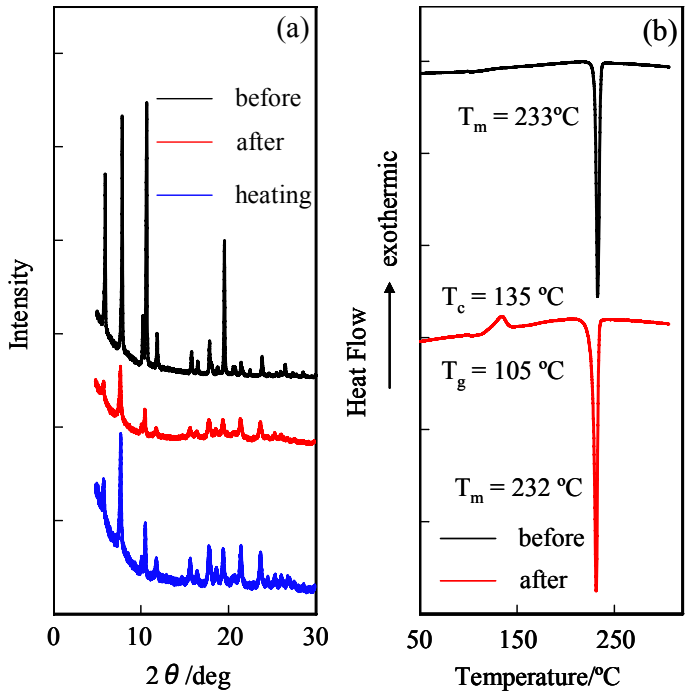

Fig. S20 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **5a** before and after grinding, and after heating the ground solid.

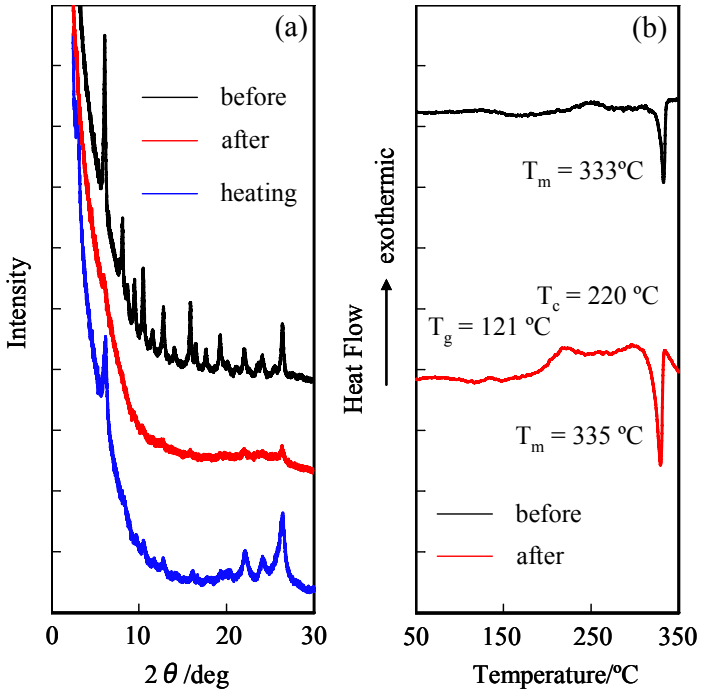

Fig. S21 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **3b** before and after grinding, and after heating the ground solid.

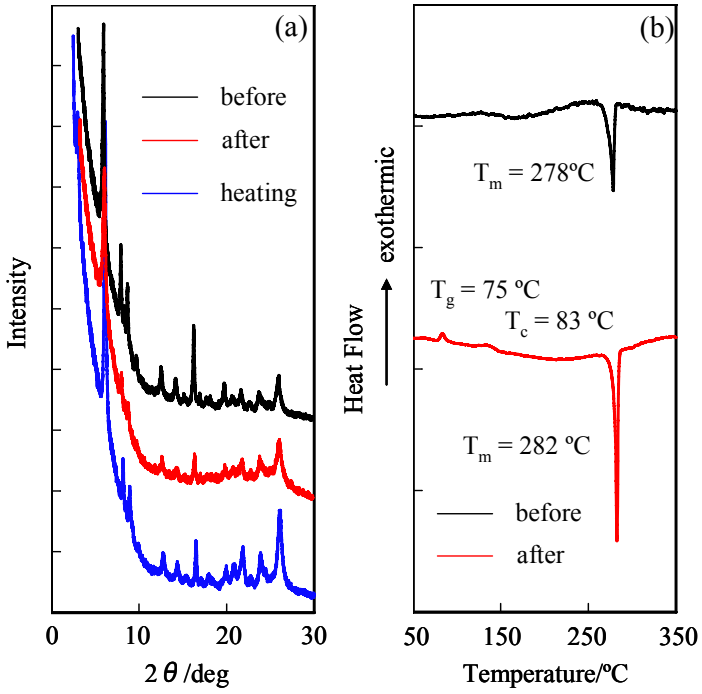

Fig. S22 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **i1b** before and after grinding, and after heating the ground solid.

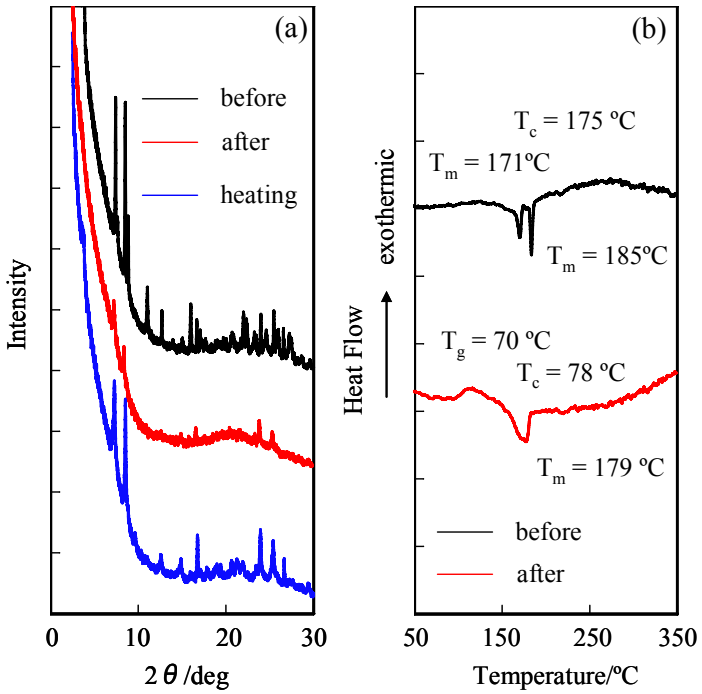

Fig. S23 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **i4a** before and after grinding, and after heating the ground solid.

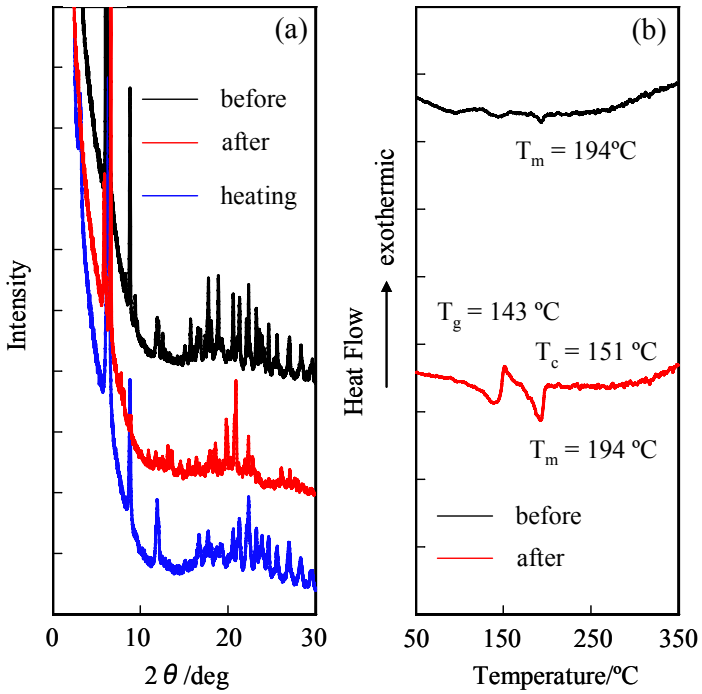

Fig. S24 (a) XRD patterns and (b) DSC curves (scan rate: 10 ºC min^{-1}) of **i5a** before and after grinding, and after heating the ground solid.