Thermal isomerization of spiropyran to merocyanine in aqueous media and its application to colorimetric temperature indication

Yasuhiro Shiraishi,* Masataka Itoh, and Takayuki Hirai

Research Center for Solar Energy Chemistry, and Division of Chemical Engineering, Graduate School of Engineering Science, Osaka University, Toyonaka 560-8531, Japan

E-mail: shiraish@cheng.es.osaka-u.ac.jp

Electronic Supplementary Information (ESI†)

Contents

page

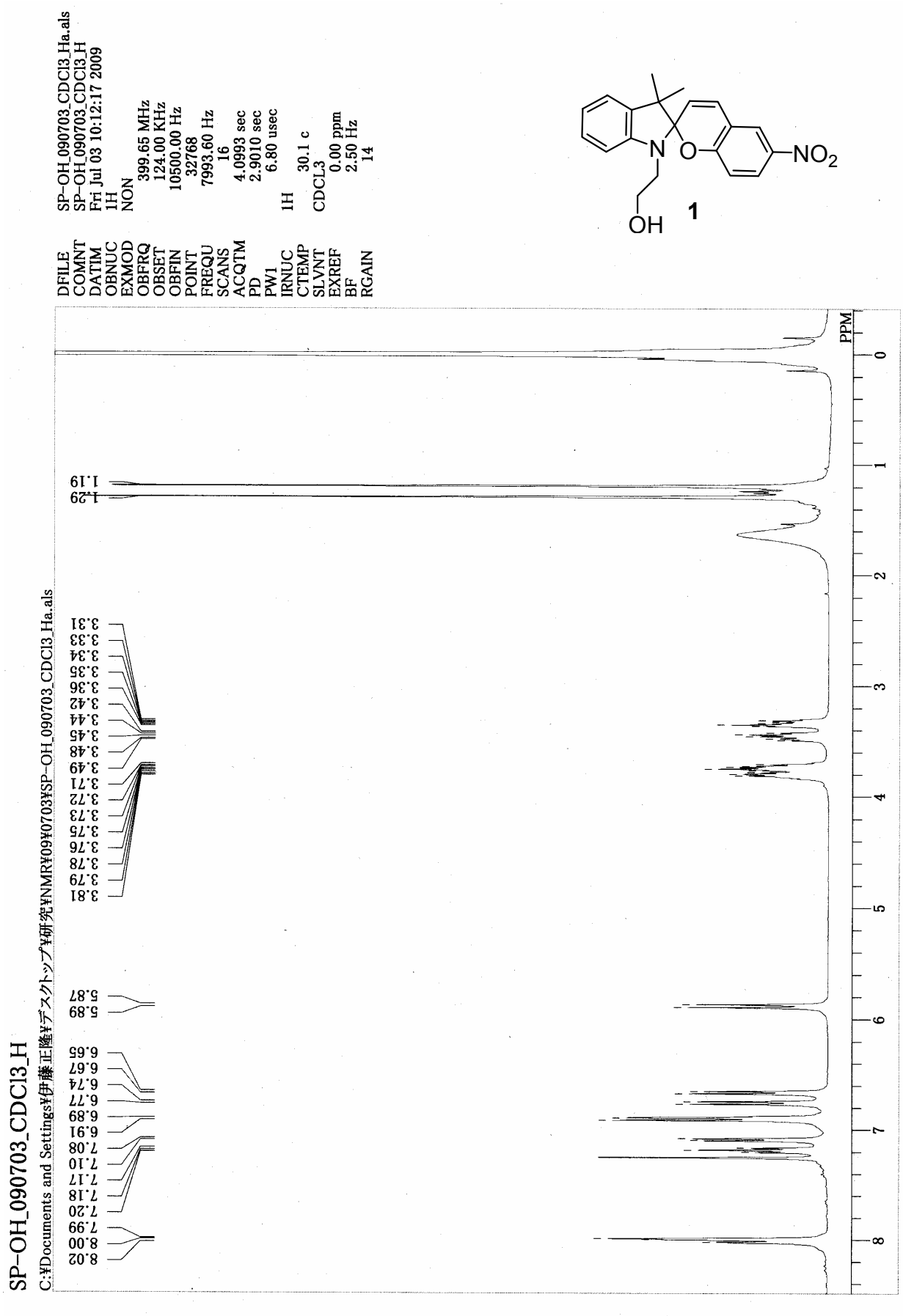


Fig. S1. ^{1}H NMR chart of **1** ($CDCl_3$, 400 MHz).

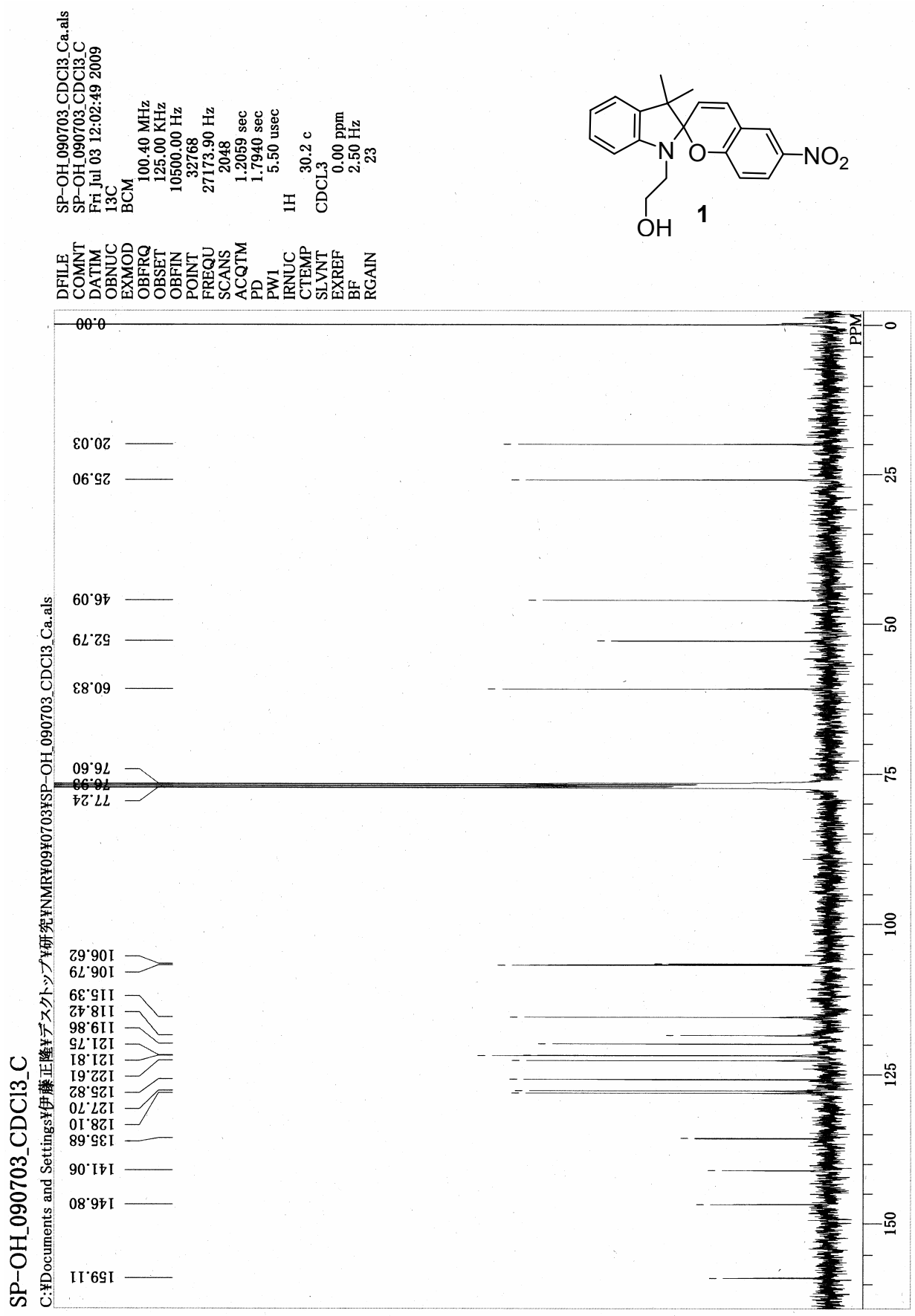


Fig. S2. ^{13}C NMR chart of **1** ($CDCl_3$, 100 MHz).

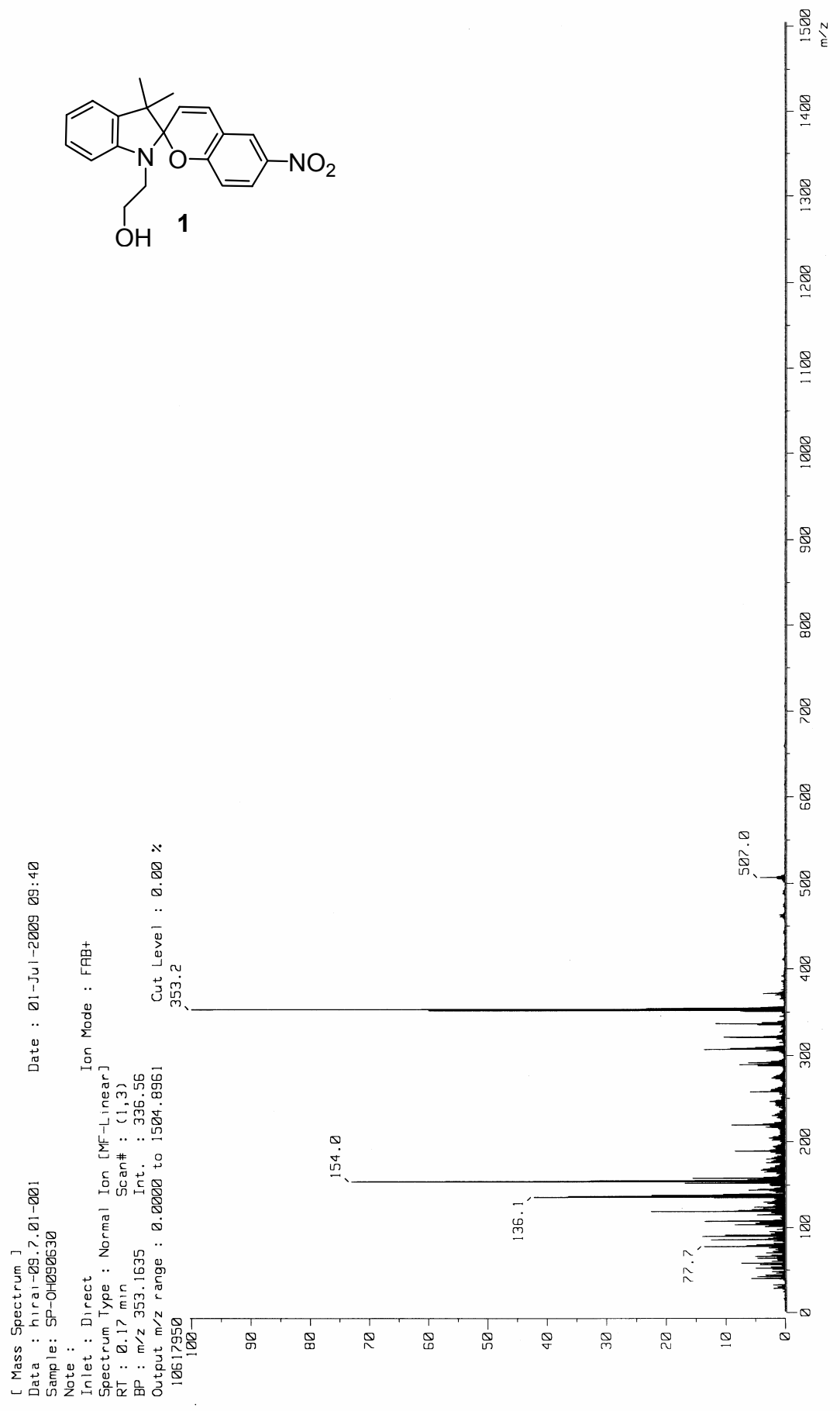


Fig. S3. FAB-MS chart of **1**.

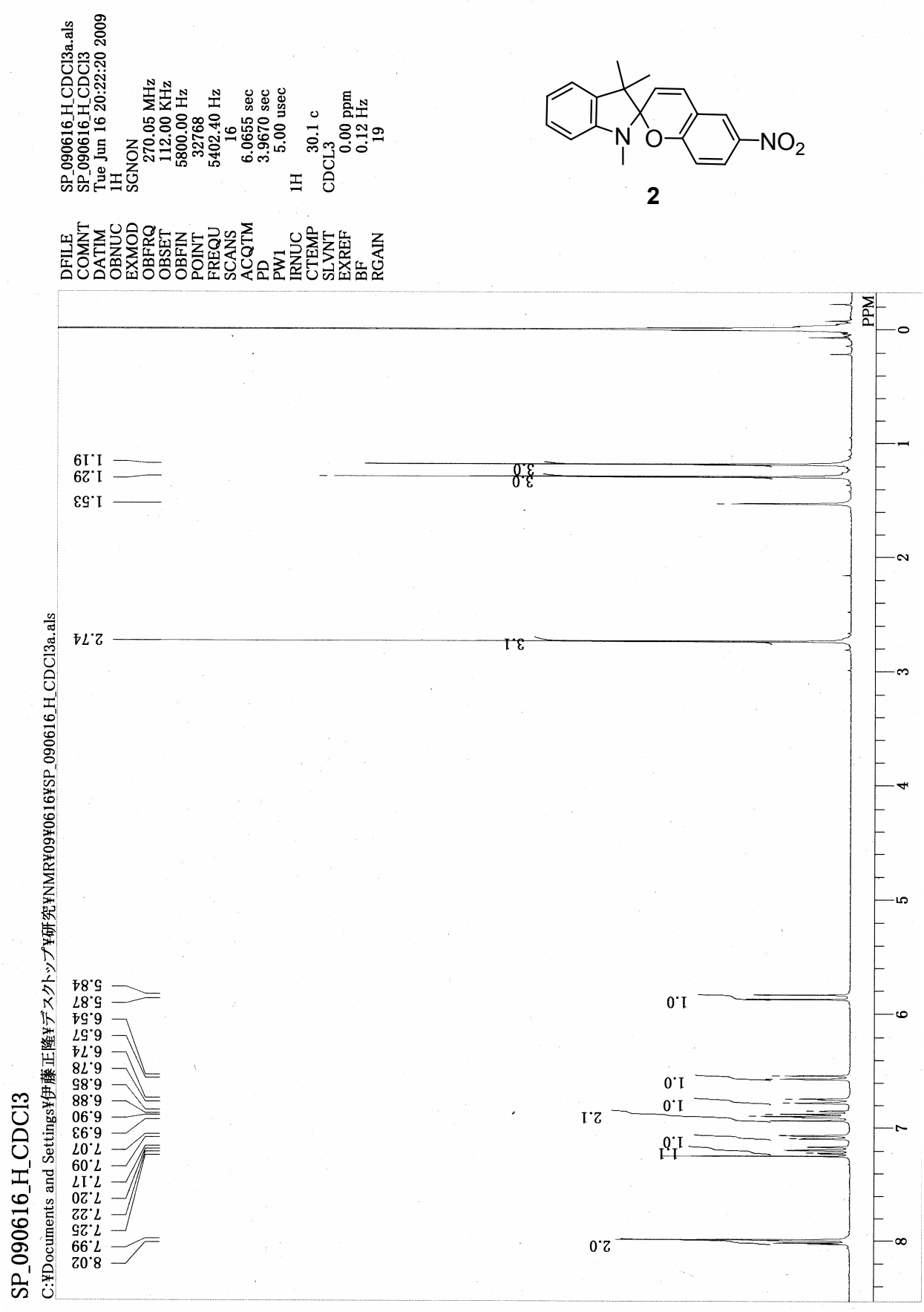


Fig. S4. ^{1}H NMR chart of **2** ($CDCl_3$, 270 MHz).

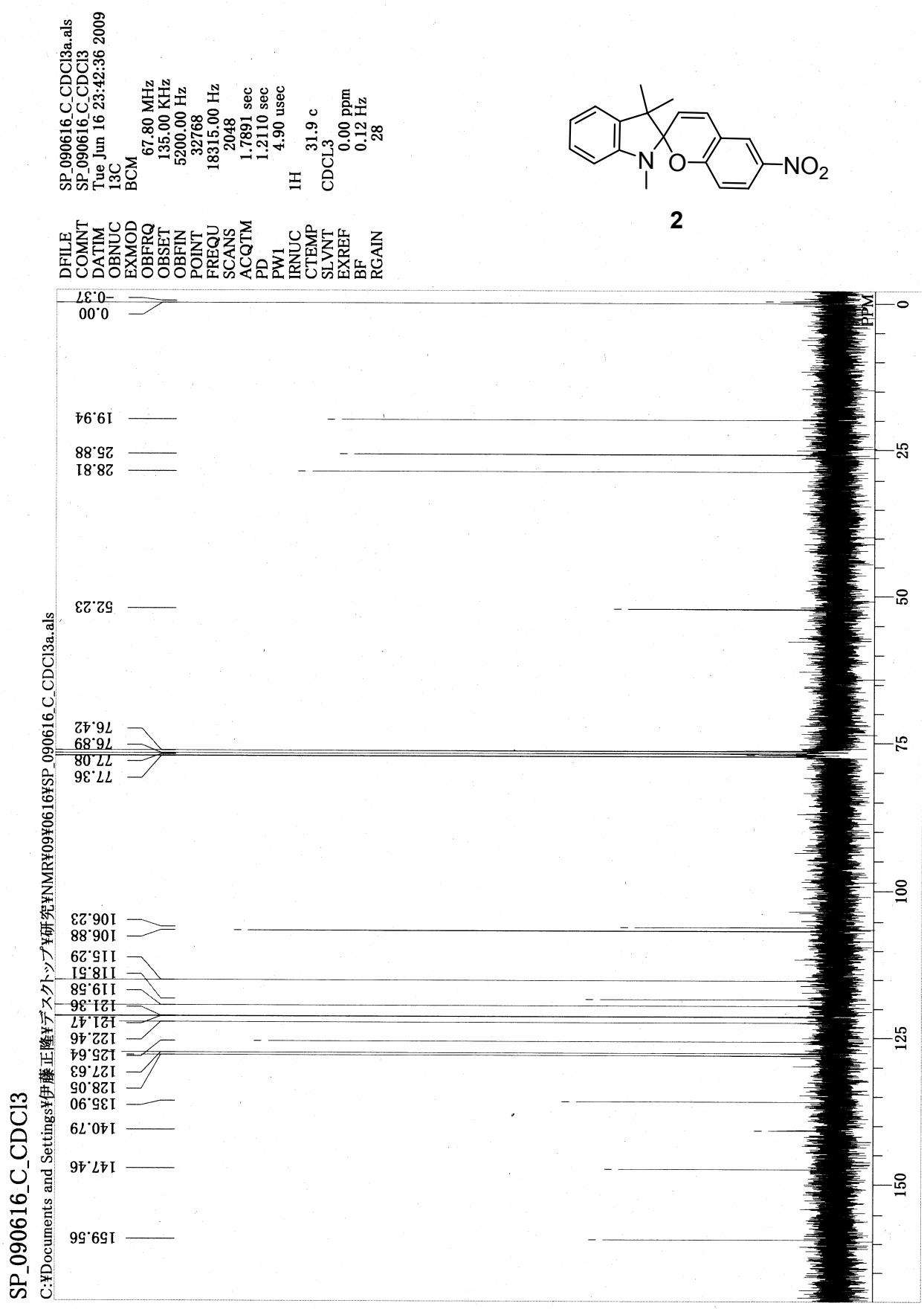
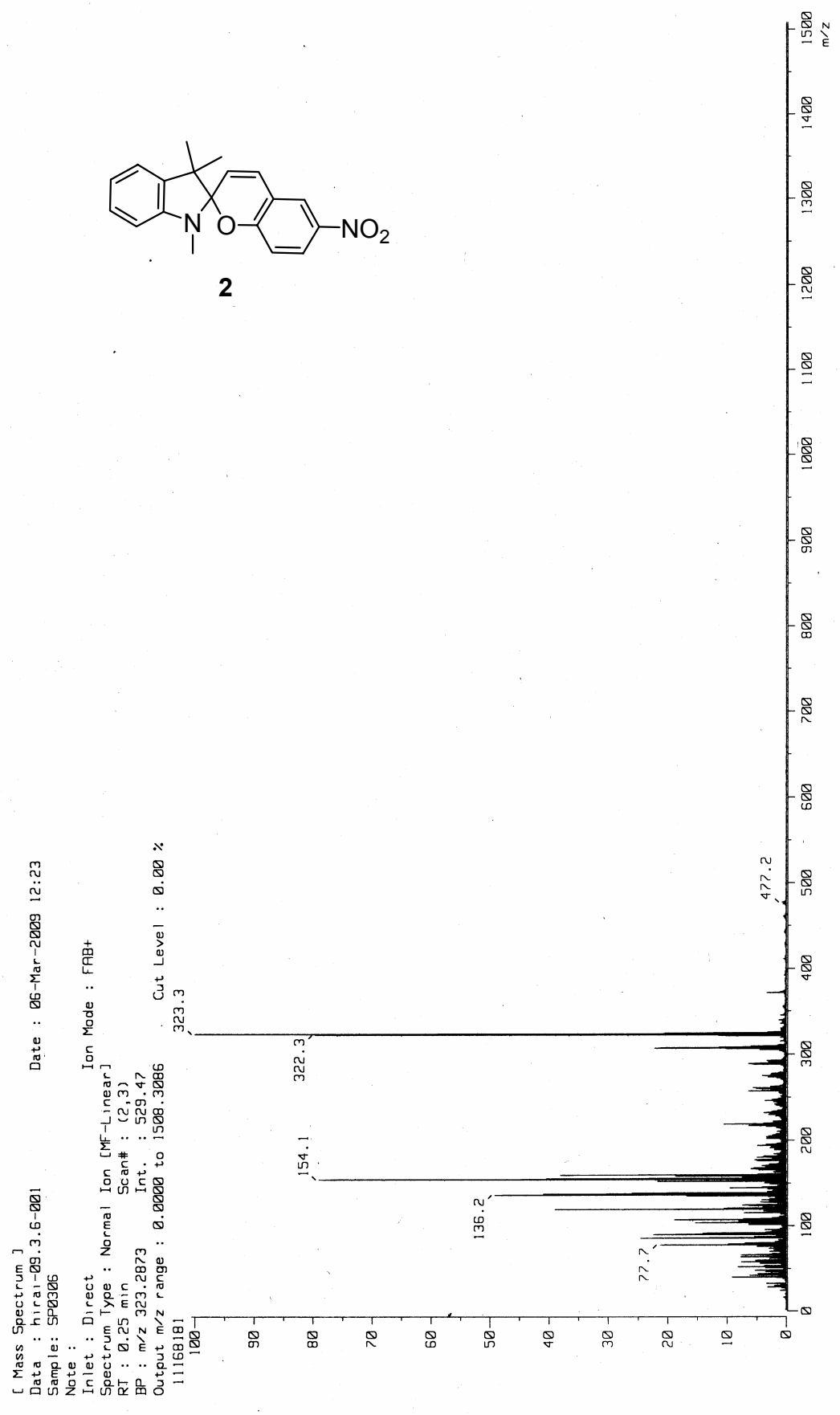


Fig. S5. ^{13}C NMR chart of **2** ($CDCl_3$, 68 MHz).



2

Fig. S6. FAB-MS chart of **2**.

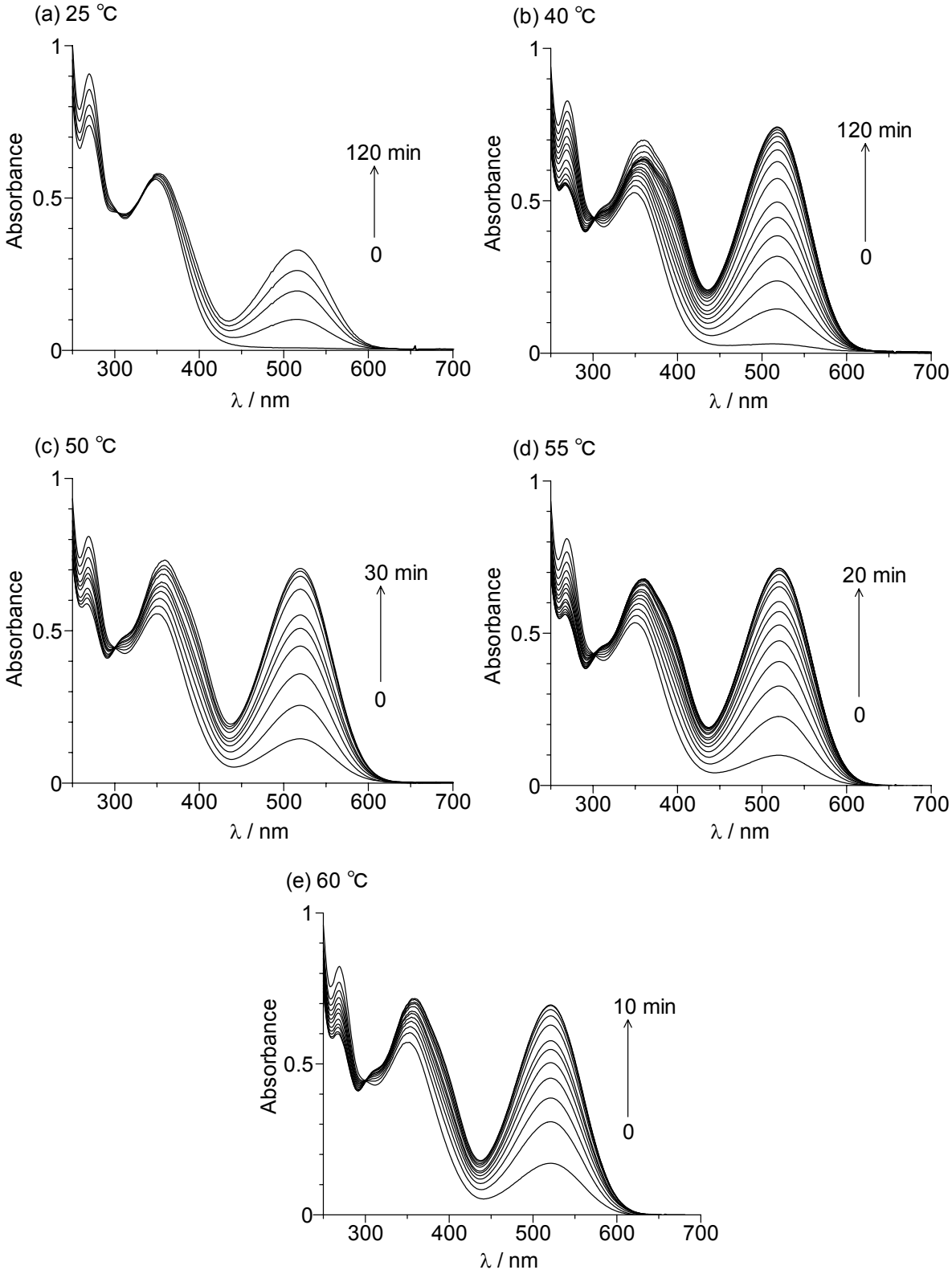


Fig. S7. Time-dependent change in absorption spectra of **1** (50 μM) measured in a water/MeOH (1/1 v/v) mixture at different temperature in the dark.

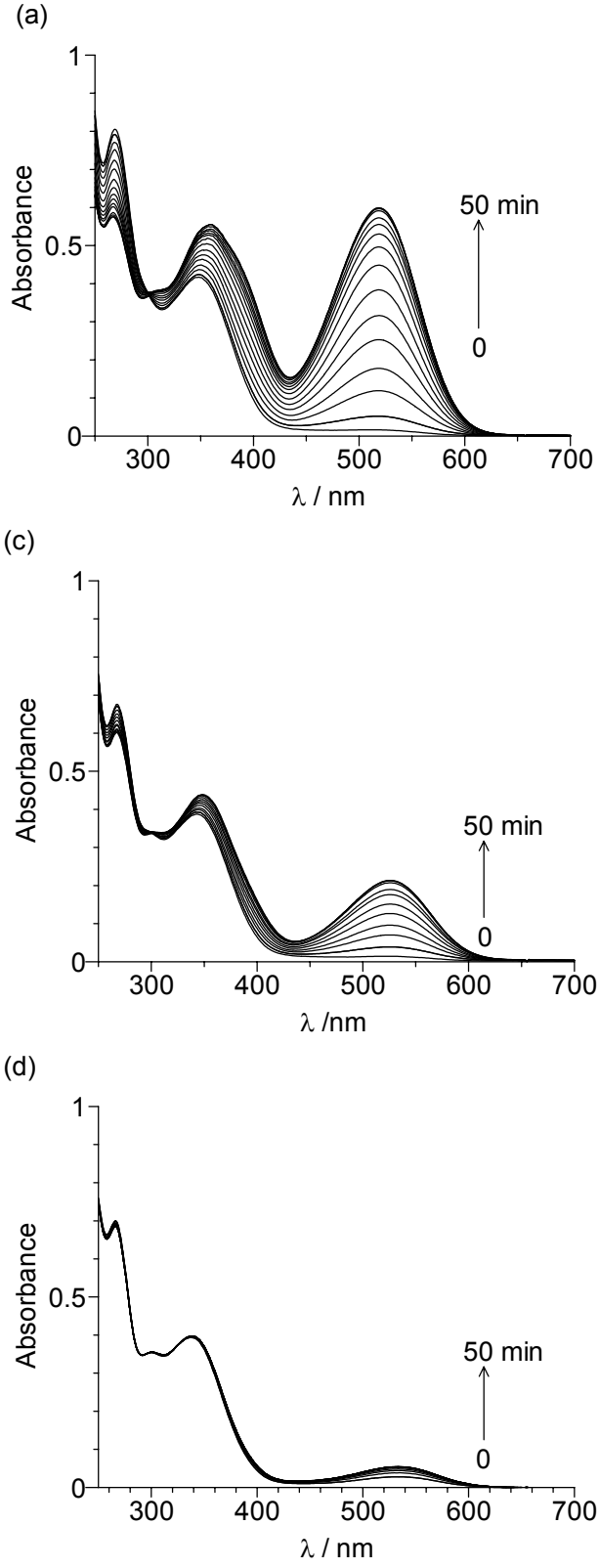


Fig. S8. Time-dependent change in absorption spectra of **1** (50 μM) measured in (a) D_2O/MeOH (1/1 v/v), (c) water/MeOH (1/4 v/v), and (d) MeOH in the dark at 45 °C.

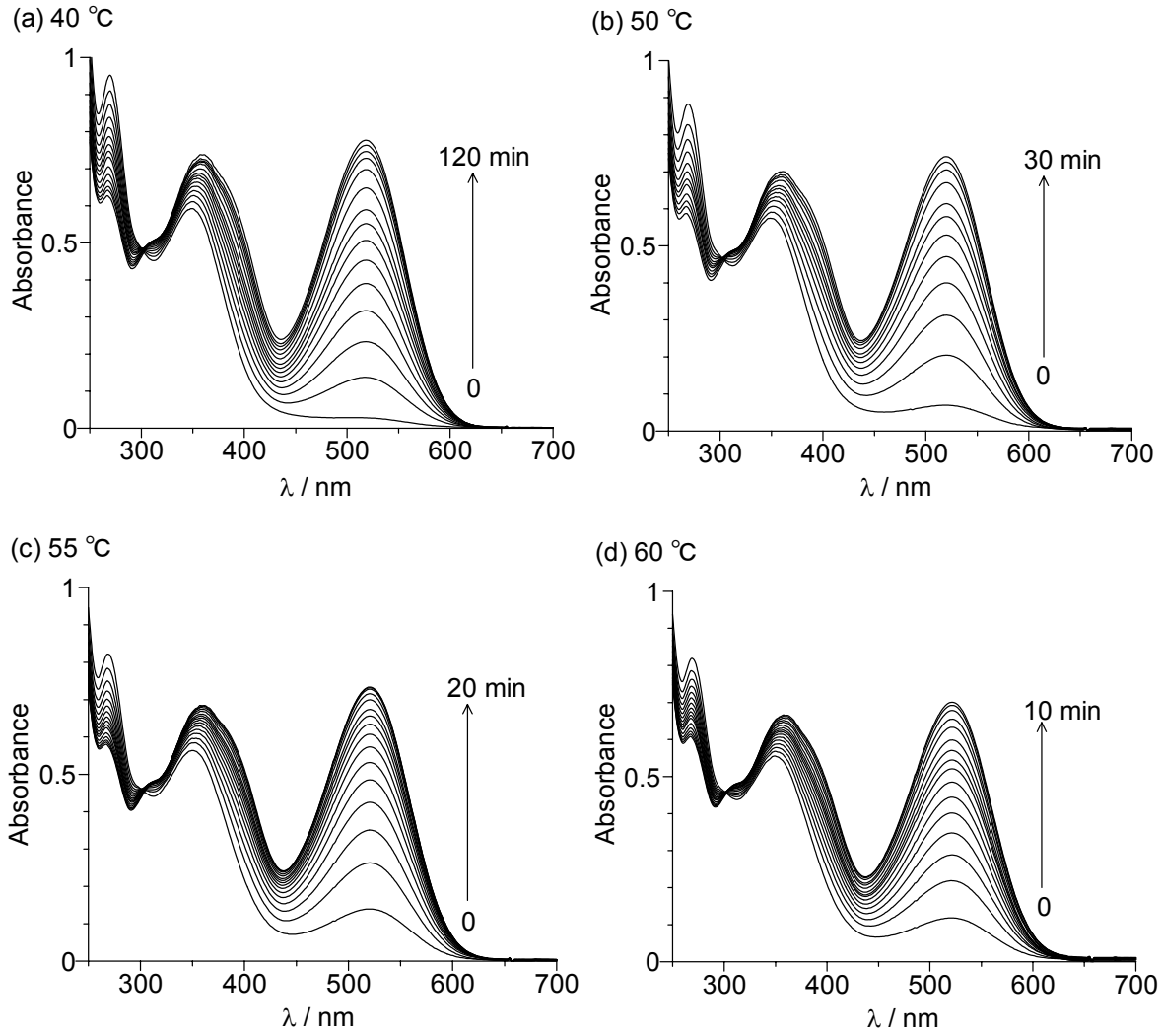


Fig. S9. Time-dependent change in absorption spectra of **1** (50 μM) measured in a D_2O/MeOH (1/1 v/v) mixture at different temperature in the dark.

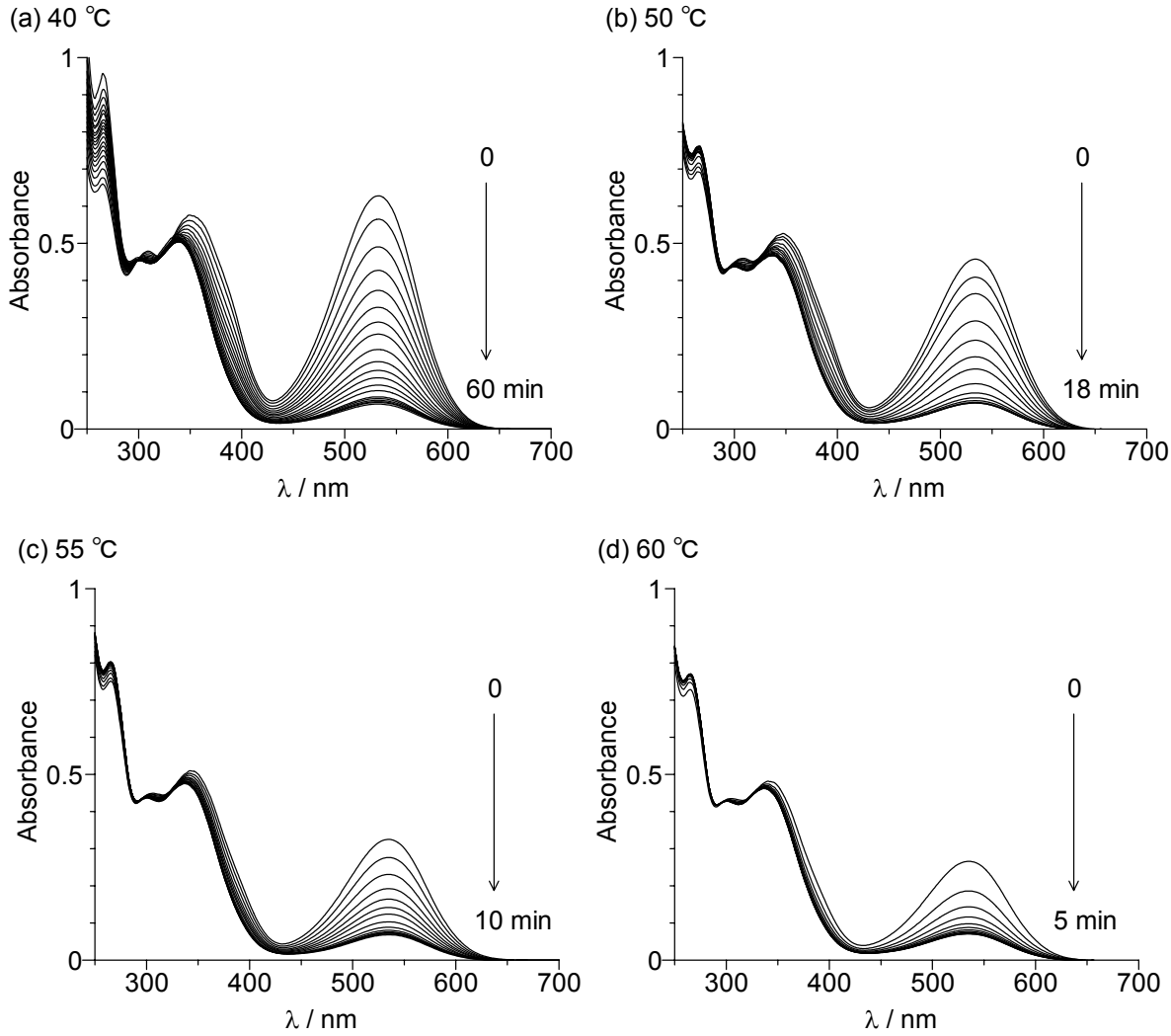


Fig. S10. Time-dependent change in absorption spectra of **1** (50 μM) measured in MeOH at different temperature in the dark. The measurement was carried out after UV irradiation (334 nm) for 15 min at the respective temperature.

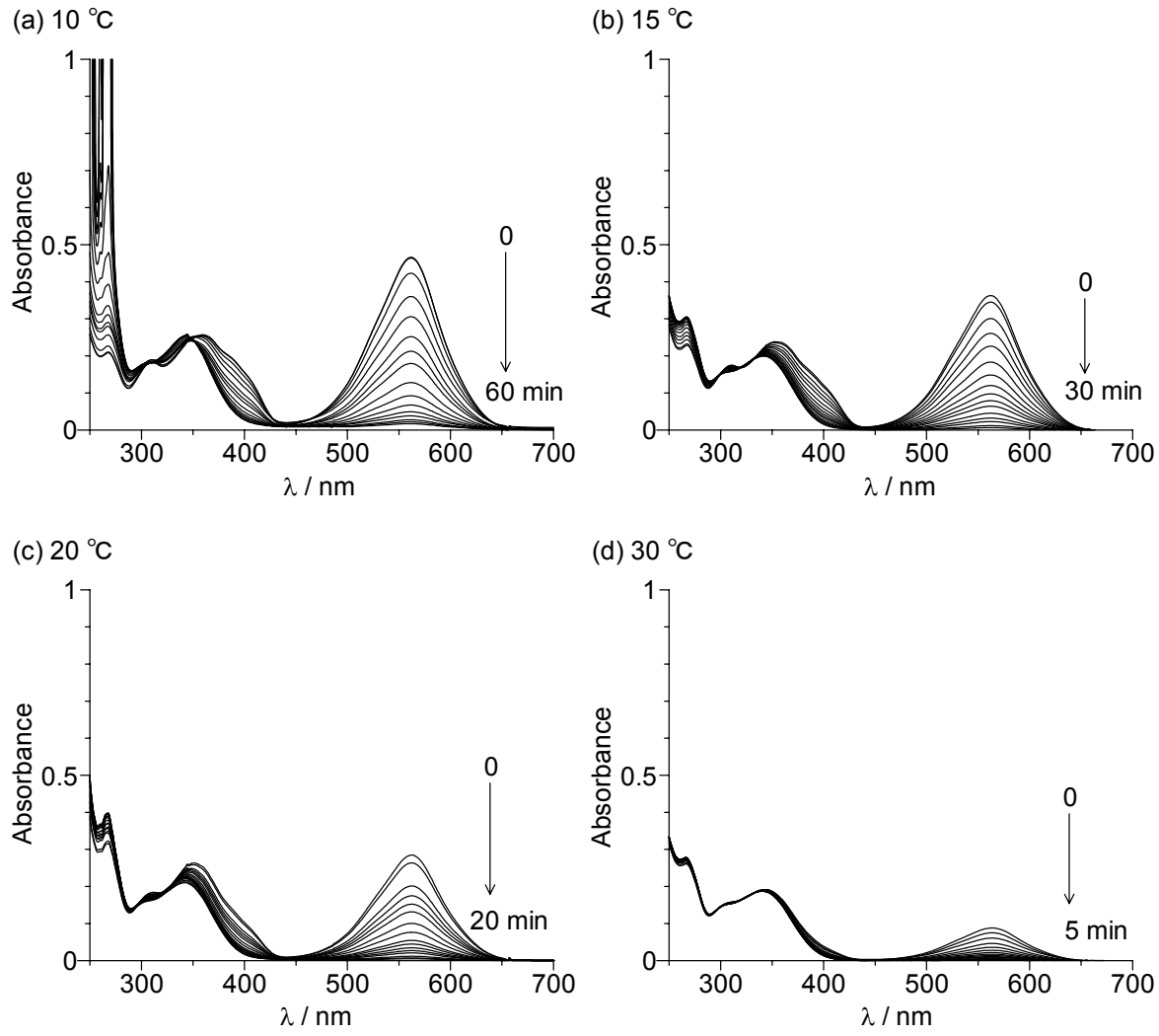


Fig. S11. Time-dependent change in absorption spectra of **1** (50 μM) measured in MeCN at different temperature in the dark. The measurement was carried out after UV irradiation (334 nm) for 15 min at the respective temperature.

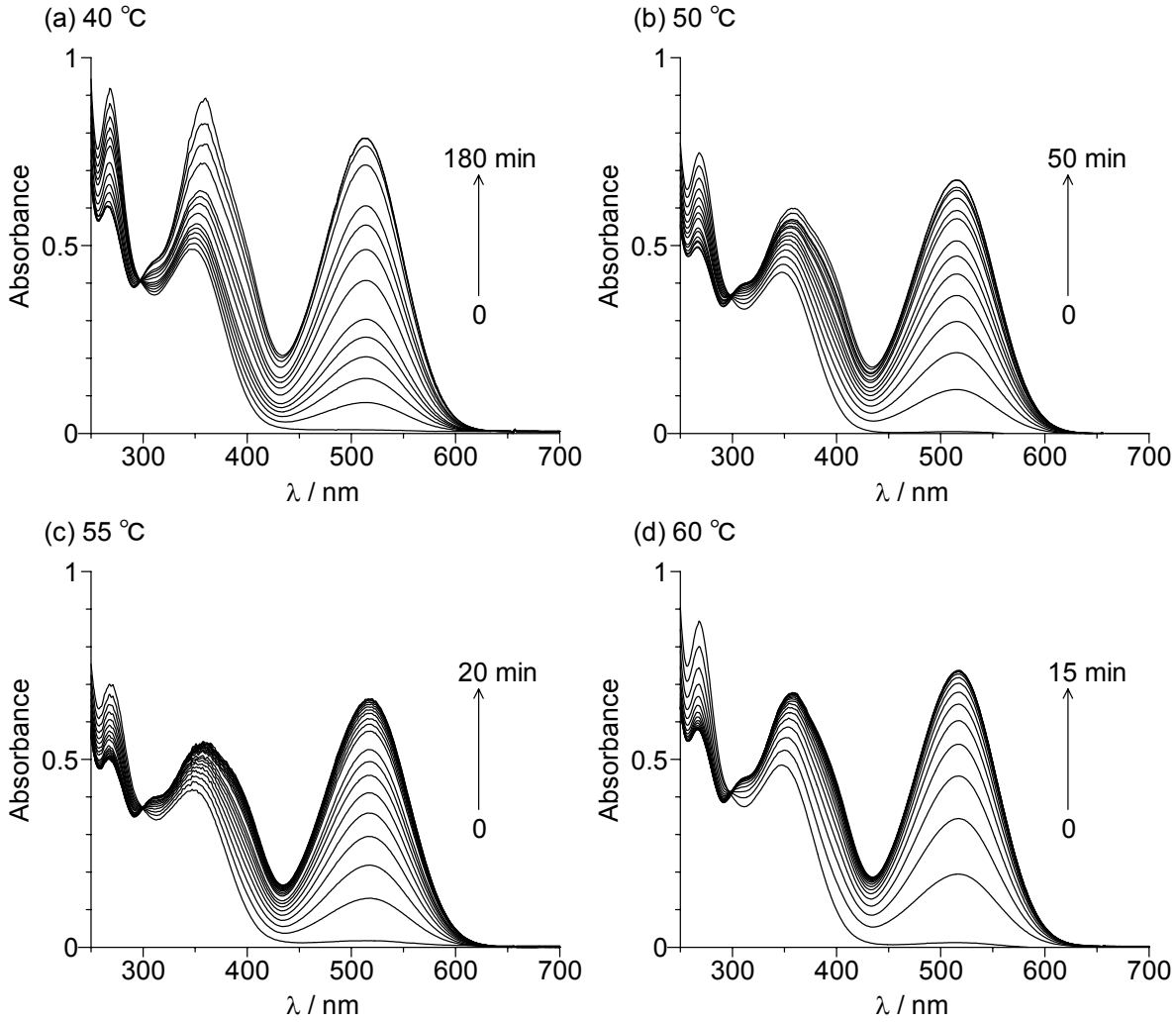


Fig. S12. Time-dependent change in absorption spectra of **2** (50 μM) measured in a D_2O/MeOH (1/1 v/v) mixture at different temperature in the dark.

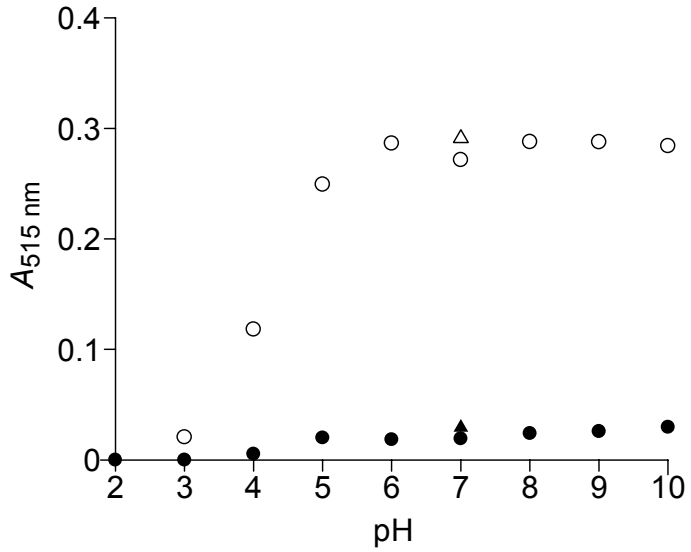


Fig. S13. Effects of pH and NaCl salt on the MC absorbance of **1** (50 μM) measured in a water/MeOH (1/1 v/v) mixture under visible light irradiation with a light intensity, 39.7 mW m^{-2} at different temperature. (closed circle) at 40 °C, (open circle) at 60 °C, (closed triangle) at 40 °C with 100 mM NaCl, and (open triangle) at 60 °C with 100 mM NaCl. The measurements were carried out after 5 min stirring at the designated temperature.