Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

High-Pressure Circular Dichroism Spectroscopy up to 400 MPa Using Polycrystalline Yttrium Aluminum Garnet (YAG) as Pressure-Resistant Optical Windows

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1. General

Circular dichroism (CD) and UV-vis absorption spectra were recorded on a JASCO J-1500 spectrometer. Pressurization experiments were carried out with a high-pressure vessel (PCI-500, Syn Corporation, Kyoto, Japan) and a high-pressure hand pump (HP-500, Syn Corporation, Kyoto, Japan) using water as pressure medium. The SiO_2 glass window (ES grade, diameter = 9.8 mm, thickness = 6.5 mm) was purchased from TOSOH Quartz Corporation. The single crystalline alumina (α-Al_2O_3, sapphire) window (diameter = 9.9 mm, thickness = 7.0 mm) was purchased from Hokushin Koki Co. Ltd. The diamond window (single crystalline diamond type IIa, diameter = 3.5 mm, thickness = 0.5 mm) was purchased from Sumitomo Electric Industries, Ltd. The polycrystalline $Y_3Al_5O_{12}$ (YAG) window (diameter = 10.0 mm, thickness = 0.5, 1.0, and 5.0 mm) was purchased from Konoshima Chemical Co., Ltd. **P1** and **P2** were prepared according to our previous report.[1-3] $CHCl_3$, 1,1,2-trichloroethane (1,1,2-TCE), 1,2-dichloroethane (1,2-DCE), and 1-chlorobutane (1-BuCl) were purchased from the commercial sources and were used without further purification.

2. CD spectra of α-Al_2O_3 window

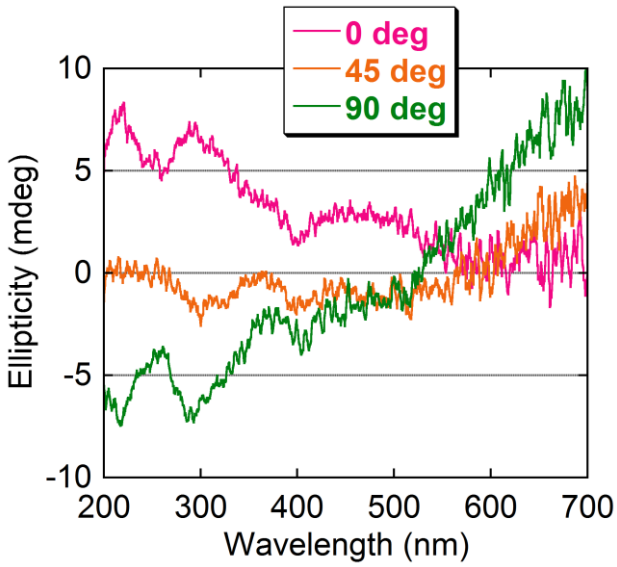

Figure S1. CD spectra of α-Al_2O_3 window with various orientation (0, 45, and 90 deg)

3. Breaking test of polycrystalline YAG windows

A polycrystalline YAG window (thickness = 0.5 or 1.0 mm) was set to a high-pressure vessel (Fig. S2a), which was placed in a water bath for safety (Fig. S2b). The vessel was pressurized by a high-pressure hand pump to burst the YAG window. For the YAG window with 0.5 mm thickness, the pressure change was recorded by a digital pressure sensor (up to 100 MPa, VALCOM Co., Ltd.) and a universal recorder (midi LOGGER GL200A, GRAPHTEC Corporation). For the YAG window with 1.0 mm thickness, the pressure was measured by a pressure gauge (up to 500 MPa, Astra Gauge Corporation) and was recorded as a movie file using a digital camera (23 frame/sec, Nikon D7000).

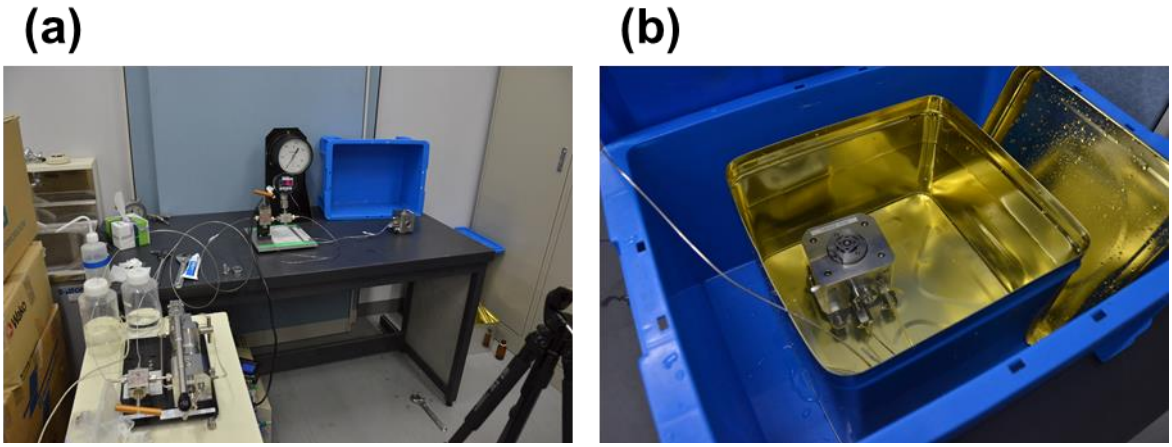

Figure S2. Breaking test of polycrystalline YAG windows. (a) A high-pressure pump, a pressure gauge, and high-pressure cell. (b) The high-pressure cell in water for safety.

4. High-pressure CD and UV-vis measurement

General procedure: A polymer was dissolved in solvent (ca. 0.1 g/L) to enclose a quartz inner cell (volume = 300 μL, light path length = 2 mm) with a diaphragm tube. The inner cell was placed in a high-pressure vessel with polycrystalline YAG windows to be pressurized by a high-pressure hand pump using water as pressure medium. The high-pressure vessel was set in JASCO J-1500 spectrometer to measure CD and UV-vis spectra.

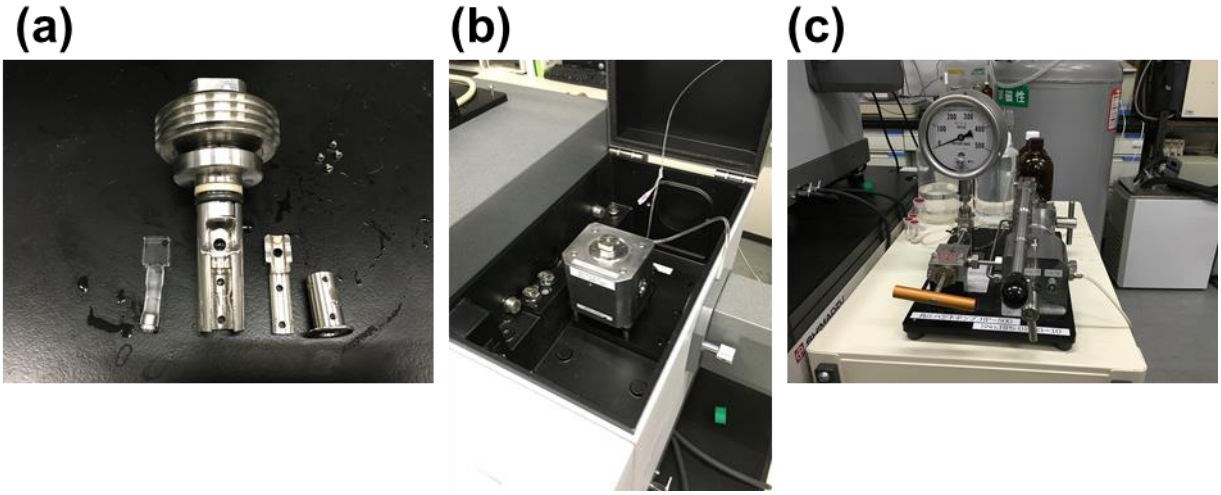

Figure S3. Photographs of (a) a quartz inner cell and a cell holder (b) a high-pressure vessel with YAG windows in a CD spectrometer (JASCO, J-1500) (c) a high-pressure hand pump with a pressure gauge (up to 500 MPa).

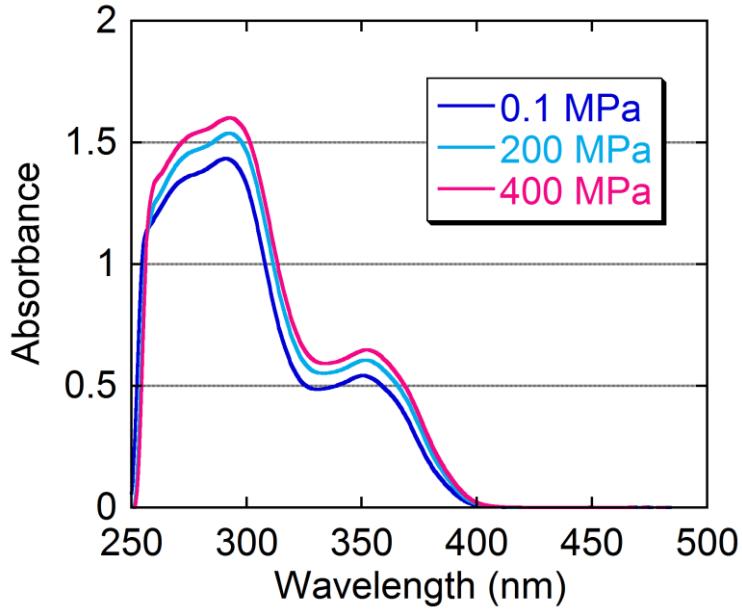

Figure S4. UV-vis absorption spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 20/80) at 0.1, 100, and 200 MPa (13.1×10^{-2} g/L, light path length = 2.0 mm).

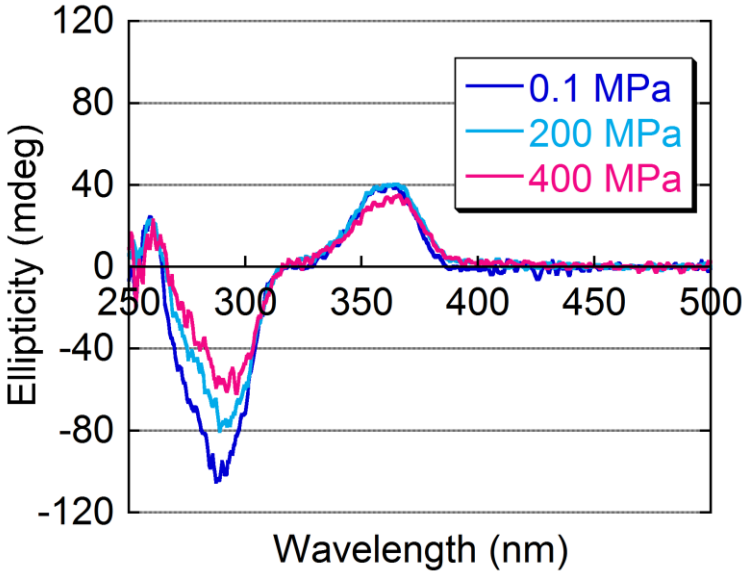

Figure S5. CD spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 20/80) at 0.1, 100, and 200 MPa (13.1×10^{-2} g/L, light path length = 2.0 mm).

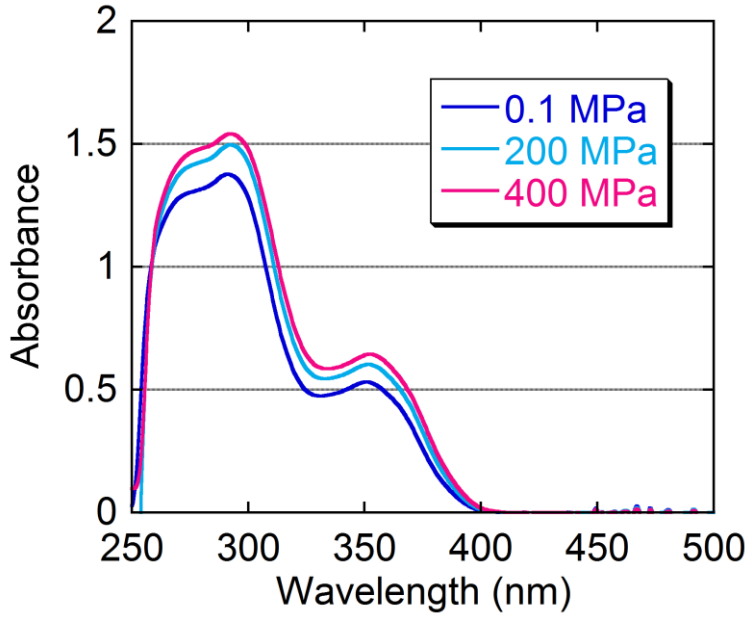

Figure S6. UV-vis absorption spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 30/70) at 0.1, 100, and 200 MPa (12.9×10^{-2} g/L, light path length = 2.0 mm).

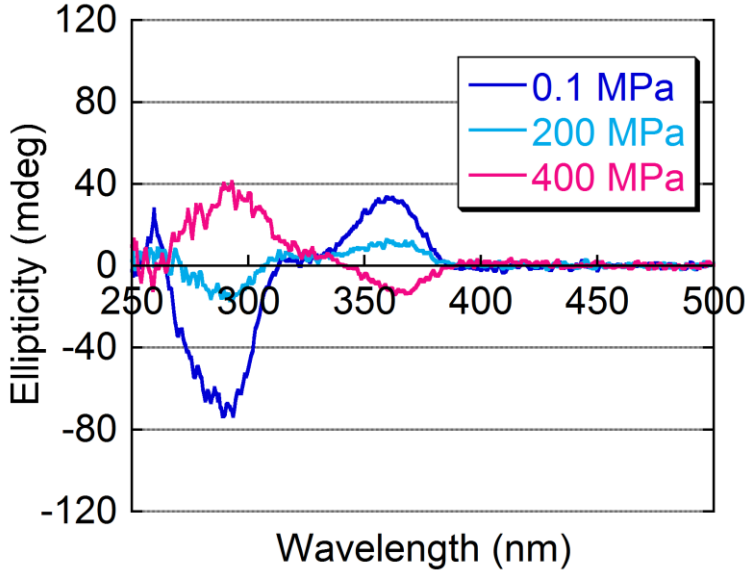

Figure S7. CD spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 30/70) at 0.1, 100, and 200 MPa (12.9×10^{-2} g/L, light path length = 2.0 mm).

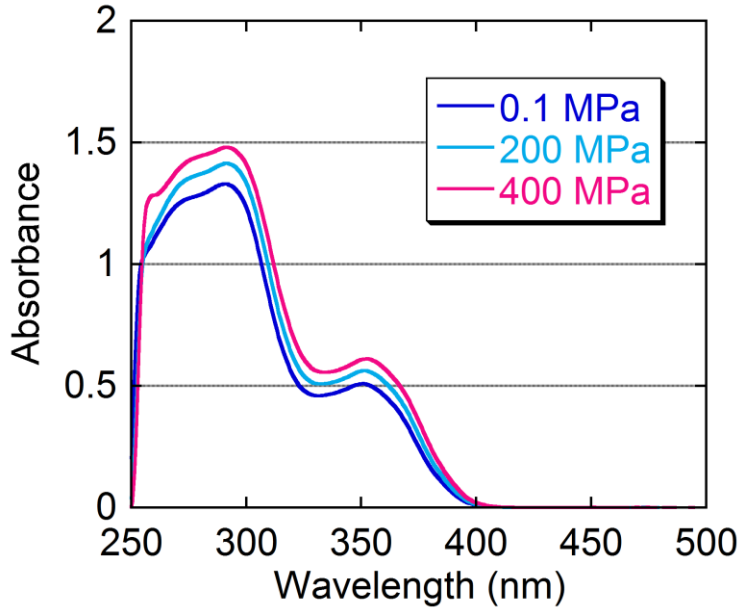

Figure S8. UV-vis absorption spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 35/65) at 0.1, 100, and 200 MPa (11.7×10^{-2} g/L, light path length = 2.0 mm).

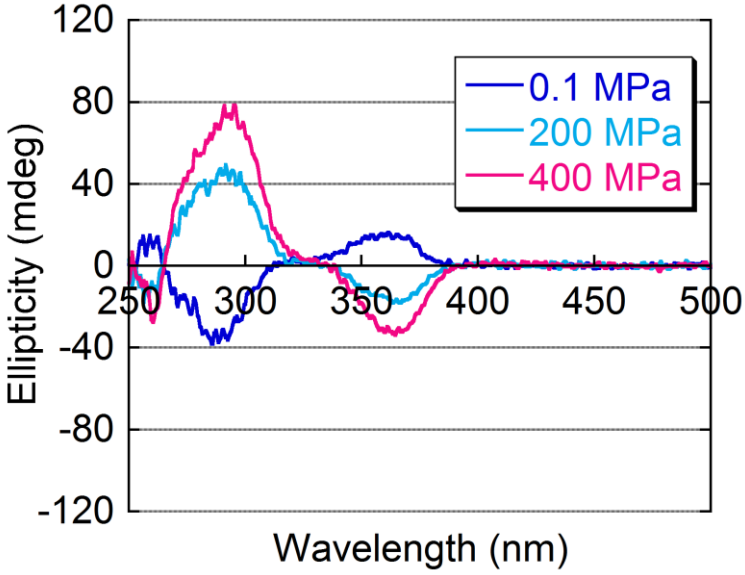

Figure S9. CD spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 35/65) at 0.1, 100, and 200 MPa (11.7×10^{-2} g/L, light path length = 2.0 mm).

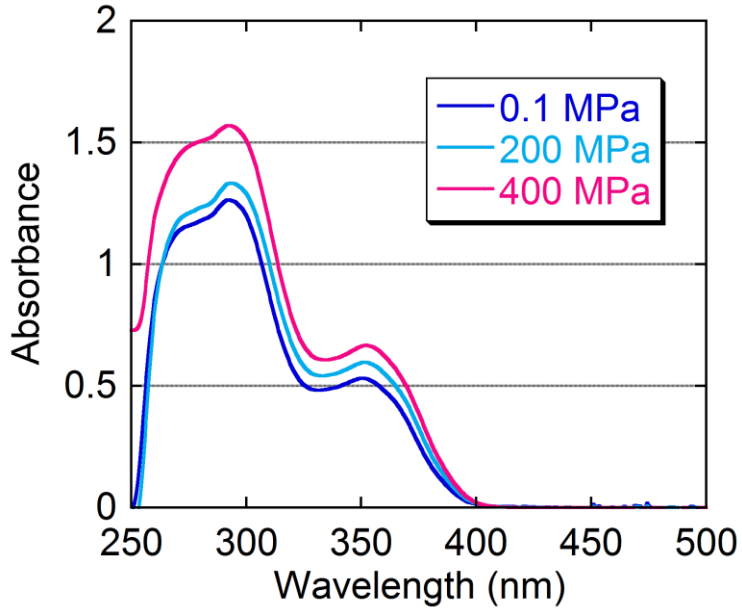

Figure S10. UV-vis absorption spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 40/60) at 0.1, 100, and 200 MPa (11.7×10^{-2} g/L, light path length = 2.0 mm).

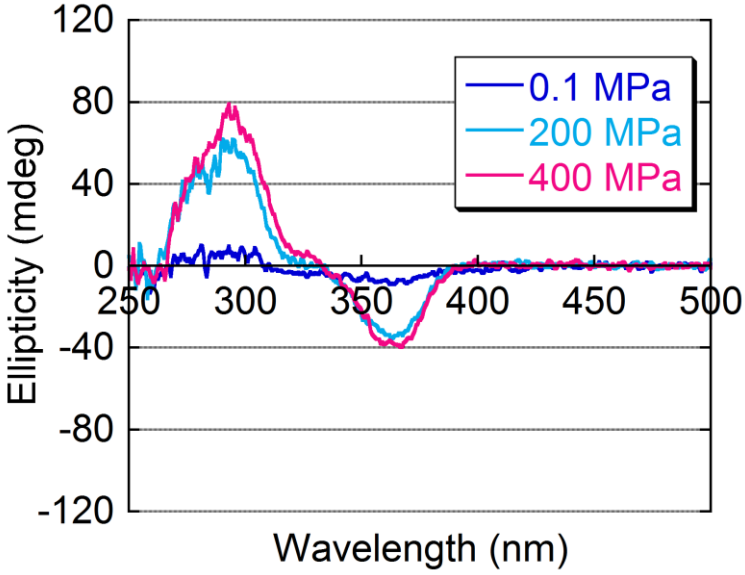

Figure S11. CD spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 40/60) at 0.1, 100, and 200 MPa (11.7×10^{-2} g/L, light path length = 2.0 mm).

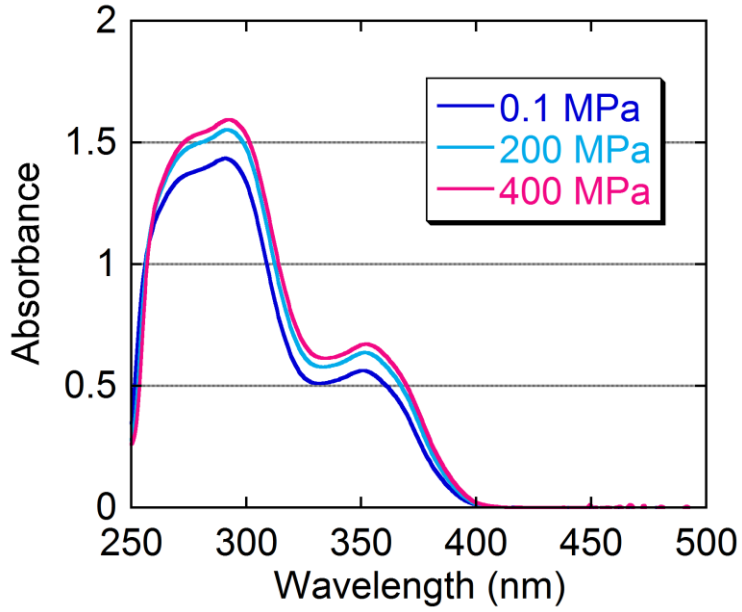

Figure S12. UV-vis absorption spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 50/50) at 0.1, 100, and 200 MPa (13.8×10^{-2} g/L, light path length = 2.0 mm).

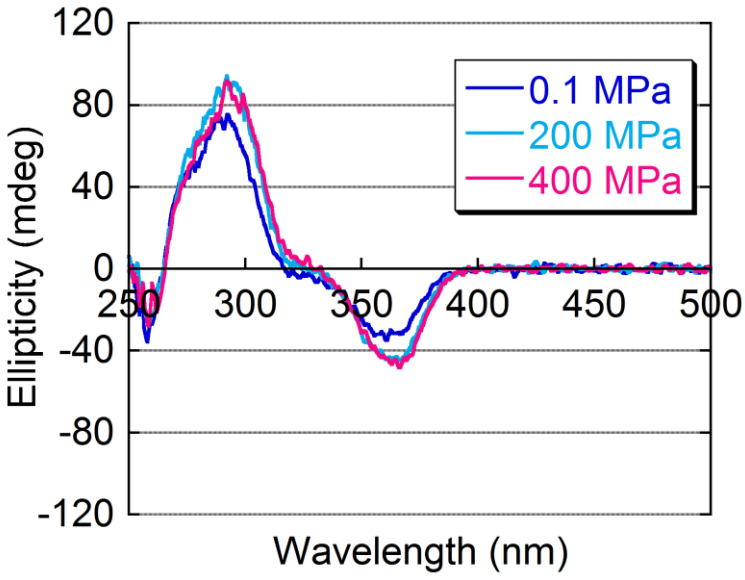

Figure S13. CD spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 50/50) at 0.1, 100, and 200 MPa (13.8×10^{-2} g/L, light path length = 2.0 mm).

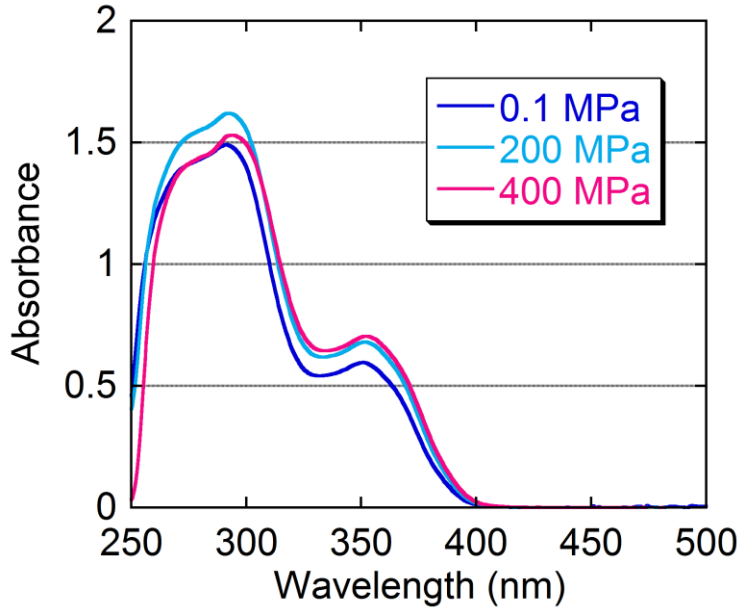

Figure S14. UV-vis absorption spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 60/40) at 0.1, 100, and 200 MPa (13.3×10^{-2} g/L, light path length = 2.0 mm).

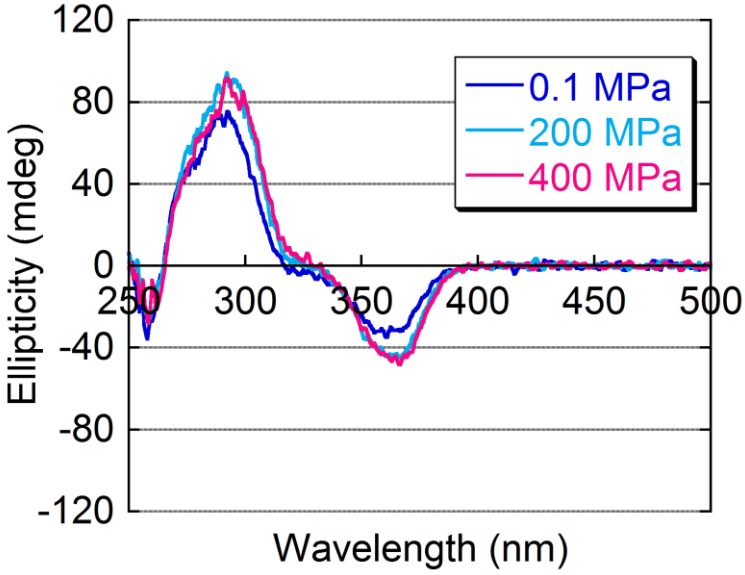

Figure S15. CD spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 60/40) at 0.1, 100, and 200 MPa (13.3×10^{-2} g/L, light path length = 2.0 mm).

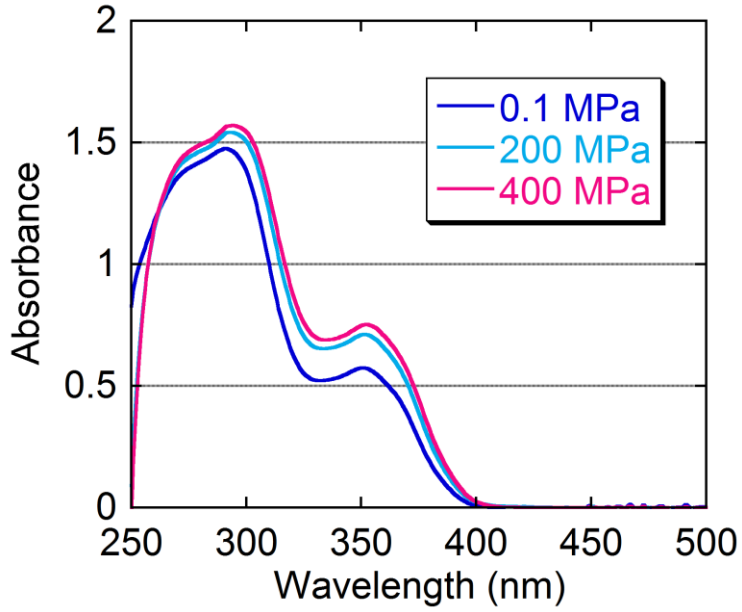

Figure S16. UV-vis absorption spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 80/20) at 0.1, 100, and 200 MPa (13.3 × 10^{-2} g/L, light path length = 2.0 mm).

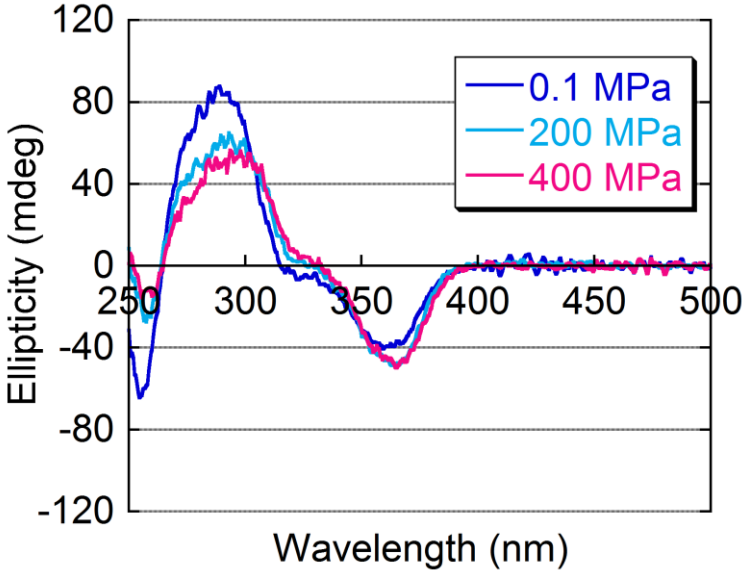

Figure S17. CD spectra of **1** in $CHCl_3$/1,1,2-TCE (v/v = 80/20) at 0.1, 100, and 200 MPa (13.3× 10^{-2} g/L, light path length = 2.0 mm).

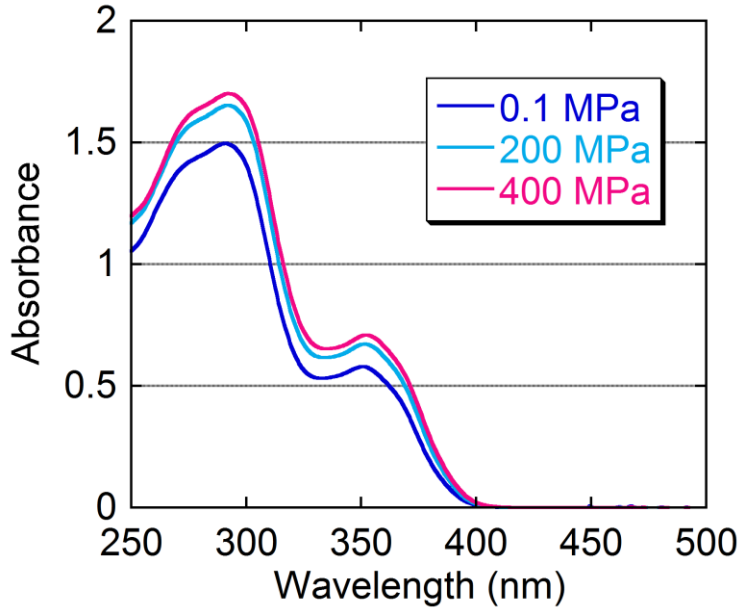

Figure S18. UV-vis absorption spectra of **1** in $CHCl_3$ at 0.1, 100, and 200 MPa (13.8×10^{-2} g/L, light path length = 2.0 mm).

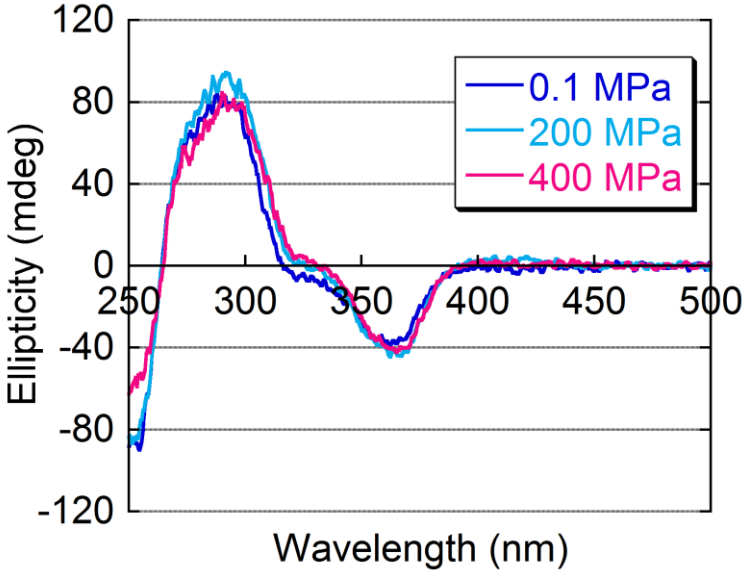

Figure S19. CD spectra of **1** in $CHCl_3$ at 0.1, 100, and 200 MPa (13.8×10^{-2} g/L, light path length = 2.0 mm).

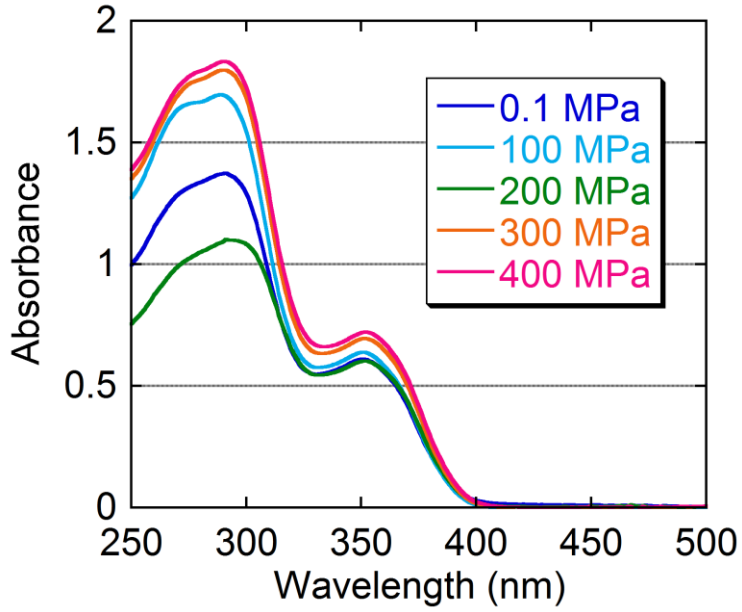

Figure S20. UV-vis absorption spectra of **1** in 1-BuCl at 0.1 to 400 MPa (13.9×10^{-2} g/L, light path length = 2.0 mm).

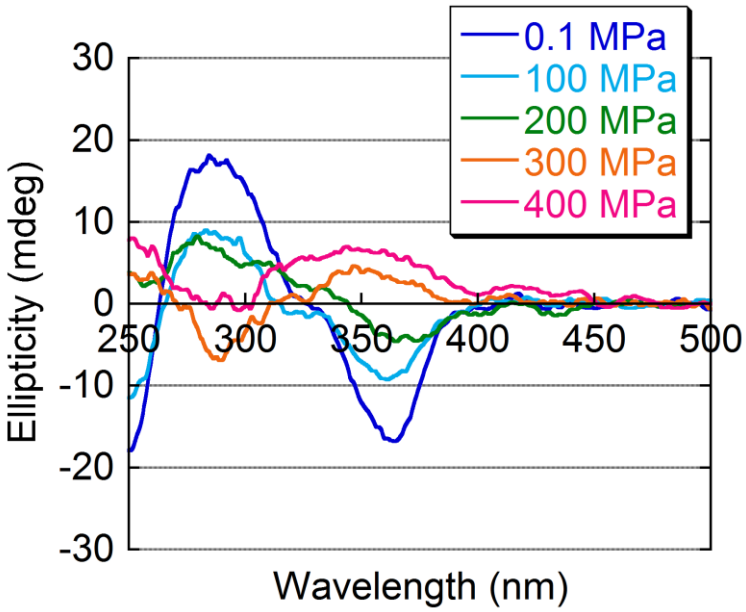

Figure S21. CD spectra of **1** of **1** in 1-BuCl at 0.1 to 400 MPa (13.9×10^{-2} g/L, light path length = 2.0 mm).

4. References

1. Yamada, T; Nagata, Y.; Suginome, M. *Chem. Commun.* **2010**, *46*, 4914-4916.
2. Nagata, Y.; Yamada, T.; Adachi, T.; Akai, Y.; Yamamoto, T.; Suginome, M. *J. Am. Chem. Soc.*, **2013**, *135*, 10104.
3. Nagata, Y.; Takeda, R.; Suginome, M. *Chem. Commun.* **2015**, *51*, 11182-11185.