Supporting Information

Pressure-Driven, Solvation-Directed Planar Chirality Switching of Cyclophano-Pillar[5]arenes (Molecular Universal Joints)

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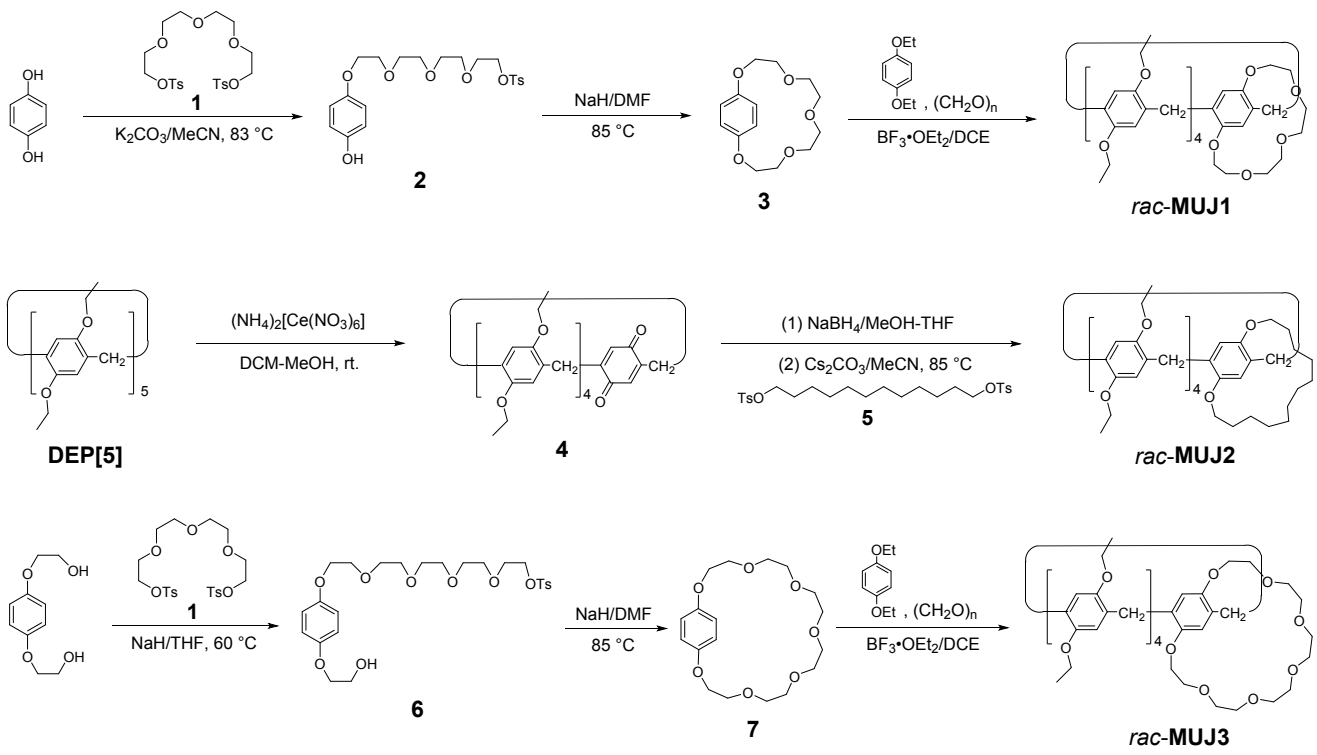
1. Synthesis



Scheme S1 Syntheses of **MUJ1**, **MUJ2**, and **MUJ3**.

2. Chiral HPLC Traces of Racemic and Optically Resolved MUJs

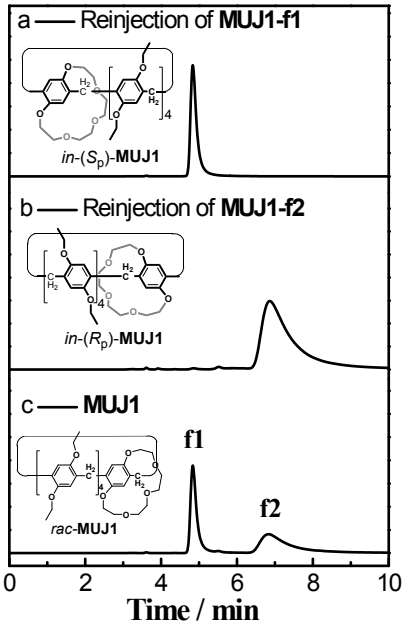


Fig. S1 Chiral HPLC chromatograms (*n*-H:THF = 9:1) for (a) *in*-(S_p)-**MUJ1** (the first fraction), (b) *in*-(R_p)-**MUJ1** (the second fraction), and (c) *rac*-**MUJ1** as prepared.

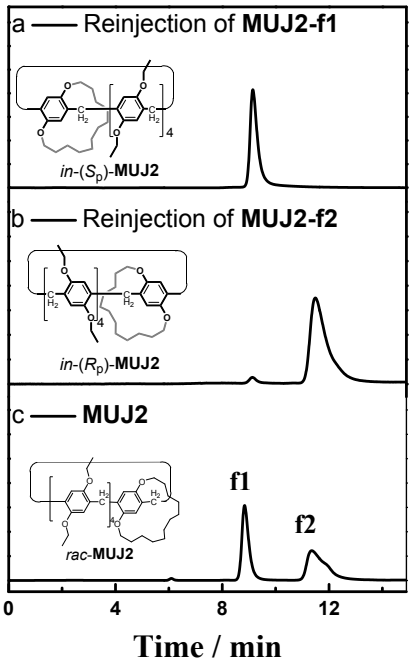


Fig. S2 Chiral HPLC chromatograms (*n*-H:DCM = 9:1) for (a) *in*-(S_p)-**MUJ2** (the first fraction), (b) *in*-(R_p)-**MUJ2** (the second fraction), and (c) *rac*-**MUJ2**.

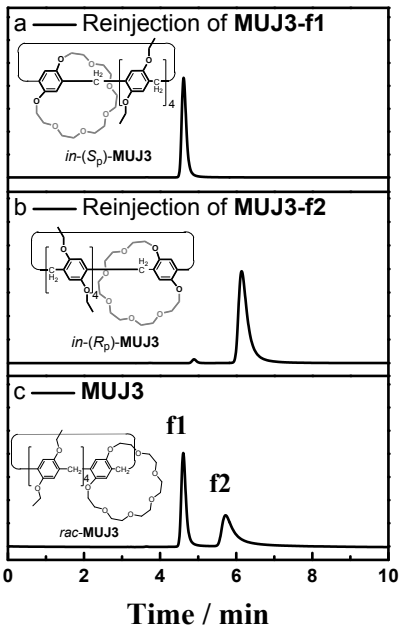


Fig. S3 Chiral HPLC chromatograms (*n*-H:THF = 9:1) for (a) *in*-(S_p)-**MUJ3** (the first fraction), (b) *in*-(R_p)-**MUJ3** (the second fraction), and (c) *rac*-**MUJ3**.

3. Pressure-Dependent CD and UV-vis Spectra of *in*-(R_p)/*out*-(S_p)-MUJs

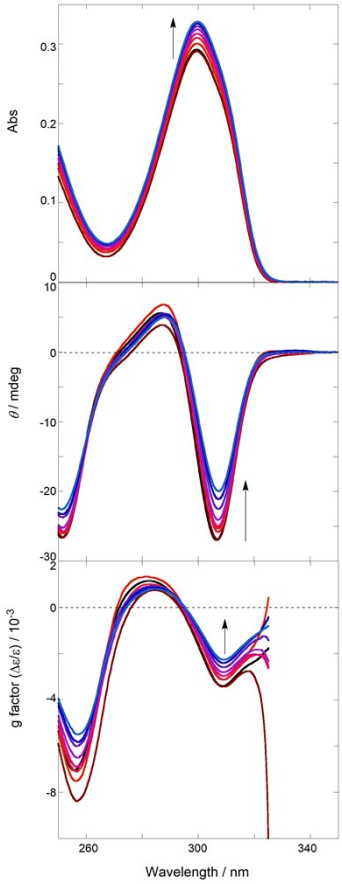


Fig. S4 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (104 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in AN at room temperature, measured in a high-pressure cell.

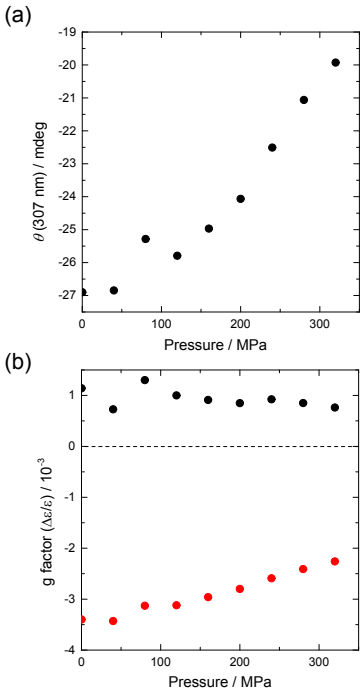


Fig. S5 Plots of (a) ellipticity changes at 307 nm and (b) anisotropy changes at 283 (black) and 309 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ1** in AN as a function of pressure.

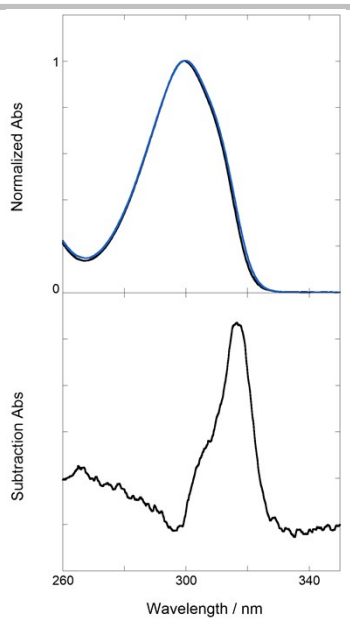


Fig. S6 Normalized UV/vis (normalized at 299 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (104 μM) at 0.1 (black) and 320 MPa (light blue) in AN at room temperature, measured in a high-pressure cell.

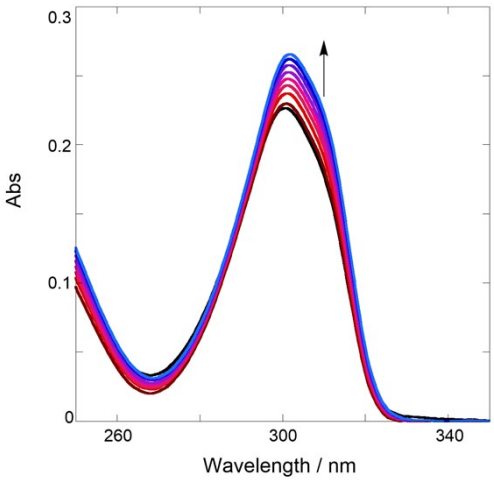


Fig. S7 UV/vis (top) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (92 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in AN at room temperature, measured in a high-pressure cell.

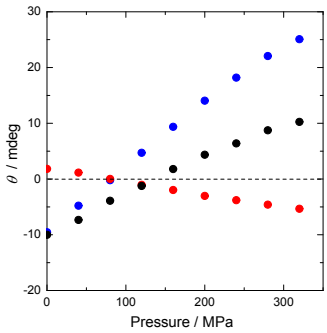


Fig. S8 Plots of ellipticity changes at 309 (blue), 290 (red), and 254 nm (black) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in AN as a function of pressure.

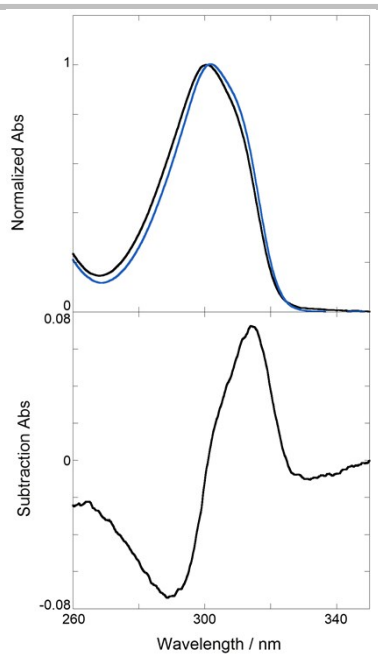


Fig. S9 Normalized UV/vis (normalized at 301 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (92 μM) at 0.1 (black) and 320 MPa (light blue) in AN at room temperature, measured in a high-pressure cell.

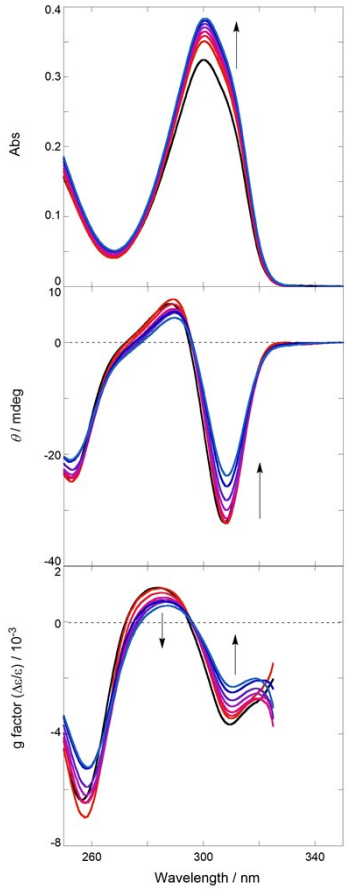


Fig. S10 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (98 μM) at 0.1, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in AN at room temperature, measured in a high-pressure cell.

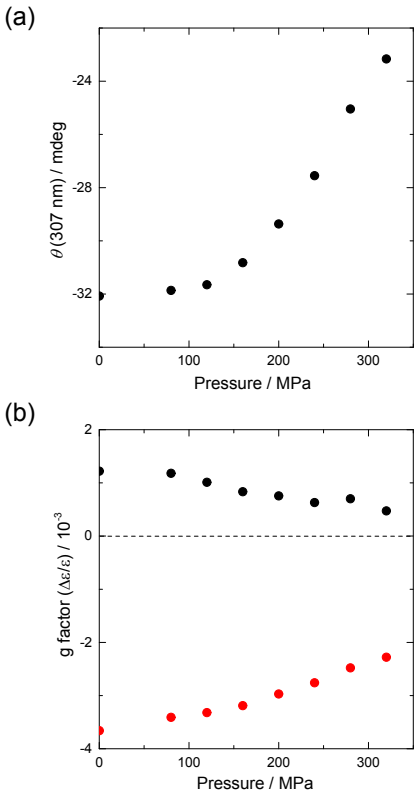


Fig. S11 Plots of (a) ellipticity changes at 307 nm and (b) anisotropy changes at 283 (black) and 309 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ3** in AN as a function of pressure.

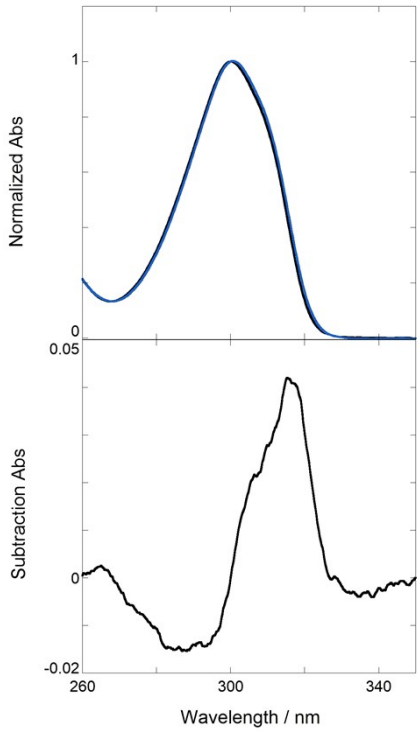


Fig. S12 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (98 μM) at 0.1 (black) and 320 MPa (light blue) in AN at room temperature, measured in a high-pressure cell.

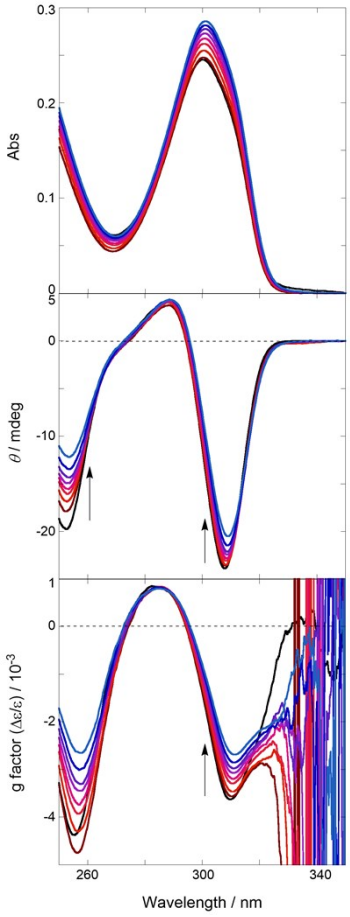


Fig. S13 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (84 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in DCM at room temperature, measured in a high-pressure cell.

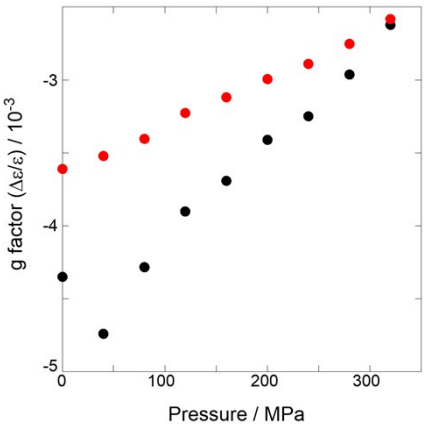


Fig. S14 Plots of anisotropy changes at 256 (black) and 309 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ1** in DCM as a function of pressure.

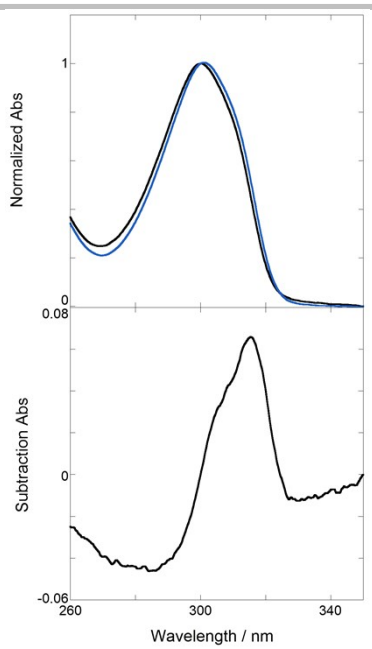


Fig. S15 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (84 μM) at 0.1 (black) and 320 MPa (light blue) in DCM at room temperature, measured in a high-pressure cell.

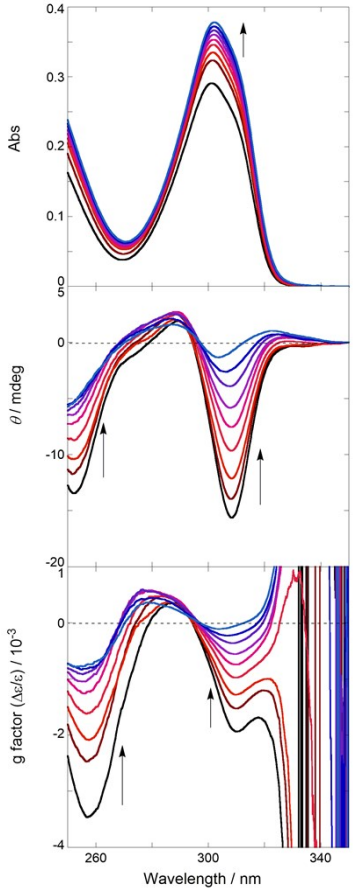


Fig. S16 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (90 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in DCM at room temperature, measured in a high-pressure cell.

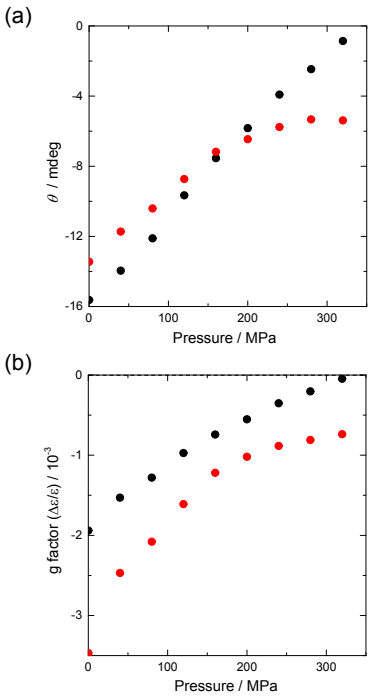


Fig. S17 Plots of (a) ellipticity changes at 308 (black) and 252 nm (red) and (b) anisotropy changes at 310 (black) and 257 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in DCM as a function of pressure.

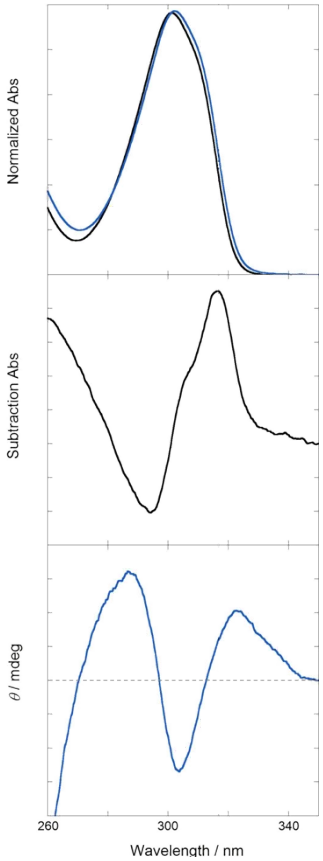


Fig. S18 Normalized UV/vis (top), subtraction UV (middle), and CD spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (90 μM) at 0.1 (black) and 320 MPa (light blue) in DCM at room temperature, measured in a high-pressure cell.

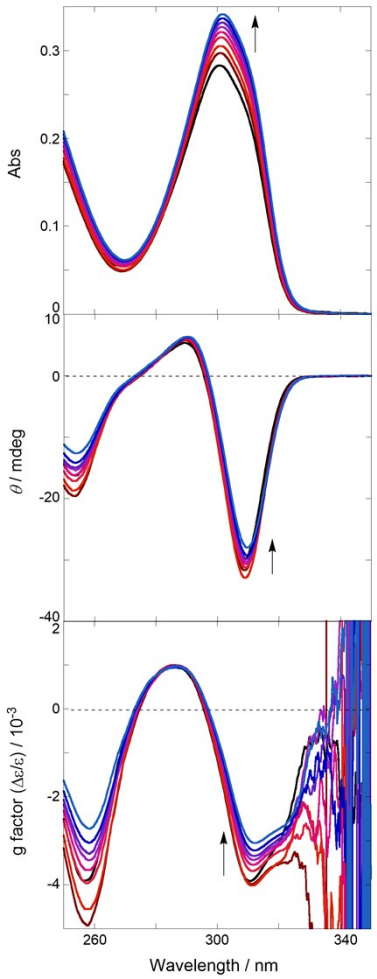


Fig. S19 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (89 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in DCM at room temperature, measured in a high-pressure cell.

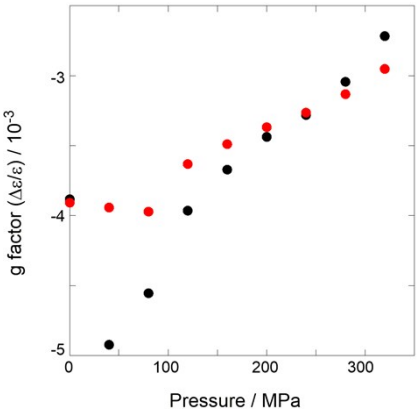


Fig. S20 Plots of anisotropy changes at 258 (black) and 310 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ3** in DCM as a function of pressure.

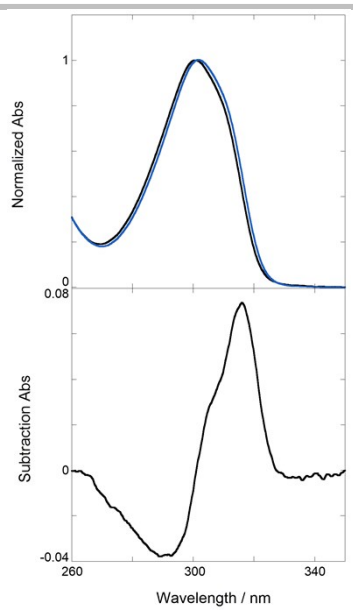


Fig. S21 Normalized UV/vis (normalized at 301 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (89 μM) at 0.1 (black) and 320 MPa (light blue) in DCM at room temperature, measured in a high-pressure cell.

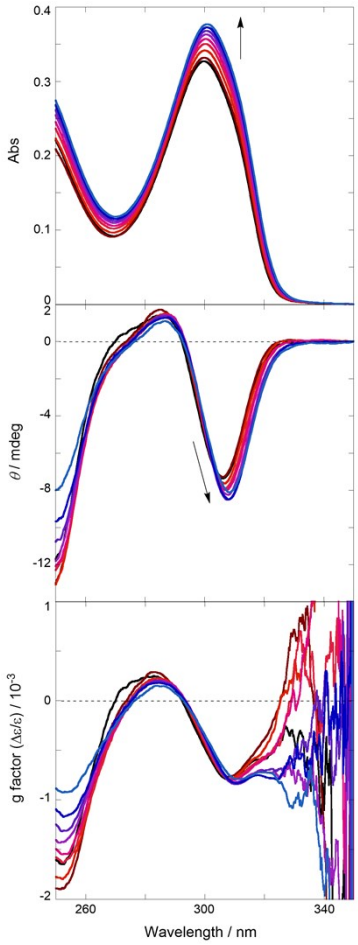


Fig. S22 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (111 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in CHL at room temperature, measured in a high-pressure cell.

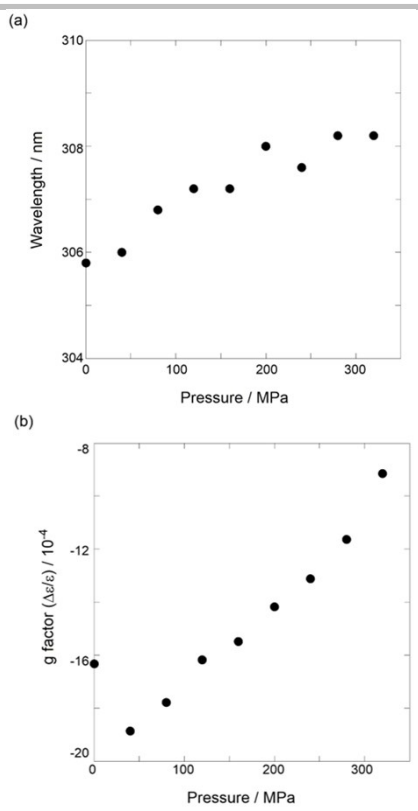


Fig. S23 Plots of (a) ellipticity maxima and (b) anisotropy changes at 253 nm for *in*-(R_p)/*out*-(S_p)-**MUJ1** in CHL as a function of pressure.

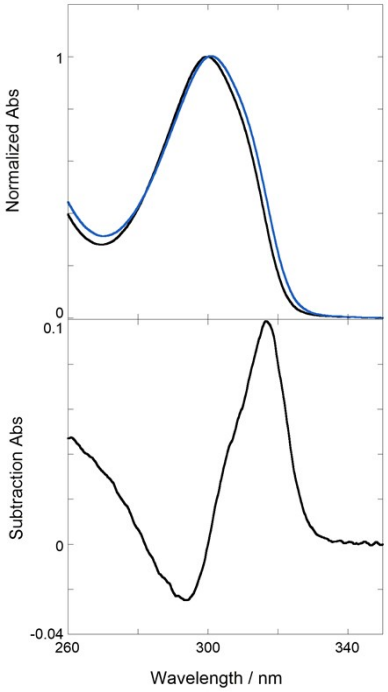


Fig. S24 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (111 μM) at 0.1 (black) and 320 MPa (light blue) in CHL at room temperature, measured in a high-pressure cell.

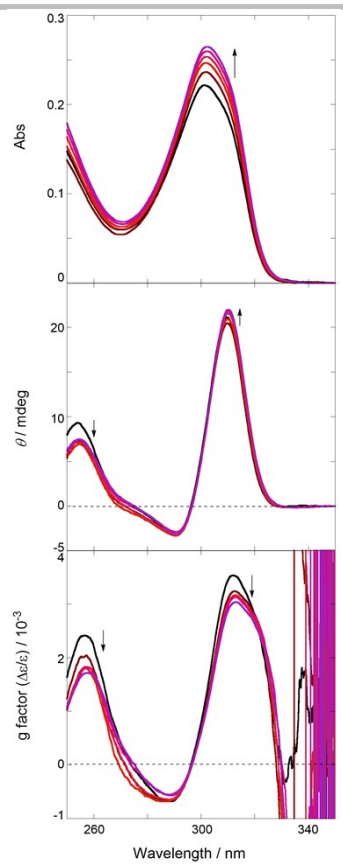


Fig. S25 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (83 μM) at 0.1, 40, 80, 120, 160, and 200 MPa (from black to purple) in CHL at room temperature, measured in a high-pressure cell.

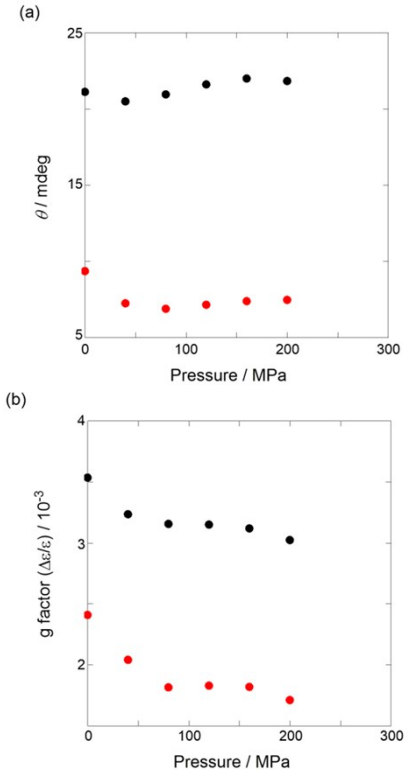


Fig. S26 Plots of (a) ellipticity changes at 310 (black) and 254 nm (red) and (b) anisotropy changes at 312 (black) and 257 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in CHL as a function of pressure.

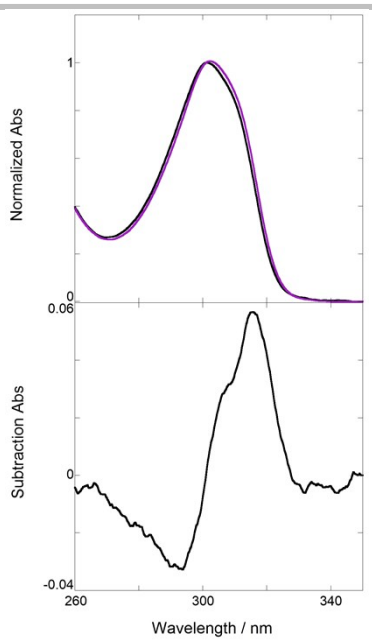


Fig. S27 Normalized UV/vis (normalized at 301 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (83 μM) at 0.1 (black) and 200 MPa (purple) in CHL at room temperature, measured in a high-pressure cell.

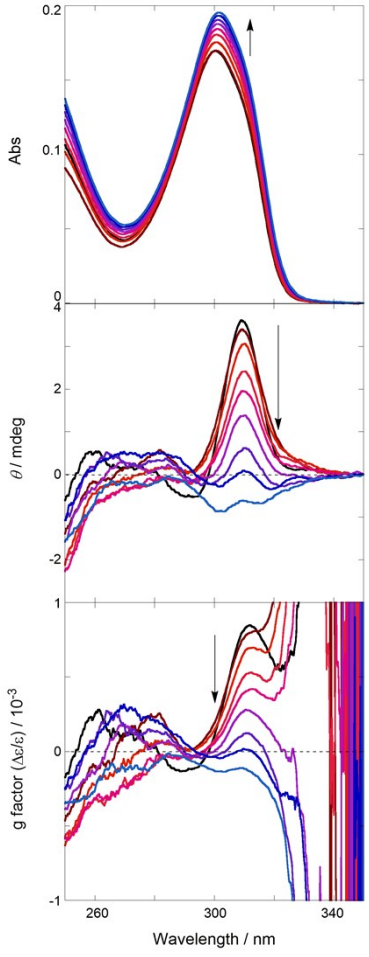


Fig. S28 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (71 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in CHL at room temperature, measured in a high-pressure cell.

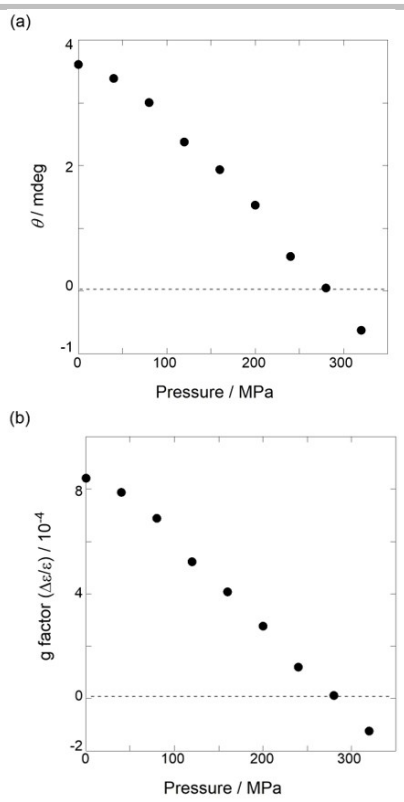


Fig. S29 Plots of (a) ellipticity changes at 309 nm and (b) anisotropy changes at 311 nm for *in*-(R_p)/*out*-(S_p)-**MUJ3** in CHL as a function of pressure.

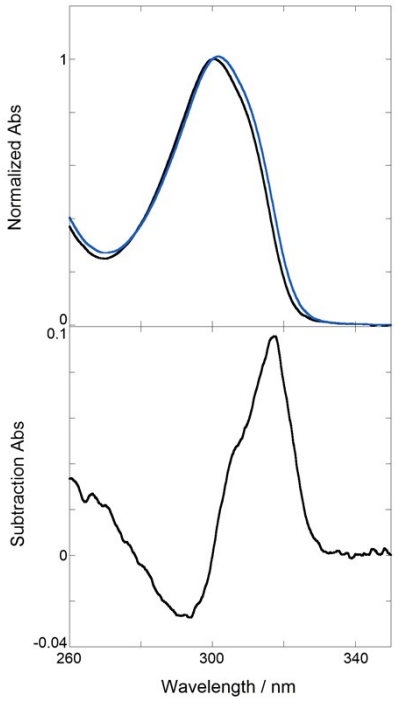


Fig. S30 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (71 μM) at 0.1 (black) and 320 MPa (light blue) in CHL at room temperature, measured in a high-pressure cell.

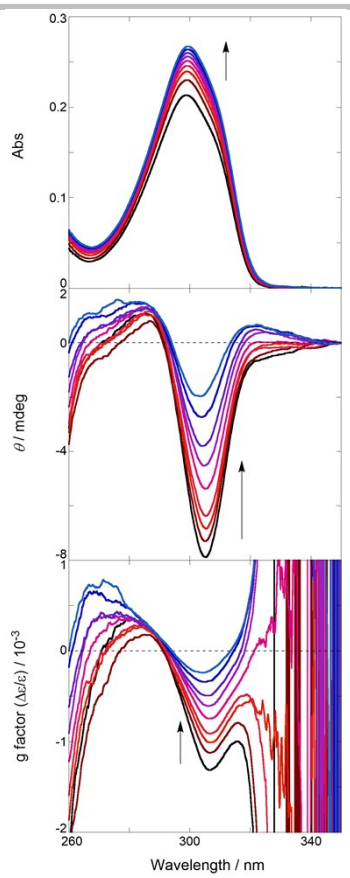


Fig. S31 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (94 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in EA at room temperature, measured in a high-pressure cell.

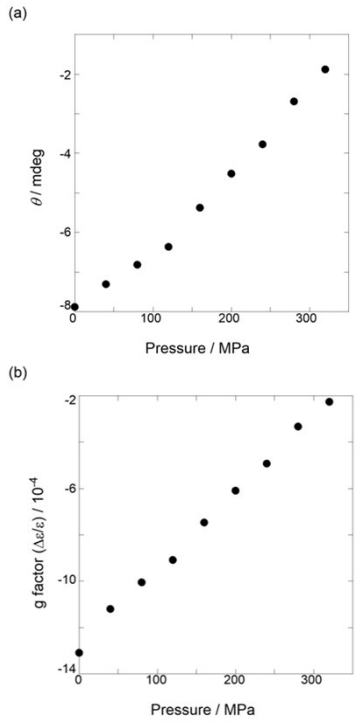


Fig. S32 Plots of (a) ellipticity changes at 305 nm (black) and (b) anisotropy changes at 306 nm (black) for *in*-(R_p)/*out*-(S_p)-**MUJ1** in EA as a function of pressure.

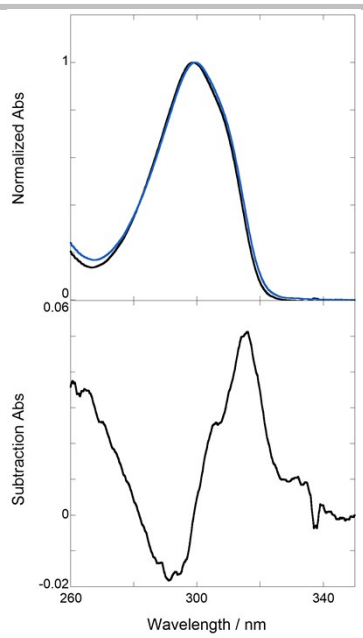


Fig. S33 Normalized UV/vis (normalized at 299 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (94 μM) at 0.1 (black) and 320 MPa (light blue) in EA at room temperature, measured in a high-pressure cell.

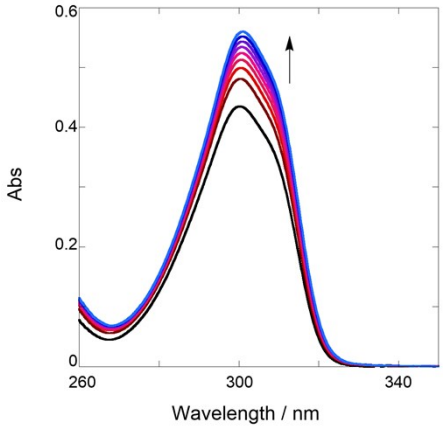


Fig. S34 UV/vis spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (136 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in EA at room temperature, measured in a high-pressure cell.

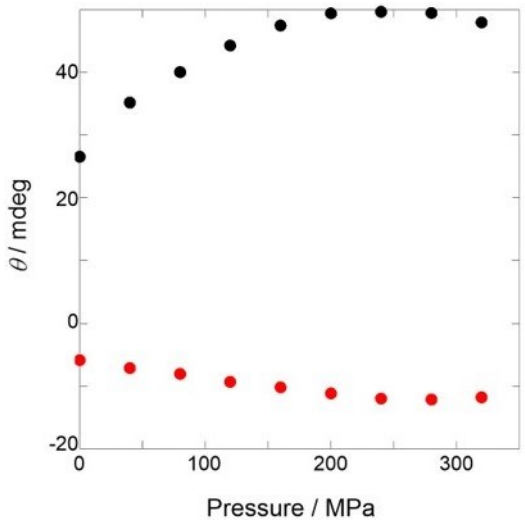


Fig. S35 Plots of ellipticity changes at 308 (black) and 290 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in EA as a function of pressure.

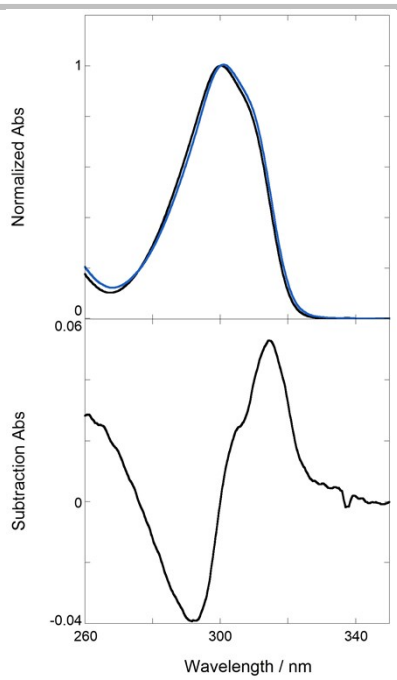


Fig. S36 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (136 μM) at 0.1 (black) and 320 MPa (light blue) in EA at room temperature, measured in a high-pressure cell.

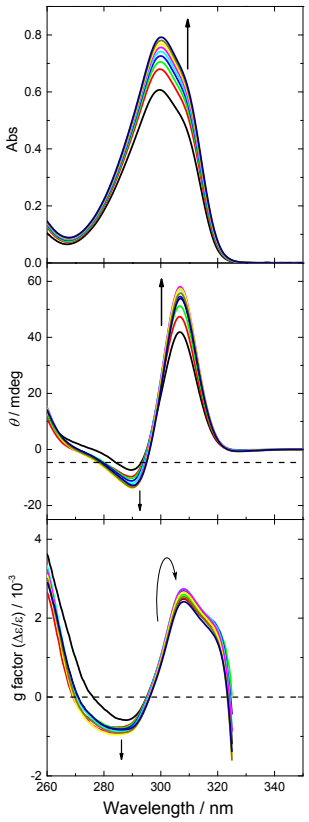


Fig. S37 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (179 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in EA at room temperature, measured in a high-pressure cell.

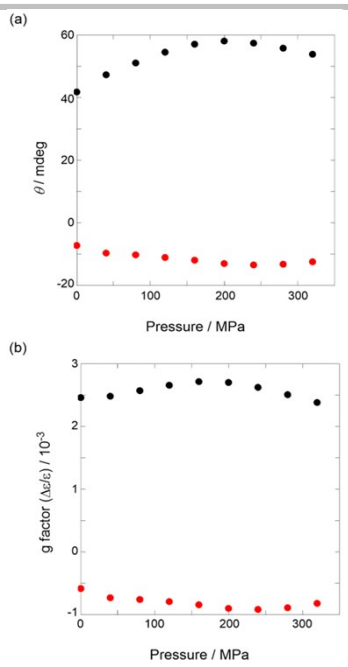


Fig. S38 Plots of (a) ellipticity changes at 307 (black) and 289 nm (red) and (b) anisotropy changes at 307 (black) and 288 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ3** in EA as a function of pressure.

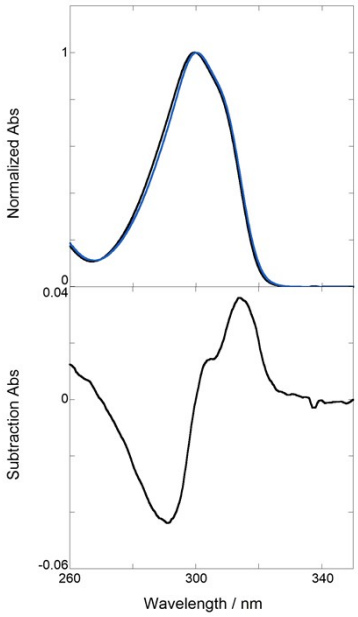


Fig. S39 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (179 μM) at 0.1 (black) and 320 MPa (light blue) in EA at room temperature, measured in a high-pressure cell.

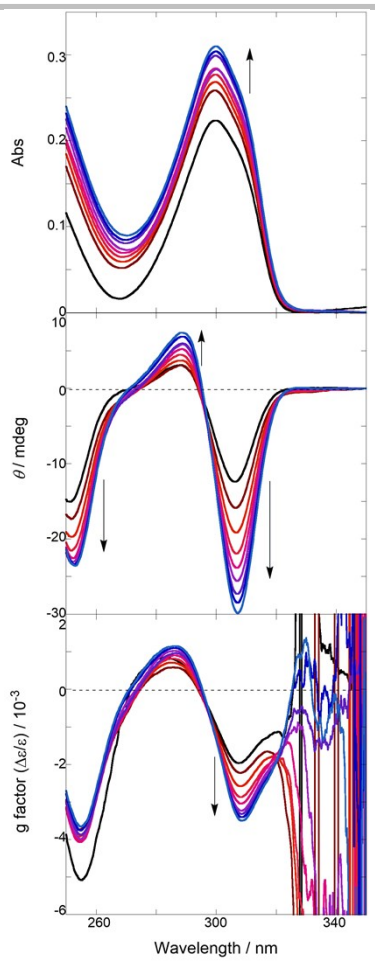


Fig. S40 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (97 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in THF at room temperature, measured in a high-pressure cell.

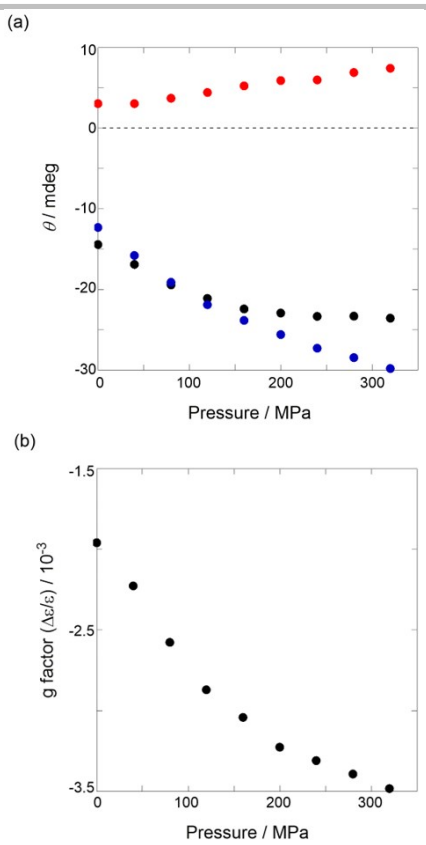


Fig. S41 Plots of (a) ellipticity changes at 307 (blue), 289 (red), and 253 nm (black) and (b) anisotropy changes at 308 nm for *in*-(R_p)/*out*-(S_p)-**MUJ1** in THF as a function of pressure.

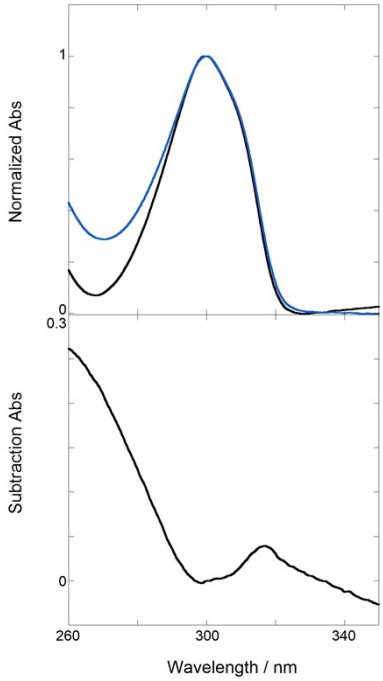


Fig. S42 Normalized UV/vis (normalized at 301 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (97 μM) at 0.1 (black) and 320 MPa (light blue) in THF at room temperature, measured in a high-pressure cell.

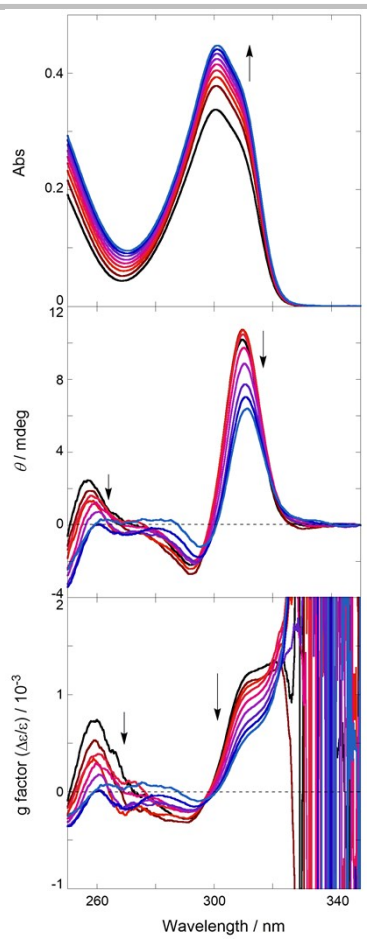


Fig. S43 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (93 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in THF at room temperature, measured in a high-pressure cell.

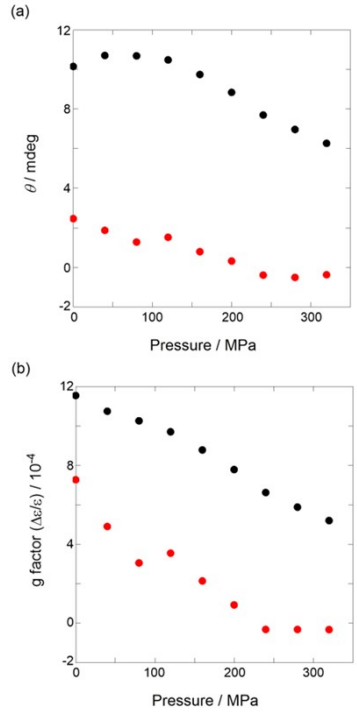


Fig. S44 Plots of (a) ellipticity changes at 310 (black) and 257 nm (red) and (b) anisotropy changes at 310 (black) and 258 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in THF as a function of pressure.

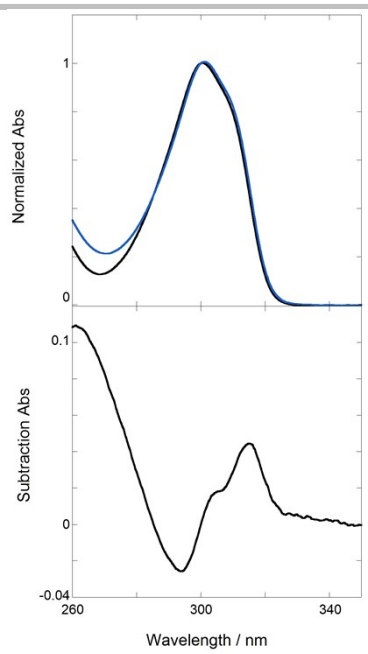


Fig. S45 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (93 μM) at 0.1 (black) and 320 MPa (light blue) in THF at room temperature, measured in a high-pressure cell.

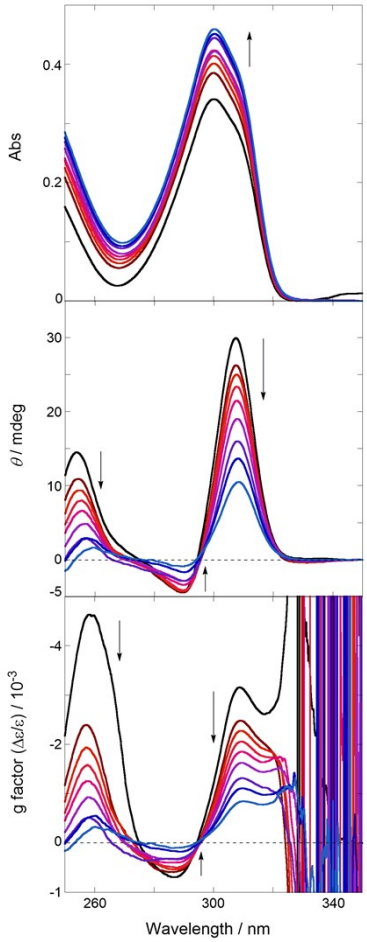


Fig. S46 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (60 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in THF at room temperature, measured in a high-pressure cell.

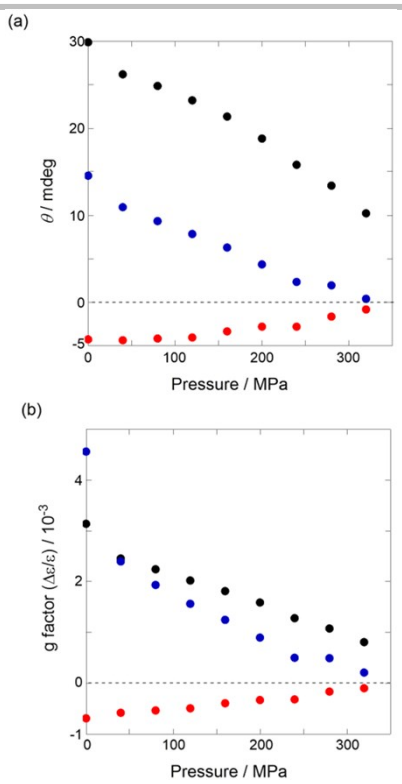


Fig. S47 Plots of (a) ellipticity changes at 307 (black), 290 (red), and 254 nm (blue) and (b) anisotropy changes at 308 (black), 287 (red), and 257 nm (blue) for *in*-(R_p)/*out*-(S_p)-**MUJ3** in THF as a function of pressure.

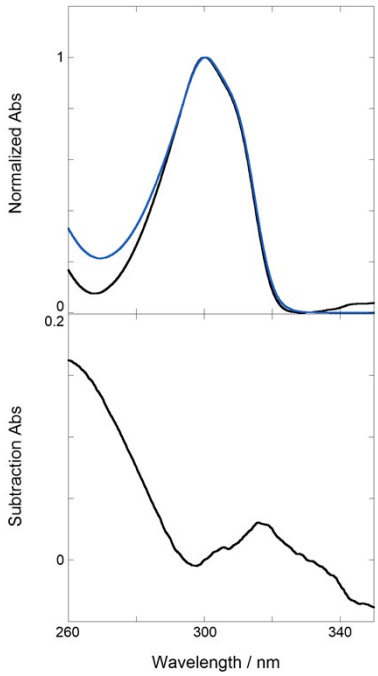


Fig. S48 Normalized UV/vis (normalized at 301 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (60 μM) at 0.1 (black) and 320 MPa (light blue) in THF at room temperature, measured in a high-pressure cell.

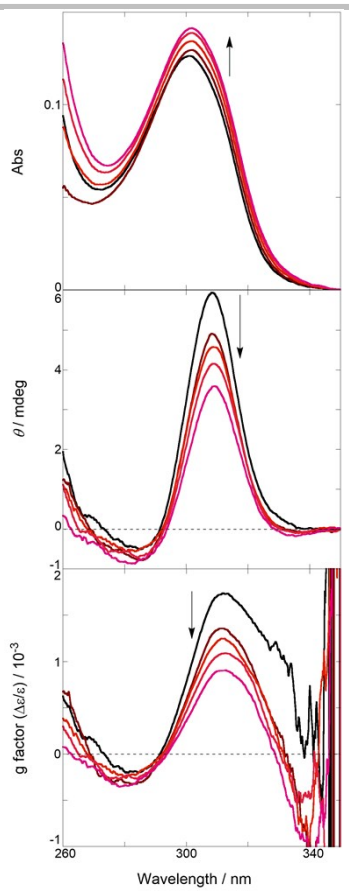


Fig. S49 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (91 μM) at 0.1, 40, 80, 120, and 160 MPa (from black to pink) in CTC at room temperature, measured in a high-pressure cell.

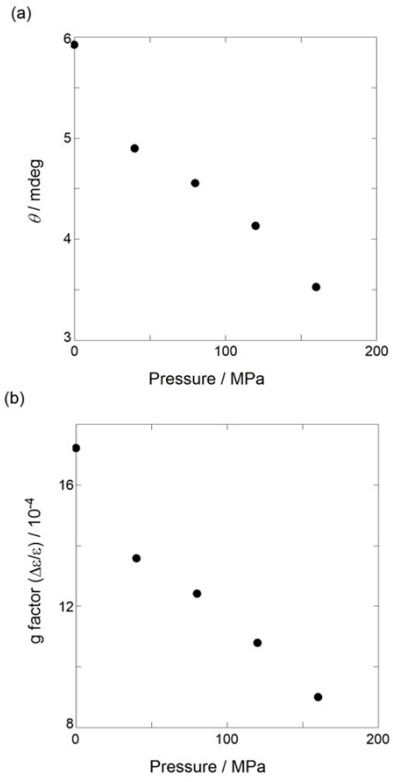


Fig. S50 Plots of (a) ellipticity changes at 308 nm (black) and (b) anisotropy changes at 311 nm (black) for *in*-(R_p)/*out*-(S_p)-**MUJ1** in CTC as a function of pressure.

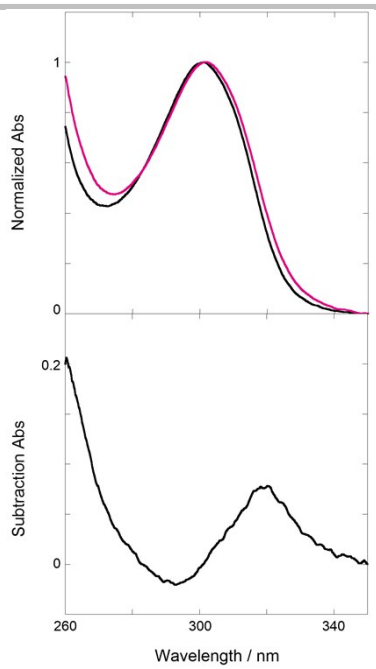


Fig. S51 Normalized UV/vis (normalized at 301 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (91 μM) at 0.1 (black) and 160 MPa (pink) in CTC at room temperature, measured in a high-pressure cell.

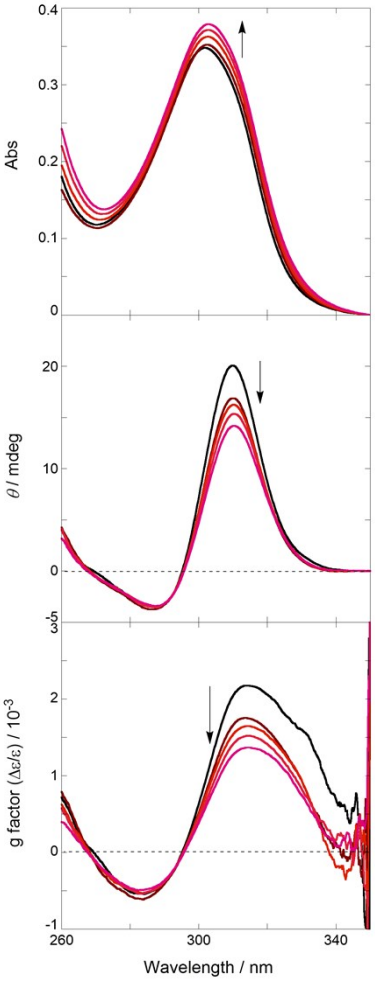


Fig. S52 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (120 μM) at 0.1, 40, 80, 120, and 160 MPa (from black to pink) in CTC at room temperature, measured in a high-pressure cell.

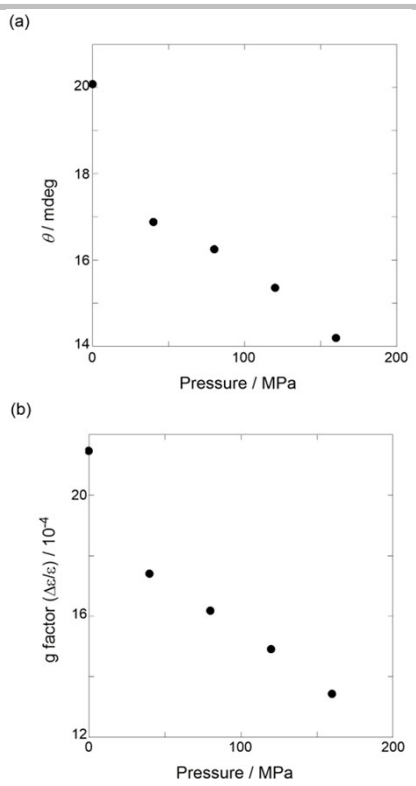


Fig. S53 Plots of (a) ellipticity changes at 310 nm (black) and (b) anisotropy changes at 312 nm (black) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in CTC as a function of pressure.

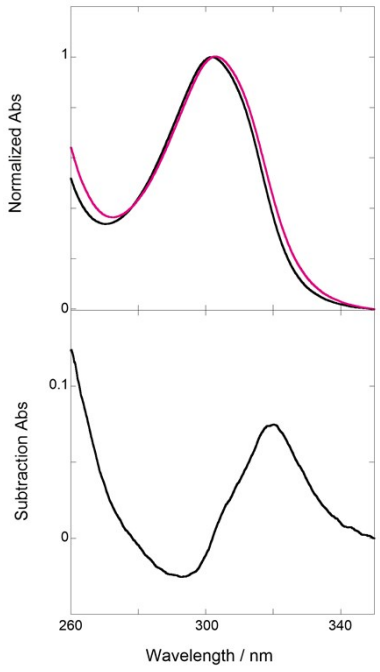


Fig. S54 Normalized UV/vis (normalized at 302 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (120 μM) at 0.1 (black) and 160 MPa (pink) in CTC at room temperature, measured in a high-pressure cell.

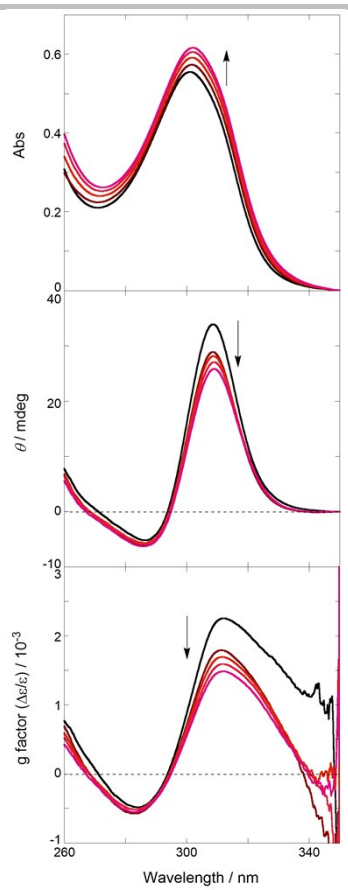


Fig. S55 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (166 μM) at 0.1, 40, 80, 120, and 160 MPa (from black to pink) in CTC at room temperature, measured in a high-pressure cell.

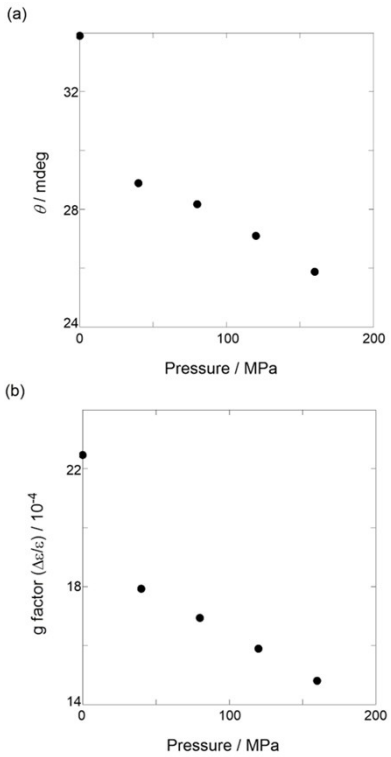


Fig. S56 Plots of (a) ellipticity changes at 309 nm (black) and (b) anisotropy changes at 311 nm (black) for *in*-(R_p)/*out*-(S_p)-**MUJ3** in CTC as a function of pressure.

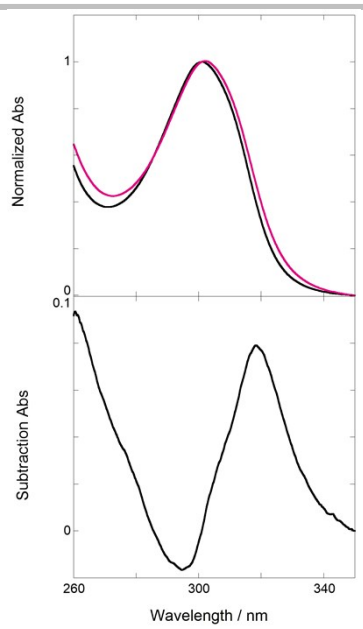


Fig. S57 Normalized UV/vis (normalized at 301 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (166 μM) at 0.1 (black) and 160 MPa (pink) in CTC at room temperature, measured in a high-pressure cell.

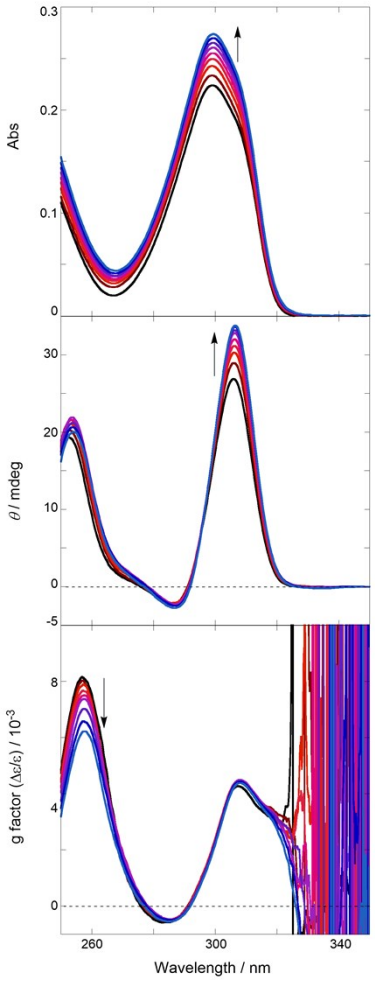


Fig. S58 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (91 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in MCH at room temperature, measured in a high-pressure cell.

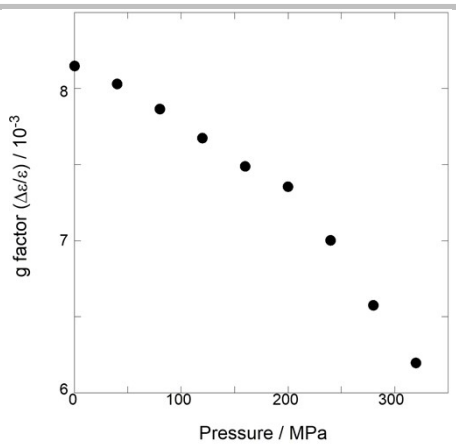


Fig. S59 Plots of anisotropy changes at 257 nm for *in*-(R_p)/*out*-(S_p)-**MUJ1** in MCH as a function of pressure.

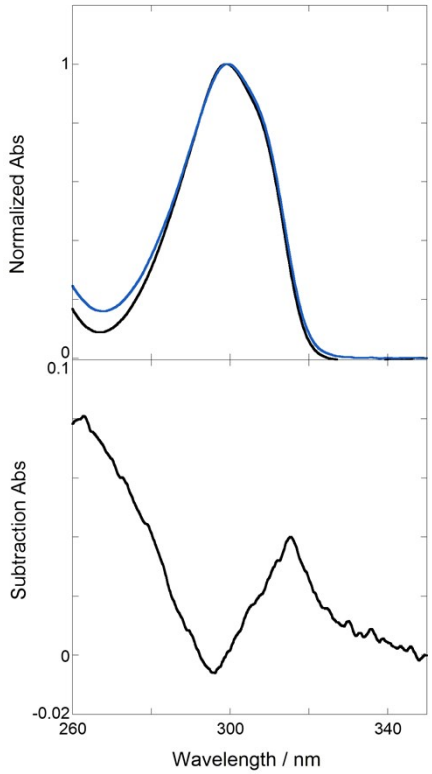


Fig. S60 Normalized UV/vis (normalized at 299 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (91 μM) at 0.1 (black) and 320 MPa (light blue) in MCH at room temperature, measured in a high-pressure cell.

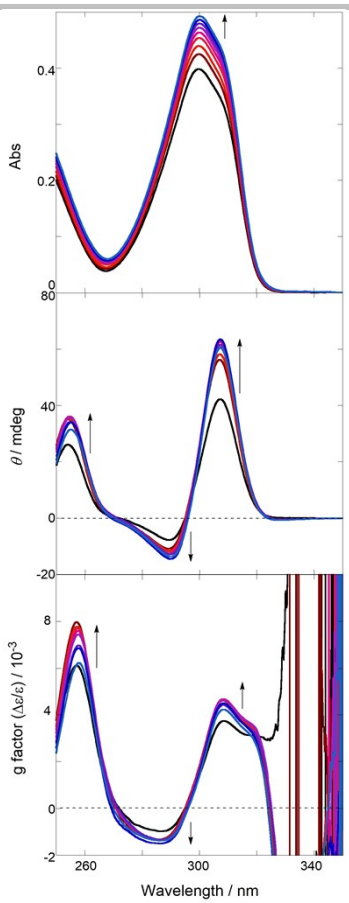


Fig. S61 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (120 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in MCH at room temperature, measured in a high-pressure cell.

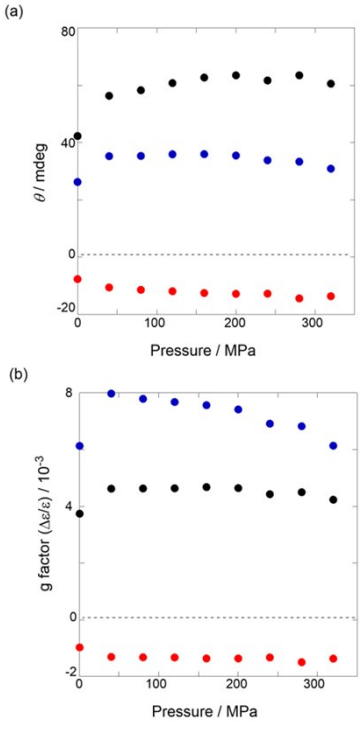


Fig. S62 Plots of (a) ellipticity changes at 307 (black), 290 (red), and 254 nm (blue) and (b) anisotropy changes at 308 (black), 287 (red), and 257 nm (blue) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in MCH as a function of pressure.

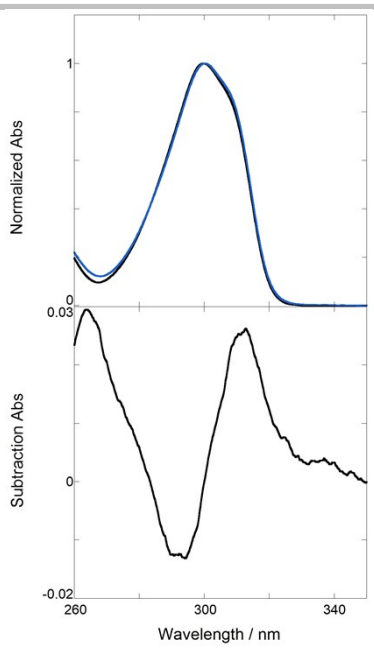


Fig. S63 Normalized UV/vis (normalized at 300 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (120 μM) at 0.1 (black) and 320 MPa (light blue) in MCH at room temperature, measured in a high-pressure cell.

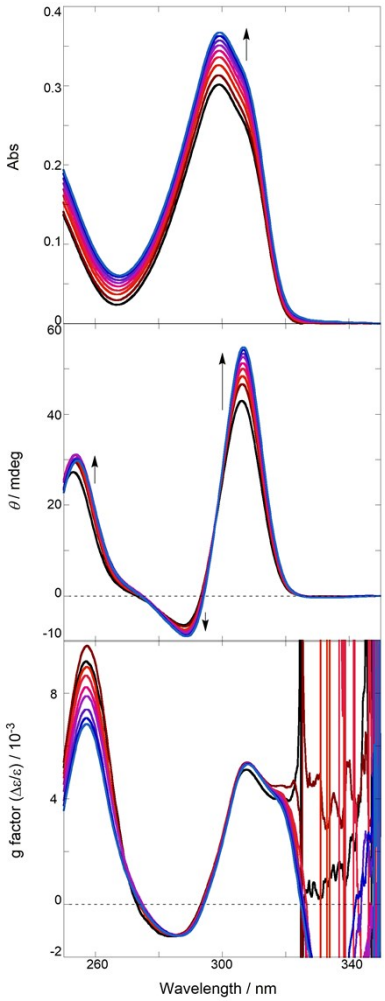


Fig. S64 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (94 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in MCH at room temperature, measured in a high-pressure cell.

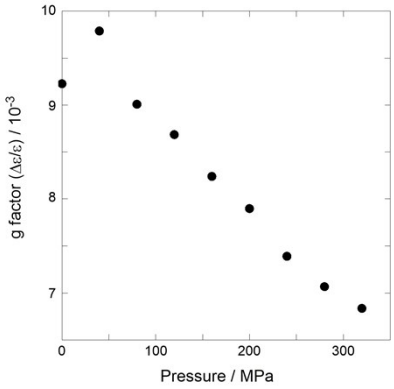


Fig. S65 Plots of anisotropy changes at 257 nm for *in*-(R_p)/*out*-(S_p)-**MUJ3** in MCH as a function of pressure.

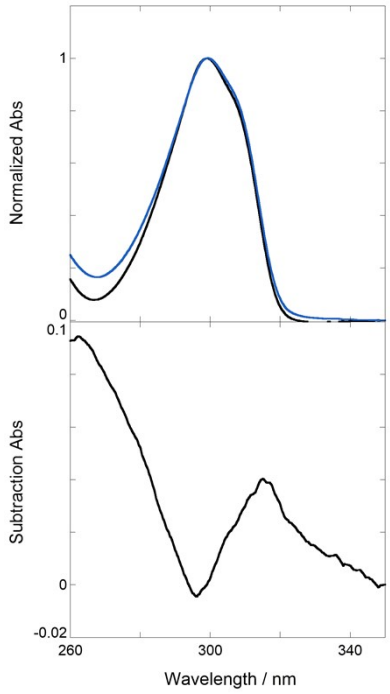


Fig. S66 Normalized UV/vis (normalized at 299 nm; top) and subtraction UV (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (94 μM) at 0.1 (black) and 320 MPa (light blue) in MCH at room temperature, measured in a high-pressure cell.

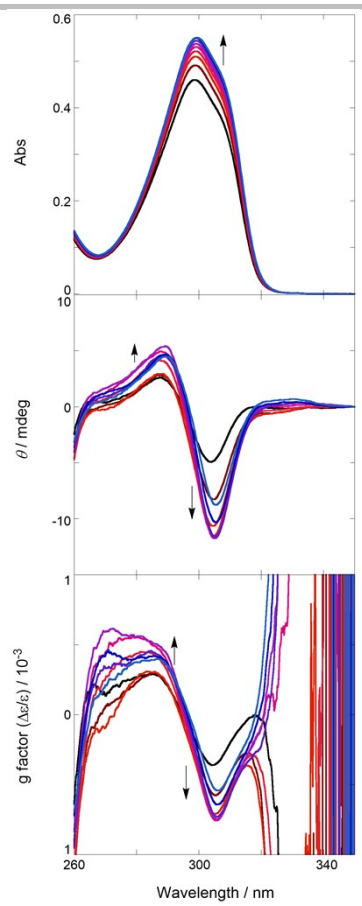


Fig. S67 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ1** (191 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in *n*-H at room temperature, measured in a high-pressure cell.

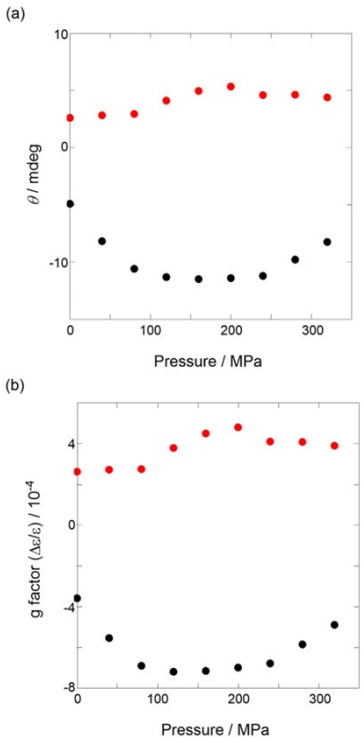


Fig. S68 Plots of (a) ellipticity changes at 304 (black) and 288 nm (red) and (b) anisotropy changes at 304 (black) and 288 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ1** in *n*-H as a function of pressure.

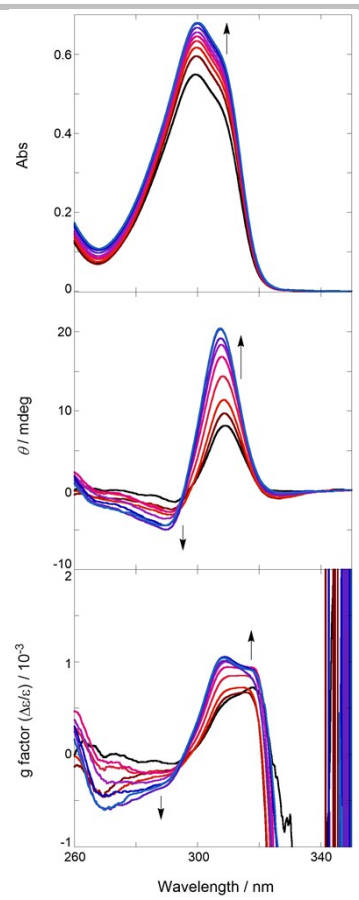


Fig. S69 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ2** (142 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to blue) in *n*-H at room temperature, measured in a high-pressure cell.

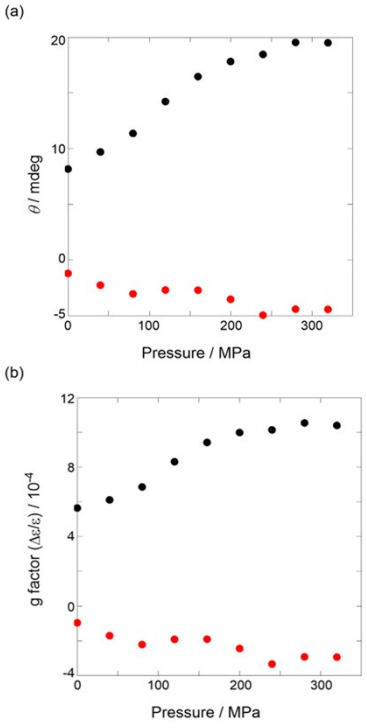


Fig. S70 Plots of (a) ellipticity changes at 309 (black) and 290 nm (red) and (b) anisotropy changes at 309 (black) and 290 nm (red) for *in*-(R_p)/*out*-(S_p)-**MUJ2** in *n*-H as a function of pressure.

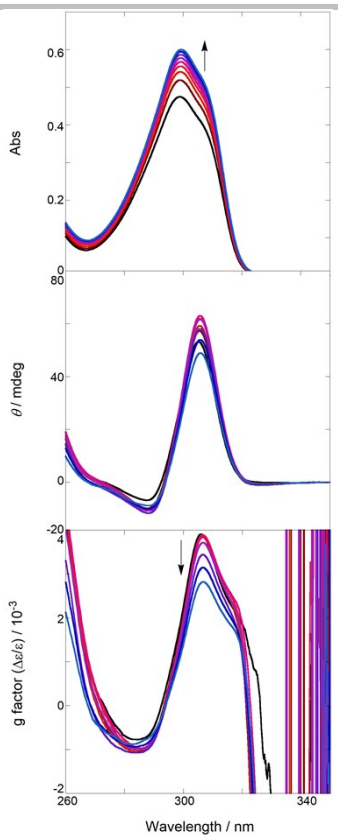


Fig. S71 UV/vis (top), CD (middle), and anisotropy (bottom) spectra of *in*-(R_p)/*out*-(S_p)-**MUJ3** (133 μM) at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue) in *n*-H at room temperature, measured in a high-pressure cell.

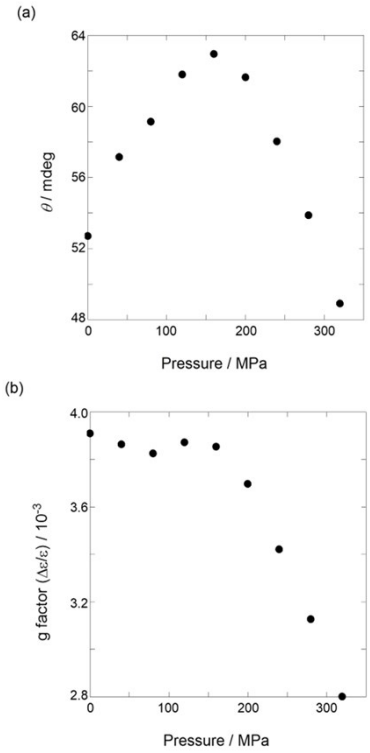


Fig. S72 Plots of (a) ellipticity changes at 306 nm and (b) anisotropy changes at 306 nm for *in*-(R_p)/*out*-(S_p)-**MUJ3** in *n*-H as a function of pressure.

4. Pressure Effects on the Anisotropy (*g*) Factors of *in*-(R_p)/*out*-(S_p)-MUJs

Table S1 Pressure Effects on the Anisotropy (*g*) Factor of **MUJ**s at the Extremum (310 ± 1 nm)

Solvent	E_T[a]	*in*-(R_p)/*out*-(S_p)-**MUJ1**			*in*-(R_p)/*out*-(S_p)-**MUJ2**			*in*-(R_p)/*out*-(S_p)-**MUJ3**		
		$g_{310}^{0.1MPa}$ /10^{-6} [b]	g_{310}^{Pmax} /10^{-6} [c]	Δg_{310} /10^{-6} [d]	$g_{310}^{0.1MPa}$ /10^{-6} [b]	g_{310}^{Pmax} /10^{-6} [c]	Δg_{310} /10^{-6} [d]	$g_{310}^{0.1MPa}$ /10^{-6} [b]	g_{310}^{Pmax} /10^{-6} [c]	Δg_{310} /10^{-6} [d]
n-H	30.9	-359	-490	*-131*	565	1040	*475*	3910	2800	*-1110*
MCH	~31	4260	4340	*80*	3740	4230	*490*	5100	5250	*150*
CTC	32.5	1720	899[e]	*-821*[f]	2170	1360[e]	*-810*[f]	2250	1480[e]	*-770*[f]
THF	37.4	-1960	-3400	*-1440*	1200	558	*-642*	3140	809	*-2330*
EA	38.1	-1310	-225	*1090*	2270	3040	*770*	2490	2420	*-70*
CHL	39.1	-798	-744	*54*	3520	2970[g]	*-550*[h]	842	-124	*-966*
DCM	41.1	-3630	-2660	*970*	-1940	47	*1987*	-3910	-2950	*960*
AN	46.0	-3390	-2240	*1150*	-1560	3440	*5000*	-3690	-2280	*1410*

[a] Reichardt's solvent polarity parameter; see reference 6.
[b] Anisotropy factor at 0.1 MPa.
[c] Anisotropy factor at the highest pressure applied, i.e., 320 MPa, unless otherwise noted.
[d] $\Delta g = g_{310}^{320MPa} - g_{310}^{0.1MPa}$, unless otherwise noted.
[e] Anisotropy factor at 160 MPa.
[f] $\Delta g = g_{310}^{160MPa} - g_{310}^{0.1MPa}$.
[g] Anisotropy factor at 200 MPa.
[h] $\Delta g = g_{310}^{200MPa} - g_{310}^{0.1MPa}$.

5. DFT Calculations of the van der Waals Volumes of the *in*- and *out*-Conformers of MUJs

The density functional theory (DFT) calculations were used for the optimization of the ground-state geometries at the B3LYP/6-31g (d) level. All the calculations were performed on Gaussian 09W. The van der Waals volumes were calculated for the geomery-optimized *in*- and *out*-conformers of **MUJ** by the Materials Studio 2017.

Table S2 DFT-Calculated Changes in Energy (ΔE) and van der Waals Volume (ΔV) upon Self-Complexation of **MUJs**.

Host	E_{in}[a]/a.u.	$\Delta E_{in\text{-}out}$[b]/kJ mol^{-1}	V_{in}[c]/Å^3	$\Delta V_{in\text{-}out}$[d]/Å^3
MUJ1	−3271.87492083	0.59	944.46[e]	−0.30
MUJ2	−3203.50573109	3.89	986.79[e]	−0.36
MUJ3	−3579.54900355	−9.25	1029.70[e]	−0.26

[a] The energy of *in*-(S_p)-**MUJ** geometry-optimized *in vacuo* by the DFT method at the B3LYP/6-31G(d) level. [b] The energy change upon self-complexation, evaluated by subtracting the energy of *out*-(S_p)-**MUJ** from that of *in*-(S_p)-**MUJ**; [c] The van der Waals volume of *in*-(S_p)-**MUJ**. [d] The volume change upon self-complexation, evaluated by subtracting the vdW volume of *out*-(S_p)-**MUJ** from that of the *in*-(S_p)-**MUJ**; [e] The van der Waals volume calculated by Materials Studio 2017.

6. Complexation of Solvent Molecules with 1,4-Diethoxypillar[5]arene (DEP[5]) in Methylcyclohexane

Isothermal titration calorimetry (ITC) expermints were performed using a Microcal VP-ITC instrument. Typically, an MCH soluton of guest solvent (300 - 350 mM) was added with stirring to an MCH solution of DEP[5] (1.0 mM) placed in a calorimeter cuvette at 25 °C under the atmospheric pressure (0.1 MPa). The thermograms obtained were analyzed by assuming the 1:1 stoichiomery to give the association constant (K_a) and the themodynamic parameters ($\Delta H°$ and $\Delta S°$).

However, some of the guest solvents did not develop any detectable heat (CTC and CHL) or mix with MCH (AN), and accordingly only the K_a values were determined for these guests by ^{1}H NMR spectral titration (**Supplementary Table 3**).

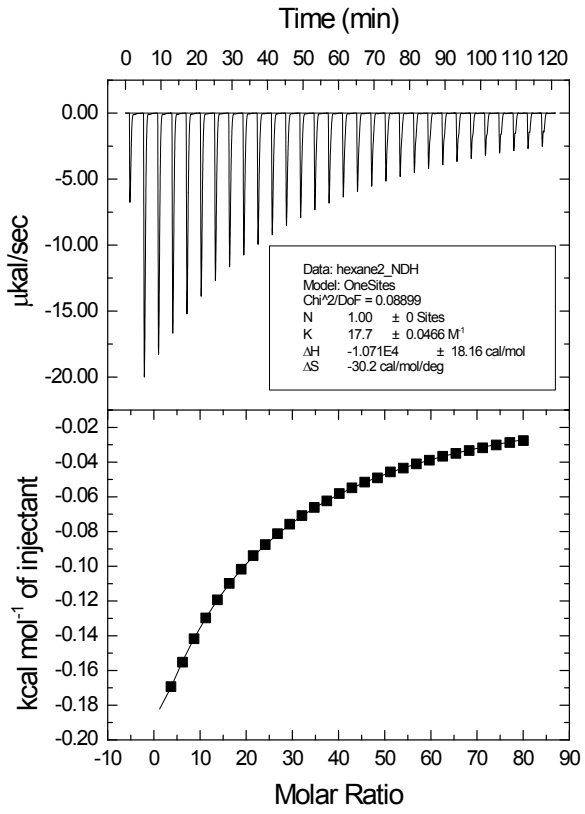


Fig. S73 Calorimetric titration data for the complexation of host **DEP[5]** (1.0 mM) with *n*-hexane (350 mM) in methylcyclohexane at 25 °C, which gave the 1:1 association constant (K_a) of 17.7 M^{-1}.

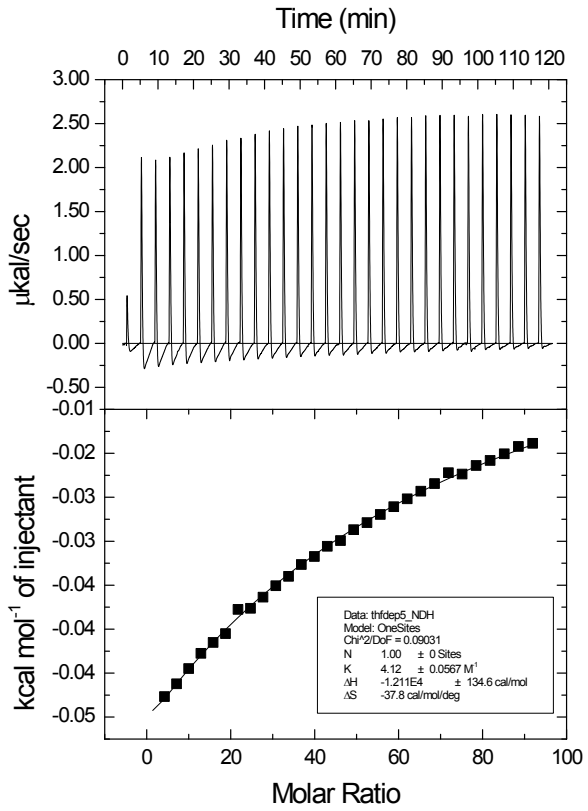


Fig. S74 Calorimetric titration data for the complexation of host **DEP[5]** (1.0 mM) with tetrahydrofuran (400 mM) in methylcyclohexane at 25 °C, which gave the 1:1 association constant (K_a) of 4.1 M^{-1}.

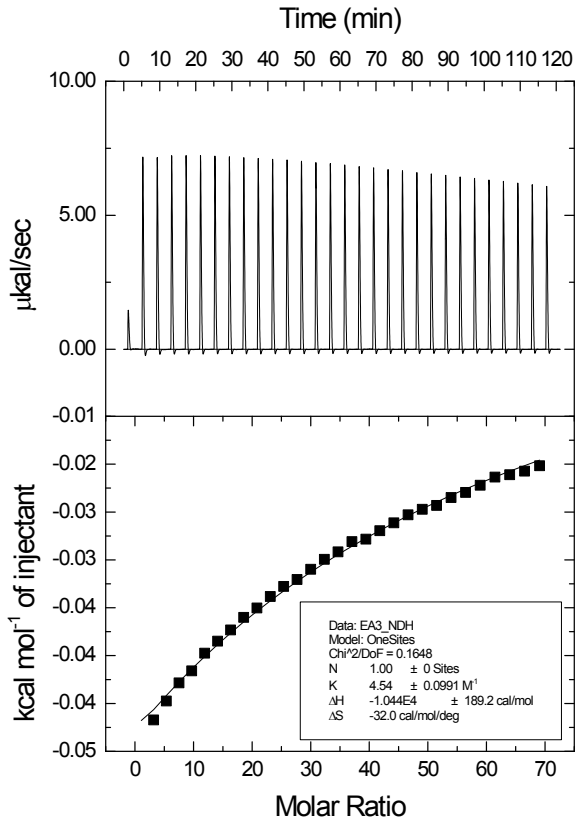


Fig. S75 Calorimetric titration data for the complexation of host **DEP[5]** (1.0 mM) with ethyl acetate (300 mM) in methylcyclohexane at 25 °C, which gave the 1:1 association constant (K_a) of 4.5 M^{-1}.

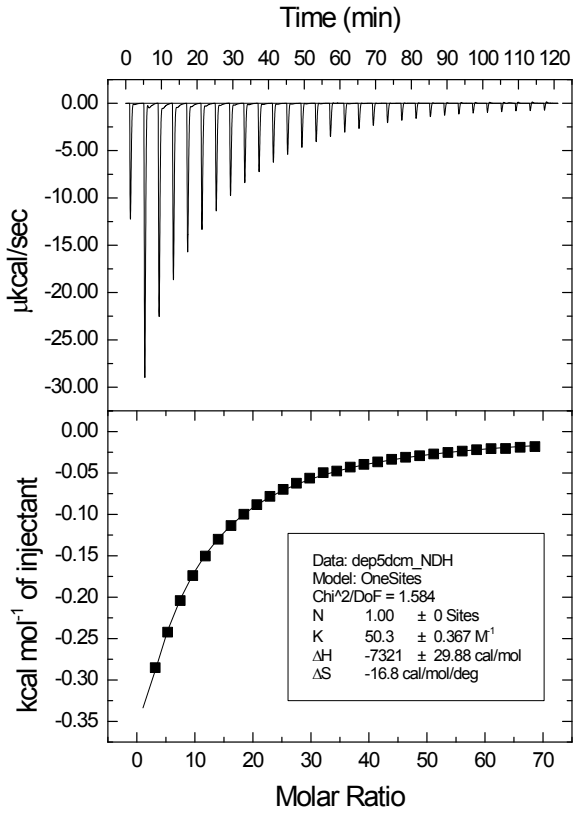


Fig. S76 Calorimetric titration data for the complexation of host **DEP[5]** (1.0 mM) with dichloromethane (300 mM) in methylcyclohexane at 25 °C, which gave the 1:1 association constant (K_a) of 50.3 M^{-1}.

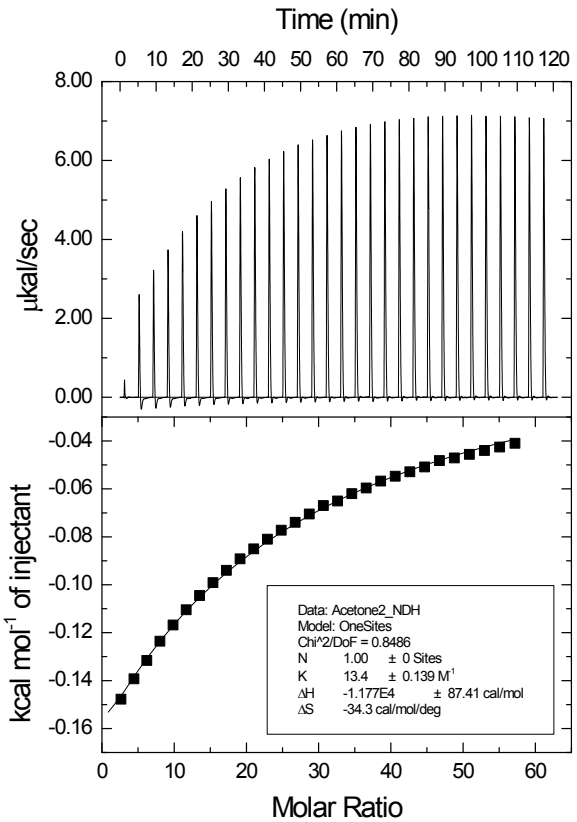


Fig. S77 Calorimetric titration data for the complexation of host **DEP[5]** (1.0 mM) with acetone (250 mM) in methylcyclohexane at 25 °C, which gave the 1:1 association constant (K_a) of 13.4 M^{-1}.

Table S3 Association Constants (K_a) and Thermodynamic Parameters for the 1:1 Complexation of Some Solvent Molecules with DEP[5] Determined by Isothermal Titration Calorimetry in MCH or by ^{1}H NMR Spectral Titration in MCH-d_{14} at 25 °C under Ambient Pressure (0.1 MPa)

Guest	K_a / M^{-1}	$\Delta H°$ / kcal mol^{-1}	$\Delta S°$ / cal mol^{-1} K^{-1}
n-Hexane (*n*-H)	17.80 ± 0.05	-10.71 ± 0.02	-30.2
Carbon Tetrachloride (CTC)	~0[a]	~0	
Tetrahydrofuran (THF)	4.12 ± 0.06	-12.1 ± 0.1	-37.8
Ethyl Acetate (EA)	4.54 ± 0.10	-10.4 ± 0.2	-32.0
Chloroform (CHL)	0.63 ± 0.02[b]	~0	
Acetone	13.4 ± 0.1	-11.77 ± 0.09	-34.3
Dichloromethane (DMC)	50.3 ± 0.4	-7.32 ± 0.03	-16.8
Acetonitrile (AN)	550 ± 30[c]		

[a] The heat effect observed was too small to determine the parameters by ITC under the condition employed, which means that K_a is very small or the $\Delta H°$ value is incidentally close to zero. Further examinations by NMR spectral titration at much higher host/guest concentrations also showed only extremely small chemical shift changes (see Fig. S 81, Supplementary Table 6, and relevant discussion) to reveal that no complexation or perching takes place between DEP[5] and CTC, i.e., K_a ~0. [b] The heat effect observed was too small to determine the parameters by ITC under the condition employed, which means that K_a is very small or the $\Delta H°$ value is incidentally close to zero. Further examinations by NMR spectral titration showed small, yet appreciable chemical shift changes (see Fig. Ss 79-80) to give the K_a value. [c] The low solubility of AN in MCH did not allow us to obtain reliable data by ITC, and hence only the K_a value was determined by NMR spectral titration in MCH-d_{14} (Fig. Ss 82-83) with sonication after each addition of AN to make the solution homogeneous.

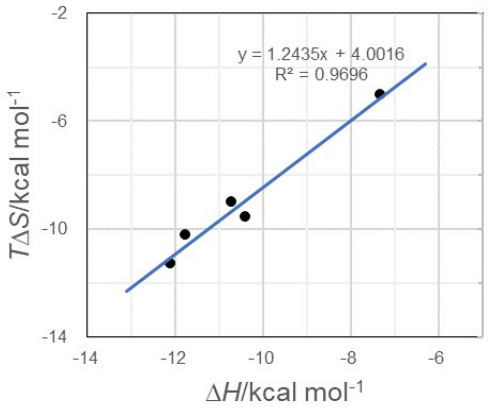


Fig. S78 Enthalpy-entropy compensation plot obtained from the thermodynamic parameters for the complexation of DEP[5] with *n*-H, THF, EA, DCM, and acetone in MCH (Supplementary Table 3); the regression line: y = 1.24x + 4.0 (r^2 = 0.9696).

Discussion: The available thermodynamic parameter listed in Supplementary Table 3 indicate that the complexation of guest solvent with DEP[5] in MCH is obiously driven by the negative enthalpy changes ($\Delta H°$) of –7 to –12 kcal mol^{-1}, which are moderately cancelled by the entropy changes ($\Delta S°$) of –17 to –38 cal mol^{-1} K^{-1} or the $T\Delta S°$ values of –5 to –11 kcal mol^{-1}. Interestingly, the thermodynamic parameters obtained exhibit a compensatory $\Delta H°$-$\Delta S°$ relationship (r^2 = 0.9696) with a slope of 1.24 and an intercept of 4.0, implying that the complexation mechanism and the controlling factors are shared among the guest molecules examined.[7]

7. Anisotropy Factors of Pure *out*-MUJs

Table S4 Anisotropy (g_{310}^{out}) Factors of Pure *out*-(R_p)-Conformers of **MUJ**s Estimated by Adding a >2000-fold Excess of Strong Binder 1,4-Dicyanobutane[a]

Solvent (E_T)	g_{310}^{out}			Average	Std. dev.	$g_{310}^{MUJ1}/g_{310}^{MUJ3}$
	MUJ1	**MUJ2**	**MUJ3**			
n-H (30.9)	0.013	0.016	0.016	0.015	0.002	0.81
MCH (~31)	0.013	0.015	0.016	0.015	0.002	0.79
CTC (32.5)	0.007	0.008	0.009	0.008	0.001	0.81
THF (37.4)	0.013	0.015	0.016	0.015	0.001	0.82
EA (38.1)	0.012	0.015	0.016	0.014	0.002	0.77
CHL (39.1)	[b]	0.013	0.014	0.014	0.001	[b]
DCM (41.1)	0.011	0.013	0.015	0.013	0.002	0.77
AN (46.0)	0.010	0.010	0.014	0.011	0.002	0.75
Average	0.011	0.013	0.015			
Std. dev.	0.002	0.003	0.003			
Average[c]	0.012	0.014	0.015			
Std. dev.[c]	0.001	0.002	0.001			
$g_{310}^{min}/g_{310}^{max}$	0.53	0.54	0.53			
$g_{310}^{min}/g_{310}^{max}$ [c]	0.79	0.63	0.85			

[a] Note that, only in this experiment, the antipodal *in*-(S_p)/*out*-(R_p)-conformers (the first-eluting enantiomers on chiral HPLC) were used and hence all the g_{310}^{out} factors shown here are positive. Logically, the g_{310}^{out} factors of the *out*-(S_P)-conformers used in all the other experiments should be negative. [b] Not determined. [c] Calculated without including the data obtained in CTC, which show significant deviations from those in other solvents, irrespective of the subring type incorporated in **MUJ**.

8. ^{1}H NMR Spectral Titration of DEP[5] in MCH-d_{14}

^{1}H NMR Spectral Titration of DEP[5] with **CHL**

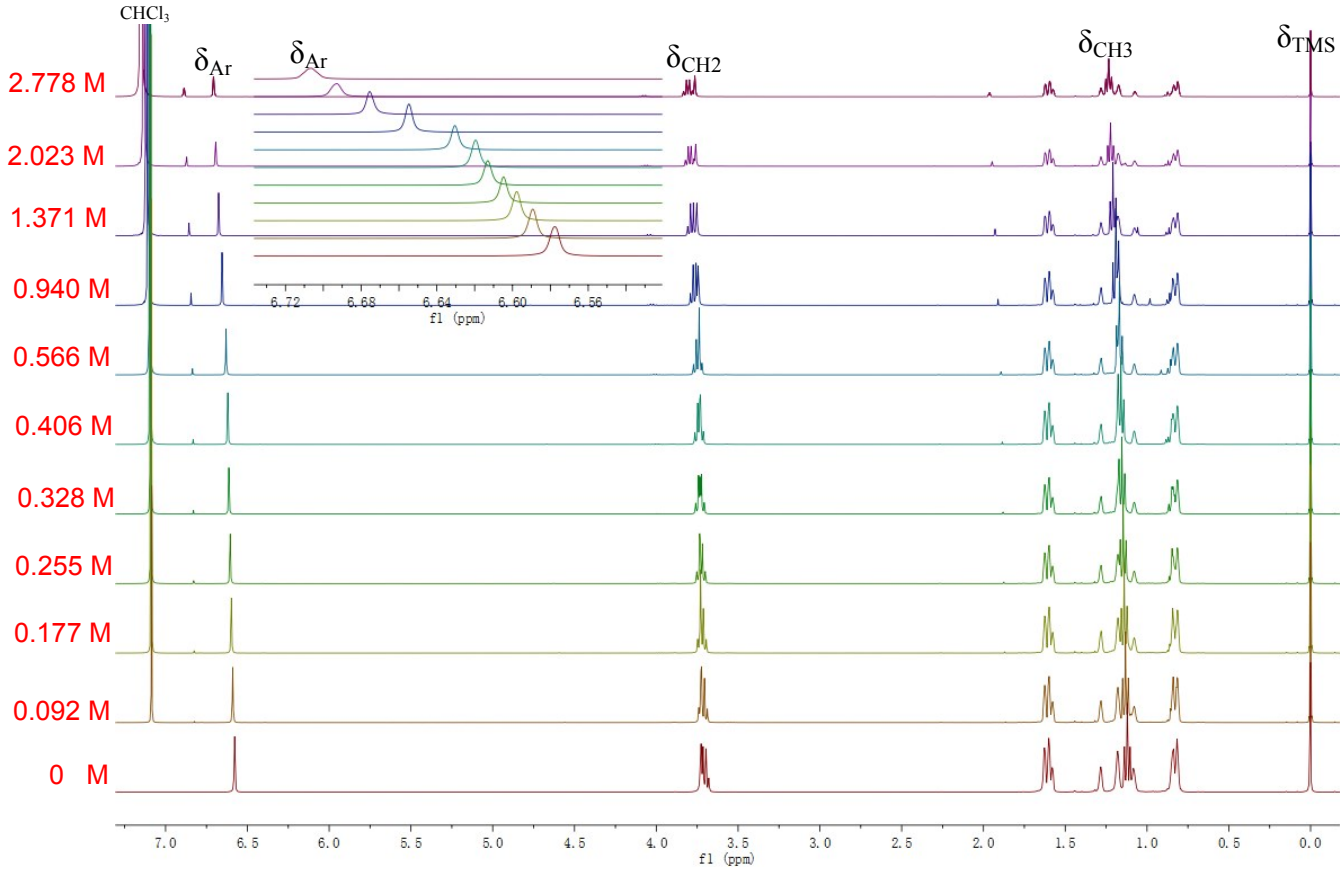


Fig. S79 ^{1}H NMR spectra (400 MHz) of DEP[5] (4.2 mM) upon titration with CHL (0-2.78 M) in MCH-d_{14} at room temperature.

Table S5 Chemical shifts of the aromatic and ethoxy protons of DEP[5] (4.2 mM) in the presence of 0-2.78 M CHL

[CHL]/M	δ_{Ar}/ppm	δ_{CH2}/ppm	δ_{CH3}/ppm
0	6.578	3.697	1.121
0.092	6.589	3.705	1.132
0.177	6.598	3.712	1.139
0.255	6.605	3.718	1.146
0.328	6.613	3.724	1.154
0.406	6.619	3.730	1.159
0.566	6.630	3.738	1.169
0.940	6.655	3.757	1.190
1.371	6.675	3.773	1.208
2.023	6.693	3.787	1.223
2.778	6.706	3.796	1.234
$\Delta\delta$[a]	*0.128*	*0.099*	*0.113*

[a] $\Delta\delta = \delta$(2.778 M) – δ(0 M).

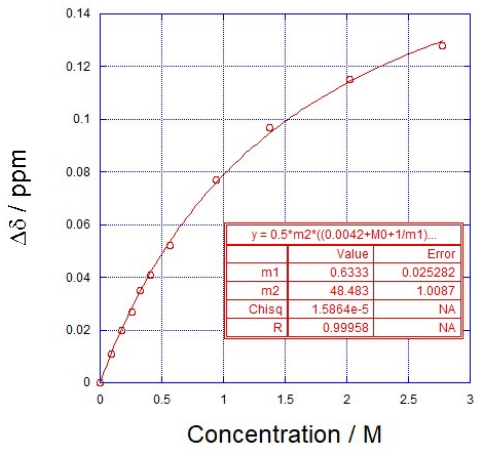


Figure S80 Chemical shift changes of the aromatic proton plotted against the CHL concentration and the least-square-means fit to the 1:1 complexation model to determine the K_a value; K_a = 0.63 ± 0.02 M^{-1}.

[1]H NMR Spectral Titration of DEP[5] with **CTC**

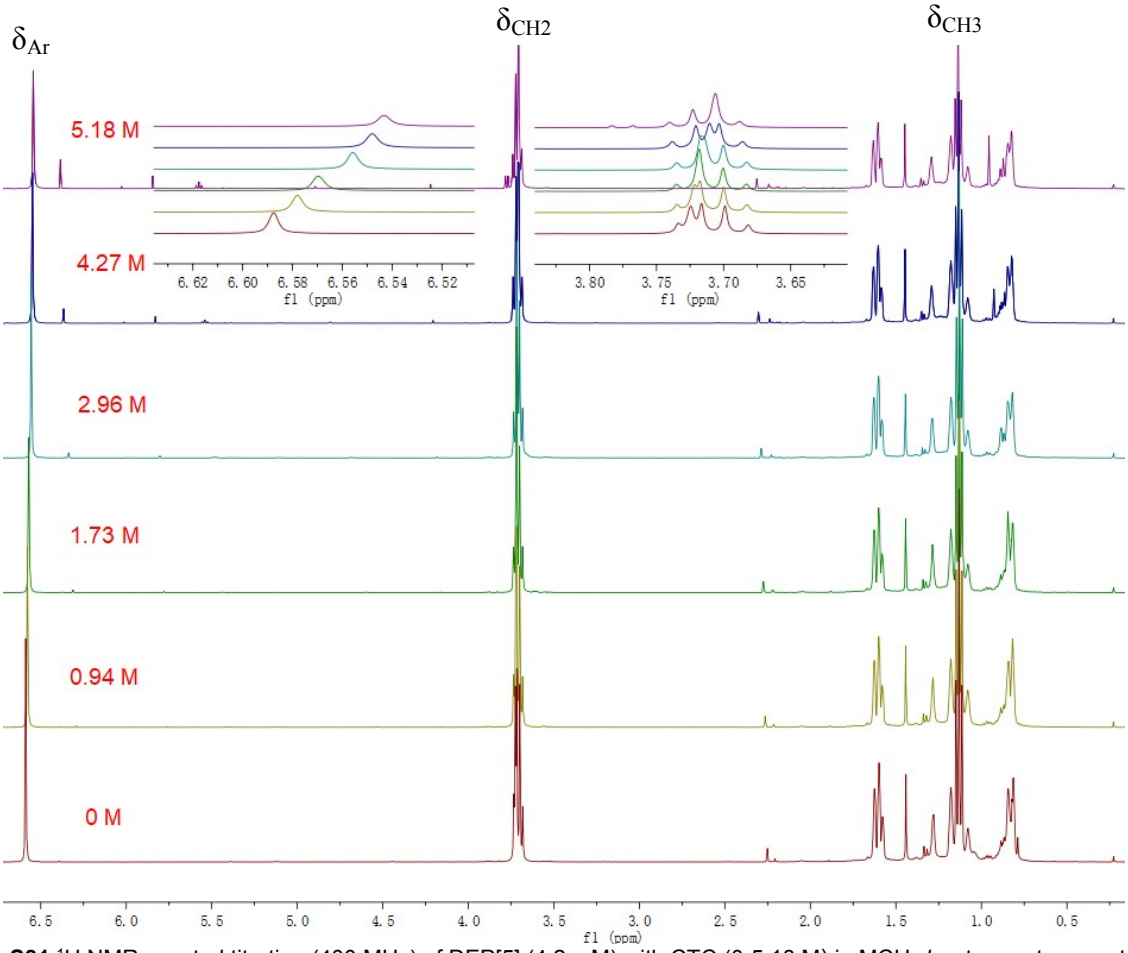


Fig. S81 [1]H NMR spectral titration (400 MHz) of DEP[5] (4.2 mM) with CTC (0-5.18 M) in MCH-d_{14} at room temperature.

Table S6 Chemical shifts of the aromatic and ethoxy protons of DEP[5] (~4.2 mM) in the presence of 0-5.18 M CTC

[CTC]/M	δ_{Ar}/ppm	δ_{CH2}/ppm	δ_{CH3}/ppm
0.0	6.588	3.699	1.131
0.94	6.578	3.700	1.131
1.73	6.570	3.700	1.130
2.96	6.556	3.700	1.129
4.27	6.548	3.703	1.133
5.18	6.543	3.706	1.136
$\Delta\delta$[a]	*–0.045*	*–0.007*	*–0.005*

[a] $\Delta\delta = \delta$(5.18 M) – δ(0 M).

^{1}H NMR Spectral Titration of DEP[5] with **AN**

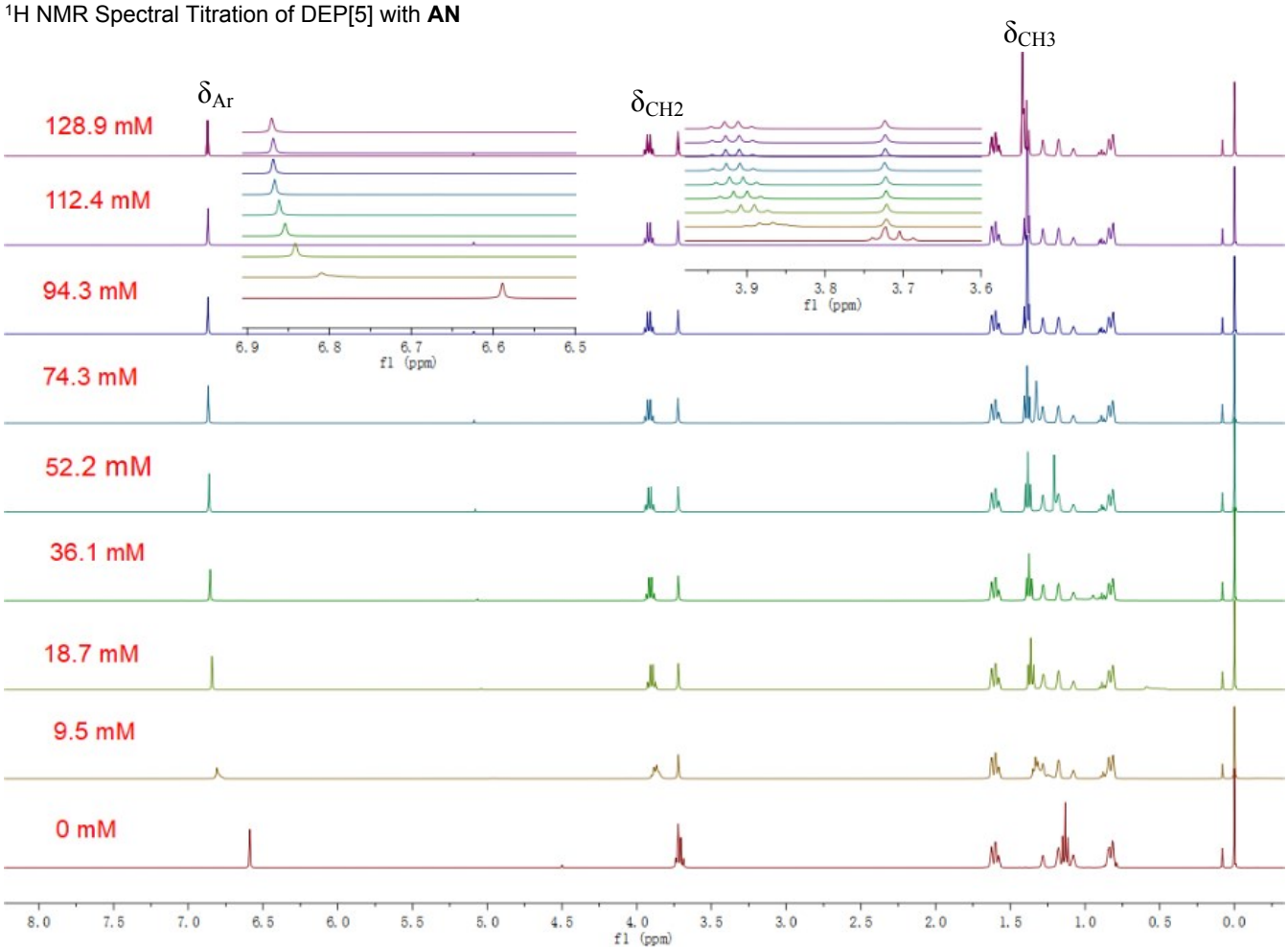


Fig. S82 ^{1}H NMR spectra (400 MHz) of DEP[5] (4.3 mM) upon titration with AN (0-128.9 mM) in MCH-d_{14} at room temperature.

Table S7 Chemical shifts of the aromatic and ethoxy protons of DEP[5] (4.3 mM) in the presence of 0-128.9 mM AN

[AN]/mM	δ_{Ar}/ppm	δ_{CH2}/ppm	δ_{CH3}/ppm
0.0	6.589	3.704	1.132
9.5	6.810	3.850	1.333
18.7	6.842	3.891	1.362
36.1	6.854	3.900	1.375
52.2	6.861	3.905	1.382
74.3	6.867	3.909	1.388
94.3	6.869	3.910	1.390
112.4	6.869	3.910	1.390
128.9	6.871	3.911	1.393
$\Delta\delta$[a]	*0.282*	*0.207*	*0.261*

[a] $\Delta\delta = \delta$(0.1289 M) – δ(0 M).

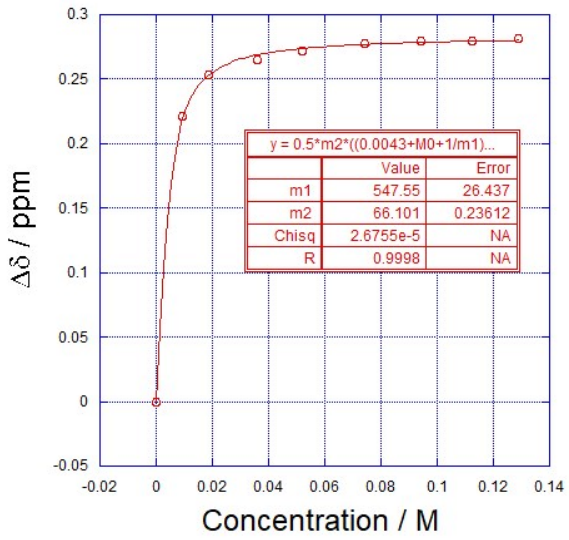


Figure S83 Chemical shift changes of the aromatic proton plotted against the AN concentration and the least-square-means fit to the 1:1 complexation model to determine the K_a value; K_a = 550 ± 30 M^{-1}.

9. Appendix

Table S8 Geometries of (a) *in*-(S_p)- and (b) *out*-(R_p)-**MUJ1**, (c) *in*-(S_p)- and (d) *out*-(R_p)-**MUJ2,** and (e) *in*-(S_p)- and (f) *out*-(R_p)-**MUJ3**, all optimized at the DFT-B3LYP/6-31G(d) Level

(a) *in*-(S_p)-**MUJ1**

Atom	x	y	x
C	-1.10711700	3.46444900	-2.15496300
C	0.28648300	3.56097300	-2.18410100
C	0.98685900	4.03711200	-1.06222000
C	0.24364100	4.43729800	0.05299700
C	-1.15330500	4.35008000	0.07605100
C	-1.84933300	3.84232200	-1.03321600
C	-3.36424600	3.67550500	-1.02906400
C	-4.37881200	-0.02172500	-1.09436800
C	-3.98583700	1.24485700	-1.53040200
C	-3.80530900	2.28178600	-0.60168000
C	-3.99128400	1.98926300	0.75162500
C	-4.24212900	0.68880600	1.19417100
C	-4.46141900	-0.33855200	0.26349900
C	-4.72302500	-1.77503800	0.69620900
O	-4.31430200	0.33060800	2.52368700
O	-3.77733300	1.56975600	-2.85366700
C	-3.58061400	0.56230100	-3.83431000
C	-2.50814300	-0.49225200	-3.52219000
O	-1.40969600	0.10627300	-2.87235800
C	-0.55009200	-0.84250500	-2.24905000
C	0.28080500	-0.20423500	-1.15459600
O	-0.51668200	0.07597000	-0.01095000
C	-3.76251700	1.15583300	3.53817100
C	-2.31201800	1.61432400	3.33022100
O	-1.54466000	0.57464700	2.76588600
C	-0.32197600	1.03691100	2.20251600
C	0.23521900	0.05148300	1.19487700
C	3.55277000	1.89660800	-1.75971000
C	4.12130900	0.64769500	-1.48837500
C	4.34034400	0.23667200	-0.16998500
C	3.99931800	1.12912200	0.85930800
C	3.43783700	2.37965100	0.58555500
C	3.18446200	2.77809500	-0.74475100
C	2.50884700	4.10668000	-1.06011800
C	4.86724400	-1.15435900	0.15349600
C	3.09975500	-2.79427800	-0.63238200
C	2.01696100	-3.65394200	-0.41690400
C	1.54459100	-3.88340800	0.88807500
C	2.21472500	-3.26248300	1.94708400
C	3.29976500	-2.40492900	1.73219000
C	3.74585000	-2.14729600	0.42687600
C	0.33023400	-4.76661200	1.14699200
C	-1.75604200	-4.07189900	-0.13216400
C	-2.96438400	-3.37678800	-0.25672200
C	-3.44663400	-2.59956800	0.80889500
C	-2.70483900	-2.58114200	1.99222200
C	-1.50660700	-3.28773400	2.12442500
C	-1.00039400	-4.03114400	1.04456900
O	-1.91445200	4.73044300	1.16733900
C	-2.41203800	6.04313100	3.08829700
C	-1.31348100	5.56016200	2.15545400
O	1.04834300	3.21202900	-3.27466000
C	1.44803100	2.45007000	-5.49280300
C	0.38303200	2.74785000	-4.45039600
O	3.09592100	3.28533600	1.56113400
C	3.04138300	4.19862600	3.75580100
C	3.43163100	2.99525100	2.91425500
O	4.41482600	-0.21561500	-2.53807800
C	5.71769700	-0.86296800	-4.43496700
C	5.56208700	0.15055600	-3.31465300
O	3.97689600	-1.76330200	2.74822700
C	4.64711200	-1.36455700	4.99412000
C	3.67525300	-2.11018000	4.09483900
O	1.35585300	-4.30849700	-1.43142100
C	1.05927700	-5.14672200	-3.63761300
C	1.89313400	-4.23939800	-2.74871200
O	-0.76541200	-3.30617500	3.28523300
C	-0.36637600	-2.92217100	5.60198800
C	-1.29757100	-2.64530300	4.43362900
O	-3.72971600	-3.39529500	-1.40940000
C	-4.61620400	-4.38384800	-3.38360600
C	-3.48694000	-4.42075200	-2.36695800
H	-1.64750700	3.05488300	-2.99748600
H	0.78550200	4.80399700	0.91712500
H	-3.80315600	4.41105000	-0.34878900
H	-3.74399400	3.88406300	-2.03316600
H	-4.58427700	-0.81116800	-1.80637100
H	-3.88865900	2.80203200	1.45990800
H	-5.23013000	-1.77659700	1.66501100
H	-5.39151200	-2.24804500	-0.02908700
H	-3.29975800	1.12906700	-4.72695000
H	-4.52331600	0.03757500	-4.05897300
H	-2.21338100	-0.95415700	-4.48368200
H	-2.91224000	-1.29346600	-2.89385300
H	0.12869200	-1.28029500	-3.00223900
H	-1.13984700	-1.65583500	-1.80618100
H	0.76091900	0.71335900	-1.52382500
H	1.07579100	-0.91965200	-0.90393500
H	-4.38402000	2.05084600	3.70372800
H	-3.83406100	0.53588500	4.43683000
H	-2.26638900	2.49674500	2.68230900
H	-1.92050300	1.92101900	4.31895400
H	-0.47785600	1.99850000	1.69567200
H	0.42342000	1.18792900	3.00440200
H	1.27629900	0.34801700	1.00591800
H	0.24875500	-0.96280100	1.61887700
H	3.35545900	2.17229400	-2.79018300
H	4.16241300	0.80749900	1.88128300
H	2.82658700	4.85273700	-0.32580200
H	2.85040200	4.44402100	-2.04390300
H	5.52180300	-1.10113600	1.02748100
H	5.46192400	-1.51587400	-0.68985300
H	3.44816300	-2.58277100	-1.63693600
H	1.84419500	-3.44095600	2.94867200
H	0.42190900	-5.19940800	2.14825000
H	0.33063000	-5.59171000	0.42839200
H	-1.36615000	-4.64760800	-0.96334600
H	-3.07160700	-1.96532900	2.80191500
H	-1.99059500	6.68866600	3.86681000
H	-3.16566700	6.61134200	2.53417200
H	-2.90936000	5.19739400	3.57494200
H	-0.80785100	6.40815800	1.67180300
H	-0.55302000	4.99599500	2.71660000
H	2.04408400	3.34350500	-5.70656700
H	0.97859400	2.11651800	-6.42509400
H	2.12106600	1.65895900	-5.14534500
H	-0.30779900	3.52318000	-4.81386400
H	-0.20173300	1.85083700	-4.21328900
H	3.57291600	5.09416300	3.41883600

H	3.29110500	4.02079500	4.80755000
H	1.96526700	4.38833100	3.68396900
H	4.50936200	2.79339600	2.99649400
H	2.89638400	2.09540900	3.25115900
H	6.58531400	-0.61312000	-5.05554600
H	5.86122200	-1.87005000	-4.02944000
H	4.82660000	-0.87235800	-5.07131500
H	6.45388900	0.16691700	-2.67035900
H	5.43121700	1.16339600	-3.72076400
H	5.67977400	-1.64269000	4.76101700
H	4.45022700	-1.60539000	6.04450300
H	4.54480900	-0.28207100	4.86341200
H	3.77067300	-3.19687800	4.23216200
H	2.63713600	-1.83454900	4.33141800
H	1.44395600	-5.12711000	-4.66318800
H	1.08989300	-6.17882000	-3.27416100
H	0.01488700	-4.81761000	-3.65509700
H	2.94488400	-4.56021000	-2.73993900
H	1.86464900	-3.20346600	-3.11625200
H	-0.75267900	-2.44834500	6.51133500
H	-0.27903400	-3.99861600	5.78227400
H	0.63483900	-2.52331300	5.40753000
H	-2.30453000	-3.03163400	4.64854300
H	-1.37996700	-1.56937200	4.23390900
H	-5.58047100	-4.55526600	-2.89498600
H	-4.46715000	-5.15902700	-4.14341300
H	-4.65508200	-3.41190200	-3.88686600
H	-3.44310900	-5.39680100	-1.86312700
H	-2.51767300	-4.25860800	-2.86231500

(b) *out*-(R_p)-**MUJ1**

Atom	x	y	x
C	-3.76175600	2.87888900	-1.34168800
C	-3.43697600	3.53447200	-0.15040300
C	-3.94172600	3.01808300	1.05289800
C	-4.73586400	1.86717900	1.04211100
C	-5.05132700	1.20327300	-0.14679600
C	-4.56106200	1.73256600	-1.35309800
C	1.00733400	3.72675400	-1.25016000
C	1.64030700	3.47325300	-0.03364000
C	0.90406100	3.69897200	1.14679400
C	-0.42057700	4.13555600	1.08378500
C	-1.05420600	4.37503800	-0.14365000
C	-0.31290400	4.18281700	-1.31621900
C	-2.52772300	4.75440500	-0.17426500
C	3.06076000	2.93080100	0.01642500
C	-0.32306100	-4.21219600	-1.14205400
C	-0.97672000	-4.41101400	0.07787900
C	-0.26140000	-4.16945400	1.26208900
C	1.06303100	-3.72595200	1.20299100
C	1.70898500	-3.50686900	-0.01693400
C	0.99946500	-3.76477500	-1.20094700
C	-2.43970900	-4.82928700	0.10671100
C	3.12948500	-0.69190700	-1.22014500
C	3.14247700	-1.42897800	-0.03129200
C	3.15797500	-0.71872700	1.17819300
C	3.09273500	0.67605000	1.18148100
C	3.10919800	1.41224700	-0.00344800
C	3.16898400	0.70285000	-1.21337900
O	3.25121900	1.45845600	-2.36542900
O	3.22867000	-1.45555600	2.34669000
C	3.12305700	-2.94846600	-0.04973100
C	-4.64924800	-1.99367400	-1.22101800
C	-5.04011000	-1.33501700	-0.05151800
C	-4.61283100	-1.86070600	1.17915600
C	-3.79328000	-2.99270900	1.21193800
C	-3.38404500	-3.63777100	0.04109500
C	-3.83706000	-3.13089800	-1.18768400
C	-5.88388900	-0.07055100	-0.12220500
C	4.02195000	0.99452000	-3.46628100
C	5.38514200	0.38941800	-3.13253600
O	6.06524900	1.19741400	-2.19389100
C	4.03871800	-0.95184500	3.40795900
C	5.45746600	-0.57515400	3.00525600
O	6.10903000	-1.72862500	2.49221000
C	7.43804000	-1.50436000	2.05919300
C	7.57392200	-0.97285700	0.63402700
C	7.37033500	0.72677800	-1.90723900
C	7.79416400	1.12662900	-0.49604900
O	7.19560000	0.39455500	0.56114600
O	-4.91841800	1.06865400	-2.50569100
C	-5.11367700	0.75574900	-4.85594000
C	-4.52220900	1.62188900	-3.75636700
O	-3.60678600	3.70156900	2.20394900
C	-3.71007100	4.24089900	4.51621600
C	-4.17320400	3.27642500	3.43684000
O	-0.90842600	4.37733500	-2.55840900
C	0.55946400	5.95720400	-3.77323900
C	-0.78758300	5.69928800	-3.10674000
O	1.56521200	3.45804800	2.32887500
C	1.85314800	3.40789200	4.68830500
C	0.88517200	3.70359400	3.55483000
O	1.67800400	-3.54778700	-2.38234000
C	1.99486700	-3.55742400	-4.73762100
C	1.01785300	-3.83767700	-3.60761500
O	-0.93552500	-4.38995800	2.44451100
C	-1.17110600	-4.59165000	4.80187900
C	-0.22660000	-4.22934000	3.66790400
O	-3.43497300	-3.81064100	-2.31868900
C	-3.43768100	-4.37150700	-4.62864400
C	-3.95168300	-3.40072700	-3.57832400
O	-5.04699700	-1.20459500	2.31157000
C	-5.42087100	-0.92143100	4.64329800
C	-4.74077300	-1.76878300	3.58068600
H	-3.34652600	3.27493600	-2.26085100
H	-5.10818400	1.44301800	1.96636100
H	1.54055700	3.53046200	-2.17466100
H	-1.00404500	4.26748600	1.98673000
H	-2.74184600	5.33211800	-1.07739900
H	-2.75478700	5.39056200	0.68566800
H	3.62091900	3.31026200	-0.84221100
H	3.55240400	3.29185200	0.92405600
H	-0.89031600	-4.38748400	-2.04773700
H	1.61522800	-3.50625300	2.10861000
H	-2.63887100	-5.49279100	-0.73963400
H	-2.63608300	-5.39115200	1.02397700
H	3.09414300	-1.23271800	-2.16027700
H	3.04731400	1.21703900	2.12064200
H	3.63029900	-3.30382400	-0.95103800
H	3.67976900	-3.31476400	0.81740400
H	-4.97654100	-1.57523000	-2.16464100
H	-3.43008600	-3.38649500	2.15346700
H	-6.50487300	-0.11013600	-1.02204800
H	-6.55354800	-0.03745100	0.74229800

H	3.46130200	0.25605700	-4.06162500
H	4.15731000	1.88602600	-4.08577400
H	5.28027900	-0.62935700	-2.73456300
H	5.94362600	0.31437000	-4.08304000
H	4.06643300	-1.76584100	4.13823300
H	3.56617600	-0.08171700	3.88864700
H	5.97821400	-0.20879200	3.90816000
H	5.45953100	0.23184600	2.26641700
H	7.93131900	-2.48369400	2.09416600
H	7.96902700	-0.83013000	2.75014100
H	8.62947900	-1.09084100	0.33103900
H	6.95727100	-1.58969200	-0.03583900
H	7.42020500	-0.36755000	-2.01495300
H	8.09268800	1.15298500	-2.62512000
H	8.89322700	1.03756400	-0.43527900
H	7.52487800	2.17332300	-0.32505800
H	-4.84770000	1.16078200	-5.83854100
H	-4.73248400	-0.26886900	-4.79189600
H	-6.20510700	0.72293800	-4.77700700
H	-3.42568000	1.64933400	-3.82738500
H	-4.88773900	2.65582800	-3.84008800
H	-4.03274900	5.26128300	4.28613200
H	-2.61801800	4.23597900	4.59831600
H	-4.13052400	3.95334000	5.48617400
H	-3.84975900	2.25030400	3.66683100
H	-5.27065600	3.27124500	3.36480000
H	1.37688000	5.91503800	-3.04696000
H	0.56451000	6.95234000	-4.23470900
H	0.75062700	5.21273700	-4.55350300
H	-0.97677900	6.44569200	-2.32248400
H	-1.59451100	5.77348000	-3.84399600
H	1.37325300	3.59963900	5.65435400
H	2.17101700	2.36020800	4.66370400
H	2.74308000	4.04058100	4.61069500
H	-0.00613800	3.06353400	3.62493500
H	0.54924800	4.75014800	3.59340600
H	1.53171500	-3.78584300	-5.70387800
H	2.29337300	-2.50366700	-4.73954200
H	2.89489000	-4.17132600	-4.62988500
H	0.11719400	-3.21442600	-3.70794800
H	0.69853600	-4.89031600	-3.62322200
H	-1.52428100	-5.62239800	4.69598300
H	-2.04277900	-3.92852500	4.80927300
H	-0.65798300	-4.49703500	5.76528100
H	0.12508600	-3.19233600	3.76777900
H	0.65841500	-4.88234300	3.67635200
H	-3.76184100	-5.39214700	-4.40184900
H	-2.34329500	-4.35884400	-4.66676100
H	-3.82058300	-4.09613900	-5.61752600
H	-3.62562800	-2.37444600	-3.80375800
H	-5.05114000	-3.40255300	-3.55229200
H	-5.22239400	-1.33346100	5.63890100
H	-5.04909100	0.10833900	4.61659300
H	-6.50387000	-0.90077500	4.48515000
H	-3.65161700	-1.78535700	3.73425000
H	-5.09922800	-2.80760800	3.62562000

(c) *in*-(S_p)-**MUJ2**

Atom	x	y	x
C	-2.20725200	-3.51181200	-0.57866100
C	-3.15522600	-2.53471100	-0.90750100
C	-3.81116100	-1.81103300	0.09872600
C	-3.51366900	-2.13837500	1.43025400
C	-2.58332200	-3.13189400	1.75418000
C	-1.89401800	-3.83315200	0.74301800
C	-0.84635100	-4.89559900	1.07121400
C	2.70933200	-3.79075700	0.13917600
C	1.46683400	-4.43073600	0.06443200
C	0.57076800	-4.33619400	1.14662000
C	0.98644600	-3.64666600	2.28599300
C	2.20397200	-2.96395800	2.33997900
C	3.08852400	-3.02710900	1.25143100
C	4.40919000	-2.25881900	1.24601600
O	2.58460400	-2.19395100	3.42511100
O	1.02617600	-5.17927200	-1.00685200
C	1.57559500	-1.49749200	4.17172900
C	1.03654400	-0.24108600	3.47351200
C	0.41148900	-0.48161800	2.09411100
C	1.77442200	-5.28594700	-2.21982800
C	1.22890800	-4.35840400	-3.30751200
C	1.22135300	-2.87531400	-2.92210000
C	-0.03061400	0.78455200	1.36380400
C	0.66888400	-1.96488900	-4.02277600
C	-0.61079200	0.49630500	-0.03075000
C	0.64036100	-0.46962500	-3.66095400
C	0.37826600	-0.00220500	-1.09618300
C	-0.28636900	-0.08344000	-2.48431500
C	-3.82108400	1.15165300	-1.65878900
C	-3.21545200	2.40010100	-1.83989900
C	-2.93587400	3.22184000	-0.73946900
C	-3.36220200	2.78474300	0.52374200
C	-3.99009300	1.54714300	0.69816500
C	-4.19994700	0.68718100	-0.39931500
C	-4.81049300	-0.69964200	-0.22117600
C	-2.11456200	4.50138800	-0.87332000
C	0.15645000	3.89272200	-1.83648600
C	1.52480200	3.61903800	-1.72647000
C	2.16743800	3.71631600	-0.47936900
C	1.40523000	4.12478900	0.62003700
C	0.03625000	4.39631800	0.51057600
C	-0.61229100	4.26799700	-0.72915000
C	3.64646400	3.37652700	-0.31731500
C	4.09382400	0.93356000	-0.87217000
C	4.29277500	-0.40739600	-0.52265500
C	4.28560400	-0.79664000	0.82906300
C	4.16701000	0.21109000	1.79124500
C	3.98958700	1.55451800	1.44300800
C	3.91456300	1.93197400	0.09204700
O	-2.27910000	-3.48265900	3.04977600
C	-2.60602100	-3.60054700	5.40240000
C	-3.05617300	-2.93717300	4.11155100
O	-3.39891600	-2.23849000	-2.24280300
C	-3.91500000	-4.37974300	-3.37761500
C	-4.41423500	-3.02465000	-2.88878800
O	-4.42360000	1.08638400	1.91873000
C	-4.94719100	1.23175800	4.23489200
C	-4.30519800	1.93915700	3.05341900
O	-2.79973100	2.77467400	-3.11287100
C	-4.83849400	2.69656400	-4.51398900
C	-3.74381200	3.54408200	-3.87554200
O	-0.74774800	4.78711900	1.57490800
C	-1.19028400	5.50850700	3.79635800
C	-0.12401200	5.01156000	2.83430300
O	2.31034400	3.24133700	-2.79221200

C	2.86225300	2.96461500	-5.08789300
C	1.75439300	3.29833700	-4.10328100
O	3.86020100	2.56350800	2.37726700
C	4.33157200	3.66079500	4.43453800
C	4.33638000	2.33006800	3.70066000
O	4.50534500	-1.40273200	-1.45242400
C	5.41312700	-2.26858300	-3.47860100
C	4.92249400	-1.02137000	-2.76226700
H	-1.69094500	-4.02696000	-1.38247400
H	-4.01204300	-1.57924100	2.21267000
H	-0.88546400	-5.67587300	0.30790800
H	-1.10112500	-5.35616800	2.03031500
H	3.39821800	-3.81698500	-0.69533100
H	0.28976700	-3.58977200	3.11288300
H	5.10006100	-2.76416900	0.56398500
H	4.84854600	-2.29699300	2.24743200
H	2.07844600	-1.22183500	5.10494200
H	0.75559300	-2.17530200	4.43914900
H	1.85032400	0.48689100	3.37510000
H	0.29609500	0.21178600	4.15238500
H	1.14111400	-0.99024000	1.46257700
H	-0.44174500	-1.16596200	2.18805500
H	2.84006900	-5.10831300	-2.04403300
H	1.66855400	-6.33139600	-2.53195700
H	1.82987500	-4.51792500	-4.21605000
H	0.20604500	-4.67586900	-3.55480300
H	2.23551100	-2.55226200	-2.65125800
H	0.61578200	-2.75537600	-2.01904100
H	0.81942300	1.47247800	1.27371900
H	-0.79300500	1.31294000	1.95734800
H	1.26380000	-2.10134900	-4.93917200
H	-0.35410400	-2.28431500	-4.27253300
H	-1.06748500	1.41568300	-0.40344700
H	-1.42570200	-0.23131500	0.06925500
H	1.66354800	-0.12250300	-3.45071300
H	0.31737200	0.07563200	-4.55916000
H	1.22986400	0.68817700	-1.15135200
H	0.79297500	-0.97628400	-0.81066300
H	-1.13487800	-0.78086100	-2.45104500
H	-0.72646900	0.89861600	-2.69844700
H	-3.94902500	0.50720200	-2.52220900
H	-3.14294700	3.41487300	1.37722200
H	-5.34550800	-0.95347000	-1.14067300
H	-5.55113500	-0.65903400	0.58340500
H	-2.30103100	4.95751200	-1.84961200
H	-2.43920500	5.21481800	-0.11089800
H	-0.35227400	3.78093100	-2.78663400
H	1.90520400	4.19124200	1.57879800
H	4.15806400	3.57478100	-1.26314000
H	4.07613500	4.03997400	0.43905400
H	4.04792200	1.22659100	-1.91469200
H	4.19200400	-0.08431100	2.83303700
H	-3.18760600	-3.21487000	6.24692000
H	-2.74727000	-4.68452500	5.34847100
H	-1.54647900	-3.40132700	5.59393000
H	-4.12329100	-3.12511000	3.92571200
H	-2.91253600	-1.84785700	4.16296900
H	-3.62373200	-5.02451500	-2.54294300
H	-3.05025800	-4.25345400	-4.03789200
H	-4.70763400	-4.88897200	-3.93938800
H	-4.74291300	-2.41558200	-3.73766000
H	-5.26991400	-3.15133800	-2.21091600
H	-6.00029700	1.01501300	4.02941100
H	-4.89001600	1.86292600	5.12845600
H	-4.43559000	0.28718300	4.44761500
H	-4.80752700	2.89663600	2.85412200
H	-3.24517100	2.15207300	3.25391000
H	-5.48419600	3.32689200	-5.13749800
H	-4.40073900	1.91673800	-5.14613800
H	-5.46351800	2.21683900	-3.75439000
H	-3.14498900	4.03625500	-4.64925800
H	-4.18369000	4.32533500	-3.23993700
H	-0.74903000	5.70818200	4.77904300
H	-1.64464700	6.43262800	3.42511700
H	-1.98142400	4.76121000	3.91953000
H	0.67918200	5.75527600	2.72744200
H	0.32975200	4.07994000	3.20182000
H	3.69066300	3.67410300	-4.99367000
H	2.48061900	3.00813800	-6.11387000
H	3.24794700	1.95592100	-4.90721700
H	1.35306500	4.30474200	-4.29225600
H	0.92640500	2.58263000	-4.19382300
H	4.68969300	3.52774500	5.46135500
H	4.98029500	4.38357400	3.92967200
H	3.31892800	4.07604100	4.47429600
H	5.34904200	1.90425900	3.66056300
H	3.69063600	1.60639500	4.21782300
H	6.25033000	-2.72071600	-2.93725000
H	5.74892800	-2.01385600	-4.48994900
H	4.61328200	-3.01169800	-3.56022700
H	5.72275400	-0.27143100	-2.68979000
H	4.08462000	-0.56652200	-3.30940500

(d) *out*-(R_p)-**MUJ2**

Atom	x	y	x
C	-0.31720300	-4.25225500	-0.96747200
C	-1.56942200	-3.64091600	-0.85370700
C	-2.05828400	-3.19807000	0.37808900
C	-1.26508800	-3.39416400	1.52119000
C	-0.01867300	-4.01681600	1.40868000
C	0.47622200	-4.44814000	0.17381000
C	1.86419600	-5.06310700	0.07762600
C	-3.29794300	-0.38072800	-0.97016200
C	-3.08173600	0.99293600	-1.09820800
C	-2.95639900	1.82781000	0.02214400
C	-3.08766700	1.24365400	1.29121400
C	-3.19183300	-0.14481400	1.41330200
C	-3.28988800	-0.98457500	0.30337700
C	-3.40280500	-2.49202000	0.46718800
O	-3.08628500	1.99851700	2.45668000
O	-3.52795900	-1.21133400	-2.04468400
C	-4.22142000	2.86005400	2.67468500
C	-5.07577600	2.42692200	3.87070400
C	-5.85884700	1.10268300	3.78178700
C	-7.08612200	1.04274200	2.84565400
C	-6.76115600	1.05482600	1.34084000
C	-7.78740900	0.37066200	0.42340300
C	-7.23358500	0.26089900	-1.00456600
C	-8.07566700	-0.53264900	-2.01294400
C	-7.28943700	-0.81244100	-3.31052100
C	4.19455300	-2.31859900	-1.22140000
C	3.24171000	-3.33821700	-1.16147500
C	2.95586900	-4.00483800	0.03406300
C	3.66620000	-3.63753200	1.18698900

C	4.62211700	-2.61747400	1.12666200	H	-8.00084300	-0.63789800	0.80783100
C	4.89356600	-1.93650300	-0.06280900	H	-7.06322700	1.27122500	-1.40609300
C	4.42187400	2.52192800	-1.32527600	H	-6.23881500	-0.19837100	-0.93590400
C	5.06317900	1.28007900	-1.28885000	H	-8.99600500	0.02030500	-2.24573400
C	5.25385100	0.57970900	-0.09954800	H	-8.39540400	-1.48666300	-1.56831400
C	4.80085700	1.18051000	1.09367300	H	-6.80792700	0.12440200	-3.62723600
C	4.14523500	2.41308400	1.06012000	H	-7.98238800	-1.07526200	-4.12014200
C	3.93684000	3.09759100	-0.14600600	H	2.68461300	-3.62890500	-2.04430900
C	5.90157100	-0.79671800	-0.09557200	H	5.15557200	-2.30947100	2.01770600
C	-0.39244100	3.59712100	-1.36253000	H	5.39093400	0.83509100	-2.22101200
C	0.97730500	3.86938100	-1.33391600	H	3.74826400	2.85461800	1.96678100
C	1.64109800	4.15223700	-0.13252600	H	6.55933000	-0.88568200	0.77477500
C	0.89728600	4.15343900	1.05399800	H	6.52484700	-0.88999300	-0.99098500
C	-0.47067600	3.86718100	1.02457100	H	1.56990400	3.84668800	-2.24141300
C	-1.14105200	3.59696400	-0.16817700	H	-1.01568200	3.82215500	1.96226800
C	-2.63463200	3.30348900	-0.17283500	H	-3.10105800	3.90217000	0.61297400
C	3.14293200	4.39483900	-0.14394800	H	-3.05976000	3.63668400	-1.12374000
C	-4.01059800	-0.65583100	-3.27152200	H	3.39662400	4.98552800	-1.02813800
C	-4.92053700	-1.68767300	-3.93904000	H	3.42684900	4.98116900	0.73379700
C	-6.23031300	-1.93332300	-3.16687300	H	-4.56284100	0.26981400	-3.06911400
O	-1.79197900	-2.94809400	2.71162300	H	-3.15896900	-0.40398600	-3.91941400
C	-1.82252900	-2.51300900	5.04798700	H	-5.13782600	-1.34513400	-4.96062300
C	-1.02253300	-3.10306700	3.89871400	H	-4.35954300	-2.62592500	-4.03632100
O	0.21240600	-4.68244600	-2.16679900	H	-6.66842200	-2.88348000	-3.49689800
C	0.19570900	-5.20241200	-4.48527200	H	-5.97242400	-2.07595700	-2.11078500
C	-0.59240000	-4.59559600	-3.33629000	H	-2.78591900	-3.02307800	5.14980900
O	3.35460900	-4.32223300	2.34390200	H	-2.01053500	-1.44760500	4.88084100
C	3.68835000	-5.08532300	4.56901000	H	-1.27047000	-2.62381000	5.98789200
C	4.15534400	-4.11169500	3.49955500	H	-0.05741300	-2.58794800	3.78989300
O	4.51411500	-1.64360900	-2.37593500	H	-0.81499400	-4.16908500	4.07484100
C	4.19372600	-0.90406000	-4.61441300	H	-0.39157900	-5.16285100	-5.40933200
C	3.72826900	-1.87402500	-3.54048100	H	1.13062600	-4.65548500	-4.64641300
O	5.04748400	0.48738500	2.25187700	H	0.44204100	-6.24782800	-4.27414700
C	5.12124500	0.15312600	4.60743200	H	-0.84300700	-3.54530800	-3.54613200
C	4.66074900	1.07535300	3.49166700	H	-1.53678900	-5.13818100	-3.18252000
O	4.20067900	3.13784100	-2.55481400	H	4.27712400	-4.95404800	5.48353600
C	6.44915700	3.39003300	-3.56325900	H	2.63329300	-4.91868500	4.80991300
C	5.21342500	4.06517500	-2.97871100	H	3.80299700	-6.11852000	4.22627700
O	1.52713900	4.37627100	2.27318600	H	4.05114400	-3.07342400	3.84876100
C	0.26735800	6.21559200	3.35345400	H	5.21550300	-4.27534200	3.25711100
C	1.56976700	5.74176000	2.71797800	H	5.25745700	-1.04943400	-4.83016600
O	-1.09680600	3.30677800	-2.50723700	H	4.04220300	0.13142700	-4.29295700
C	-0.27565500	4.71736300	-4.34699900	H	3.62901700	-1.06759200	-5.53918500
C	-0.43784600	3.31227500	-3.77482700	H	2.66491100	-1.71997400	-3.30927200
H	-2.18187600	-3.46616100	-1.72983800	H	3.85014800	-2.91465000	-3.87712500
H	0.60996600	-4.16191700	2.27973400	H	4.64329900	-0.82815500	4.52175600
H	1.92198700	-5.67922900	-0.82356700	H	4.85790800	0.58059100	5.58112100
H	2.03077500	-5.71519500	0.93874900	H	6.20652400	0.01363700	4.57100400
H	-2.98240400	1.43998800	-2.08088800	H	3.57072600	1.21091300	3.51973300
H	-3.21619400	-0.57586700	2.40874000	H	5.12411400	2.06731500	3.59340900
H	-3.85981500	-2.70994800	1.43628700	H	7.15175700	4.14894800	-3.92851500
H	-4.06237500	-2.89026600	-0.30973900	H	6.96432100	2.78417400	-2.81165500
H	-4.81928200	2.92292800	1.76195500	H	6.17411800	2.74171100	-4.40208900
H	-3.82195900	3.86150100	2.88229300	H	5.49442600	4.71597800	-2.13887400
H	-5.77907800	3.24984300	4.07322400	H	4.72547900	4.68605800	-3.73789900
H	-4.40930300	2.37560200	4.74202600	H	0.38987900	7.23477000	3.73993100
H	-6.20715300	0.87402800	4.79844900	H	-0.55038300	6.22473500	2.62631500
H	-5.16794900	0.29340800	3.51464400	H	-0.01517900	5.56162700	4.18528200
H	-7.78521200	1.85426800	3.09606100	H	1.84800700	6.39640400	1.88000000
H	-7.61863600	0.10900600	3.07740500	H	2.38158100	5.77157600	3.45267000
H	-6.61406600	2.08587700	0.99156500	H	-1.25113700	5.20779400	-4.42938500
H	-5.80098900	0.54814600	1.19014700	H	0.17179400	4.66656700	-5.34663300
H	-8.74450800	0.91264300	0.42954000	H	0.36677100	5.33808800	-3.71564500

H	-1.09035200	2.71625500	-4.42068100
H	0.52370600	2.78908500	-3.70719900

(e) *in*-(S_p)-**MUJ3**

Atom	x	y	x
O	-1.23700100	0.68660800	-4.72701400
O	-3.14163800	1.87980000	-2.76957800
O	-1.10354300	1.64941500	-0.56701300
O	1.34449100	-1.07128100	-0.04708200
O	3.50202800	-2.09762800	1.61011000
O	5.75668600	-1.74027100	-0.22691000
O	3.95327800	-0.44933100	-3.10798000
O	1.24808300	4.32206000	-2.40194300
O	4.10499600	2.11795200	1.81452700
O	-0.76136000	4.42136200	2.48386700
O	0.68884400	-0.48125700	4.64795400
O	-4.25161300	0.60047700	2.81158700
O	-1.62227900	-4.22145900	2.00881100
O	-4.55529800	-1.67160800	-1.73867900
O	0.32296000	-4.06740600	-2.86227300
C	-1.76487500	2.00872600	-4.73537500
C	-2.05378800	2.58484800	-3.35622600
C	-3.31283300	2.13653600	-1.38073500
C	-2.46286600	1.25604100	-0.47560100
C	-0.19467200	0.83812600	0.18236900
C	0.17235100	-0.44617200	-0.56873600
C	1.15414700	-1.87422000	1.10074000
C	2.33414500	-2.81803300	1.24167100
C	4.69027400	-2.87296200	1.60005500
C	5.31337200	-3.01492300	0.21334100
C	5.51576200	-1.42763300	-1.59303500
C	4.03384800	-1.16883600	-1.87162700
C	2.66118400	-0.12967600	-3.50183600
C	1.78018600	-1.14590200	-3.88893300
C	0.46746300	-0.88257700	-4.27661600
C	0.06123300	0.46777300	-4.32521000
C	0.95558900	1.48565000	-3.98713500
C	2.25552600	1.21009000	-3.53564400
C	3.16318900	2.34725000	-3.07523400
C	2.90123100	2.80106300	-1.64247300
C	1.91408300	3.75276000	-1.33529500
C	1.64361500	4.08174100	-0.00264500
C	2.35393300	3.50941700	1.05652000
C	3.39050500	2.60988100	0.75034500
C	3.64237700	2.26520400	-0.58297900
C	5.20852900	1.24673500	1.55837200
C	5.86744200	0.93640200	2.89130700
C	0.43581000	5.46600900	-2.15720900
C	0.05768900	6.06801900	-3.50060800
C	1.98526700	3.82411700	2.50042900
C	0.93187200	2.87802500	3.06559800
C	-0.43692500	3.19470500	3.01892100
C	-1.38567700	2.28626900	3.50204600
C	-1.01471200	1.04614500	4.03553600
C	0.35573100	0.73964300	4.10013400
C	1.30399000	1.64906600	3.61876100
C	-2.12595900	4.81967400	2.46348300
C	-2.19053100	6.21696000	1.86935500
C	2.06561700	-0.76167400	4.90703900
C	2.12903800	-2.05986200	5.69459200
C	-2.07208800	0.05921500	4.51771000
C	-2.53736300	-0.90988200	3.43789100
C	-3.60681200	-0.59732700	2.58133100
C	-3.95827100	-1.46540600	1.54261900
C	-3.28082200	-2.67043100	1.32717600
C	-2.25472500	-3.01273300	2.22322100
C	-1.89266600	-2.13696100	3.25206900
C	-5.53062100	0.80781400	2.21740400
C	-6.12436800	2.06911200	2.82220900
C	-0.88155200	-4.79718800	3.08186600
C	-0.52678900	-6.22148700	2.68856500
C	-3.63035800	-3.55812100	0.13867200
C	-2.85418700	-3.20279700	-1.12412900
C	-3.33057700	-2.23488300	-2.02447700
C	-2.56597000	-1.87416900	-3.13998700
C	-1.33032400	-2.46769700	-3.41064500
C	-0.87633300	-3.47334700	-2.53828900
C	-1.63067300	-3.82096800	-1.41175600
C	-5.22440300	-0.94636800	-2.77572400
C	-6.62839800	-0.63555800	-2.28434700
C	0.75315300	-5.19309800	-2.10859600
C	2.02400900	-5.72233200	-2.75257500
C	-0.49824900	-2.01471600	-4.60511400
H	-2.70097400	1.92744100	-5.29589100
H	-1.09705600	2.68706100	-5.28461500
H	-1.17473700	2.53218100	-2.71061000
H	-2.32517400	3.64868000	-3.48634800
H	-4.36913700	1.93268700	-1.16555800
H	-3.12151800	3.19843400	-1.15868300
H	-2.82182600	1.36469100	0.56179100
H	-2.60396100	0.20865100	-0.76977100
H	-0.60982100	0.62852200	1.17671400
H	0.70775300	1.43751600	0.30775800
H	0.41479800	-0.18178700	-1.59809100
H	-0.65880200	-1.16378000	-0.58331800
H	0.24507600	-2.48536700	0.99804300
H	1.05007800	-1.26929400	2.01225400
H	2.10727400	-3.57636200	2.01184600
H	2.47618400	-3.34267300	0.28505400
H	4.51052300	-3.87493600	2.02541200
H	5.39934600	-2.35061400	2.25058600
H	6.16767300	-3.70963700	0.27448300
H	4.58849600	-3.44985100	-0.48631700
H	5.91366100	-2.20924100	-2.25830300
H	6.07704500	-0.50908400	-1.79018600
H	3.46581200	-2.10509300	-1.94387500
H	3.59091200	-0.58931500	-1.05645800
H	2.11984600	-2.17648600	-3.85867400
H	0.65188600	2.52344000	-4.01505100
H	3.02932200	3.20008200	-3.74872400
H	4.20259800	2.01933300	-3.15612400
H	0.84145500	4.76783800	0.24192900
H	4.42695300	1.55733300	-0.82064200
H	5.92165800	1.74331000	0.88423300
H	4.86201800	0.32657500	1.07585000
H	6.73328300	0.28414800	2.73313500
H	6.20713500	1.85342000	3.38410300
H	5.16676900	0.42390000	3.55913000
H	0.99300500	6.19427800	-1.55126500
H	-0.46148400	5.17521200	-1.59139400
H	-0.56474500	6.95752200	-3.35282700
H	0.95366700	6.35880100	-4.05803100
H	-0.50653900	5.35203100	-4.10731900
H	1.61041200	4.84943000	2.55798900

H	2.88495100	3.76259700	3.11907900
H	-2.44312300	2.51703200	3.45462000
H	2.35897900	1.40404100	3.63437400
H	-2.53541200	4.81213500	3.48445700
H	-2.71606100	4.11289000	1.86154600
H	-3.22693600	6.57158900	1.84812600
H	-1.59584400	6.91682900	2.46492400
H	-1.80296600	6.22046200	0.84521300
H	2.50817600	0.06317000	5.48302400
H	2.61656400	-0.85549100	3.96130800
H	3.17077100	-2.30960600	5.92401600
H	1.57652500	-1.97156600	6.63557800
H	1.69808700	-2.88604600	5.11861500
H	-1.66506600	-0.51512300	5.35493800
H	-2.93533700	0.62036000	4.88690100
H	-4.75091100	-1.20405900	0.85192900
H	-1.07219200	-2.38061500	3.91652100
H	-5.43131400	0.91334800	1.12707400
H	-6.17376400	-0.06253700	2.40977700
H	-7.11279400	2.26455900	2.39218300
H	-6.23056800	1.96421400	3.90651300
H	-5.48427200	2.93465500	2.62118600
H	-1.48500500	-4.77865900	4.00027600
H	0.03096700	-4.21331600	3.27260400
H	0.05100000	-6.70122400	3.48618400
H	-1.43219900	-6.81044500	2.51163600
H	0.07441200	-6.23202300	1.77312500
H	-3.42569700	-4.60007400	0.40021300
H	-4.70100600	-3.46818000	-0.06679600
H	-2.90542900	-1.08814100	-3.80256100
H	-1.27121800	-4.57221200	-0.71829100
H	-5.25812600	-1.56123400	-3.68651200
H	-4.67614600	-0.02525900	-3.00627500
H	-7.18162200	-0.08346400	-3.05203600
H	-7.17464900	-1.55642000	-2.05551900
H	-6.59702700	-0.02097800	-1.37775500
H	-0.03204600	-5.96322500	-2.10251300
H	0.94019500	-4.90081100	-1.06431600
H	2.38997400	-6.59783300	-2.20490400
H	1.83722800	-6.01463700	-3.79064000
H	2.80802100	-4.95763300	-2.74830700
H	-1.17522100	-1.69046800	-5.40088400
H	0.07552100	-2.86555300	-4.98324800

(f) *out*-(R_p)-**MUJ3**

Atom	x	y	x
C	1.31627200	4.19303800	-0.92497300
C	-0.00881100	3.83153500	-1.18388900
C	-0.36311000	3.12313200	-2.33560800
C	0.64809700	2.78439600	-3.24788100
C	1.97352800	3.14645100	-2.98911100
C	2.33149500	3.84390300	-1.83169300
C	3.78936100	4.18209900	-1.55532400
C	-2.60040600	1.29809300	-0.58327200
C	-2.79546200	0.06624700	0.04180700
C	-2.57513900	-1.14056500	-0.62861800
C	-2.15603600	-1.06801300	-1.96835900
C	-1.92071300	0.16506100	-2.57977300
C	-2.13405400	1.37178300	-1.90357000
C	-1.80761700	2.70312600	-2.56237900
O	-1.92362400	-2.25805800	-2.63853000
O	-2.85188700	2.46275800	0.13870000
C	-4.22672100	2.85737000	0.13059700
C	-4.41603100	3.94157200	1.19115000
O	-5.71686100	4.50716000	1.11037400
C	-2.58572100	-2.44944400	-3.88965600
C	-4.09759500	-2.56330300	-3.77482300
O	-4.41503000	-3.73850900	-3.03976400
C	-5.80080000	-4.00335700	-2.89378000
C	-6.44211800	-3.30368800	-1.70189100
O	-6.58920700	-1.91693100	-1.98073900
C	-6.57973200	-1.06334800	-0.84958700
C	-7.91845200	-1.01887000	-0.11009900
O	-7.72514600	-0.16009500	0.99881600
C	-8.89100400	0.10831900	1.75778900
C	-8.52101300	1.01453500	2.92782800
O	-8.27847200	2.36704000	2.58887700
C	-7.11334100	2.60172300	1.80754500
C	-6.66921700	4.04421800	2.05656900
C	5.14061000	2.07133700	1.34321800
C	4.52709500	3.09174700	0.61087800
C	4.51348900	3.08645500	-0.78705500
C	5.15760300	2.03066400	-1.45240300
C	5.76608500	1.00722100	-0.72007700
C	5.76015600	1.00063600	0.67791700
C	3.62889200	-2.22508400	3.13964500
C	4.59756600	-1.24958200	2.88683500
C	5.37530900	-1.27087100	1.72536300
C	5.17791900	-2.32078800	0.81352600
C	4.20442100	-3.29249600	1.06307400
C	3.41110400	-3.25833500	2.21367400
C	6.37618000	-0.15895700	1.44716500
C	-1.11727700	-2.64844800	2.02074000
C	0.09075900	-3.09340200	2.56482400
C	0.98528800	-3.87300400	1.82515400
C	0.63431900	-4.22082300	0.51040600
C	-0.57701300	-3.78113500	-0.03178300
C	-1.46235100	-2.98711300	0.70246900
C	-2.74904000	-2.48081600	0.06850200
C	2.31787300	-4.29480200	2.42739700
O	0.25122200	2.09481100	-4.37374100
C	0.51699800	1.07868500	-6.50545900
C	1.22659000	1.78379800	-5.36138500
O	1.70679300	4.89311100	0.19571000
C	1.38928200	6.12886900	2.20258400
C	0.70327800	5.33441600	1.10374200
O	5.14501000	2.07476900	-2.83092100
C	5.80741200	1.44782600	-5.02677700
C	5.89680500	1.10411500	-3.54899300
O	5.17940600	2.04338600	2.72146800
C	4.91386200	2.91668300	4.91730900
C	4.66428400	3.15885000	3.43785000
O	5.98362000	-2.32165100	-0.30547900
C	6.95490800	-3.22839300	-2.27748600
C	5.90208800	-3.42493300	-1.19919600
O	2.84375000	-2.24072200	4.27375600
C	2.19870600	-1.60628600	6.47268700
C	3.11780700	-1.29769600	5.30221900
O	1.53690500	-4.99960100	-0.18154500
C	2.31713500	-6.32569700	-1.99352200
C	1.18961600	-5.43995900	-1.48979800
O	-2.02601700	-1.87574400	2.71149700
C	-2.88639200	-0.67595000	4.57356200
C	-1.73122000	-1.51689800	4.05560200

H	-0.79563700	4.06818900	-0.47755100
H	2.76655300	2.86976200	-3.67274200
H	4.30065600	4.35160800	-2.50725600
H	3.83908200	5.11143700	-0.98084100
H	-3.11230000	0.05005500	1.08022600
H	-1.53555700	0.19813700	-3.59413800
H	-1.99892400	2.63013400	-3.63636100
H	-2.46540500	3.47946000	-2.16110200
H	-4.86546600	1.98961700	0.33627000
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H	-5.88777600	-5.08625300	-2.74214700
H	-5.80741800	-3.45395100	-0.81639200
H	-7.42183000	-3.76898700	-1.50063500
H	-5.78732700	-1.35303500	-0.14505300
H	-6.34488900	-0.06119300	-1.22090400
H	-8.22080400	-2.02452000	0.22796800
H	-8.70806000	-0.64010900	-0.77843200
H	-9.66105600	0.59312400	1.13612700
H	-9.31679100	-0.83105300	2.15255000
H	-9.35931900	1.03610400	3.63295000
H	-7.64837800	0.57967400	3.44214800
H	-6.32188800	1.89194300	2.08553300
H	-7.31947600	2.46380800	0.73824300
H	-7.53665500	4.70328800	1.95217300
H	-6.28661100	4.14957500	3.08372700
H	4.01922900	3.90552900	1.11345300
H	6.23730700	0.17228200	-1.22364900
H	4.75120100	-0.42861400	3.57645900
H	4.01995300	-4.08824800	0.35161100
H	6.77240500	0.20957400	2.39766200
H	7.21354500	-0.56324100	0.87148800
H	0.37909400	-2.82078300	3.57239900
H	-0.84745100	-4.02061900	-1.05267700
H	-3.09886400	-3.21296900	-0.66476700
H	-3.51454200	-2.38148400	0.84411600
H	2.18647800	-4.46248400	3.50021200
H	2.63115200	-5.24129700	1.97833600
H	1.23150600	0.83116800	-7.29819900
H	0.05114200	0.15031900	-6.15876900
H	-0.26317600	1.71954100	-6.92849800
H	1.71127400	2.70618200	-5.71358100
H	2.00716200	1.13969800	-4.93064600
H	0.64759700	6.50227400	2.91721500
H	2.10596600	5.50329100	2.74518100
H	1.92803100	6.98397400	1.78199400
H	-0.03122100	5.95941000	0.57493300
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H	4.76764400	1.42149500	-5.36956800
H	6.20637100	2.44971000	-5.21462900
H	6.94304600	1.11421400	-3.21025900
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H	6.93329800	-4.06599700	-2.98336100
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H	7.95457800	-3.17203500	-1.83506500
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H	-2.70804600	-0.38966300	5.61600200
H	-2.99720500	0.23652200	3.97863300
H	-3.82492300	-1.23746800	4.52352300
H	-1.60417400	-2.42217300	4.66776800
H	-0.78877600	-0.95156600	4.09659700

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