Electronic Supplementary Information

for

Pseudohelicene chemosensor displaying ternary signaling stimulated by hydrostatic pressure and solvent

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Experimental Section

Materials. All commercial reagents and solvents were used without further purification. The sample solutions were dissolved in spectroscopic grade toluene, chloroform, dichloromethane (DCM), and methanol (MeOH). The target material (**[2]HA$_2$**) was synthesized according to the literature.[1]

Instruments. UV/vis spectra were acquired by using a JASCO V-550 or V-770 spectrometer. Fluorescence spectra were acquired by using a JASCO FP-8500 spectrofluorometer. The absolute fluorescence quantum yields at 0.1 MPa ($\Phi_{F,0.1\ MPa}$) were evaluated using a spectrofluorometer (FP-8500) fitted with an integrating sphere. Fluorescence lifetime decays were obtained using a Hamamatsu Quantaurus-Tau single-photon counting apparatus with an LED light source (λ_{ex} = 405 nm); photons were collected up to 10000 counts.

Hydrostatic pressure spectroscopy. The spectroscopic experiments under hydrostatic pressure were conducted using a custom-built high-pressure apparatus; the details are summarized in our previous publications.[2,3] In this apparatus (Figure S1), a quartz inner cell (2 mm path length) with a Teflon tube was filled with the sample solution. The cell was set into the outer cell, which was filled with H_2O that can be hydrostatically pressurized by a hand pump. The outer cell was placed in the spectrometers, enabling acquisition of the hydrostatic pressure spectroscopy data (range: 0.1–400 MPa) through the sapphire windows.

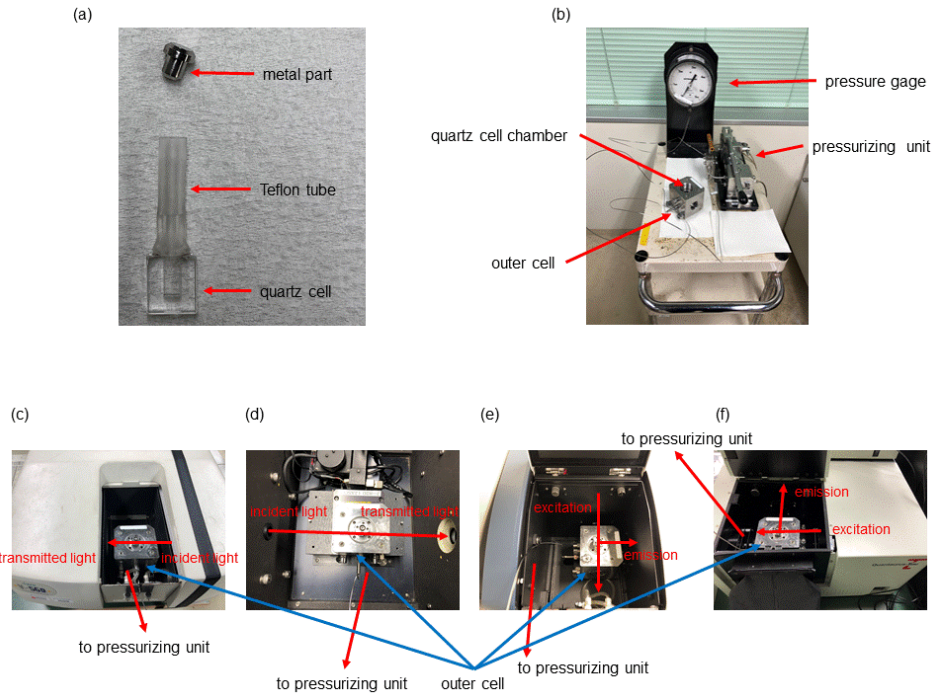

Figure S1. Photographs of (a) inner quartz cell, (b) pressurizing units, and setup for (c) UV/vis, (d) circular dichroism, (e) fluorescence, and (d) lifetime measurements. Reproduced with permission from Ref. 3. Copyright 2020, John Wiley & Sons.

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[1] K. Watanabe, E. Tsurumaki, M. Hasegawa and S. Toyota, *Chem. Eur. J.* 2024, **30**, e202400929.
[2] H. Mizuno and G. Fukuhara, *Acc. Chem. Res.* 2022, **55**, 1748–1762.
[3] H. Mizuno, M. Kitamatsu, Y. Imai and G. Fukuhara, *ChemPhotoChem* 2020, **4**, 502–507.

Characterization Data of [2]HA$_2$

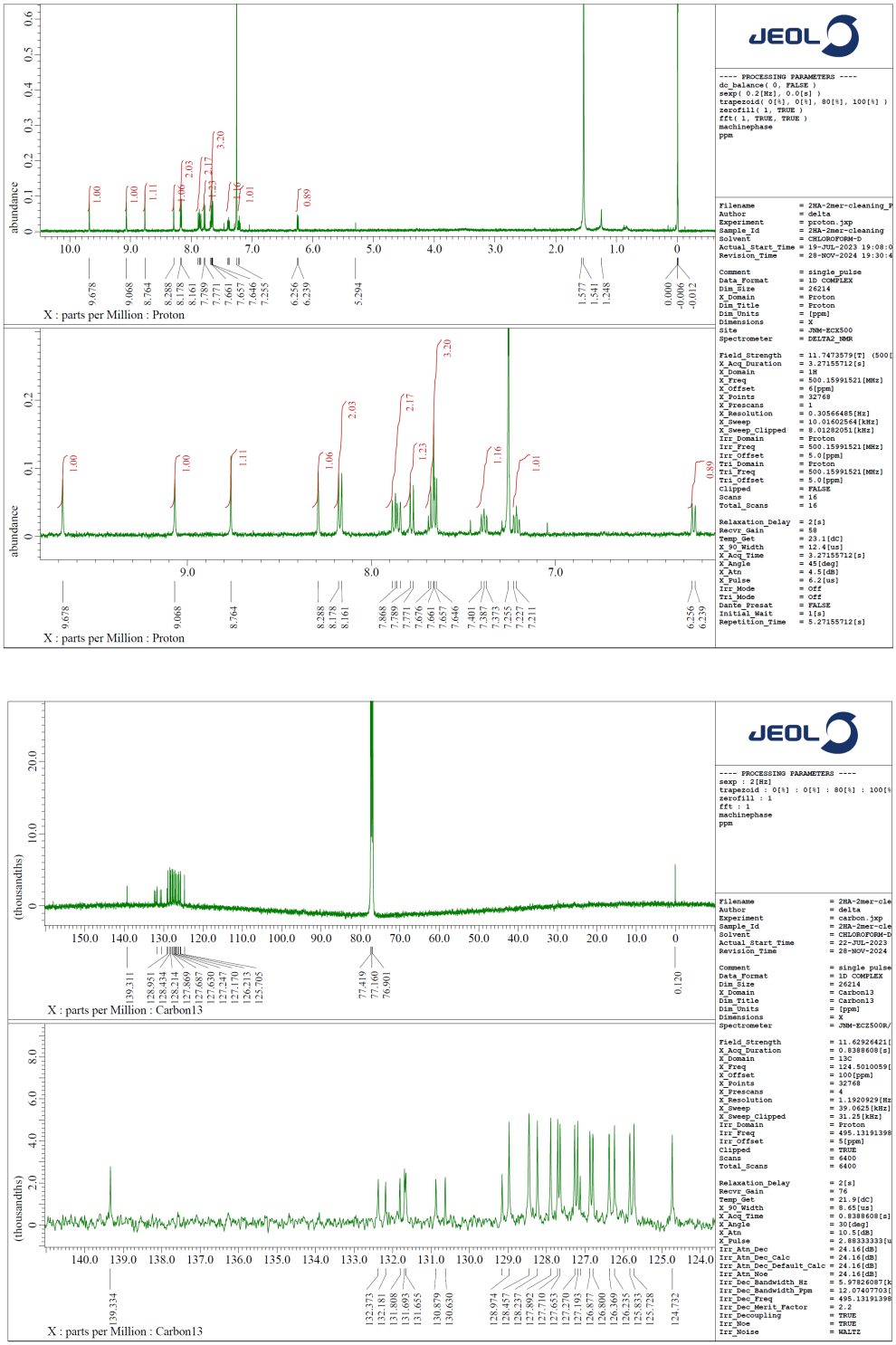

Figure S2. ^{1}H (top, 500 MHz, $CDCl_3$) and ^{13}C NMR spectra (bottom, 125 MHz, $CDCl_3/CS_2$ 10:1) of **[2]HA$_2$**.

Compound data: mp 280–300 °C (dec.); R_f 0.14 (hexane/CH_2Cl_2 5:1); HRMS (FAB): *m/z* calcd. for $C_{52}H_{30}$ $[M]^+$: 654.2348; found: 654.2394.

Concentration-Dependent Optical Properties of [2]HA_2

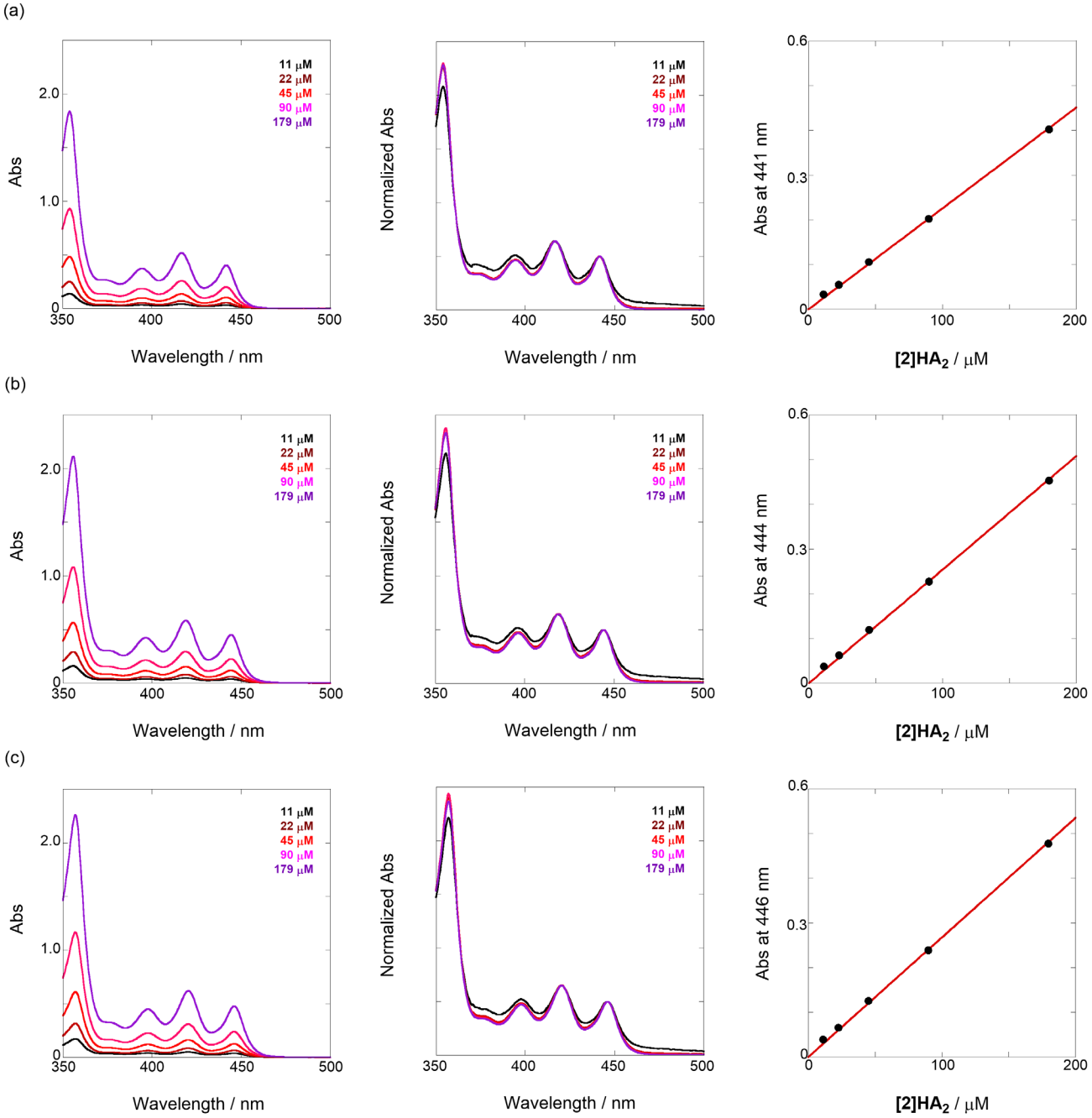

Figure S3. Concentration-dependent (11–179 μM, from black to purple) UV/vis absorption spectra (left), normalized UV/vis absorption spectra (center), and absorbance–concentration plots (right) of **[2]HA_2** at (a) 0.1 MPa (correlation coefficient r = 0.999), (b) 160 MPa (r = 0.999), and (c) 320 MPa (r = 0.999) in toluene at room temperature in a high-pressure cell.

UV/vis Absorption and Fluorescence Spectra of [2]HA$_2$

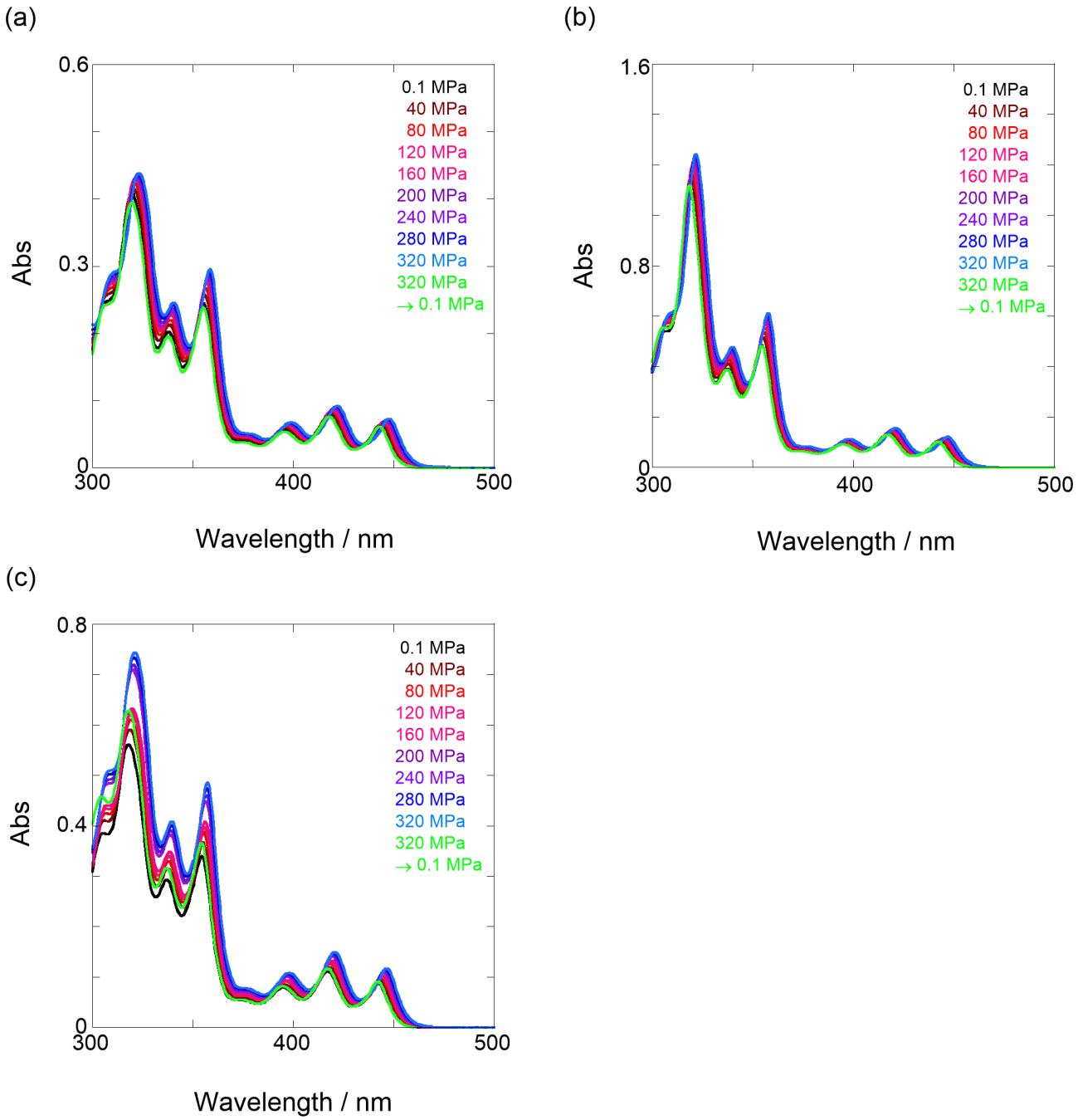

Figure S4. Pressure-dependent UV/vis absorption spectra of **[2]HA$_2$** in (a) toluene (66 μM), (b) chloroform (58 μM), and (c) DCM (57 μM) at room temperature in a high-pressure cell. Pressure applied: 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue). The green line shows the spectrum at 0.1 MPa after depressurization from 320 MPa.

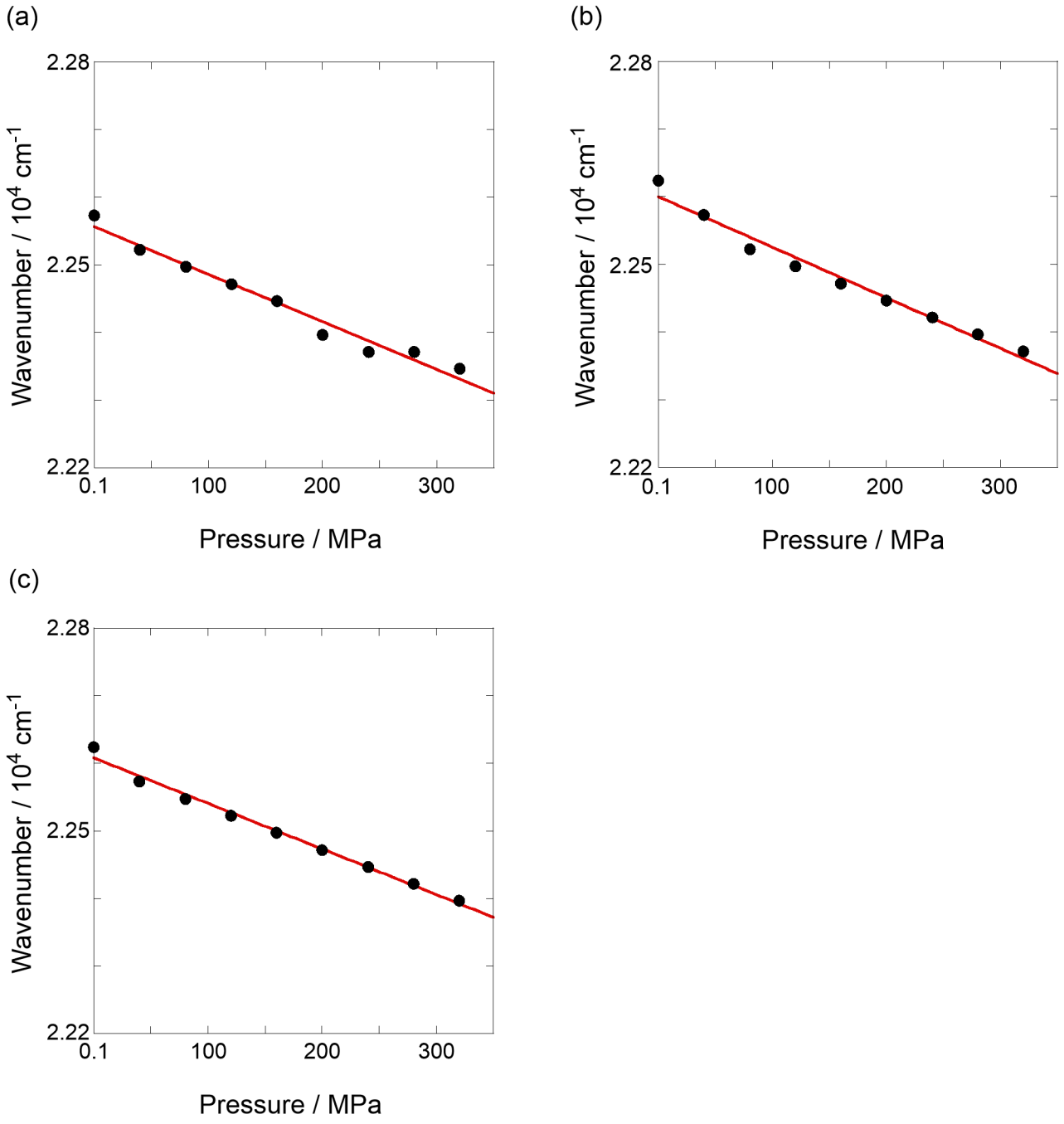

Figure S5. Plots of wavenumber changes for the pressure-induced absorption maxima of **[2]HA$_2$** in (a) toluene (r = 0.986, slope; −0.70 cm^{-1} MPa^{-1}), (b) chloroform (r = 0.988, slope; −0.75 cm^{-1} MPa^{-1}), and (c) DCM (r = 0.995, slope; −0.68 cm^{-1} MPa^{-1}).

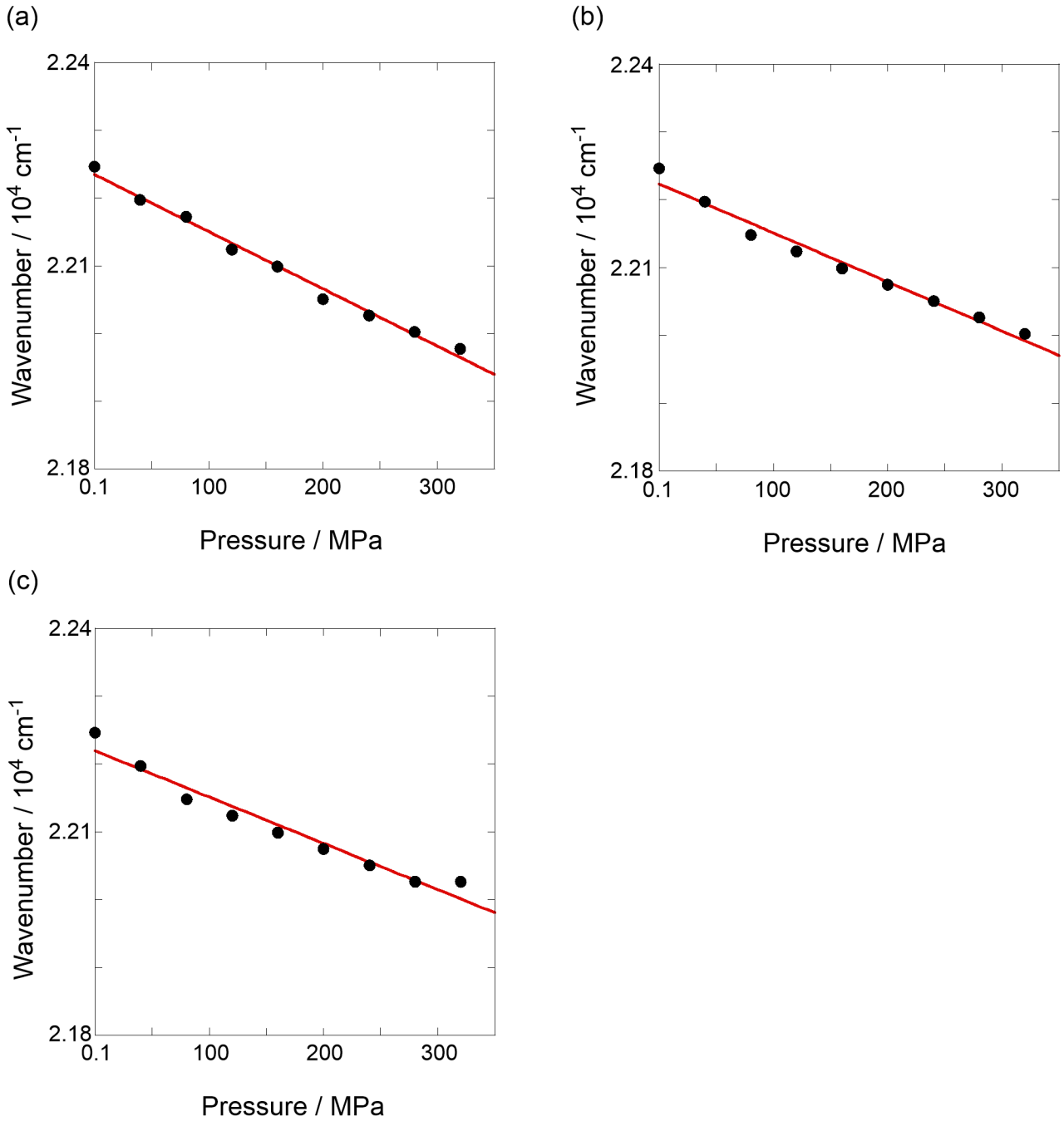

Figure S6. Plots of wavenumber changes for the pressure-induced fluorescence maxima of **[2]HA$_2$** in (a) toluene (r = 0.995, slope; −0.85 cm^{-1} MPa^{-1}), (b) chloroform (r = 0.988, slope; −0.72 cm^{-1} MPa^{-1}), and (c) DCM (r = 0.977, slope; −0.68 cm^{-1} MPa^{-1}).

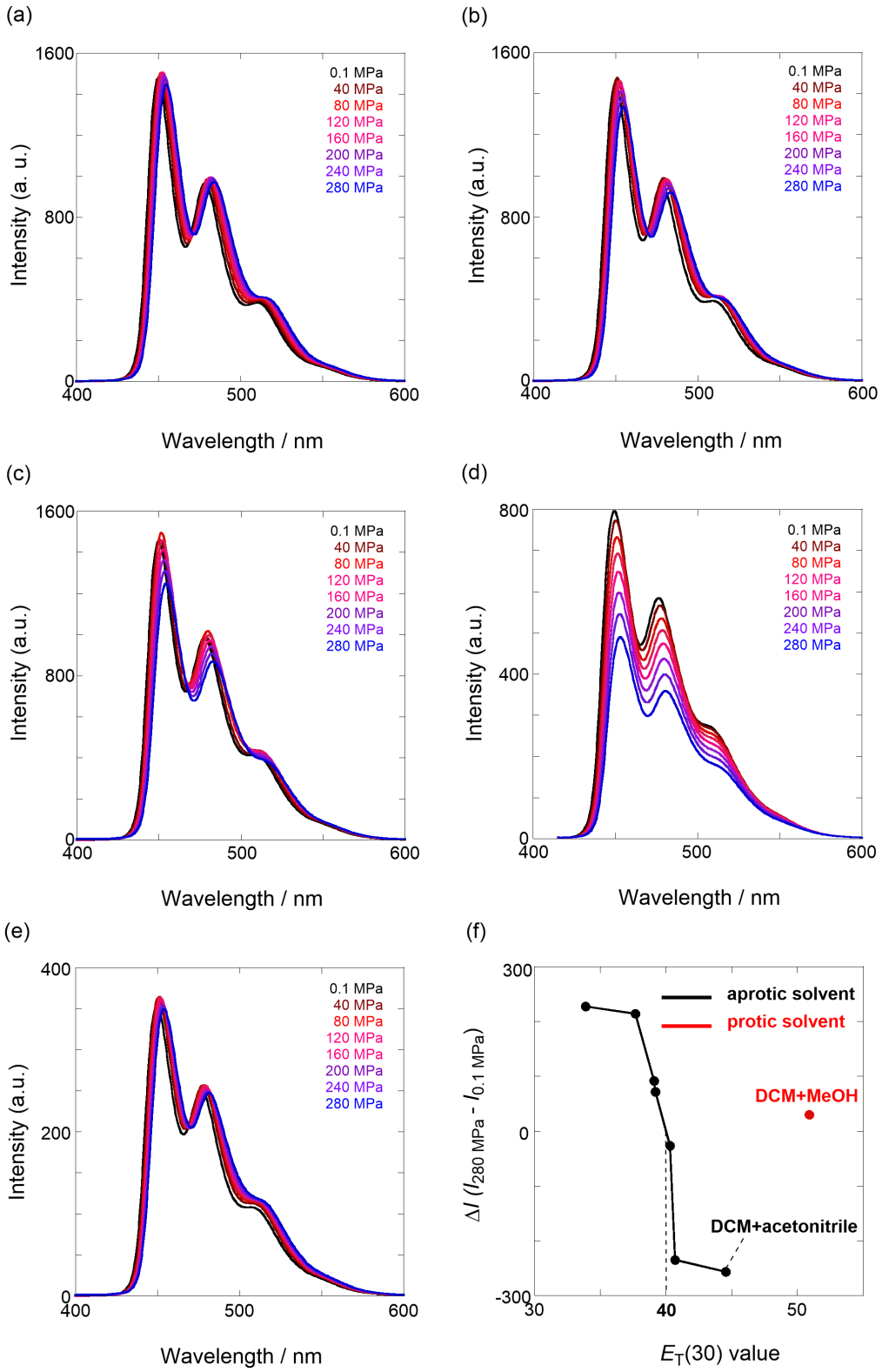

Figure S7. Pressure-dependent fluorescence spectra (λ_{ex} 390–409 nm) of **[2]HA$_2$** in (a) 75:25 (v/v) toluene-DCM (59 μM), (b) 50:50 (v/v) toluene-DCM (59 μM), (c) 25:75 (v/v) toluene-DCM (59 μM), (d) 50:50 (v/v) DCM-acetonitrile (61 μM), and (e) 75:25 (v/v) DCM-MeOH (57 μM) at room temperature in a high-pressure cell. Pressure applied: 0.1, 40, 80, 120, 160, 200, 240, and 280 MPa (from black to blue). (d) Hydrostatic pressure-induced ΔI ($I_{280\ MPa} - I_{0.1\ MPa}$) against $E_T(30)$.

Discussion: About a similar foldamer chemosensor (see ref. 26 in the main text), the effect of methanol as a protic solvent was closely investigated, revealing the appropriate interactions between methanol and the chemosensor. Indeed, in the literature, the addition of methanol causes the decreases of binding constants of targeted ion pairs, but ΔV° did not alter significantly. This and the present data indicate that methanol may affect to not the ground-state ion-pairing volume but the excited-state fluorescence quenching critically.

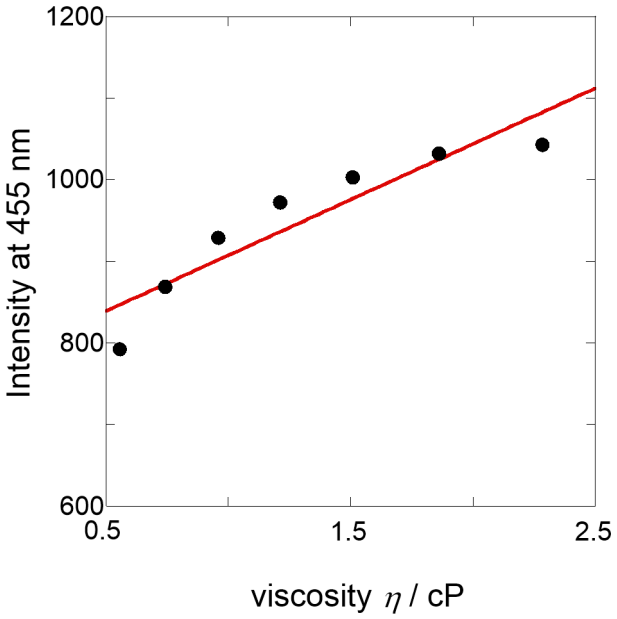

Figure S8. Pressure dependence of fluorescence intensity (λ_{obs} 455 nm) of **[2]HA$_2$** in toluene as a function of toluene viscosity (r = 0.925).

Discussion: In order to investigate the extent of a viscosity effect in **[2]HA$_2$**, we plotted the fluorescence intensity (455 nm) in toluene against toluene viscosity, and then investigated the correlation. As shown in Fig. S8, a slight correlation (r = 0.925) was observed, but deviated in the initial and late stage of the applied pressures. It can be therefore concluded that the correlation for considering effects on hydrostatic pressure seems to be better using data shown in Fig. 3, rather than the viscosity.

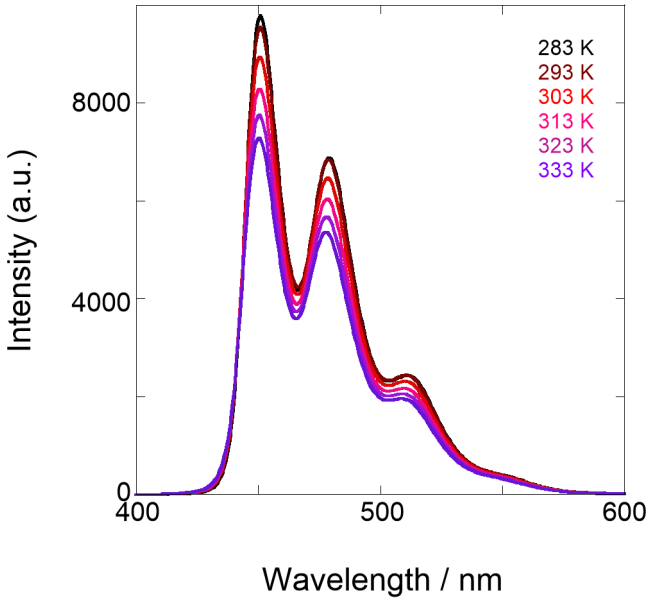

Figure S9. Temperature-dependent fluorescence spectra (λ_{ex} 391 nm) of **[2]HA$_2$** in toluene at 0.1 MPa in a regular 1 cm cell.

Excitation Spectra of [2]HA$_2$

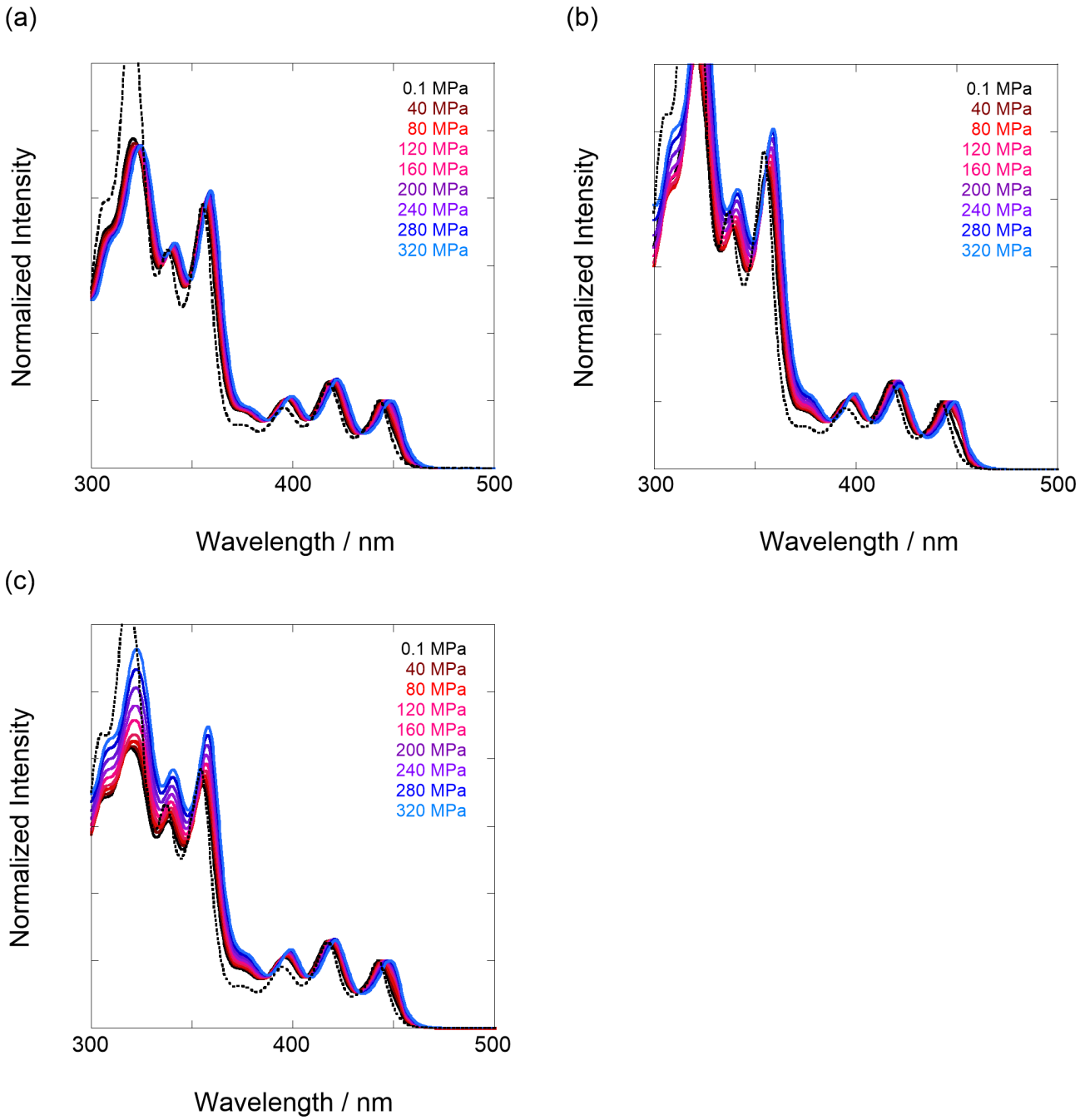

Figure S10. Pressure-dependent excitation spectra (λ_{em} 450 nm) of **[2]HA$_2$** in (a) toluene (66 µM), (b) chloroform (61 µM), and (c) DCM (57 µM) at room temperature in a high-pressure cell. Black dotted lines show the normalized UV/vis absorption spectra at 0.1 MPa. Pressure applied: 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to light blue).

Fluorescence Lifetime Decays of [2]HA_2

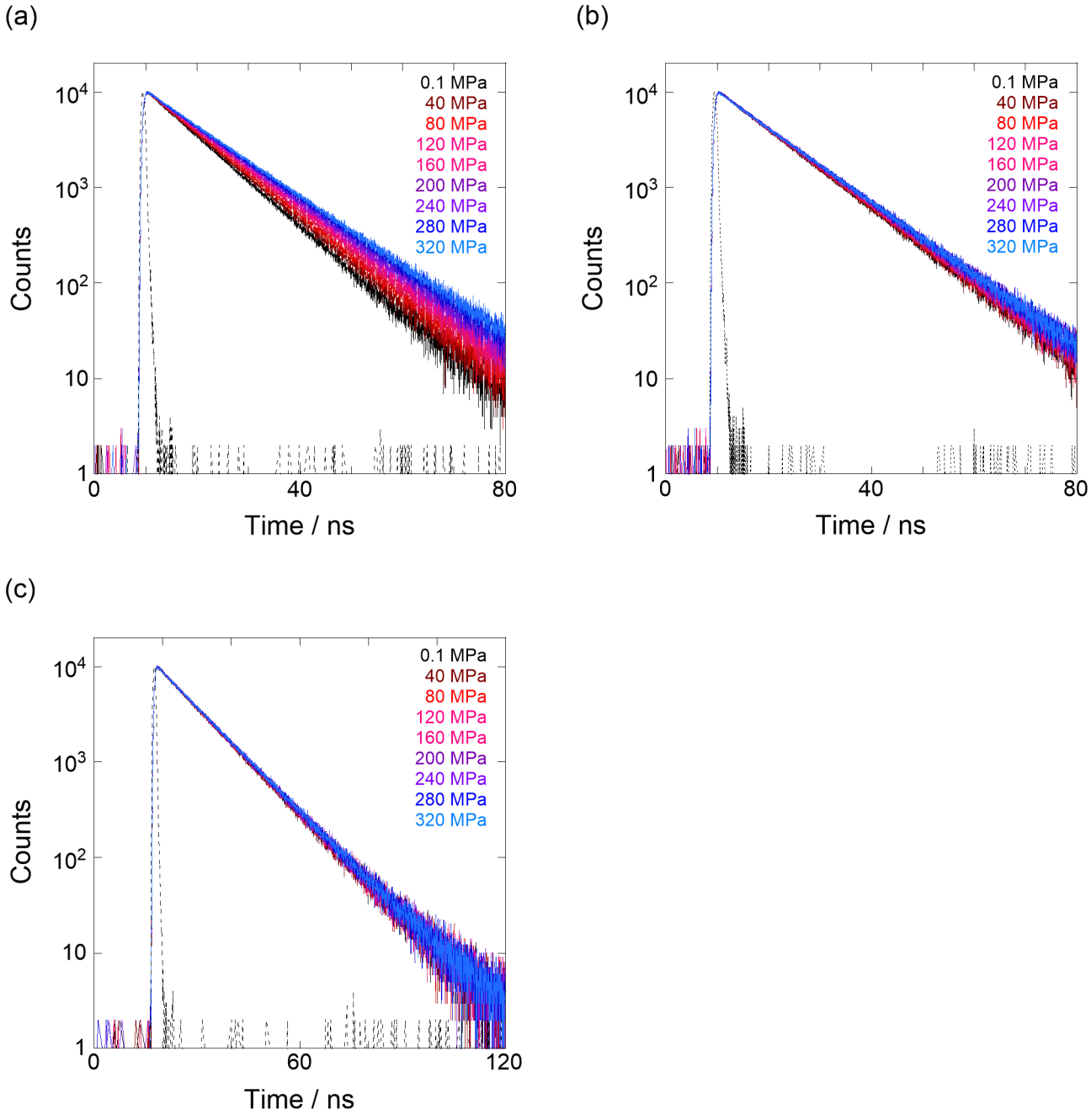

Figure S11. Time-correlated fluorescence decay (λ_{ex} 405 nm, λ_{em} 450 nm) of **[2]HA_2** at 0.1, 40, 80, 120, 160, 200, 240, 280, and 320 MPa (from black to sky blue lines) in (a) toluene (66 μM), (b) chloroform (61 μM), and (c) DCM (57 μM) at room temperature in a high-pressure cell. The black dotted line represents the instrument response function.

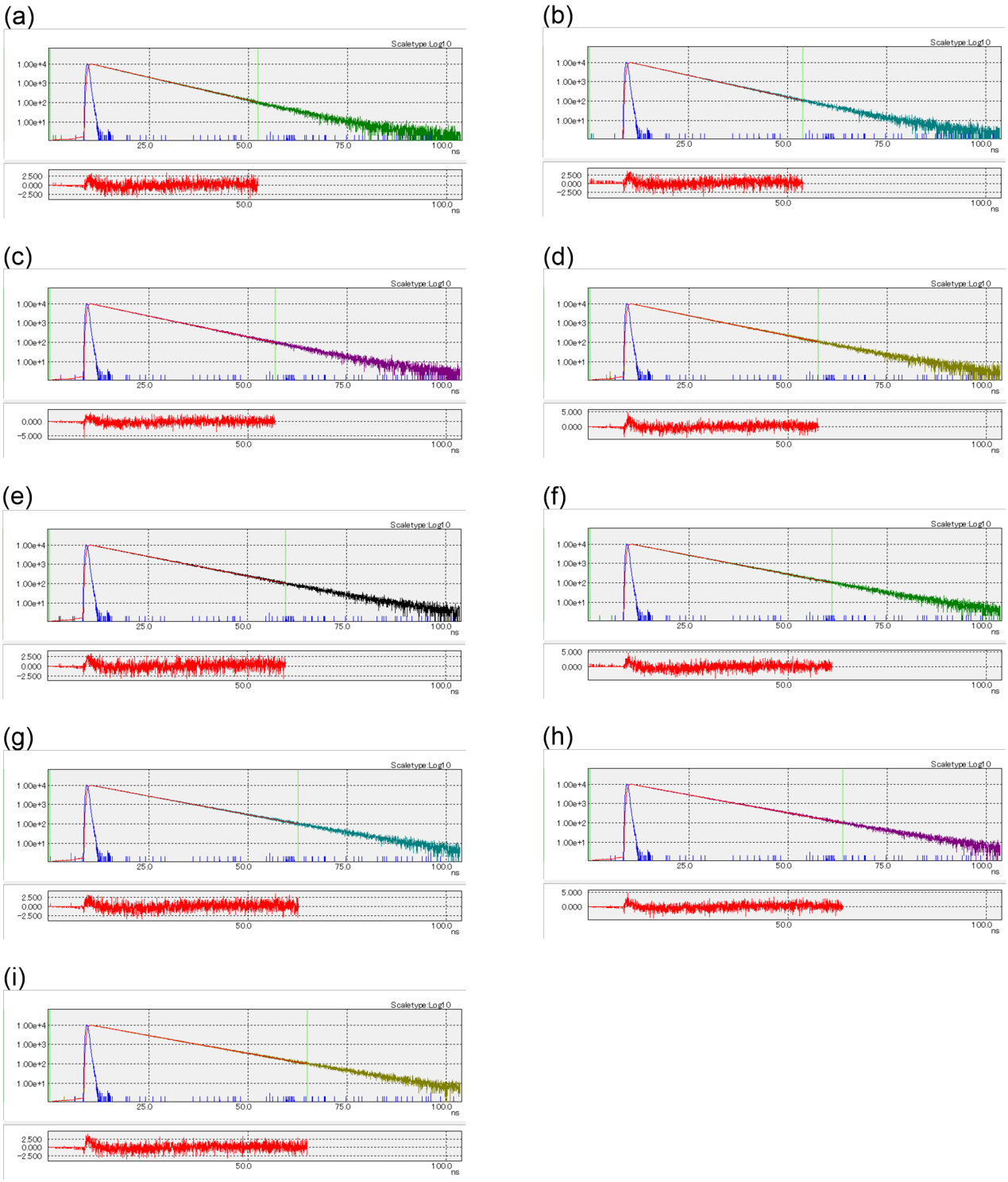

Figure S12. Time-correlated fluorescence decay of **[2]HA$_2$** (66 μM) monitored at 450 nm at (a) 0.1, (b) 40, (c) 80, (d) 120, (e) 160, (f) 200, (g) 240, (h) 280, and (i) 320 MPa in toluene at room temperature in a high-pressure cell. The colored, red, and blue lines represent fluorescence decay, fitting result, and the instrument response function, respectively.

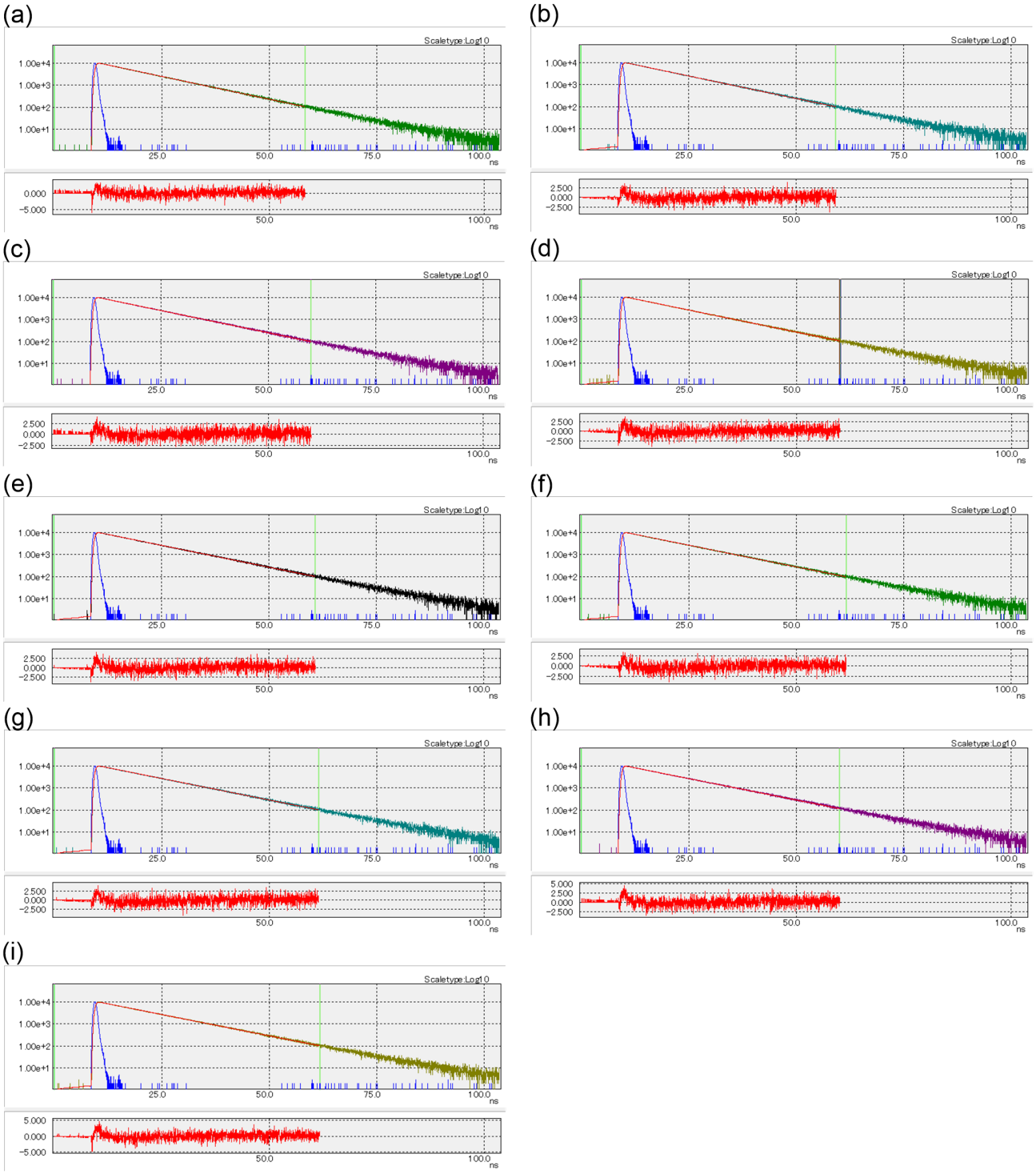

Figure S13. Time-correlated fluorescence decay of **[2]HA$_2$** (61 μM) monitored at 450 nm at (a) 0.1, (b) 40, (c) 80, (d) 120, (e) 160, (f) 200, (g) 240, (h) 280, and (i) 320 MPa in chloroform at room temperature in a high-pressure cell. The colored, red, and blue lines represent fluorescence decay, fitting result, and the instrument response function, respectively.

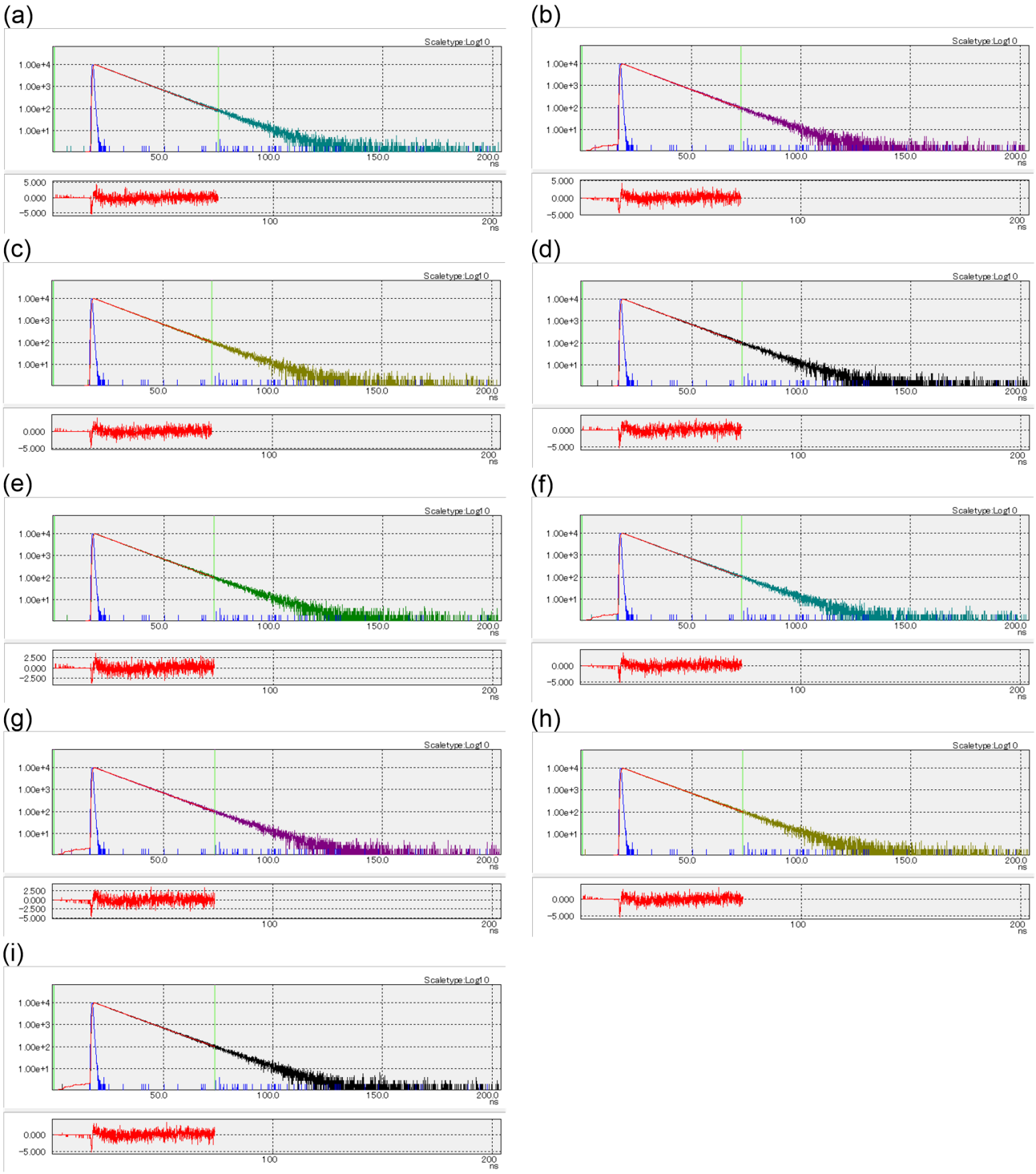

Figure S14. Time-correlated fluorescence decay of **[2]HA$_2$** (57 μM) monitored at 450 nm at (a) 0.1, (b) 40, (c) 80, (d) 120, (e) 160, (f) 200, (g) 240, (h) 280, and (i) 320 MPa in DCM at room temperature in a high-pressure cell. The colored, red, and blue lines represent fluorescence decay, fitting result, and the instrument response function, respectively.

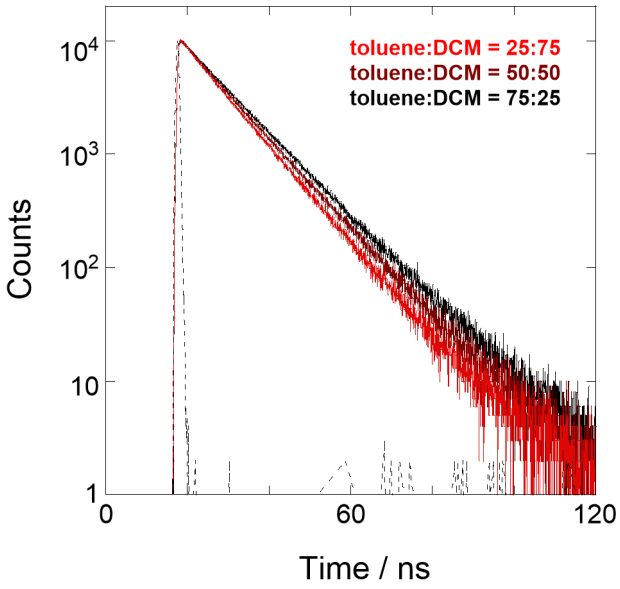

Figure S15. Time-correlated fluorescence decay (λ_{ex} 405 nm, λ_{em} 450 nm) of **[2]HA$_2$** in each solvent (black: 75:25 (v/v) toluene-DCM, brown: 50:50 (v/v) toluene-DCM, red: 25:75 (v/v) toluene-DCM) at 0.1 MPa at room temperature in a high-pressure cell. The black dotted line represents the instrument response function.

Table S1. Fluorescence Lifetimes of [2]HA$_2$ in Toluene-DCM Mixtures at 0.1 MPa[a]

Solvent	λ_{em}[b]/nm	τ/ns	χ^2
Toluene	450	9.1	1.1
75:25 (v/v) toluene-DCM	450	10.1	1.3
50:50 (v/v) toluene-DCM	450	10.9	1.3
25:75 (v/v) toluene-DCM	450	11.6	1.3
DCM	450	11.6	1.3

[a]Fluorescence lifetime determined using hydrostatic pressure time-correlated single-photon counting method at room temperature; λ_{ex} = 405 nm. [b]Monitoring wavelength.

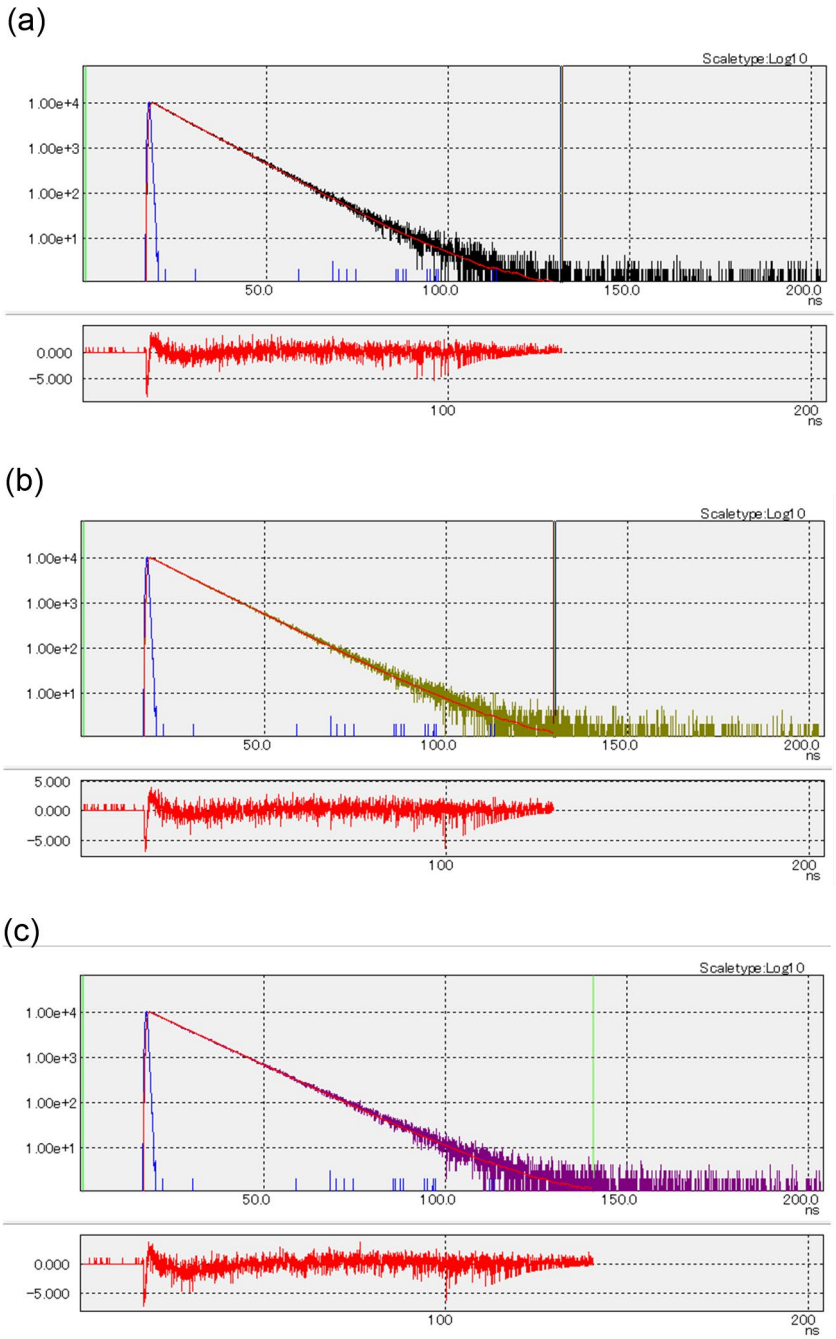

Figure S16. Time-correlated fluorescence decay of **[2]HA$_2$** (57 μM) monitored at 450 nm in (a) 75:25 (v/v) toluene-DCM, (b) 50:50 (v/v) toluene-DCM, and (c) 25:75 (v/v) toluene-DCM at 0.1 MPa at room temperature in a high-pressure cell. The colored, red, and blue lines represent fluorescence decay, fitting result, and the instrument response function, respectively.

Determination of Fluorescence Quantum Yields ($\Phi_{F,X\ MPa}$) under Hydrostatic Pressure

As described in the Experimental Section, the $\Phi_{F,0.1\ MPa}$ values were evaluated using a spectrofluorometer (FP-8500) fitted with an integrating sphere, after which the relative fluorescence quantum yields under hydrostatic pressure ($\Phi_{F,X\ MPa}$) were determined using Eq. S1:[4]

$$\Phi_{\mathrm{F,X\ MPa}} = \Phi_{\mathrm{F,0.1\ MPa}} \cdot \frac{A_{\mathrm{P_0}}}{A_{\mathrm{P}}} \cdot \frac{I_{\mathrm{P_0}}}{I_{\mathrm{P}}} \cdot \frac{n_{\mathrm{P}}^2}{n_{\mathrm{P_0}}^2} \cdot \frac{D_{\mathrm{P}}}{D_{\mathrm{P_0}}} \quad \text{(S1)}$$

where A, I, n, and D are the absorbance at the excitation wavelength, intensity of the excitation light, refractive index, and area ratio in the fluorescence spectrum, respectively (Table S3–S5). The data for A were extracted from Figure S4. The value of I_P/I_{P0} was set at unity because the measurements were performed at the same excitation wavelength under each pressure (Figure 2). The refractive indices at 0.1 MPa at 298.15 K (n_{P_0}) were identical to the literature values,[5,6] and the refractive indices under pressure (n_P) were calculated from the change in the densities of each solvent using the Eykman equation (Eq. S2). The densities of each solvent were calculated by fitting previous data obtained by applying Eq. S3 (see Figure S17 and Table S2). The constant C was calculated using known density data at 0.1 MPa.[7–9] The data for D were obtained by integrating the area of the fluorescence spectra using MATLAB software.[10]

$$\frac{n^2 - 1}{n + 0.4} \cdot \frac{1}{d} = \mathrm{C} \quad \text{(S2)}$$

$$d(P) = \sum_{i=1}^{5} \mathrm{a}_i \, P^{i-1} \quad \text{(S3)}$$

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[4] J. N. Demas and G. A. Crosby, *J. Phys. Chem.* 1971, **75**, 991–1024.
[5] B. González, I. Domínguez, E. J. González and A. Domínguez, *J. Chem. Eng. Data* 2010, **55**, 1003–1011.
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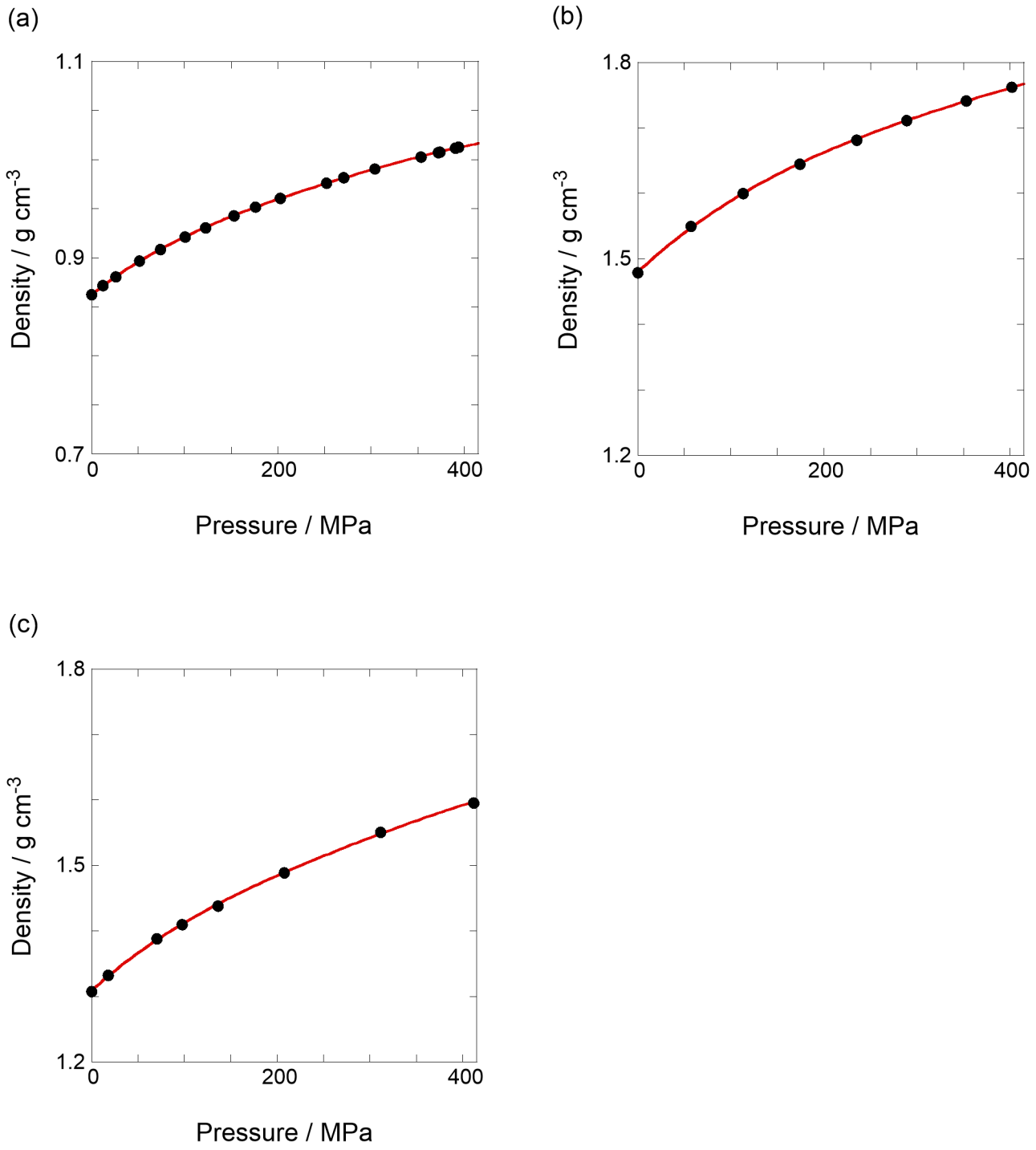

Figure S17. Pressure-dependent solvent densities in (a) toluene (298.15 K, extracted from Ref. 7), (b) chloroform (298.15 K, extracted from Ref. 10), and (c) DCM (303.15 K, extracted from Ref. 9).

Table S2. Fitting Parameters of Pressure-Dependent Solvent Density Plots

Solvent	a_1	a_2	a_3	a_4	a_5
Toluene	0.863	0.750×10^{-3}	-2.001×10^{-6}	4.141×10^{-6}	-3.653×10^{-12}
Chloroform	1.480	1.325×10^{-3}	-2.708×10^{-6}	3.702×10^{-6}	-2.041×10^{-12}
DCM	1.309	1.284×10^{-3}	-3.015×10^{-6}	5.904×10^{-6}	-4.909×10^{-12}

Table S3. Relative Fluorescence Quantum Yields of [2]HA$_2$ in Toluene

Pressure / MPa	Density[a] / g cm^{-3}	Refractive index (n_{P_0})[c]	Area (D_{P_0})[e]	Abs (A_{P_0})[f]	Fluorescence quantum yield (Φ_{P_0})[g]
0.1	0.862	1.494	1.751×10^6	0.048	0.334
Pressure / MPa	Density[b] / g cm^{-3}	Refractive index (n_P)[d]	Area (D_P)[e]	Abs (A_P)[f]	Fluorescence quantum yield (Φ_P)[h]
40	0.890	1.511	1.824×10^6	0.049	0.351
80	0.912	1.524	1.885×10^6	0.049	0.366
120	0.930	1.536	1.933×10^6	0.049	0.383
160	0.946	1.545	1.976×10^6	0.048	0.400
200	0.960	1.554	2.023×10^6	0.048	0.415
240	0.972	1.562	2.054×10^6	0.048	0.425
280	0.984	1.569	2.079×10^6	0.048	0.435
320	0.995	1.576	2.090×10^6	0.048	0.441

[a]Ref. 7. [b]Data calculated from the fitting results (Figure S17a and Table S2). [c]Ref. 5. [d]Data calculated using Eq. S2. [e]Data extracted from Figure 2a. [f]Data extracted from Figure S4a. [g]Measured using spectrofluorometer (FP-8500). [h]Data calculated using Eq. S1.

Table S4. Relative Fluorescence Quantum Yields of [2]HA$_2$ in Chloroform

Pressure / MPa	Density[a] / g cm^{-3}	Refractive index (n_{P_0})[c]	Area (D_{P_0})[e]	Abs (A_{P_0})[f]	Fluorescence quantum yield (Φ_{P_0})[g]
0.1	1.479	1.443	1.074×10^6	0.077	0.334
Pressure / MPa	Density[b] / g cm^{-3}	Refractive index (n_P)[d]	Area (D_P)[e]	Abs (A_P)[f]	Fluorescence quantum yield (Φ_P)[h]
40	1.529	1.459	1.127×10^6	0.078	0.356
80	1.570	1.473	1.163×10^6	0.078	0.372
120	1.606	1.484	1.180×10^6	0.078	0.383
160	1.636	1.494	1.192×10^6	0.079	0.392
200	1.663	1.502	1.193×10^6	0.079	0.396
240	1.686	1.510	1.202×10^6	0.078	0.404
280	1.707	1.517	1.181×10^6	0.078	0.402
320	1.726	1.523	1.142×10^6	0.078	0.392

[a]Ref. 8. [b]Data calculated from the fitting results (Figure S17b and Table S2). [c]Ref. 6. [d]Data calculated using Eq. S2. [e]Data extracted from Figure 2b. [f]Data extracted from Figure S4b. [g]Measured using spectrofluorometer (FP-8500). [h]Data calculated using Eq. S1.

Table S5. Relative Fluorescence Quantum Yields of [2]HA_2 in DCM

Pressure / MPa	Density[a] / g cm^{-3}	Refractive index (n_{P_0})[c]	Area (D_{P_0})[e]	Abs (A_{P_0})[f]	Fluorescence quantum yield (Φ_{P_0})[g]
0.1	1.308[a]	1.442	2.560×10^6	0.085	0.360
Pressure / MPa	Density[b] / g cm^{-3}	Refractive index (n_P)[d]	Area (D_P)[e]	Abs (A_P)[f]	Fluorescence quantum yield (Φ_P)[h]
40	1.356	1.439	2.478×10^6	0.085	0.354
80	1.395	1.453	2.391×10^6	0.085	0.336
120	1.429	1.465	2.351×10^6	0.088	0.350
160	1.458	1.475	2.284×10^6	0.085	0.343
200	1.485	1.484	2.173×10^6	0.088	0.318
240	1.509	1.492	2.019×10^6	0.088	0.299
280	1.532	1.500	1.845×10^6	0.088	0.276
320	1.553	1.508	1.668×10^6	0.088	0.254

[a]Ref. 9. [b]Data calculated from the fitting results (Figure S17c and Table S2). [c]Ref. 6. [d]Data calculated using Eq. S2. [e]Data extracted from Figure 2c. [f]Data extracted from Figure S4c. [g]Measured using spectrofluorometer (FP-8500). [h]Data calculated using Eq. S1.

Table S6. Quantum Yields, Fluorescence Lifetimes, and Kinetic Rate Constants of [2]HA_2

Solvent	P / MPa	Φ_F	τ_F / ns	χ^2	k_F / 10^7 s^{-1}	k_{nr} / 10^7 s^{-1}
Toluene	0.1	0.334	9.1	1.1	3.7	7.3
	40	0.351	9.6	1.1	3.7	6.8
	80	0.366	10.0	1.2	3.7	6.4
	120	0.383	10.3	1.1	3.7	6.0
	160	0.400	10.7	1.1	3.8	5.6
	200	0.415	11.0	1.2	3.8	5.3
	240	0.425	11.3	1.1	3.8	5.1
	280	0.435	11.5	1.2	3.8	4.9
	320	0.441	11.7	1.1	3.8	4.8
Chloroform	0.1	0.334	10.5	1.2	3.2	6.4
	40	0.356	10.6	1.1	3.4	6.1
	80	0.372	10.7	1.1	3.5	5.9
	120	0.383	10.8	1.1	3.5	5.7
	160	0.392	10.9	1.1	3.6	5.6
	200	0.396	11.0	1.1	3.6	5.5
	240	0.404	11.1	1.2	3.6	5.4
	280	0.402	11.2	1.2	3.6	5.4
	320	0.392	11.2	1.2	3.5	5.4
DCM	0.1	0.360	11.6	1.3	3.1	5.5
	40	0.354	11.6	1.2	3.1	5.6
	80	0.336	11.6	1.2	2.9	5.7
	120	0.350	11.7	1.3	3.0	5.6
	160	0.343	11.7	1.2	2.9	5.6
	200	0.318	11.8	1.2	2.7	5.8
	240	0.299	11.8	1.2	2.5	5.9
	280	0.276	11.8	1.2	2.3	6.1
	320	0.254	11.9	1.2	2.1	6.3

DFT Calculations

DFT calculations were carried out with Orca 5.0.3.[11] on a Windows computer. The structures were optimized by the hybrid DFT method at the (TD-)CAM-B3LYP/def2-SVP level. Solvent effects were incorporated using the implicit solvation model based on density (SMD).[12] Molecular van der Waals volumes were calculated using MultiWFN 3.8[13] with the Monte Carlo method.

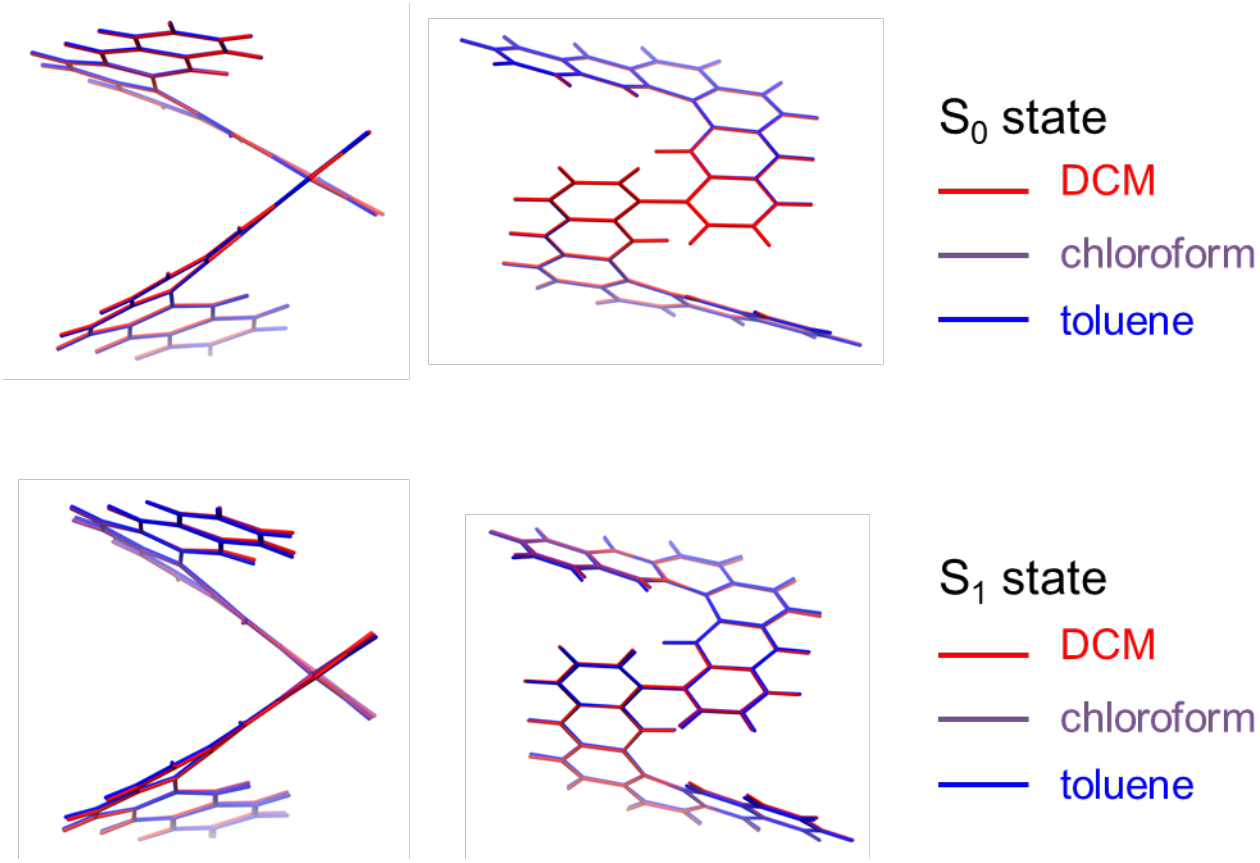

Figure S18. Calculated structures of **[2]HA$_2$** with (*P*,*P*$_a$,*P*) conformations in S_0 and S_1 states. The calculated structures in DCM (red), chloroform (purple), and toluene (blue) were superimposed for comparison.

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Table S7. Calculated Molecular Volumes of [2]HA_2 in S_0 State

	P,P_a,*P* / Å^3	*M*,P_a,*P* / Å^3	*M*,P_a,*M* / Å^3
toluene	902.32	900.48	901.98
chloroform	902.50	900.50	902.29
DCM	902.58	900.52	902.10

Table S8. Calculated Molecular Volumes of [2]HA_2 in S_1 State

	P,P_a,*P* / Å^3	*M*,P_a,*P* / Å^3	*M*,P_a,*M* / Å^3
toluene	902.20	898.52	897.00
chloroform	902.48	898.69	897.15
DCM	902.54	898.87	897.22

Table S9. Calculated Relative Energies of [2]HA_2 in S_0 State

	P,P_a,*P* / kJ mol^{-1}	*M*,P_a,*P* / kJ mol^{-1}	*M*,P_a,*M* / kJ mol^{-1}
toluene	0	+0.80	−0.47
chloroform	0	+0.98	−0.05
DCM	0	+1.11	+0.21

Table S10. Calculated Relative Energies of [2]HA_2 in S_1 State

	P,P_a,*P* / kJ mol^{-1}	*M*,P_a,*P* / kJ mol^{-1}	*M*,P_a,*M* / kJ mol^{-1}
toluene	0	+1.79	+1.73
chloroform	0	+1.88	+2.11
DCM	0	+1.90	+2.29

Table S11. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (M,P_a,M) Conformer in Toluene (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	-0.0892	-1.6681	3.8528	42	C	-5.0026	-2.9435	-1.8985
2	C	0.5749	-2.9240	3.9156	43	C	-3.6015	-3.0881	-1.6243
3	C	1.6928	-3.1488	3.1671	44	C	-2.9012	-2.0382	-0.9250
4	C	2.2006	-2.1299	2.3059	45	C	-2.9108	-4.1962	-2.1089
5	C	1.5233	-0.8716	2.2194	46	C	-1.5195	-4.3064	-2.0037
6	C	0.3572	-0.6561	3.0412	47	C	-0.8019	-3.2256	-1.4035
7	C	3.3770	-2.3037	1.5680	48	C	-1.5079	-2.1294	-0.8828
8	C	3.8782	-1.3137	0.7277	49	C	-0.7904	-5.4237	-2.5153
9	C	3.1423	-0.0898	0.5332	50	C	0.5735	-5.4557	-2.4450
10	C	2.0126	0.1054	1.3343	51	C	1.2914	-4.3719	-1.8621
11	C	5.1667	-1.4736	0.1164	52	C	0.6253	-3.2905	-1.3588
12	C	5.7196	-0.4561	-0.5815	53	H	-0.9762	-1.5051	4.4690
13	C	4.9879	0.7523	-0.8458	54	H	0.1846	-3.7019	4.5753
14	C	3.6663	0.9036	-0.4076	55	H	2.2183	-4.1053	3.2147
15	C	5.6473	1.7993	-1.5770	56	H	3.9415	-3.2322	1.6838
16	C	5.0053	2.9458	-1.8957	57	H	1.5034	1.0641	1.3219
17	C	3.6035	3.0900	-1.6244	58	H	5.7083	-2.4087	0.2750
18	C	2.9016	2.0379	-0.9303	59	H	6.7278	-0.5450	-0.9924
19	C	2.9134	4.1992	-2.1074	60	H	6.6957	1.6541	-1.8472
20	C	1.5218	4.3082	-2.0057	61	H	5.5223	3.7552	-2.4157
21	C	0.8029	3.2245	-1.4120	62	H	3.4741	4.9866	-2.6176
22	C	1.5082	2.1272	-0.8930	63	H	0.9167	1.3077	-0.4948
23	C	0.7934	5.4269	-2.5152	64	H	1.3495	6.2533	-2.9646
24	C	-0.5708	5.4575	-2.4492	65	H	-1.1202	6.3154	-2.8435
25	C	-1.2898	4.3708	-1.8732	66	H	-2.3807	4.4081	-1.8358
26	C	-0.6245	3.2880	-1.3720	67	H	-1.1738	2.4540	-0.9295
27	C	0.0910	1.6698	3.8527	68	H	0.9804	1.5080	4.4658
28	C	-0.5748	2.9248	3.9176	69	H	-0.1833	3.7032	4.5760
29	C	-1.6952	3.1484	3.1724	70	H	-2.2213	4.1045	3.2214
30	C	-2.2043	2.1292	2.3125	71	H	-3.9469	3.2299	1.6919
31	C	-1.5262	0.8715	2.2251	72	H	-1.5060	-1.0645	1.3290
32	C	-0.3571	0.6573	3.0428	73	H	-5.7128	2.4057	0.2823
33	C	-3.3816	2.3018	1.5757	74	H	-6.7289	0.5431	-0.9894
34	C	-3.8820	1.3117	0.7350	75	H	-6.6937	-1.6528	-1.8498
35	C	-3.1454	0.0883	0.5400	76	H	-5.5182	-3.7515	-2.4221
36	C	-2.0158	-0.1062	1.3411	77	H	-3.4705	-4.9815	-2.6232
37	C	-5.1701	1.4712	0.1229	78	H	-0.9162	-1.3130	-0.4783
38	C	-5.7212	0.4544	-0.5773	79	H	-1.3457	-6.2478	-2.9697
39	C	-4.9883	-0.7530	-0.8426	80	H	1.1235	-6.3124	-2.8409
40	C	-3.6674	-0.9047	-0.4023	81	H	2.3821	-4.4103	-1.8211
41	C	-5.6458	-1.7983	-1.5778	82	H	1.1739	-2.4590	-0.9109

Table S12. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (M,P_a,M) Conformer in Chloroform (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	-0.0930	-1.6705	3.8445	42	C	-5.0267	-2.9500	-1.8811
2	C	0.5758	-2.9238	3.9145	43	C	-3.6220	-3.0879	-1.6206
3	C	1.7031	-3.1439	3.1782	44	C	-2.9203	-2.0366	-0.9245
4	C	2.2146	-2.1230	2.3213	45	C	-2.9302	-4.1908	-2.1163
5	C	1.5324	-0.8676	2.2268	46	C	-1.5370	-4.2929	-2.0252
6	C	0.3579	-0.6562	3.0377	47	C	-0.8193	-3.2096	-1.4291
7	C	3.3990	-2.2930	1.5950	48	C	-1.5259	-2.1190	-0.8970
8	C	3.9022	-1.3022	0.7565	49	C	-0.8070	-5.4050	-2.5478
9	C	3.1614	-0.0828	0.5519	50	C	0.5580	-5.4295	-2.4914
10	C	2.0242	0.1095	1.3431	51	C	1.2760	-4.3428	-1.9131
11	C	5.1968	-1.4581	0.1565	52	C	0.6090	-3.2662	-1.4000
12	C	5.7499	-0.4406	-0.5417	53	H	-0.9863	-1.5114	4.4528
13	C	5.0131	0.7625	-0.8173	54	H	0.1820	-3.7028	4.5709
14	C	3.6874	0.9092	-0.3896	55	H	2.2334	-4.0975	3.2323
15	C	5.6729	1.8087	-1.5498	56	H	3.9670	-3.2186	1.7175
16	C	5.0272	2.9501	-1.8802	57	H	1.5091	1.0649	1.3225
17	C	3.6224	3.0881	-1.6201	58	H	5.7414	-2.3901	0.3237
18	C	2.9204	2.0366	-0.9244	59	H	6.7618	-0.5252	-0.9446
19	C	2.9308	4.1911	-2.1158	60	H	6.7240	1.6667	-1.8114
20	C	1.5377	4.2932	-2.0253	61	H	5.5433	3.7595	-2.4013
21	C	0.8197	3.2097	-1.4297	62	H	3.4917	4.9780	-2.6266
22	C	1.5260	2.1191	-0.8974	63	H	0.9345	1.3005	-0.4969
23	C	0.8079	5.4053	-2.5480	64	H	1.3640	6.2312	-2.9985
24	C	-0.5572	5.4298	-2.4922	65	H	-1.1081	6.2825	-2.8958
25	C	-1.2754	4.3429	-1.9145	66	H	-2.3669	4.3757	-1.8859
26	C	-0.6086	3.2663	-1.4013	67	H	-1.1564	2.4314	-0.9585
27	C	0.0923	1.6704	3.8446	68	H	0.9856	1.5114	4.4530
28	C	-0.5766	2.9236	3.9147	69	H	-0.1828	3.7026	4.5712
29	C	-1.7039	3.1438	3.1784	70	H	-2.2342	4.0974	3.2325
30	C	-2.2153	2.1229	2.3214	71	H	-3.9677	3.2184	1.7175
31	C	-1.5330	0.8676	2.2269	72	H	-1.5094	-1.0649	1.3224
32	C	-0.3585	0.6562	3.0378	73	H	-5.7419	2.3897	0.3234
33	C	-3.3997	2.2928	1.5950	74	H	-6.7619	0.5249	-0.9452
34	C	-3.9027	1.3020	0.7565	75	H	-6.7237	-1.6668	-1.8125
35	C	-3.1617	0.0827	0.5518	76	H	-5.5426	-3.7594	-2.4025
36	C	-2.0246	-0.1096	1.3431	77	H	-3.4908	-4.9777	-2.6273
37	C	-5.1972	1.4578	0.1563	78	H	-0.9345	-1.3005	-0.4960
38	C	-5.7501	0.4404	-0.5422	79	H	-1.3629	-6.2308	-2.9986
39	C	-5.0131	-0.7626	-0.8179	80	H	1.1091	-6.2821	-2.8949
40	C	-3.6874	-0.9092	-0.3898	81	H	2.3674	-4.3756	-1.8841
41	C	-5.6726	-1.8088	-1.5507	82	H	1.1566	-2.4315	-0.9567

Table S13. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (M,P_a,M) Conformer in DCM (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	-0.0867	-1.6682	3.8525	42	C	-4.9996	-2.9449	-1.9066
2	C	0.5795	-2.9235	3.9161	43	C	-3.5993	-3.0925	-1.6274
3	C	1.6971	-3.1484	3.1662	44	C	-2.8967	-2.0408	-0.9324
4	C	2.2019	-2.1294	2.3026	45	C	-2.9117	-4.2070	-2.1031
5	C	1.5229	-0.8718	2.2159	46	C	-1.5208	-4.3210	-1.9925
6	C	0.3576	-0.6565	3.0389	47	C	-0.8004	-3.2377	-1.3994
7	C	3.3770	-2.3037	1.5622	48	C	-1.5034	-2.1349	-0.8878
8	C	3.8749	-1.3135	0.7197	49	C	-0.7949	-5.4465	-2.4920
9	C	3.1382	-0.0896	0.5266	50	C	0.5691	-5.4837	-2.4166
10	C	2.0093	0.1052	1.3291	51	C	1.2901	-4.3968	-1.8417
11	C	5.1616	-1.4753	0.1043	52	C	0.6270	-3.3074	-1.3508
12	C	5.7132	-0.4586	-0.5967	53	H	-0.9732	-1.5065	4.4701
13	C	4.9811	0.7507	-0.8581	54	H	0.1910	-3.7005	4.5781
14	C	3.6609	0.9040	-0.4151	55	H	2.2250	-4.1036	3.2145
15	C	5.6409	1.7968	-1.5912	56	H	3.9425	-3.2319	1.6769
16	C	5.0008	2.9460	-1.9055	57	H	1.4969	1.0620	1.3154
17	C	3.6003	3.0935	-1.6273	58	H	5.7020	-2.4114	0.2621
18	C	2.8972	2.0417	-0.9330	59	H	6.7198	-0.5475	-1.0115
19	C	2.9131	4.2079	-2.1035	60	H	6.6878	1.6478	-1.8656
20	C	1.5220	4.3217	-1.9945	61	H	5.5172	3.7554	-2.4263
21	C	0.8012	3.2381	-1.4023	62	H	3.4749	4.9950	-2.6129
22	C	1.5038	2.1355	-0.8896	63	H	0.9092	1.3185	-0.4904
23	C	0.7963	5.4468	-2.4951	64	H	1.3549	6.2726	-2.9427
24	C	-0.5678	5.4835	-2.4216	65	H	-1.1157	6.3460	-2.8080
25	C	-1.2892	4.3963	-1.8478	66	H	-2.3798	4.4393	-1.8049
26	C	-0.6262	3.3072	-1.3558	67	H	-1.1761	2.4724	-0.9152
27	C	0.0866	1.6681	3.8534	68	H	0.9736	1.5066	4.4703
28	C	-0.5806	2.9228	3.9185	69	H	-0.1922	3.6996	4.5808
29	C	-1.6990	3.1473	3.1698	70	H	-2.2277	4.1021	3.2193
30	C	-2.2036	2.1287	2.3057	71	H	-3.9453	3.2304	1.6816
31	C	-1.5236	0.8717	2.2174	72	H	-1.4966	-1.0613	1.3156
32	C	-0.3575	0.6567	3.0394	73	H	-5.7040	2.4103	0.2654
33	C	-3.3792	2.3027	1.5660	74	H	-6.7202	0.5473	-1.0108
34	C	-3.8764	1.3130	0.7224	75	H	-6.6868	-1.6470	-1.8671
35	C	-3.1389	0.0897	0.5281	76	H	-5.5155	-3.7542	-2.4282
36	C	-2.0097	-0.1049	1.3302	77	H	-3.4732	-4.9939	-2.6131
37	C	-5.1630	1.4746	0.1068	78	H	-0.9091	-1.3178	-0.4882
38	C	-5.7137	0.4584	-0.5956	79	H	-1.3531	-6.2721	-2.9403
39	C	-4.9810	-0.7503	-0.8579	80	H	1.1172	-6.3465	-2.8021
40	C	-3.6609	-0.9035	-0.4145	81	H	2.3807	-4.4404	-1.7972
41	C	-5.6401	-1.7960	-1.5921	82	H	1.1766	-2.4729	-0.9092

Table S14. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (P,P_a,M) Conformer in Toluene (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	-1.5601	-2.0253	2.9637	42	C	-4.0423	2.5976	-2.9364
2	C	-2.1155	-3.2748	2.5712	43	C	-4.1812	1.4040	-2.1521
3	C	-1.5188	-4.0150	1.5932	44	C	-3.5118	1.3066	-0.8775
4	C	-0.3270	-3.5480	0.9612	45	C	-5.0248	0.3846	-2.5861
5	C	0.2318	-2.2864	1.3429	46	C	-5.3141	-0.7277	-1.7878
6	C	-0.4231	-1.5263	2.3801	47	C	-4.7459	-0.7818	-0.4772
7	C	0.3558	-4.3185	0.0139	48	C	-3.8645	0.2292	-0.0610
8	C	1.5405	-3.8884	-0.5756	49	C	-6.1891	-1.7757	-2.2090
9	C	2.0650	-2.5788	-0.2787	50	C	-6.4932	-2.8089	-1.3688
10	C	1.4052	-1.8408	0.7094	51	C	-5.9441	-2.8546	-0.0550
11	C	2.2895	-4.7844	-1.4092	52	C	-5.0989	-1.8720	0.3772
12	C	3.5207	-4.4370	-1.8454	53	H	-2.0503	-1.4501	3.7525
13	C	4.0552	-3.1252	-1.6044	54	H	-3.0192	-3.6368	3.0663
14	C	3.3004	-2.1500	-0.9401	55	H	-1.9319	-4.9787	1.2868
15	C	5.3870	-2.8430	-2.0645	56	H	-0.0280	-5.3101	-0.2385
16	C	5.9442	-1.6225	-1.8982	57	H	1.8299	-0.9036	1.0553
17	C	5.1650	-0.5373	-1.3744	58	H	1.8686	-5.7677	-1.6305
18	C	3.8056	-0.7753	-0.9521	59	H	4.1284	-5.1403	-2.4192
19	C	5.6950	0.7503	-1.3547	60	H	5.9516	-3.6556	-2.5271
20	C	4.9244	1.8632	-0.9995	61	H	6.9723	-1.4246	-2.2094
21	C	3.5451	1.6547	-0.6866	62	H	6.7328	0.8972	-1.6646
22	C	3.0268	0.3496	-0.6709	63	H	1.9636	0.2450	-0.4716
23	C	5.4459	3.1934	-0.9859	64	H	6.5023	3.3441	-1.2215
24	C	4.6383	4.2548	-0.6899	65	H	5.0449	5.2686	-0.6813
25	C	3.2590	4.0510	-0.3970	66	H	2.6250	4.9108	-0.1698
26	C	2.7287	2.7918	-0.3988	67	H	1.6725	2.6345	-0.1703
27	C	1.0393	-0.2051	3.8818	68	H	1.3587	-1.1508	4.3249
28	C	1.5717	1.0116	4.3906	69	H	2.2900	0.9776	5.2125
29	C	1.1905	2.2062	3.8542	70	H	1.5977	3.1475	4.2305
30	C	0.2544	2.2466	2.7774	71	H	0.3574	4.3778	2.4955
31	C	-0.2949	1.0269	2.2679	72	H	-1.5851	0.1408	0.8189
32	C	0.1329	-0.2210	2.8522	73	H	-0.7160	5.6283	0.7536
33	C	-0.1073	3.4479	2.1581	74	H	-2.0401	5.6591	-1.3364
34	C	-0.9975	3.4926	1.0893	75	H	-3.2963	4.5892	-3.0146
35	C	-1.6380	2.2861	0.6280	76	H	-4.5539	2.6514	-3.8999
36	C	-1.2221	1.0850	1.2122	77	H	-5.5047	0.4784	-3.5636
37	C	-1.2055	4.7246	0.3836	78	H	-3.4906	0.1660	0.9576
38	C	-1.9350	4.7409	-0.7544	79	H	-6.6147	-1.7306	-3.2144
39	C	-2.6256	3.5680	-1.2153	80	H	-7.1646	-3.6051	-1.6979
40	C	-2.5929	2.3760	-0.4801	81	H	-6.2037	-3.6845	0.6060
41	C	-3.3490	3.6532	-2.4541	82	H	-4.6716	-1.9073	1.3815

Table S15. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (P,P_a,M) Conformer in Chloroform (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	-1.5625	-2.0274	2.9573	42	C	-4.0449	2.5878	-2.9424
2	C	-2.1173	-3.2767	2.5623	43	C	-4.1860	1.3972	-2.1534
3	C	-1.5185	-4.0164	1.5848	44	C	-3.5161	1.3028	-0.8785
4	C	-0.3254	-3.5481	0.9557	45	C	-5.0321	0.3780	-2.5837
5	C	0.2326	-2.2867	1.3397	46	C	-5.3237	-0.7305	-1.7802
6	C	-0.4242	-1.5277	2.3768	47	C	-4.7557	-0.7805	-0.4691
7	C	0.3585	-4.3176	0.0079	48	C	-3.8712	0.2297	-0.0570
8	C	1.5437	-3.8857	-0.5801	49	C	-6.2011	-1.7784	-2.1977
9	C	2.0676	-2.5762	-0.2807	50	C	-6.5077	-2.8074	-1.3528
10	C	1.4066	-1.8397	0.7079	51	C	-5.9594	-2.8486	-0.0381
11	C	2.2926	-4.7808	-1.4152	52	C	-5.1120	-1.8660	0.3906
12	C	3.5235	-4.4320	-1.8520	53	H	-2.0557	-1.4533	3.7451
13	C	4.0574	-3.1201	-1.6089	54	H	-3.0225	-3.6384	3.0550
14	C	3.3032	-2.1461	-0.9416	55	H	-1.9304	-4.9801	1.2765
15	C	5.3889	-2.8376	-2.0707	56	H	-0.0247	-5.3090	-0.2463
16	C	5.9469	-1.6175	-1.9026	57	H	1.8295	-0.9022	1.0550
17	C	5.1686	-0.5334	-1.3743	58	H	1.8715	-5.7639	-1.6372
18	C	3.8095	-0.7714	-0.9503	59	H	4.1318	-5.1337	-2.4272
19	C	5.7007	0.7536	-1.3516	60	H	5.9519	-3.6499	-2.5360
20	C	4.9317	1.8661	-0.9907	61	H	6.9745	-1.4185	-2.2148
21	C	3.5526	1.6580	-0.6757	62	H	6.7382	0.9001	-1.6628
22	C	3.0323	0.3535	-0.6637	63	H	1.9695	0.2507	-0.4611
23	C	5.4554	3.1957	-0.9728	64	H	6.5115	3.3455	-1.2103
24	C	4.6496	4.2570	-0.6702	65	H	5.0573	5.2704	-0.6577
25	C	3.2703	4.0538	-0.3750	66	H	2.6385	4.9139	-0.1422
26	C	2.7380	2.7951	-0.3814	67	H	1.6821	2.6375	-0.1515
27	C	1.0372	-0.2051	3.8794	68	H	1.3566	-1.1499	4.3249
28	C	1.5703	1.0125	4.3863	69	H	2.2881	0.9791	5.2089
29	C	1.1906	2.2067	3.8472	70	H	1.5984	3.1487	4.2214
30	C	0.2546	2.2454	2.7699	71	H	0.3613	4.3764	2.4826
31	C	-0.2962	1.0251	2.2632	72	H	-1.5908	0.1372	0.8190
32	C	0.1310	-0.2222	2.8495	73	H	-0.7073	5.6227	0.7357
33	C	-0.1050	3.4463	2.1478	74	H	-2.0330	5.6500	-1.3551
34	C	-0.9952	3.4891	1.0787	75	H	-3.2940	4.5781	-3.0274
35	C	-1.6384	2.2824	0.6216	76	H	-4.5572	2.6388	-3.9057
36	C	-1.2247	1.0819	1.2085	77	H	-5.5119	0.4690	-3.5615
37	C	-1.2000	4.7195	0.3688	78	H	-3.4971	0.1685	0.9618
38	C	-1.9300	4.7339	-0.7692	79	H	-6.6261	-1.7361	-3.2035
39	C	-2.6243	3.5609	-1.2253	80	H	-7.1807	-3.6038	-1.6786
40	C	-2.5941	2.3713	-0.4859	81	H	-6.2217	-3.6750	0.6264
41	C	-3.3486	3.6437	-2.4642	82	H	-4.6864	-1.8968	1.3960

Table S16. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*M*) Conformer in DCM (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	-1.5645	-2.0253	2.9500	42	C	-4.0574	2.5857	-2.9419
2	C	-2.1192	-3.2745	2.5538	43	C	-4.1968	1.3955	-2.1516
3	C	-1.5186	-4.0149	1.5777	44	C	-3.5242	1.3016	-0.8780
4	C	-0.3240	-3.5470	0.9510	45	C	-5.0439	0.3760	-2.5800
5	C	0.2340	-2.2857	1.3361	46	C	-5.3335	-0.7321	-1.7752
6	C	-0.4245	-1.5263	2.3720	47	C	-4.7630	-0.7816	-0.4650
7	C	0.3611	-4.3167	0.0041	48	C	-3.8775	0.2289	-0.0550
8	C	1.5472	-3.8847	-0.5824	49	C	-6.2116	-1.7805	-2.1908
9	C	2.0714	-2.5755	-0.2818	50	C	-6.5161	-2.8095	-1.3448
10	C	1.4092	-1.8390	0.7062	51	C	-5.9653	-2.8500	-0.0309
11	C	2.2962	-4.7800	-1.4174	52	C	-5.1174	-1.8668	0.3960
12	C	3.5274	-4.4315	-1.8539	53	H	-2.0598	-1.4508	3.7361
13	C	4.0616	-3.1197	-1.6097	54	H	-3.0260	-3.6352	3.0443
14	C	3.3081	-2.1457	-0.9414	55	H	-1.9300	-4.9786	1.2686
15	C	5.3935	-2.8381	-2.0717	56	H	-0.0221	-5.3079	-0.2510
16	C	5.9527	-1.6186	-1.9026	57	H	1.8312	-0.9013	1.0538
17	C	5.1755	-0.5345	-1.3724	58	H	1.8744	-5.7628	-1.6398
18	C	3.8161	-0.7714	-0.9481	59	H	4.1360	-5.1328	-2.4292
19	C	5.7098	0.7517	-1.3478	60	H	5.9551	-3.6508	-2.5380
20	C	4.9425	1.8646	-0.9839	61	H	6.9804	-1.4199	-2.2148
21	C	3.5633	1.6580	-0.6680	62	H	6.7473	0.8971	-1.6591
22	C	3.0408	0.3542	-0.6584	63	H	1.9781	0.2532	-0.4543
23	C	5.4687	3.1934	-0.9633	64	H	6.5248	3.3417	-1.2017
24	C	4.6649	4.2554	-0.6569	65	H	5.0741	5.2681	-0.6421
25	C	3.2853	4.0536	-0.3606	66	H	2.6554	4.9143	-0.1244
26	C	2.7508	2.7958	-0.3698	67	H	1.6948	2.6390	-0.1390
27	C	1.0378	-0.2024	3.8734	68	H	1.3583	-1.1467	4.3193
28	C	1.5714	1.0158	4.3787	69	H	2.2900	0.9831	5.2006
29	C	1.1910	2.2098	3.8390	70	H	1.5988	3.1523	4.2118
30	C	0.2534	2.2473	2.7628	71	H	0.3599	4.3783	2.4732
31	C	-0.2982	1.0264	2.2581	72	H	-1.5964	0.1371	0.8181
32	C	0.1302	-0.2205	2.8445	73	H	-0.7098	5.6224	0.7265
33	C	-0.1068	3.4478	2.1401	74	H	-2.0404	5.6482	-1.3622
34	C	-0.9987	3.4894	1.0723	75	H	-3.3061	4.5761	-3.0295
35	C	-1.6431	2.2823	0.6176	76	H	-4.5721	2.6359	-3.9040
36	C	-1.2288	1.0822	1.2051	77	H	-5.5256	0.4666	-3.5569
37	C	-1.2041	4.7193	0.3614	78	H	-3.5013	0.1673	0.9629
38	C	-1.9366	4.7329	-0.7753	79	H	-6.6385	-1.7383	-3.1959
39	C	-2.6325	3.5595	-1.2284	80	H	-7.1895	-3.6063	-1.6689
40	C	-2.6011	2.3704	-0.4881	81	H	-6.2262	-3.6762	0.6344
41	C	-3.3597	3.6419	-2.4659	82	H	-4.6902	-1.8968	1.4009

Table S17. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*P*) Conformer in Toluene (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.7319	-1.5181	0.9865	42	C	-4.6842	0.2136	-2.4683
2	H	1.2857	-0.5879	0.9365	43	H	-5.1675	0.0447	-3.4340
3	C	4.5411	0.1929	-0.0810	44	C	-5.1293	-0.4972	-1.3479
4	C	3.5002	-0.7468	-0.0077	45	C	5.0320	0.8639	1.0818
5	H	3.1208	-0.9809	0.9831	46	H	4.5850	0.6272	2.0501
6	C	-0.2048	-1.6528	2.0244	47	C	-2.4577	2.9813	-3.4198
7	C	0.3968	0.6329	3.0301	48	H	-2.2548	3.6371	-4.2694
8	C	0.9266	-2.4893	0.0003	49	C	-1.9210	-3.0201	3.1643
9	C	-0.7319	1.5179	0.9866	50	H	-2.5106	-3.9389	3.2032
10	H	-1.2856	0.5877	0.9365	51	C	-5.0324	-0.8635	1.0818
11	C	0.0478	-3.6308	0.0268	52	H	-4.5855	-0.6268	2.0502
12	C	-0.9933	-2.8454	2.0932	53	C	-3.3450	1.9670	-3.5277
13	C	-0.9265	2.4892	0.0005	54	H	-3.8674	1.7731	-4.4671
14	C	2.9912	-1.4005	-1.1325	55	C	6.1695	1.4747	-1.4129
15	C	-1.8851	2.3608	-1.0997	56	H	6.6119	1.7048	-2.3852
16	C	1.8853	-2.3609	-1.0998	57	C	-1.2973	-0.8566	4.0423
17	C	-0.8519	-3.7958	1.0758	58	H	-1.4358	-0.0908	4.8085
18	H	-1.4945	-4.6797	1.0844	59	C	0.8520	3.7955	1.0761
19	C	-2.9912	1.4006	-1.1324	60	H	1.4947	4.6794	1.0847
20	C	-3.5004	0.7469	-0.0076	61	C	-2.0622	-2.0536	4.1166
21	H	-3.1210	0.9811	0.9832	62	H	-2.7681	-2.1855	4.9395
22	C	-4.5413	-0.1926	-0.0809	63	C	1.2973	0.8561	4.0424
23	C	0.2048	1.6525	2.0246	64	H	1.4358	0.0904	4.8085
24	C	3.6690	-1.1631	-2.3840	65	C	6.0286	1.7934	0.9839
25	C	0.8057	-4.3105	-2.1637	66	H	6.3898	2.3056	1.8783
26	H	0.7577	-4.9693	-3.0337	67	C	-6.1697	-1.4743	-1.4129
27	C	1.7213	-3.2038	-2.2063	68	H	-6.6121	-1.7044	-2.3853
28	C	4.6842	-0.2134	-2.4683	69	C	1.9211	3.0197	3.1646
29	H	5.1675	-0.0445	-3.4339	70	H	2.5106	3.9385	3.2035
30	C	-0.3967	-0.6332	3.0301	71	C	-0.8054	4.3104	-2.1635
31	C	2.4579	-2.9812	-3.4200	72	H	-0.7574	4.9692	-3.0334
32	H	2.2551	-3.6371	-4.2696	73	C	2.0623	2.0532	4.1168
33	C	5.1291	0.4975	-1.3478	74	H	2.7682	2.1850	4.9397
34	C	0.0462	-4.5532	-1.0719	75	C	-6.0290	-1.7929	0.9839
35	H	-0.6215	-5.4164	-1.0286	76	H	-6.3904	-2.3051	1.8783
36	C	-3.6689	1.1632	-2.3840	77	C	6.6038	2.1054	-0.2816
37	C	0.9934	2.8451	2.0934	78	H	7.3988	2.8522	-0.3401
38	C	3.3452	-1.9669	-3.5278	79	C	-0.0460	4.5531	-1.0716
39	H	3.8677	-1.7730	-4.4671	80	H	0.6218	5.4163	-1.0283
40	C	-0.0477	3.6307	0.0270	81	C	-6.6043	-2.1049	-0.2817
41	C	-1.7211	3.2038	-2.2062	82	H	-7.3993	-2.8517	-0.3402

Table S18. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*P*) Conformer in Chloroform (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.7314	-1.5171	0.9910	42	C	-4.6775	0.2086	-2.4716
2	H	1.2881	-0.5885	0.9441	43	H	-5.1585	0.0386	-3.4383
3	C	4.5395	0.1950	-0.0827	44	C	-5.1247	-0.5010	-1.3509
4	C	3.4986	-0.7447	-0.0078	45	C	5.0334	0.8645	1.0801
5	H	3.1217	-0.9787	0.9842	46	H	4.5895	0.6253	2.0494
6	C	-0.2057	-1.6521	2.0288	47	C	-2.4492	2.9757	-3.4215
7	C	0.3969	0.6329	3.0357	48	H	-2.2445	3.6313	-4.2709
8	C	0.9236	-2.4867	0.0025	49	C	-1.9235	-3.0197	3.1673
9	C	-0.7313	1.5169	0.9911	50	H	-2.5138	-3.9383	3.2047
10	H	-1.2879	0.5883	0.9441	51	C	-5.0339	-0.8640	1.0801
11	C	0.0434	-3.6275	0.0277	52	H	-4.5901	-0.6249	2.0495
12	C	-0.9957	-2.8440	2.0960	53	C	-3.3368	1.9614	-3.5299
13	C	-0.9234	2.4866	0.0027	54	H	-3.8581	1.7661	-4.4697
14	C	2.9872	-1.3972	-1.1325	55	C	6.1646	1.4792	-1.4178
15	C	-1.8808	2.3574	-1.0989	56	H	6.6042	1.7102	-2.3912
16	C	1.8809	-2.3575	-1.0991	57	C	-1.2974	-0.8572	4.0479
17	C	-0.8560	-3.7936	1.0773	58	H	-1.4358	-0.0929	4.8155
18	H	-1.4991	-4.6772	1.0852	59	C	0.8561	3.7933	1.0775
19	C	-2.9872	1.3973	-1.1324	60	H	1.4993	4.6769	1.0855
20	C	-3.4988	0.7449	-0.0077	61	C	-2.0634	-2.0540	4.1209
21	H	-3.1220	0.9789	0.9843	62	H	-2.7693	-2.1859	4.9439
22	C	-4.5398	-0.1947	-0.0827	63	C	1.2974	0.8568	4.0479
23	C	0.2058	1.6518	2.0289	64	H	1.4359	0.0924	4.8155
24	C	3.6625	-1.1586	-2.3855	65	C	6.0294	1.7949	0.9805
25	C	0.7980	-4.3053	-2.1649	66	H	6.3931	2.3063	1.8746
26	H	0.7489	-4.9624	-3.0362	67	C	-6.1649	-1.4788	-1.4179
27	C	1.7146	-3.1989	-2.2066	68	H	-6.6045	-1.7098	-2.3913
28	C	4.6775	-0.2084	-2.4716	69	C	1.9236	3.0193	3.1675
29	H	5.1586	-0.0384	-3.4382	70	H	2.5139	3.9378	3.2050
30	C	-0.3969	-0.6332	3.0356	71	C	-0.7977	4.3052	-2.1647
31	C	2.4495	-2.9757	-3.4216	72	H	-0.7486	4.9623	-3.0359
32	H	2.2449	-3.6313	-4.2711	73	C	2.0635	2.0535	4.1210
33	C	5.1245	0.5013	-1.3509	74	H	2.7694	2.1853	4.9440
34	C	0.0393	-4.5487	-1.0723	75	C	-6.0300	-1.7943	0.9805
35	H	-0.6295	-5.4112	-1.0289	76	H	-6.3938	-2.3056	1.8745
36	C	-3.6624	1.1587	-2.3854	77	C	6.6013	2.1090	-0.2865
37	C	0.9958	2.8436	2.0962	78	H	7.3956	2.8565	-0.3457
38	C	3.3370	-1.9613	-3.5299	79	C	-0.0391	4.5485	-1.0721
39	H	3.8583	-1.7660	-4.4697	80	H	0.6298	5.4110	-1.0286
40	C	-0.0432	3.6273	0.0279	81	C	-6.6017	-2.1084	-0.2866
41	C	-1.7144	3.1989	-2.2065	82	H	-7.3962	-2.8559	-0.3458

Table S19. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*P*) Conformer in DCM (S_0 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.7300	-1.5166	0.9945	42	C	-4.6713	0.2061	-2.4748
2	H	1.2883	-0.5889	0.9493	43	H	-5.1507	0.0361	-3.4422
3	C	4.5363	0.1978	-0.0854	44	C	-5.1197	-0.5037	-1.3545
4	C	3.4955	-0.7423	-0.0087	45	C	5.0316	0.8674	1.0768
5	H	3.1203	-0.9754	0.9841	46	H	4.5895	0.6276	2.0468
6	C	-0.2070	-1.6515	2.0326	47	C	-2.4421	2.9737	-3.4218
7	C	0.3972	0.6327	3.0403	48	H	-2.2361	3.6296	-4.2707
8	C	0.9203	-2.4853	0.0046	49	C	-1.9254	-3.0193	3.1708
9	C	-0.7298	1.5164	0.9947	50	H	-2.5162	-3.9375	3.2075
10	H	-1.2881	0.5887	0.9494	51	C	-5.0322	-0.8669	1.0769
11	C	0.0394	-3.6256	0.0295	52	H	-4.5902	-0.6271	2.0469
12	C	-0.9979	-2.8430	2.0992	53	C	-3.3297	1.9593	-3.5312
13	C	-0.9202	2.4851	0.0048	54	H	-3.8503	1.7637	-4.4713
14	C	2.9829	-1.3952	-1.1329	55	C	6.1591	1.4826	-1.4234
15	C	-1.8764	2.3556	-1.0980	56	H	6.5971	1.7132	-2.3976
16	C	1.8766	-2.3557	-1.0981	57	C	-1.2972	-0.8576	4.0528
17	C	-0.8594	-3.7922	1.0797	58	H	-1.4351	-0.0940	4.8214
18	H	-1.5028	-4.6756	1.0875	59	C	0.8596	3.7919	1.0800
19	C	-2.9829	1.3952	-1.1328	60	H	1.5031	4.6752	1.0878
20	C	-3.4958	0.7426	-0.0086	61	C	-2.0641	-2.0540	4.1253
21	H	-3.1206	0.9757	0.9842	62	H	-2.7697	-2.1857	4.9485
22	C	-4.5366	-0.1974	-0.0854	63	C	1.2973	0.8570	4.0529
23	C	0.2071	1.6512	2.0327	64	H	1.4352	0.0935	4.8214
24	C	3.6565	-1.1564	-2.3869	65	C	6.0271	1.7985	0.9755
25	C	0.7917	-4.3029	-2.1642	66	H	6.3920	2.3103	1.8688
26	H	0.7419	-4.9592	-3.0360	67	C	-6.1594	-1.4821	-1.4234
27	C	1.7088	-3.1967	-2.2060	68	H	-6.5973	-1.7127	-2.3977
28	C	4.6713	-0.2059	-2.4748	69	C	1.9256	3.0188	3.1711
29	H	5.1508	-0.0359	-3.4422	70	H	2.5163	3.9371	3.2079
30	C	-0.3971	-0.6332	3.0402	71	C	-0.7913	4.3027	-2.1640
31	C	2.4425	-2.9738	-3.4219	72	H	-0.7414	4.9590	-3.0358
32	H	2.2366	-3.6297	-4.2708	73	C	2.0642	2.0535	4.1254
33	C	5.1194	0.5041	-1.3545	74	H	2.7698	2.1851	4.9487
34	C	0.0336	-4.5464	-1.0710	75	C	-6.0278	-1.7978	0.9755
35	H	-0.6358	-5.4084	-1.0270	76	H	-6.3929	-2.3095	1.8688
36	C	-3.6564	1.1565	-2.3869	77	C	6.5970	2.1128	-0.2926
37	C	0.9980	2.8426	2.0995	78	H	7.3908	2.8608	-0.3529
38	C	3.3300	-1.9593	-3.5312	79	C	-0.0333	4.5462	-1.0708
39	H	3.8506	-1.7636	-4.4713	80	H	0.6361	5.4081	-1.0267
40	C	-0.0391	3.6254	0.0298	81	C	-6.5976	-2.1121	-0.2926
41	C	-1.7085	3.1966	-2.2058	82	H	-7.3915	-2.8600	-0.3530

Table S20. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (M,P_a,M) Conformer in Toluene (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.8417	1.4547	3.9477	42	C	5.5809	0.0183	-2.0054
2	C	0.8906	2.8758	3.9990	43	C	4.4546	0.8412	-1.6938
3	C	0.0780	3.6228	3.1968	44	C	3.3316	0.2687	-0.9736
4	C	-0.8200	2.9859	2.2880	45	C	4.4055	2.1601	-2.1225
5	C	-0.8533	1.5573	2.2120	46	C	3.2551	2.9732	-1.9579
6	C	-0.0029	0.7942	3.0916	47	C	2.1041	2.3862	-1.3514
7	C	-1.7126	3.7139	1.4926	48	C	2.1739	1.0470	-0.8890
8	C	-2.5874	3.0944	0.6040	49	C	3.1923	4.3108	-2.4027
9	C	-2.5455	1.6648	0.4253	50	C	2.0283	5.0479	-2.2611
10	C	-1.7124	0.9427	1.2854	51	C	0.8899	4.4671	-1.6754
11	C	-3.5865	3.8660	-0.0788	52	C	0.9257	3.1574	-1.2298
12	C	-4.5246	3.2490	-0.8331	53	H	1.4897	0.8754	4.6093
13	C	-4.4743	1.8336	-1.0785	54	H	1.5793	3.3610	4.6940
14	C	-3.4340	1.0506	-0.5626	55	H	0.0970	4.7144	3.2372
15	C	-5.5196	1.2439	-1.8687	56	H	-1.7482	4.8014	1.5958
16	C	-5.5168	-0.0759	-2.1648	57	H	-1.7472	-0.1421	1.2860
17	C	-4.3973	-0.8976	-1.8021	58	H	-3.6028	4.9479	0.0701
18	C	-3.3078	-0.3246	-1.0496	59	H	-5.3289	3.8211	-1.3012
19	C	-4.3322	-2.2164	-2.2458	60	H	-6.3361	1.8889	-2.2012
20	C	-3.1981	-3.0113	-2.0427	61	H	-6.3342	-0.5285	-2.7306
21	C	-2.0715	-2.4223	-1.3895	62	H	-5.1791	-2.6271	-2.8015
22	C	-2.1555	-1.1033	-0.9158	63	H	-1.2569	-0.6877	-0.4679
23	C	-3.1059	-4.3616	-2.5010	64	H	-3.9722	-4.8066	-2.9967
24	C	-1.9551	-5.0781	-2.3279	65	H	-1.8920	-6.1095	-2.6822
25	C	-0.8262	-4.4872	-1.6896	66	H	0.0878	-5.0716	-1.5631
26	C	-0.8814	-3.1989	-1.2371	67	H	-0.0194	-2.7469	-0.7415
27	C	-0.9514	-1.3370	3.9570	68	H	-1.6101	-0.7310	4.5827
28	C	-1.0188	-2.7349	4.0277	69	H	-1.7306	-3.2094	4.7062
29	C	-0.1767	-3.5109	3.2476	70	H	-0.2105	-4.6011	3.3099
30	C	0.7442	-2.9057	2.3720	71	H	1.6565	-4.7527	1.7049
31	C	0.8044	-1.4793	2.2792	72	H	1.8013	0.1885	1.3685
32	C	-0.0552	-0.6983	3.1045	73	H	3.5715	-4.9530	0.2526
33	C	1.6607	-3.6650	1.5968	74	H	5.3395	-3.8968	-1.1261
34	C	2.5760	-3.0828	0.7335	75	H	6.4106	-1.9549	-2.0150
35	C	2.5649	-1.6452	0.5339	76	H	6.4090	0.4608	-2.5634
36	C	1.7230	-0.8958	1.3688	77	H	5.2775	2.5810	-2.6300
37	C	3.5652	-3.8757	0.0722	78	H	1.2570	0.6171	-0.4904
38	C	4.5378	-3.2919	-0.6962	79	H	4.0745	4.7548	-2.8703
39	C	4.5338	-1.9030	-0.9545	80	H	1.9917	6.0818	-2.6111
40	C	3.4482	-1.0739	-0.4503	81	H	-0.0274	5.0505	-1.5719
41	C	5.5842	-1.3163	-1.6949	82	H	0.0430	2.7076	-0.7702

Table S21. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (M,P_a,M) Conformer in Chloroform (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.8382	1.4557	3.9552	42	C	5.5731	0.0095	-2.0138
2	C	0.8854	2.8773	4.0081	43	C	4.4469	0.8341	-1.7020
3	C	0.0727	3.6242	3.2055	44	C	3.3251	0.2643	-0.9765
4	C	-0.8231	2.9866	2.2945	45	C	4.3989	2.1513	-2.1345
5	C	-0.8542	1.5578	2.2164	46	C	3.2495	2.9675	-1.9674
6	C	-0.0042	0.7950	3.0968	47	C	2.0998	2.3840	-1.3548
7	C	-1.7155	3.7152	1.4992	48	C	2.1685	1.0457	-0.8889
8	C	-2.5885	3.0952	0.6088	49	C	3.1880	4.3036	-2.4154
9	C	-2.5442	1.6659	0.4280	50	C	2.0254	5.0442	-2.2708
10	C	-1.7109	0.9433	1.2875	51	C	0.8882	4.4675	-1.6791
11	C	-3.5878	3.8673	-0.0736	52	C	0.9232	3.1581	-1.2304
12	C	-4.5247	3.2507	-0.8302	53	H	1.4859	0.8773	4.6180
13	C	-4.4719	1.8355	-1.0779	54	H	1.5723	3.3622	4.7051
14	C	-3.4313	1.0525	-0.5622	55	H	0.0891	4.7158	3.2471
15	C	-5.5162	1.2465	-1.8709	56	H	-1.7525	4.8025	1.6036
16	C	-5.5117	-0.0728	-2.1699	57	H	-1.7422	-0.1416	1.2846
17	C	-4.3914	-0.8940	-1.8074	58	H	-3.6043	4.9490	0.0773
18	C	-3.3031	-0.3217	-1.0522	59	H	-5.3295	3.8219	-1.2983
19	C	-4.3250	-2.2119	-2.2544	60	H	-6.3324	1.8922	-2.2027
20	C	-3.1899	-3.0059	-2.0515	61	H	-6.3277	-0.5257	-2.7376
21	C	-2.0645	-2.4173	-1.3955	62	H	-5.1709	-2.6220	-2.8121
22	C	-2.1498	-1.0994	-0.9186	63	H	-1.2516	-0.6846	-0.4686
23	C	-3.0964	-4.3556	-2.5129	64	H	-3.9620	-4.7996	-3.0107
24	C	-1.9451	-5.0717	-2.3396	65	H	-1.8806	-6.1024	-2.6957
25	C	-0.8171	-4.4812	-1.6984	66	H	0.0968	-5.0662	-1.5718
26	C	-0.8737	-3.1936	-1.2433	67	H	-0.0130	-2.7408	-0.7458
27	C	-0.9490	-1.3361	3.9664	68	H	-1.6075	-0.7301	4.5927
28	C	-1.0141	-2.7339	4.0408	69	H	-1.7236	-3.2078	4.7224
29	C	-0.1718	-3.5110	3.2610	70	H	-0.2025	-4.6011	3.3263
30	C	0.7458	-2.9056	2.3822	71	H	1.6607	-4.7536	1.7183
31	C	0.8033	-1.4796	2.2854	72	H	1.7930	0.1877	1.3662
32	C	-0.0554	-0.6977	3.1105	73	H	3.5692	-4.9560	0.2620
33	C	1.6627	-3.6662	1.6071	74	H	5.3348	-3.9012	-1.1236
34	C	2.5745	-3.0843	0.7405	75	H	6.4028	-1.9643	-2.0186
35	C	2.5610	-1.6470	0.5366	76	H	6.3997	0.4510	-2.5751
36	C	1.7190	-0.8968	1.3710	77	H	5.2696	2.5693	-2.6466
37	C	3.5628	-3.8791	0.0790	78	H	1.2515	0.6198	-0.4862
38	C	4.5334	-3.2962	-0.6931	79	H	4.0694	4.7442	-2.8876
39	C	4.5284	-1.9081	-0.9544	80	H	1.9898	6.0774	-2.6230
40	C	3.4422	-1.0766	-0.4503	81	H	-0.0271	5.0537	-1.5730
41	C	5.5774	-1.3241	-1.6988	82	H	0.0417	2.7104	-0.7661

Table S22. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (M,P_a,M) Conformer in DCM (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.8360	1.4561	3.9596	42	C	5.5689	0.0057	-2.0196
2	C	0.8820	2.8778	4.0135	43	C	4.4430	0.8313	-1.7071
3	C	0.0694	3.6247	3.2105	44	C	3.3219	0.2631	-0.9783
4	C	-0.8249	2.9866	2.2981	45	C	4.3956	2.1476	-2.1416
5	C	-0.8548	1.5578	2.2189	46	C	3.2469	2.9657	-1.9727
6	C	-0.0050	0.7952	3.0998	47	C	2.0982	2.3844	-1.3562
7	C	-1.7170	3.7155	1.5026	48	C	2.1661	1.0466	-0.8885
8	C	-2.5887	3.0953	0.6109	49	C	3.1862	4.3011	-2.4224
9	C	-2.5433	1.6660	0.4292	50	C	2.0246	5.0438	-2.2756
10	C	-1.7101	0.9433	1.2886	51	C	0.8884	4.4695	-1.6800
11	C	-3.5876	3.8677	-0.0719	52	C	0.9228	3.1604	-1.2297
12	C	-4.5237	3.2514	-0.8300	53	H	1.4834	0.8781	4.6231
13	C	-4.4698	1.8362	-1.0787	54	H	1.5676	3.3627	4.7118
14	C	-3.4294	1.0531	-0.5624	55	H	0.0842	4.7164	3.2528
15	C	-5.5133	1.2478	-1.8735	56	H	-1.7548	4.8028	1.6075
16	C	-5.5085	-0.0713	-2.1736	57	H	-1.7395	-0.1417	1.2841
17	C	-4.3881	-0.8926	-1.8103	58	H	-3.6042	4.9493	0.0800
18	C	-3.3006	-0.3208	-1.0534	59	H	-5.3284	3.8223	-1.2987
19	C	-4.3215	-2.2102	-2.2585	60	H	-6.3291	1.8941	-2.2054
20	C	-3.1865	-3.0044	-2.0546	61	H	-6.3236	-0.5243	-2.7425
21	C	-2.0618	-2.4163	-1.3969	62	H	-5.1669	-2.6198	-2.8173
22	C	-2.1472	-1.0985	-0.9190	63	H	-1.2494	-0.6845	-0.4677
23	C	-3.0929	-4.3539	-2.5169	64	H	-3.9581	-4.7971	-3.0161
24	C	-1.9418	-5.0705	-2.3425	65	H	-1.8769	-6.1011	-2.6990
25	C	-0.8142	-4.4805	-1.6994	66	H	0.0991	-5.0663	-1.5719
26	C	-0.8710	-3.1929	-1.2437	67	H	-0.0111	-2.7401	-0.7449
27	C	-0.9473	-1.3363	3.9713	68	H	-1.6056	-0.7306	4.5982
28	C	-1.0110	-2.7341	4.0472	69	H	-1.7190	-3.2079	4.7305
29	C	-0.1686	-3.5113	3.2672	70	H	-0.1976	-4.6014	3.3336
30	C	0.7469	-2.9055	2.3867	71	H	1.6632	-4.7538	1.7236
31	C	0.8029	-1.4798	2.2882	72	H	1.7887	0.1877	1.3650
32	C	-0.0553	-0.6977	3.1136	73	H	3.5676	-4.9569	0.2649
33	C	1.6639	-3.6664	1.6112	74	H	5.3320	-3.9026	-1.1242
34	C	2.5737	-3.0844	0.7428	75	H	6.3983	-1.9685	-2.0221
35	C	2.5590	-1.6473	0.5372	76	H	6.3946	0.4466	-2.5828
36	C	1.7169	-0.8969	1.3717	77	H	5.2655	2.5638	-2.6566
37	C	3.5614	-3.8801	0.0809	78	H	1.2492	0.6230	-0.4830
38	C	4.5309	-3.2976	-0.6931	79	H	4.0671	4.7397	-2.8976
39	C	4.5254	-1.9099	-0.9556	80	H	1.9896	6.0766	-2.6291
40	C	3.4392	-1.0771	-0.4510	81	H	-0.0258	5.0574	-1.5721
41	C	5.5735	-1.3273	-1.7023	82	H	0.0422	2.7140	-0.7623

Table S23. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (P,P_a,M) Conformer in Toluene (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	1.4790	2.2329	2.9565	42	C	3.9589	-2.5786	-2.8224
2	C	1.9768	3.4953	2.5289	43	C	4.0606	-1.3492	-2.1003
3	C	1.3435	4.1832	1.5350	44	C	3.4216	-1.2300	-0.8019
4	C	0.1798	3.6405	0.9116	45	C	4.8083	-0.2955	-2.6058
5	C	-0.3128	2.3603	1.3211	46	C	5.0522	0.8902	-1.8667
6	C	0.3666	1.6659	2.3867	47	C	4.5245	0.9725	-0.5430
7	C	-0.5375	4.3491	-0.0587	48	C	3.7356	-0.0969	-0.0463
8	C	-1.6817	3.8309	-0.6579	49	C	5.8219	1.9607	-2.3691
9	C	-2.1215	2.4946	-0.3450	50	C	6.0724	3.0778	-1.5899
10	C	-1.4444	1.8273	0.6806	51	C	5.5641	3.1556	-0.2814
11	C	-2.4736	4.6562	-1.5245	52	C	4.8047	2.1198	0.2340
12	C	-3.6615	4.2088	-1.9909	53	H	1.9897	1.7049	3.7651
13	C	-4.0989	2.8615	-1.7481	54	H	2.8636	3.9114	3.0120
14	C	-3.2945	1.9605	-1.0390	55	H	1.7078	5.1590	1.2055
15	C	-5.3824	2.4626	-2.2565	56	H	-0.2122	5.3574	-0.3272
16	C	-5.8392	1.1992	-2.0987	57	H	-1.8186	0.8753	1.0449
17	C	-4.9932	0.1895	-1.5289	58	H	-2.1219	5.6655	-1.7491
18	C	-3.6811	0.5485	-1.0481	59	H	-4.3036	4.8549	-2.5940
19	C	-5.4096	-1.1397	-1.5188	60	H	-5.9940	3.2196	-2.7528
20	C	-4.5625	-2.1777	-1.1134	61	H	-6.8318	0.9099	-2.4510
21	C	-3.2253	-1.8459	-0.7328	62	H	-6.4145	-1.3793	-1.8760
22	C	-2.8231	-0.5009	-0.7105	63	H	-1.7843	-0.3043	-0.4584
23	C	-4.9636	-3.5492	-1.1117	64	H	-5.9887	-3.7952	-1.3998
24	C	-4.0804	-4.5322	-0.7633	65	H	-4.3947	-5.5784	-0.7660
25	C	-2.7418	-4.2041	-0.3999	66	H	-2.0454	-5.0015	-0.1312
26	C	-2.3268	-2.9021	-0.3871	67	H	-1.3036	-2.6476	-0.1031
27	C	-1.0133	0.3801	4.0047	68	H	-1.3345	1.3409	4.4124
28	C	-1.4724	-0.8092	4.5862	69	H	-2.1532	-0.7679	5.4389
29	C	-1.0611	-2.0319	4.0811	70	H	-1.4180	-2.9645	4.5243
30	C	-0.1864	-2.0909	2.9799	71	H	-0.1641	-4.2510	2.8405
31	C	0.2842	-0.8810	2.3787	72	H	1.4393	-0.0401	0.7777
32	C	-0.1436	0.3663	2.9178	73	H	0.8923	-5.5582	1.1216
33	C	0.2238	-3.3245	2.4092	74	H	2.1801	-5.6819	-0.9935
34	C	1.0639	-3.4007	1.3096	75	H	3.3299	-4.6243	-2.7975
35	C	1.6249	-2.1876	0.7433	76	H	4.4602	-2.6558	-3.7897
36	C	1.1608	-0.9708	1.2658	77	H	5.2481	-0.3928	-3.6018
37	C	1.3345	-4.6589	0.6870	78	H	3.4038	-0.0245	0.9879
38	C	2.0543	-4.7277	-0.4768	79	H	6.2265	1.8911	-3.3818
39	C	2.6508	-3.5775	-1.0387	80	H	6.6709	3.8990	-1.9900
40	C	2.5629	-2.2998	-0.3451	81	H	5.7694	4.0373	0.3295
41	C	3.3266	-3.6642	-2.2764	82	H	4.4008	2.1819	1.2468

Table S24. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*M*) Conformer in Chloroform (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	1.4823	2.2322	2.9415	42	C	3.9801	-2.5774	-2.8217
2	C	1.9785	3.4951	2.5118	43	C	4.0819	-1.3484	-2.0970
3	C	1.3400	4.1844	1.5221	44	C	3.4375	-1.2290	-0.8005
4	C	0.1728	3.6416	0.9042	45	C	4.8330	-0.2962	-2.5995
5	C	-0.3178	2.3611	1.3153	46	C	5.0756	0.8901	-1.8584
6	C	0.3667	1.6659	2.3774	47	C	4.5429	0.9726	-0.5366
7	C	-0.5483	4.3508	-0.0631	48	C	3.7496	-0.0954	-0.0433
8	C	-1.6945	3.8317	-0.6585	49	C	5.8484	1.9592	-2.3579
9	C	-2.1325	2.4950	-0.3445	50	C	6.0978	3.0765	-1.5769
10	C	-1.4515	1.8276	0.6786	51	C	5.5857	3.1544	-0.2702
11	C	-2.4888	4.6573	-1.5230	52	C	4.8227	2.1190	0.2426
12	C	-3.6776	4.2092	-1.9876	53	H	1.9986	1.7040	3.7463
13	C	-4.1132	2.8611	-1.7439	54	H	2.8688	3.9094	2.9901
14	C	-3.3076	1.9604	-1.0356	55	H	1.7021	5.1605	1.1909
15	C	-5.3977	2.4623	-2.2514	56	H	-0.2245	5.3593	-0.3327
16	C	-5.8544	1.1988	-2.0930	57	H	-1.8226	0.8745	1.0431
17	C	-5.0076	0.1895	-1.5227	58	H	-2.1376	5.6669	-1.7474
18	C	-3.6948	0.5483	-1.0429	59	H	-4.3220	4.8544	-2.5891
19	C	-5.4256	-1.1395	-1.5107	60	H	-6.0089	3.2198	-2.7473
20	C	-4.5790	-2.1774	-1.1031	61	H	-6.8471	0.9084	-2.4440
21	C	-3.2414	-1.8460	-0.7230	62	H	-6.4310	-1.3784	-1.8670
22	C	-2.8374	-0.5014	-0.7035	63	H	-1.7986	-0.3064	-0.4507
23	C	-4.9822	-3.5487	-1.0983	64	H	-6.0076	-3.7934	-1.3862
24	C	-4.1002	-4.5320	-0.7464	65	H	-4.4154	-5.5779	-0.7458
25	C	-2.7610	-4.2044	-0.3829	66	H	-2.0667	-5.0027	-0.1110
26	C	-2.3440	-2.9027	-0.3739	67	H	-1.3206	-2.6478	-0.0902
27	C	-1.0162	0.3783	3.9923	68	H	-1.3399	1.3385	4.3998
28	C	-1.4771	-0.8116	4.5712	69	H	-2.1607	-0.7712	5.4218
29	C	-1.0640	-2.0344	4.0661	70	H	-1.4220	-2.9677	4.5069
30	C	-0.1854	-2.0915	2.9681	71	H	-0.1646	-4.2523	2.8249
31	C	0.2882	-0.8812	2.3707	72	H	1.4539	-0.0383	0.7782
32	C	-0.1420	0.3656	2.9086	73	H	0.8935	-5.5571	1.1072
33	C	0.2257	-3.3254	2.3966	74	H	2.1882	-5.6789	-1.0050
34	C	1.0689	-3.3998	1.2995	75	H	3.3456	-4.6219	-2.8020
35	C	1.6342	-2.1863	0.7376	76	H	4.4853	-2.6538	-3.7871
36	C	1.1707	-0.9699	1.2616	77	H	5.2770	-0.3938	-3.5937
37	C	1.3392	-4.6580	0.6755	78	H	3.4138	-0.0209	0.9895
38	C	2.0625	-4.7256	-0.4865	79	H	6.2564	1.8889	-3.3692
39	C	2.6627	-3.5756	-1.0446	80	H	6.6990	3.8969	-1.9749
40	C	2.5757	-2.2974	-0.3483	81	H	5.7906	4.0353	0.3422
41	C	3.3426	-3.6623	-2.2800	82	H	4.4170	2.1802	1.2549

Table S25. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (P,P_a,M) Conformer in DCM (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	1.4824	2.2322	2.9379	42	C	3.9878	-2.5783	-2.8205
2	C	1.9779	3.4953	2.5079	43	C	4.0898	-1.3488	-2.0954
3	C	1.3379	4.1850	1.5192	44	C	3.4440	-1.2288	-0.7994
4	C	0.1699	3.6419	0.9028	45	C	4.8418	-0.2977	-2.5981
5	C	-0.3199	2.3610	1.3139	46	C	5.0838	0.8897	-1.8571
6	C	0.3661	1.6658	2.3752	47	C	4.5499	0.9732	-0.5359
7	C	-0.5523	4.3515	-0.0636	48	C	3.7555	-0.0941	-0.0424
8	C	-1.6990	3.8321	-0.6580	49	C	5.8572	1.9580	-2.3568
9	C	-2.1365	2.4951	-0.3441	50	C	6.1063	3.0761	-1.5760
10	C	-1.4541	1.8273	0.6779	51	C	5.5934	3.1550	-0.2697
11	C	-2.4942	4.6582	-1.5216	52	C	4.8296	2.1200	0.2432
12	C	-3.6833	4.2102	-1.9856	53	H	2.0005	1.7039	3.7417
13	C	-4.1185	2.8618	-1.7420	54	H	2.8691	3.9092	2.9849
14	C	-3.3124	1.9607	-1.0345	55	H	1.6991	5.1614	1.1879
15	C	-5.4035	2.4635	-2.2492	56	H	-0.2290	5.3602	-0.3331
16	C	-5.8605	1.1999	-2.0910	57	H	-1.8238	0.8734	1.0418
17	C	-5.0135	0.1903	-1.5212	58	H	-2.1431	5.6680	-1.7456
18	C	-3.7002	0.5485	-1.0418	59	H	-4.3285	4.8554	-2.5863
19	C	-5.4324	-1.1385	-1.5092	60	H	-6.0146	3.2216	-2.7445
20	C	-4.5861	-2.1768	-1.1017	61	H	-6.8535	0.9096	-2.4416
21	C	-3.2480	-1.8462	-0.7220	62	H	-6.4381	-1.3768	-1.8651
22	C	-2.8432	-0.5017	-0.7025	63	H	-1.8043	-0.3076	-0.4492
23	C	-4.9904	-3.5479	-1.0964	64	H	-6.0161	-3.7917	-1.3842
24	C	-4.1089	-4.5318	-0.7442	65	H	-4.4248	-5.5775	-0.7431
25	C	-2.7692	-4.2050	-0.3812	66	H	-2.0758	-5.0040	-0.1087
26	C	-2.3512	-2.9035	-0.3728	67	H	-1.3275	-2.6489	-0.0896
27	C	-1.0175	0.3770	3.9890	68	H	-1.3425	1.3368	4.3965
28	C	-1.4785	-0.8132	4.5672	69	H	-2.1632	-0.7732	5.4170
29	C	-1.0642	-2.0360	4.0624	70	H	-1.4220	-2.9697	4.5026
30	C	-0.1839	-2.0921	2.9657	71	H	-0.1621	-4.2535	2.8219
31	C	0.2901	-0.8817	2.3694	72	H	1.4597	-0.0376	0.7805
32	C	-0.1417	0.3650	2.9064	73	H	0.8971	-5.5572	1.1059
33	C	0.2285	-3.3263	2.3945	74	H	2.1937	-5.6785	-1.0061
34	C	1.0729	-3.3997	1.2984	75	H	3.3517	-4.6226	-2.8012
35	C	1.6391	-2.1860	0.7378	76	H	4.4940	-2.6545	-3.7855
36	C	1.1751	-0.9697	1.2621	77	H	5.2870	-0.3962	-3.5917
37	C	1.3436	-4.6582	0.6746	78	H	3.4190	-0.0178	0.9900
38	C	2.0676	-4.7254	-0.4872	79	H	6.2661	1.8867	-3.3677
39	C	2.6683	-3.5755	-1.0445	80	H	6.7080	3.8962	-1.9741
40	C	2.5816	-2.2966	-0.3476	81	H	5.7984	4.0361	0.3423
41	C	3.3490	-3.6627	-2.2795	82	H	4.4239	2.1813	1.2556

Table S26. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*P*) Conformer in Toluene (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.8283	-1.5155	0.8187	42	C	-5.0525	0.3450	-2.2914
2	H	1.3698	-0.5759	0.7575	43	H	-5.6188	0.2089	-3.2164
3	C	4.7284	0.0665	0.0966	44	C	-5.4031	-0.4001	-1.1597
4	C	3.6770	-0.8864	0.0837	45	C	5.1248	0.7269	1.2818
5	H	3.2315	-1.1400	1.0437	46	H	4.6061	0.4935	2.2145
6	C	-0.1461	-1.6383	1.8399	47	C	-2.9076	3.1409	-3.3421
7	C	0.4282	0.6428	2.8177	48	H	-2.7772	3.8246	-4.1840
8	C	1.0797	-2.5119	-0.1360	49	C	-1.8856	-2.9954	2.9181
9	C	-0.8232	1.5532	0.8636	50	H	-2.4854	-3.9081	2.9424
10	H	-1.3634	0.6138	0.8251	51	C	-5.0945	-0.8490	1.2386
11	C	0.1906	-3.6581	-0.1363	52	H	-4.5592	-0.6487	2.1698
12	C	-0.9348	-2.8308	1.8934	53	C	-3.8019	2.1285	-3.4063
13	C	-1.0996	2.5508	-0.0756	54	H	-4.4034	1.9631	-4.3029
14	C	3.2377	-1.5237	-1.0792	55	C	6.4392	1.3307	-1.1155
15	C	-2.1410	2.4478	-1.0995	56	H	6.9576	1.5567	-2.0505
16	C	2.1140	-2.4329	-1.1341	57	C	-1.3016	-0.8337	3.8240
17	C	-0.7456	-3.8031	0.8748	58	H	-1.4525	-0.0569	4.5765
18	H	-1.3811	-4.6924	0.8807	59	C	0.7361	3.8508	0.9102
19	C	-3.2451	1.4854	-1.0691	60	H	1.3687	4.7419	0.8980
20	C	-3.6565	0.7941	0.0733	61	C	-2.0609	-2.0108	3.8780
21	H	-3.1916	0.9928	1.0350	62	H	-2.7956	-2.1453	4.6747
22	C	-4.7044	-0.1405	0.0597	63	C	1.3799	0.8527	3.7847
23	C	0.1739	1.6789	1.8446	64	H	1.5618	0.0744	4.5291
24	C	4.0105	-1.2905	-2.2858	65	C	6.1420	1.6656	1.2622
25	C	1.1087	-4.4021	-2.2659	66	H	6.4345	2.1714	2.1848
26	H	1.0938	-5.0810	-3.1217	67	C	-6.4531	-1.3693	-1.1653
27	C	2.0201	-3.3216	-2.2833	68	H	-6.9807	-1.5639	-2.1023
28	C	5.0258	-0.3438	-2.2879	69	C	1.9395	3.0383	2.9126
29	H	5.5689	-0.1571	-3.2181	70	H	2.5241	3.9608	2.9361
30	C	-0.3600	-0.6235	2.8200	71	C	-1.1612	4.4386	-2.1839
31	C	2.8302	-3.0959	-3.4175	72	H	-1.1863	5.1235	-3.0345
32	H	2.7015	-3.7490	-4.2836	73	C	2.1409	2.0542	3.8369
33	C	5.4052	0.3703	-1.1230	74	H	2.8908	2.1768	4.6214
34	C	0.2610	-4.6010	-1.2095	75	C	-6.1039	-1.7696	1.1985
35	H	-0.4289	-5.4479	-1.2016	76	H	-6.3892	-2.3103	2.1037
36	C	-4.0286	1.2890	-2.2647	77	C	6.8006	1.9708	0.0582
37	C	0.9520	2.8785	1.8940	78	H	7.6030	2.7117	0.0504
38	C	3.7519	-2.0813	-3.4470	79	C	-0.3203	4.6553	-1.1472
39	H	4.3564	-1.9062	-4.3397	80	H	0.3425	5.5232	-1.1285
40	C	-0.2326	3.7020	-0.0784	81	C	-6.7920	-2.0351	-0.0212
41	C	-2.0723	3.3271	-2.1877	82	H	-7.5956	-2.7748	-0.0337

Table S27. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*P*) Conformer in Chloroform (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.8229	-1.5563	0.8614	42	C	-5.0237	0.3631	-2.2843
2	H	1.3687	-0.6199	0.8288	43	H	-5.5663	0.1834	-3.2162
3	C	4.7107	0.1245	0.0489	44	C	-5.4029	-0.3614	-1.1243
4	C	3.6579	-0.8048	0.0624	45	C	5.1118	0.8223	1.2310
5	H	3.1972	-1.0064	1.0257	46	H	4.5822	0.6163	2.1644
6	C	-0.1730	-1.6833	1.8439	47	C	-2.8294	3.1245	-3.3934
7	C	0.3682	0.6140	2.8282	48	H	-2.7007	3.7842	-4.2546
8	C	1.0911	-2.5491	-0.0855	49	C	-1.9416	-3.0426	2.9089
9	C	-0.8268	1.5186	0.8360	50	H	-2.5292	-3.9634	2.9283
10	H	-1.3720	0.5813	0.7749	51	C	-5.1240	-0.7360	1.2781
11	C	0.2193	-3.6968	-0.0924	52	H	-4.6075	-0.5075	2.2135
12	C	-0.9556	-2.8803	1.8886	53	C	-3.7513	2.1099	-3.4300
13	C	-1.0784	2.5193	-0.1148	54	H	-4.3561	1.9401	-4.3236
14	C	3.2372	-1.4866	-1.0827	55	C	6.4586	1.3537	-1.1784
15	C	-2.1138	2.4454	-1.1128	56	H	6.9812	1.5520	-2.1174
16	C	2.1286	-2.4440	-1.1139	57	C	-1.3725	-0.8629	3.7908
17	C	-0.7467	-3.8483	0.8988	58	H	-1.5513	-0.0880	4.5395
18	H	-1.3826	-4.7370	0.8837	59	C	0.7524	3.8034	0.8972
19	C	-3.2367	1.5355	-1.0646	60	H	1.3893	4.6917	0.9057
20	C	-3.6757	0.8872	0.0934	61	C	-2.1374	-2.0625	3.8387
21	H	-3.2314	1.1316	1.0565	62	H	-2.8862	-2.1860	4.6243
22	C	-4.7270	-0.0665	0.0980	63	C	1.3145	0.8175	3.8294
23	C	0.1526	1.6342	1.8540	64	H	1.4675	0.0371	4.5777
24	C	4.0153	-1.2860	-2.2815	65	C	6.1254	1.7387	1.1912
25	C	1.1348	-4.4239	-2.2074	66	H	6.4192	2.2714	2.0984
26	H	1.1535	-5.1027	-3.0630	67	C	-6.4353	-1.3229	-1.1258
27	C	2.0505	-3.3158	-2.2077	68	H	-6.9524	-1.5419	-2.0633
28	C	5.0436	-0.3464	-2.3081	69	C	1.8992	2.9830	2.9317
29	H	5.6053	-0.2067	-3.2354	70	H	2.5005	3.8947	2.9579
30	C	-0.4222	-0.6511	2.8226	71	C	-1.1088	4.4231	-2.2345
31	C	2.8807	-3.1259	-3.3657	72	H	-1.0958	5.1071	-3.0862
32	H	2.7423	-3.8041	-4.2108	73	C	2.0765	1.9929	3.8861
33	C	5.4037	0.3893	-1.1729	74	H	2.8150	2.1215	4.6803
34	C	0.2979	-4.6440	-1.1677	75	C	-6.1404	-1.6763	1.2502
35	H	-0.3687	-5.5091	-1.1508	76	H	-6.4335	-2.1893	2.1688
36	C	-4.0095	1.3106	-2.2736	77	C	6.8073	2.0100	-0.0313
37	C	0.9438	2.8245	1.9105	78	H	7.6142	2.7463	-0.0432
38	C	3.7791	-2.1168	-3.4280	79	C	-0.2593	4.6154	-1.1782
39	H	4.3770	-1.9473	-4.3263	80	H	0.4310	5.4620	-1.1652
40	C	-0.1873	3.6646	-0.1109	81	C	-6.7970	-1.9732	0.0434
41	C	-2.0197	3.3424	-2.2578	82	H	-7.5983	-2.7153	0.0290

Table S28. Cartesian Coordinates (Å) of Optimized Structure of [2]HA_2 (*P*,P_a,*P*) Conformer in DCM (S_1 State) Calculated by TD-DFT Method at CAM-B3LYP/def2-SVP Level

Label	Element	x	y	z	Label	Element	x	y	z
1	C	0.8247	-1.5587	0.8651	42	C	-5.0241	0.3689	-2.2876
2	H	1.3716	-0.6229	0.8332	43	H	-5.5667	0.1923	-3.2200
3	C	4.7101	0.1266	0.0450	44	C	-5.4036	-0.3596	-1.1293
4	C	3.6584	-0.8042	0.0617	45	C	5.1115	0.8274	1.2255
5	H	3.1992	-1.0038	1.0261	46	H	4.5838	0.6216	2.1601
6	C	-0.1721	-1.6845	1.8470	47	C	-2.8291	3.1321	-3.3898
7	C	0.3695	0.6132	2.8302	48	H	-2.6997	3.7938	-4.2495
8	C	1.0929	-2.5521	-0.0812	49	C	-1.9432	-3.0423	2.9111
9	C	-0.8278	1.5201	0.8402	50	H	-2.5309	-3.9630	2.9303
10	H	-1.3745	0.5836	0.7808	51	C	-5.1255	-0.7412	1.2722
11	C	0.2212	-3.7001	-0.0871	52	H	-4.6099	-0.5149	2.2087
12	C	-0.9554	-2.8812	1.8919	53	C	-3.7515	2.1180	-3.4285
13	C	-1.0791	2.5211	-0.1106	54	H	-4.3565	1.9498	-4.3223
14	C	3.2378	-1.4890	-1.0818	55	C	6.4547	1.3564	-1.1872
15	C	-2.1146	2.4478	-1.1091	56	H	6.9757	1.5533	-2.1274
16	C	2.1301	-2.4479	-1.1104	57	C	-1.3739	-0.8616	3.7915
17	C	-0.7457	-3.8506	0.9037	58	H	-1.5538	-0.0863	4.5395
18	H	-1.3813	-4.7396	0.8892	59	C	0.7537	3.8039	0.9007
19	C	-3.2370	1.5378	-1.0635	60	H	1.3910	4.6920	0.9092
20	C	-3.6763	0.8852	0.0929	61	C	-2.1399	-2.0608	3.8395
21	H	-3.2328	1.1257	1.0572	62	H	-2.8901	-2.1827	4.6239
22	C	-4.7280	-0.0683	0.0940	63	C	1.3177	0.8151	3.8300
23	C	0.1535	1.6342	1.8570	64	H	1.4714	0.0342	4.5778
24	C	4.0147	-1.2900	-2.2817	65	C	6.1234	1.7457	1.1823
25	C	1.1375	-4.4309	-2.2006	66	H	6.4175	2.2809	2.0880
26	H	1.1572	-5.1109	-3.0553	67	C	-6.4359	-1.3208	-1.1343
27	C	2.0524	-3.3218	-2.2026	68	H	-6.9526	-1.5368	-2.0727
28	C	5.0417	-0.3488	-2.3117	69	C	1.9030	2.9808	2.9328
29	H	5.6021	-0.2103	-3.2398	70	H	2.5049	3.8922	2.9586
30	C	-0.4220	-0.6514	2.8247	71	C	-1.1091	4.4280	-2.2287
31	C	2.8820	-3.1337	-3.3616	72	H	-1.0966	5.1133	-3.0795
32	H	2.7436	-3.8143	-4.2049	73	C	2.0809	1.9897	3.8863
33	C	5.4015	0.3899	-1.1782	74	H	2.8209	2.1169	4.6793
34	C	0.3004	-4.6495	-1.1607	75	C	-6.1421	-1.6818	1.2411
35	H	-0.3660	-5.5148	-1.1420	76	H	-6.4356	-2.1973	2.1581
36	C	-4.0100	1.3162	-2.2733	77	C	6.8034	2.0159	-0.0417
37	C	0.9458	2.8236	1.9131	78	H	7.6089	2.7538	-0.0559
38	C	3.7792	-2.1236	-3.4266	79	C	-0.2593	4.6190	-1.1721
39	H	4.3767	-1.9549	-4.3254	80	H	0.4310	5.4655	-1.1576
40	C	-0.1874	3.6662	-0.1063	81	C	-6.7981	-1.9750	0.0332
41	C	-2.0197	3.3473	-2.2535	82	H	-7.5994	-2.7172	0.0160