

Supporting Information

AIE-active auronones for circularly polarized luminescence and trace water detection

Wenzeng Duan,^{*,a} Wenjing Liu,^a Houting Liu,^a Honghan Ji,^a Yanmin Huo,^a Huaiwei Wang,^a and Shuwen Gong^{*,a}

^a School of Chemistry and Chemical Engineering, Shandong Provincial Key Laboratory of Chemical Energy Storage and Novel Cell Technology, Liaocheng University, No.1 Hunan Road, Liaocheng, 252000, China; *E-mail: duanwenzeng@lcu.edu.cn; gongshw@lcu.edu.cn.

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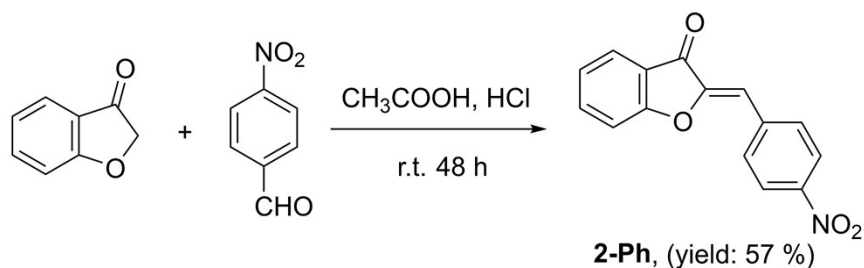
1. General Information

All the solvents were of analytical grade without further purification. Column flash chromatography was carried out on silica gel (200–400 mesh). Thin-layer chromatography (TLC) was performed on silica gel GF254. ^1H , ^{13}C NMR and 2D NOESY spectra were recorded on Bruker AVANCE NEO 500 MHz spectrometer and referenced to the residual proton signals of the solvent. HRMS spectra were recorded on an Agilent 100 ABI-API4000 spectrometer. X-ray data were collected on Bruker Smart APEX II CCD diffractometer. Chiral HPLC analysis of $(R_p)/(S_p)$ -**2-PCP** was performed using the Waters e2695 HPLC system with 2998PDA detector and (R, R) Whelk-O2 column (250 × 4.6 mm, 5 μm); Mobile phase: mixed solvents of hexane and *iso*-propanol with the ratio of 98.5% : 1.5% as an eluent; Flow rate: 0.4 mL/min; Column temperature: 35 °C. The absorbance spectra measurements were performed on a T9CS UV–vis spectrophotometer (Persee Instrument Co., Ltd. Beijing, China). The fluorescence spectra were measured on F-7100 spectrofluorimeter (Hitachi, Japan) luminescence spectrophotometer (the pathlength of the quartz cell is 1 cm) with a xenon arc lamp as the light source. Circular dichroism spectra of $(R_p)/(S_p)$ -**2-PCP** in THF/H₂O mixture solutions (5.0×10^{-5} mol/L) were measured using a J-810-150s spectropolarimeter (JASCO Co., Japan), at room temperature (cell length: 10 mm, bandwidth: 1 nm, scanning speed: 100 nm/min, data pitch: 1 nm, accumulations: 2). The CD spectra were approximated using the simple moving average (SMA) method. Circularly polarized luminescence (CPL) spectra in THF/H₂O mixture solutions (5.0×10^{-5} mol/L) for $(R_p)/(S_p)$ -**2-PCP** were recorded with a JASCO CPL-300 spectrofluoropolarimeter at room temperature. The CPL spectra were approximated using the SMA method. ($\lambda_{\text{ex}} = 360$ nm, cell length: 10 mm, E_x & E_m slit width: 3000 μm , scanning speed: 100 nm/min, data pitch: 1 nm, accumulations: 8).

2. Experimental section

2.1 General procedure for the preparation of **2-Ph**.^[1]

Compound **2-Ph** was readily prepared according to Scheme S1.



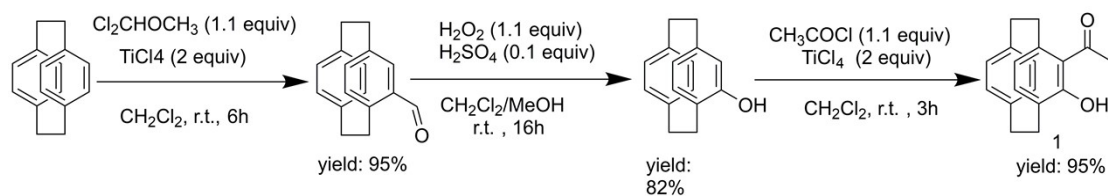
Scheme S1. Synthetic route for **2-Ph**

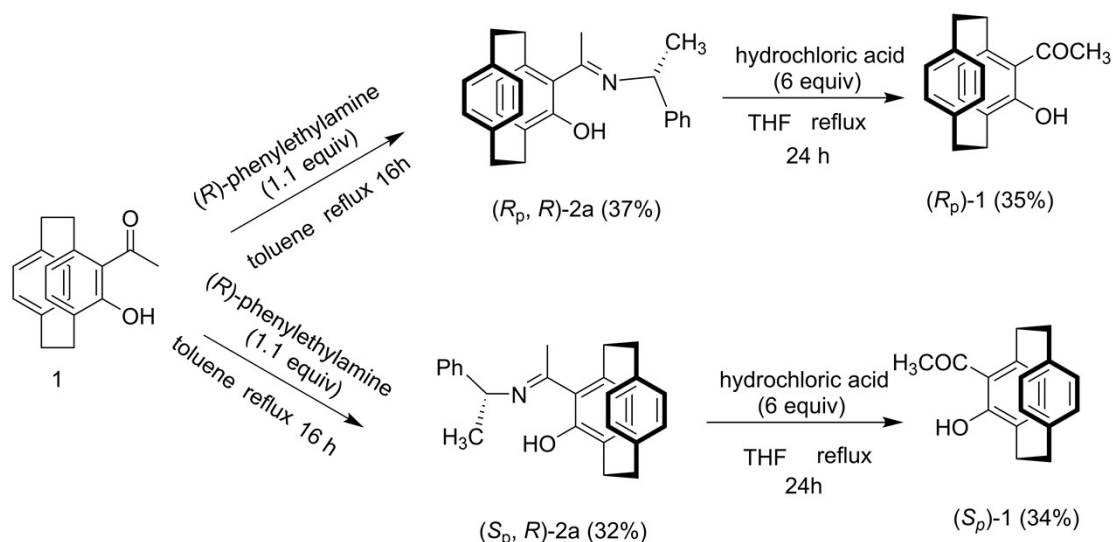
Benzofuran-3(2*H*)-one (0.1 g, 0.75 mmol) was dissolved in glacial acetic acid (5 mL) at room temperature under argon. Subsequently, the *p*-nitrobenzaldehyde (0.113 g, 0.75 mmol) and hydrochloric acid (12 mol/L, 75 μ L) were added, and the reaction mixture was stirred at room temperature for 48 h. An orange precipitate was formed, and the precipitate was isolated by filtration. The crude product was washed by ethanol to obtain **2-Ph** (0.11 g, 57%) as a light yellow powder.

¹H NMR (500 MHz, CDCl₃) δ 8.33 – 8.28 (m, 2H), 8.09 – 8.04 (m, 2H), 7.84 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.72 (ddd, *J* = 8.5, 7.2, 1.4 Hz, 1H), 7.39 – 7.36 (m, 1H), 7.29 (td, *J* = 7.6, 0.9 Hz, 1H), 6.88 (s, 1H); ¹³C{¹H} NMR (126 MHz, CDCl₃) δ 184.5, 166.4, 148.4, 147.7, 138.7, 137.6, 131.8, 125.0, 124.2, 124.0, 121.1, 113.1, 109.4. HRMS (ESI⁺): calcd for C₁₅H₉NO₄: [M+ K]⁺ 306.0163; found: [M+ K]⁺ 306.0172.

2.2 General procedure for the preparation of (*R*_p)/(*S*_p)-**1**.

(*R*_p)/(*S*_p)-**1** were easily prepared according to literature methods (Scheme S2).^[2]

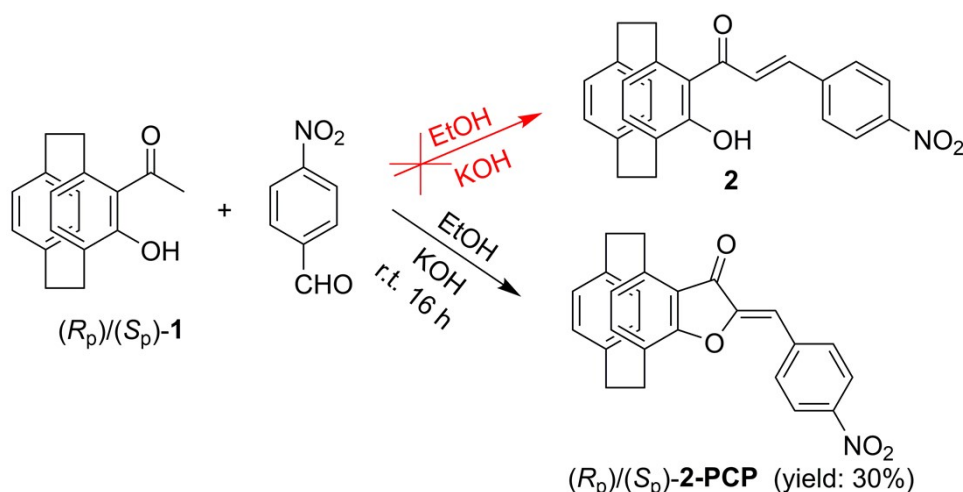




Scheme S2. Synthetic routes for $(R_p)/(S_p)$ -5-acetyl-4-hydroxy[2.2]paracyclophane ($(R_p)/(S_p)$ -1).

2.3 General procedure for the preparation of $(R_p)/(S_p)$ -2-PCP.

Compounds $(R_p)/(S_p)$ -2-PCP were readily prepared according to Scheme S3.



Scheme S3. Synthetic route for $(R_p)/(S_p)$ -2-PCP

Solution of KOH (0.36 g, 6.5 mmol in 2 mL H₂O) was added to a solution of compound **1** (0.2 g, 0.75 mmol) in ethanol (20 mL). After the mixture was stirred at room temperature for 30 minutes, p -nitrobenzaldehyde (0.14 g, 0.92 mmol) was added, and the reaction mixture was stirred at room temperature for another 16 h. Then the pH value of the mixed solution was adjusted to 7–8 by adding dilute hydrochloric acid (1.2 mol/L) in an ice water bath. The resulting precipitate was isolated by filtration, purified by column chromatography on silica gel (petroleum

ether / dichloromethane (1:1) to give the product **2-PCP** (0.09 g, 30% yield) as a yellow powder.

The procedure of adding H₂O₂: solution of KOH (0.18 g, 3.3 mmol in 1 mL H₂O) was added to a solution of compound **1** (0.1 g, 0.38 mmol) in ethanol (10 mL). After the mixture was stirred at room temperature for 30 minutes, *p*-nitrobenzaldehyde (0.07 g, 0.46 mmol) and H₂O₂ (35%, 65 μL, 0.76 mmol) were added, and the reaction mixture was stirred at room temperature for another 16 h. Then the pH value of the mixed solution was adjusted to 7–8 by adding dilute hydrochloric acid (1.2 mol/L) in an ice water bath. The resulting precipitate was isolated by filtration, purified by column chromatography on silica gel (petroleum ether / dichloromethane (1:1) to give the product **2-PCP** (0.07 g, 49 % yield) as a yellow powder.

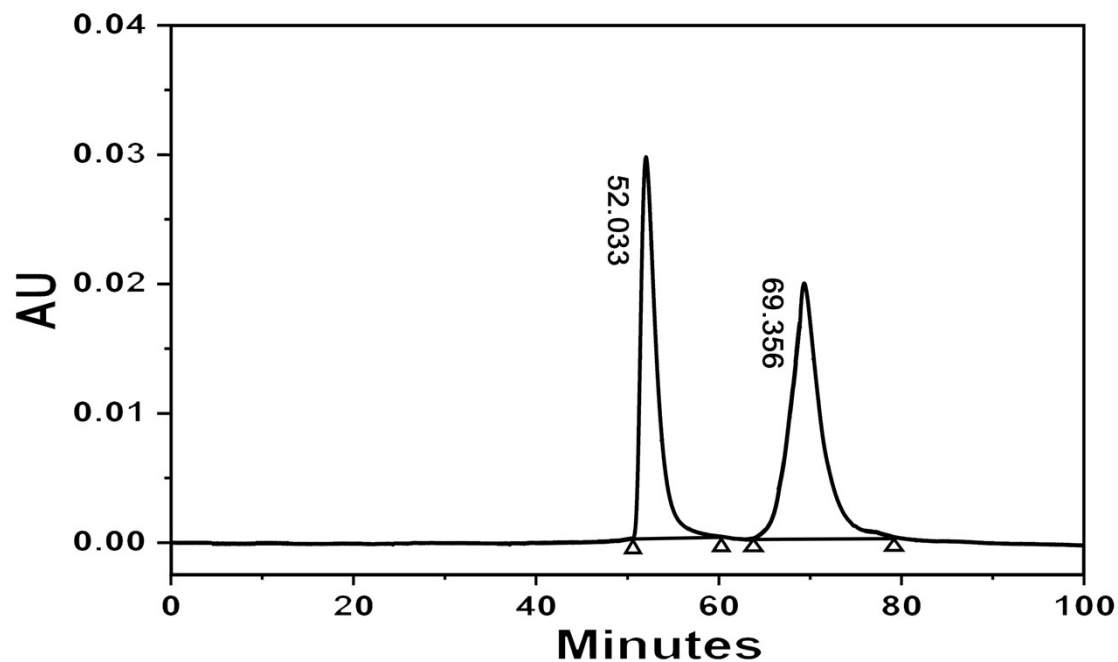
(*R*_p)/(*S*_p)-**2-PCP**: *R*_p [α]₂₅ D = 392 (*c* = 0.05, CH₂Cl₂), *S*_p [α]₂₅ D = -420 (*c* = 0.05, CH₂Cl₂); ¹H NMR (500 MHz, CDCl₃) δ 8.36 (d, *J* = 8.8 Hz, 2H), 8.11 (d, *J* = 8.8 Hz, 2H), 6.82 – 6.75 (m, 2H), 6.64 (dd, *J* = 7.8, 1.7 Hz, 1H), 6.58 – 6.51 (m, 2H), 6.46 (dd, *J* = 7.8, 1.7 Hz, 1H), 6.39 (dd, *J* = 7.8, 1.8 Hz, 1H), 4.04 (ddd, *J* = 13.1, 9.8, 3.5 Hz, 1H), 3.57 (ddd, *J* = 13.7, 9.7, 3.9 Hz, 1H), 3.24 – 3.09 (m, 4H), 2.96 – 2.85 (m, 2H); ¹³C{¹H} NMR (126 MHz, CDCl₃) δ 185.6, 165.7, 148.3, 147.5, 143.4, 142.6, 139.4, 139.2, 139.1, 133.7, 133.4, 131.5, 130.1, 129.7, 127.5, 124.2, 124.1, 123.5, 108.5, 34.2, 33.8, 31.1, 29.5. HRMS (ESI⁺): calcd for C₂₅H₁₉NO₄: [M + K]⁺ 436.0946; found: [M + K]⁺ 436.0954.

3. References

- [1] Kafle, A.; Bhattarai, S.; Miller, J. M.; Handy, S. T. Hydrogen sulfide sensing using an aurone-based fluorescent probe. *RSC Adv.* **2020**, *10*, 45180-45188.
- [2] (a) Cakici, M.; Gu, Z. G.; Nieger, M.; Bürck, J.; Heinke, L.; Bräse, S. Planar-chiral building blocks for metal–organic frameworks. *Chem. Commun.* **2015**, *51*, 4796-4798. (b) Friedmann, C. J.; Ay, S.; Bräse, S. Improved synthesis of enantiopure 4-hydroxy[2.2]paracyclophane. *J. Org. Chem.* **2010**, *75*, 4612-4614. (c) He, F. Y.; Ma, Y. D.; Zhao, L.; Duan, W. Z.; Chen, J. Q.; Zhao, Z. X. Synthesis of planar chiral [2.2]paracyclophane Schiff bases for the enantioselective Henry reaction. *Tetrahedron: Asymmetry* **2012**, *23*, 809-817. (d) Duan, W. Z. Ji, H. H. Yang, Z. R.; Yao, Q. X.; Huo, Y. M.; Ren, X. R.; Zhao, J. J.; Gong, S. W. Planar chiral [2.2]paracyclophanyl-based

boron fluoride complexes: synthesis, crystal structure and photophysical properties.
Dalton Trans. **2021**, *50*, 12963-12969.

4. HPLC chromatograms

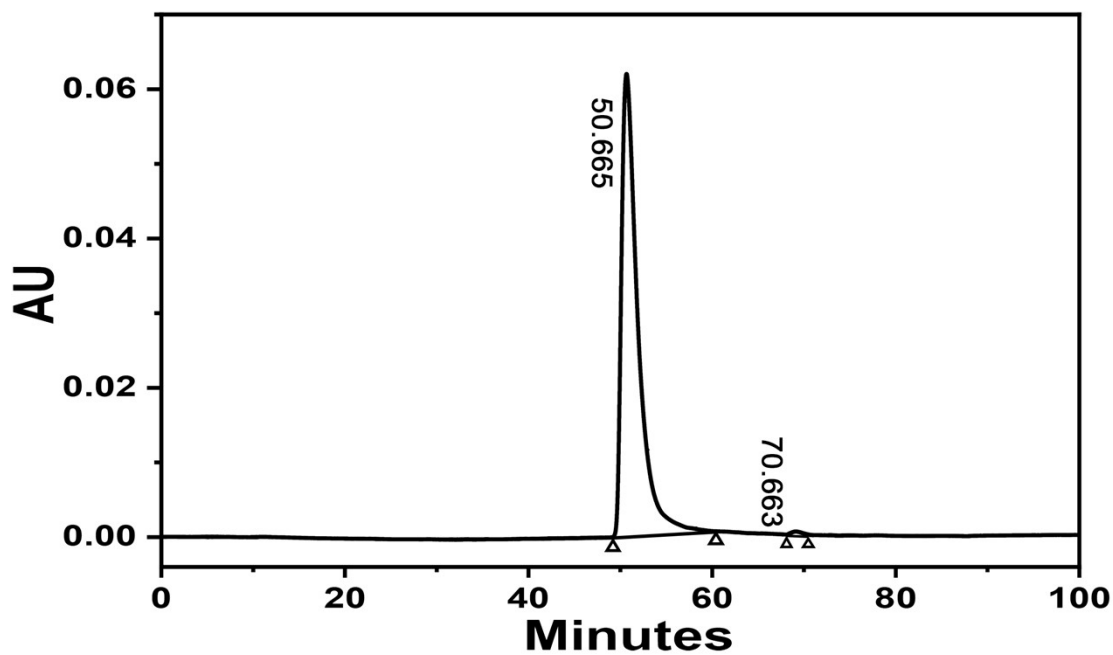


<Peak Table>

PDA Ch1 420 nm

Peak Name	Retention Time	Area	Peak Height	Area %
1	52.033	3592544	29581	49.57
2	69.356	3654239	19733	50.43
Total		7246783	49314	100.00

Figure S1. Chromatogram of the racemic of **2-PCP**.

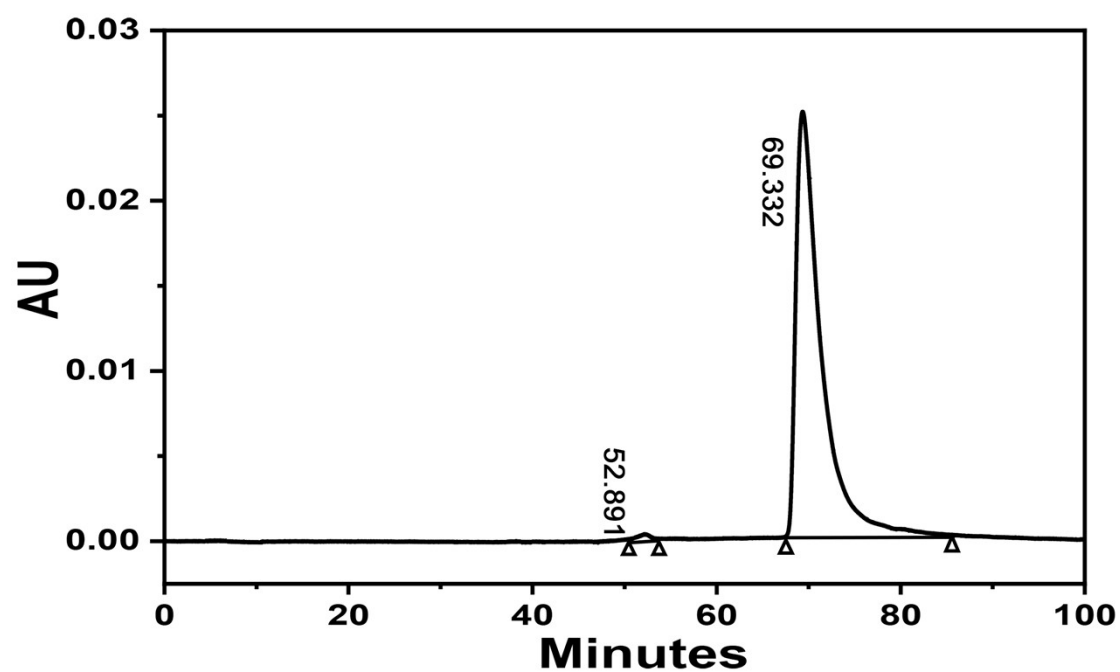


<Peak Table>

PDA Ch1 420 nm

Peak Name	Retention Time	Area	Peak Height	Area %
1	50.665	7878986	62467	99.78
2	70.663	17519	296	0.22
Total		7896505	62763	100.00

Figure S2. Chromatogram of the racemic of (*R_p*)-2-PCP.



<Peak Table>

PDA Ch1 420 nm

Peak Name	Retention Time	Area	Peak Height	Area %
1	52.891	8340	166	0.18

2	69.332	4694088	25154	99.82
Total		4702428	25320	100.00

Figure S3. Chromatogram of the racemic of (*S_p*)-**2-PCP**.

5. General Procedure for crystal measurement.

Single crystals of **2-Ph** and **2-PCP** suitable for X-ray diffraction were obtained by evaporation of their CH₂Cl₂ solutions at room temperature. X-ray data were collected on Bruker Smart APEX II CCD diffractometer. The structure was solved by direct methods (SHELXL-2018) and refined by the full-matrix least-squares on *F*² (SHELXL-2018). All the non-hydrogen atoms were refined anisotropically and all the hydrogen atoms were placed by using AFIX instructions.

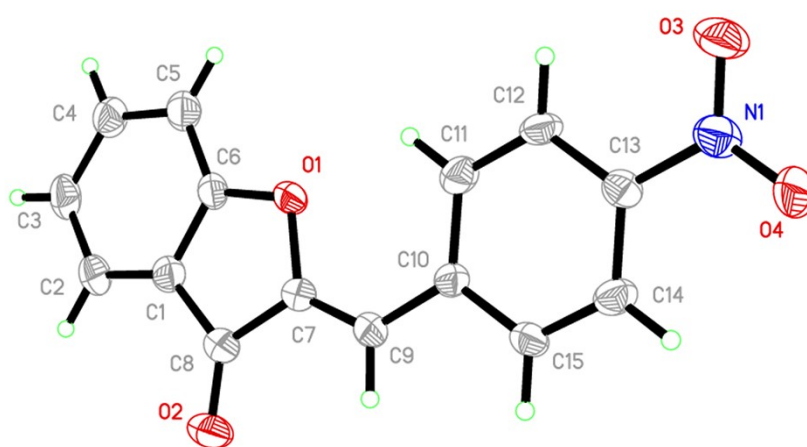


Figure S4. Single crystals of compound **2-Ph** (Ellipsoids are drawn to 30% probability).

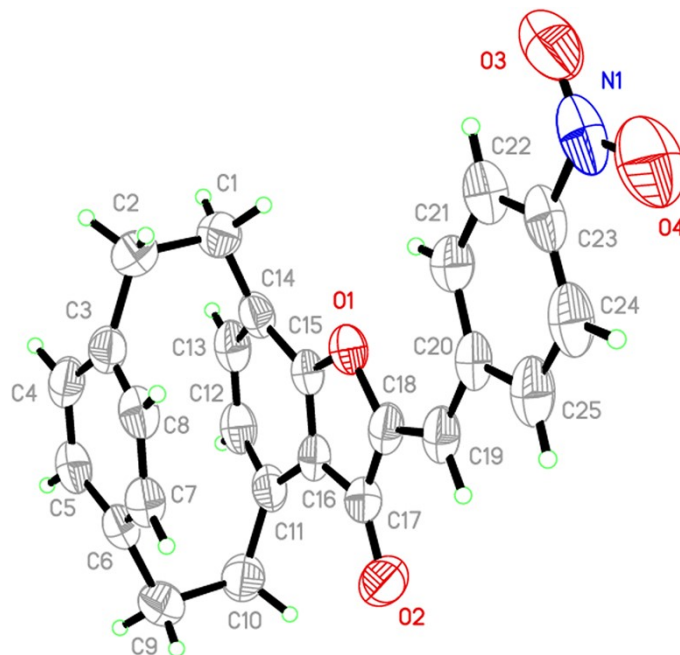


Figure S5. Single crystals of compound **2-PCP** (Ellipsoids are drawn to 30% probability).

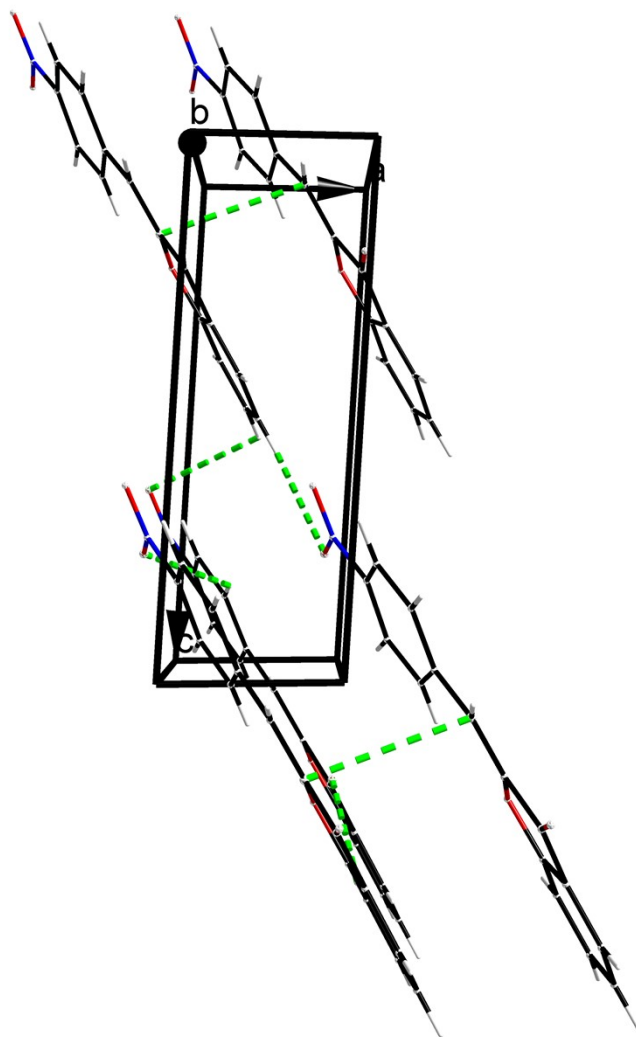


Figure S6. Molecular packing structure of **2-Ph** along *b* axis. The bright green dotted lines show weak intermolecular interactions.

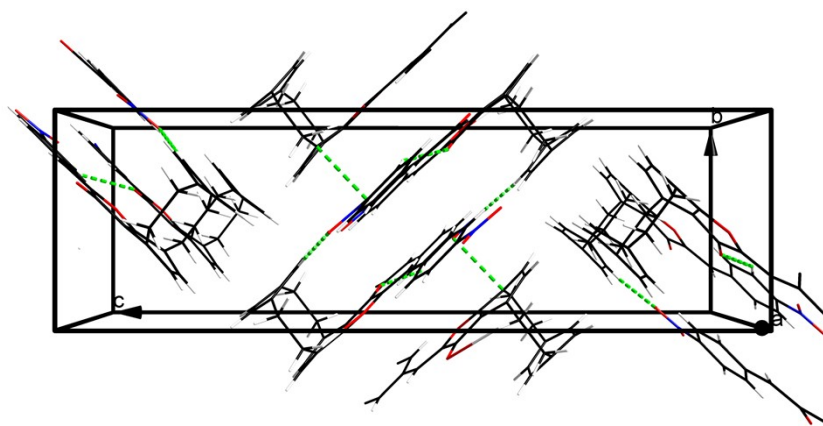


Figure S7. Molecular packing structure of **2-PCP** along *a* axis. The bright green dotted lines show weak intermolecular interactions.

Table S1. Crystallographic data and structure refinement for **2-Ph** and **2-PCP**.

Compound	2-Ph	2-PCP
Empirical formula	C ₁₅ H ₉ NO ₄	C ₂₅ H ₁₉ NO ₄
CCDC number	2202112	2183638
Formula weight	267.23	397.41
Temperature	298(2) K	293(2) K
Crystal system	Triclinic	Monoclinic
space group	P1	P2(1)/n
Unit cell dimensions	a = 3.8550 (4) Å;	a = 9.1268 (8) Å;
	$\alpha = 91.025 (2)^\circ$	$\alpha = 90^\circ$
	b = 6.9039 (7) Å;	b = 8.0238 (7) Å;
	$\beta = 93.364(3)^\circ$	$\beta = 89.960 (6)^\circ$
Volume	c = 11.2145 (11) Å;	c = 26.1099 (14) Å;
	$\gamma = 96.825(4)^\circ$	$\gamma = 90^\circ$
	295.75(5) Å ³	1912.1(3) Å ³
Z	1	4
Cal. Density	1.500 g/cm ³	1.381 g/cm ³
Index ranges	-4 ≤ h ≤ 4	-10 ≤ h ≤ 10
	-8 ≤ k ≤ 8	-9 ≤ k ≤ 9
	-8 ≤ l ≤ 13	0 ≤ l ≤ 31
F (000)	138	832
Crystal size	0.360 x 0.270 x 0.070 mm ³	0.120 x 0.110 x 0.110 mm ³
GOF	1.081	1.144
R indices	R ₁ = 0.0961,	R ₁ = 0.0622,
	wR ₂ = 0.2301	wR ₂ = 0.1746

Table S2. Hydrogen bonds for **2-Ph** and **2-PCP** [Å and °]

Compound	C-H...A	D(H...A)	∠(DHA)
2-Ph	C3-H3...O3	2.67(7) Å	168.1(6)°

2-PCP	C4-H4...O4	2.59(8) Å	163.7(6)°
	C5-H5...O2	2.63(7) Å	145.8(6)°
	C15-H15...O3	2.61(8) Å	130.3(3)°
	C8-H8...O4	2.66(5) Å	159.6(3)°
	C22-H22...O2	2.63(4) Å	153.4(3)°

Table S3. $\pi\cdots\pi$ for **2-Ph** and **2-PCP** [Å]

Compound	$\pi\cdots\pi$	D($\pi\cdots\pi$)
2-Ph	C7...C9	3.40(1) Å
2-PCP	O3...C4	3.11(6) Å

6. Photophysical Properties

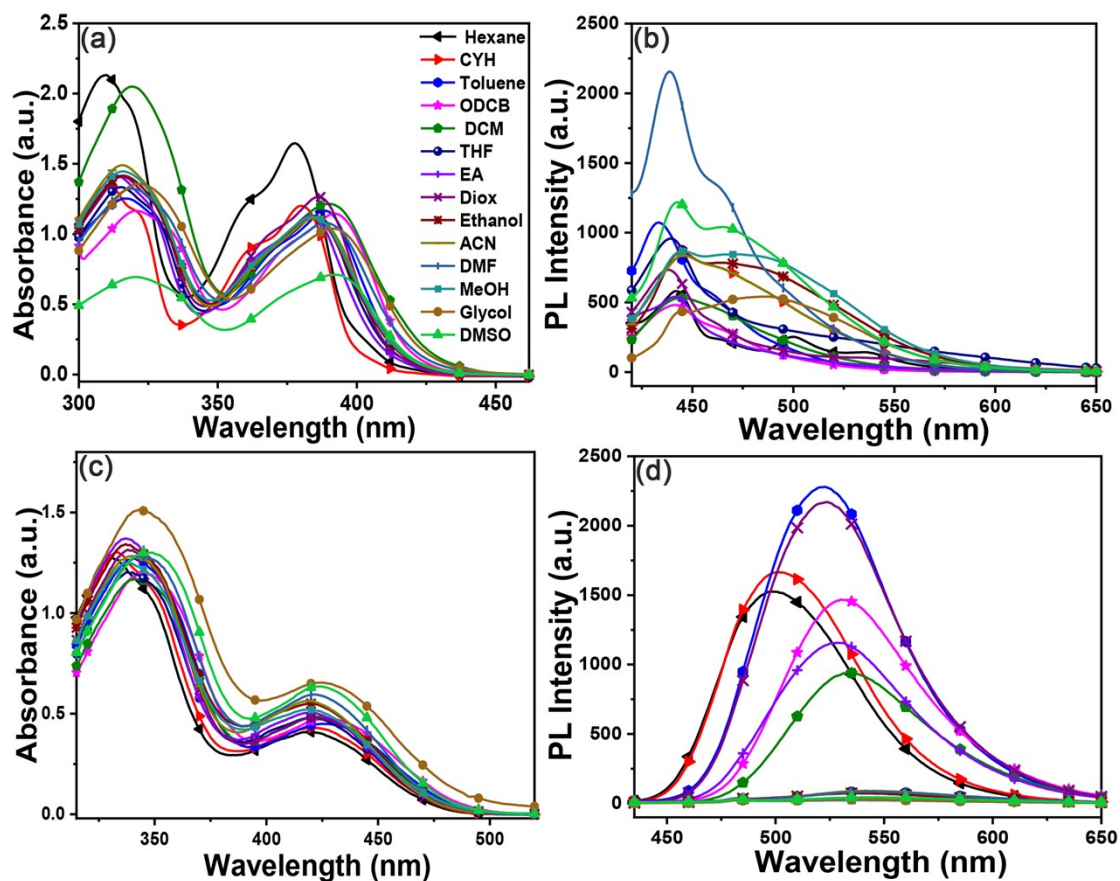


Figure S8. Absorption spectra of compounds (a) **2-Ph**, (c) **2-PCP** and fluorescence spectra of compounds (b) **2-Ph**, (d) **2-PCP** in various solvents (50 μM) such as hexane, cyclohexane (CYH), toluene, 1,2-dichlorobenzene (ODCB), dichloromethane (DCM), tetrahydrofuran (THF), ethyl acetate (EA), 1,4-dioxane (Diox), ethanol, acetonitrile (ACN), *N,N*-dimethylformamide (DMF), methanol (MeOH), ethylene glycol (Glycol) and dimethyl sulfoxide (DMSO), respectively.

Theoretical calculations

All the calculations were based on density functional theory (DFT) with B3LYP functional and 6-31G(d) basis set. Solvent (dichloromethane) was considered in all the calculations. The UV-vis absorptions of the compounds (vertical excitation) were calculated with the TD-DFT method based on the optimized ground state geometry (S_0 state). All these calculations were performed with Gaussian 09 software.

Computational details

The time-dependent density functional theory (TD-DFT) calculations were performed at the hybrid density functional theory level (B3LYP) with the 6-31G(d) basis set, using the Gaussian09 software package.⁴² The calculations were carried out in the gas phase, using the crystal structures of 2-Ph and 2-PCP as model structures and CH₂Cl₂ as the optimized solvent.

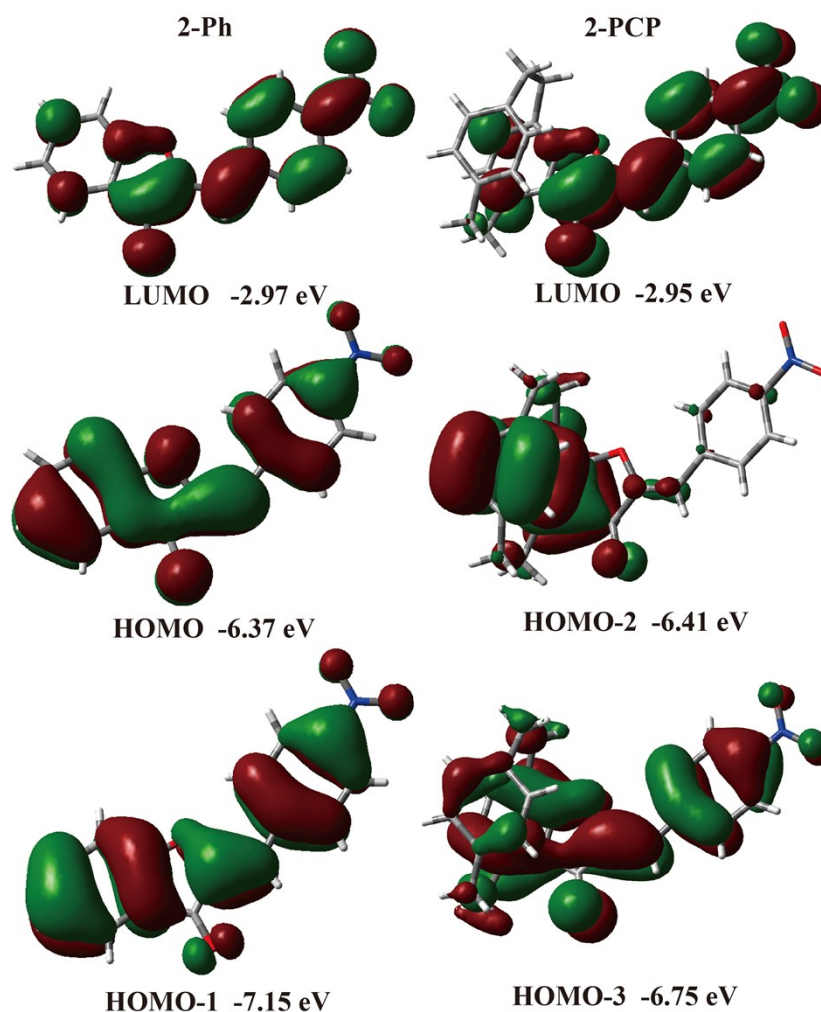


Figure S9. The angular nodal patterns of the LUMO, HOMO and HOMO-1 of **2-Ph** and the angular nodal patterns of the LUMO, HOMO-2 and HOMO-3 of **2-PCP**, calculated by using B3LYP/6-31G(d) basis set with the G09 program package.

Table S4. Related wave functions, oscillator strengths, and calculated electronic excitation energies of **2-Ph** and **2-PCP**.

Compound	State ^[a] ^[b]	λ [nm]	$f^{[c]}$	E_g (eV)	Orbital
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						(coefficient) ^[d]
2-Ph	S ₁	411.79	0.3375	3.01	H-L (68.3 %)	
	S ₃	333.24	0.7095	3.72	H ₁ -L (66.5 %)	
2-PCP	S ₄	415.96	0.1523	2.98	H ₂ -L (60.6 %)	
	S ₆	355.40	0.3477	3.49	H ₃ -L (57.3 %)	

^[a]Only selected excited states were considered. ^[b]DCM was employed as the solvent for the DFT calculations. ^[c]Oscillator strength. ^[d]MOs involved in the transitions. H = HOMO; L = LUMO. Coefficient of the wavefunction for each excitation.

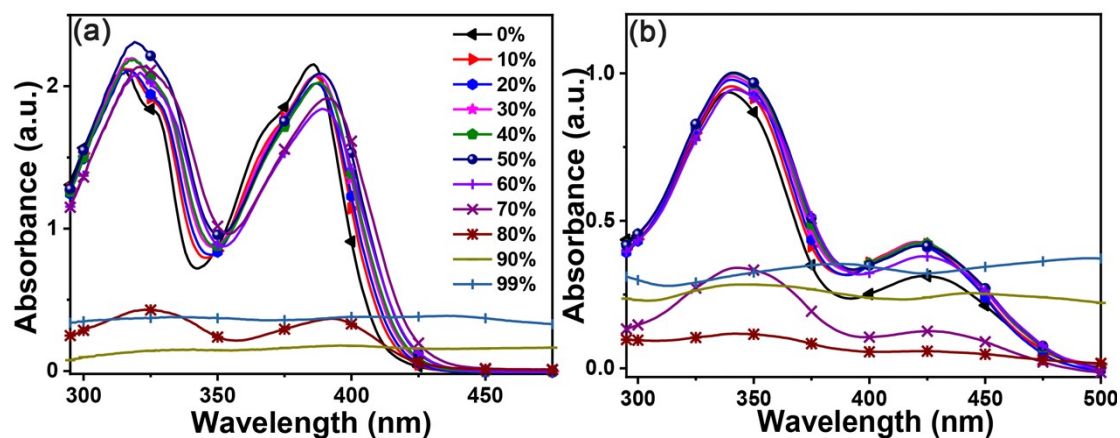


Figure S10. Absorption spectra of compounds (a) 2-Ph and (b) 2-PCP in THF/water mixtures (50 μM) with varied volumetric fractions of water (f_w).

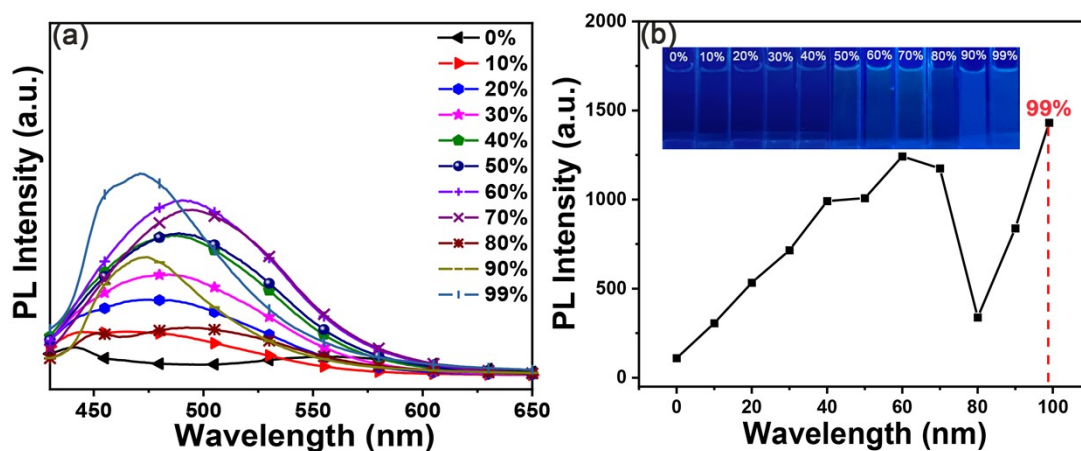


Figure S11. (a) Fluorescence spectra of compound 2-Ph in THF/water mixtures (50 μM) with varied volumetric fractions of water (f_w). (b) Changes in the F_{max} of 2-Ph in THF/water mixtures (50 μM) with varied volumetric fractions of water (f_w). Inset: The emission pictures of the solution of 2-Ph with different f_w under UV light (365 nm).

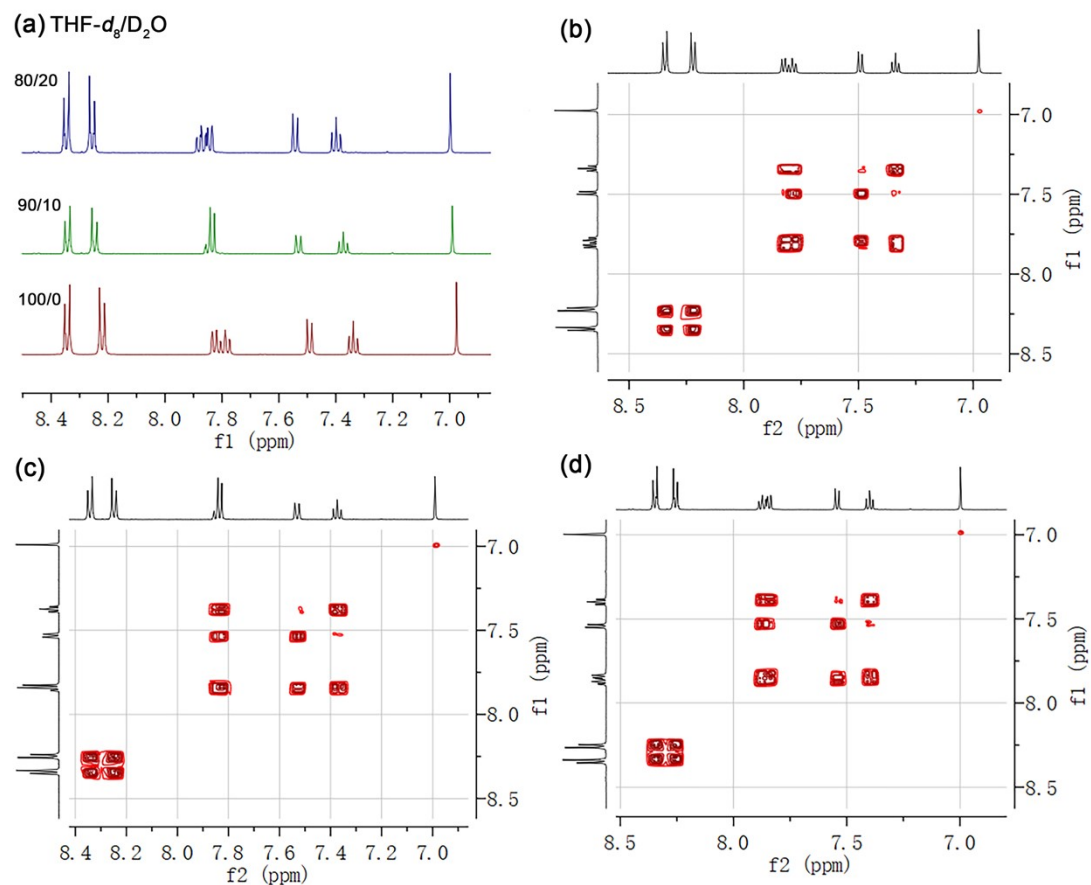


Figure S12 (a) ^1H NMR spectra of **2-Ph** in mixed THF- d_8 /D $_2$ O (5×10^{-3} M) with various ratios of 80/20, 90/10, and 100/0. 2D NOESY spectra of **2-Ph** in mixed THF- d_8 /D $_2$ O (5×10^{-3} M) with various ratios of (b) 100/0, (c) 90/10, and (d) 80/20.

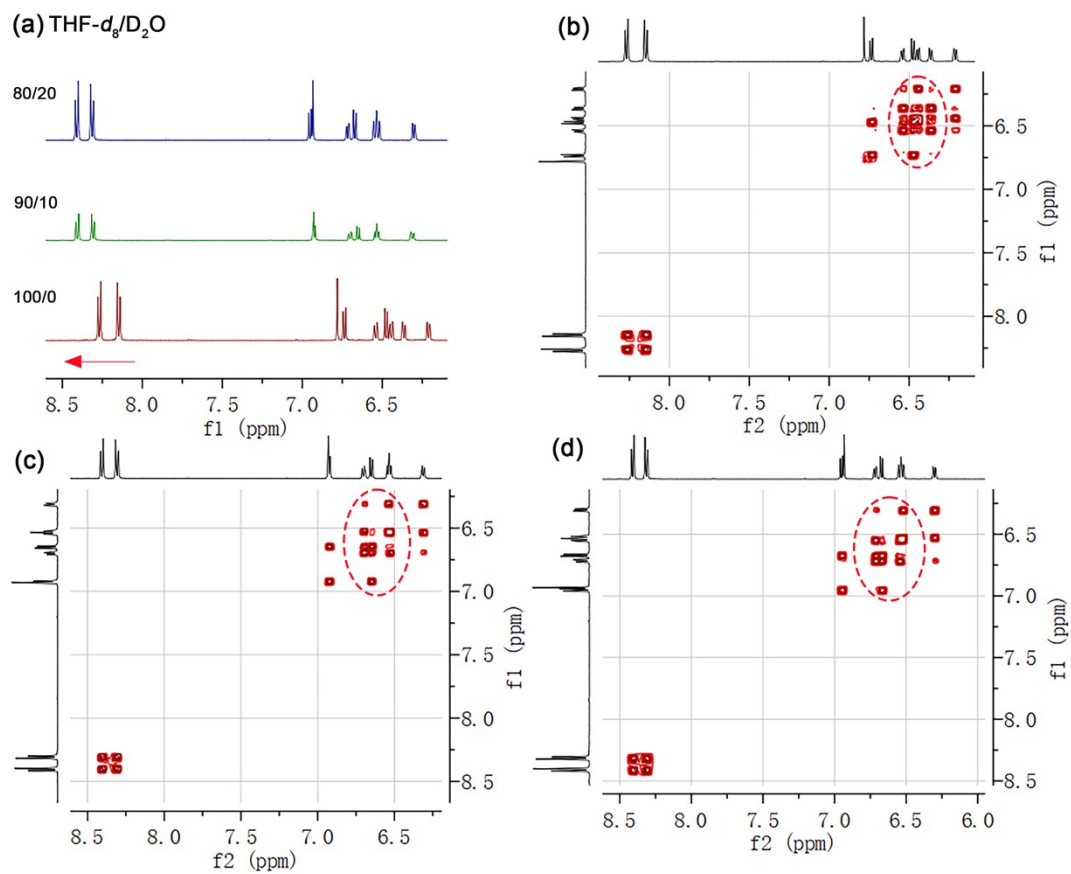


Figure S13 (a) ¹H NMR spectra of **2-PCP** in mixed THF-*d*₈/D₂O (5×10^{-3} M) with various ratios of 80/20, 90/10, and 100/0. 2D NOESY spectra of **2-PCP** in mixed THF-*d*₈/D₂O (5×10^{-3} M) with various ratios of (b) 100/0, (c) 90/10, and (d) 80/20.

Table S5. Photophysical data of **2-Ph** in various solvents.^a Molar absorption coefficients, measured at a concentration of 5×10^{-5} mol/L.

Solvent	λ_{abs} (nm)	ϵ (mol ⁻¹ cm ⁻¹) ^a	λ_{em} (nm)	Φ_{f} (%) ^b
Hexane	309/378	43400/33300	—	—
Cyclohexane	311/380	27200/24200	—	—
Toluene	317/389	25200/23400	—	—
1,2-Dichlorobenzene	321/392	23400/23000	—	—
Dichloromethane	320/390	41300/24300	—	—
Tetrahydrofuran	316/386	26800/22700	—	—
Ethyl acetate	314/384	28400/22700	—	—
1,4-Dioxane	316/387	28300/25400	—	—
Ethanol	316/385	28400/22300	463	< 1
Acetonitrile	316/385	30000/22300	—	—
<i>N,N</i> -Dimethylformamide	319/389	26600/21600	—	—
Methanol	315/384	29000/22600	472	< 1
Ethylene glycol	322/392	27200/20800	482	< 1
Dimethyl sulfoxide	321/392	13900/14200	—	—

^b The fluorescence quantum yields measured using the absolute method with an integrating sphere.**Table S6.** Photophysical data of **2-PCP** in various solvents.

Solvent	λ_{abs} (nm)	ϵ (mol ⁻¹ cm ⁻¹) ^a	λ_{em} (nm)	Φ_{f} (%) ^b
Hexane	331/419	25500/8200	498	< 1
Cyclohexane	333/420	26000/8600	501	< 1
Toluene	340/425	25000/9000	523	1.3
1,2-Dichlorobenzene	346/428	23900/9500	530	1.9
Dichloromethane	341/423	23400/9700	534	< 1
Tetrahydrofuran	338/420	24000/9600	—	—
Ethyl acetate	337/419	27400/10100	531	1.8
1,4-Dioxane	338/421	26300/9600	524	1.9
Ethanol	337/420	26800/11000	—	—
Acetonitrile	340/419	25700/11300	—	—
<i>N,N</i> -Dimethylformamide	343/422	25600/11900	—	—
Methanol	337/419	25000/10400	—	—
Ethylene glycol	344/424	30300/13100	—	—
Dimethyl sulfoxide	346/423	26000/12700	—	—

^a Molar absorption coefficients, measured at a concentration of 5×10^{-5} mol/L.^b The fluorescence quantum yields measured using the absolute method with an integrating sphere.

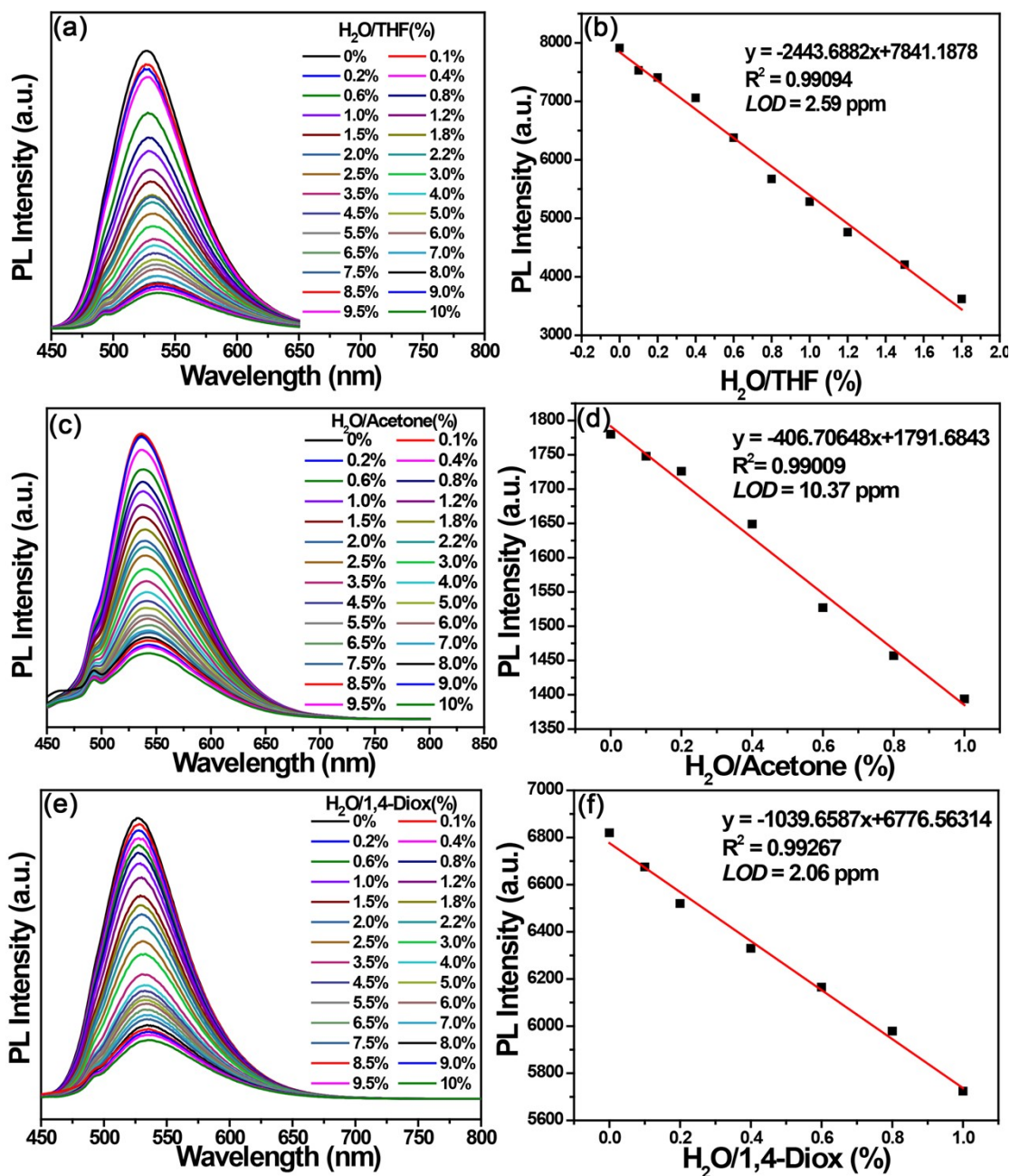
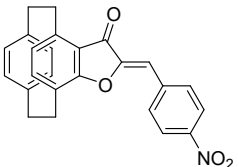
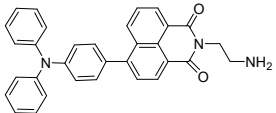
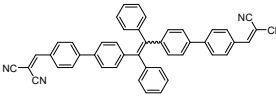
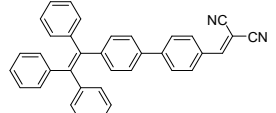
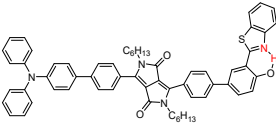
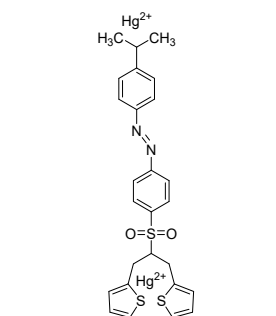
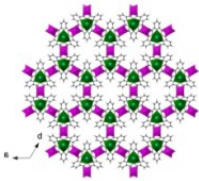
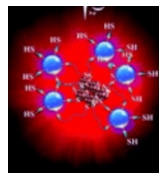
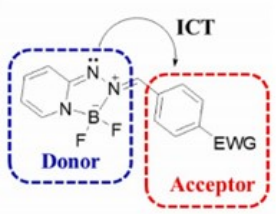
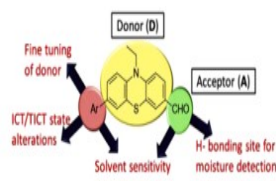
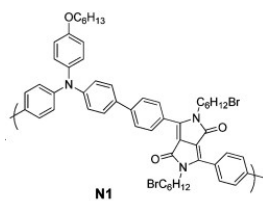


Figure S14. PL spectra of compound 2-PCP (50 μM) in (a) THF, (c) acetone and (e) 1,4-dioxane solution with increasing f_w (0-1.8 % v/v). The linear relationship between PL intensity and f_w in (b) THF, (d) acetone and (f) 1,4-dioxane solutions.

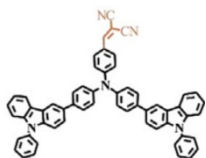
Table. S7. Comparison of trace water detection methods.

Sensors	Detecting system	Detection limit (ppm)	Linear scope (v/v %)	Reference
	THF	2.59	0-1.8%	This work
	Acetone	10.37	0-1.0%	
	1,4-dioxane	2.065	0-1.0%	

	THF	17	0–1%	Sens. Actuators B Chem., 2021, 344, 130120.
	1,4-dioxane	31	0–1.2%	
	Acetone	14	0–1%	
	THF	109	0–1%	Chem. Sci., 2014, 5, 2710.
	THF	63	0–1%	Anal. Chem., 2019, 91, 5261.
	THF	64	0–1.25%	Anal. Chem., 2019, 91, 5261.
	Acetone	420	0–2.5%	
	THF	41	0.0125–0.0780 %	Anal. Chim. Acta., 2020, 1136, 178.
	Acetone	144	0.0437–0.1980 %	
	THF	1300	0–6.25%	J. Photochem. Photobiol. A Chem., 2020, 402, 112830.
	THF	500	0.3–5%	Analyst, 2018, 143, 3068.
	THF	280	0–3.8%	Dyes Pigments, 2020, 181, 108554.
	Acetone	210	0–3.8%	
	THF	80	0–1.32 %	J. Photochem. Photobiol. A Chem., 2020, 402, 112804.
	DMSO	210	0–2.9%	



THF 50 0–2% New J. Chem., 2016, 40, 6706.



THF 130 0–0.5% Dyes Pigments, 2019, 166, 1.

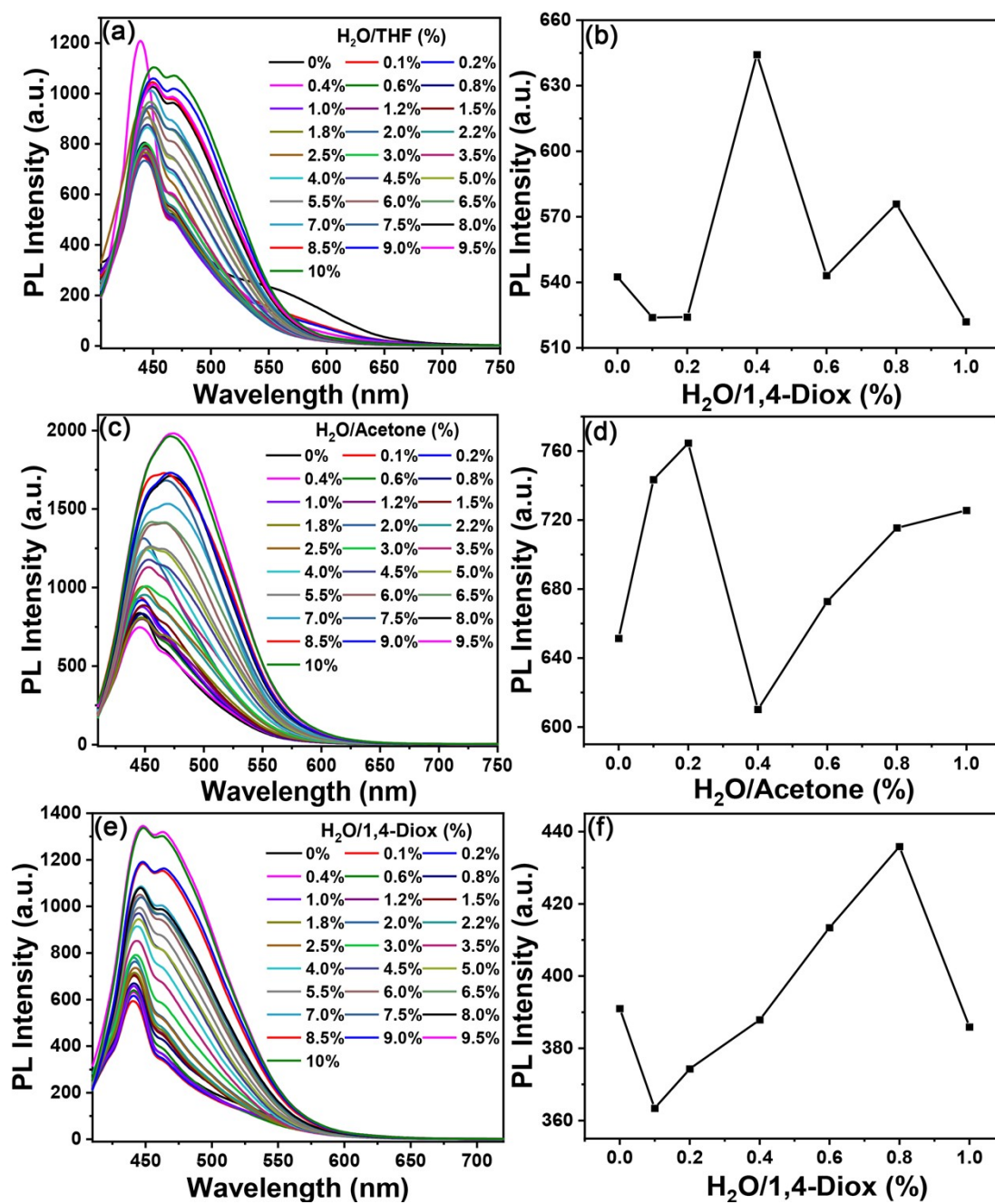


Figure S15. PL spectra of compound 2-Ph (50 μ M) in (a) THF, (c) acetone and (e) 1,4-dioxane

solution with increasing f_w (0-1.0 % v/v). The relationship between PL intensity and f_w in (b) THF, (d) acetone and (f) 1,4-dioxane solutions.

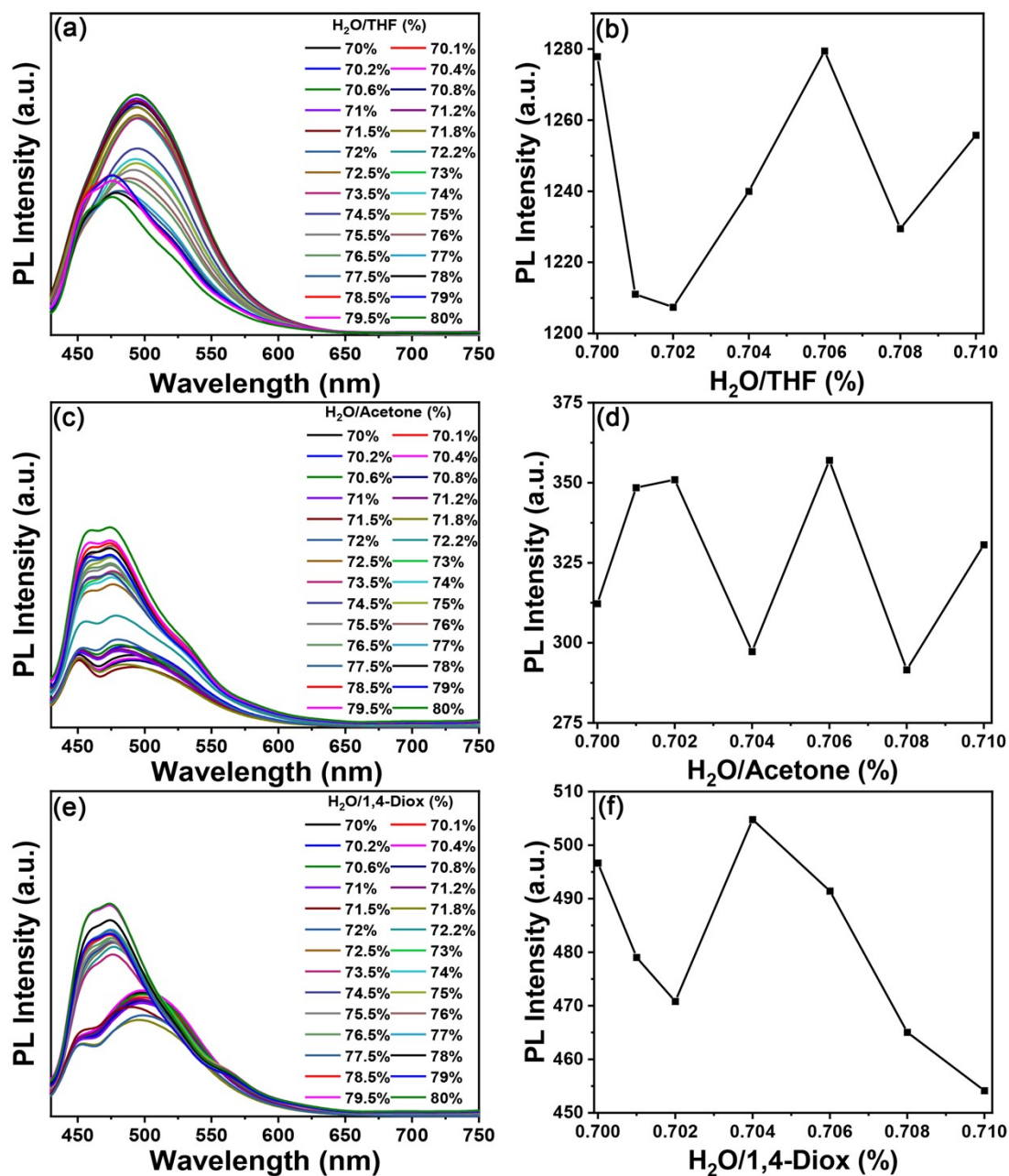


Figure S16. PL spectra of compound 2-Ph (50 μM) in (a) THF, (c) acetone and (e) 1,4-dioxane solution with increasing f_w (70-80 % v/v). The relationship between PL intensity and f_w in (b) THF, (d) acetone and (f) 1,4-dioxane solutions.

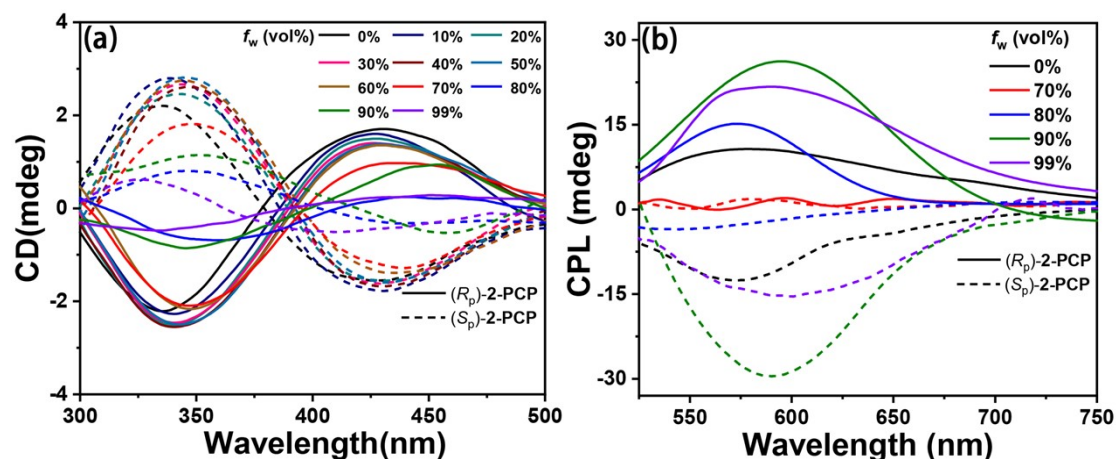


Figure S17. (a) CD and (b) CPL spectra of compounds $(R_p)/(S_p)$ -2-PCP in THF/water mixture ($50 \mu\text{M}$) with varied f_w .

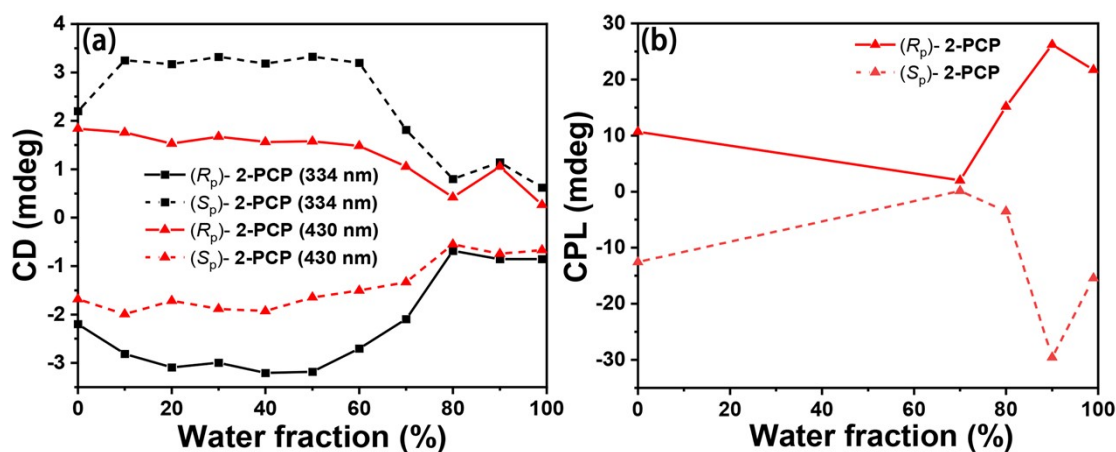


Figure S18. (a) Changes of CD intensity at 334 nm and 430 nm of $(R_p)/(S_p)$ -2-PCP in THF/water mixture with varied f_w . (b) Changes of CPL intensity at 578 nm of $(R_p)/(S_p)$ -2-PCP in THF/water mixture with varied f_w .

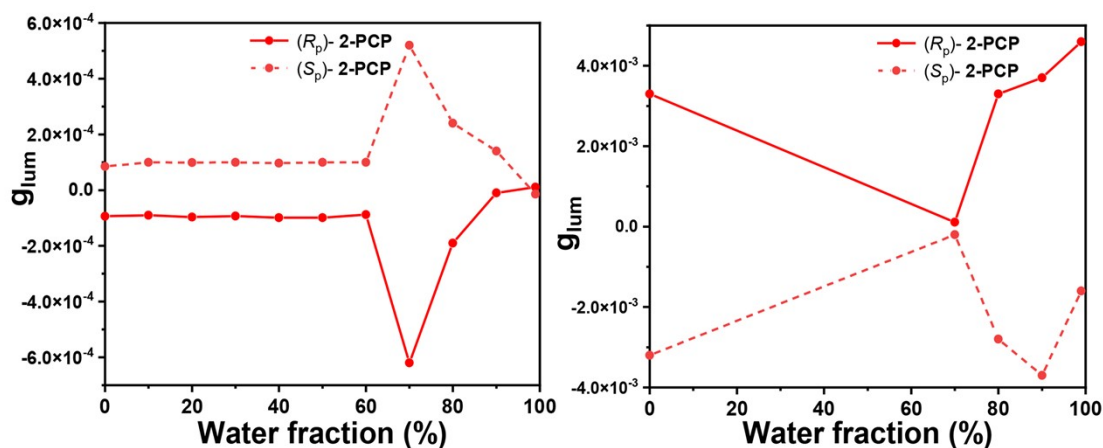


Figure S19. (a) Changes of g_{abs} value for $(R_p)/(S_p)$ -2-PCP (430 nm) in THF/water mixture with varied f_w and (b) changes of g_{lum} value for $(R_p)/(S_p)$ -2-PCP (578 nm) in THF/water mixture with varied f_w .

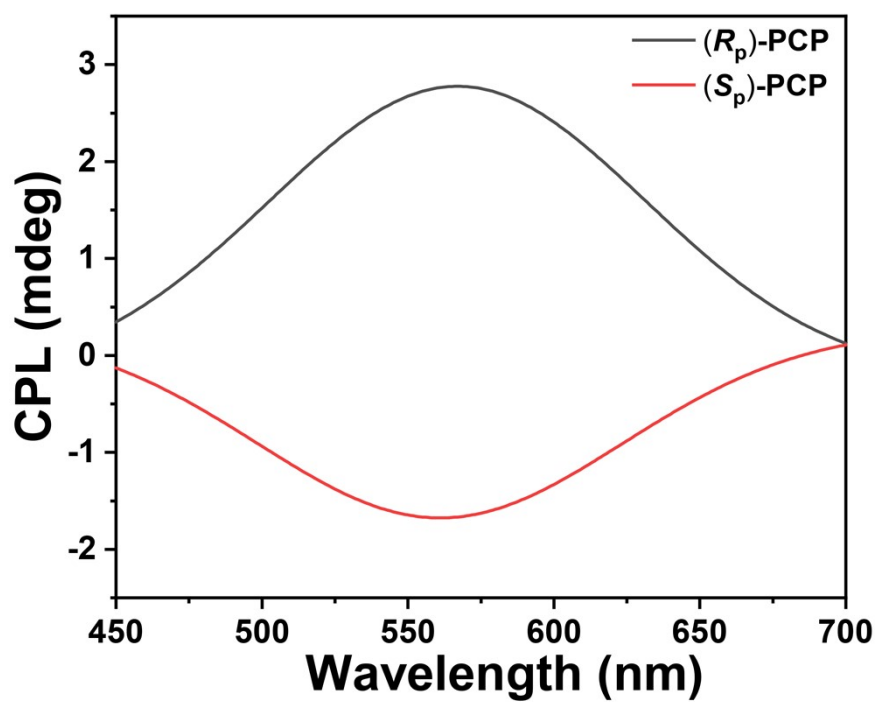
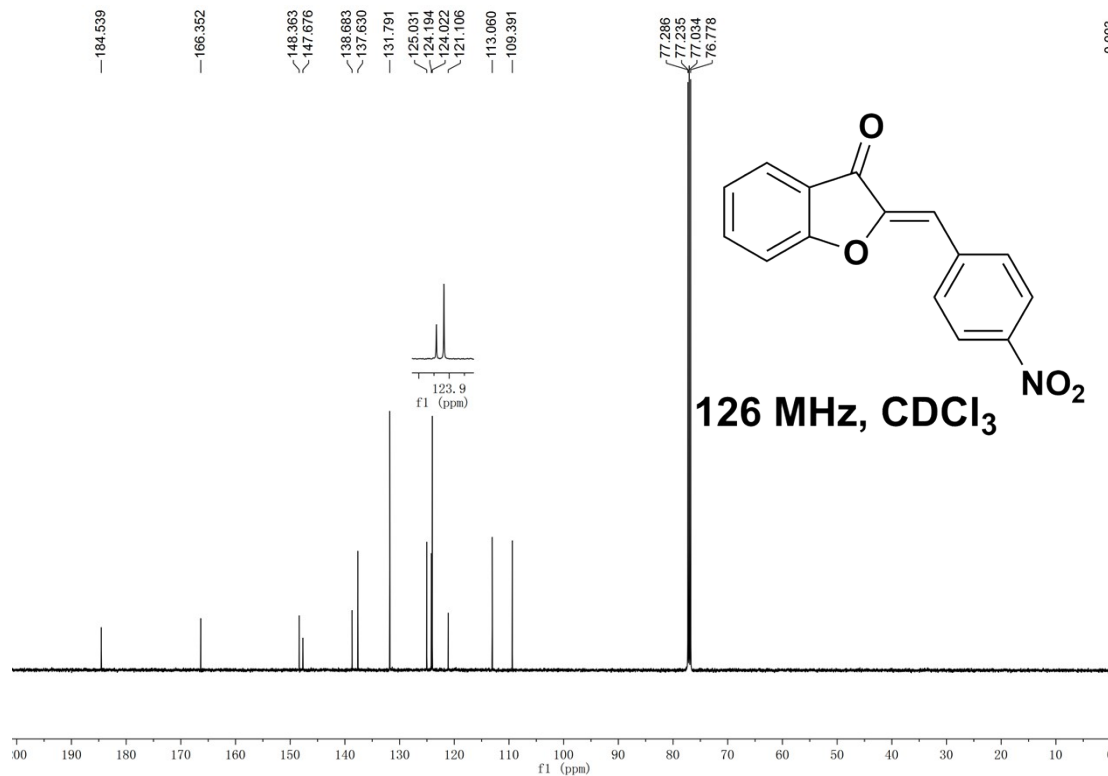
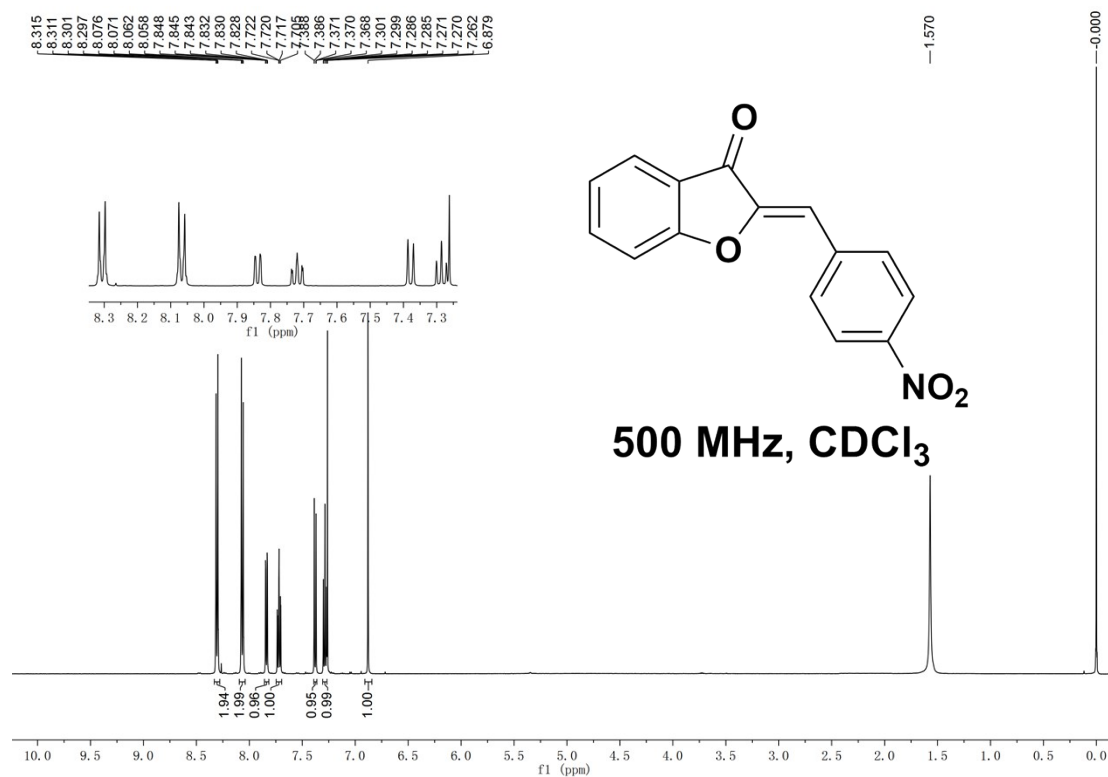
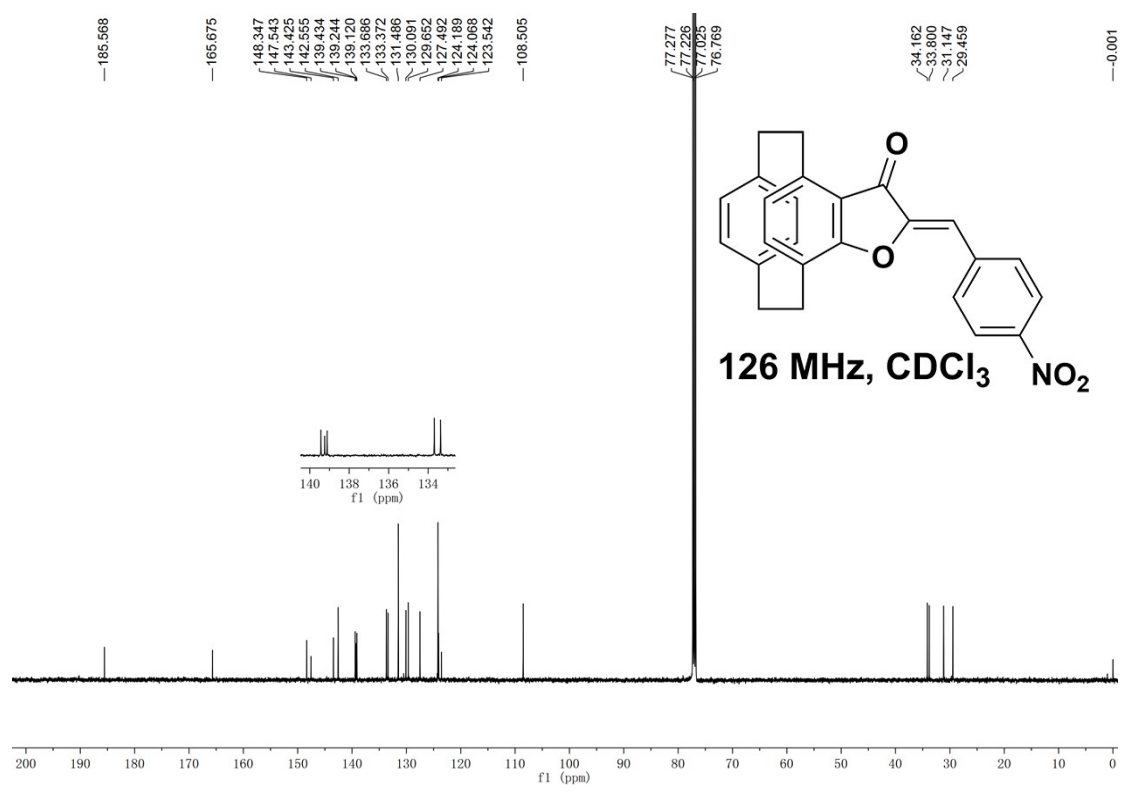
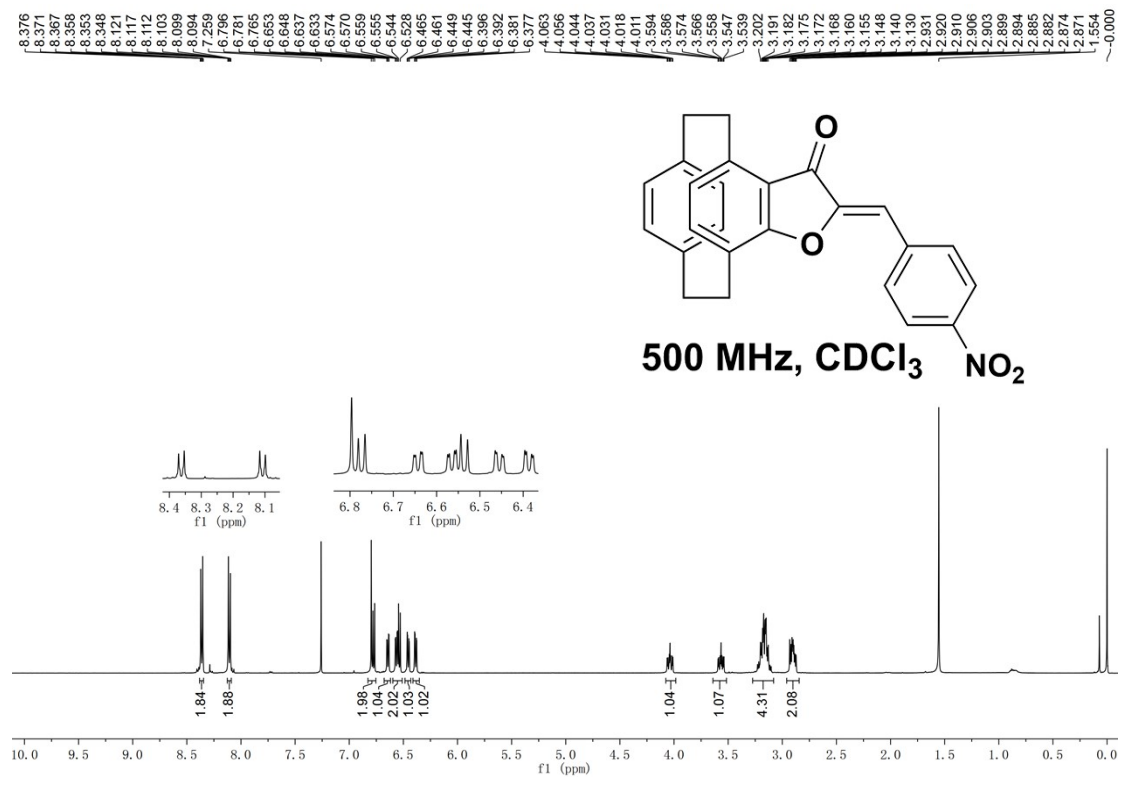
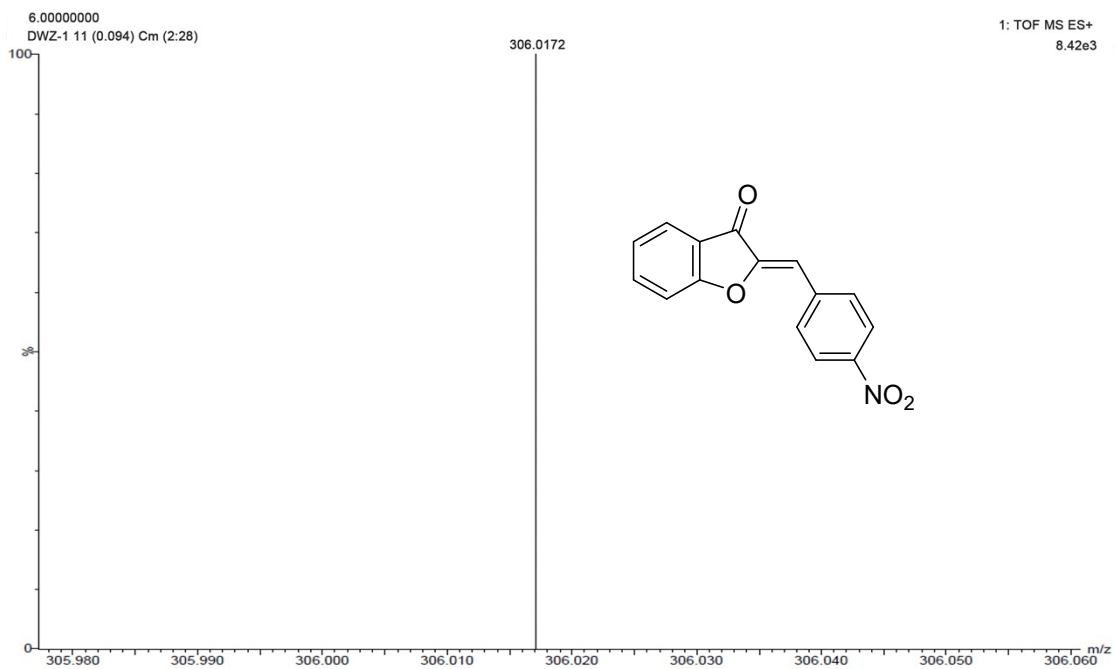


Figure S20. CPL spectra of $(R_p)/(S_p)$ -2-PCP in the powder solid-state.

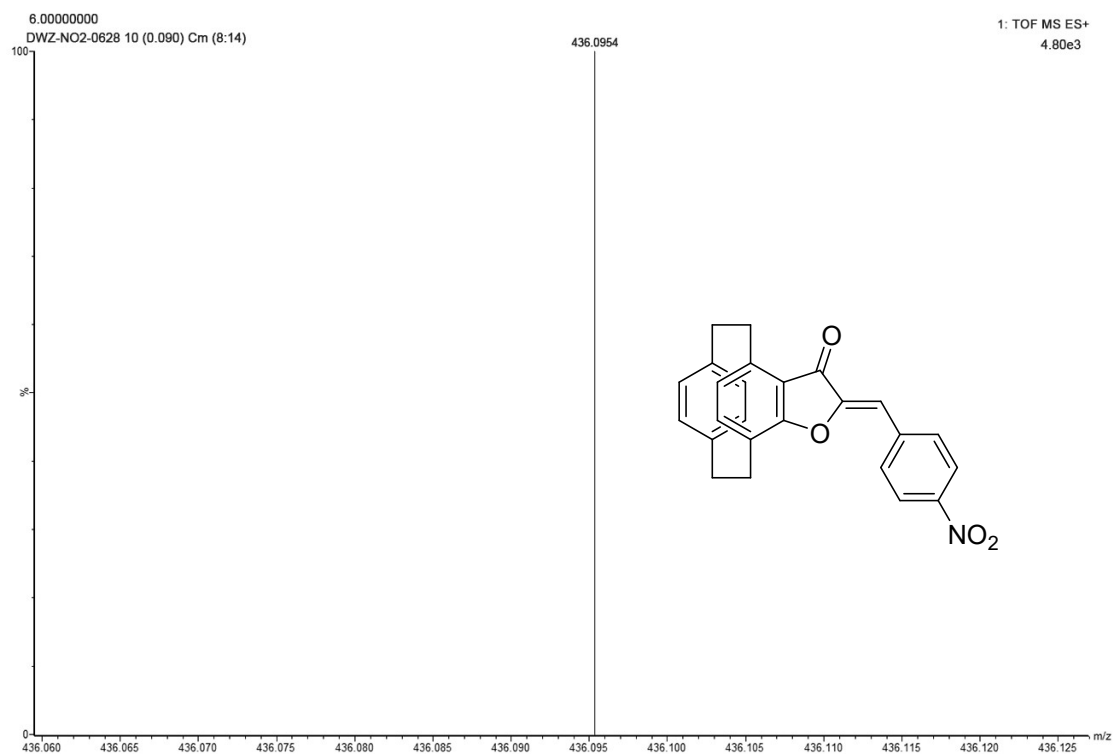
7. NMR and HRMS spectra







HRMS data for **2-Ph**



HRMS data for **2-PCP**

8. Theoretical calculations

Optimized structure of **2-Ph** in the ground state

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	-0.1396	-0.6532	-2.9815
O	2.9741	1.9781	2.1701
O	2.9808	5.4597	2.1689
O	-0.1617	-1.8035	-2.6244
O	-0.6043	-0.3015	-4.0469
C	3.7291	3.6462	3.578
C	4.301	4.0839	4.7106
H	4.3588	4.997	4.8792
C	4.7957	3.185	5.6193
H	5.198	3.4744	6.4067
C	4.6792	1.8267	5.3328
H	5.0132	1.2149	5.9496
C	4.1146	1.3586	4.2092
H	4.0614	0.4473	4.0316
C	3.6162	2.2901	3.3396
C	2.6419	3.185	1.578
C	3.1004	4.2797	2.4252
C	1.9822	3.2516	0.4275
H	1.8274	4.1147	0.1167
C	1.4662	2.2135	-0.4096
C	1.4435	0.8746	-0.0492
H	1.8037	0.6089	0.7659
C	0.8996	-0.0479	-0.8774
H	0.8516	-0.9396	-0.6165
C	0.4186	0.34	-2.1052
C	0.4096	1.6546	-2.4778
H	0.0438	1.9151	-3.2917
C	0.9451	2.5719	-1.6351
H	0.9613	3.4659	-1.8894

Optimized structure of **2-PCP** in the ground state

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	5.6936	0.3555	-2.1697
O	1.3868	3.6003	1.8851
O	-1.9933	2.7	1.3185
O	6.6924	0.796	-1.6867

O	5.5469	-0.4413	-3.1149
C	2.7446	4.8111	4.1619
H	3.1268	5.5871	4.602
H	3.275	4.6204	3.3734
C	2.7918	3.6027	5.1175
H	3.3479	2.9207	4.7141
H	3.2254	3.885	5.9385
C	1.4431	2.9776	5.4779
C	0.6361	3.6227	6.4256
H	1.0515	4.122	7.0906
C	-0.6517	3.5594	6.4256
H	-1.14	4.0193	7.0687
C	-1.3543	2.7538	5.3969
C	-0.5434	1.9121	4.6658
H	-0.9315	1.2486	4.1429
C	0.8201	2.0284	4.6972
H	1.3368	1.4545	4.1782
C	-2.7017	3.0972	5.0418
H	-3.1897	3.3091	5.8512
H	-3.1224	2.3156	4.6437
C	-2.8274	4.2606	4.0758
H	-3.2956	3.9554	3.2822
H	-3.3684	4.9488	4.4902
C	-1.5061	4.8632	3.658
C	-0.8183	5.8518	4.4282
H	-1.3202	6.4344	4.9491
C	0.4686	5.9817	4.4439
H	0.8517	6.6755	4.9323
C	1.3032	5.116	3.7494
C	0.6919	4.3962	2.7833
C	-0.6543	4.2293	2.705
C	-0.9197	3.2376	1.6945
C	0.3905	2.883	1.188
C	0.7257	2.0027	0.2063
H	0.0084	1.546	-0.1711
C	2.046	1.6569	-0.3603
C	3.2637	2.2547	-0.0261
H	3.2814	2.9463	0.5947
C	4.4516	1.8262	-0.6162
H	5.2693	2.1834	-0.3539
C	4.388	0.873	-1.5849
C	3.1784	0.2672	-1.9948
H	3.1783	-0.3787	-2.6631
C	2.0069	0.6411	-1.3917

H

1.2032 0.2508 -1.6431