Supporting Information

A General Structural Decoupling Strategy Toward Ultra-Long Blue Circularly Polarized Room-Temperature Phosphorescence

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EXPERIMENTAL SECTION

Reagents and materials

4-Biphenylcarboxylic acid (BPCA), 4-biphenylacetic acid (BPAA), and L/D-4,4'-biphenylalanine (D/L-BPAla) were purchased from Adamas Reagent Ltd (commercially available), all samples underwent purification and spectroscopic characterization prior to optical property measurements. Polyvinyl alcohol (PVA), hydrochloric acid (HCl), acetonitrile (AN), and tetrahydrofuran (THF) were purchased from Adamas Reagent Ltd. Ultrapure water was prepared using an Asura AXLM1820 water purification system.

Measurements

Nuclear magnetic resonance (^{1}H NMR and ^{13}C NMR) spectra were tested on the Bruker AVANCE III HD-500 spectrometer or Bruker Magnet System 400′ 54 Ascend. The chemical shifts in ^{1}H NMR spectra are reported using tetramethyl silane as a standard, and those in ^{13}C NMR spectra are reported using the solvent signals as a standard. Data for both high-performance liquid chromatography (HPLC) and high-resolution mass spectrometry (HRMS) was generated using a Waters ultra-performance liquid chromatography-quadrupole time-of-flight mass spectrometer, model Acquity 2D-UPLC/Xevo G2-XS QTOF. Ultraviolet spectrum obtained via PerkinElmer Instruments Lambda 365 in the United States. Fluorescent spectra, phosphorescent spectra and time attenuation curves were tested on Horiba Jobin Yvon QM-8000, and Absolute quantum yields were measured on an Edinburgh FLS1000 fluorescence spectrophotometer equipped with a continuous xenon lamp. Circular Dichroism

spectrum and circularly polarized luminescence spectrum obtained on Jasco J-1500 circular dichroism spectrophotometer and Jasco CPL-300 circularly polarized luminescence spectrophotometer, respectively.

Preparation of polymer-based films

Doping D/L-BPAla PVA films: Dissolve 15 g of PVA in 150 mL of deionized water at 60° C to prepare a 10% PVA aqueous solution. Dissolve the organic chromophore (1.0 mg) in water (10 mL), add a drop of HCl, heating and stirring 15 min. Then add 5 mL chromophore solution (0.1 mg/mL) into 5 mL of the aforementioned 10% PVA aqueous solution. Thoroughly mix the mixture at 60° C to obtain a transparent solution, pour it into a plastic petri dish (60 mm in diameter), cover with a lid, and dry in an oven at 80° C to obtain a high-transparency phosphorescent film.

Doping BPAA and BPCA PVA films: Dissolve 15 g of PVA in 150 mL of deionized water at 60° C to prepare a 10% PVA aqueous solution. Dissolve the organic chromophore (5.0 mg) in THF (10 mL), stirring 15 min. Then add 5 mL of the aforementioned 10% PVA aqueous solution. Thoroughly mix the mixture at 60° C to obtain a transparent solution, pour it into a plastic petri dish (60 mm in diameter), cover with a lid, and dry in an oven at 80℃ to obtain a high-transparency phosphorescent film.

Co-doping PVA films: Dissolve 1 mg of Rhodamine 6g (R6g) in 10 mL of water. Dissolve the guest molecule (**D/L-BPAla**) (1 mg) in 10 mL of water, add a drop of HCl, heating and stirring 15 min. Then add 0.25 mL of the R6g aqueous solution (0.1 mg/mL) and 5 mL of the PVA aqueous solution into the 5 mL guest molecule solution.

Thoroughly mix the mixture at 60° C to obtain a transparent solution. Pour the solution into a plastic petri dish (60 mm in diameter), cover it with a lid, and dry in an oven at 80° C to yield a 5% R6g-co-doped film. Phosphorescent films with other R6g doping concentrations were prepared following the same method.

Computational Methods

Geometry optimizations and frequency calculations were performed by using the density functional theory (DFT), and the time-dependent density functional theory (TD-DFT) was applied to study the low-lying excited states with the B3LYP functional and 6-31G(d) basis set. All above calculations were carried out with the Gaussian 16 B.01 package[1]. Gaussian calculation results were analyzed by Multiwfn 3.8[2, 3] and VMD 1.9.3 software[4]. The spin-orbit coupling (SOC) constants between singlet and triplet states were obtained using ORCA 4.2[5] with Gaussian-optimized structures and the B3LYP/6-31G(d) method.

Supporting Figures

BPCA

^{1}H NMR (500 MHz, DMSO-d6) δ 13.05 (s, 1H), 8.03 (d, J = 8.2 Hz, 2H), 7.79 (d, J = 8.3 Hz, 2H), 7.73 (d, J = 7.6 Hz, 2H), 7.49 (s, 2H), 7.42 (t, J = 7.4 Hz, 1H). MS (BPCA) (m/z): [M-H]- cacl. for $[C_{13}H_9O_2]^-$, 197.06; found, 197.0605.

BPAA

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.40 (s, 1H), 7.65 (d, J = 7.8 Hz, 2H), 7.61 (d, J = 8.1 Hz, 2H), 7.46 (t, J = 7.7 Hz, 2H), 7.35 (d, J = 8.0 Hz, 3H), 3.62 (s, 2H).

MS (BPAA) (m/z): [M-H]- cacl. for $[C_{14}H_{11}O_2]$-,211.07; found, 211.0763.

D-BPAla

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.57 (s, 2H), 7.67 – 7.60 (m, 4H), 7.45 (t, J = 7.6 Hz, 2H), 7.36 (dd, J = 17.5, 7.8 Hz, 3H), 4.17 (s, 1H), 3.20 (d, J = 6.3 Hz, 2H). MS (L-BPAla) (m/z): [M+H]+ cacl. for $[C_{15}H_{16}NO_2]^+$, 242.11; found, 242.1182.

L-BPAla

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.62 – 8.51 (m, 2H), 7.67 – 7.61 (m, 4H), 7.46 (t, J = 7.6 Hz, 2H), 7.37 (dd, J = 16.9, 7.9 Hz, 3H), 4.18 (t, J = 6.3 Hz, 1H), 3.20 (s, 2H)..

MS (L-BPAla) (m/z): [M+H]+ cacl. for $[C_{15}H_{16}NO_2]^+$,242.11; found,242.1182.

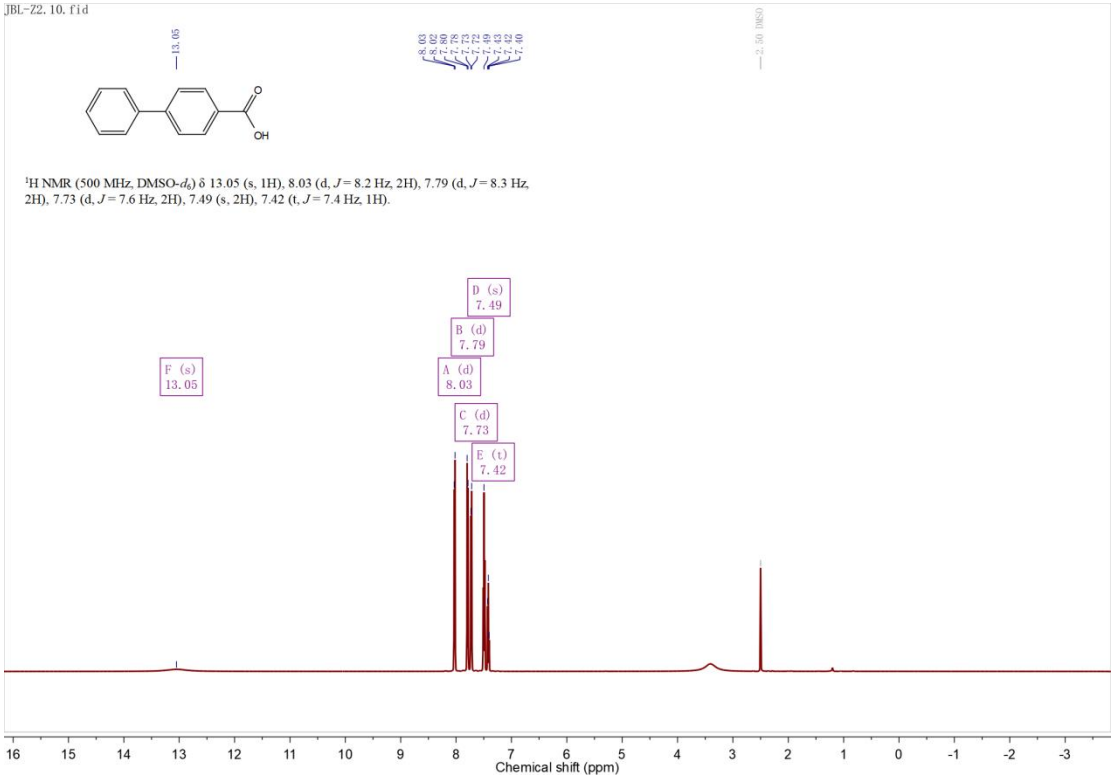

Figure S1. ^{1}H-NMR spectra of BPCA

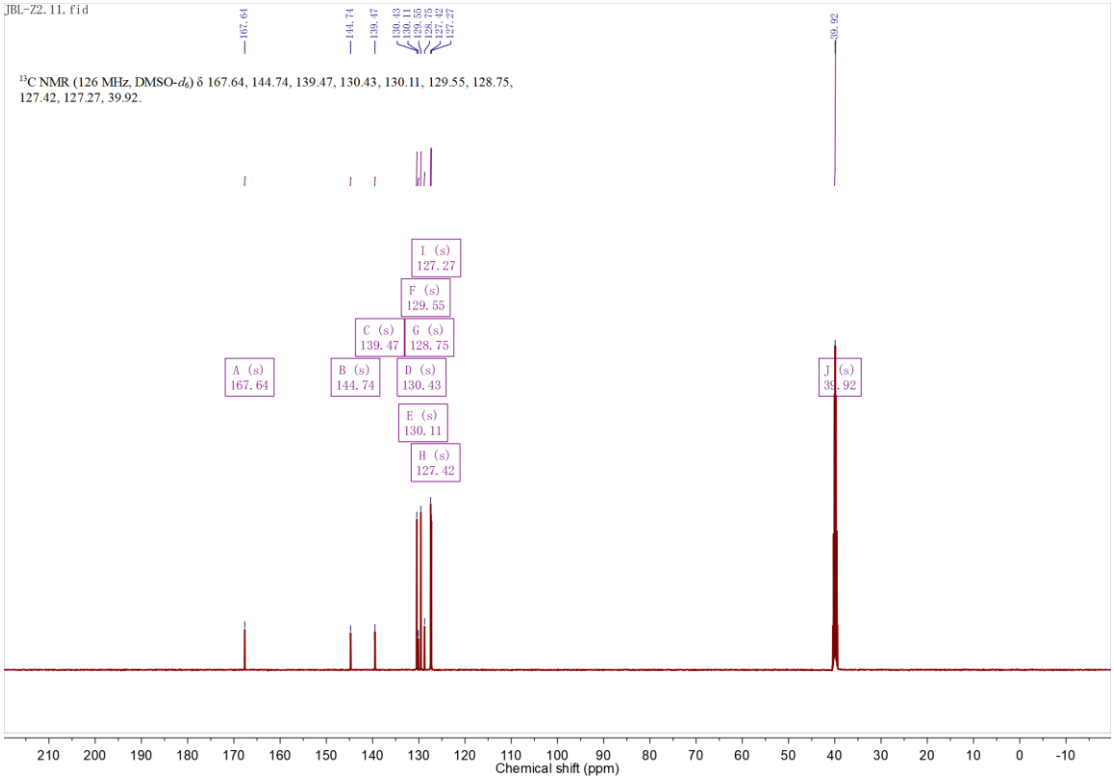

Figure S2. ^{13}C-NMR spectra of BPCA

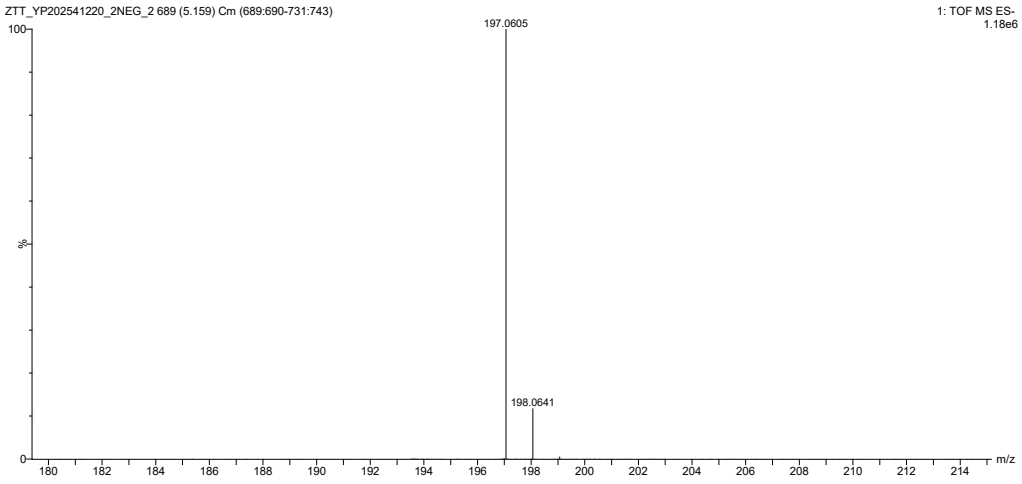

Figure S3. Time of Flight Mass Spectra of BPCA

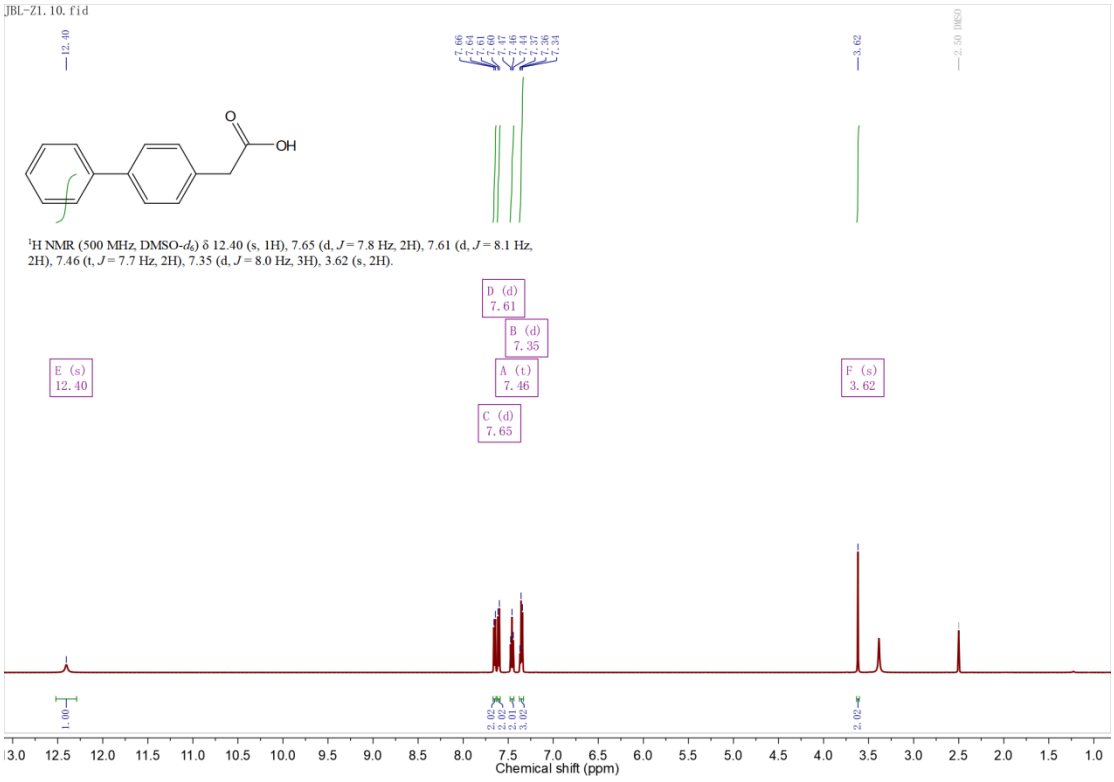

Figure S4. ^{1}H-NMR spectra of BPAA

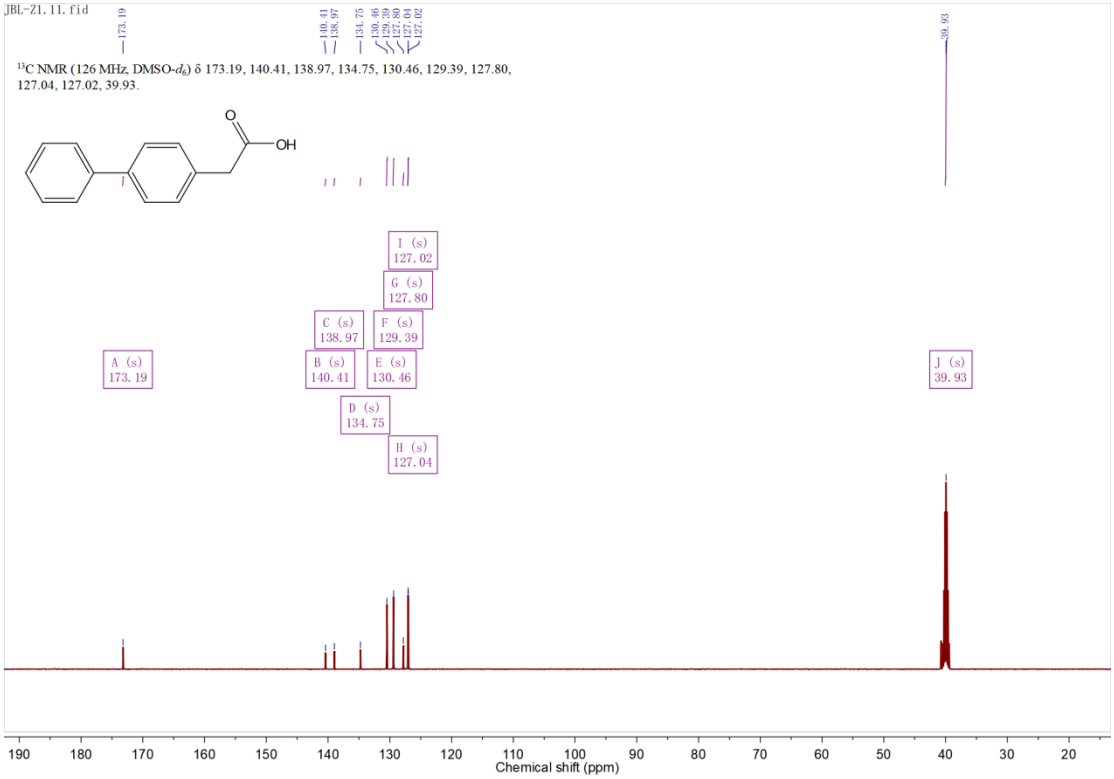

Figure S5. ^{13}C-NMR spectra of BPAA

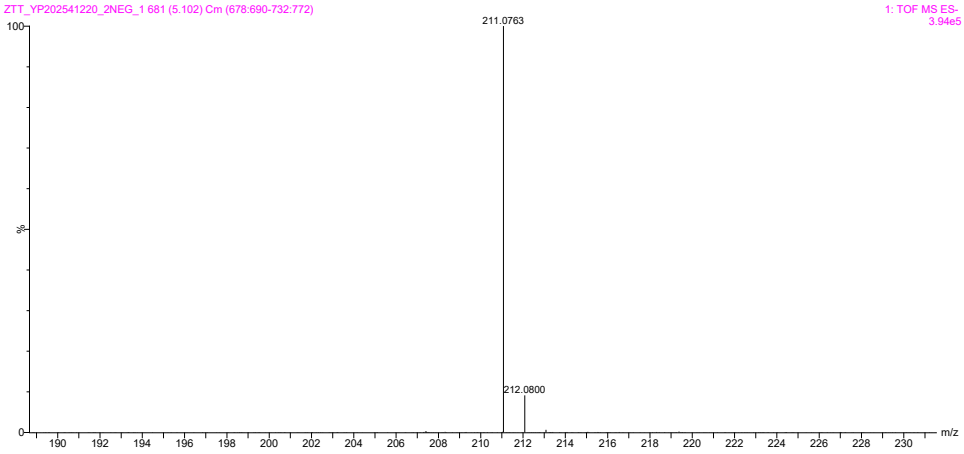

Figure S6. Time of Flight Mass Spectra of BPAA

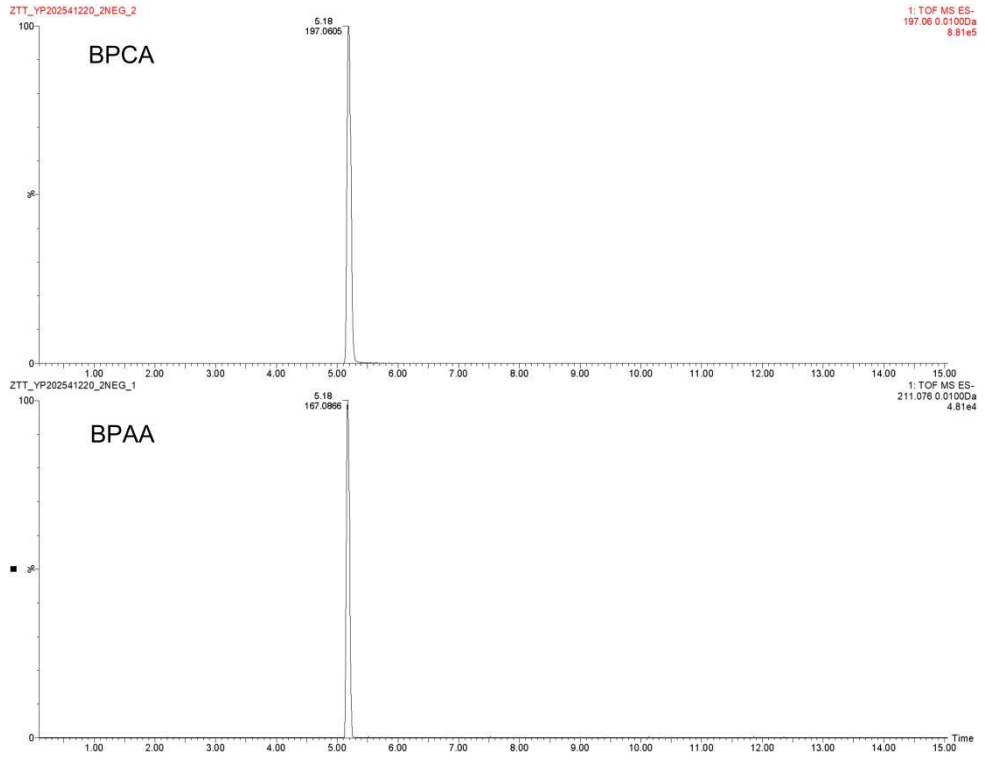

Figure S7. HPLC of BPCA and BPAA

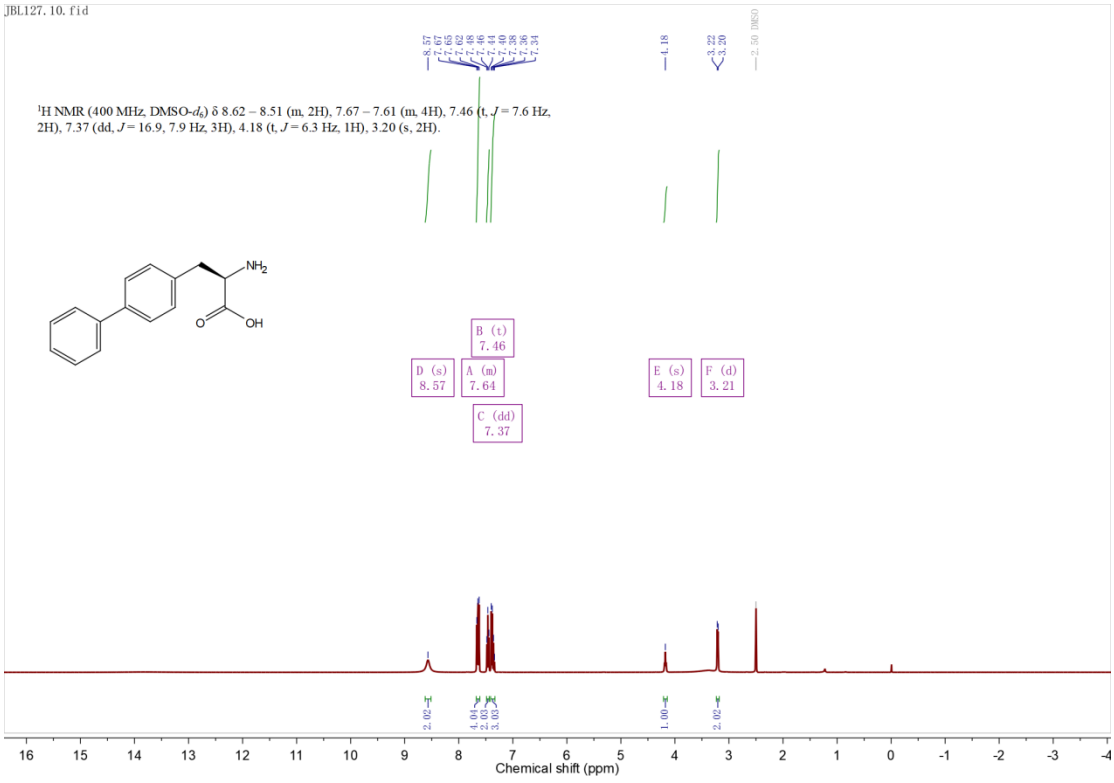

Figure S8 ^{1}H-NMR spectra of L-BPAla

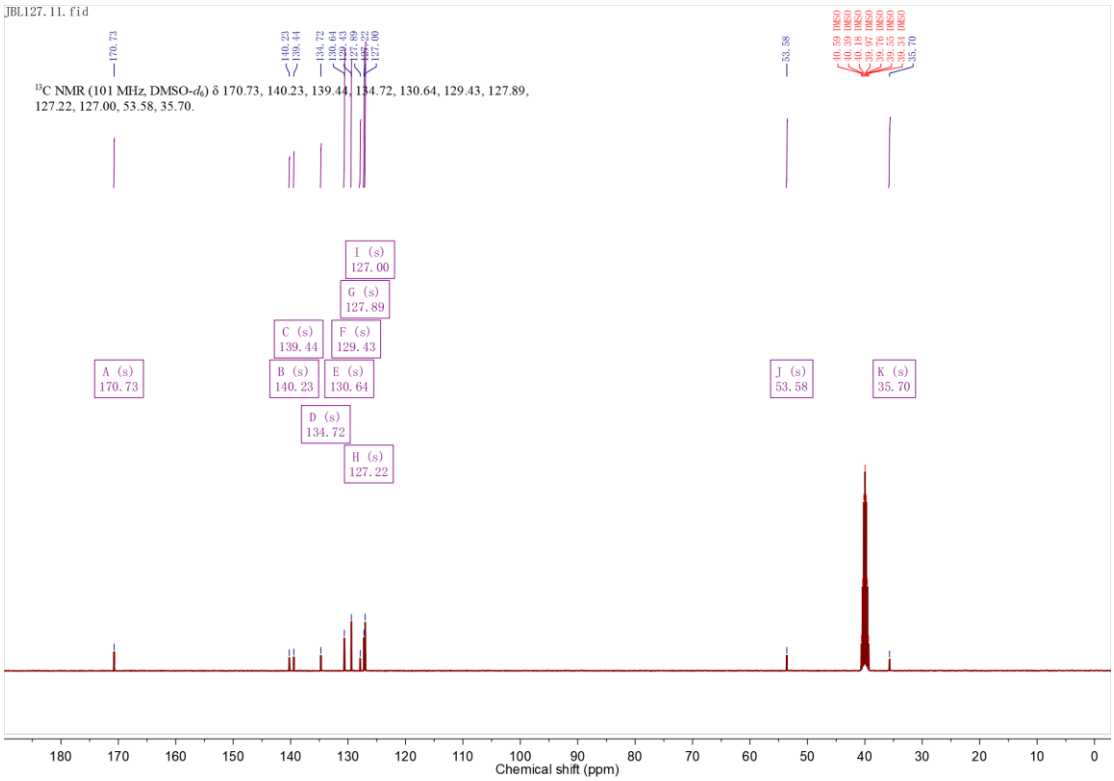

Figure S9 ^{13}C-NMR spectra of L-BPAla.

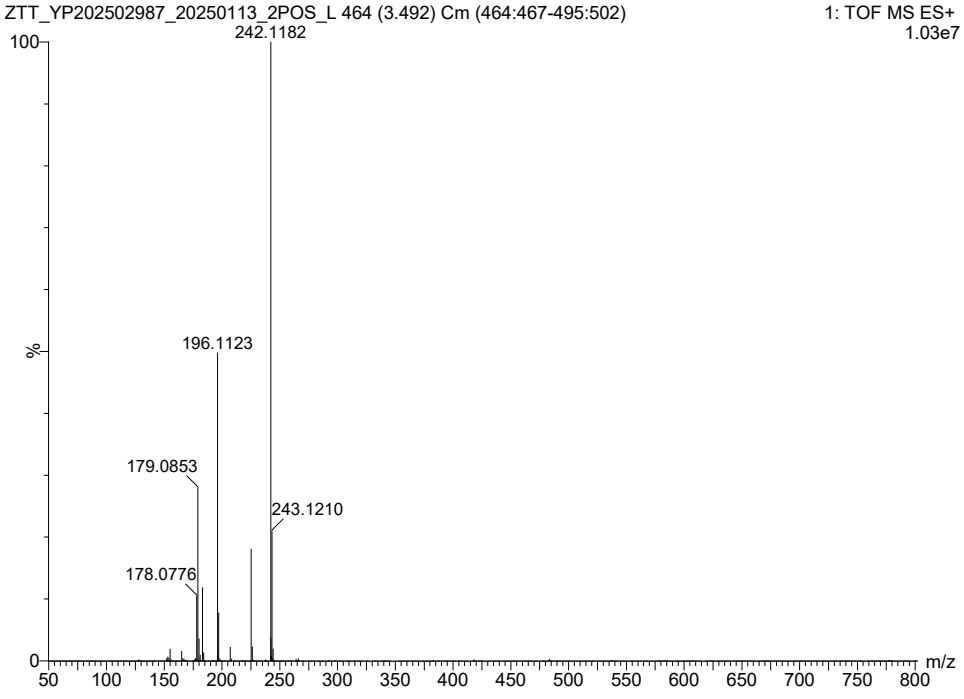

Figure S10. Time of Flight Mass Spectra of L-BPAla.

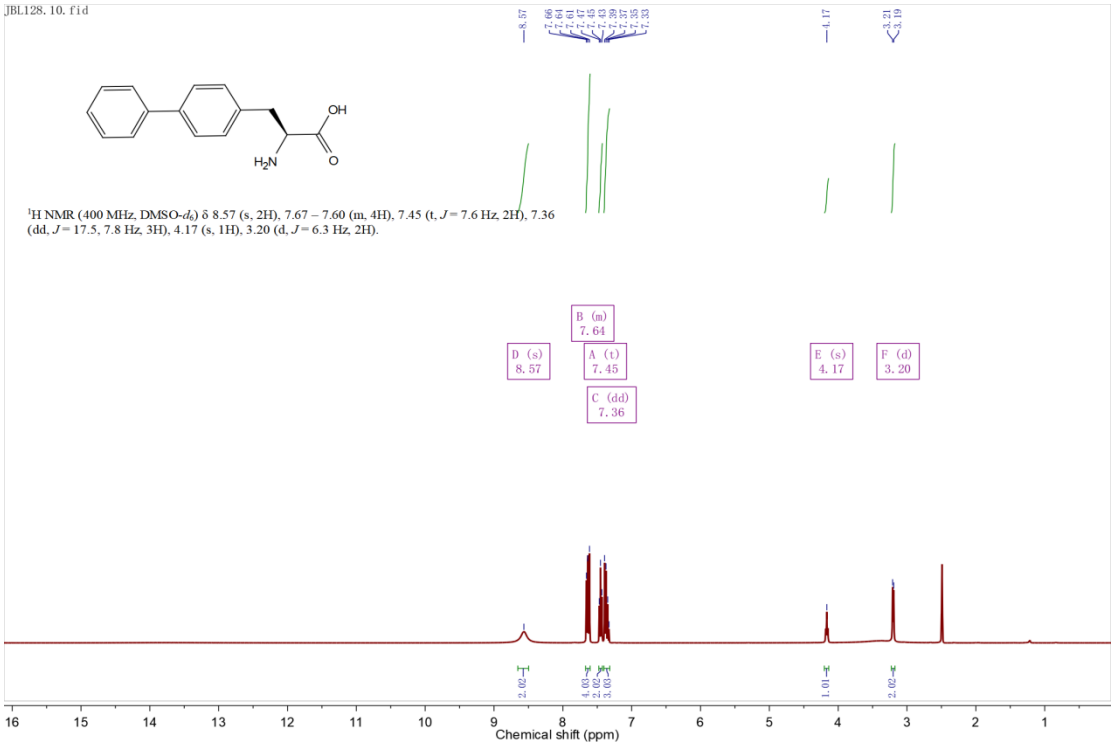

Figure S11. [1]H-NMR spectra of D-BPAla

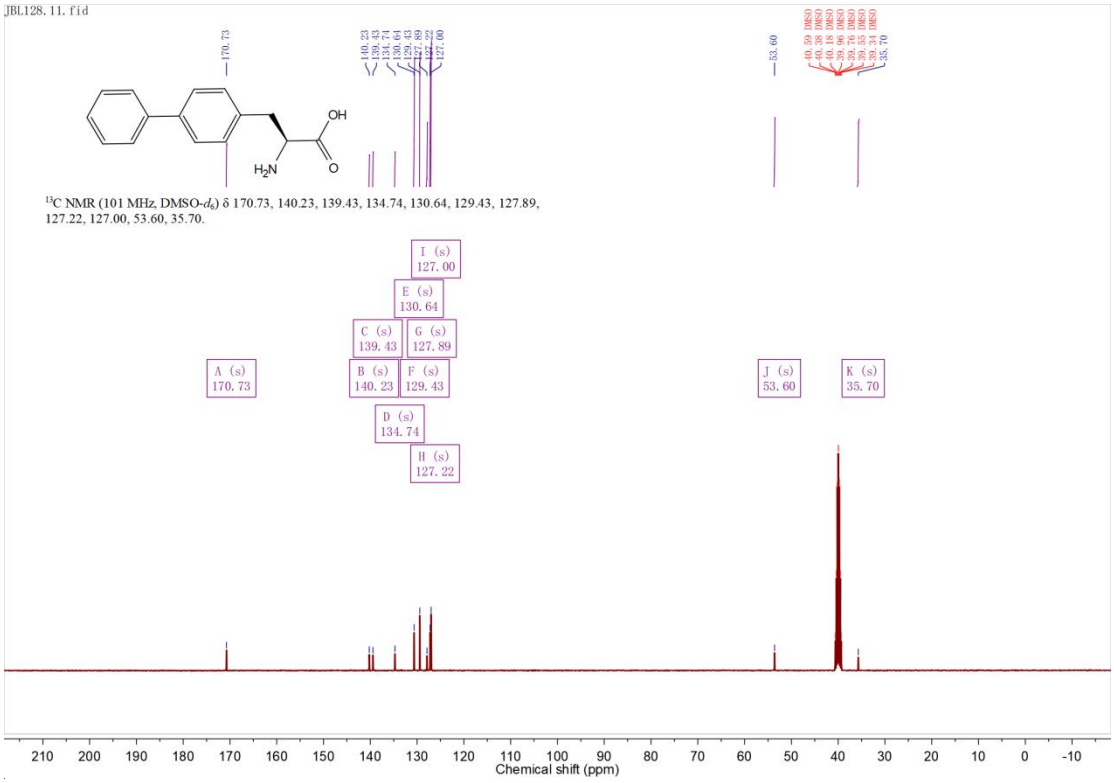

Figure S12. [13]C-NMR spectra of D-BPAla.

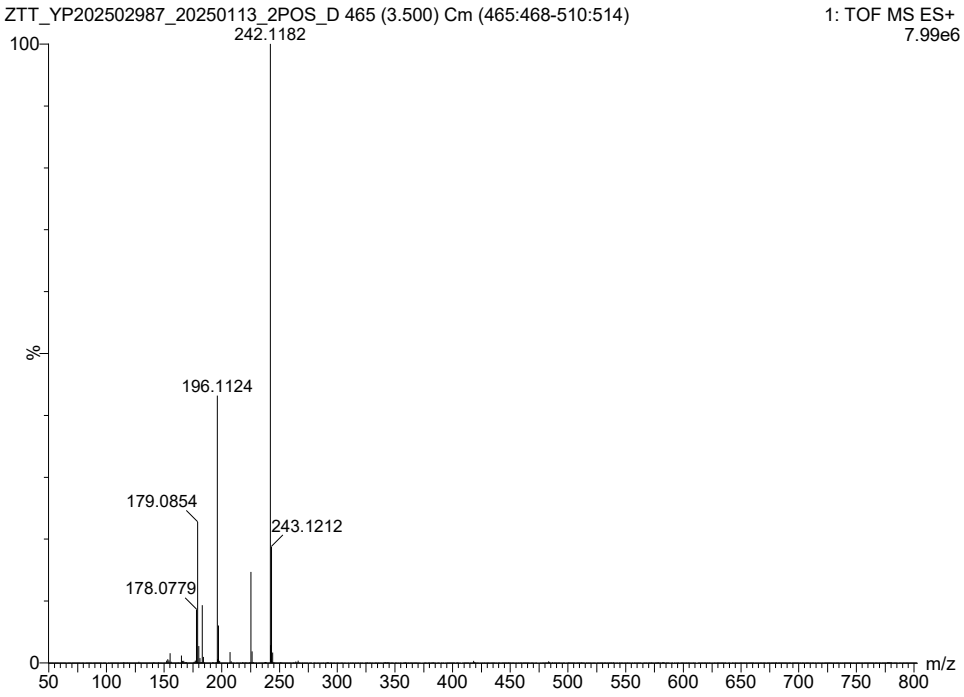

Figure S13. Time of Flight Mass Spectra of D-BPAla.

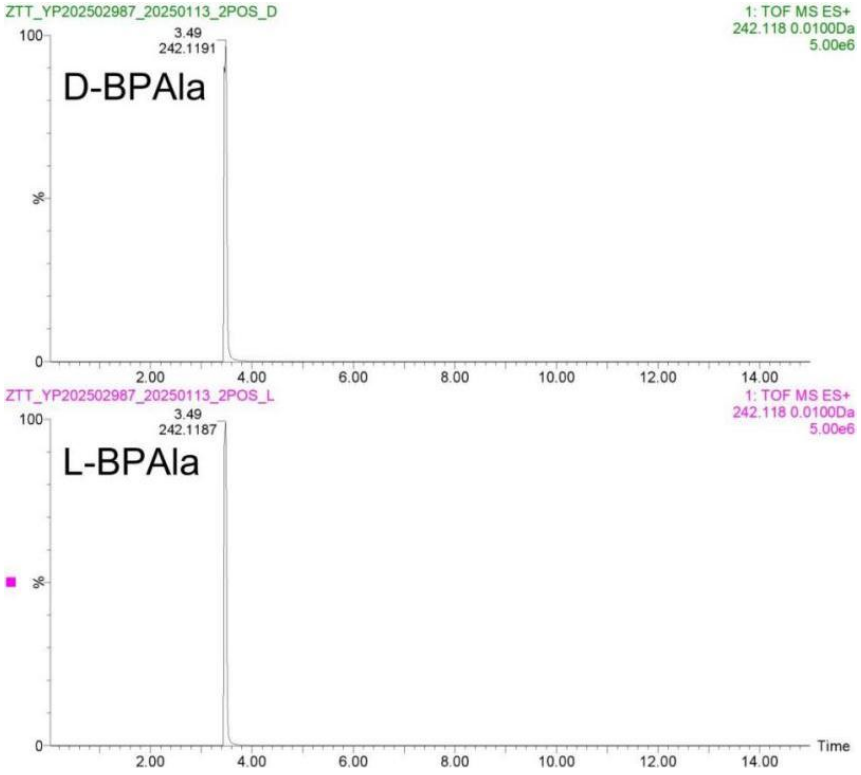

Figure S14. HPLC of D-BPAla and L-BPAla

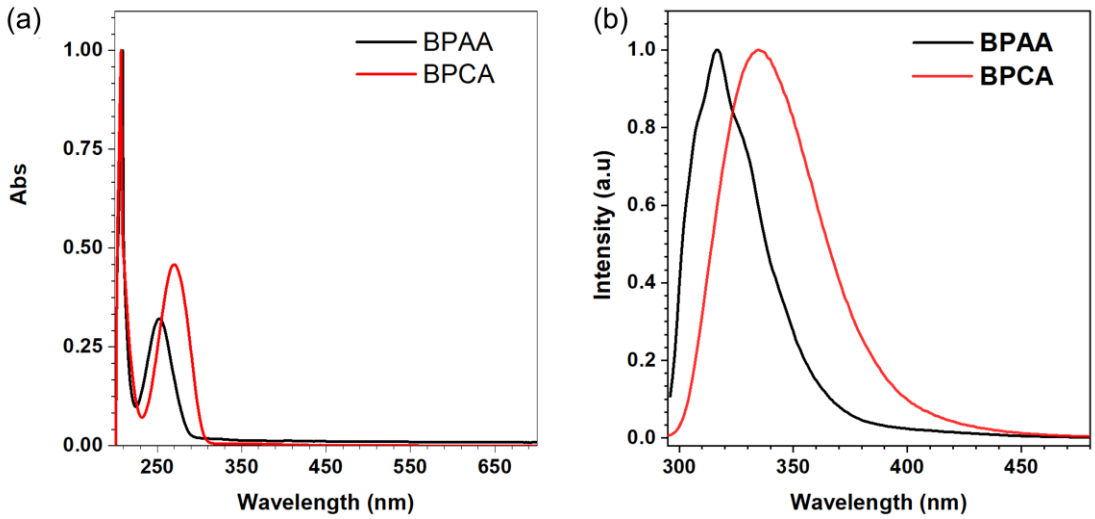

Figure S15. (a) UV-Vis spectrum and (b) photoluminescence emission spectra of BPCA and BPAA solution. Concentrations = 1×10^{-5} M, solvent is acetonitrile.

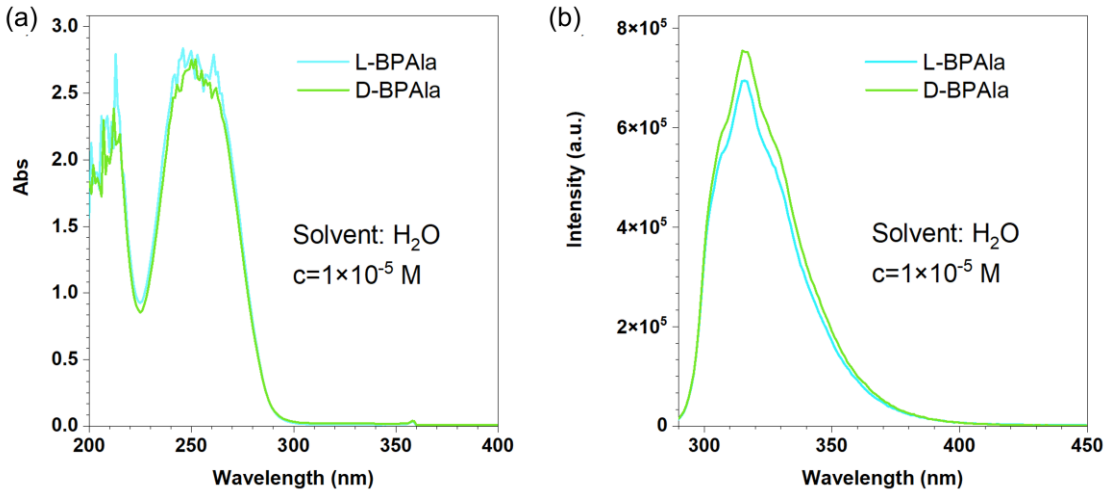

Figure S16. (a) UV-Vis spectrum and (b) photoluminescence emission spectra of L-BPAla and D-BPAla aqueous solution. Concentrations = 1×10^{-5} M.

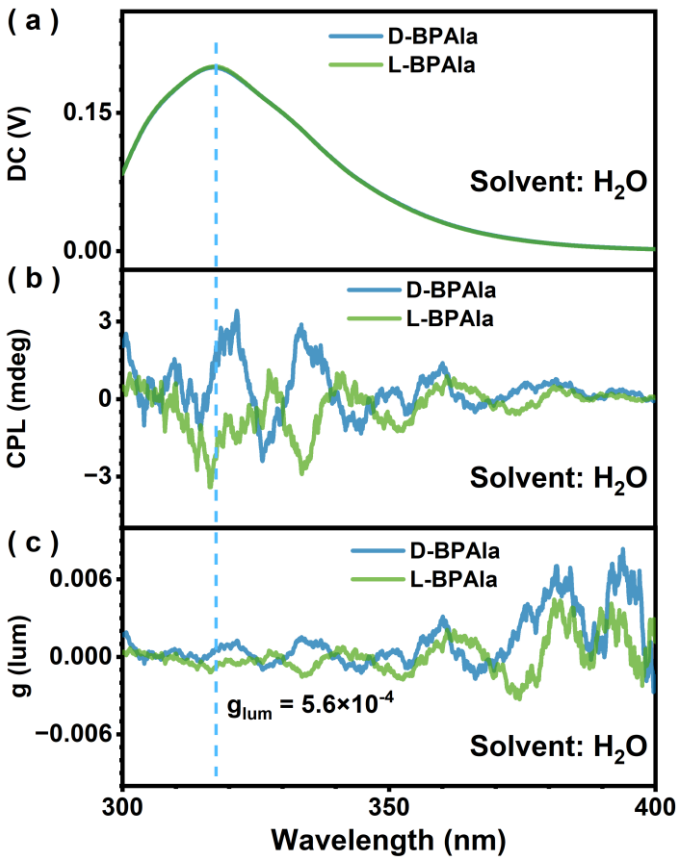

Figure S17. DC (a), CPL (b), glum values-wavelength (c) of D-BPAla and L-BPAla aqueous solution. Concentrations = 1×10^{-5} M.

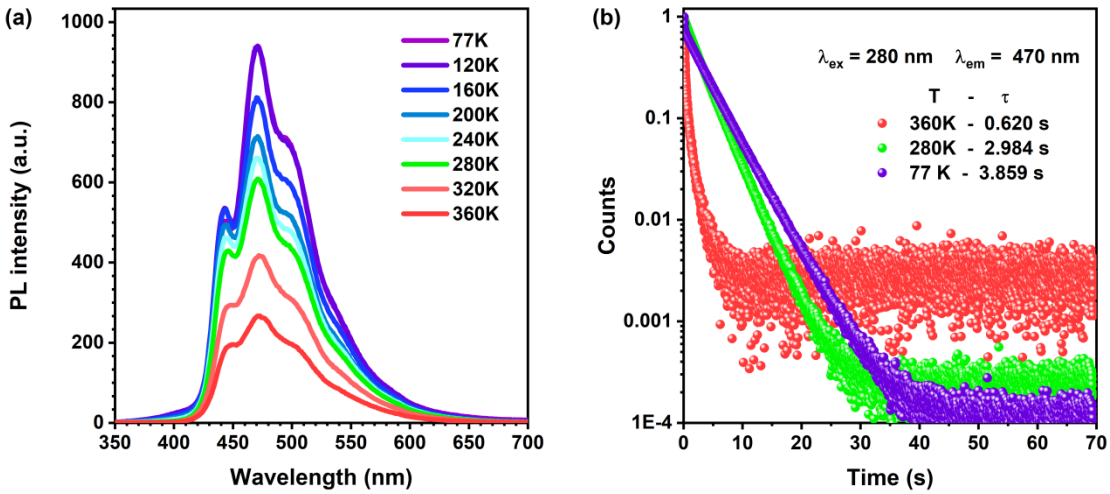

Figure S18. (a) Phosphorescence emission spectra of L-BPAla@PVA film with different temperatures, (b) phosphorescence decay curves at 77 K, 280 K and 360 K, t_d = 1 ms.

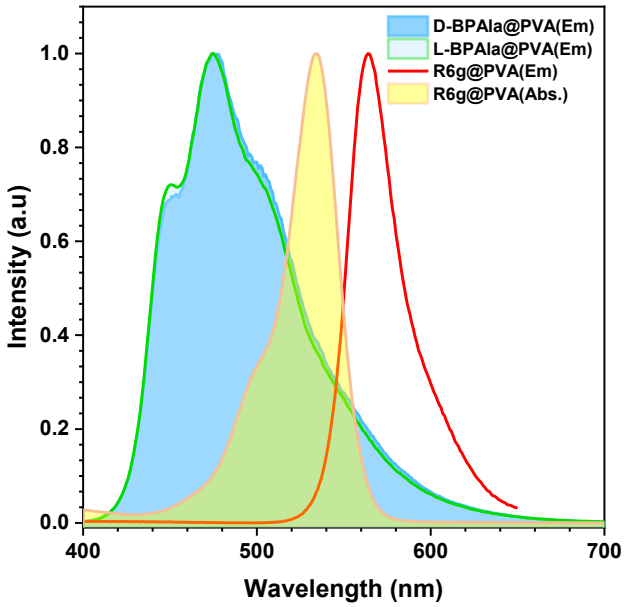

Figure S19. Phosphorescence emission spectra of 0.1 wt% D/L-BPAla@PVA, fluorescence emission spectra and UV-Vis spectrum of 1 wt% R6g@PVA film. The spectral overlap ratios to be 36.17% and 36.83% between the emission spectra of D/L-BPAla@PVA and the absorption spectrum of R6g, respectively.

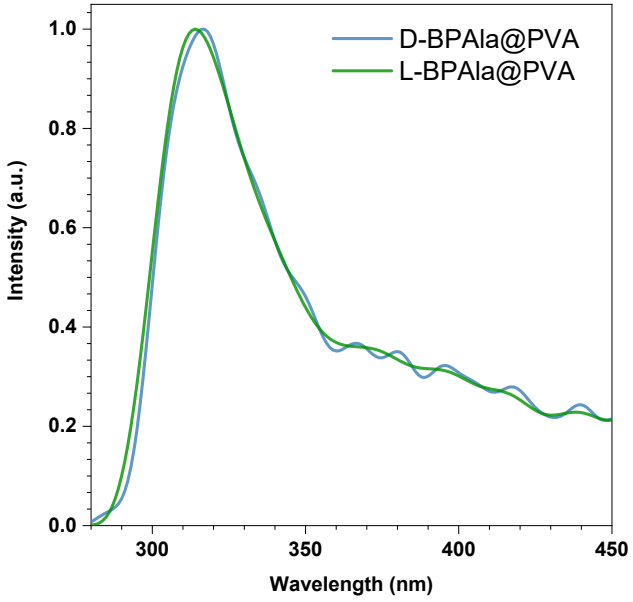

Figure S20. Photoluminescence emission spectra of D/L-BPAla@PVA films

Table S1. Photophysical data of room temperature phosphorescence of PVA doped films.

Compound	EM_p/nm	τ_p/s	Φ_P	CIE (x, y)
BPCA	487	1.06	23.48	0.18,0.32
BPAA	478	2.63	11.40	0.18,0.30
D-BPAla	475	2.91	7.91	0.17,0.26
L-BPAla	475	2.91	9.10	0.17,0.27

6 Theoretically calculated optimized molecular structures

Cartesian coordinates of Compound BPCA in the ground state

C	-4.02498900	-1.13331800	-0.44948300
C	-2.63200800	-1.12348500	-0.45152600
C	-1.92014000	-0.00036700	-0.00061000
C	-2.64624800	1.11247600	0.45307700
C	-4.03922000	1.10217000	0.45681700
C	-4.73443600	-0.02065500	0.00517200

H	-4.55731000	-2.00845200	-0.81138500
H	-2.08747200	-1.98253900	-0.83194100
H	-2.11259500	1.97947300	0.83083300
H	-4.58257700	1.96966100	0.82068300
H	-5.82058600	-0.02845200	0.00735600
C	-0.43960100	0.01060400	-0.00338300
C	0.27223900	1.18215400	-0.31535100
C	0.29011000	-1.14975900	0.30611400
C	1.66044600	1.19382800	-0.31682500
H	-0.27294500	2.08151200	-0.58408400
C	1.67993700	-1.14452400	0.30409600
H	-0.24156600	-2.05662300	0.57676100
C	2.37623300	0.03038100	-0.00763100
H	2.21303400	2.09364200	-0.56475500
H	2.23081800	-2.04434300	0.55271200
C	3.85645900	0.09575000	-0.02450500
O	4.50907600	1.08687900	-0.28715700
O	4.44517900	-1.08863100	0.28990200
H	5.40446600	-0.92138800	0.24609500

Cartesian coordinates of Compound BPCA in the first triplet state

C	-4.02136700	-1.23273000	-0.00033000
C	-2.64752900	-1.23478300	-0.00024400
C	-1.88214300	-0.00022200	0.00004200
C	-2.66644200	1.22237800	0.00017300
C	-4.03994400	1.19922000	0.00009600
C	-4.74706600	-0.02233900	-0.00014400
H	-4.55610300	-2.17845700	-0.00056000
H	-2.13013200	-2.18516400	-0.00049000
H	-2.16324600	2.18032500	0.00040400
H	-4.58914500	2.13660600	0.00022600
H	-5.83201900	-0.03065800	-0.00019600
C	-0.48169600	0.01149800	0.00019600
C	0.29505200	1.25685900	0.00010000
C	0.31345300	-1.22301600	0.00038100
C	1.65203400	1.25884100	-0.00001300
H	-0.22370300	2.20687100	0.00004000
C	1.67207800	-1.20925900	0.00029200
H	-0.19241800	-2.17996100	0.00070000
C	2.39747800	0.03032200	0.00003400
H	2.21253400	2.18704600	-0.00013400
H	2.23026200	-2.13827600	0.00044700

C	3.85040300	0.09746700	-0.00013200
O	4.50608300	1.13257600	-0.00035400
O	4.45261400	-1.13012700	-0.00001800
H	5.40851800	-0.94333700	-0.00017100

Cartesian coordinates of Compound BPAA in the ground state

C	4.32133300	1.12385100	-0.69070200
C	2.94512000	1.13658100	-0.47407000
C	2.28331600	0.00242800	0.02284600
C	3.04421200	-1.14572800	0.29479200
C	4.42023800	-1.15983900	0.07687900
C	5.06527000	-0.02477400	-0.41650100
H	4.81219000	2.01002000	-1.08351200
H	2.36945700	2.02496500	-0.71674100
H	2.55436700	-2.02406600	0.70470500
H	4.99111800	-2.05659200	0.30147000
H	6.13814300	-0.03531500	-0.58609000
C	0.82012600	0.01638600	0.25397100
C	0.03495200	-1.11824300	-0.00942400
C	0.17553800	1.16264800	0.74167900
C	-1.33808400	-1.10816100	0.21064100
H	0.50477100	-2.00883900	-0.41592900
C	-1.20036600	1.17432500	0.95838600
H	0.76179500	2.04586000	0.97700800
H	-1.93255900	-1.98782700	-0.01930400
H	-1.67709200	2.07297600	1.34120600
C	-4.20050000	-0.13332900	-0.38627500

O	-4.46358300	-1.19720900	-0.90171100
O	-4.48893200	1.05564800	-0.96755400
H	-4.90119200	0.84302500	-1.82627600
C	-1.97264400	0.03885800	0.70258800
C	-3.47369600	0.04445400	0.93177700
H	-3.78294600	0.98116900	1.40161800
H	-3.76683500	-0.78962000	1.57644100

Cartesian coordinates of Compound BPAA in the first triplet state

C	-4.38746800	-1.14289300	-0.32646300
C	-3.03491100	-1.20610600	-0.11921100
C	-2.22312800	0.00060800	0.03360300
C	-2.95780500	1.26200700	-0.05201000
C	-4.31103600	1.29465000	-0.25982200
C	-5.06104500	0.10088100	-0.40254000
H	-4.95396000	-2.06398400	-0.43499500
H	-2.56051500	-2.17761200	-0.06859700
H	-2.42389600	2.19769000	0.05252400
H	-4.81889000	2.25377000	-0.31652400
H	-6.13246900	0.13896200	-0.56795300
C	-0.84780700	-0.04842700	0.24739000
C	-0.02810400	1.15971300	0.39613800
C	-0.10813100	-1.31407000	0.33915500
C	1.31451000	1.09636500	0.61893500
H	-0.49631900	2.13280300	0.32362200
C	1.23774200	-1.34683600	0.56193600
H	-0.63885700	-2.25076100	0.22908900
H	1.89226800	2.01250100	0.70794900
H	1.74949400	-2.30432100	0.61882000
C	4.17015800	0.17789500	-0.38583100

O	4.47296300	1.29965100	-0.72567300
O	4.34446400	-0.90703500	-1.17999200
H	4.71697200	-0.57160900	-2.01727900
C	1.99773900	-0.15404700	0.72760600
C	3.48989900	-0.19101100	0.92322900
H	3.81534900	-1.18643600	1.23792200
H	3.80773700	0.54569000	1.66804800

Cartesian coordinates of Compound D- BPAla in the ground state

O	-4.36651100	0.94645500	-1.81777400
O	-3.39623400	1.87338700	-0.01098200
N	-4.99538600	-1.03189900	0.11543500
C	-2.77010200	-0.67963700	1.11947900
C	-1.29219900	-0.50451700	0.85561100
C	-3.62560500	-0.56466400	-0.15082300
C	1.47260200	-0.20100400	0.29791200
C	-0.52224500	-1.58550900	0.40806200
C	-0.65790900	0.73204100	1.02108000
C	0.83396500	-1.43989700	0.13261200
C	0.69921200	0.88009800	0.74780800
C	2.91675500	-0.04172100	0.00888900
C	-3.74972000	0.88442400	-0.60955700
C	3.72346100	0.78971700	0.80224200
C	3.51562000	-0.71799100	-1.06607800
C	5.08144800	0.94079500	0.52976600
C	4.87397100	-0.56938500	-1.33808300
C	5.66344300	0.26137200	-0.54152100
H	-2.94649700	-1.67662700	1.54319900
H	-3.13245600	0.05133700	1.84682400
H	-3.12545200	-1.11452800	-0.96722500

H	-0.98923000	-2.56111600	0.28838800
H	-1.24318900	1.58707000	1.34169000
H	1.41396300	-2.30214700	-0.18319100
H	1.16226300	1.85617600	0.85940700
H	-4.96186100	-2.01305500	0.38732800
H	-5.54058800	-0.98361100	-0.74341800
H	3.28443900	1.30026600	1.65428000
H	2.90279400	-1.34428500	-1.70777700
H	5.68835900	1.58360500	1.16152200
H	5.31479600	-1.09631500	-2.17995300
H	6.72237300	0.37831900	-0.75370200
H	-4.45623900	1.89473100	-2.02976600

Cartesian coordinates of Compound D- BPAla in the first triplet state

O	-4.37250100	1.08598400	-1.74516500
O	-3.32367200	1.85370400	0.09251400
N	-5.00825600	-1.02597900	0.01725500
C	-2.78078200	-0.77646300	1.05429600
C	-1.31084800	-0.57941800	0.82184300
C	-3.63191700	-0.55948900	-0.21049800
C	1.51301500	-0.22013600	0.28888300
C	-0.52857400	-1.61372100	0.22227200
C	-0.64581200	0.63707200	1.15479700
C	0.80186800	-1.46186100	-0.03519400
C	0.68474700	0.81960000	0.91236400
C	2.86835800	-0.04347100	0.02483600
C	-3.72592200	0.92081000	-0.56255400
C	3.57563500	1.19395100	0.35684500
C	3.68759100	-1.08058200	-0.60357900
C	4.91024400	1.35314800	0.09524400
C	5.02056000	-0.89265700	-0.85358600
C	5.66828000	0.32152900	-0.51321800
H	-2.96359400	-1.80714500	1.39003700
H	-3.15347100	-0.10731000	1.83462800
H	-3.13521300	-1.05641800	-1.06247300

H	-1.01400000	-2.55534700	-0.02788500
H	-1.22933200	1.43836600	1.59570800
H	1.34358400	-2.28545500	-0.48243400
H	1.13577300	1.76449900	1.18657600
H	-4.98990000	-2.02546200	0.21315900
H	-5.55103700	-0.90321200	-0.83564300
H	3.03435200	2.00740600	0.82242600
H	3.23285100	-2.02260800	-0.88217500
H	5.39751700	2.28825200	0.35880000
H	5.59286400	-1.68901600	-1.32226700
H	6.72514200	0.45893900	-0.71562400
H	-4.43702200	2.04898800	-1.88891400

Cartesian coordinates of Compound L- BPAla in the ground state

O	2.68557900	1.04544600	-1.78226200
O	3.85076000	1.87516800	-0.04079900
N	5.17743600	-0.65077700	-0.14176800
C	2.90290900	-0.85890400	0.96909000
C	1.41779000	-0.67380700	0.78361200
C	3.73118200	-0.52049600	-0.30454300
C	-1.35005600	-0.27538600	0.31494500
C	0.79990800	0.53923500	1.11149800
C	0.63087700	-1.68356400	0.21783400

C	-0.55865500	0.73553900	0.88165800
C	-0.72784700	-1.49062000	-0.01169100
C	-2.79643500	-0.06812400	0.07129400
C	3.45313900	0.92538600	-0.68275400
C	-3.58209600	0.66482800	0.97509200
C	-3.41747500	-0.59873400	-1.07072200
C	-4.94200900	0.86162600	0.74463700
C	-4.77772800	-0.40418600	-1.30093500
C	-5.54636600	0.32749900	-0.39439100
H	3.27028700	-0.21938500	1.77978500
H	3.12908700	-1.89823400	1.23845100
H	3.40399800	-1.16621400	-1.12478000
H	1.39628900	1.34240200	1.53666300
H	1.08656500	-2.63838000	-0.03497500
H	-1.00965200	1.69355900	1.12316400
H	-1.32291400	-2.30051100	-0.42318100
H	5.39630500	-1.56218500	0.25674900
H	5.49111700	0.05325200	0.52562100
H	-3.12571200	1.05987900	1.87793300
H	-2.82087000	-1.14517500	-1.79529200
H	-5.53284600	1.42548400	1.46126100
H	-5.23629700	-0.81707100	-2.19526500

H	-6.60676500	0.48002800	-0.57393200
H	2.52581100	2.00132400	-1.90307200

Cartesian coordinates of Compound L- BPAla in the first triplet state

O	-2.59024900	1.10627600	1.70305400
O	-3.86570400	1.87316500	0.00967500
N	-5.17896900	-0.63524000	0.21825700
C	-2.91502900	-0.91733500	-0.90928700
C	-1.43856700	-0.72917400	-0.76417400
C	-3.73393600	-0.50950000	0.36399100
C	1.38751200	-0.28726000	-0.31597100
C	-0.80764700	0.49041100	-1.15617500
C	-0.62124200	-1.72289800	-0.14624600
C	0.52304300	0.71182700	-0.95619100
C	0.71169800	-1.53247800	0.06827600
C	2.74408500	-0.06995800	-0.08887500
C	-3.43224700	0.94830500	0.66454300
C	3.41434100	1.17024700	-0.47867600
C	3.60006500	-1.06553700	0.55551200
C	4.75080400	1.36821300	-0.25409900
C	4.93411700	-0.83962600	0.76766400
C	5.54562700	0.37550300	0.37092500
H	-3.30146500	-0.31817300	-1.74257900

H	-3.15453500	-1.96944800	-1.11353100
H	-3.40049900	-1.12070200	1.20741100
H	-1.41550600	1.26109400	-1.62424000
H	-1.08135300	-2.66159600	0.15560000
H	0.94791400	1.65223300	-1.28287200
H	1.28270600	-2.32644200	0.53201600
H	-5.41229300	-1.55680600	-0.14656900
H	-5.49829600	0.05303900	-0.46242500
H	2.84466600	1.95548900	-0.95879200
H	3.17335900	-2.00677500	0.87748100
H	5.21020900	2.30425300	-0.56070800
H	5.53464500	-1.60629900	1.25016100
H	6.60333400	0.54334900	0.54370000
H	-2.40823100	2.06348200	1.76840900

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