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## **Supporting Information For:**

## Pteridine derivatives: novel low molecular weight

## organogelators and Piezofluorochromism

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Dye	solvents	$\lambda_{abs}(nm)^a$	$\lambda_{em}(nm)^{b}$	∆v <sub>st</sub> <sup>c</sup> /cm <sup>-1</sup>	${\cal D}_{\it F}{}^{\sf d}$	${\cal D}_{F}^{e}$
НСР	Cyclohexane	338, 375	481	5877	0.11	
	Toluene	340, 383	484	5449		
	DCM	340, 382	485	5559		
	DMF	341, 382	497	6057		
FCP	Cyclohexane	337, 376	480	5762	0.35	
	Toluene	340, 382	480	5345		
	DCM	340, 383	484	5449		
	DMF	340, 381	492	5922		
ССР	Cyclohexane	339, 377	484	5864	0.27	
	Toluene	343, 383	487	5576	0.51	
	DCM	343, 383	491	5743	0.38	
	DMF	344, 383	499	6070	0.63	
BCP	Cyclohexane	339, 379	486	5809	0.20	
	Toluene	344, 385	490	5566		
	DCM	343, 385	495	5772		
	DMF	344, 385	501	6014		
OHP	Toluene	333,346,400	504	5159	0.76	
	DCM	333,345,396	508	5567		
	DMF	333,345,390	510	6033		
ΡΥΡ	Cyclohexane	352	490	8001	0.02	0.24
	Toluene	356	508	8405		
	DCM	357	518	8706		
	DMF	358	520	8702		
PIP	Cyclohexane	352	489	7959	0.07	0.49
	Toluene	356	505	8288		
	DCM	357	515	8594		
	DMF	358	522	8776		
BNP	Cyclohexane	348	491	8369	0.01	0.19
	Toluene	351	500	8490		
	DCM	351	506	8727		
	DMF	354	520	9018		
DBP	Cyclohexane	358	493	7649	0.11	
	Toluene	361	502	7781		
	DCM	363	513	8055		
	DMF	364	521	8279		

 Table S1 Photophysical data of synthesized ptridine derivatives.

<sup>a</sup> Concentration is maintained at 1.0 × 10<sup>-5</sup> M; <sup>b</sup> Excited at 350 nm, 380 nm and 390 nm; <sup>c</sup>  $\Delta v_{st} = v_{abs}$ - v<sub>f</sub>; <sup>d</sup> Using 9,10-diphenylanthracene in toluene ( $\Phi_F = 85\%$ ) and cyclohexanone ( $\Phi_F = 100\%$ ) as the standard; <sup>e</sup> in solid-state.

Compounds	$\lambda_{abs}^{[a]}(nm)$	$\lambda_{abs}^{[b]}$ (nm)	$f^{[c]}$	Transition (%) <sup>[d]</sup>
ССР	383	367.44	0.1630	$H \rightarrow L (92.8)$
				$H \rightarrow L+1(2.5)$
	343	335.25	0.1273	H-3→L (51.1)
				$H-1 \rightarrow L(41.5)$
				$H \rightarrow L+1(2.4)$
		328.69	0.2245	$\text{H-2} \rightarrow \text{L}(5.5)$
				$\text{H-1}{\rightarrow}\text{L}(45.5)$
				H→L+1 (5.8)
НСР	383	366.07	0.1541	H-4→L (92.8)
				$H\rightarrow L+1(2.7)$
	340	333.67	0.0262	H-2→L (55.9)
				H-1→L (14.7)
		324.44	0.2122	H-2→L (6.7)
				$H-1 \rightarrow L(66.5)$
				$H \rightarrow L+1(14.3)$
PIP		378.09	0.1650	H→L (94.7)
	356	352.91	0.0791	H-1→L (87.4)
				$H \rightarrow L(2.1)$
				$H \rightarrow L+1(6.6)$
		332.28	0.0058	H-6→L (2.6)
				H-4→L (2.4)
				H-3→L (78.8)

Table S2. Main orbital transitions calculated with TD-DFT.

 $H-3 \rightarrow L (78.8)$ <sup>a</sup> Experimental absorption in toluene; <sup>b</sup> Compound transition wavelength *in vacuo*; <sup>c</sup> Compound oscillator strength *in vacuo*; <sup>d</sup> H represents HOMO, L represents LUMO.

ССР	Solvent	Acetone 1	Methanol	Ethanol	Isopropanol	a hutonol	Amylene
						<i>n</i> -outanoi	alcohol
	Concentration(mg/mL)	8	6.7	5	10	8	5
	T <sub>gel</sub> (°C)	56	50	53	60	70	55
НСР	Solvent	Toluene/Petroleum			Toluene/Cyclohexane		
	Concentration(mg/mL)	13.3			13.3		
	T <sub>gel</sub> (°C)	88			82		
FCP	Solvent	Toluen	e/ T	oluene/	Chlorobenzen	ne/ Chlor	obenzene/
		Petroleum	<sup>im</sup> Cyc	lohexane	Petroleum	Cycl	lohexane
	Concentration (mg/mL)	13.3		10	12.5		12.5
	T <sub>gel</sub> (°C)	58		70	50		77

Table S3  $T_{gel} \mbox{ of } CCP, FCP \mbox{ and } HCP \mbox{ in different solvents}$ 



**Figure S1** Normalized A) UV/Vis absorbance and B) fluorescence emission spectra of **CCP** ( $\lambda_{ex}$  = 380 nm) in different solvents; C) UV/Vis absorbance and D) fluorescence emission spectra of **PIP** ( $\lambda_{ex}$  = 350 nm) in different solvents. The concentrations are maintained at 1.0 × 10<sup>-5</sup> M.



Figure S2 Normalized UV/Vis absorbance HCP (A), FCP (C), BCP (E) fluorescence emission spectra of HCP (B), FCP (D), BCP (F) ( $\lambda_{ex}$  = 380 nm) in different solvents. The concentrations are maintained at 1.0 × 10<sup>-5</sup> M.



Figure S3 Normalized a) UV/Vis absorbance and b) fluorescence emission spectra of OHP ( $\lambda_{ex}$  = 390 nm) in different solvents. The concentrations are maintained at 1.0 × 10<sup>-5</sup> M.



**Figure S4.** Normalized UV/Vis absorbance **DBP** (A), **BNP** (C), **PYP** (E) fluorescence emission spectra of **DBP** (B), **BNP** (D), **PYP** (F) ( $\lambda_{ex}$  = 350 nm) in different solvents. The concentrations are maintained at 1.0 × 10<sup>-5</sup> M.



**FigureS5** Excitation (record every 10 s) and fluorescence emission spectra (recorded every 5s) (B) ( $\lambda$ ex = 380 nm) of compound **CCP** upon cooling the hot solutions in amylene alcohol which had first been stimulated by ultrasound to room temperature. The arrows indicated the spectral changes from the sol to the gel.



Figure S6 Time-dependent UV-vis absorption (A) and fluorescence emission spectra (B) ( $\lambda_{ex}$  = 380 nm) of compound FCP upon cooling the hot solutions in toluene/cyclohexan v/v = 5/11, which have first been stimulated by ultrasound to room temperature. The arrows indicate the spectral changes from the sol to the gel. Insets: Photographs of the solutions and gels irradiated by 365 nm light.



**Figure S7** Time-dependent UV-vis absorption (A) and fluorescence emission spectra (B) ( $\lambda_{ex}$  = 380 nm) of compound **HCP** upon cooling the hot solutions in toluene/petroleum ether v/v = 5/11, which have first been stimulated by ultrasound to room temperature. The arrows indicate the spectral changes from the sol to the gel. Insets: Photographs of the solutions and gels irradiated by 365 nm light.



**FigureS8** SEM images of xerogel **FCP** obtained from toluene/cyclohexane (A) and xerogel **HCP** obtained from toluene/petroleum ether (B).



**Figure S9** Sheer dependence of storage modulus G' and loss modulus G'' of **CCP** in amylene alcohol (5.0 mg/mL)(a), **HCP** in Toluene /Petroleum ether (13.3 mg/mL) (b) and **FCP** in Toluene/Cyclohexane (13.3 mg/mL);



Figure S10 XRD pattern of xerogel CCP obtained from amylene alcohol.



**Figure S11** (A) XRD pattern of xerogel **HCP** obtained from toluene/petroleum ether and (B) the proposed molecular packing mode of **HCP** in the gel phase.



**Figure S12** (A) XRD pattern of xerogel **FCP** obtained from Toluene/Cyclohexane and (B) the proposed molecular packing mode of **FCP** in the gel phase.



**Figure S13** Normalized fluorescence spectra (left) and the XRD patterns (right) of **BNP** (A/B) and **DBP** (C/D) upon stimulated by mechanical forces ( $\lambda_{ex}$  = 360 nm). Inset photographs taken under UV illumination.



**Figure S14** Normalized fluorescence spectra (left) and the XRD patterns (right) of **OHP** (A/B) upon stimulated by mechanical forces ( $\lambda_{ex}$  = 360 nm). Inset photographs taken under UV illumination.



Figure S15 UV-Vis absorption spectra of PYP (A), PIP (B), DBP (C), BNP (D) and OHP (E) in different solid states.



**Figure S16** Maximum fluorescent emission of **PYP** (A), **PIP** (B), **DAP** (C), **BAE** (D) upon repeating treated by grinding and fuming with DCM and **HP** (E) upon repeating treated by grinding and heating.



Figure S17 The torsional angle ( $C_1$ ,  $C_6$  with  $C_7$ ,  $C_8$ ) of compound PYP (A) and PIP (B) in single crystal.



Figure S18 The CH…N distance of compound PYP (A) and PIP (B) in single crystal.



**Figure S19** Molecular stacking structures of **PYP** along the *b*-axis and *c*-axis (top) and molecular stacking structures of **PIP** along the *a*-axis and *c*-axis (bottom).



Figure S20 <sup>1</sup>H NMR (400 MHz) spectrum of HCP in CDCl<sub>3</sub>.



Figure 21 <sup>13</sup>C NMR (100 MHz) spectrum of HCP in CDCl<sub>3</sub>.



Figure S22 MALDI/TOF MS spectrum of HCP.



Figure S23 <sup>1</sup>H NMR (400 MHz) spectrum of FCP in CDCl<sub>3</sub>.



Figure S24 <sup>13</sup>C NMR (100 MHz) spectrum of FCP in CDCl<sub>3</sub>



Figure S25 MALDI/TOF MS spectrum of FCP.



Figure S26 <sup>1</sup>H NMR (400 MHz) spectrum of CCP in CDCl<sub>3</sub>.



Figure S27 <sup>13</sup>C NMR (100 MHz) spectrum of CCP in CDCl<sub>3</sub>.



Figure S28 MALDI/TOF MS spectrum of CCP.







Figure S30 <sup>13</sup>C NMR (100 MHz) spectrum of BCP in CDCl<sub>3</sub>.



Figure S31 MALDI/TOF MS spectrum of BCP.



Figure S32 <sup>1</sup>H NMR (400 MHz) spectrum of PYP in CDCl<sub>3</sub>.



Figure S33 <sup>13</sup>C NMR (100 MHz) spectrum of PYP in CDCl<sub>3</sub>.



Figure S34 MALDI/TOF MS spectrum of PYP.



Figure S35  $^1\text{H}$  NMR (400 MHz) spectrum of PIP in CDCl\_3.



Figure S36 <sup>13</sup>C NMR (100 MHz) spectrum of PIP in CDCl<sub>3</sub>.



Figure S37 MALDI/TOF MS spectrum of PIP.



Figure S38 <sup>1</sup>H NMR (400 MHz) spectrum of DBP in DMSO-d<sub>6</sub>.



Figure S39 <sup>13</sup>C NMR (100 MHz) spectrum of DBP in CDCl<sub>3</sub>.



Figure S40 MALDI/TOF MS spectrum of DBP.



Figure S41 <sup>1</sup>H NMR (400 MHz) spectrum of BNP in CDCl<sub>3</sub>.



Figure S42 <sup>13</sup>C NMR (100 MHz) spectrum of BNP in CDCl<sub>3</sub>.



Figure S43 MALDI/TOF MS spectrum of BNP.



Figure S44 <sup>1</sup>H NMR (400 MHz) spectrum of OHP in DMSO-d<sub>6</sub>.



Figure S45 <sup>13</sup>C NMR (100 MHz) spectrum of OHP in DMSO-d<sub>6</sub>.



Figure S46 MALDI/TOF MS spectrum of OHP.