Six novel coordination polymers based on 5-(1H-tetrazol-5-yl)isophthalic acid ligand: structures, luminescence, and magnetic properties

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Table S1. Selected bond lengths [Å] and angles [°] for CPs **1-6**.

CP **1**			
Mn1-O6	2.089(2)	Mn1-O5A	2.143(2)
Mn1-O3B	2.152(2)	Mn1-O1	2.184(2)
Mn1-N4C	2.392(3)	Mn1-N1	2.401(3)
Mn2-O4D	2.060(2)	Mn2-O1	2.105(2)
Mn2-O2B	2.148(2)	Mn2-O1E	2.158(2)
Mn2-N2	2.235(3)		
O6-Mn1-O5A	87.19(11)	O6-Mn1-O3B	88.61(11)
O5A-Mn1-O3B	175.17(9)	O6-Mn1-O1	179.13(10)
O5A-Mn1-O1	93.31(9)	O3B-Mn1-O1	90.86(9)
O6-Mn1-N4C	94.82(10)	O5A-Mn1-N4C	90.39(10)
O3B-Mn1-N4C	87.60(10)	O1-Mn1-N4C	84.47(8)
O6-Mn1-N1	92.59(10)	O5A-Mn1-N1	95.63(9)
O3B-Mn1-N1	86.92(9)	O1-Mn1-N1	88.08(8)
N4C-Mn1-N1	170.68(9)	O4D-Mn2-O1	147.71(11)
O4D-Mn2-O2B	86.74(10)	O1-Mn2-O2B	93.41(9)
O4D-Mn2-O1E	93.12(9)	O1-Mn2-O1E	82.43(9)
O2B-Mn2-O1E	171.98(9)	O4D-Mn2-N2	121.94(12)
O1-Mn2-N2	90.19(9)	O2B-Mn2-N2	95.91(10)

O1E-Mn2-N2	90.98(9)		

A -x+1,-y+1,-z+1; B x+1/2,-y+3/2,z-1/2; C x+1,y,z; D x,y,z-1; E -x+1,-y+1,-z.

CP **2**			
Cu1-O1	1.936(4)	Cu1-O2	1.943(4)
Cu1-O5A	1.944(4)	Cu1-N2	1.980(4)
Cu1-O4B	2.236(4)	Cu2-O3B	2.111(4)
Cu2-O6A	1.921(4)	Cu2-O1C	1.945(4)
Cu2-O1	2.041(4)	Cu2-N3C	2.048(4)
O1-Cu1-O2	178.26(18)	O1-Cu1-O5A	93.44(16)
O2-Cu1-O5A	87.71(17)	O1-Cu1-N2	88.48(17)
O2-Cu1-N2	90.10(18)	O5A-Cu1-N2	166.3(2)
O1-Cu1-O4B	86.54(15)	O2-Cu1-O4B	94.43(19)
O5A-Cu1-O4B	104.76(17)	N2-Cu1-O4B	88.94(17)
N3C-Cu2-O3B	107.21(17)	O6A-Cu2-O1C	172.85(17)
O6A-Cu2-O1	93.13(16)	O1C-Cu2-O1	81.87(17)
O6A-Cu2-N3C	91.63(16)	O1C-Cu2-N3C	89.02(16)
O1-Cu2-N3C	140.31(17)	O6A-Cu2-O3B	89.93(17)
O1C-Cu2-O3B	96.68(16)	O1-Cu2-O3B	112.17(15)

A x+1,y,z+1; B x+1,-y+3/2,z+1/2; C -x+2,-y+1,-z+1.

CP **3**			
Co1-O3A	1.993(2)	Co1-O1	2.029(2)
Co1-O6	2.064(2)	Co1-O5	2.259(3)
Co1-N4B	2.269(3)	Co1-N1C	2.347(3)
Co2-O6D	2.031(2)	Co2-O4E	2.044(3)
Co2-O6	2.053(2)	Co2-N3B	2.104(3)
Co2-N2F	2.122(3)	Co2-O7	2.219(3)
O3A-Co1-O1	95.89(10)	O3A-Co1-O6	88.83(10)
O1-Co1-O6	175.26(9)	O3A-Co1-O5	168.11(11)
O1-Co1-O5	93.49(10)	O6-Co1-O5	81.89(10)

O3A-Co1-N4B	100.99(11)	O1-Co1-N4B	91.88(10)
O6-Co1-N4B	86.73(9)	O5-Co1-N4B	85.95(13)
O3A-Co1-N1C	84.98(11)	O1-Co1-N1C	89.41(10)
O6-Co1-N1C	91.48(9)	O5-Co1-N1C	87.83(12)
N4B-Co1-N1C	173.72(11)	O6D-Co2-O4E	90.86(10)
O6D-Co2-O6	165.59(13)	O4E-Co2-O6	103.33(10)
O6D-Co2-N3B	93.18(10)	O4E-Co2-N3B	90.03(11)
O6-Co2-N3B	84.43(10)	O6D-Co2-N2F	89.16(10)
O4E-Co2-N2F	89.82(11)	O6-Co2-N2F	93.33(10)
N3B-Co2-N2F	177.66(11)	O6D-Co2-O7	83.60(11)
O4E-Co2-O7	174.45(11)	O6-Co2-O7	82.22(10)
N3B-Co2-O7	90.59(11)	N2F-Co2-O7	89.78(11)

A -x+1,y-1/2,-z+3/2; B x,-y+3/2,z-1/2; C x,-y+3/2,z+1/2; D x,-y+1/2,z-1/2; E -x+1,-y+1,-z+1; F x,y-1,z.

CP **4**

Zn1-O1	1.912(2)	Zn1-O3A	1.935(2)
Zn1-O5B	1.957(2)	Zn1-N1	2.050(2)
Zn2-O1	1.937(2)	Zn2-N5	2.099(3)
Zn2-N6	2.126(3)	Zn2-N4B	2.214(2)
Zn2-N2	2.254(2)		
O1-Zn1-O3A	126.66(9)	O1-Zn1-O5B	111.18(10)
O3A-Zn1-O5B	96.42(9)	O1-Zn1-N1	94.79(9)
N5-Zn2-N6	77.89(10)	O1-Zn2-N4B	103.45(9)
N5-Zn2-N4B	98.45(10)	N6-Zn2-N4B	89.18(9)
O1-Zn2-N2	86.58(9)	N5-Zn2-N2	94.64(10)
N6-Zn2-N2	172.38(9)	N4B-Zn2-N2	90.42(9)

A -x+2,-y,-z+1; B x,-y+1/2,z-1/2.

CP **5**

Zn1-O5	1.9051(16)	Zn1-O1	1.9734(14)

Zn1-O4A	1.9916(14)	Zn1-N1B	2.0392(18)
Zn2-O5	1.9306(15)	Zn2-N4C	2.0474(18)
Zn2-N5	2.0941(18)	Zn2-O3A	2.1306(15)
Zn2-N6	2.1883(18)		
O5-Zn1-O1	122.57(7)	O5-Zn1-O4A	108.06(7)
O1-Zn1-O4A	104.64(6)	O5-Zn1-N1B	106.83(7)
O1-Zn1-N1B	111.59(7)	O4A-Zn1-N1B	100.98(7)
O5-Zn2-N4C	106.27(7)	O5-Zn2-N5	134.18(7)
N4C-Zn2-N5	119.46(7)	O5-Zn2-O3A	91.40(6)
N4C-Zn2-O3A	96.41(7)	N5-Zn2-O3A	86.48(7)
O5-Zn2-N6	96.16(7)	N4C-Zn2-N6	95.82(7)
N5-Z2-N6	77.49(7)	O3A-Zn2-N6	163.21(7)

A x,y-1,z; B -x,-y+1,-z+1; C -x+1,-y+1,-z+1.

CP **6**

Zn1-O5	1.9430(18)	Zn1-O3A	1.9656(18)
Zn1-O2	1.985(2)	Zn1-N4B	2.040(2)
Zn1-O1	2.554(2)	Zn2-N5	2.054(2)
Zn2-O5	1.8858(18)	Zn2-O4C	1.9685(18)
Zn2-N1D	2.029(2)		
O5-Zn1-O3A	105.07(8)	O5-Zn1-O2	103.15(8)
O3A-Zn1-O2	116.10(9)	O5-Zn1-N4B	101.86(8)
O3A-Zn1-N4B	105.87(8)	O2-Zn1-N4B	122.42(9)
O5-Zn1-O1	155.15(7)	O3A-Zn1-O1	97.42(8)
O2-Zn1-O1	56.39(8)	N4B-Zn1-O1	81.63(8)
N1D-Zn2-N5	108.04(8)	O5-Zn2-O4C	122.11(8)
O5-Zn2-N1D	107.88(8)	O4C-Zn2-N1D	105.79(9)
O5-Zn2-N5	116.47(8)	O4C-Zn2-N5	95.27(8)

A -x+1,-y+2,-z+1; B -x+1,-y+1,-z+1; C x-1,y-1,z-1; D -x,-y+1,-z+1.

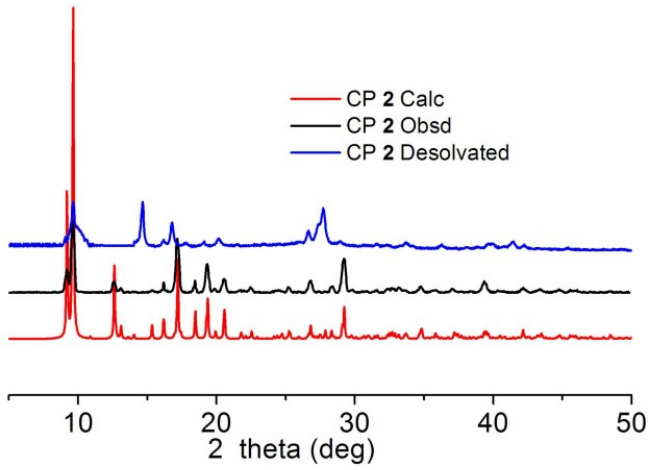

Fig. S1. PXRD patterns for CP **2** (simulated: red; experimental: black;desolvated sample: blue).

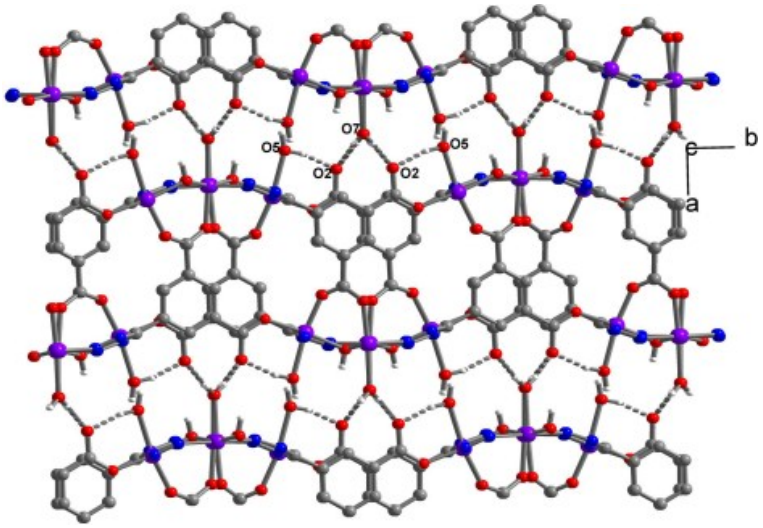

Fig. S2. The 3D architecture with hydrogen bonds between the layers in CP **3**. (O5-H···O2 = 1.768 Å, O5-H···O2 = 166°, O5···O2 = 2.593 Å; O7-H···O2 [-x+2, -y+1, -z+1] = 2.006 Å, O7-H···O2 = 177°, O7···O2 = 2.699 Å; O7-H···O2 [-x+2, y-1/2, -z+3/2] = 1.841 Å, O7-H···O2 = 176°, O7···O2 = 2.711 Å).

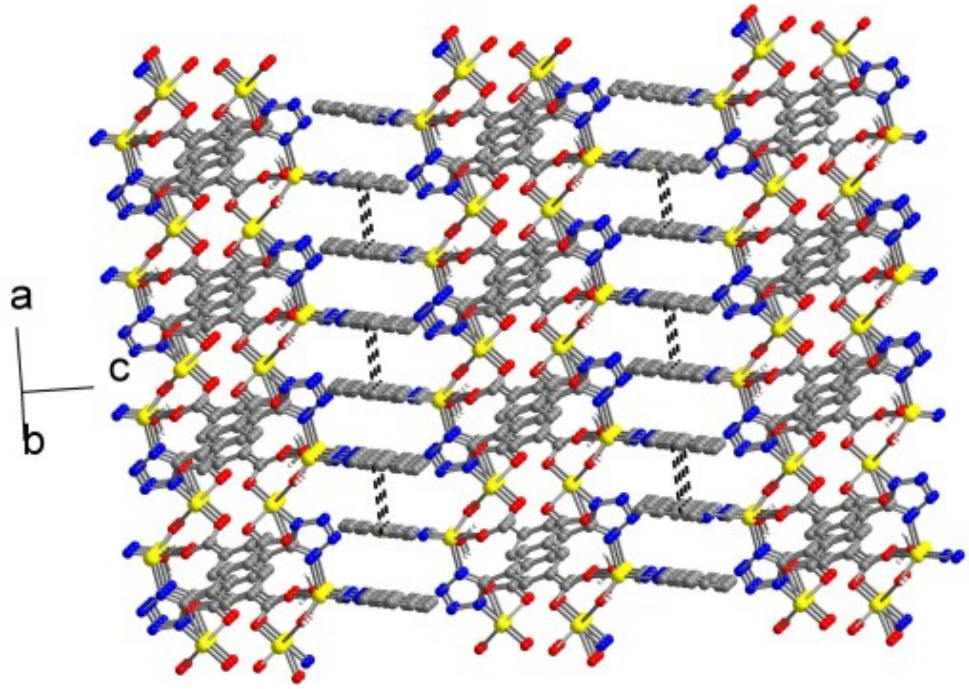

Fig. S3. The 3D architecture by π-π stacking in CP **5**.

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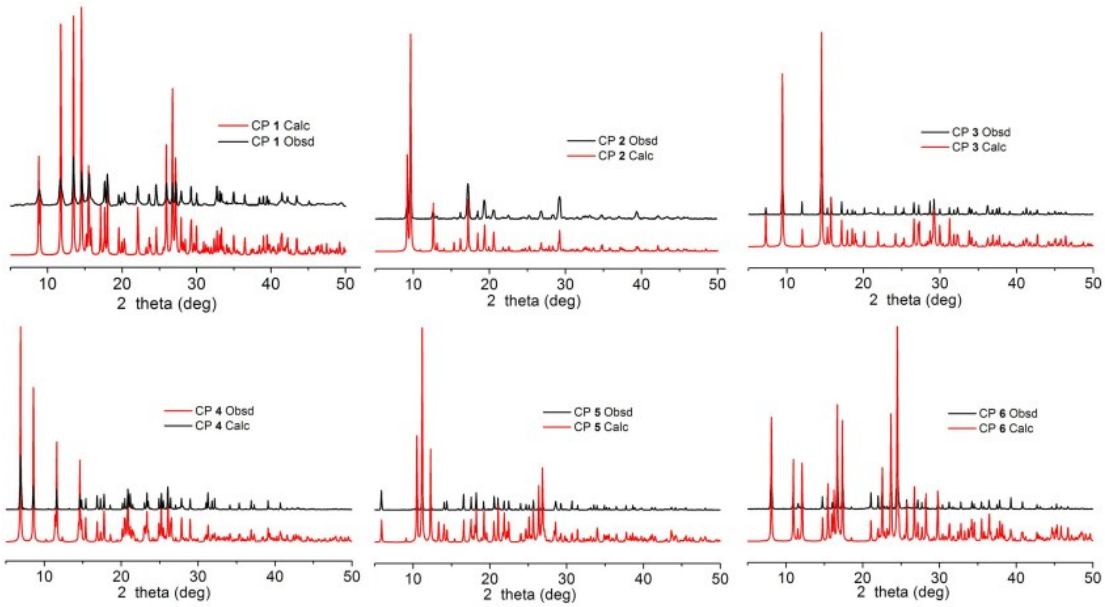

Fig. S4. PXRD patterns for CPs **1-6** (simulated: red; experimental: black)

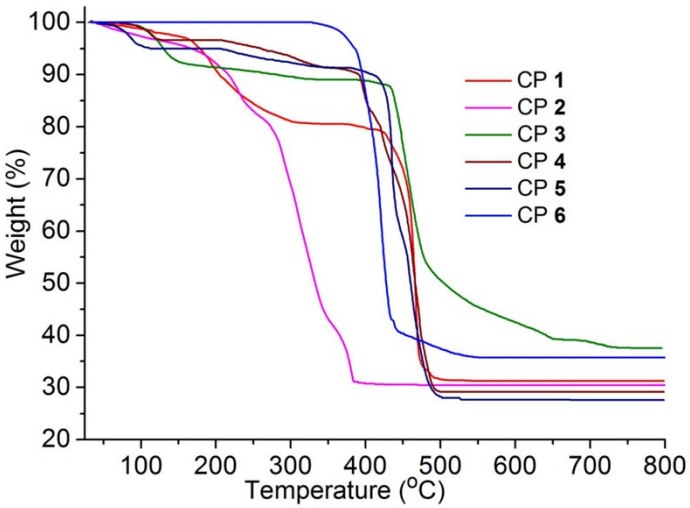

Fig. S5. TGA curves of CPs **1-6**.

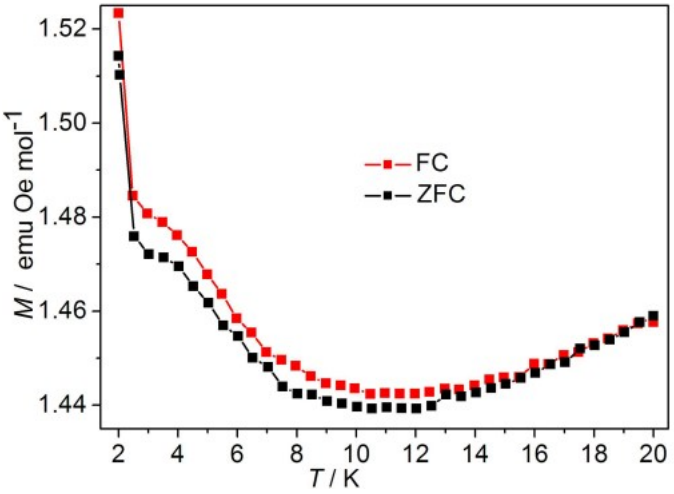

Fig. S6. The FCM and ZFCM curves at 20 Oe for CP **1**.

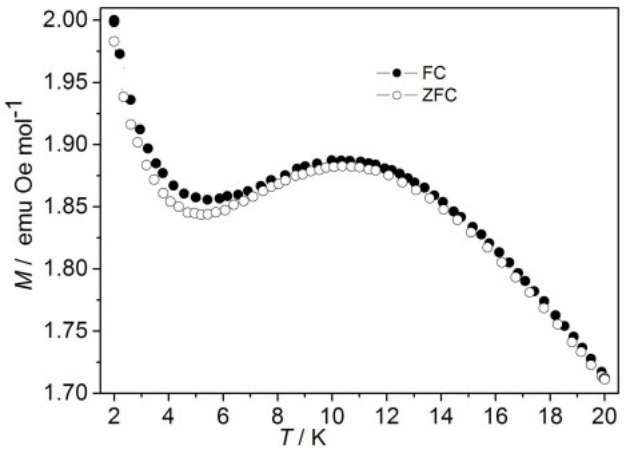

Fig. S7. The FCM and ZFCM curves at 20 Oe for CP **3**.

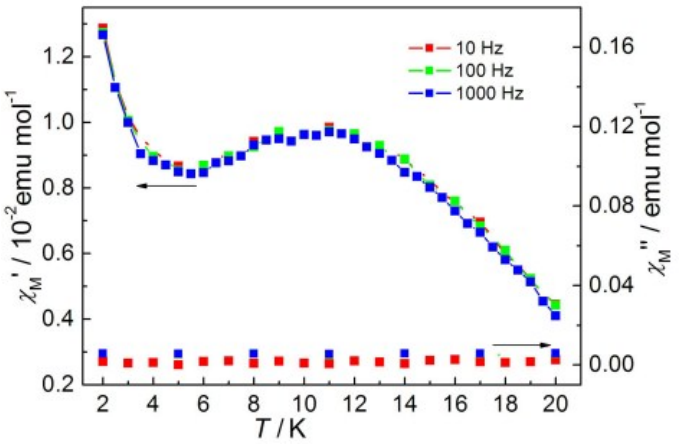

Fig. S8. The AC curves obtained at 3 Oe eld for CP **3**.

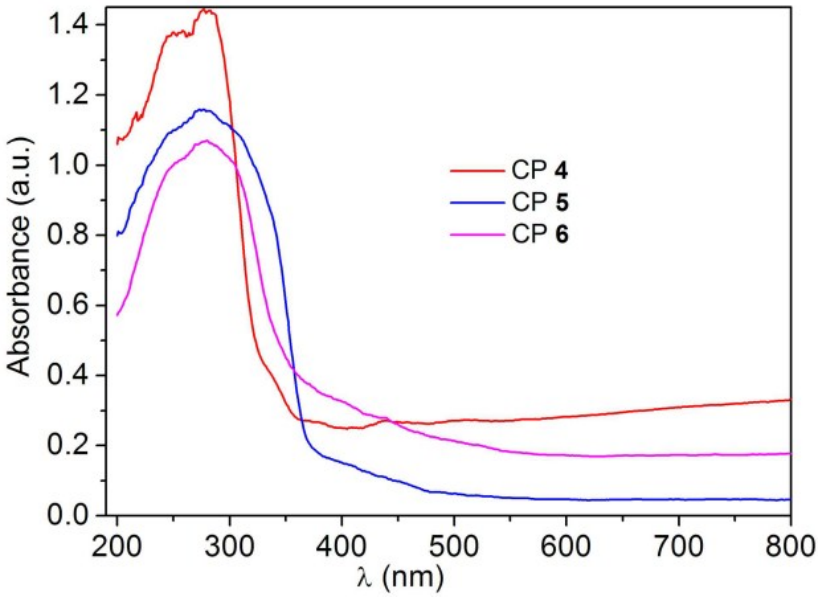

Fig. S9. UV-vis spectra of CPs **4-6**.

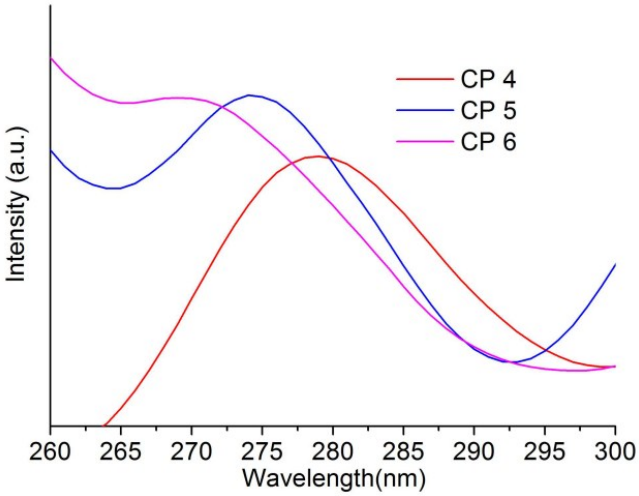

Fig. S10. Excitation spectra of CPs **4-6** at room temperature in the solid state.

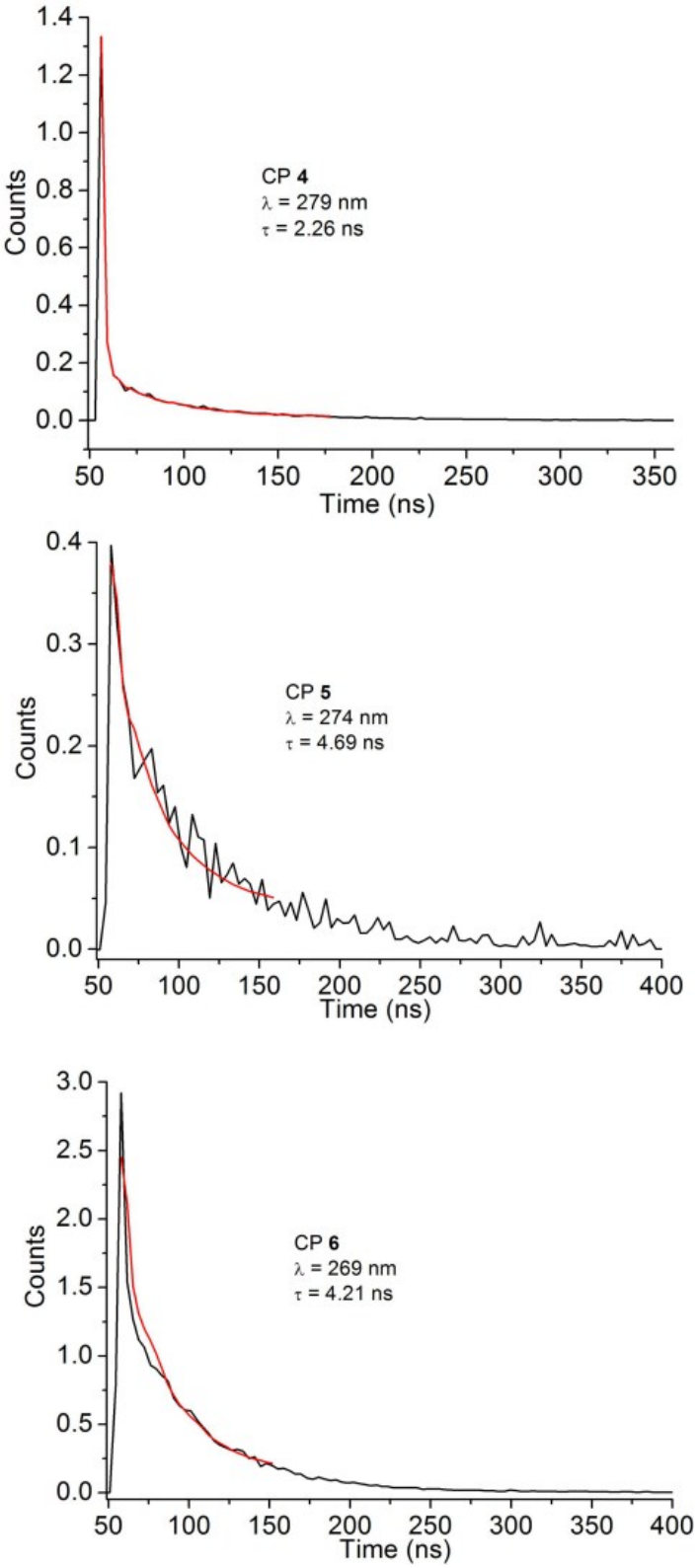

Fig. S11. Decay curves and fitting curves of CPs **4-6**