Supporting Information for the Manuscript:

Novel Coordination Polymers of Zn(II) and Cd(II) Tuned by different Aromatic Polycarboxylates: Synthesis, Structures and Photocatalytic Properties

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Table S1. **Crystallographic data and structure refinement details for complex 1−6[a,b]**

Complex	**1**	**2**	**3**	**4**	**5**	**6**
Formula	$C_{27}H_{24}CdN_4O_4$	$C_{56}H_{58}Zn_3N_8O_{18}$	$C_{75}H_{74}Cd_3N_6O_{16}$	$C_{28}H_{26}Zn_2N_4O_8$	$C_{24}H_{21}CdN_4O_4$	$C_{33}H_{32}CdN_4O_8S$
fw	580.90	1327.21	1736.66	677.27	541.85	757.09
T/K	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)
λ (Mo K), Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Cryst syst	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group	*P2(1)/c*	*P-1*	*P-1*	*P2(1)/c*	*P-1*	*P2(1)/c*
a (Å)	12.761(3)	9.4806(19)	12.156(2)	11.650(2)	9.4698(19)	12.0052(2)
b (Å)	14.961(3)	18.127(4)	18.590(4)	15.490(3)	11.079(2)	18.834(4)
c (Å)	17.532(3)	18.693(4)	21.024(4)	17.108(6)	11.161(2)	16.723(6)
α(°)	90	61.88(3)	74.05(3)	90	77.45(3)	90
β(°)	132.259(19)	83.98(3)	75.94(3)	115.37(2)	78.01(3)	123.27
γ(°)	90	86.35(3)	75.58(3)	90	85.11(3)	90
V (Å^3)	2477.3(11)	2817.3(10)	4345.8(14)	2789.5(12)	1117.1(4)	3161.4(14)
Z	4	2	2	4	2	4
$D_{calcd.}$(g·cm^{-3})	1.558	1.565	1.263	1.613	1.611	1.591
abs coeff (mm^{-1})	0.923	1.349	0.786	1.778	1.017	0.816
F(000)	1176	1368	1676	1384	546	1544
θ (°)	2.08-28.05	2.15-25.50	1.36-25.50	1.86-25.49	1.88-27.91	2.03-25.50
R(int)	0.0357	0.0528	0.0970	0.0778	0.0553	0.0278
GOF	1.002	1.032	0.999	1.050	0.959	0.999
R_1(I>2sigma(I))[a]	0.0411	0.0643	0.0685	0.0824	0.0567	0.0419
wR_2(I>2sigma(I))[b]	0.1337	0.1983	0.1950	0.3068	0.1407	0.1658

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$. [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

Table S2. Selected Bond Lengths (Å) and Bond Angles (deg) for 1−6

Compound **1**			
Cd(1)-O(3)#1	2.278(3)	O(3)#1-Cd(1)-O(1)	152.52(11)
Cd(1)-N(4)#2	2.287(3)	N(4)#2-Cd(1)-O(1)	93.24(10)
Cd(1)-N(1)	2.292(3)	N(1)-Cd(1)-O(1)	104.94(11)
Cd(1)-O(1)	2.304(3)	O(3)#1-Cd(1)-O(2)	101.24(10)
Cd(1)-O(2)	2.446(2)	N(4)#2-Cd(1)-O(2)	145.35(9)
Cd(1)-O(4)#1	2.459(3)	N(1)-Cd(1)-O(2)	93.51(9)
O(3)-Cd(1)#3	2.277(3)	O(1)-Cd(1)-O(2)	55.16(8)
O(4)-Cd(1)#3	2.459(3)	O(3)#1-Cd(1)-O(4)#1	55.00(9)
N(4)-Cd(1)#4	2.287(3)	N(4)#2-Cd(1)-O(4)#1	95.87(9)
O(3)#1-Cd(1)-N(4)#2	104.30(11)	N(1)-Cd(1)-O(4)#1	140.52(10)
O(3)#1-Cd(1)-N(1)	89.02(11)	O(1)-Cd(1)-O(4)#1	102.89(10)
N(4)#2-Cd(1)-N(1)	109.83(9)	O(2)-Cd(1)-O(4)#1	80.03(8)
Symmetry codes: #1 = x+1, -y-1/2, z+1/2; #2 = x, -y+1/2, z-1/2; #3 = x-1, -y-1/2, z-1/2; #4 = x, -y+1/2, z+1/2.			
Compound **2**			
Zn(1)-O(4)	1.928(3)	O(4)-Zn(1)-O(12)	108.85(16)
Zn(1)-O(12)	1.966(3)	O(4)-Zn(1)-O(5)#1	97.08(16)
Zn(1)-O(5)#1	1.993(4)	O(12)-Zn(1)-O(5)#1	112.74(15)
Zn(1)-N(4)	1.997(4)	O(4)-Zn(1)-N(4)	122.74(17)
Zn(2)-O(6)	1.934(3)	O(12)-Zn(1)-N(4)	110.70(16)
Zn(2)-O(9)#2	1.967(4)	O(5)#1-Zn(1)-N(4)	103.79(17)
Zn(2)-O(11)#1	1.991(4)	O(6)-Zn(2)-O(9)#2	116.67(17)
Zn(2)-N(5)	1.993(4)	O(6)-Zn(2)-O(11)#1	111.03(17)
Zn(3)-O(1)	1.929(4)	O(9)#2-Zn(2)-O(11)#1	90.17(16)
Zn(3)-O(7)#3	1.940(4)	O(6)-Zn(2)-N(5)	118.57(17)
Zn(3)-N(1)#4	1.997(4)	O(9)#2-Zn(2)-N(5)	111.16(18)
Zn(3)-N(8)#5	2.008(4)	O(11)#1-Zn(2)-N(5)	104.86(18)
O(5)-Zn(1)#1	1.993(4)	O(1)-Zn(3)-O(7)#3	100.93(16)
O(7)-Zn(3)#3	1.940(4)	O(1)-Zn(3)-N(1)#4	111.56(16)
O(9)-Zn(2)#6	1.967(4)	O(7)#3-Zn(3)-N(1)#4	113.71(16)
O(11)-Zn(2)#1	1.991(4)	O(1)-Zn(3)-N(8)#5	112.93(18)
N(1)-Zn(3)#7	1.997(4)	O(7)#3-Zn(3)-N(8)#5	113.08(16)
N(8)-Zn(3)#5	2.008(4)	N(1)#4-Zn(3)-N(8)#5	104.91(18)
Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z.			
Compound **3**			
Cd(1)-N(1)	2.265(5)	O(2)-Cd(1)-O(1)	55.29(17)
Cd(1)-N(9)	2.276(5)	N(1)-Cd(1)-O(8)	151.10(17)
Cd(1)-O(7)	2.297(4)	N(9)-Cd(1)-O(8)	87.51(18)
Cd(1)-O(2)	2.366(5)	O(7)-Cd(1)-O(8)	55.14(15)
Cd(1)-O(1)	2.391(5)	O(2)-Cd(1)-O(8)	115.98(18)
Cd(1)-O(8)	2.424(5)	O(1)-Cd(1)-O(8)	94.92(18)
Cd(2)-O(5)#1	2.200(5)	O(5)#1-Cd(2)-N(4)#2	108.55(19)

Cd(2)-N(4)#2	2.246(5)	O(5)#1-Cd(2)-N(12)#3	95.1(2)
Cd(2)-N(12)#3	2.318(5)	N(4)#2-Cd(2)-N(12)#3	98.3(2)
Cd(2)-O(13)	2.363(5)	O(5)#1-Cd(2)-O(13)	146.97(18)
Cd(2)-O(12)	2.371(5)	N(4)#2-Cd(2)-O(13)	99.80(18)
Cd(3)-O(9)	2.199(5)	N(12)#3-Cd(2)-O(13)	97.3(2)
Cd(3)-O(11)	2.278(5)	O(5)#1-Cd(2)-O(12)	92.12(18)
Cd(3)-O(4)#4	2.284(5)	N(4)#2-Cd(2)-O(12)	147.30(19)
Cd(3)-N(5)	2.294(5)	N(12)#3-Cd(2)-O(12)	104.96(19)
Cd(3)-O(3)#4	2.404(5)	O(13)-Cd(2)-O(12)	55.10(16)
Cd(3)-O(10)	2.619(7)	O(9)-Cd(3)-O(11)	109.2(2)
O(3)-Cd(3)#4	2.404(5)	O(9)-Cd(3)-O(4)#4	142.1(2)
O(4)-Cd(3)#4	2.284(5)	O(11)-Cd(3)-O(4)#4	91.83(19)
O(5)-Cd(2)#5	2.200(5)	O(9)-Cd(3)-N(5)	100.8(2)
N(4)-Cd(2)#2	2.246(5)	O(11)-Cd(3)-N(5)	91.76(19)
N(12)-Cd(2)#3	2.318(5)	O(4)#4-Cd(3)-N(5)	110.00(19)
N(1)-Cd(1)-N(9)	97.92(19)	O(9)-Cd(3)-O(3)#4	103.7(2)
N(1)-Cd(1)-O(7)	96.46(17)	O(11)-Cd(3)-O(3)#4	145.73(18)
N(9)-Cd(1)-O(7)	107.88(19)	O(4)#4-Cd(3)-O(3)#4	55.24(16)
N(1)-Cd(1)-O(2)	91.7(2)	N(5)-Cd(3)-O(3)#4	91.4(2)
N(9)-Cd(1)-O(2)	96.86(18)	O(9)-Cd(3)-O(10)	51.3(2)
O(7)-Cd(1)-O(2)	152.54(18)	O(11)-Cd(3)-O(10)	90.0(3)
N(1)-Cd(1)-O(1)	94.27(19)	O(4)#4-Cd(3)-O(10)	99.3(2)
N(9)-Cd(1)-O(1)	149.95(19)	N(5)-Cd(3)-O(10)	150.6(2)
O(7)-Cd(1)-O(1)	97.84(17)	O(3)#4-Cd(3)-O(10)	103.4(3)

Symmetry codes: #1 = x, y-1, z; #2 = -x+1, -y, -z+1; #3 = -x, -y, -z+1; #4 = -x, -y, -z+2; #5 = x, y+1, z.

Compound **4**

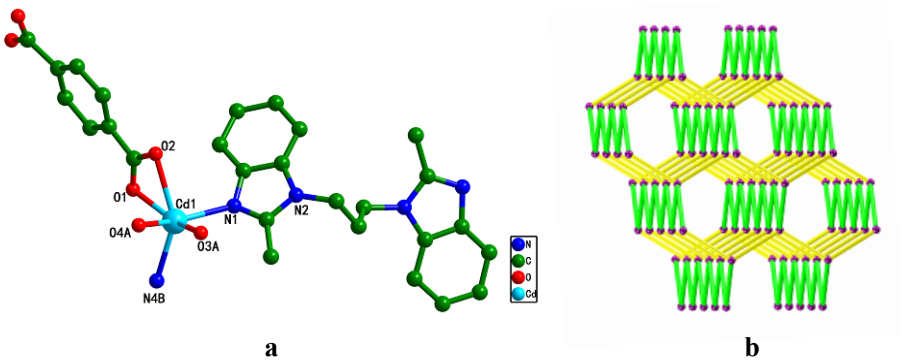
Zn(1)-O(5)#1	1.942(6)	O(5)#1-Zn(1)-O(7)#2	116.4(3)
Zn(1)-O(1)	1.944(5)	O(1)-Zn(1)-O(7)#2	105.2(2)
Zn(1)-O(7)#2	1.961(6)	O(5)#1-Zn(1)-N(1)	112.8(3)
Zn(1)-N(1)	2.010(7)	O(1)-Zn(1)-N(1)	116.6(3)
Zn(2)-O(1)	1.946(5)	O(7)#2-Zn(1)-N(1)	102.7(3)
Zn(2)-O(2)	1.964(5)	O(1)-Zn(2)-O(2)	108.6(2)
Zn(2)-O(6)#2	2.004(6)	O(1)-Zn(2)-O(6)#2	111.6(2)
Zn(2)-N(4)#1	2.008(6)	O(2)-Zn(2)-O(6)#2	111.9(2)
O(5)-Zn(1)#3	1.942(6)	O(1)-Zn(2)-N(4)#1	116.7(3)
O(6)-Zn(2)#2	2.004(6)	O(2)-Zn(2)-N(4)#1	109.2(2)
O(7)-Zn(1)#2	1.961(6)	O(6)#2-Zn(2)-N(4)#1	98.7(3)
N(4)-Zn(2)#3	2.008(6)	Zn(1)-O(1)-Zn(2)	112.9(3)
O(5)#1-Zn(1)-O(1)	103.4(2)		

Symmetry codes: #1 = -x+1, y+1/2, -z+1/2; #2 = -x+1, -y+2, -z; #3 = -x+1, y-1/2, -z+1/2.

Compound **5**

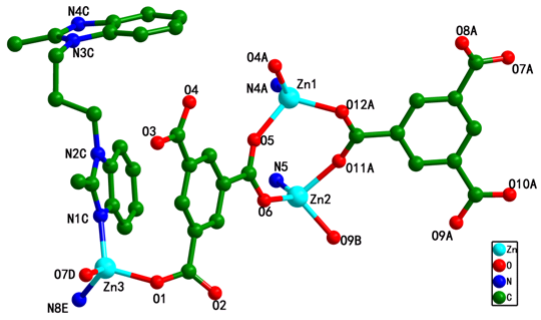
Cd(1)-N(4)#1	2.277(4)	N(4)#1-Cd(1)-N(1)	90.37(17)
Cd(1)-O(4)#2	2.290(4)	O(4)#2-Cd(1)-N(1)	97.36(15)
Cd(1)-O(1)	2.306(4)	O(1)-Cd(1)-N(1)	102.85(16)

Cd(1)-N(1)	2.321(4)	N(4)#1-Cd(1)-O(2)	100.73(15)
Cd(1)-O(2)	2.429(4)	O(4)#2-Cd(1)-O(2)	141.17(14)
Cd(1)-O(3)#2	2.557(4)	O(1)-Cd(1)-O(2)	55.00(13)
O(3)-Cd(1)#2	2.557(4)	N(1)-Cd(1)-O(2)	99.33(15)
O(4)-Cd(1)#2	2.290(4)	N(4)#1-Cd(1)-O(3)#2	88.32(15)
N(4)-Cd(1)#1	2.277(4)	O(4)#2-Cd(1)-O(3)#2	53.90(13)
N(4)#1-Cd(1)-O(4)#2	113.99(15)	O(1)-Cd(1)-O(3)#2	92.43(14)
N(4)#1-Cd(1)-O(1)	153.61(17)	N(1)-Cd(1)-O(3)#2	147.03(15)
O(4)#2-Cd(1)-O(1)	87.19(14)	O(2)-Cd(1)-O(3)#2	113.28(14)
Symmetry codes: #1 = -x, -y+1, -z+1; #2 = -x, -y, -z; #3 = -x+1, -y, -z.			
Compound **6**			
Cd(1)-O(2)	2.268(3)	O(2)-Cd(1)-O(6)#2	137.30(11)
Cd(1)-N(1)#1	2.268(3)	N(1)#1-Cd(1)-O(6)#2	95.34(11)
Cd(1)-N(4)	2.291(3)	N(4)-Cd(1)-O(6)#2	103.49(11)
Cd(1)-O(6)#2	2.293(3)	O(2)-Cd(1)-O(1)	55.05(10)
Cd(1)-O(1)	2.486(3)	N(1)#1-Cd(1)-O(1)	93.84(11)
Cd(1)-O(5)#2	2.505(3)	N(4)-Cd(1)-O(1)	153.20(10)
O(5)-Cd(1)#3	2.506(3)	O(6)#2-Cd(1)-O(1)	99.15(11)
O(6)-Cd(1)#3	2.293(3)	O(2)-Cd(1)-O(5)#2	91.46(10)
N(1)-Cd(1)#1	2.268(3)	N(1)#1-Cd(1)-O(5)#2	149.16(10)
O(2)-Cd(1)-N(1)#1	117.55(10)	N(4)-Cd(1)-O(5)#2	87.05(11)
O(2)-Cd(1)-N(4)	98.22(10)	O(6)#2-Cd(1)-O(5)#2	54.05(10)
N(1)#1-Cd(1)-N(4)	98.10(10)	O(1)-Cd(1)-O(5)#2	94.88(12)
Symmetry codes: #1 = -x+1, -y+2, -z+1; #2 = -x+2, y+1/2, -z+1/2; #3 = -x+2, y-1/2, -z+1/2.			



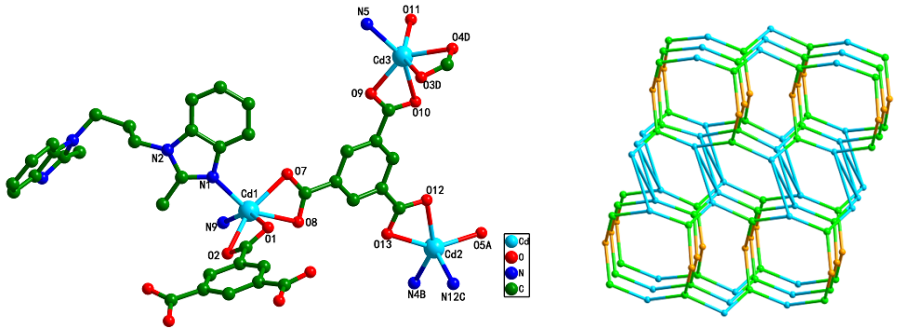
a **b**

Figure S1. (a) Coordination environment of Cd(II) ion in **1** with hydrogen atoms omitted for clarity. Symmetry operator: A = 0.5+x, 1.5−y, -0.5+z ; B = 0.5+x, 0.5−y, 0.5+z; (b) Schematic illustrating the 3D topology in complex **1**. Color code: purple ball, Cd atom; green stick, *p*-bdc^{2-}linker; yellow stick, pbmb linker.



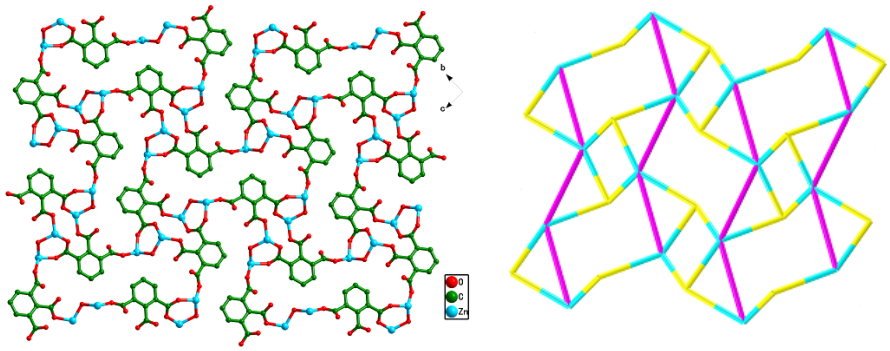
a

Figure S2. (a) Coordination environment of Zn(II) ion in **2.** Hydrogen atoms and the free water molecule are omitted for clarity. Symmetry operator: A = 1-x, 2−y, -z ; B = x, y, 1+z; C=1+x, y, z; D=1-x, 1-y, -z; E=2-x, 1-y, 1-z.



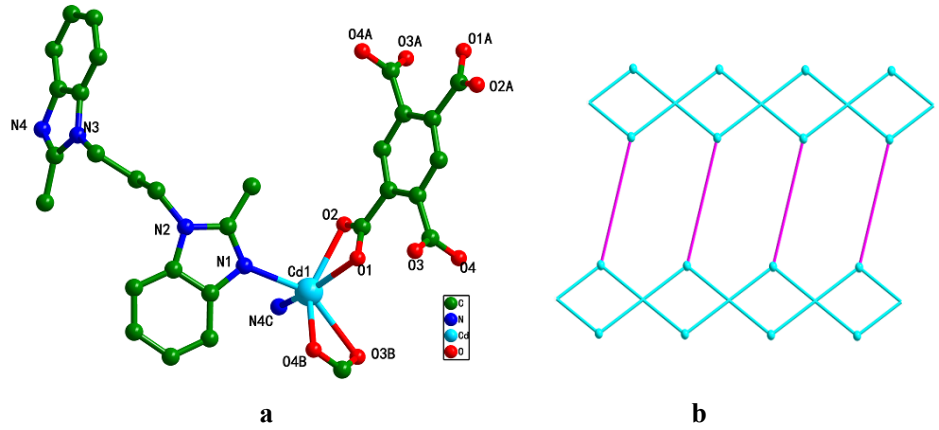
a **b**

Figure S3. (a) Coordination environment of Cd(II) ion in **3.** Hydrogen atoms and the free water molecule are omitted for clarity. Symmetry operator: A = x, -1+y, z ; B = 1-x, -y, 1-z; C=-x, -y, 1-z; D=-x, -y, 2-z; (b) Schematic illustrating the (2, 3, 4)-connected topology with the topological notation of $(6^5.8)_2(6^3)_2$. Color code: light blue ball, Cd1 or Cd2 atom; orange ball, Cd3 atom; green ball, 3-connected node.



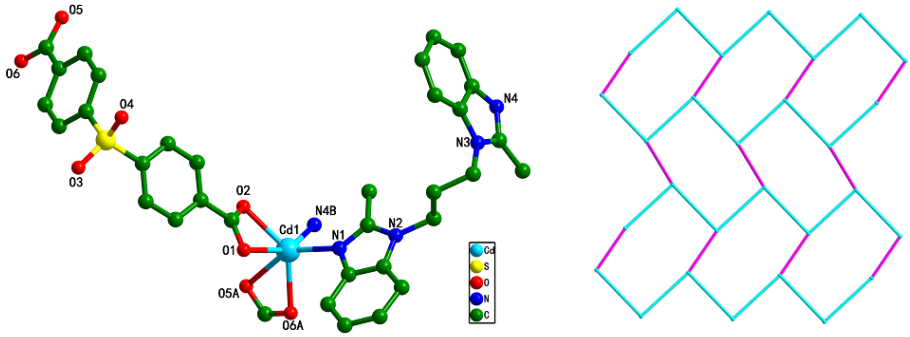
a **b**

Figure S4. (a) 2D layer of **4** formed by Zn and 1,2,3-btc^{3-}; (b) Schematic illustrating the (3,5)-connected topology with the topological notation of $(3.6^2)(3.6.7)(3.4.5)(3^2.4.5.6^2.7^4)$. Color code: yellow ball, 3-connected node; light blue ball, 5-connected node; pink stick, pbmb linker.



a b

Figure S5. (a) Coordination environment of Cd(II) ion in **5.** Hydrogen atoms are omitted for clarity. Symmetry operator: A = 1-x, −y, -z ; B = -x, -y, -z; (b) Schematic illustrating the (3,4)-connected topology with the topological notation of $(4.6^2)(4^2.6^2.8^2)$. Color code: pink stick, pbmb linker; light blue stick, $btec^{4-}$ linker.



a b

Figure S6. (a) Coordination environment of Cd(II) ion in **6.** Hydrogen atoms and the free water molecule are omitted for clarity. Symmetry operator: A=-0.5-x, 0.5+y, 1.5-z; B=1-x, 1-y, 2-z; (b) Schematic illustrating the topology with the topological notation of 6^3. Color code: pink stick, pbmb linker; light blue stick, $sdba^{2-}$ linker.

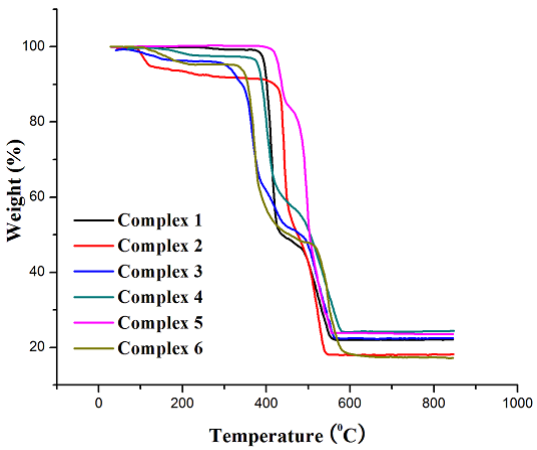
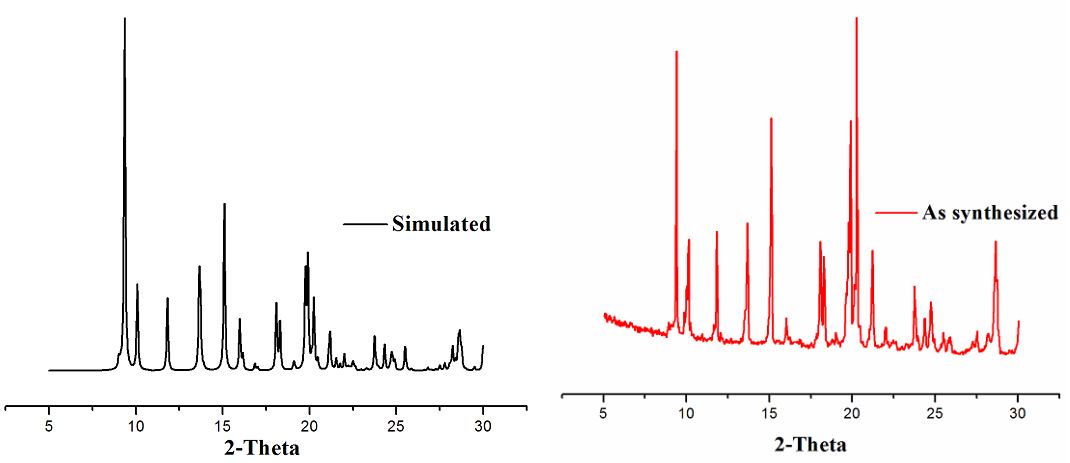
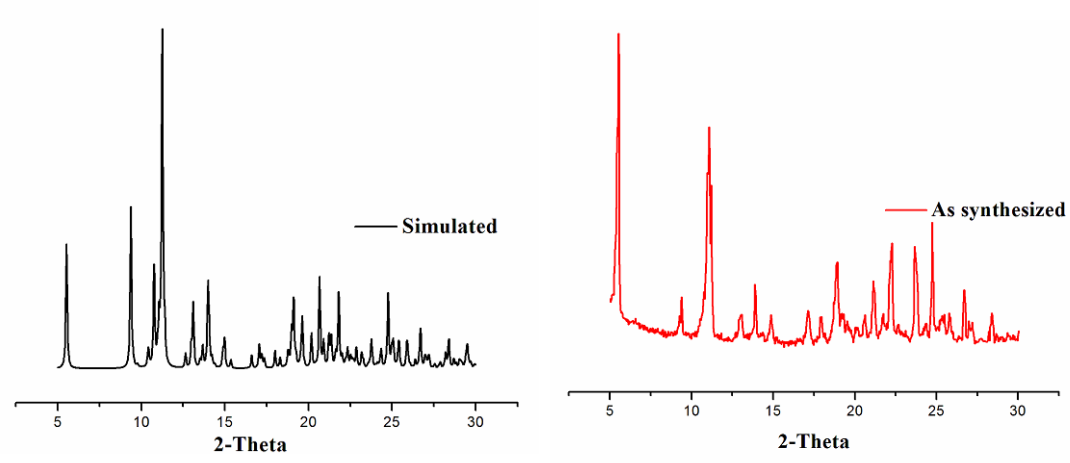


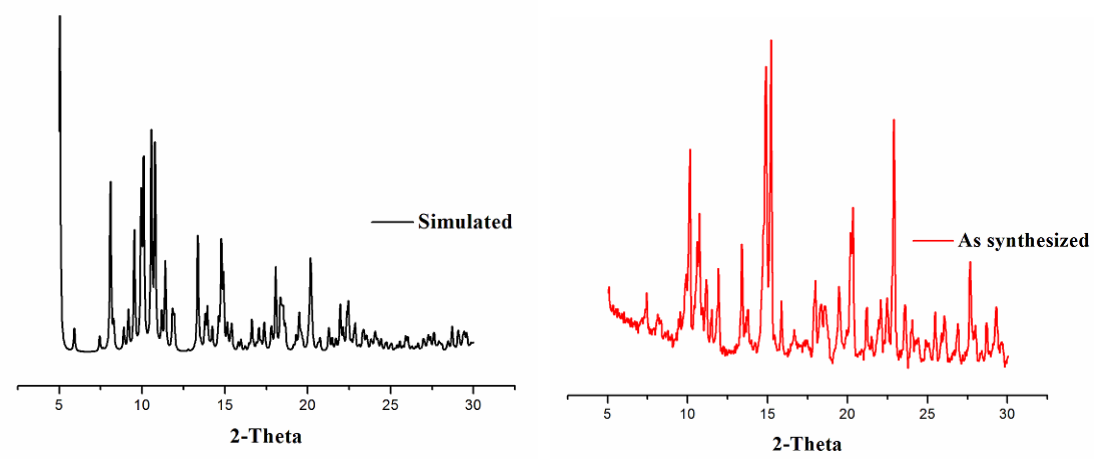
Figure S7. TGA curves of complexes **1-6**.



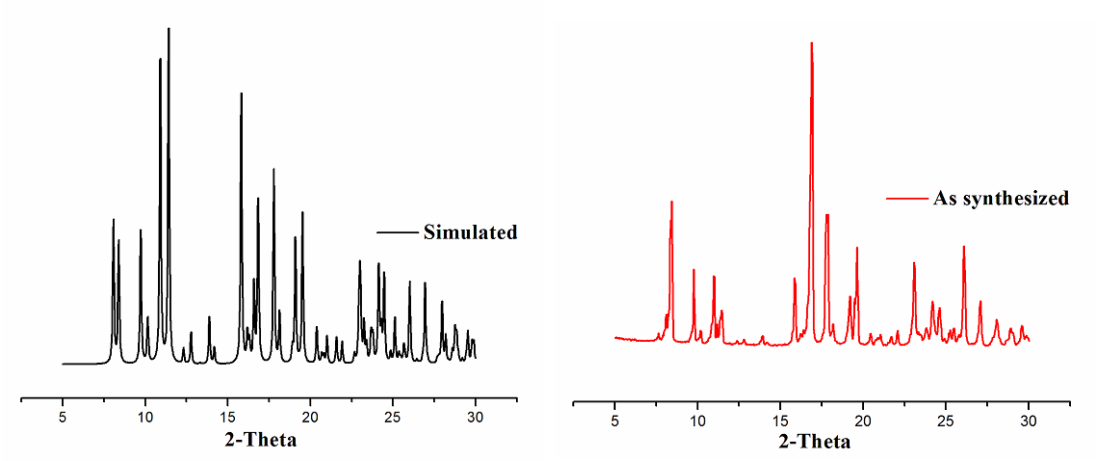
Complex 1



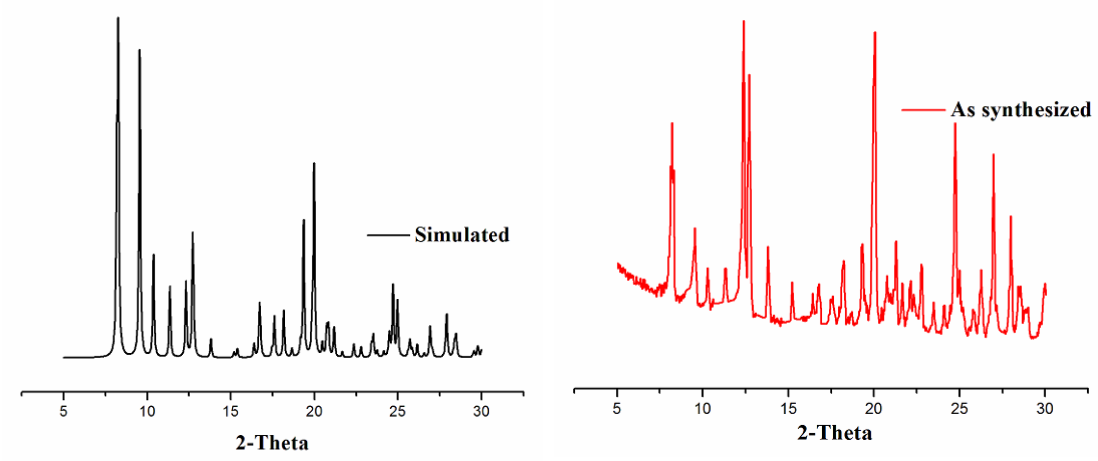
Complex 2



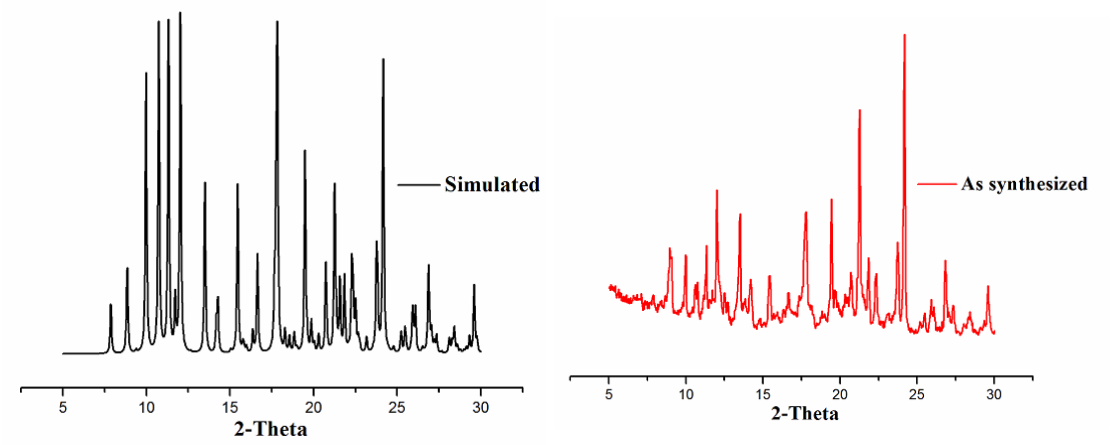
Complex 3



Complex 4



Complex 5



Complex 6

Figure S8. The simulated (black) and experimental (red) PXRD patterns for compounds **1-6**.

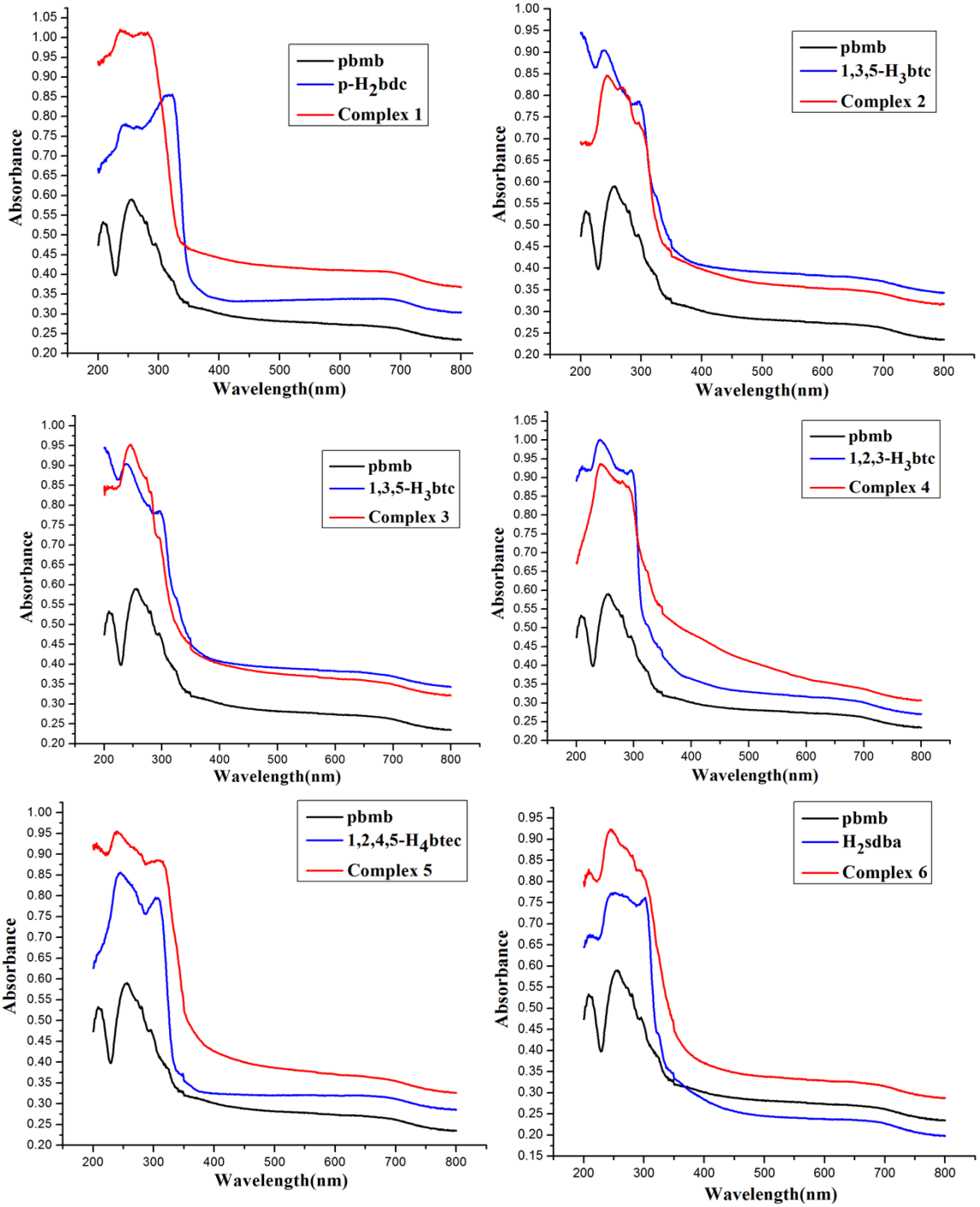


Figure S9. The diffuse-reflectance UV-vis spectra for compounds **1**−**6** and the relative ligands

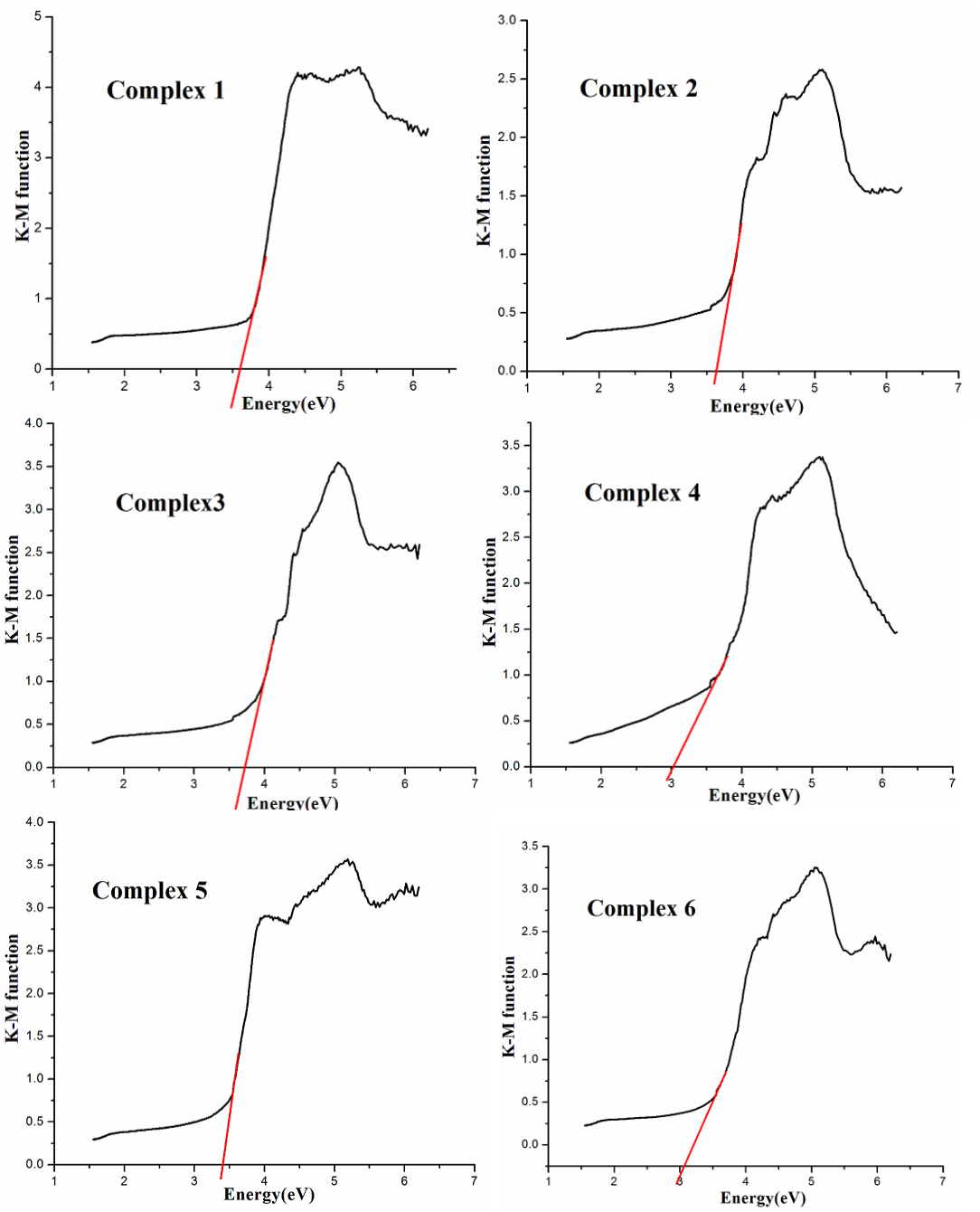


Figure S10. Kubelka-Munk-transformed diffuse reflectance of complexes **1-6**.

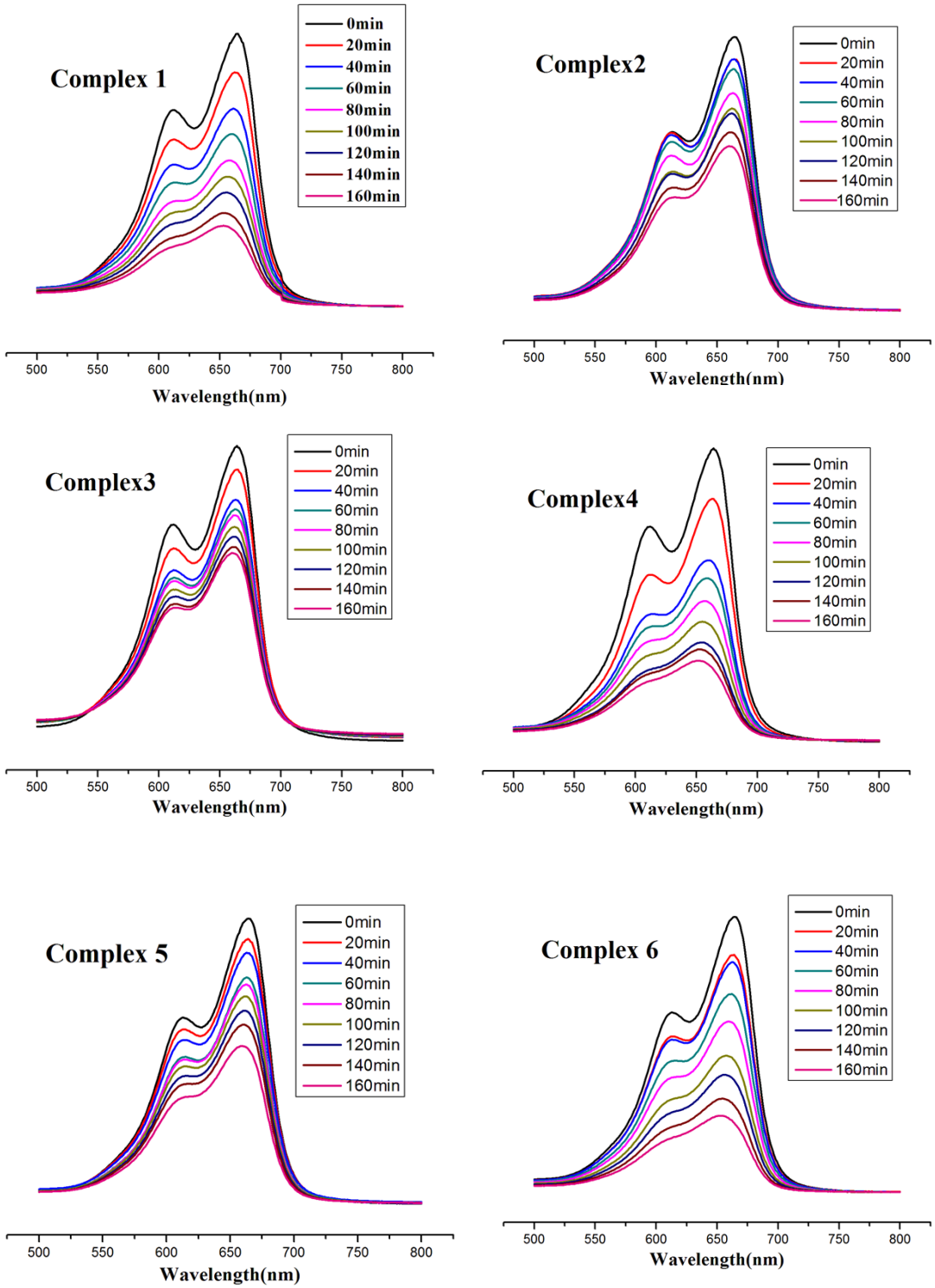


Figure S11. Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation with the use of complexes **1**−**6**.