Table S1. Selected bond lengths (Å) and angles (°) for **1**

N(1)-Mn(1)	2.201(4)	N(18)-Mn(1)	2.287(3)
N(19)-Mn(1)	2.279(3)	N(20)-Mn(1)	2.268(4)
O(2)-Mn(1)	2.157(4)	N(17)-Mn(1)	2.259(3)
N(6)-Mn(2)	2.229(4)	N(21)-Mn(2)	2.242(3)
N(22)-Mn(2)	2.249(4)	N(24)-Mn(2)	2.250(3)
O(1)-Mn(2)	2.212(3)	N(23)-Mn(2)	2.236(3)
N(1)-Mn(1)-N(18)	99.30(13)	N(17)-Mn(1)-N(18)	72.30(13)
N(1)-Mn(1)-N(19)	91.08(13)	N(17)-Mn(1)-N(19)	96.78(13)
N(1)-Mn(1)-N(20)	91.74(14)	N(17)-Mn(1)-N(20)	86.67(13)
N(1)-Mn(1)-O(2)	95.38(14)	N(17)-Mn(1)-O(2)	89.01(13)
N(1)-Mn(1)-N(17)	171.04(15)	N(19)-Mn(1)-N(20)	71.74(13)
N(18)-Mn(1)-N(19)	166.61(13)	N(19)-Mn(1)-O(2)	89.44(12)
N(18)-Mn(1)-N(20)	99.33(13)	N(20)-Mn(1)-O(2)	160.01(13)
N(18)-Mn(1)-O(2)	97.92(12)	N(6)-Mn(2)-N(21)	90.89(12)
N(23)-Mn(2)-N(21)	95.64(13)	N(6)-Mn(2)-N(22)	90.66(14)
N(23)-Mn(2)-N(22)	89.48(13)	N(6)-Mn(2)-N(24)	100.11(13)
N(23)-Mn(2)-N(24)	73.14(13)	N(6)-Mn(2)-O(1)	90.72(13)
N(23)-Mn(2)-O(1)	90.08(12)	N(6)-Mn(2)-N(23)	173.21(13)
N(22)-Mn(2)-N(24)	96.71(13)	N(21)-Mn(2)-N(22)	72.94(13)
N(22)-Mn(2)-O(1)	171.94(14)	N(21)-Mn(2)-N(24)	165.08(13)
N(24)-Mn(2)-O(1)	90.87(13)	N(21)-Mn(2)-O(1)	99.10(14)

Table S2. Selected bond lengths (Å) and angles (°) for **2**

N(1)-Mn	2.302(3)	N(1)^{a}-Mn	2.302(3)
O(1)-Mn	2.145(3)	O(1)^{a}-Mn	2.145(3)
O(2)-Mn	2.175(3)	O(2)^{a}-Mn	2.175(3)
N(1)-Mn-O(1)	90.9(1)	N(1)^{a}-Mn-O(1)	89.1(1)
N(1)-Mn-O(1)^{a}	89.1(1)	N(1)^{a}-Mn-O(1)^{a}	90.9(1)
N(1)-Mn-O(2)	90.72(9)	N(1)^{a}-Mn-O(2)	89.28(9)
N(1)-Mn-O(2)^{a}	89.28(9)	N(1)^{a}-Mn-O(2)^{a}	90.72(9)
N(1)-Mn-N(1)^{a}	180.000(1)	O(1)^{a}-Mn-O(2)	90.23(11)
O(1)-Mn-O(1)^{a}	180.000(1)	O(1)^{a}-Mn-O(2)^{a}	89.77(11)
O(1)-Mn-O(2)	89.77(11)	O(2)-Mn-O(2)^{a}	180.000(1)
O(1)-Mn-O(2)^{a}	90.23(11)		

Symmetry code: ^{a}2-x, 1-y, 2-z

Table S3. Selected bond lengths (Å) and angles (°) for **3**

N(1)-Co	2.160(3)	N(1)^{a}-Co	2.160(3)

N(9)-Co	2.095(3)	N(9)^{a}-Co	2.095(3)
N(10)-Co	2.094(3)	N(10)^{a}-Co	2.094(3)
N(1)-Co(1)-N(9)	90.51(13)	N(1)^{a}-Co(1)-N(9)	90.62(14)
N(1)-Co(1)-N(10)	89.03(13)	N(1)^{a}-Co(1)-N(10)	89.89(13)
N(1)-Co(1)-N(9)^{a}	90.62(13)	N(1)^{a}-Co(1)-N(9)^{a}	90.51(13)
N(1)-Co(1)-N(10)^{a}	89.89(13)	N(1)^{a}-Co(1)-N(10)^{a}	89.03(13)
N(1)-Co(1)-N(1)^{a}	178.33(19)	N(10)-Co(1)-N(9)^{a}	177.88(14)
N(9)-Co(1)-N(10)	83.27(15)	N(10)-Co(1)-N(10)^{a}	98.8(2)
N(9)-Co(1)-N(9)^{a}	94.6(2)	N(9)^{a}-Co(1)-N(10)^{a}	83.27(15)
N(9)-Co(1)-N(10)^{a}	177.88(14)		

Symmetry code: ^{a}1-x, y, 1.5-z

Table S4. Selected bond lengths (Å) and angles (°) for **4**

N(1)-Cd(1)	2.475(2)	N(5)-Cd(1)	2.326(3)
N(6)-Cd(1)	2.301(3)	N(7)-Cd(1)	2.331(3)
N(8)-Cd(1)	2.309(3)	N(1)^{a}-Cd(1)	2.642(3)
N(1)-Cd(1)-N(5)	110.15(9)	N(1)^{a}-Cd(1)-N(5)	82.53(9)
N(1)-Cd(1)-N(6)	90.65(9)	N(1)^{a}-Cd(1)-N(6)	91.16(9)
N(1)-Cd(1)-N(7)	86.95(9)	N(1)^{a}-Cd(1)-N(7)	80.41(9)
N(1)-Cd(1)-N(8)	89.10(9)	N(1)^{a}-Cd(1)-N(8)	89.45(10)
N(1)-Cd(1)-N(1)^{a}	167.28(8)	N(6)-Cd(1)-N(7)	104.57(10)
N(5)-Cd(1)-N(6)	77.56(10)	N(6)-Cd(1)-N(8)	178.33(10)
N(5)-Cd(1)-N(7)	162.83(10)	N(7)-Cd(1)-N(8)	77.06(10)
N(5)-Cd(1)-N(8)	100.97(10)		

Symmetry code: ^{a}1-x,-0.5+y, 0.5-z

Table S5. Selected bond lengths (Å) and angles (°) for **5**

N(1)-Zn(1)	2.126(5)	N(2)-Zn(1)	2.107(5)
N(3)-Zn(1)	2.107(5)	N(4)-Zn(1)	2.130(5)
N(8)-Zn(1)	2.324(5)	N(5)^{a}-Zn(1)	2.622(5)
N(8)-Zn(1)-N(1)	90.97(18)	N(5)^{a}-Zn(1)-N(1)	95.237(191)
N(8)-Zn(1)-N(2)	95.81(18)	N(5)^{a}-Zn(1)-N(2)	83.950(186)
N(8)-Zn(1)-N(3)	96.89(19)	N(5)^{a}-Zn(1)-N(3)	83.614(190)
N(8)-Zn(1)-N(4)	88.39(9)	N(5)^{a}-Zn(1)-N(4)	85.458(190)
N(8)-Zn(1)-N(5)^{a}	173.680(176)	N(2)-Zn(1)-N(3)	167.2(2)
N(1)-Zn(1)-N(2)	81.7(2)	N(2)-Zn(1)-N(4)	99.59(19)
N(1)-Zn(1)-N(3)	96.4(2)	N(3)-Zn(1)-N(4)	82.5(2)
N(1)-Zn(1)-N(4)	178.60(19)		

Symmetry code: ^{a} 2-x, 0.5+y, 0.5-z

Table S6. Selected bond lengths (Å) and angles (°) for **6**

N(3)-Cu	2.5853(26)	N(3)^{a}-Cu	2.5853(26)
N(9)-Cu	1.998(2)	N(9)^{a}-Cu	1.998(2)
N(8)-Cu	2.0281(19)	N(8)^{a}-Cu	2.0281(19)
N(3)-Cu(1)-N(9)	87.35(9)	N(3)^{a}-Cu(1)-N(9)	92.65(9)
N(3)-Cu(1)-N(8)	92.713(80)	N(3)^{a}-Cu(1)-N(8)	87.287(80)
N(3)-Cu(1)-N(9)^{a}	92.65(9)	N(3)^{a}-Cu(1)-N(9)^{a}	87.35(9)
N(3)-Cu(1)-N(8)^{a}	87.287(80)	N(3)^{a}-Cu(1)-N(8)^{a}	92.713(80)
N(3)-Cu(1)-N(3)^{a}	180.000	N(8)-Cu(1)-N(9)^{a}	95.55(8)
N(9)-Cu(1)-N(8)	84.45(8)	N(8)-Cu(1)-N(8)^{a}	180.0(1)
N(9)-Cu(1)-N(9)^{a}	180.00(5)	N(9)^{a}-Cu(1)-N(8)^{a}	84.45(8)
N(9)-Cu(1)-N(8)^{a}	95.55(8)		

Symmetry code: ^{a} -x,-y,-z

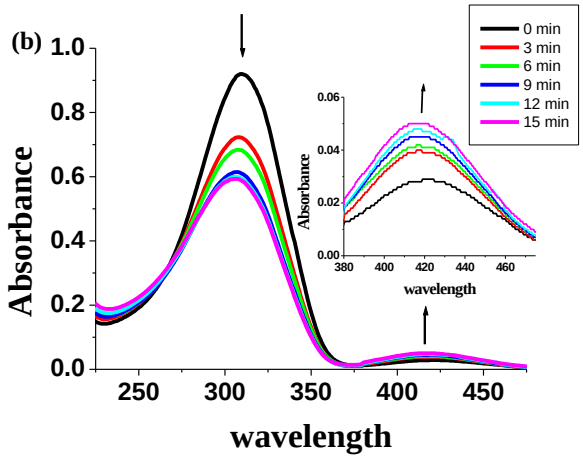
Table S7. Relevant H-Bonds in complex

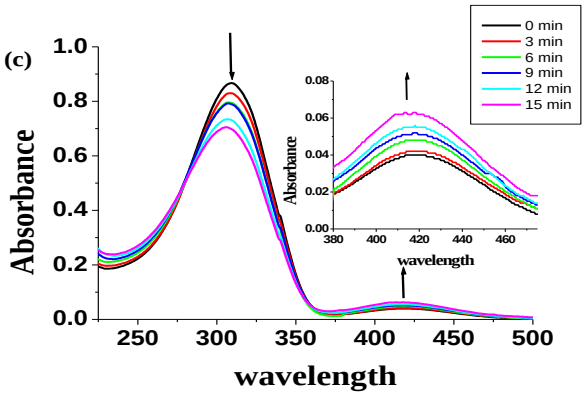
D-H…A	D-H [Å]	H…A [Å]	D…A [Å]	D-H…A[°]
Relevant H-Bonds in complex 1				
O2-H6…O3	0.80	1.937	2.7220(48)	169
C8a-H8a…O2b	0.93	1.823	2.7121(43)	159
Symmetry codes: a 0.5 + x, 0.5 - y,-0.5 + z. b 0.5 + x, 0.5 + y, z.				
Relevant H-Bonds in complex 2				
O1a-H3a…N3	0.86	2.264	2.8452(43)	125
O3a-H7a…N2	0.86	2.131	2.8466(39)	150
C1-H1…O3	0.93	1.995	2.8551(34)	162
Symmetry codes: a x, y, -1+z.				
Relevant H-Bonds in complex 5				
C8-H8…O2	0.93	1.976	2.9040(81)	174
O1-H20…O2e	0.80	2.027	2.8520(76)	173
Symmetry codes: a x, 1.5 - y, 0.5 + z.				

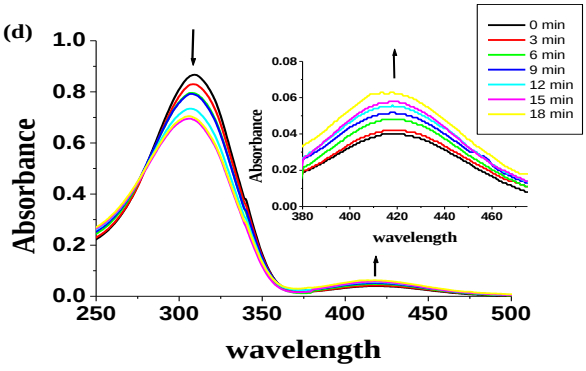
Table S8. The results of interaction energies calculation of **1**–**6**

compound	**1**	**2**	**3**	**4**	**5**	**6**
$E_{(AB)}$/u	-1086.68224991	-1182.53522111	-1182.54256798	-1182.56242568	-1182.35105496	-1182.53081402
$E_{(A,bAB)}$ /u	-591.465042458	-591.272268109	-591.276524220	-591.286178601	-591.180551884	-591.267197939
$E_{(B,bAB)}$ /u	-495.226431581	-591.272742304	-591.274983639	-591.282562596	-591.177513328	-591.266211344
$E_{(A)}$ /u	-591.461521953	-591.268871250	-591.278869794	-591.278869976	-591.156677105	-591.268871239
$E_{(B)}$ /u	-495.233070856	-591.268088953	-591.278087934	-591..27808839	-591.170665937	-591.268088779
$E_{(corrected)}$ /u	-1086.67736867	-1182.52117090	-1182.53001785	-1182.55444285	-1182.34333278	-1182.51586475
$E_{(BSSE)}$ /u	0.004881230205	0.014050209985	0.012550130569	0.007982831861	0.007722180401	0.014949265210

E(interaction energy) = $E_{(corrected)}$ - ($E_{(A)}$ + $E_{(B)}$) = $E_{(AB)}$ – ($E_{(A,bAB)}$ + $E_{(B,bAB)}$







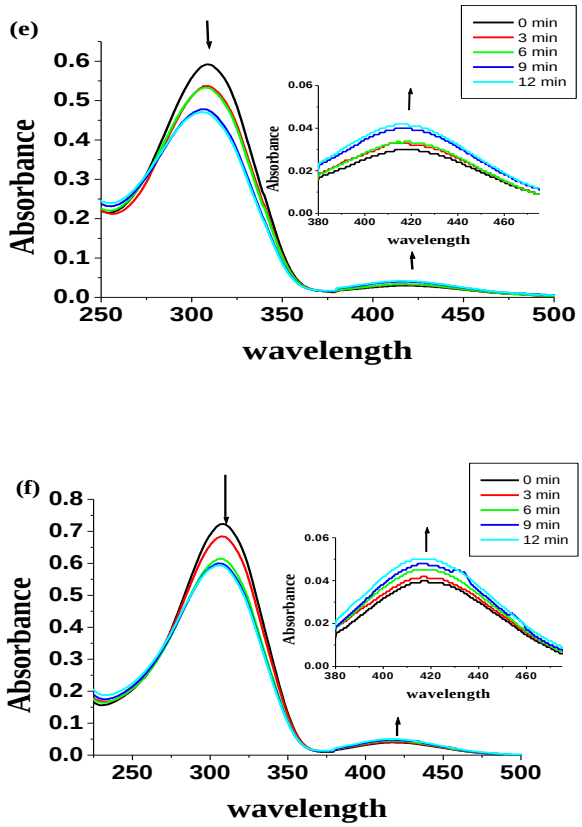
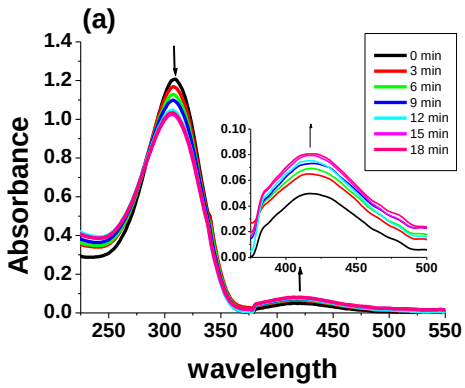


Figure S1. (b)–(e) UV-vis spectral change of **2–6** in aqueous solution with the concentration of 6.0×10^{-5} mol·L^{-1} upon repeated irradiation at 310 nm at 3 min interval at room temperature.



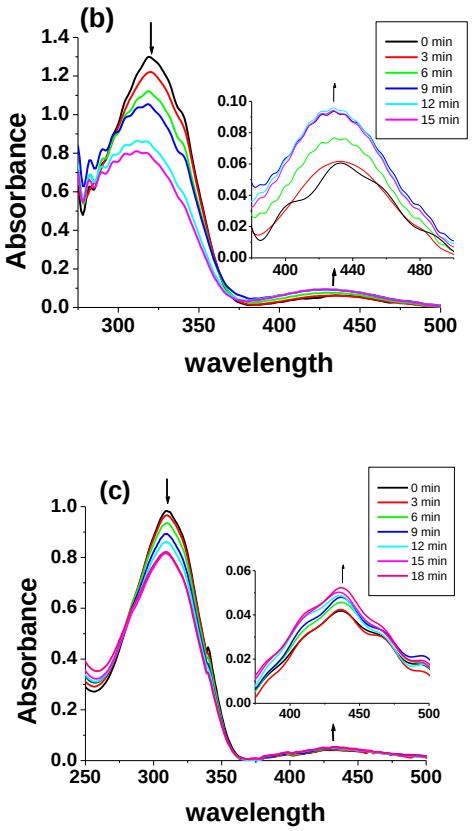
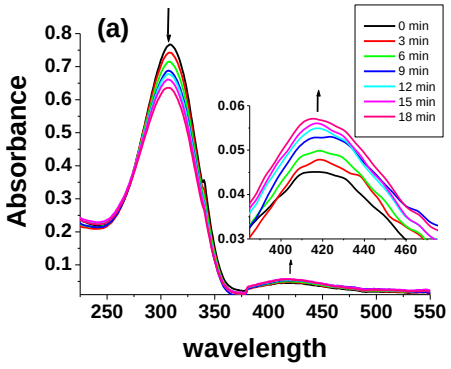


Figure S2. (a)–(c) UV-vis spectral changes in solution of water, DMF and ethanol with the concentration of 1×10^{-4} mol·L^{-1} upon repeated irradiation at 310 nm at 3 min interval at room temperature, respectively.



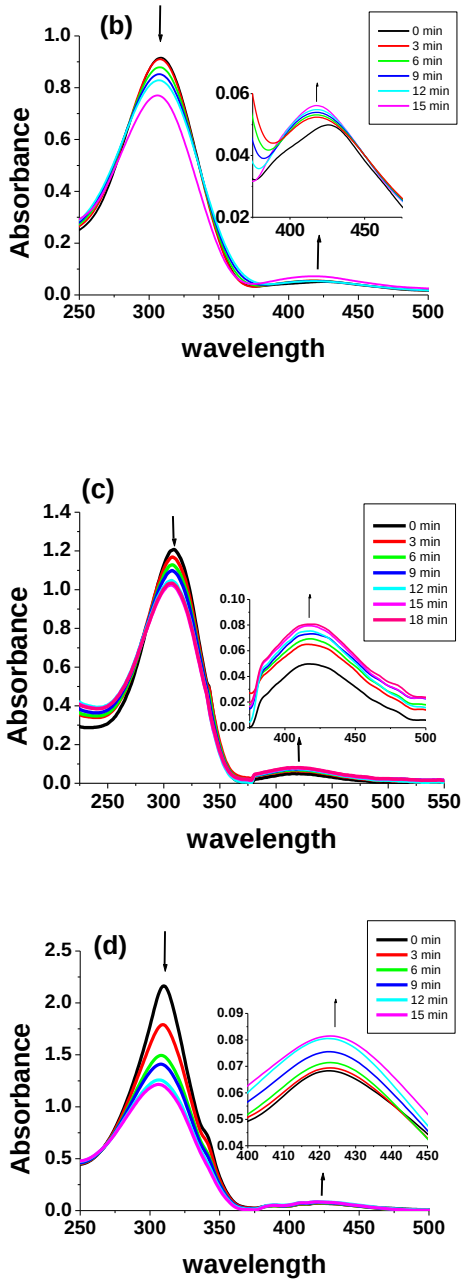


Figure S3. (a)–(d) UV-vis spectral changes in aqueous solution with the concentration of 2×10^{-5}, 5×10^{-5}, 1×10^{-4}, 5×10^{-4} mol·L^{-1} upon repeated irradiation at 310 nm at 3 min interval at room temperature, respectively.