Supporting Information

A series of temperature-dependent Cd^{II}-complexes containing an important family of N-rich heterocycles from in situ conversion of pyridine-type Schiff base

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Content

Table S**1** Crystal data and structure refinement of three compounds **1**-**3**.

	1	**2**	**3**
Chemical formula	$C_{72}H_{70}Cd_7Cl_{14}N_{18}O_2$	$C_{50}H_{42}Cd_2Cl_2N_{12}O_4$	$C_{48}H_{32}Cd_2Cl_4N_{12}$
M	2502.56	1170.66	1143.46
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	*P*2(1)/*c*	*P*-1	*P*-1
a /Å	19.5538(15)	9.5160(8)	9.471(5)
b /Å	16.2417(12)	10.9133(9)	10.437(6)
c /Å	27.985(2)	12.1129(10)	13.576(8)
α/°	90	94.787(2)	72.174(7)
β/°	94.8630(10)	90.019(2)	78.698(7)
γ/°	90	108.440(2)	81.504(7)
V/Å^3	8855.7(11)	1188.71(17)	1247.3(12)
Z	4	1	1
T /*K*	298(2)	298(2)	298(2)
F(000)	4872	588	568
D_{calcd} / gcm^{-3}	1.877	1.635	1.522
μ /mm^{-1}	2.125	1.067	1.113
λ /Å	0.71073	0.71073	0.71073
R_{int}	0.0706	0.0295	0.0471
data/restraint/parm	16034 / 7 / 982	4272 / 0 / 318	4422 / 0 / 299
GOF	1.016	1.080	1.037
R_1 [$I = 2\sigma(I)$]^a	0.0554	0.0552	0.0590
wR_2 [$I = 2\sigma(I)$]^b	0.1273	0.0853	0.0857
R_1 [all data]^a	0.1302	0.1253	0.1372
wR_2 [all data]^b	0.1642	0.1445	0.1724
Largest diff. peak and hole(e·Å^{-3})	0.915 and -1.160	0.508 and -0.503	1.208 and -1.000

0

(to be continued) Table S**1** Crystal data and structure refinement of three compounds **4-6**.

	4	**5**	**6**
Chemical formula	$C_{24}H_{18}Cd_2Cl_4N_6O$	$C_{74}H_{58}Cd_4Cl_4N_{20}O_3$	$C_{18}H_{14}CdCl_2N_4$
M	773.04	1866.80	469.63
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$C2/c$	$P2(1)/c$	$P2(1)/c$
a /Å	20.685(3)	12.900(4)	7.5806(12)
b /Å	12.3021(16)	13.916(4)	17.674(3)
c /Å	13.7360(18)	21.676(7)	13.270(2)
α/°	90	90	90
β/°	125.5010(10)	98.187(4)	90.756(2)
γ/°	90	90	90
V/Å^3	2845.6(6)	3852(2)	1777.8(5)
Z	4	2	4
T /K	298(2)	298(2)	298(2)
F(000)	1504	1852	928
D_{calcd} / gcm^{-3}	1.804	1.610	1.755
μ /mm^{-1}	1.899	1.288	1.537
λ /Å	0.71073	0.71073	0.71073
R_{int}	0.0245	0.0636	0.0478
data/restraint/parm	2584 / 1 / 171	6977 / 3 / 486	3194 / 0 / 226
GOF	1.081	1.018	1.014
R_1 [$I = 2\sigma(I)$]^a	0.0365	0.0518	0.0420
wR_2 [$I = 2\sigma(I)$]^b	0.0460	0.0927	0.0769
R_1 [all data]^a	0.1007	0.1177	0.0806
wR_2 [all data]^b	0.1082	0.1421	0.0965
Largest diff. peak and hole(e·Å^{-3})	1.015 and -0.597	0.680 and -0.667	0.469 and -0.426

(to be continued) Table S**1** Crystal data and structure refinement of three compounds **7**-**9**.

	7	**8**	**9**
Chemical formula	$C_{37}H_{31}Cd_2Cl_4N_8O$	$C_{36}H_{26}Cd_2Cl_4N_8$	$C_{18}H_{12}Cd_2Cl_3N_4O_2$
M	970.30	937.25	647.47
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$C2/c$	P-1	$P2(1)/c$
a /Å	24.137(4)	9.617(15)	11.7730(13)
b /Å	15.255(4)	9.698(16)	19.686(2)
c /Å	23.410(6)	10.175(16)	9.4109(10)
α/°	90	89.54(3)	90
β/°	114.065(5)	79.24(2)	107.0280(10)
γ/°	90	86.21(3)	90
V/Å^3	7870(3)	930(3)	2085.5(4)
Z	8	1	4
T /K	298(2)	298(2)	298(2)
F(000)	3848	462	1244
D_{calcd} / gcm^{-3}	1.638	1.673	2.062
μ /mm^{-1}	1.393	1.468	2.446
λ /Å	0.71073	0.71073	0.71073
R_{int}	0.0886	0.0522	0.0570
data/restraint/parm	7107/ 0 / 471	3295 / 0 / 227	3632 / 0 / 262
GOF	0.974	1.017	1.003
R_1 [$I = 2\sigma(I)$]^a	0.0544	0.0592	0.0475
wR_2 [$I = 2\sigma(I)$]^b	0.1484	0.0832	0.0955
R_1 [all data]^a	0.0996	0.1445	0.1013
wR_2 [all data]^b	0.1290	0.1590	0.1217
Largest diff. peak and hole(e·Å^{-3})	0.680 and -0.490	1.104 and -1.186	0.782 and -0.561

^{a} $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, ^{b} $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

(to be continued) Table S**1** Crystal data and structure refinement of two compounds **1′and 2′**

	1′	**2′**
Chemical formula	$C_{26}H_{30}Cd_2Cl_4N_6O_2$	$C_{14}H_{11}CdClN_4S$
M	825.16	415.18
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a /Å	7.3515(10)	8.41(2)
b /Å	9.4349(12)	9.44(2)
c /Å	12.6530(16)	10.76(3)
α/°	100.021(2)	68.21(3)
β/°	102.220(2)	67.16(3)
γ/°	112.091(2)	86.97(3)
V/Å^3	762.96(17)	727(3)
Z	1	2
T /K	298(2)	298(2)
F(000)	408	408
D_{calcd} / gcm^{-3}	1.796	1.897
μ /mm^{-1}	1.779	1.826
λ /Å	0.71073	0.71073
R_{int}	0.0186	0.0393
data/restraint/parm	2499 / 3 / 188	2478 / 0 / 192
GOF	1.070	1.089
R_1 [$I = 2\sigma(I)$]^a	0.0381	0.0656
wR_2 [$I = 2\sigma(I)$]^b	0.0467	0.1104
R_1 [all data]^a	0.0983	0.1774
wR_2 [all data]^b	0.1058	0.1253
Largest diff. peak and hole(e·Å^{-3})	0.799 and -0.838	1.262 and -1.091

^{a} $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, ^{b} $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where w = $1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table S**2**. Selected atomic distances (Å) and bond angles (°) for compounds **1-9**.

1			
N(17)-Cd(7)	2.334(3)	Cl(1)-Cd(2)-Cl(5)	88.84(10)
N(7)-Cd(3)	2.442(3)	Cl(6)-Cd(2)-Cl(5)	171.43(10)
N(18)-Cd(7)	2.310(4)	Cl(7)-Cd(2)-Cl(5)	84.14(4)
Cd(1)-N(6)#1	2.299(4)	Cl(2)-Cd(2)-Cl(5)	118.72(8)
Cd(1)-N(3)#1	2.304(4)	Cl(1)-Cd(2)-Cl(3)	95.10(4)
Cd(1)-N(1)#1	2.411(4)	Cl(6)-Cd(2)-Cl(3)	171.34(4)
Cd(1)-Cl(2)	2.5150(12)	Cl(7)-Cd(2)-Cl(3)	89.53(4)
Cd(1)-N(2)#1	2.547(3)	Cl(2)-Cd(2)-Cl(3)	83.18(4)
Cd(1)-Cl(1)	2.7049(12)	Cl(5)-Cd(2)-Cl(3)	93.67(4)
Cd(2)-Cl(1)	2.6202(12)	N(9)-Cd(3)-N(12)	89.23(4)
Cd(2)-Cl(6)	2.6298(12)	N(9)-Cd(3)-N(7)	96.57(4)
Cd(2)-Cl(7)	2.6380(12)	N(12)-Cd(3)-N(7)	83.40(4)
Cd(2)-Cl(2)	2.6527(13)	N(9)-Cd(3)-Cl(4)	91.22(4)
Cd(2)-Cl(5)	2.6582(12)	N(12)-Cd(3)-Cl(4)	177.04(4)
Cd(2)-Cl(3)	2.6994(13)	N(7)-Cd(3)-Cl(4)	89.60(4)
Cd(3)-N(9)	2.293(4)	N(9)-Cd(3)-N(8)	174.51(4)
Cd(3)-N(12)	2.356(4)	N(12)-Cd(3)-N(8)	86.17(4)
Cd(3)-Cl(4)	2.4530(18)	N(7)-Cd(3)-N(8)	89.68(4)
Cd(3)-N(8)	2.493(4)	Cl(4)-Cd(3)-N(8)	93.27(4)
Cd(3)-Cl(3)	2.6982(14)	N(9)-Cd(3)-Cl(3)	138.56(14)
Cd(4)-N(10)	2.311(4)	N(12)-Cd(3)-Cl(3)	94.91(13)
Cd(4)-Cl(8)	2.4441(14)	N(7)-Cd(3)-Cl(3)	78.89(12)
Cd(4)-Cl(9)	2.5612(13)	Cl(4)-Cd(3)-Cl(3)	107.33(11)
Cd(4)-Cl(7)	2.5738(13)	N(8)-Cd(3)-Cl(3)	113.76(11)
Cd(5)-N(4)	2.395(4)	N(10)-Cd(4)-Cl(8)	105.78(10)
Cd(5)-Cl(6)	2.5949(13)	N(10)-Cd(4)-Cl(9)	96.57(10)
Cd(5)-Cl(9)	2.5974(12)	Cl(8)-Cd(4)-Cl(9)	100.77(5)
Cd(5)-Cl(10)	2.6499(14)	N(10)-Cd(4)-Cl(7)	138.26(10)
Cd(5)-Cl(5)	2.6700(11)	Cl(8)-Cd(4)-Cl(7)	112.82(5)
Cd(6)-Cl(11)	2.4409(16)	Cl(9)-Cd(4)-Cl(7)	91.42(4)
Cd(6)-Cl(12)	2.4431(14)	N(4)-Cd(5)-Cl(6)	163.44(9)
Cd(6)-Cl(13)	2.4505(17)	N(4)-Cd(5)-Cl(9)	90.41(9)
Cd(6)-Cl(10)	2.5288(15)	Cl(6)-Cd(5)-Cl(9)	106.13(4)
Cd(7)-N(15)	2.341(5)	N(4)-Cd(5)-Cl(10)	89.80(9)
Cd(7)-N(13)	2.425(5)	Cl(6)-Cd(5)-Cl(10)	90.94(4)
Cd(7)-Cl(14)	2.4340(16)	Cl(9)-Cd(5)-Cl(10)	84.66(4)
Cd(7)-N(14)	2.629(7)	N(4)-Cd(5)-Cl(5)	96.67(9)
N(1)-Cd(1)#2	2.411(4)	Cl(6)-Cd(5)-Cl(5)	83.84(4)

N(2)-Cd(1)#2	2.547(3)	Cl(9)-Cd(5)-Cl(5)	91.83(4)
N(3)-Cd(1)#2	2.304(4)	Cl(10)-Cd(5)-Cl(5)	172.67(4)
N(6)-Cd(1)#2	2.299(4)	Cl(11)-Cd(6)-Cl(12)	111.73(5)
N(6)#1-Cd(1)-N(3)#1	92.07(10)	Cl(11)-Cd(6)-Cl(13)	115.66(6)
N(6)#1-Cd(1)-N(1)#1	69.47(13)	Cl(12)-Cd(6)-Cl(13)	114.73(6)
N(3)#1-Cd(1)-N(1)#1	69.78(13)	Cl(11)-Cd(6)-Cl(10)	113.54(5)
N(6)#1-Cd(1)-Cl(2)	71.27(12)	Cl(12)-Cd(6)-Cl(10)	100.13(5)
N(3)#1-Cd(1)-Cl(2)	162.32(10)	Cl(13)-Cd(6)-Cl(10)	99.35(6)
N(1)#1-Cd(1)-Cl(2)	87.45(10)	N(17)-Cd(7)-N(18)	83.30(11)
N(6)#1-Cd(1)-N(2)#1	95.02(10)	N(17)-Cd(7)-N(15)	104.51(14)
N(3)#1-Cd(1)-N(2)#1	173.06(8)	N(18)-Cd(7)-N(15)	146.78(15)
N(1)#1-Cd(1)-N(2)#1	93.46(6)	N(17)-Cd(7)-N(13)	149.82(13)
Cl(2)-Cd(1)-N(2)#1	103.62(10)	N(18)-Cd(7)-N(13)	80.78(14)
N(6)#1-Cd(1)-Cl(1)	137.39(13)	N(15)-Cd(7)-N(13)	76.82(16)
N(3)#1-Cd(1)-Cl(1)	88.85(13)	N(17)-Cd(7)-Cl(14)	98.88(9)
N(1)#1-Cd(1)-Cl(1)	97.08(14)	N(18)-Cd(7)-Cl(14)	109.22(11)
Cl(2)-Cd(1)-Cl(1)	121.22(10)	N(15)-Cd(7)-Cl(14)	101.50(12)
N(2)#1-Cd(1)-Cl(1)	101.14(10)	N(13)-Cd(7)-Cl(14)	110.51(11)
Cl(1)-Cd(2)-Cl(6)	88.64(9)	N(17)-Cd(7)-N(14)	89.1(2)
Cl(1)-Cd(2)-Cl(7)	71.79(12)	N(18)-Cd(7)-N(14)	73.45(14)
Cl(6)-Cd(2)-Cl(7)	71.15(12)	N(15)-Cd(7)-N(14)	74.43(14)
Cl(1)-Cd(2)-Cl(2)	69.28(12)	N(13)-Cd(7)-N(14)	61.8(2)
Cl(6)-Cd(2)-Cl(2)	154.88(8)	Cl(14)-Cd(7)-N(14)	171.77(18)
Cl(7)-Cd(2)-Cl(2)	90.97(9)		
2			
Cd(1)-N(2)	2.160(5)	N(2)-Cd(1)-Cl(1)	127.53(13)
Cd(1)-N(4)#1	2.255(5)	N(4)#1-Cd(1)-Cl(1)	98.56(14)
Cd(1)-N(3)	2.428(5)	N(3)-Cd(1)-Cl(1)	102.71(13)
Cd(1)-Cl(1)	2.4504(18)	N(2)-Cd(1)-N(1)	66.81(17)
Cd(1)-N(1)	2.572(5)	N(4)#1-Cd(1)-N(1)	92.00(18)
N(2)-Cd(1)-N(4)#1	131.11(18)	N(3)-Cd(1)-N(1)	137.05(18)
N(2)-Cd(1)-N(3)	70.35(18)	Cl(1)-Cd(1)-N(1)	100.68(13)
N(4)#1-Cd(1)-N(3)	119.14(18)		
3			
Cd(1)-N(2)	2.345(8)	N(3)-Cd(1)-Cl(2)	109.4(2)
Cd(1)-N(1)	2.365(7)	N(2)-Cd(1)-Cl(1)	93.7(2)
Cd(1)-N(3)	2.370(7)	N(1)-Cd(1)-Cl(1)	90.0(2)
Cd(1)-Cl(2)	2.470(3)	N(3)-Cd(1)-Cl(1)	98.1(2)
Cd(1)-Cl(1)	2.525(3)	Cl(2)-Cd(1)-Cl(1)	101.44(9)
Cd(1)-Cl(2)#1	2.863(3)	N(2)-Cd(1)-Cl(2)#1	81.24(19)

Cl(2)-Cd(1)#1	2.863(3)	N(1)-Cd(1)-Cl(2)#1	88.1(2)
N(2)-Cd(1)-N(1)	68.8(2)	N(3)-Cd(1)-Cl(2)#1	80.2(2)
N(2)-Cd(1)-N(3)	68.5(3)	Cl(2)-Cd(1)-Cl(2)#1	83.60(9)
N(1)-Cd(1)-N(3)	136.9(3)	Cl(1)-Cd(1)-Cl(2)#1	174.96(8)
N(2)-Cd(1)-Cl(2)	164.8(2)	Cd(1)-Cl(2)-Cd(1)#1	96.40(9)
N(1)-Cd(1)-Cl(2)	110.22(19)		
4			
Cd(1)-N(3)	2.3424(18)	N(3)-Cd(1)-Cl(2)	113.69(5)
Cd(1)-N(1)	2.3679(19)	N(1)-Cd(1)-Cl(2)	106.79(5)
Cd(1)-N(2)	2.4268(13)	N(2)-Cd(1)-Cl(2)	146.23(6)
Cd(1)-Cl(2)	2.4298(8)	N(3)-Cd(1)-Cl(1)	96.12(6)
Cd(1)-Cl(1)	2.4996(10)	N(1)-Cd(1)-Cl(1)	91.64(6)
N(3)-Cd(1)-N(1)	135.57(5)	N(2)-Cd(1)-Cl(1)	110.03(5)
N(3)-Cd(1)-N(2)	68.48(6)	Cl(2)-Cd(1)-Cl(1)	103.32(3)
N(1)-Cd(1)-N(2)	67.77(6)		
5			
Cd(1)-N(7)	2.224(5)	N(1)-Cd(1)-N(9)	157.61(19)
Cd(1)-N(2)	2.328(5)	N(7)-Cd(1)-Cl(1)	122.56(15)
Cd(1)-N(1)	2.359(5)	N(2)-Cd(1)-Cl(1)	106.57(15)
Cd(1)-N(9)	2.418(5)	N(1)-Cd(1)-Cl(1)	98.53(14)
Cd(1)-Cl(1)	2.442(2)	N(9)-Cd(1)-Cl(1)	103.66(15)
Cd(2)-N(4)	2.208(5)	N(4)-Cd(2)-N(10)	131.28(19)
Cd(2)-N(10)	2.299(5)	N(4)-Cd(2)-N(6)	98.34(19)
Cd(2)-N(6)	2.363(5)	N(10)-Cd(2)-N(6)	82.94(19)
Cd(2)-N(5)	2.425(6)	N(4)-Cd(2)-N(5)	72.2(2)
Cd(2)-Cl(2)	2.440(2)	N(10)-Cd(2)-N(5)	86.5(2)
N(7)-Cd(1)-N(2)	130.05(19)	N(6)-Cd(2)-N(5)	155.2(2)
N(7)-Cd(1)-N(1)	98.15(18)	N(4)-Cd(2)-Cl(2)	122.63(15)
N(2)-Cd(1)-N(1)	81.88(18)	N(10)-Cd(2)-Cl(2)	105.10(14)
N(7)-Cd(1)-N(9)	72.40(18)	N(6)-Cd(2)-Cl(2)	98.11(14)
N(2)-Cd(1)-N(9)	88.87(18)	N(5)-Cd(2)-Cl(2)	106.30(16)
6			
Cd(1)-N(2)	2.240(5)	N(2)-Cd(1)-Cl(2)	98.16(13)
Cd(1)-N(1)	2.393(5)	N(1)-Cd(1)-Cl(2)	100.50(12)
Cd(1)-Cl(1)	2.4158(17)	Cl(1)-Cd(1)-Cl(2)	112.06(6)
Cd(1)-Cl(2)	2.4676(17)	N(2)-Cd(1)-N(4)	67.5(2)
Cd(1)-N(4)	2.477(5)	N(1)-Cd(1)-N(4)	134.20(17)
N(2)-Cd(1)-N(1)	79.6(2)	Cl(1)-Cd(1)-N(4)	92.43(15)

N(2)-Cd(1)-Cl(1)	148.92(13)	Cl(2)-Cd(1)-N(4)	114.57(12)
N(1)-Cd(1)-Cl(1)	101.03(15)		
7			
Cd(1)-N(2)	2.251(4)	Cl(1)-Cd(1)-Cl(2)	116.90(7)
Cd(1)-N(3)	2.417(4)	N(2)-Cd(1)-N(1)	67.76(17)
Cd(1)-Cl(1)	2.430(2)	N(3)-Cd(1)-N(1)	143.95(17)
Cd(1)-Cl(2)	2.437(2)	Cl(1)-Cd(1)-N(1)	102.09(13)
Cd(1)-N(1)	2.452(6)	Cl(2)-Cd(1)-N(1)	93.81(15)
Cd(2)-N(6)	2.270(4)	N(6)-Cd(2)-N(5)	77.64(16)
Cd(2)-N(5)	2.427(5)	N(6)-Cd(2)-Cl(4)	137.26(14)
Cd(2)-Cl(4)	2.431(2)	N(5)-Cd(2)-Cl(4)	99.33(14)
Cd(2)-N(7)	2.434(5)	N(6)-Cd(2)-N(7)	69.45(17)
Cd(2)-Cl(3)	2.461(2)	N(5)-Cd(2)-N(7)	142.32(15)
N(2)-Cd(1)-N(3)	81.32(16)	Cl(4)-Cd(2)-N(7)	92.86(15)
N(2)-Cd(1)-Cl(1)	102.66(12)	N(6)-Cd(2)-Cl(3)	108.20(14)
N(3)-Cd(1)-Cl(1)	102.40(13)	N(5)-Cd(2)-Cl(3)	99.97(13)
N(2)-Cd(1)-Cl(2)	139.32(13)	Cl(4)-Cd(2)-Cl(3)	114.23(6)
N(3)-Cd(1)-Cl(2)	98.22(13)	N(7)-Cd(2)-Cl(3)	107.21(15)
8			
Cd(1)-N(2)	2.319(5)	N(2)-Cd(1)-Cl(2)	142.06(18)
Cd(1)-N(1)	2.450(7)	N(1)-Cd(1)-Cl(2)	91.30(15)
Cd(1)-Cl(1)	2.480(4)	Cl(1)-Cd(1)-Cl(2)	112.33(8)
Cd(1)-Cl(2)	2.481(4)	N(2)-Cd(1)-N(3)	77.58(17)
Cd(1)-N(3)	2.529(6)	N(1)-Cd(1)-N(3)	135.22(19)
N(2)-Cd(1)-N(1)	69.81(18)	Cl(1)-Cd(1)-N(3)	107.52(18)
N(2)-Cd(1)-Cl(1)	105.10(17)	Cl(2)-Cd(1)-N(3)	96.38(12)
N(1)-Cd(1)-Cl(1)	110.0(2)		
9			
Cd(1)-N(2)	2.319(5)	N(2)-Cd(1)-Cl(2)	142.06(18)
Cd(1)-N(1)	2.450(7)	N(1)-Cd(1)-Cl(2)	91.30(15)
Cd(1)-Cl(1)	2.480(4)	Cl(1)-Cd(1)-Cl(2)	112.33(8)
Cd(1)-Cl(2)	2.481(4)	N(2)-Cd(1)-N(3)	77.58(17)
Cd(1)-N(3)	2.529(6)	N(1)-Cd(1)-N(3)	135.22(19)
N(2)-Cd(1)-N(1)	69.81(18)	Cl(1)-Cd(1)-N(3)	107.52(18)
N(2)-Cd(1)-Cl(1)	105.10(17)	Cl(2)-Cd(1)-N(3)	96.38(12)
N(1)-Cd(1)-Cl(1)	110.0(2)		

Table S**3** Distances (Å) and angles (°) of hydrogen bonds for compounds **1-8**.

D-H…A	Distance(D-H)	Distance(H···A)	Distance(D···A)	Angle(D-H···A)
		1		
N(11)-H(11)...Cl(7)	0.86	2.491(3)	3.339(4)	171.1(4)
N(5)-H(5)...Cl(10)	0.86	2.870(2)	3.705(3)	164.7(3)
N(16)-H(16A···Cl(11)#1	0.86	2.823(2)	3.329(9)	119.3(2)
		2		
C(1)-H(1)···Cl(1)#2	0.93	2.455(3)	3.741(3)	157.1(5)
C(13)-H(13)···Cl(1)#2	0.93	2.927(3)	3.624(3)	132.9(4)
C(11)-H(11)···O(1)#3	0.93	2.563(3)	3.749(3)	158.5(5)
C(22)-H(22)#4···Cl(1)	0.93	2.948(3)	3.675(3)	136.2(7)
		3		
C(22)-H(22)···Cl(1)#5	0.93	2.928(2)	3.723(3)	144.2(8)
		4		
C(4)-H(4)···Cl(1)#6	0.93	2.861(3)	3.548(3)	131.7(1)
C(2)-H(2)···Cl(2)#7	0.93	2.713(3)	3.635(3)	171.6(1)
		5		
C(31)-H(31)···Cl(1)#8	0.93	2.939(3)	3.486(3)	119.1(2)
C(10)-H(10)···Cl(2)#9	0.93	2.862(3)	3.777(3)	167.8(2)
C(36)-H(36)···Cl(2)#10	0.93	2.940(3)	3.528(3)	122.5(2)
		6		
C(12)-H(12)···Cl(1)#11	0.93	2.737(2)	3.580(3)	151.1(3)
C(15)-H(15)···Cl(1)#11	0.93	2.904(2)	3.774(3)	156.3(3)
$\pi^a \cdots \pi^a$		3.770(3)		
$\pi^a \cdots \pi^a$		3.608(3)		
$\pi^a \cdots \pi^b$		3.964(3)		
$\pi^a \cdots \pi^b$		3.802(3)		
$\pi^a \cdots \pi^b$		3.821(3)		
		7		
C(17)-H(17)···Cl(2)#12	0.93	2.934(3)	3.622(3)	131.9(3)
C(1)-H(1)···Cl(2)#14	0.93	2.921(3)	3.496(3)	121.3(3)
C(1)-H(1)···Cl(1)	0.93	2.931(3)	3.563(3)	126.4(2)
C(12)-H(12)···Cl(3)#13	0.93	2.877(3)	3.494(3)	125.0(3)
C(19)-H(19)···Cl(3)	0.93	2.877(3)	3.565(3)	131.7(3)
C(2)-H(2)···Cl(4)#15	0.93	2.922(3)	3.551(3)	126.3(3)
C(6)-H(6)···Cl(4)	0.93	2.707(3)	3.680(3)	172.7(2)
C(9)-H(9)···Cl(4)	0.93	2.872(3)	3.770(3)	162.7(2)

		8		
C(10)-H(10)···Cl(1)#16	0.93	2.865(3)	3.777(3)	167.3(5)
C(13)-H(13)···Cl(1)#16	0.93	2.886(3)	3.859(3)	171.6(3)
C(16)-H(16)···Cl(1)#17	0.93	2.871(3)	3.649(3)	141.9(5)
C(18)-H(18)···Cl(2)	0.93	2.849(3)	3.552(3)	133.3(4)

*Symmetry transformations used to generate equivalent atoms: **#1** -x+1,y+1/2,-z+1/2; **#2** 1-x,2-y,2-z; **#3** 1+x, 1+y,z; **#4** -x,2-y,1-z; **#5** x,-1+y,z; **#6** 0.5-x,-0.5+1,0.5-z; **#7** -x,-y,-z; **#8** 1-x,1-y,-z; **#9** 2-x,0.5+y,0.5-z; **#10** 1-x,0.5+y,0.5-z; **#11** 2-x,-y,1-z; **#12** –x, y,0.5-z; **#13** x,1-y,-0.5+z; **#14** –x,2-y,1-z; **#15** 0.5-x,0.5+y,1.5-z; **#16** –x,2-y,2-z; **#17** x,y,1+z; #18.

*Sign π^a represents the centroid of the pyridine ring, and π^b represents the centroid of the imidazole ring.

Figure S1

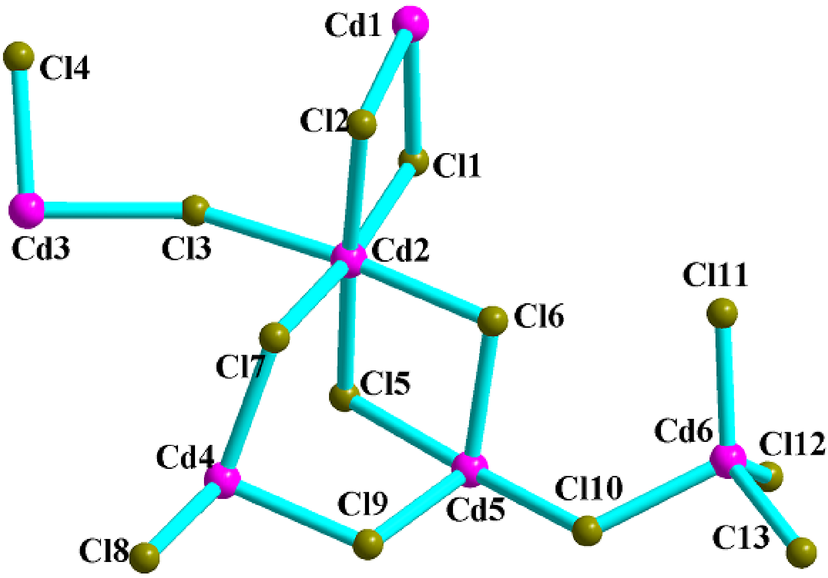


Figure S2

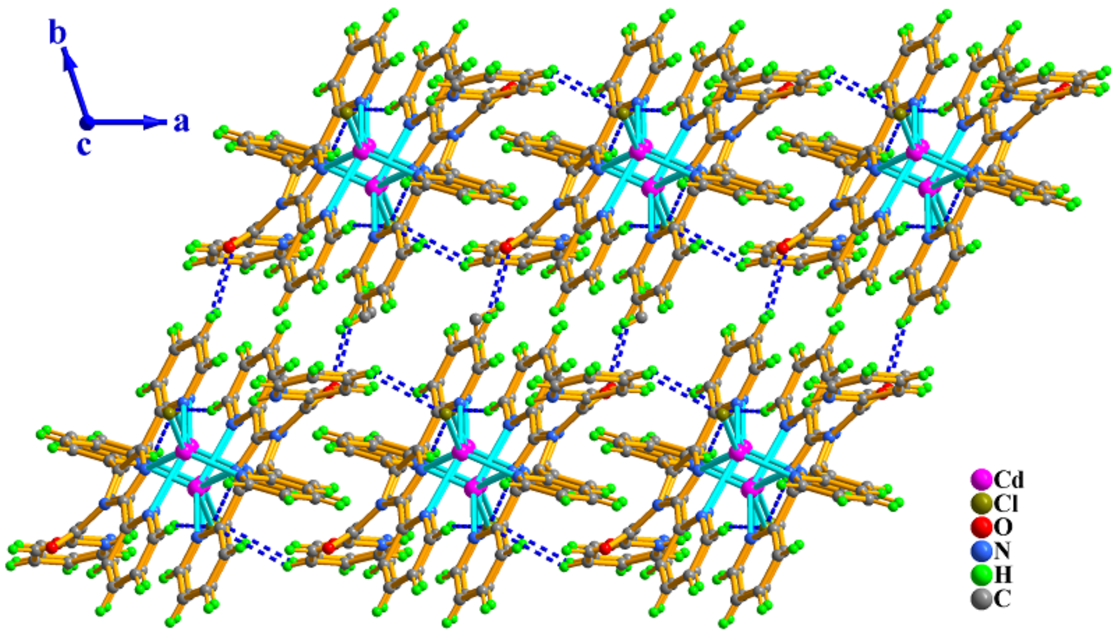


Figure S3

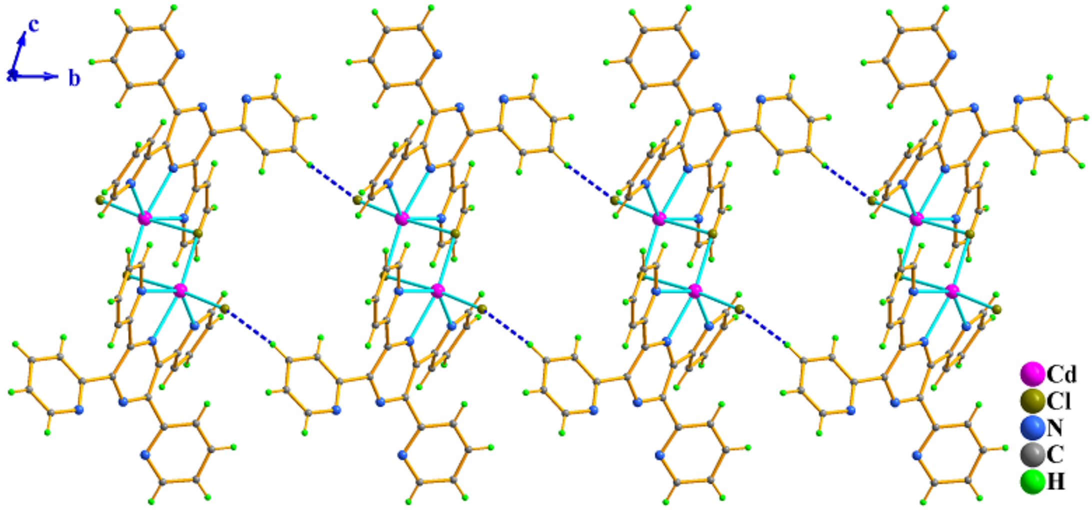


Figure S4

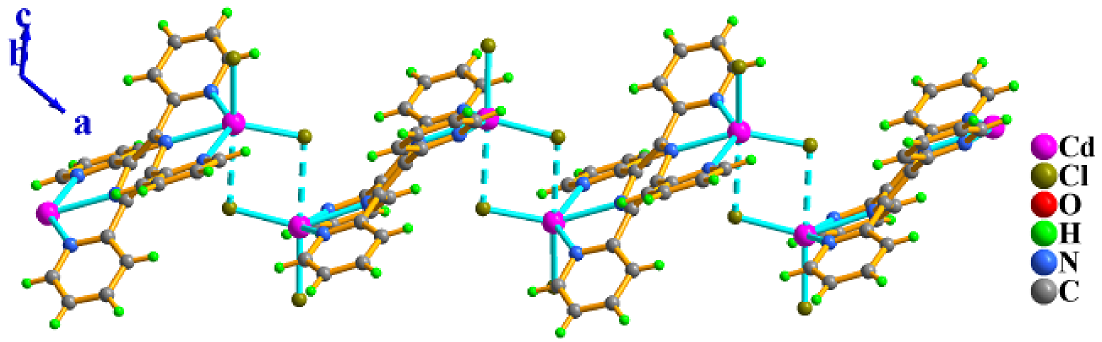
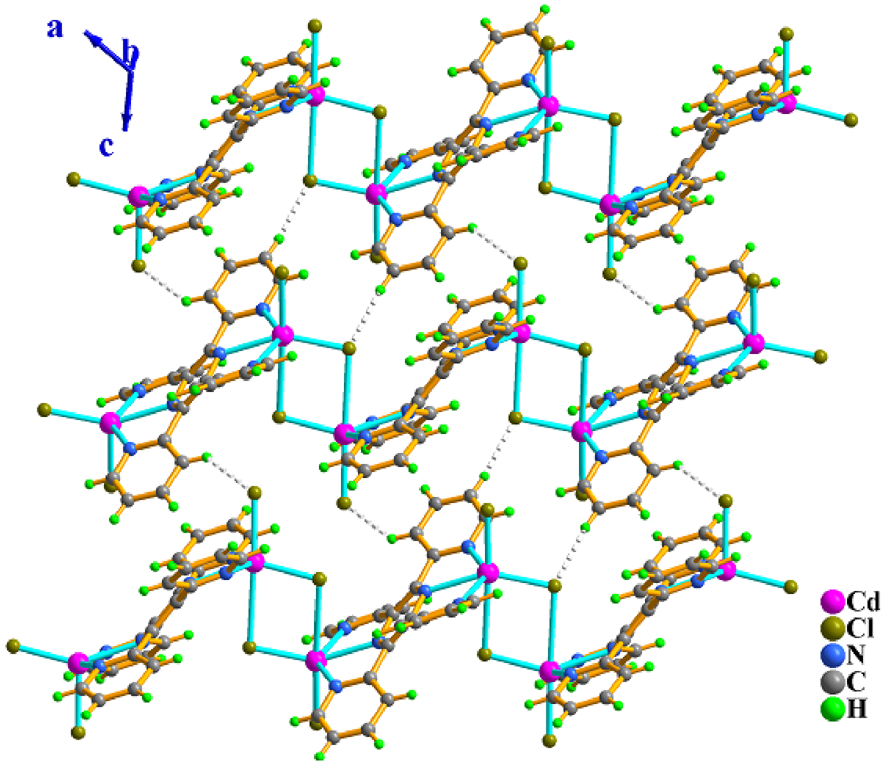


Figure S5



Scheme S1

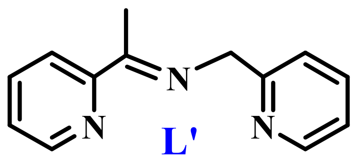


Figure S6

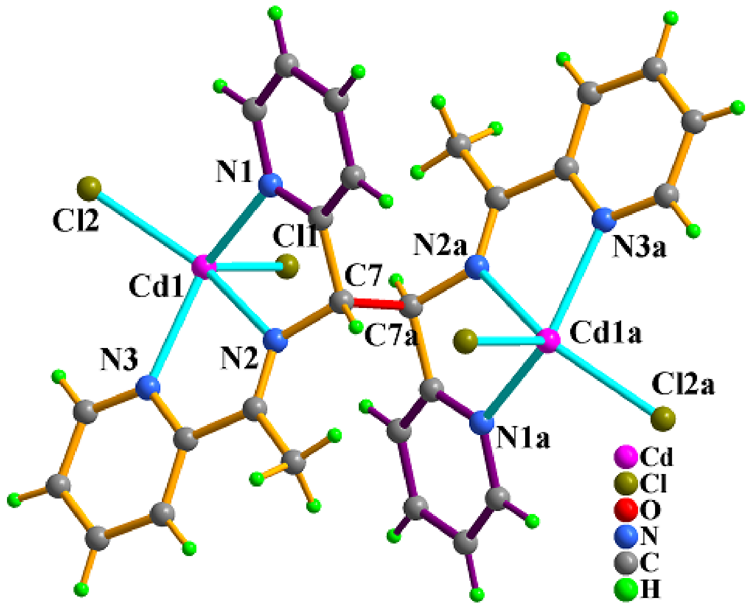


Figure S7

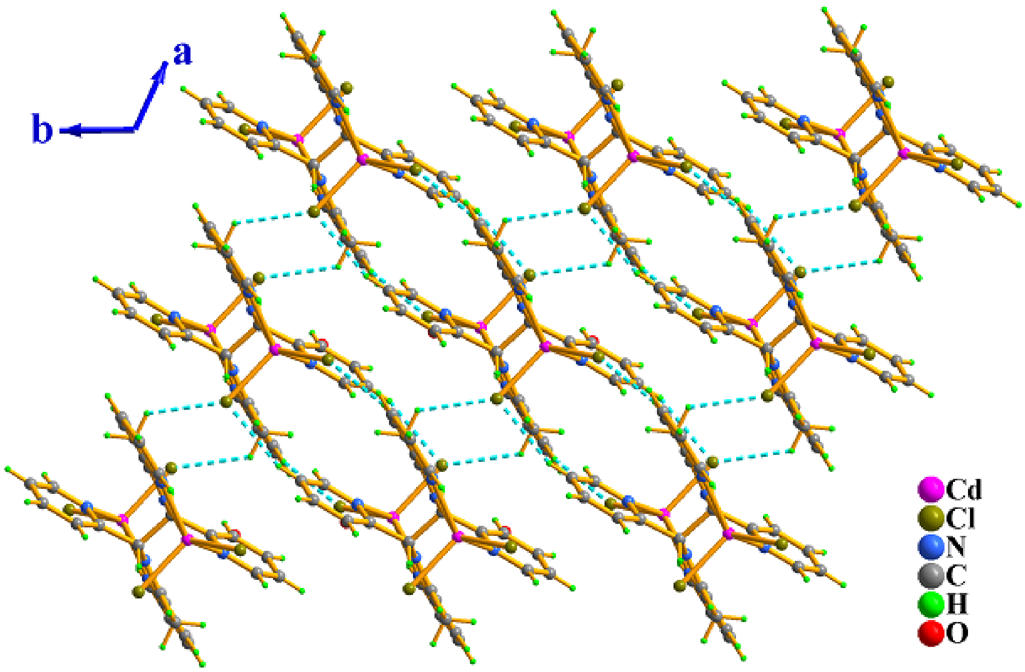


Figure S8

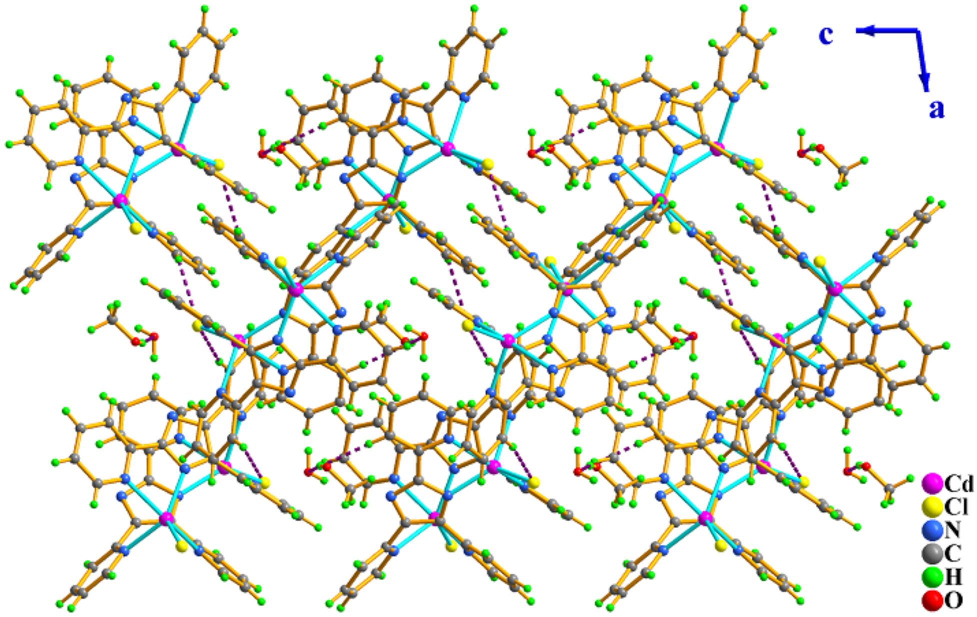


Figure S9

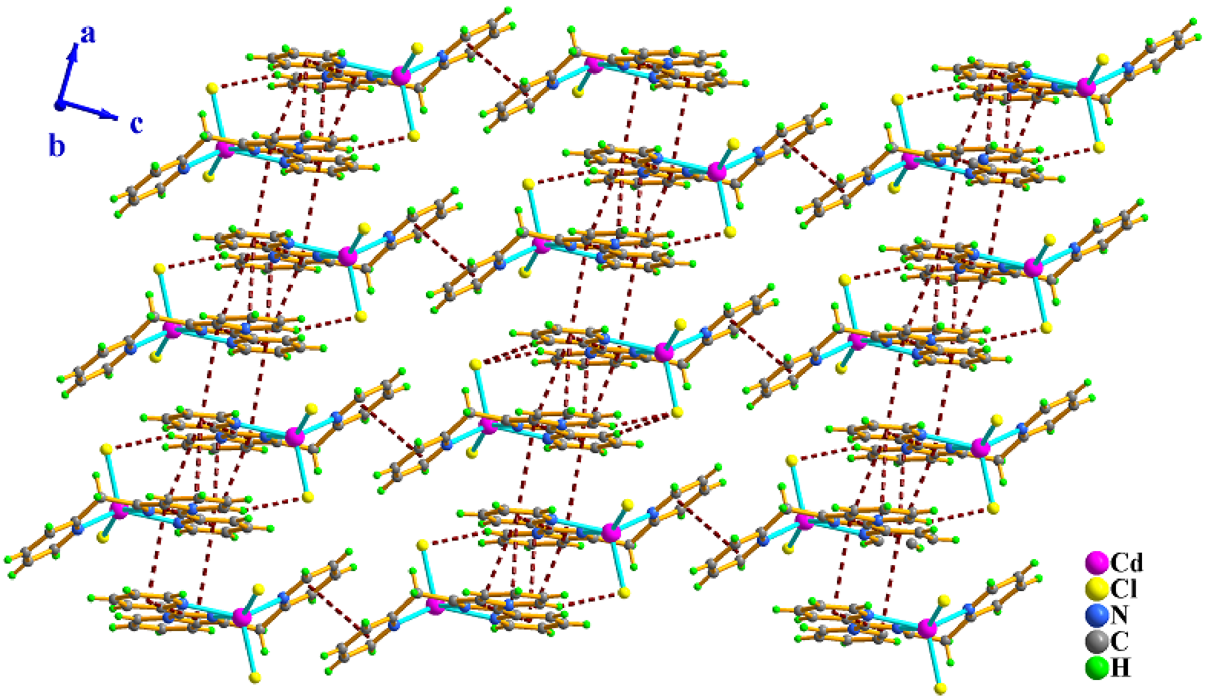


Figure S10

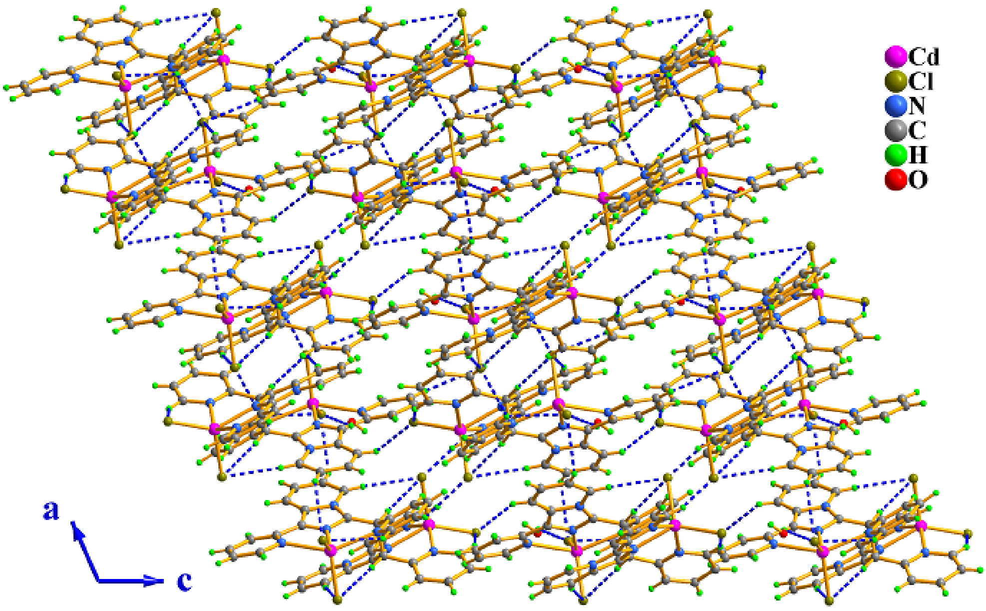


Figure S11

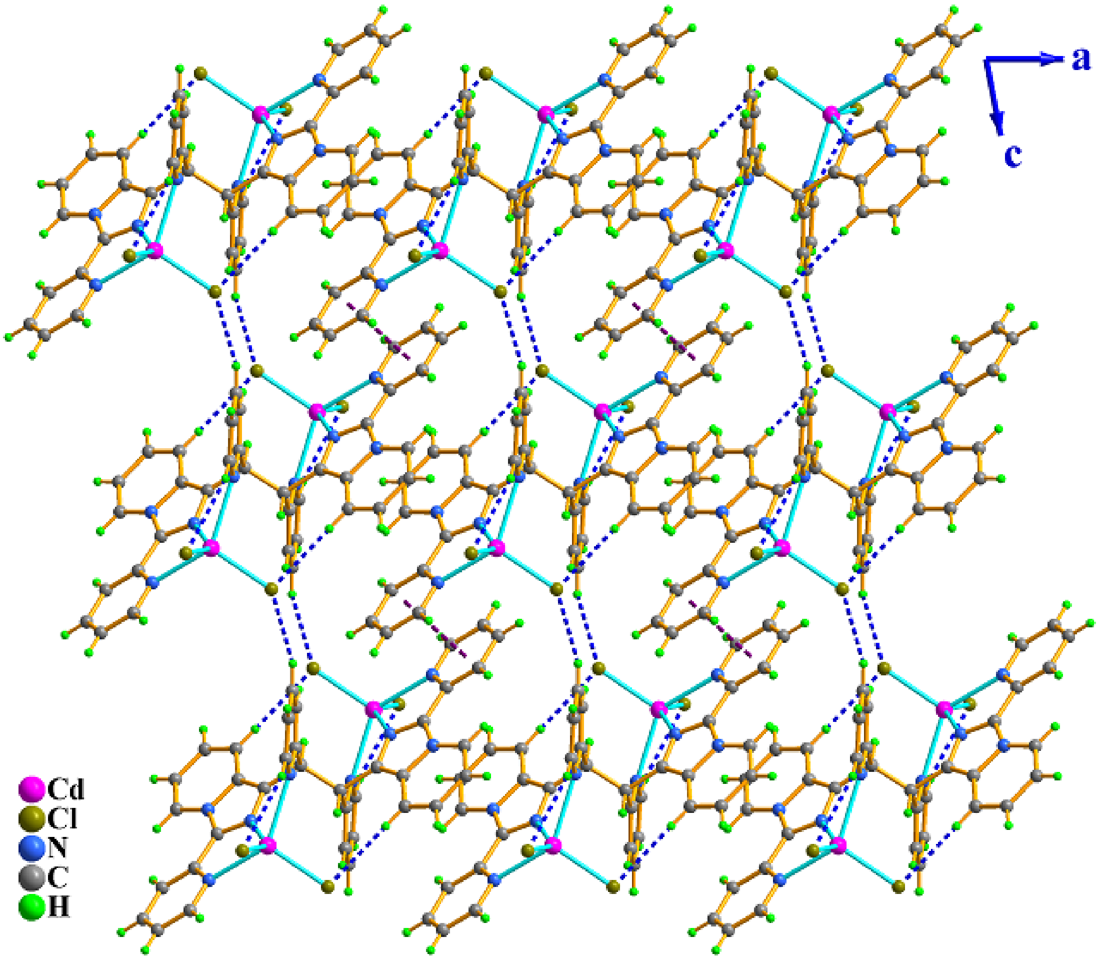


Figure S12

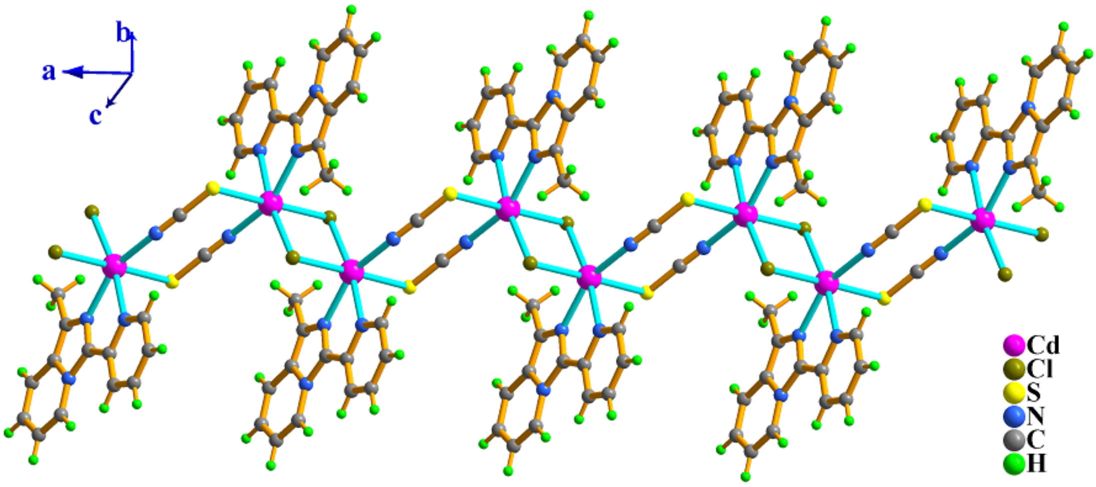
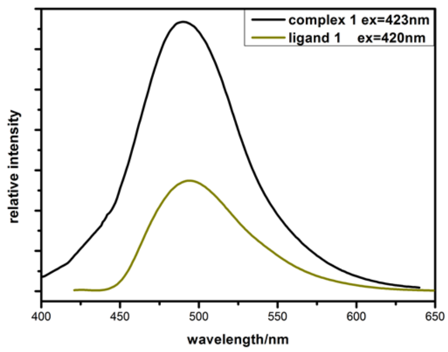
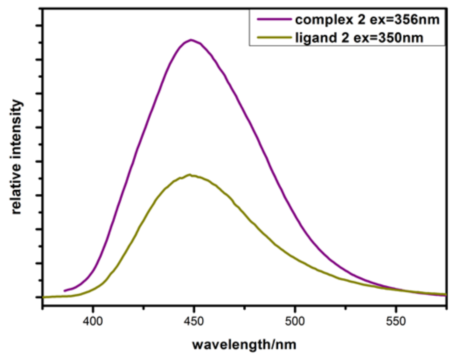


Figure S13

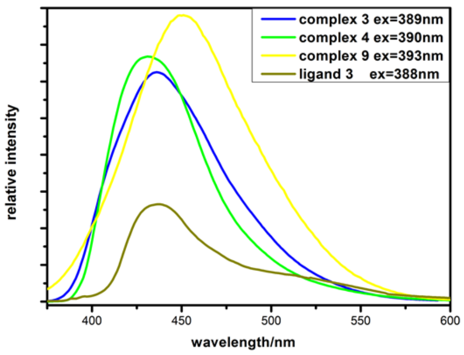
(a)



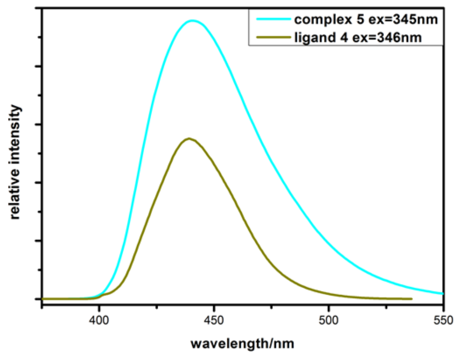
(b)



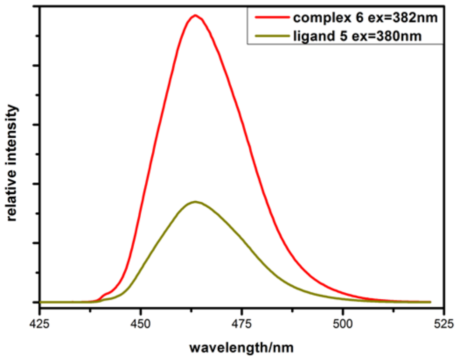
(c)



(d)



(e)



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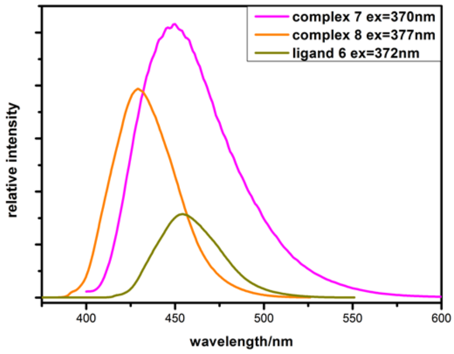
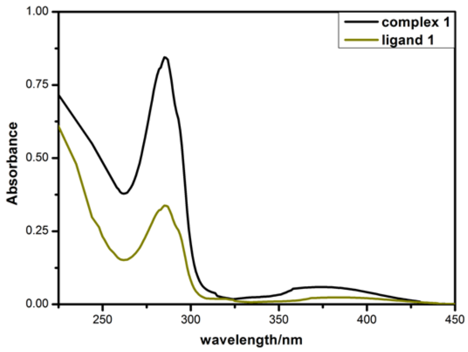


Figure S14

(a)



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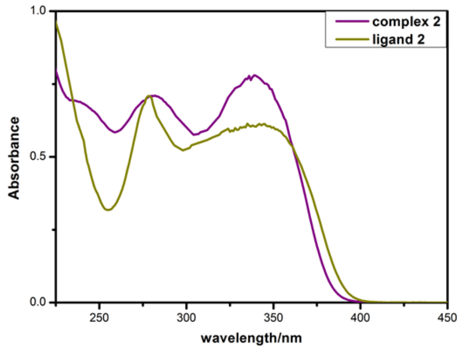

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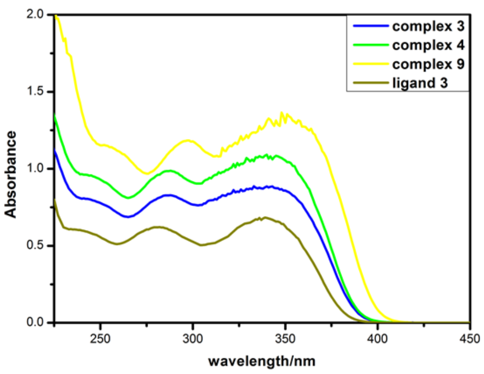

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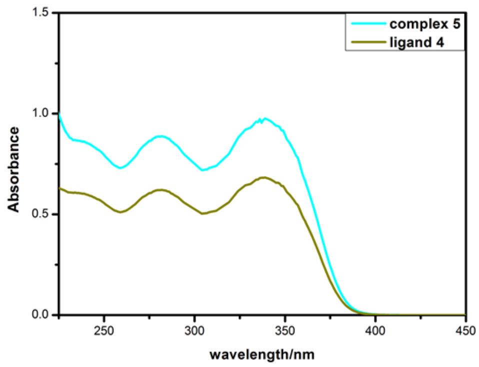

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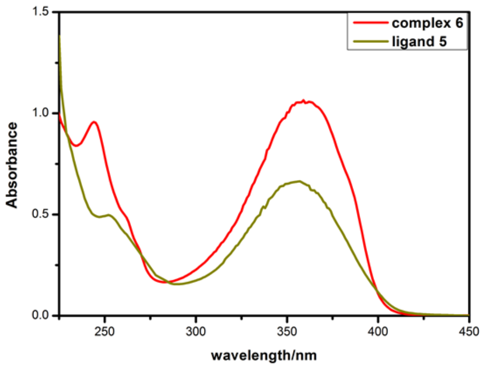

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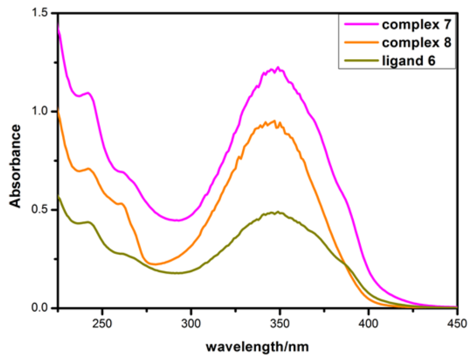


Figure S15

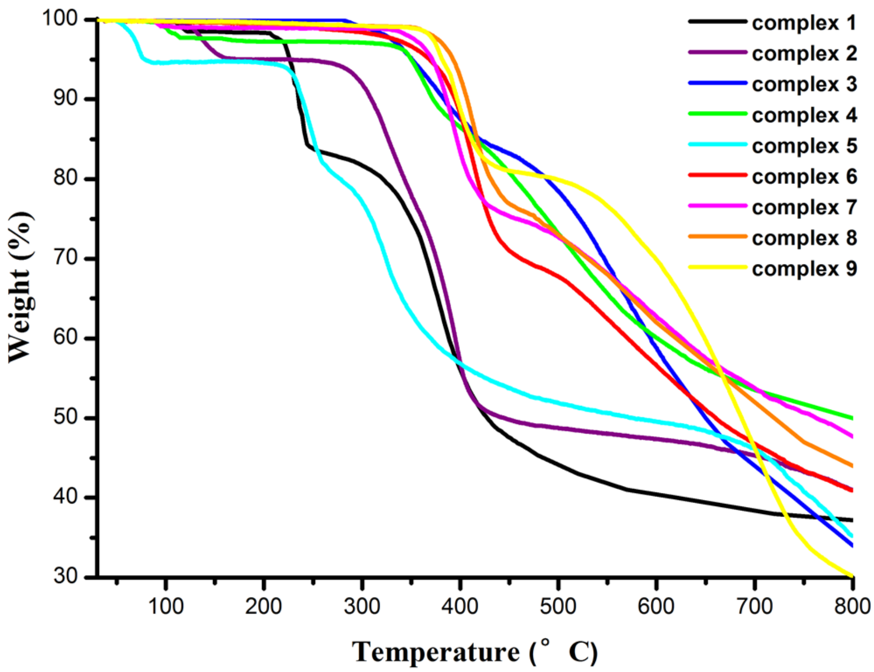
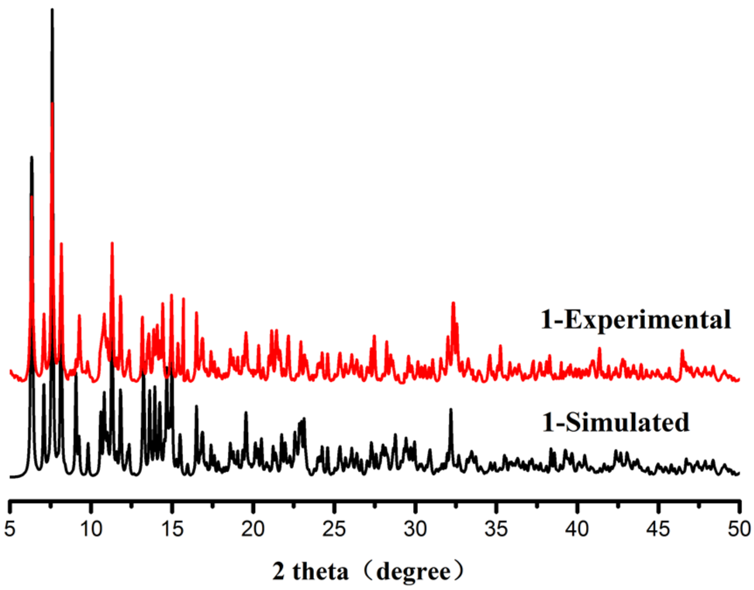
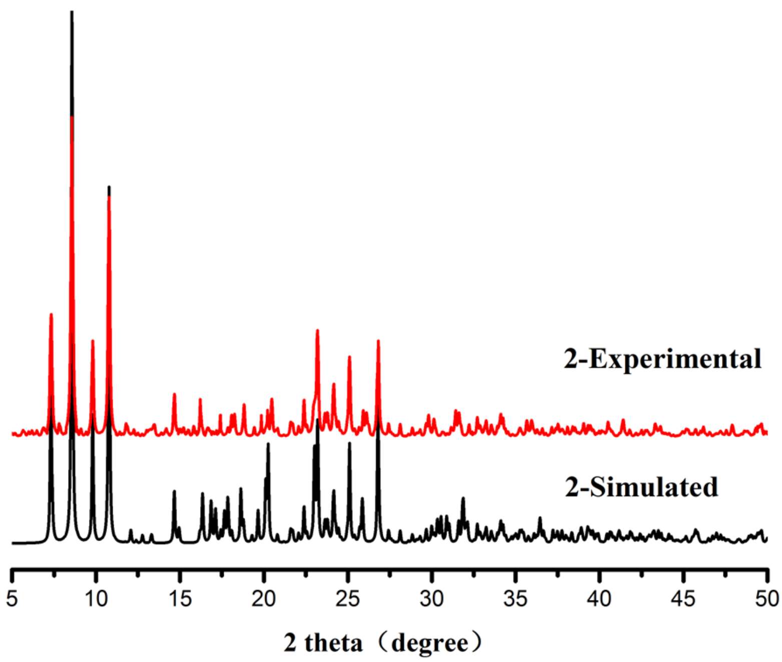


Figure S16

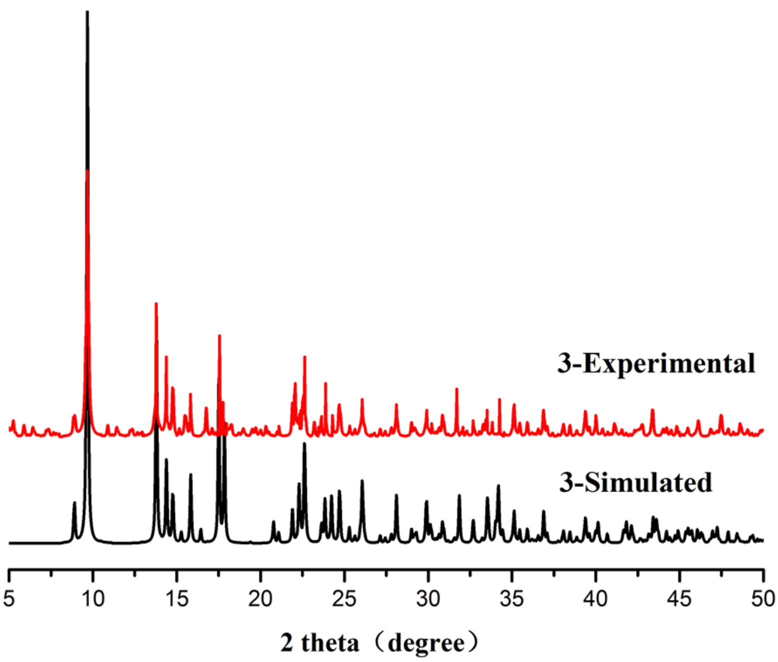
(a)



(b)



(c)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3-Simulated
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10
15
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30
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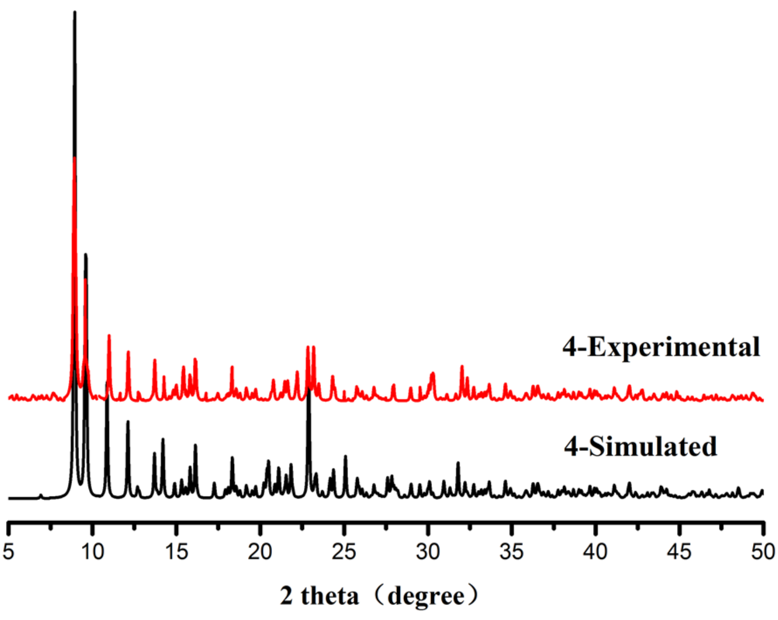
45
50
2 theta（degree）

(d)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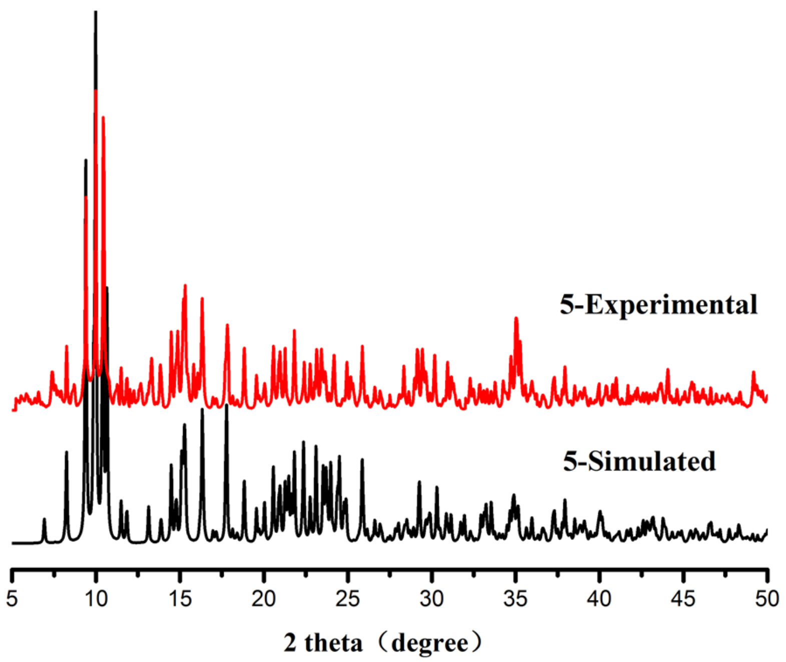
2 theta（degree）

(e)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5-Simulated
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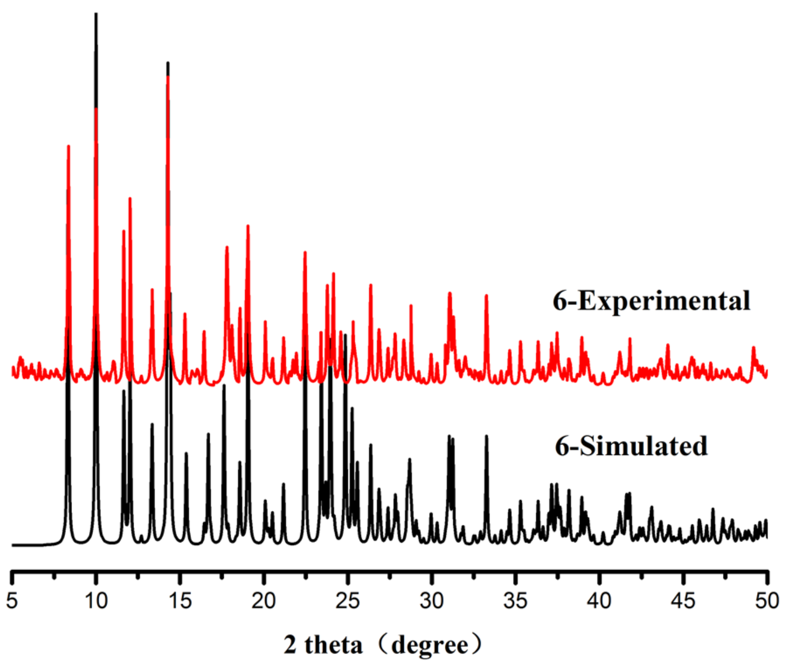
2 theta（degree）

(f)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6-Simulated
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10
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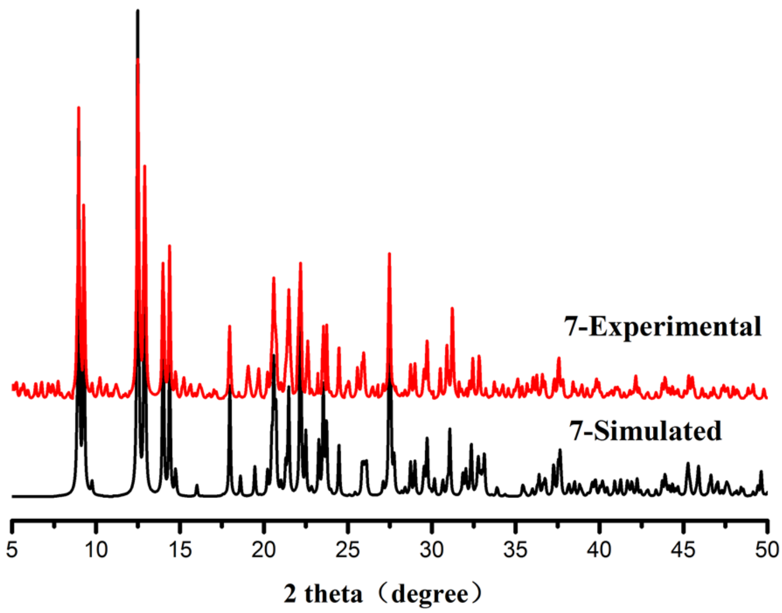
2 theta（degree）

(g)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7-Simulated
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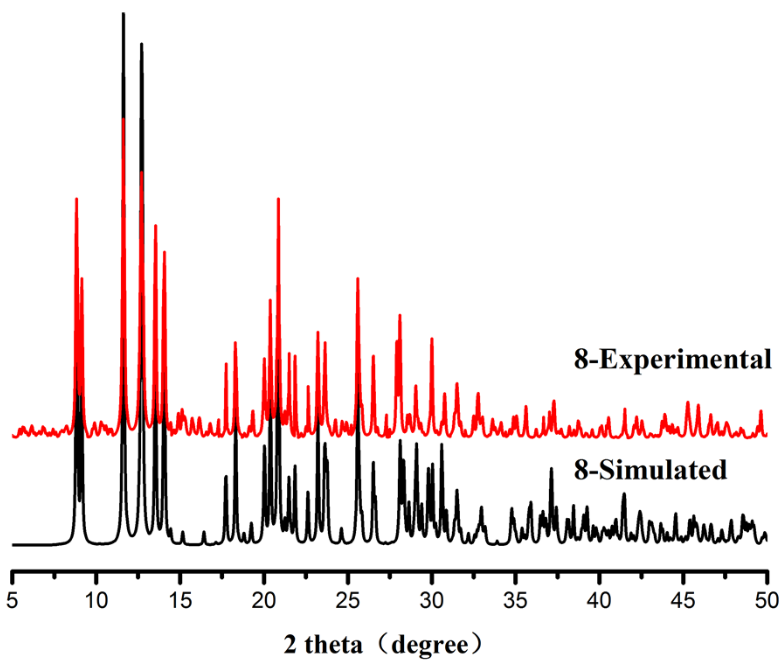
2 theta（degree）

(h)


8-Experimental
8-Simulated
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2 theta（degree）

(i)

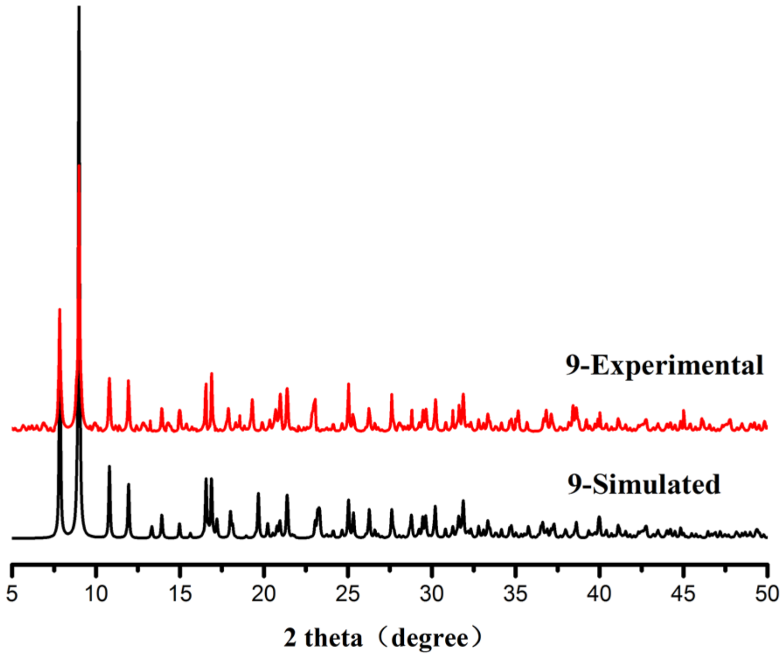
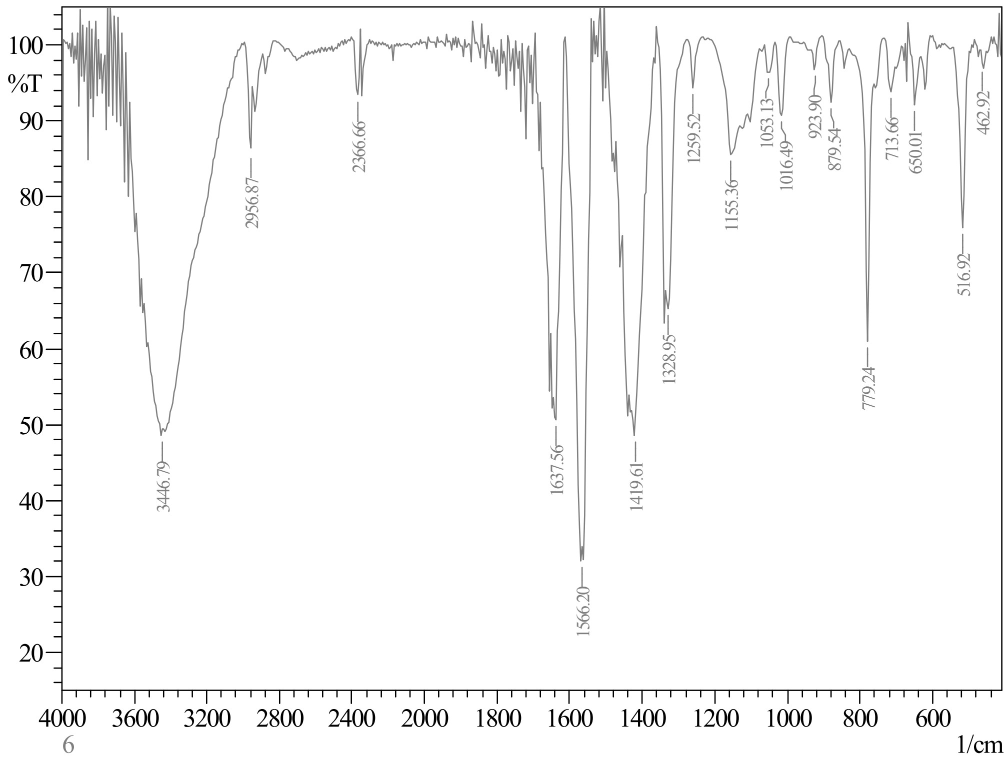
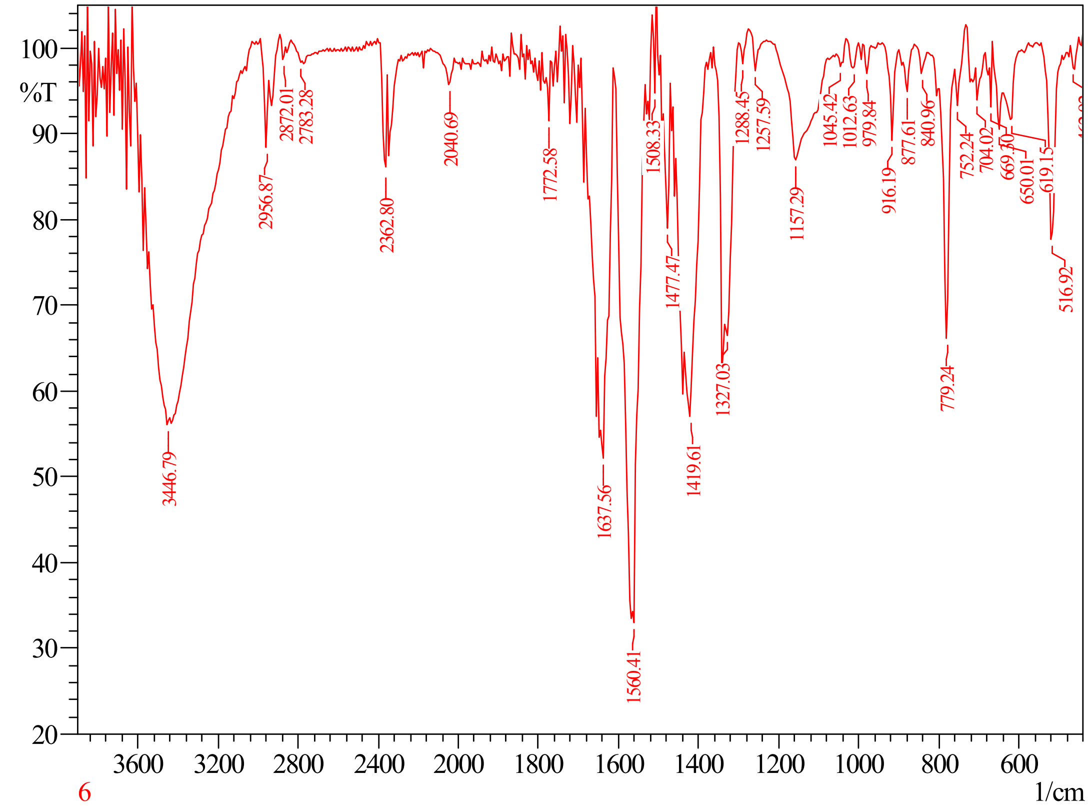


Figure S17

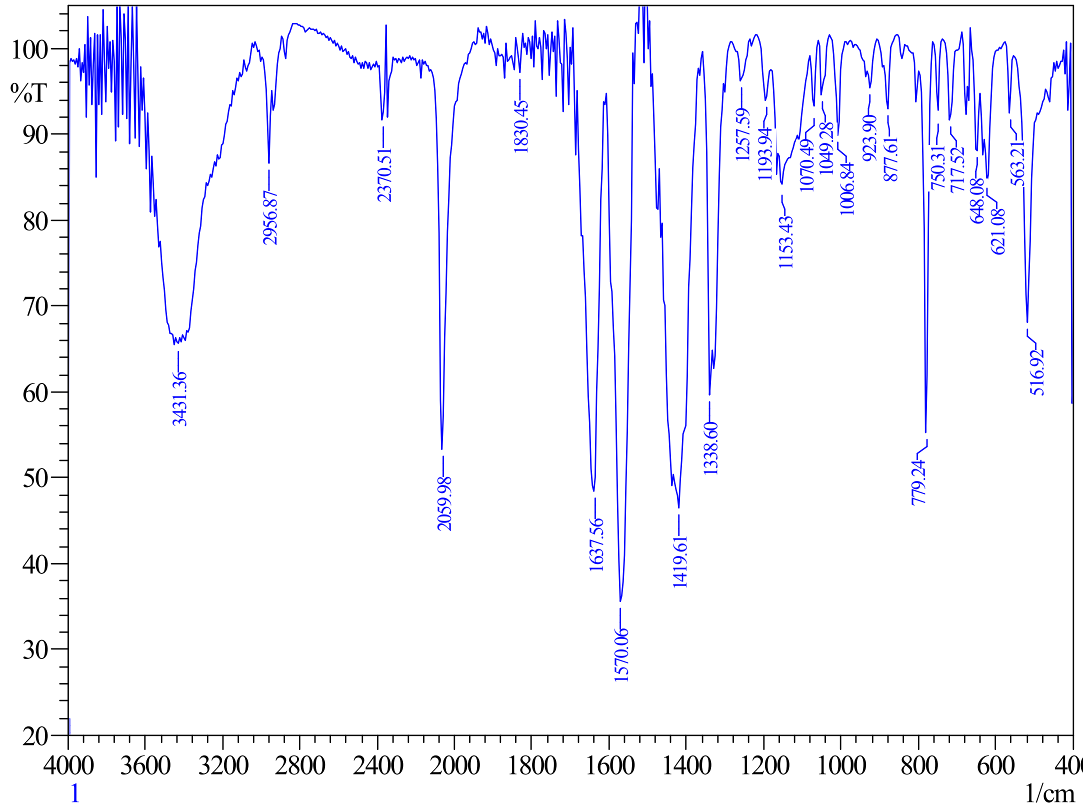
(a) For compound **1**



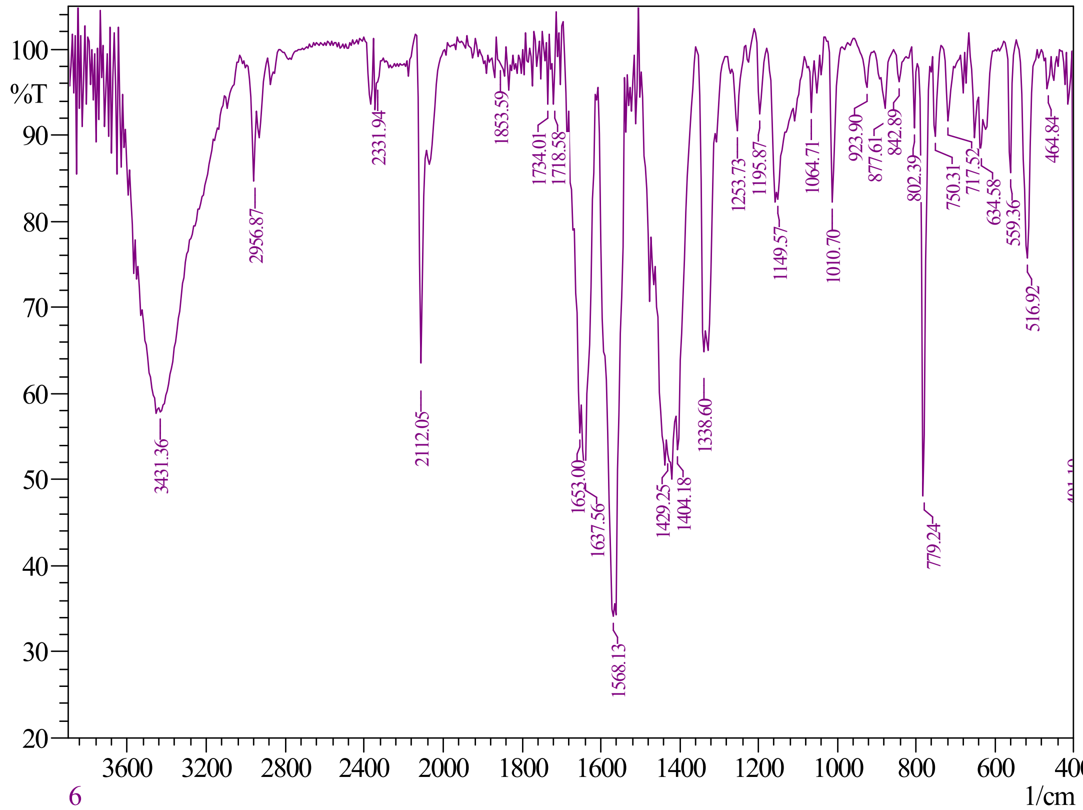
(b) For compound **2**



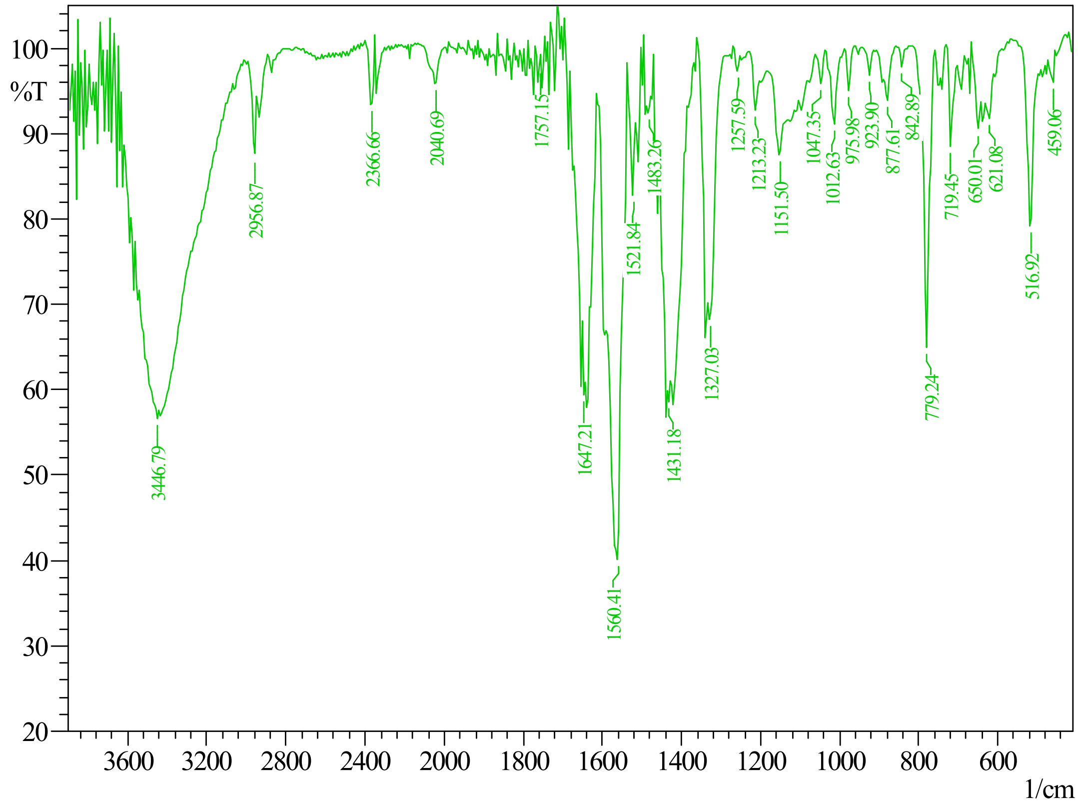
(c) For compound **3**



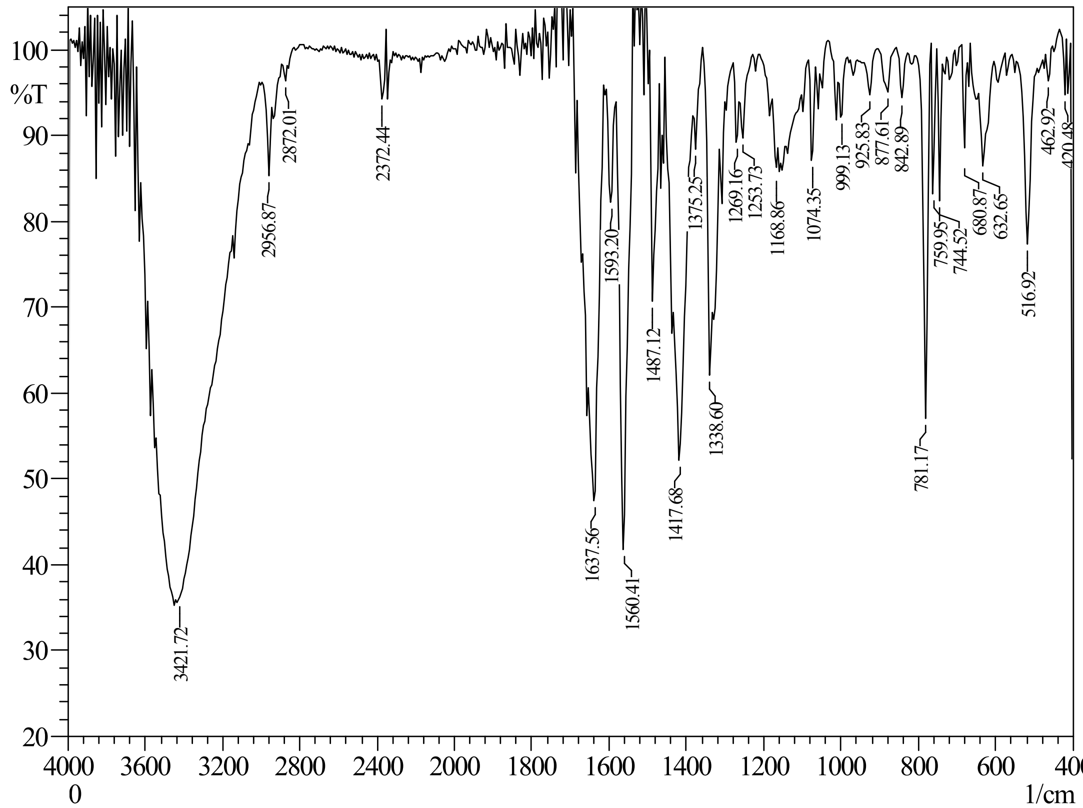
(d) For compound **4**



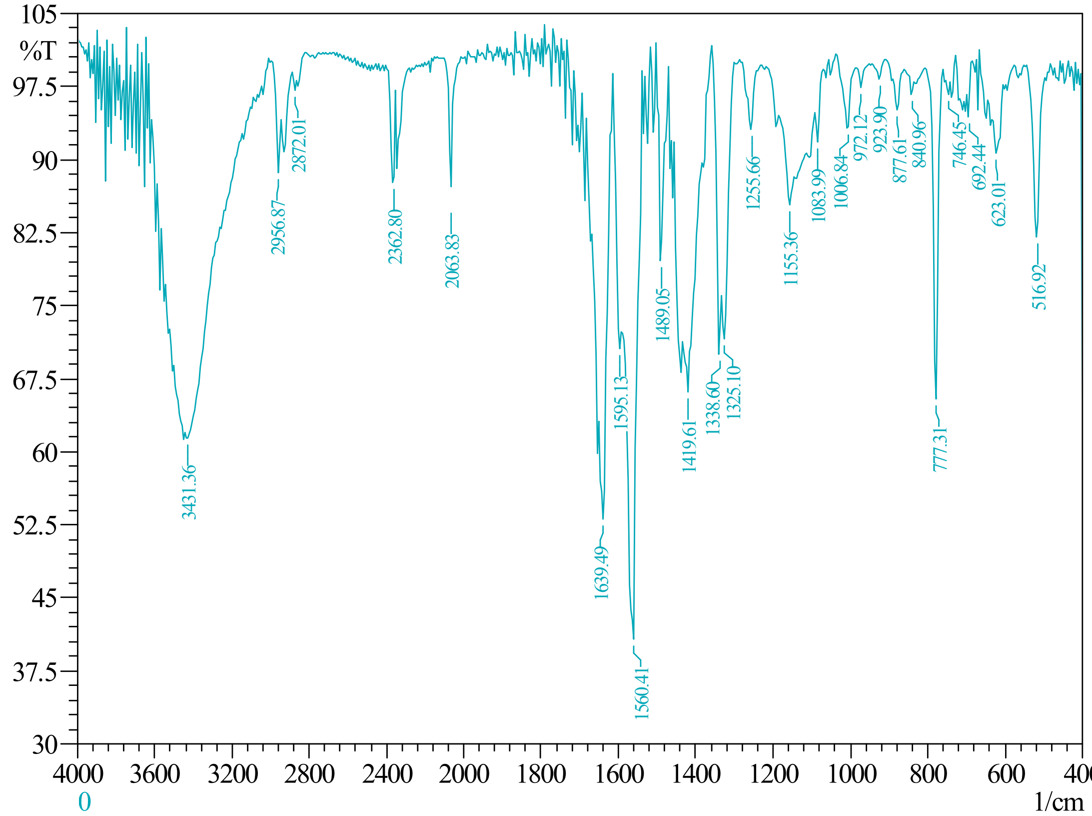
(e) For compound **5**



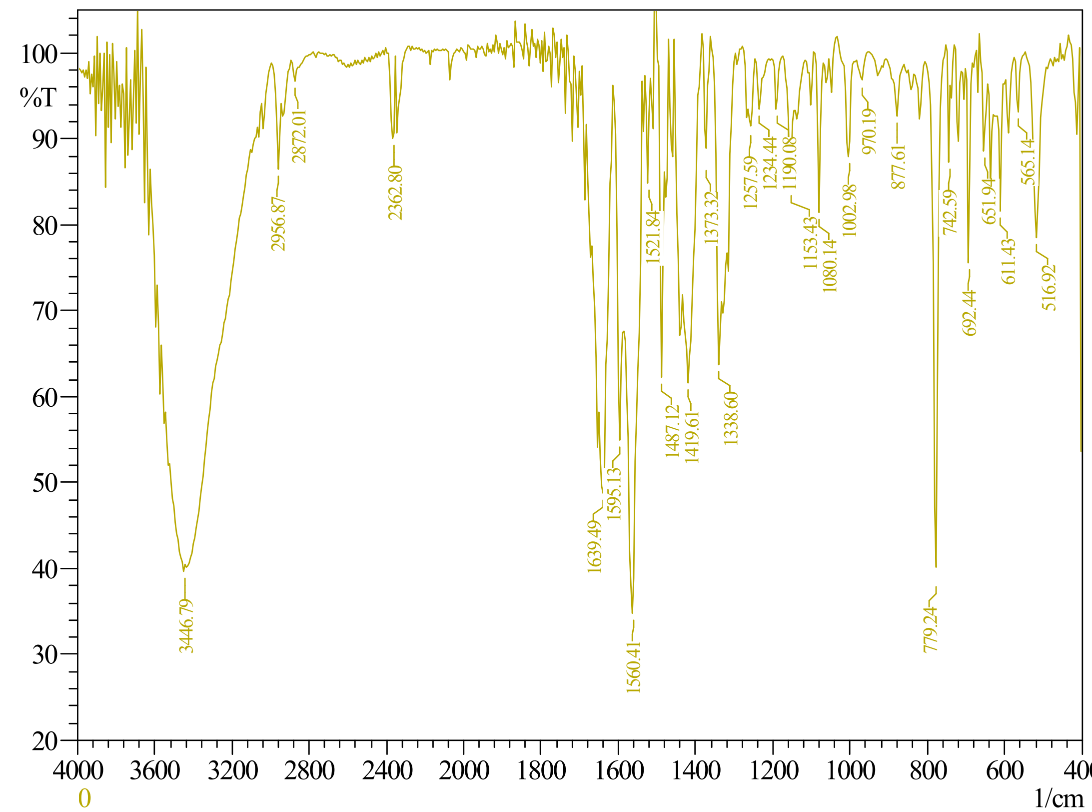
(f) For compound **6**



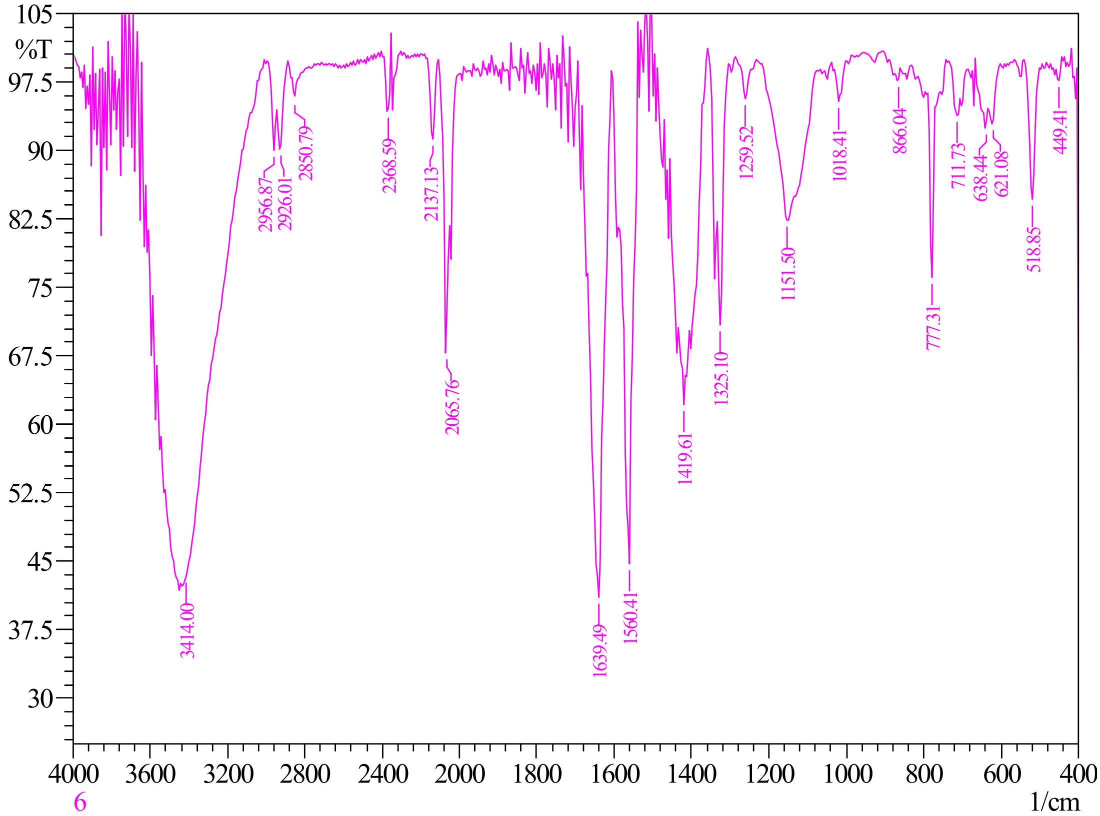
(g) For compound **7**



(h) For comound **8**



(i) For compound **9**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90
82.5
75
67.5
60
52.5
45
37.5
30
4000
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2000
1800
1600
1400
1200
1000
800
600
400
1/cm
6
3414.00
2956.87
2926.01
2850.79
2368.59
2137.13
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1639.49
1560.41
1419.61
1325.10
1259.52
1151.50
1018.41
866.04
777.31
711.73
638.44
621.08
518.85
449.41