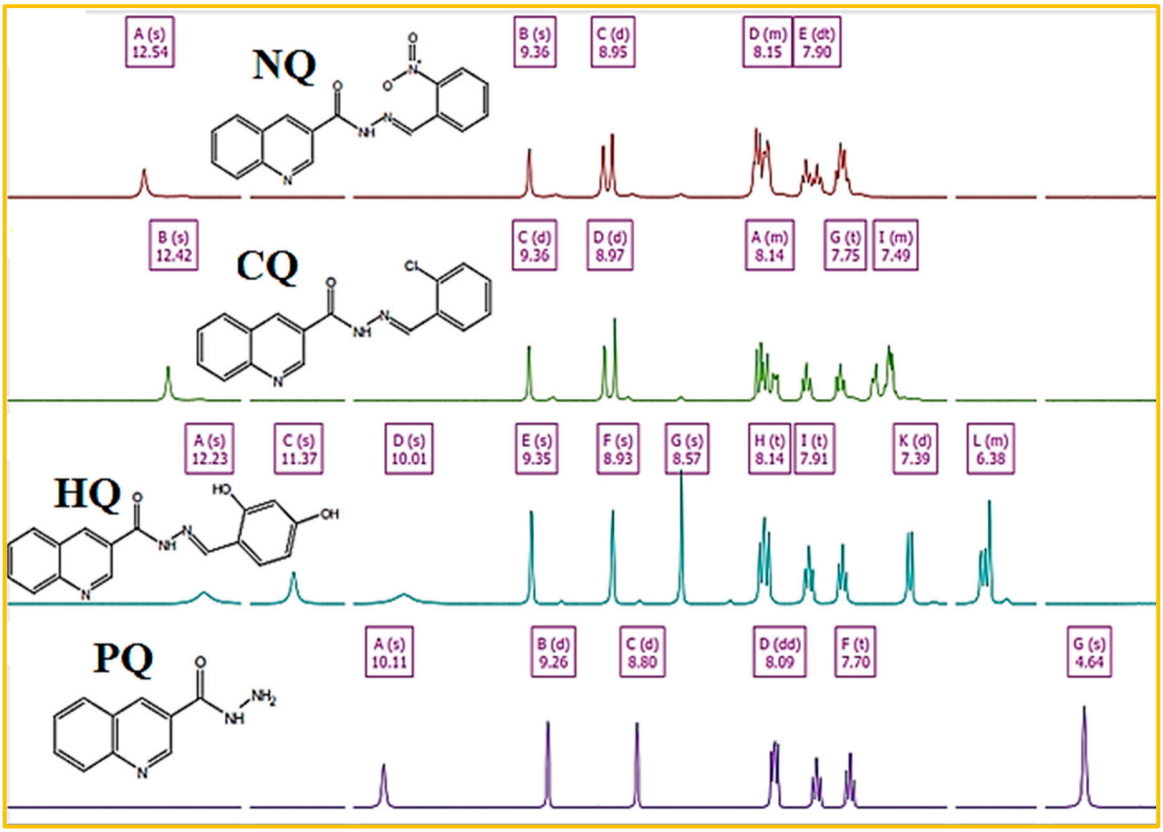

Figure S1. Comparison of the ^{1}H-NMR spectra of NQ, CQ and HQ Ligands with the amine (quinoline-3-carbohydrazide, PQ).

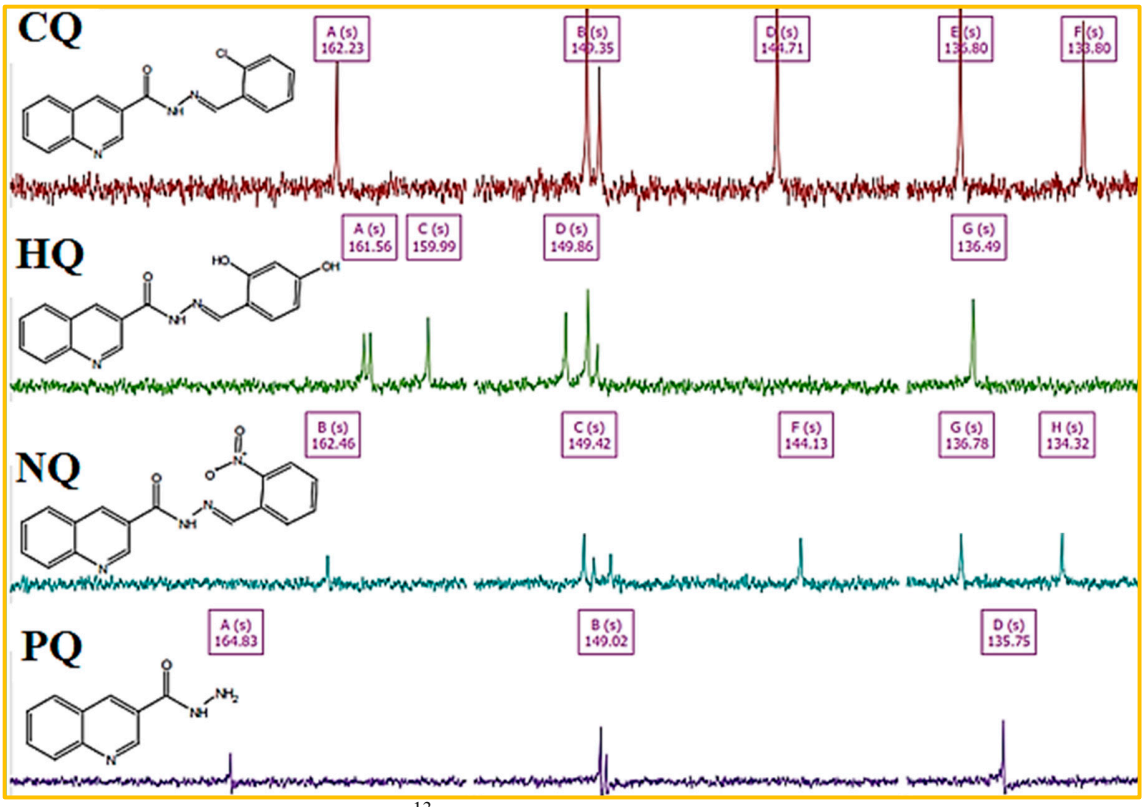

Figure S2. Comparison of the ^{13}C-NMR spectra of NQ, CQ and HQ Ligands with the amine (quinoline-3-carbohydrazide, PQ)

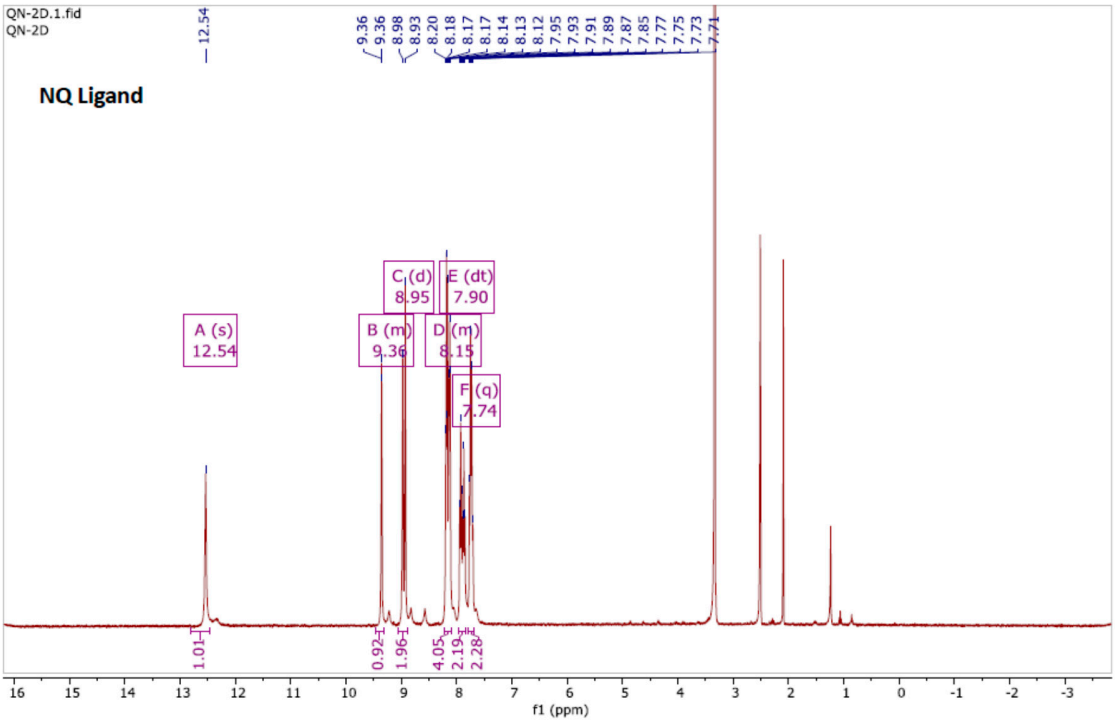

Figure S3. 1H-NMR spectrum of NQ ligand.

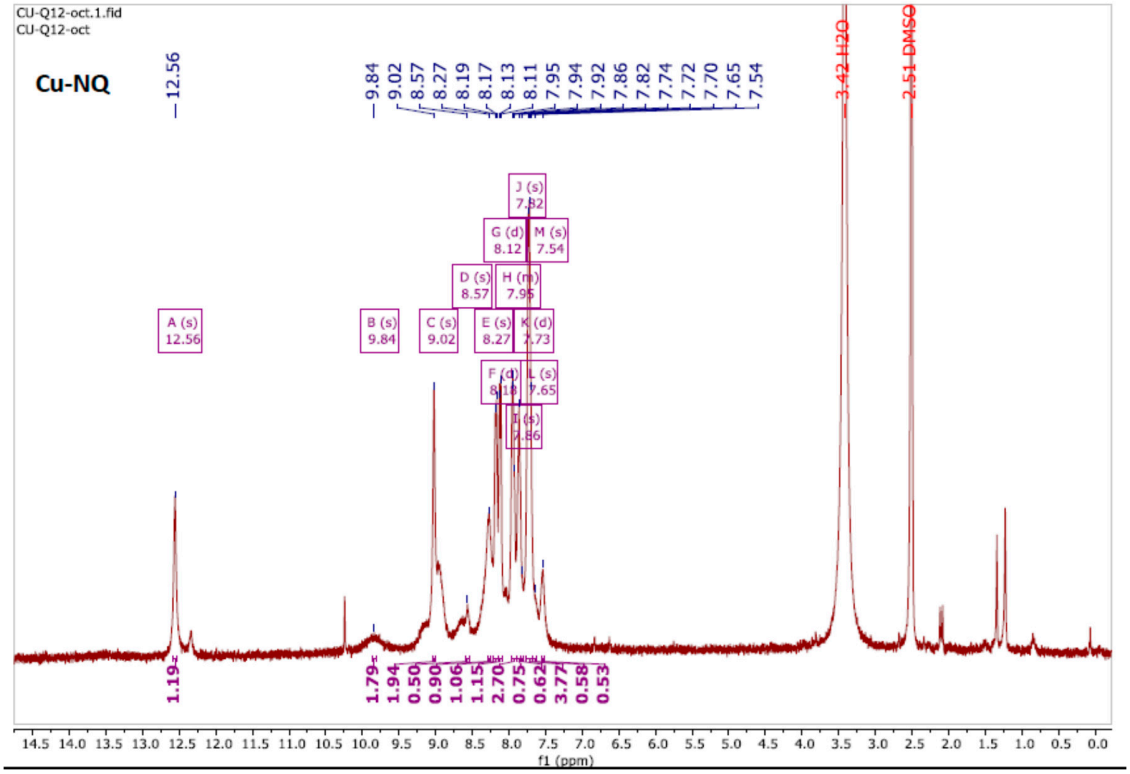

Figure S4. 1H-NMR spectrum of Cu-NQ complex.

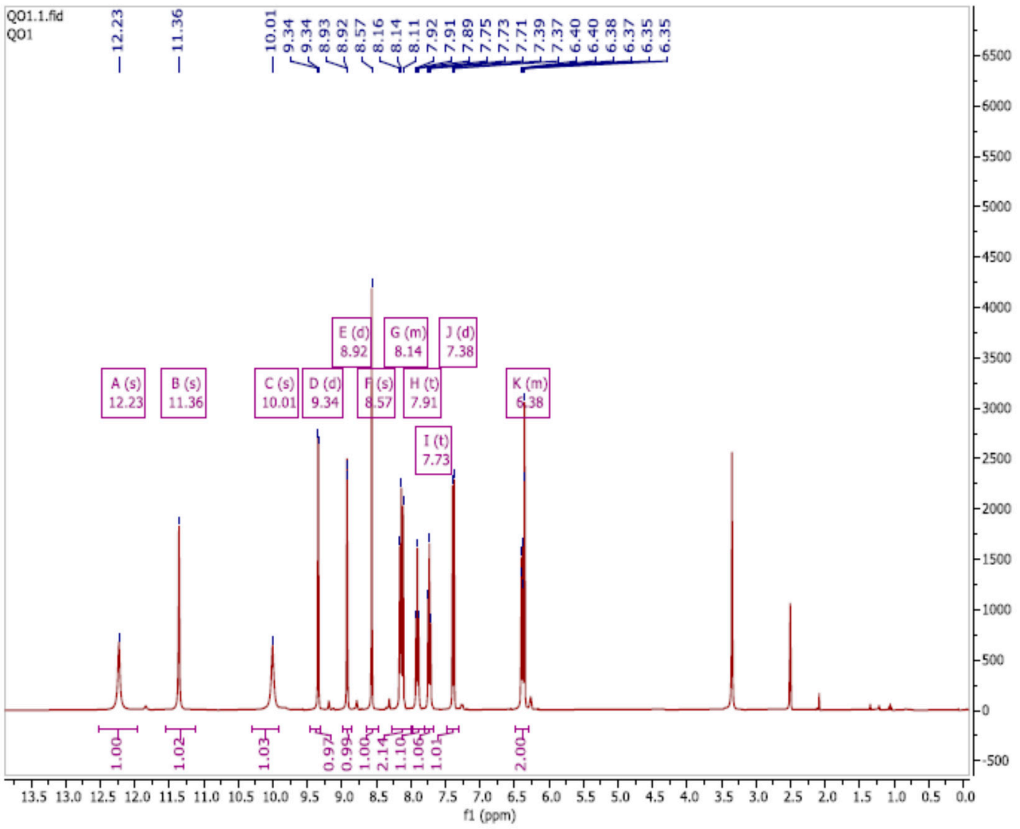

Figure S5. ^{1}H-NMR spectrum of HQ ligand.

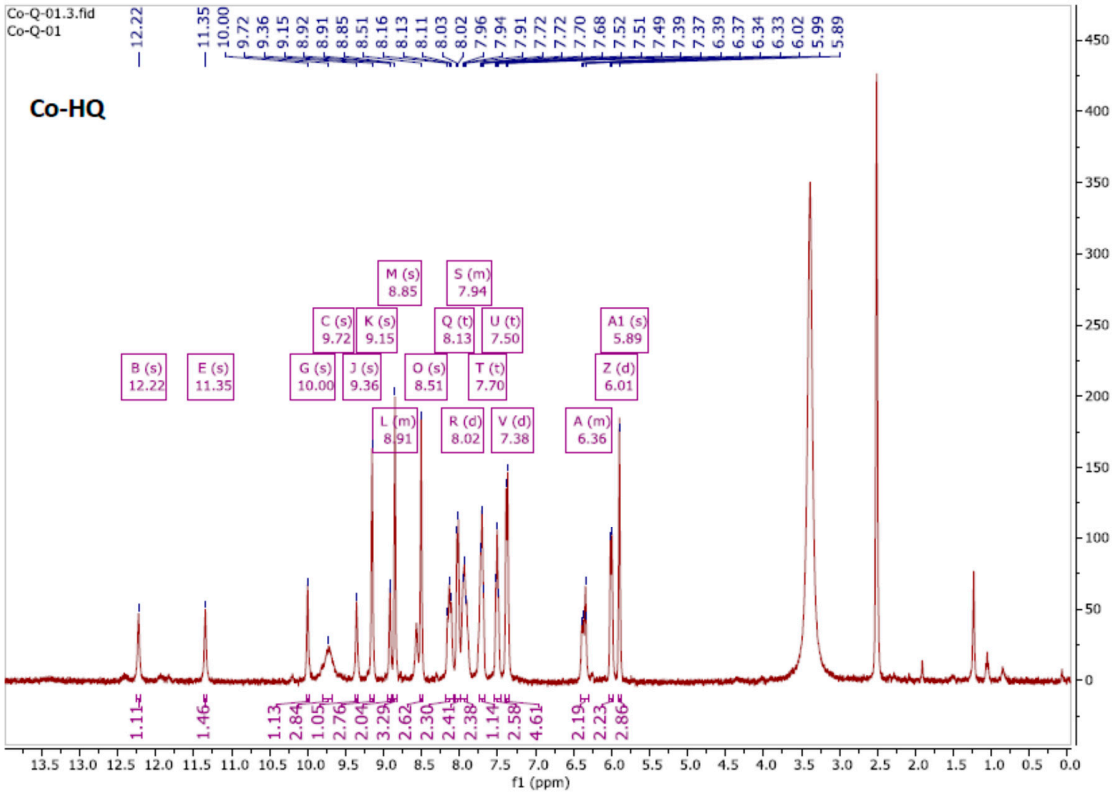

Figure S6. ^{1}H-NMR spectrum of Co-HQ complex.

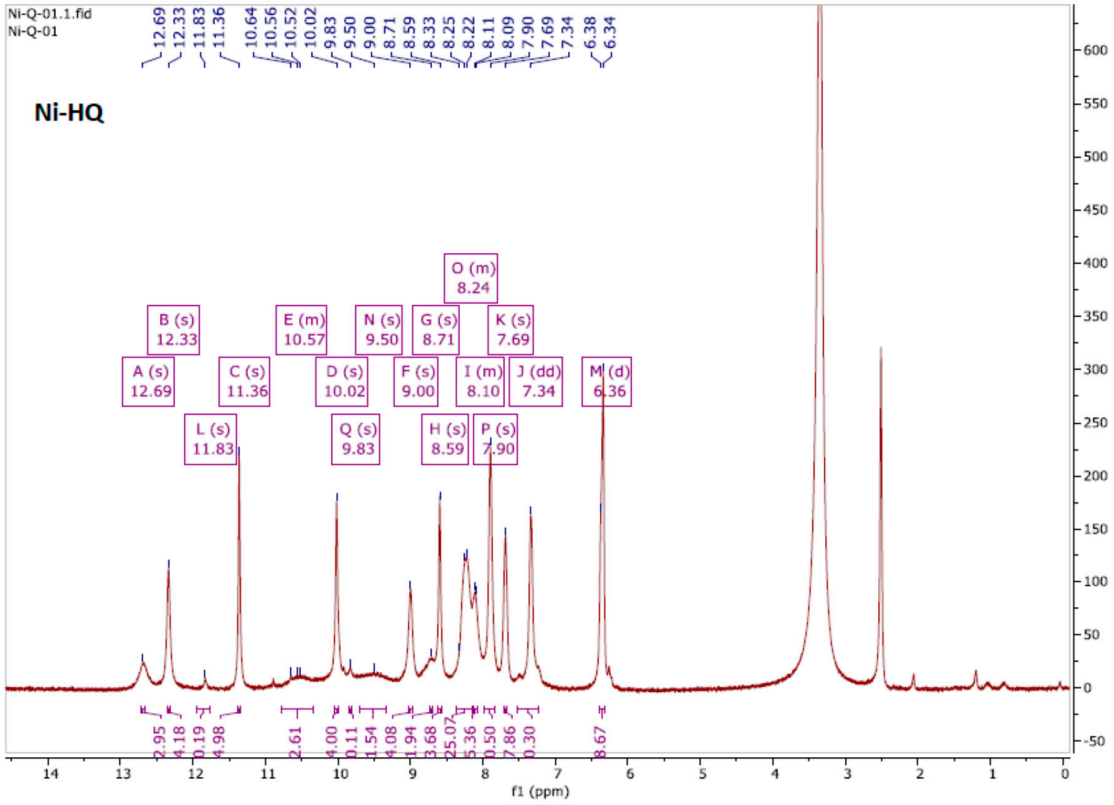

Figure S7. ^{1}H-NMR spectrum of Ni-HQ complex.

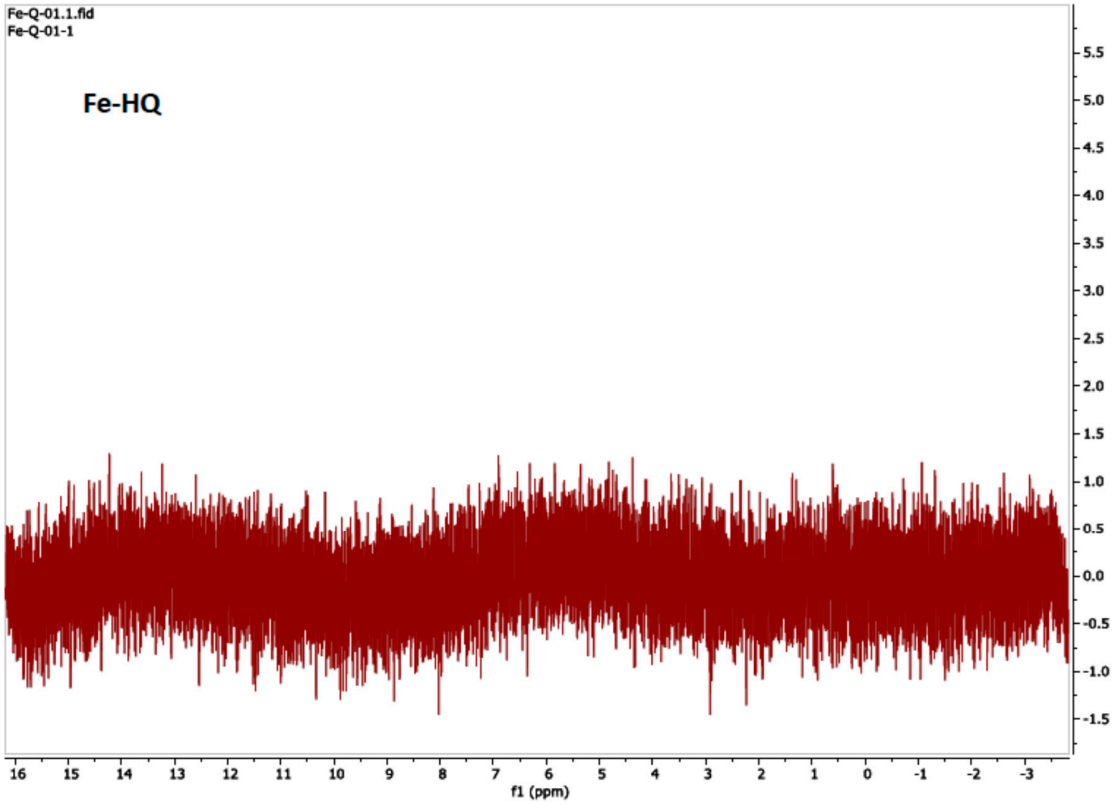

Figure S8. ^{1}H-NMR spectrum of Fe-HQ complex.

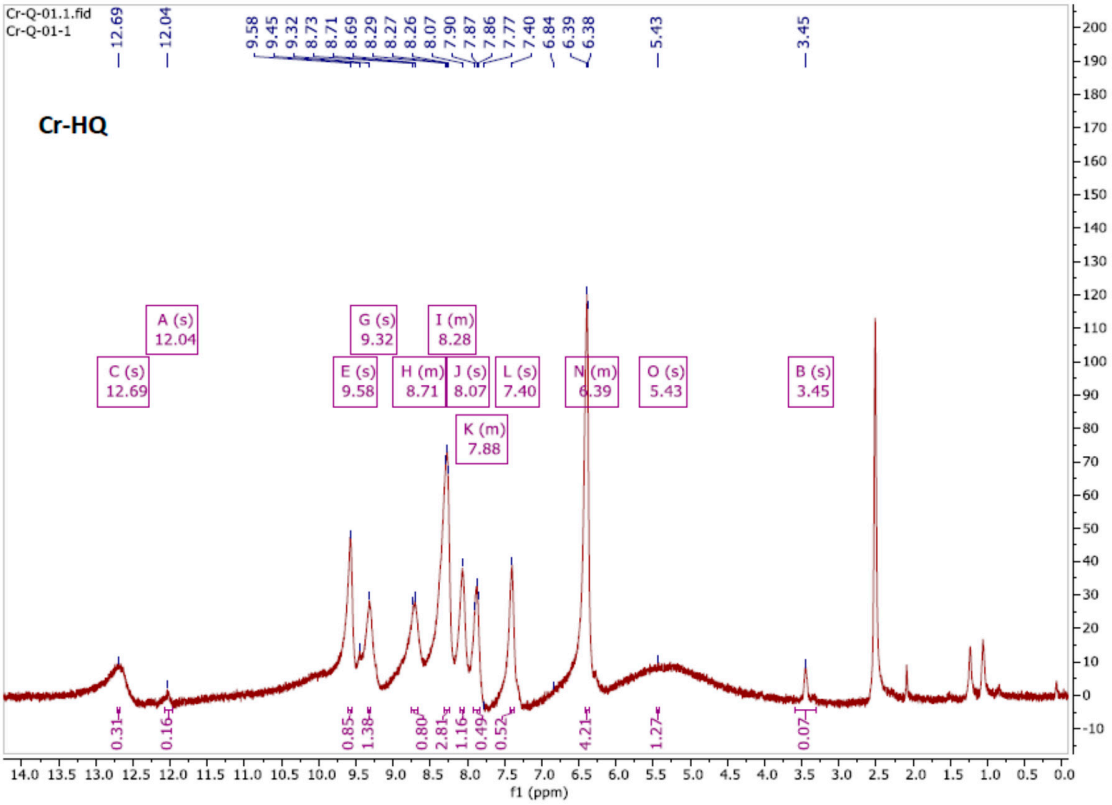

Figure S9. ^{1}H-NMR spectrum of Cr-HQ complex.

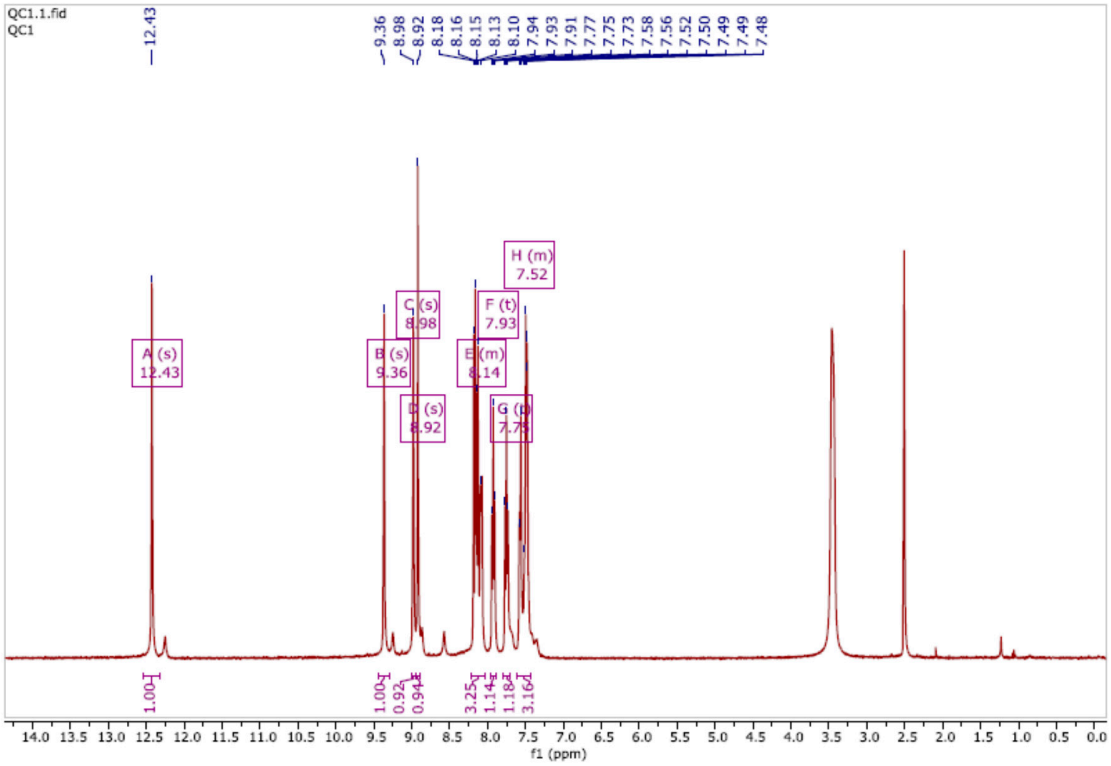

Figure S10. ^{1}H-NMR spectrum of CQ ligand.

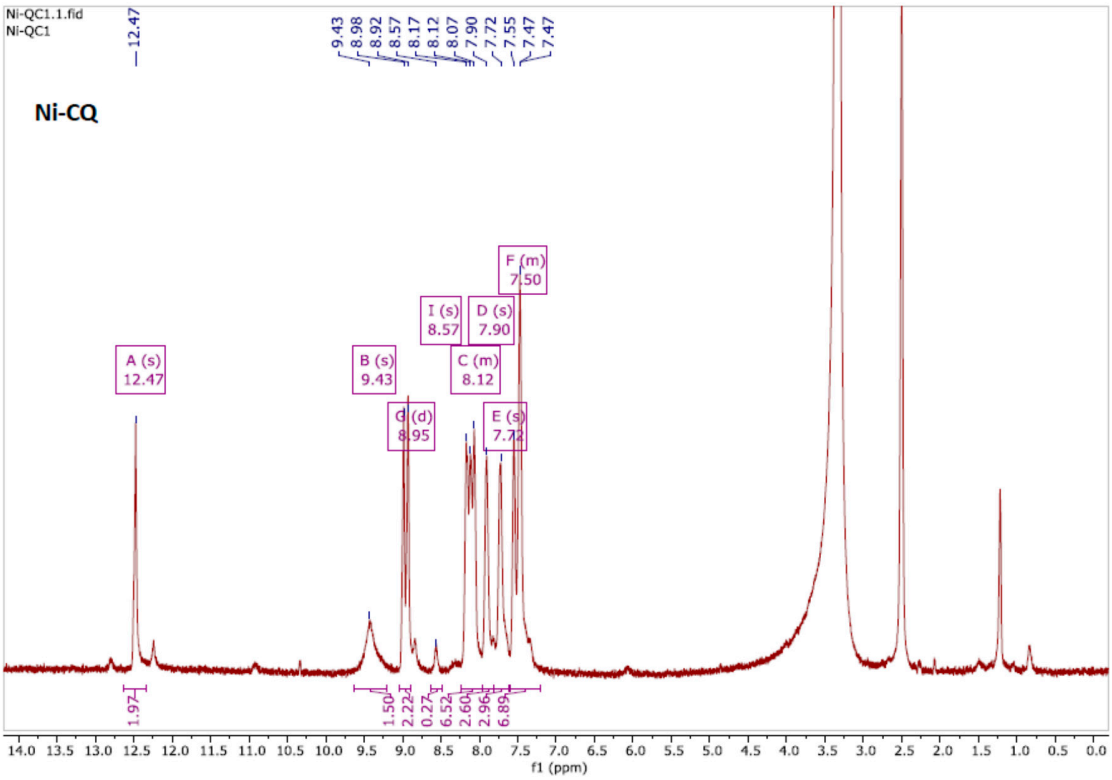

Figure S11. ^{1}H-NMR spectrum of Ni-CQ complex.

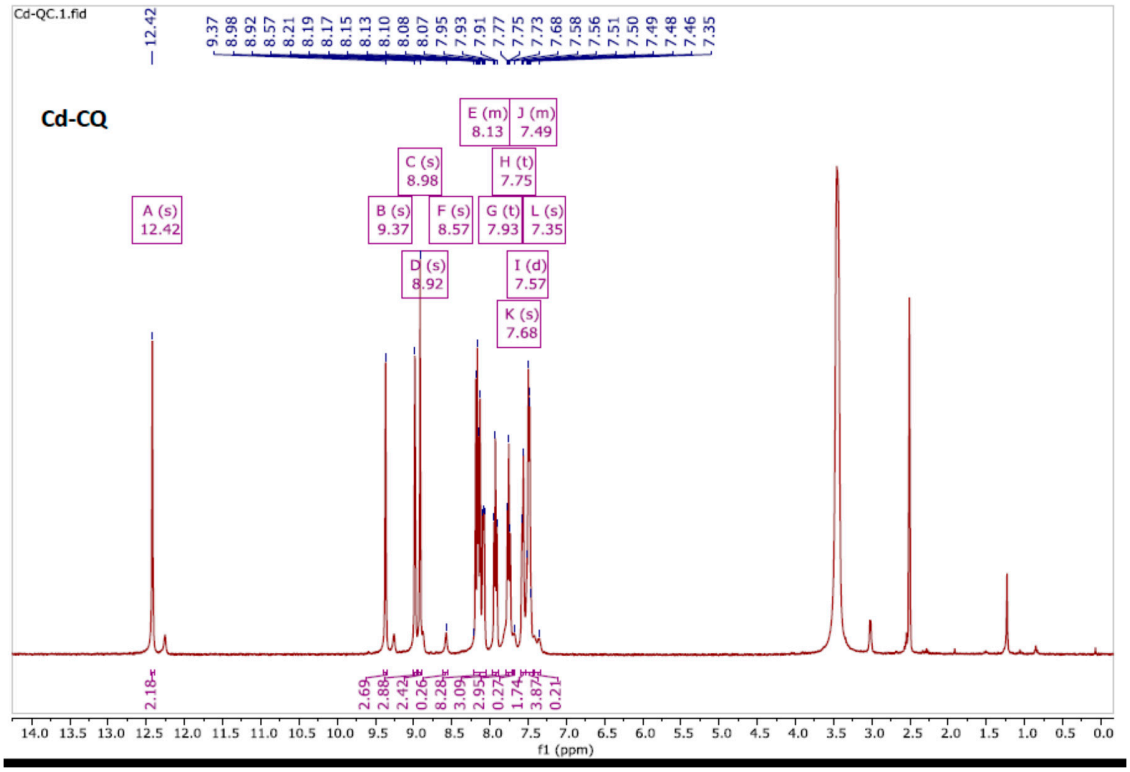

Figure S12. ^{1}H-NMR spectrum of Cd-CQ complex.

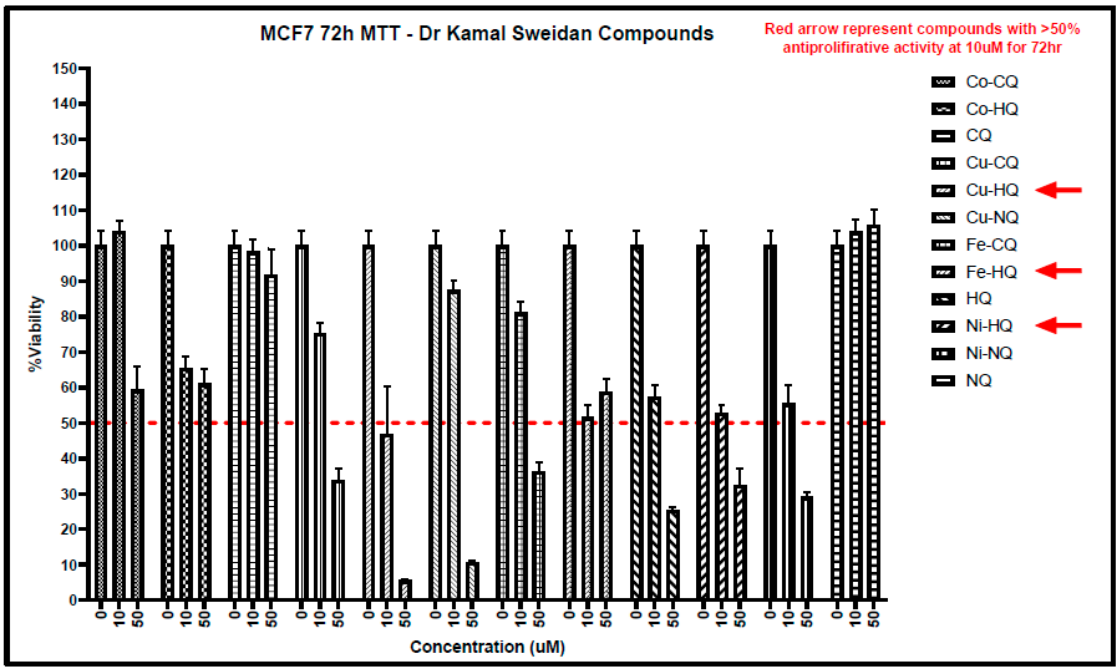

Figure S13. The 50% inhibitory concentration (IC50) values for tested compounds treatment in MCF7 cell lines. Experiments were carried out for 72 hours treatment duration. Experiments were run in triplicates for at least three independent trials (n=6). Concentrations are expressed in micromolar. NA: not applicable; SD: standard deviation; h: hour; µM: micromolar.

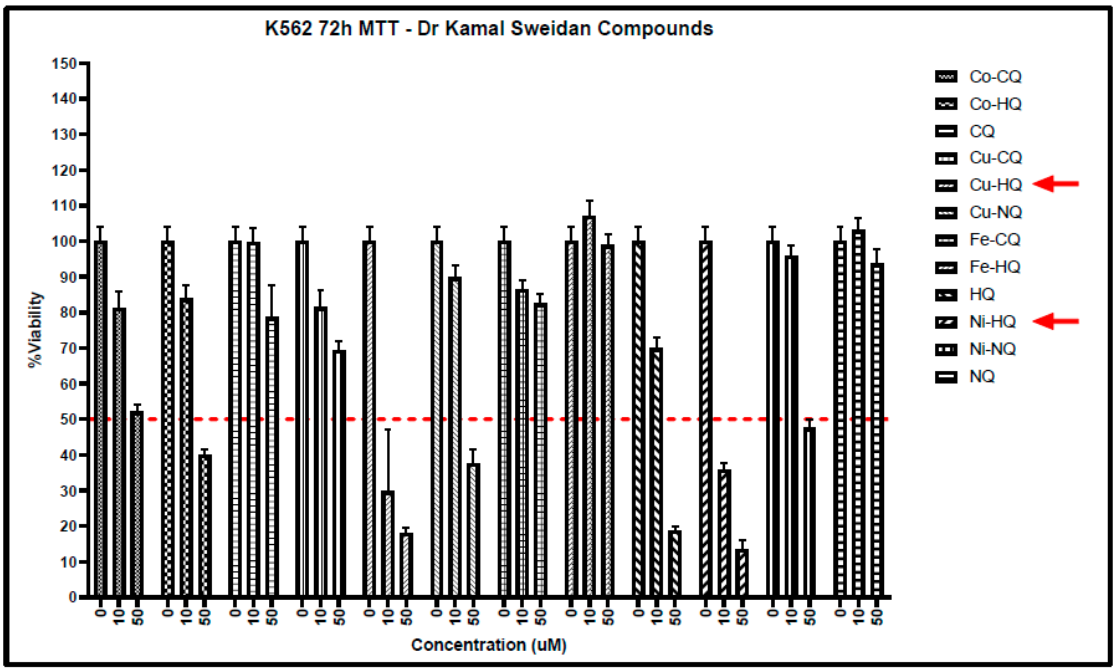

Figure S14. The 50% inhibitory concentration (IC50) values for tested compounds treatment in K562 cell lines. Experiments were carried out for 72 hours treatment duration. Experiments were run in triplicates for at least three independent trials (n=6). Concentrations are expressed in micromolar. NA: not applicable; SD: standard deviation; h: hour; µM: micromolar.

Table S1. Crystal data and structure refinement for CQ·H_2O.

Identification code	2112coqc	
Empirical formula	$C_{17}H_{14}ClN_3O_2$	
Formula weight	327.76	
Temperature	190(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	*Pbca*	
Unit cell dimensions	a = 12.7287(6) Å	α= 90°.
	b = 12.9558(5) Å	β= 90°.
	c = 18.8331(12) Å	γ = 90°.
Volume	3105.8(3) $Å^3$	
Z	8	
Density (calculated)	1.402 Mg/m^3	
Absorption coefficient	2.294 mm^{-1}	
F(000)	1360	
Crystal size	0.300 x 0.200 x 0.100 mm^3	
Theta range for data collection	4.696 to 61.648°.	
Index ranges	-14<=h<=13, -13<=k<=14, -21<=l<=21	
Reflections collected	8638	
Independent reflections	2409 [R(int) = 0.0536]	
Completeness to theta = 61.648°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.899	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2409 / 0 / 209	
Goodness-of-fit on F^2	1.090	
Final R indices [I>2sigma(I)]	R1 = 0.0495, wR2 = 0.1271	
R indices (all data)	R1 = 0.0659, wR2 = 0.1383	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.381 and -0.361 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for CQ·H_2O.

C(1)-N(1)	1.316(4)
C(1)-C(2)	1.422(4)
C(2)-C(3)	1.371(4)
C(2)-C(10)	1.492(4)
C(3)-C(4)	1.410(4)
C(4)-C(9)	1.406(4)
C(4)-C(5)	1.425(4)
C(5)-C(6)	1.364(4)
C(6)-C(7)	1.407(5)
C(7)-C(8)	1.363(5)
C(8)-C(9)	1.421(4)
C(9)-N(1)	1.379(4)
C(10)-O(1)	1.230(3)
C(10)-N(2)	1.350(4)
C(11)-N(3)	1.276(4)
C(11)-C(12)	1.466(4)
C(12)-C(13)	1.391(4)
C(12)-C(17)	1.402(4)
C(13)-C(14)	1.385(5)
C(13)-Cl(1)	1.747(3)
C(14)-C(15)	1.379(5)
C(15)-C(16)	1.386(5)
C(16)-C(17)	1.372(5)
N(2)-N(3)	1.378(3)

N(1)-C(1)-C(2)	123.9(3)
C(3)-C(2)-C(1)	117.8(3)
C(3)-C(2)-C(10)	117.9(2)
C(1)-C(2)-C(10)	124.2(2)
C(2)-C(3)-C(4)	120.1(3)
C(9)-C(4)-C(3)	118.2(2)
C(9)-C(4)-C(5)	118.8(3)
C(3)-C(4)-C(5)	123.0(3)
C(6)-C(5)-C(4)	120.3(3)

C(5)-C(6)-C(7)	120.3(3)
C(8)-C(7)-C(6)	121.1(3)
C(7)-C(8)-C(9)	119.6(3)
N(1)-C(9)-C(4)	121.8(3)
N(1)-C(9)-C(8)	118.4(3)
C(4)-C(9)-C(8)	119.8(3)
O(1)-C(10)-N(2)	122.1(3)
O(1)-C(10)-C(2)	120.5(2)
N(2)-C(10)-C(2)	117.4(2)
N(3)-C(11)-C(12)	119.3(3)
C(13)-C(12)-C(17)	117.2(3)
C(13)-C(12)-C(11)	121.8(3)
C(17)-C(12)-C(11)	121.1(3)
C(14)-C(13)-C(12)	122.1(3)
C(14)-C(13)-Cl(1)	117.4(3)
C(12)-C(13)-Cl(1)	120.4(2)
C(15)-C(14)-C(13)	119.0(3)
C(14)-C(15)-C(16)	120.3(3)
C(17)-C(16)-C(15)	120.1(3)
C(16)-C(17)-C(12)	121.3(3)
C(1)-N(1)-C(9)	118.2(2)
C(10)-N(2)-N(3)	118.0(2)
C(11)-N(3)-N(2)	115.9(2)

Table S3. Torsion angles [°] for CQ·H_2O.

N(1)-C(1)-C(2)-C(3)	1.0(4)
N(1)-C(1)-C(2)-C(10)	-178.2(3)
C(1)-C(2)-C(3)-C(4)	-0.9(4)
C(10)-C(2)-C(3)-C(4)	178.3(2)
C(2)-C(3)-C(4)-C(9)	0.2(4)
C(2)-C(3)-C(4)-C(5)	-179.4(3)
C(9)-C(4)-C(5)-C(6)	-0.2(4)
C(3)-C(4)-C(5)-C(6)	179.5(3)
C(4)-C(5)-C(6)-C(7)	0.1(5)
C(5)-C(6)-C(7)-C(8)	0.1(5)
C(6)-C(7)-C(8)-C(9)	-0.2(5)
C(3)-C(4)-C(9)-N(1)	0.5(4)
C(5)-C(4)-C(9)-N(1)	-179.8(3)
C(3)-C(4)-C(9)-C(8)	-179.6(3)
C(5)-C(4)-C(9)-C(8)	0.1(4)
C(7)-C(8)-C(9)-N(1)	-180.0(3)
C(7)-C(8)-C(9)-C(4)	0.1(4)
C(3)-C(2)-C(10)-O(1)	-6.0(4)
C(1)-C(2)-C(10)-O(1)	173.2(3)
C(3)-C(2)-C(10)-N(2)	174.4(2)
C(1)-C(2)-C(10)-N(2)	-6.5(4)
N(3)-C(11)-C(12)-C(13)	175.7(3)
N(3)-C(11)-C(12)-C(17)	-5.0(4)
C(17)-C(12)-C(13)-C(14)	-0.1(4)
C(11)-C(12)-C(13)-C(14)	179.3(3)
C(17)-C(12)-C(13)-Cl(1)	179.1(2)
C(11)-C(12)-C(13)-Cl(1)	-1.5(4)
C(12)-C(13)-C(14)-C(15)	0.2(5)
Cl(1)-C(13)-C(14)-C(15)	-179.1(3)
C(13)-C(14)-C(15)-C(16)	0.2(5)
C(14)-C(15)-C(16)-C(17)	-0.6(5)
C(15)-C(16)-C(17)-C(12)	0.6(5)
C(13)-C(12)-C(17)-C(16)	-0.3(5)
C(11)-C(12)-C(17)-C(16)	-179.7(3)

C(2)-C(1)-N(1)-C(9)	-0.3(4)
C(4)-C(9)-N(1)-C(1)	-0.5(4)
C(8)-C(9)-N(1)-C(1)	179.6(3)
O(1)-C(10)-N(2)-N(3)	1.2(4)
C(2)-C(10)-N(2)-N(3)	-179.2(2)
C(12)-C(11)-N(3)-N(2)	179.9(2)
C(10)-N(2)-N(3)-C(11)	177.8(3)

Table S4. Hydrogen bonds for CQ·H_2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1)-H(1)...O(2)	0.95	2.42	3.356(4)	168.8
C(11)-H(11)...O(2)	0.95	2.49	3.284(4)	141.2
N(2)-H(2)...O(2)	0.88	2.03	2.877(3)	162.1
O(2)-H(2A)...O(1)#1	0.81	2.08	2.862(3)	162.8
O(2)-H(2B)...N(1)#2	0.81	2.06	2.846(3)	166.6

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3/2,-z+1 #2 -x+1,-y+1,-z+1

Table S5. Crystal data and structure refinement for NQ·H_2O.

Identification code	2110niqn	
Empirical formula	C_{17} H_{14} N_4 O_4	
Formula weight	338.32	
Temperature	190(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.7148(13) Å	α= 90°.
	b = 12.6343(18) Å	β= 101.402(13)°.
	c = 12.9992(14) Å	γ = 90°.
Volume	1564.0(4) $Å^3$	
Z	4	
Density (calculated)	1.437 Mg/m^3	
Absorption coefficient	0.106 mm^{-1}	
F(000)	704	
Crystal size	0.400 x 0.200 x 0.030 mm^3	
Theta range for data collection	3.329 to 25.000°.	
Index ranges	-11<=h<=11, -15<=k<=12, -10<=l<=15	
Reflections collected	6436	
Independent reflections	2750 [R(int) = 0.0471]	
Completeness to theta = 25.000°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2750 / 0 / 226	
Goodness-of-fit on F^2	1.121	
Final R indices [I>2sigma(I)]	R1 = 0.0649, wR2 = 0.1114	
R indices (all data)	R1 = 0.1059, wR2 = 0.1267	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.219 and -0.214 e.$Å^{-3}$	

Table S6. Bond lengths [Å] and angles [°] for NQ·H_2O.

C(1)-N(1)	1.323(3)
C(1)-C(2)	1.413(4)
C(2)-C(3)	1.364(4)
C(2)-C(10)	1.502(3)
C(3)-C(4)	1.411(3)
C(4)-C(9)	1.412(4)
C(4)-C(5)	1.418(4)
C(5)-C(6)	1.372(4)
C(6)-C(7)	1.396(4)
C(7)-C(8)	1.364(4)
C(8)-C(9)	1.415(3)
C(9)-N(1)	1.379(3)
C(10)-O(1)	1.232(3)
C(10)-N(2)	1.354(3)
C(11)-N(3)	1.277(3)
C(11)-C(12)	1.475(3)
C(12)-C(17)	1.393(4)
C(12)-C(13)	1.395(4)
C(13)-C(14)	1.382(4)
C(13)-N(4)	1.472(4)
C(14)-C(15)	1.372(5)
C(15)-C(16)	1.384(4)
C(16)-C(17)	1.380(4)
N(2)-N(3)	1.386(3)
N(4)-O(3)	1.226(3)
N(4)-O(2)	1.238(3)

N(1)-C(1)-C(2)	123.7(3)
C(3)-C(2)-C(1)	118.6(2)
C(3)-C(2)-C(10)	117.7(3)
C(1)-C(2)-C(10)	123.8(2)
C(2)-C(3)-C(4)	120.1(3)
C(3)-C(4)-C(9)	117.6(2)
C(3)-C(4)-C(5)	123.2(3)

C(9)-C(4)-C(5)	119.2(2)
C(6)-C(5)-C(4)	119.6(3)
C(5)-C(6)-C(7)	120.9(3)
C(8)-C(7)-C(6)	121.0(3)
C(7)-C(8)-C(9)	119.7(3)
N(1)-C(9)-C(4)	122.2(2)
N(1)-C(9)-C(8)	118.2(3)
C(4)-C(9)-C(8)	119.6(3)
O(1)-C(10)-N(2)	122.6(2)
O(1)-C(10)-C(2)	120.4(3)
N(2)-C(10)-C(2)	117.0(3)
N(3)-C(11)-C(12)	118.8(3)
C(17)-C(12)-C(13)	116.3(2)
C(17)-C(12)-C(11)	120.6(3)
C(13)-C(12)-C(11)	123.1(3)
C(14)-C(13)-C(12)	123.1(3)
C(14)-C(13)-N(4)	116.1(3)
C(12)-C(13)-N(4)	120.7(2)
C(15)-C(14)-C(13)	118.5(3)
C(14)-C(15)-C(16)	120.6(3)
C(17)-C(16)-C(15)	119.9(3)
C(16)-C(17)-C(12)	121.6(3)
C(1)-N(1)-C(9)	117.8(3)
C(10)-N(2)-N(3)	117.8(2)
C(11)-N(3)-N(2)	114.5(2)
O(3)-N(4)-O(2)	123.7(3)
O(3)-N(4)-C(13)	118.6(2)
O(2)-N(4)-C(13)	117.6(2)

Table S7. Torsion angles [°] for NQ·H_2O.

N(1)-C(1)-C(2)-C(3)	-0.6(4)
N(1)-C(1)-C(2)-C(10)	179.2(2)
C(1)-C(2)-C(3)-C(4)	0.7(4)
C(10)-C(2)-C(3)-C(4)	-179.1(2)
C(2)-C(3)-C(4)-C(9)	-0.3(4)
C(2)-C(3)-C(4)-C(5)	-179.1(2)
C(3)-C(4)-C(5)-C(6)	179.3(2)
C(9)-C(4)-C(5)-C(6)	0.5(4)
C(4)-C(5)-C(6)-C(7)	0.6(4)
C(5)-C(6)-C(7)-C(8)	-0.7(4)
C(6)-C(7)-C(8)-C(9)	-0.4(4)
C(3)-C(4)-C(9)-N(1)	-0.4(4)
C(5)-C(4)-C(9)-N(1)	178.5(2)
C(3)-C(4)-C(9)-C(8)	179.6(2)
C(5)-C(4)-C(9)-C(8)	-1.6(4)
C(7)-C(8)-C(9)-N(1)	-178.5(2)
C(7)-C(8)-C(9)-C(4)	1.5(4)
C(3)-C(2)-C(10)-O(1)	4.8(4)
C(1)-C(2)-C(10)-O(1)	-175.0(3)
C(3)-C(2)-C(10)-N(2)	-175.0(2)
C(1)-C(2)-C(10)-N(2)	5.2(4)
N(3)-C(11)-C(12)-C(17)	16.5(4)
N(3)-C(11)-C(12)-C(13)	-166.2(2)
C(17)-C(12)-C(13)-C(14)	2.5(4)
C(11)-C(12)-C(13)-C(14)	-174.9(3)
C(17)-C(12)-C(13)-N(4)	-175.0(2)
C(11)-C(12)-C(13)-N(4)	7.6(4)
C(12)-C(13)-C(14)-C(15)	-3.0(4)
N(4)-C(13)-C(14)-C(15)	174.6(3)
C(13)-C(14)-C(15)-C(16)	1.0(5)
C(14)-C(15)-C(16)-C(17)	1.2(5)
C(15)-C(16)-C(17)-C(12)	-1.7(4)
C(13)-C(12)-C(17)-C(16)	-0.1(4)
C(11)-C(12)-C(17)-C(16)	177.4(3)

C(2)-C(1)-N(1)-C(9)	-0.1(4)
C(4)-C(9)-N(1)-C(1)	0.6(4)
C(8)-C(9)-N(1)-C(1)	-179.4(2)
O(1)-C(10)-N(2)-N(3)	-3.5(4)
C(2)-C(10)-N(2)-N(3)	176.3(2)
C(12)-C(11)-N(3)-N(2)	-179.8(2)
C(10)-N(2)-N(3)-C(11)	178.7(2)
C(14)-C(13)-N(4)-O(3)	31.3(4)
C(12)-C(13)-N(4)-O(3)	-151.1(3)
C(14)-C(13)-N(4)-O(2)	-145.1(2)
C(12)-C(13)-N(4)-O(2)	32.5(4)

Table S8. Hydrogen bonds for NQ·H_2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1)-H(1)...O(4)#1	0.95	2.33	3.276(3)	170.9
C(8)-H(8)...O(2)#2	0.95	2.46	3.352(4)	156.6
C(11)-H(11)...O(4)#1	0.95	2.52	3.323(3)	142.2
N(2)-H(2)...O(4)#1	0.88	2.02	2.884(3)	165.4
O(4)-H(4A)...N(1)#3	0.82	2.05	2.861(3)	168.2
O(4)-H(4B)...O(1)	0.82	2.03	2.830(3)	164.7

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z+3/2 #2 -x+1,-y+2,-z+1 #3 x,-y+3/2,z+1/2