Supplementary

Enhanced photocatalytic degradation of 2-thiobenzimidazole by *Tris*(8-quinolinolato)cobalt(III) complex through peroxide adduct formation: Theoretical and experimental investigation

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Fig. S1. FTIR of 8-hydroxyquinoline

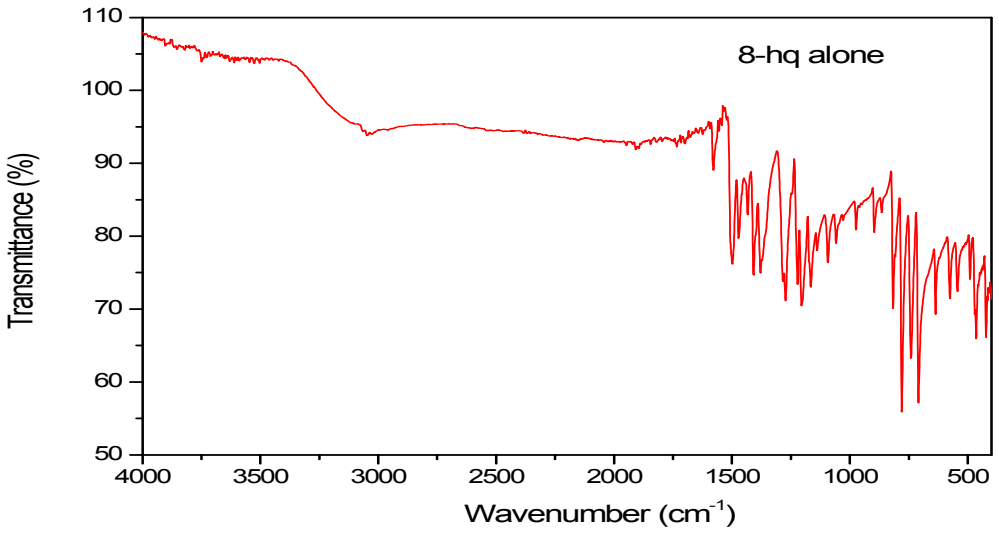

Fig. S1. FTIR of [$CrQ3.C_2H_5OH$]

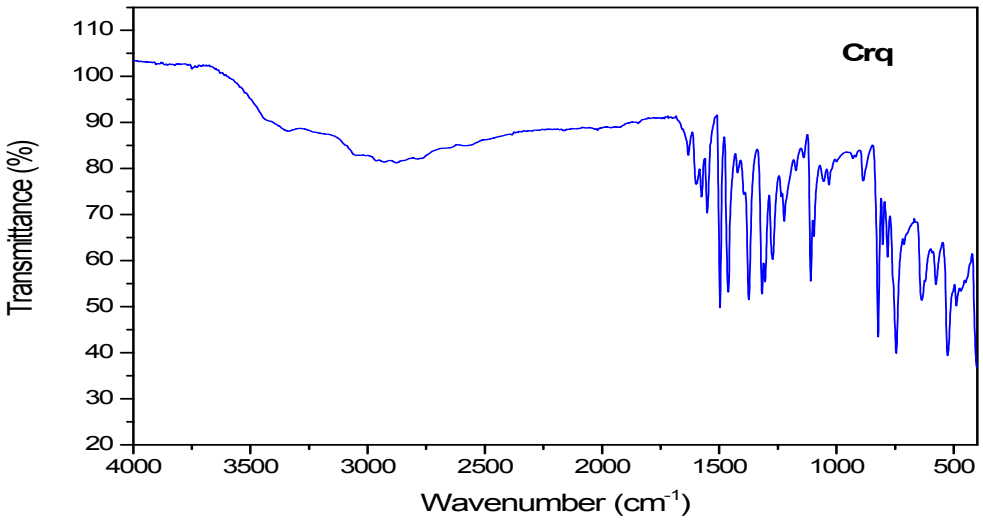

Fig. S1. FTIR of [$CoQ3.C_2H_5OH$]

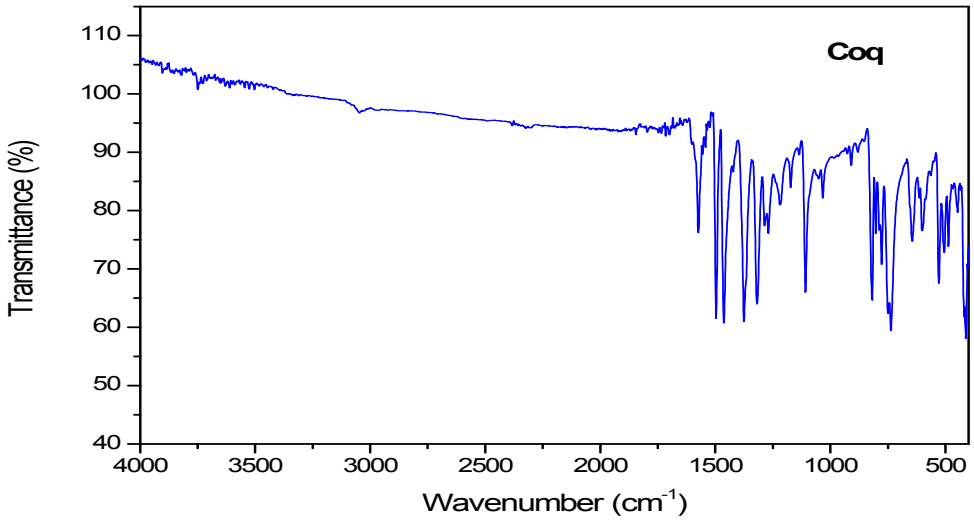

Fig. S1. FTIR of [FeQ3.C_2H_5OH]

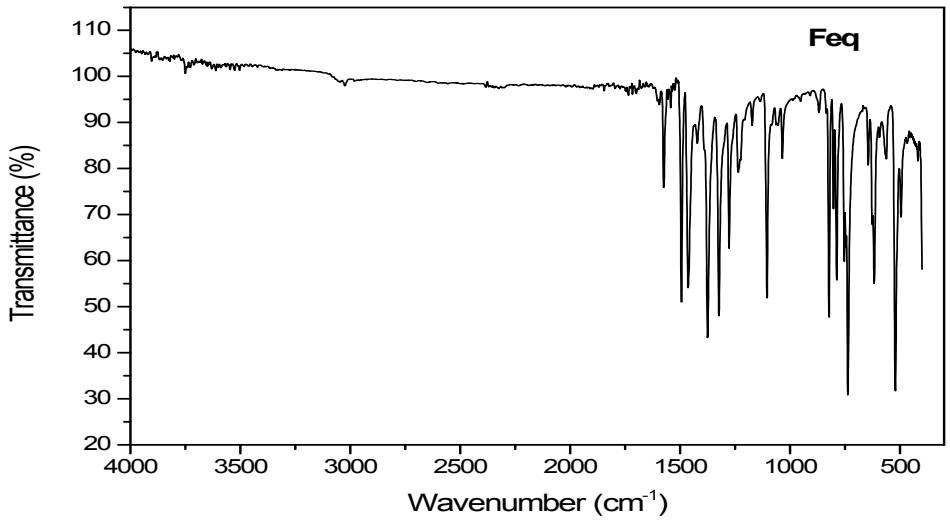

Figure S2. ^{1}H NMR (Full) spectra of the metal complexes of 8-hydroxyquinoline with Cr^{3+}, Fe^{3+}, and Co^{3+}.

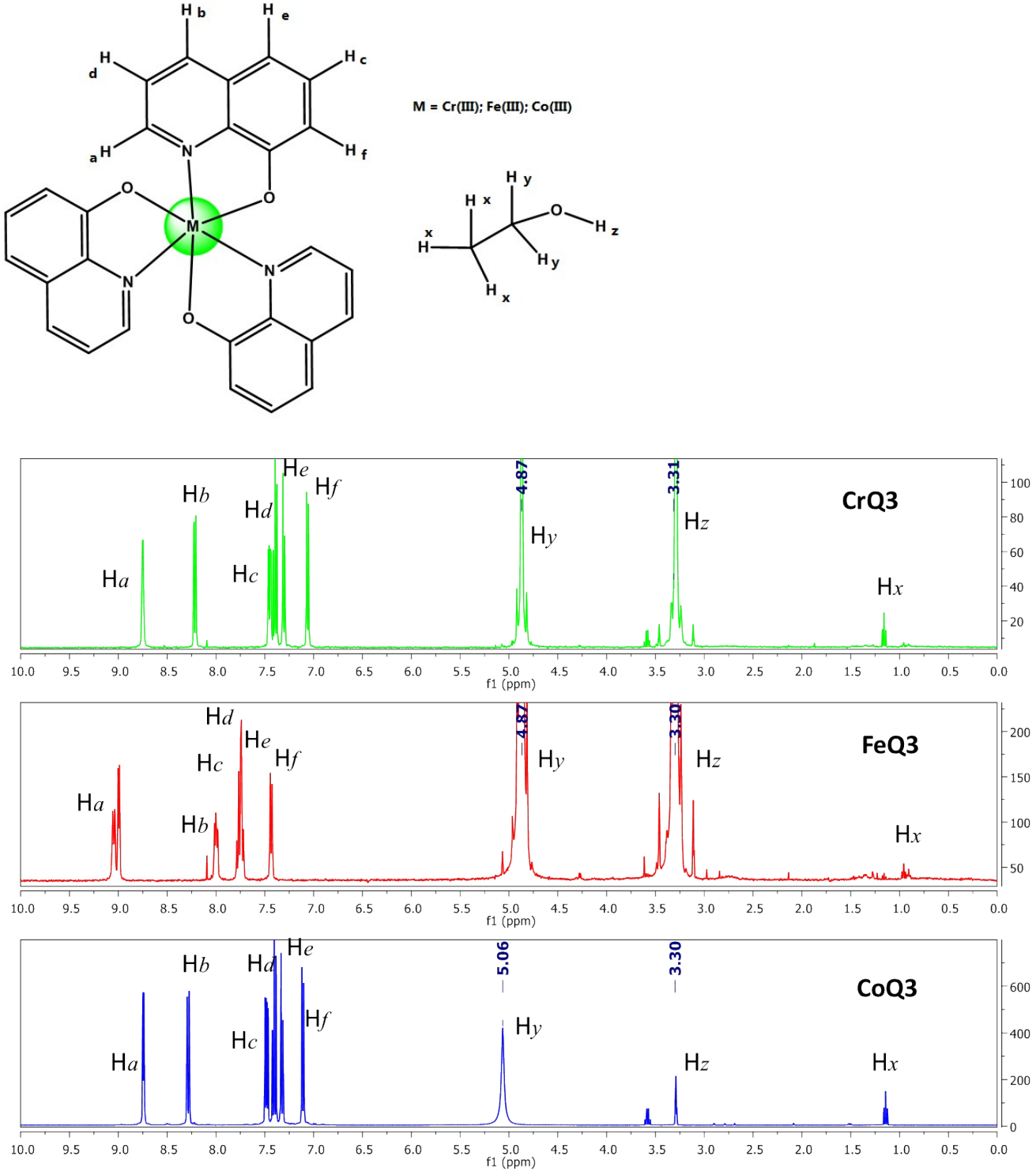

Figure S2. ^{1}H NMR (Aromatic region) spectra of the metal complexes of 8-hydroxyquinoline with Cr^{3+}, Fe^{3+}, and Co^{3+}.

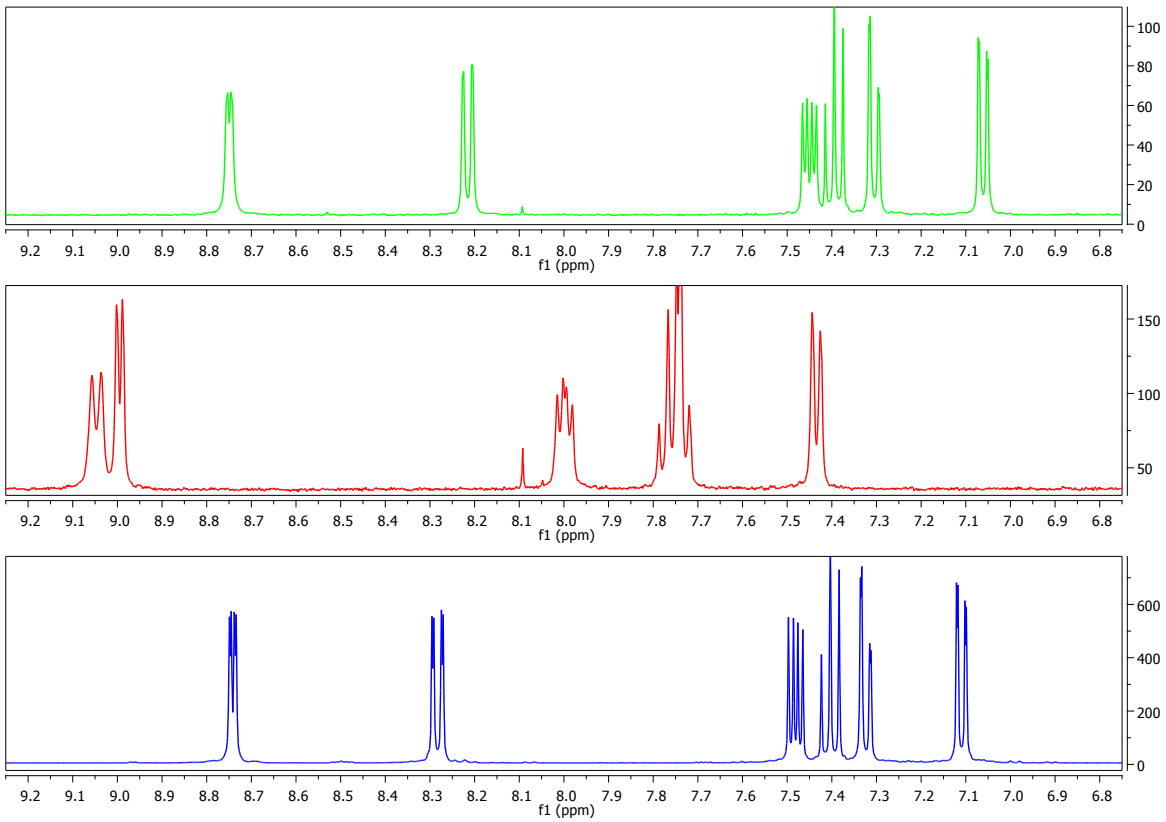

Figure S2. ^{1}H NMR (Aliphatic region) spectra of the metal complexes of 8-hydroxyquinoline with Cr^{3+}, Fe^{3+}, and Co^{3+}.

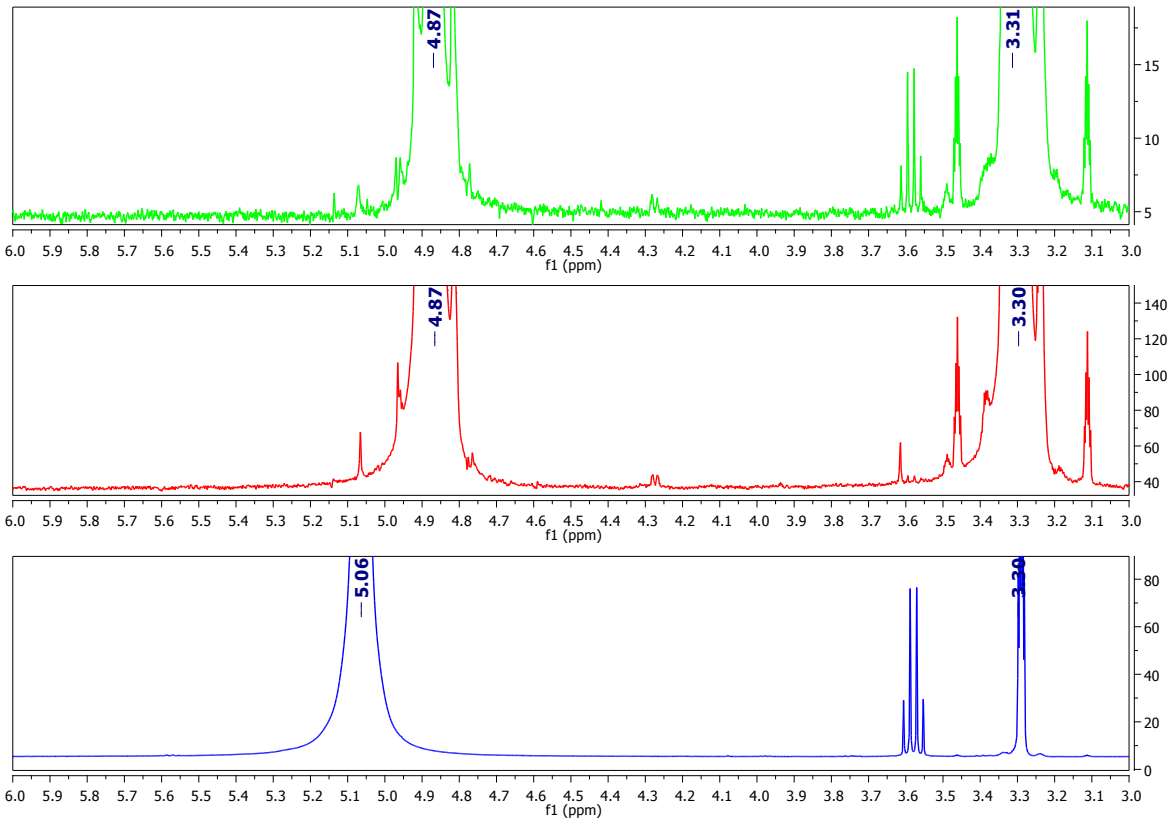

Figure. S3 Pseudo first order kinetics for 2-TBI during the degradation by metal complexes at neutral pH (pH=4.0± 0.5) without the visible light irradiation.

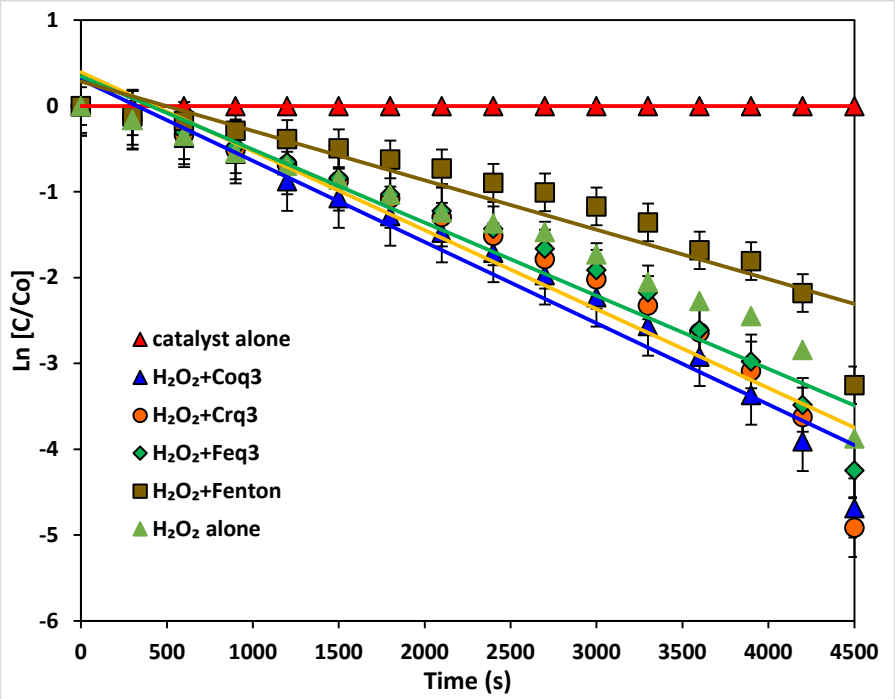

Figure. S4. Pseudo first order kinetics for 2-TBI during the degradation by metal complexes at neutral pH (pH=4.0± 0.5) under visible light irradiation.

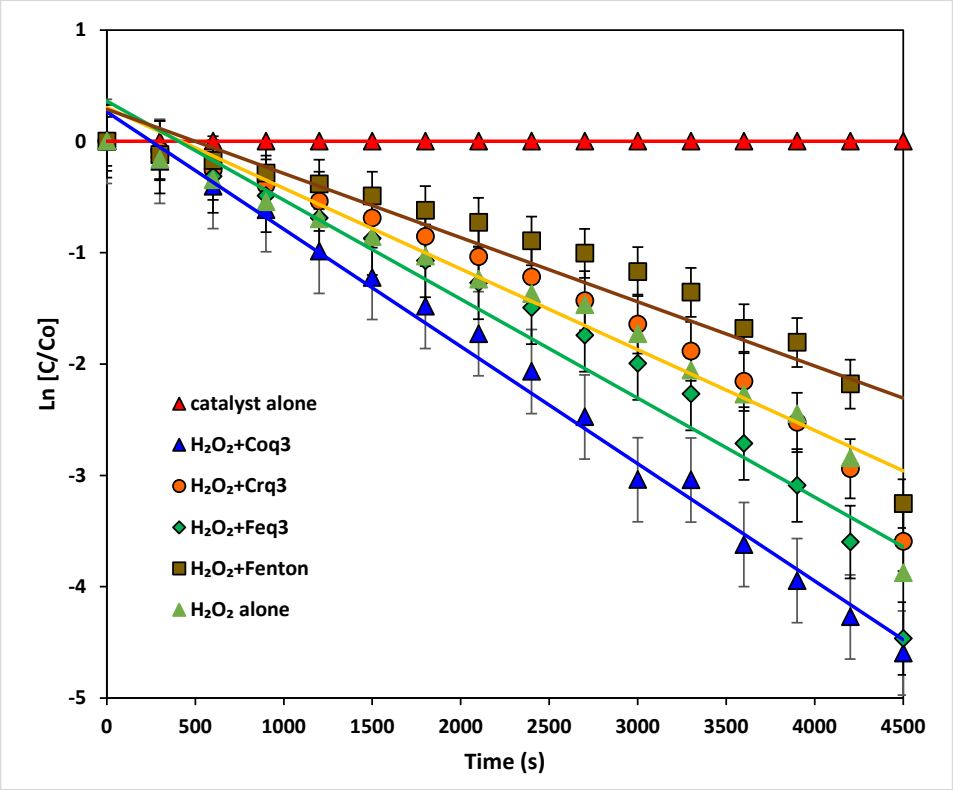
1
0
-1
-2
-3
-4
-5
Ln [C/Co]
0
500
1000
1500
2000
2500
3000
3500
4000
4500
Time (s)
catalyst alone
H₂O₂+Coq3
H₂O₂+Crq3
H₂O₂+Feq3
H₂O₂+Fenton
H₂O₂ alone

Figure S5. ^{1}H NMR (400 MHz) spectra for oxidized product of 2-TBI; a) aromatic region of 2-TBI standard; b) aliphatic region of 2-TBI standard; c) aromatic region of 2-TBI after 3hrs photocatalysed oxidation with **CoQ3**; d) aliphatic region of 2-TBI after 3hrs photocatalysed oxidation with **CoQ3**.

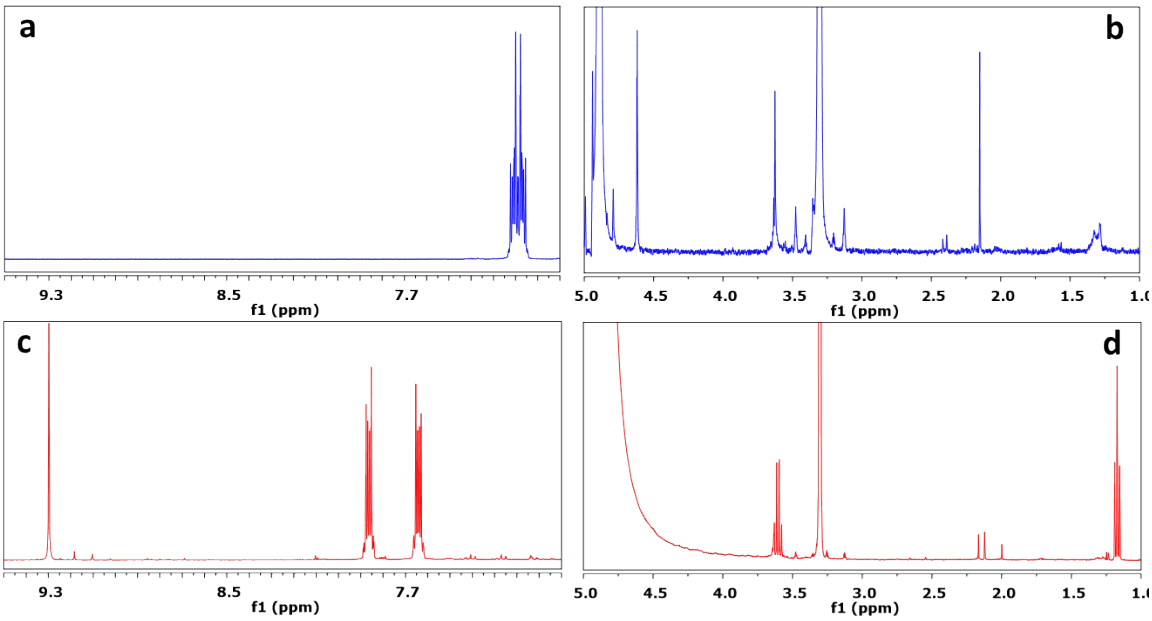

Figure S6. Electronic configuration for the metal complexes of HQ ligand (Degeneracy threshold 0.004 Hf)

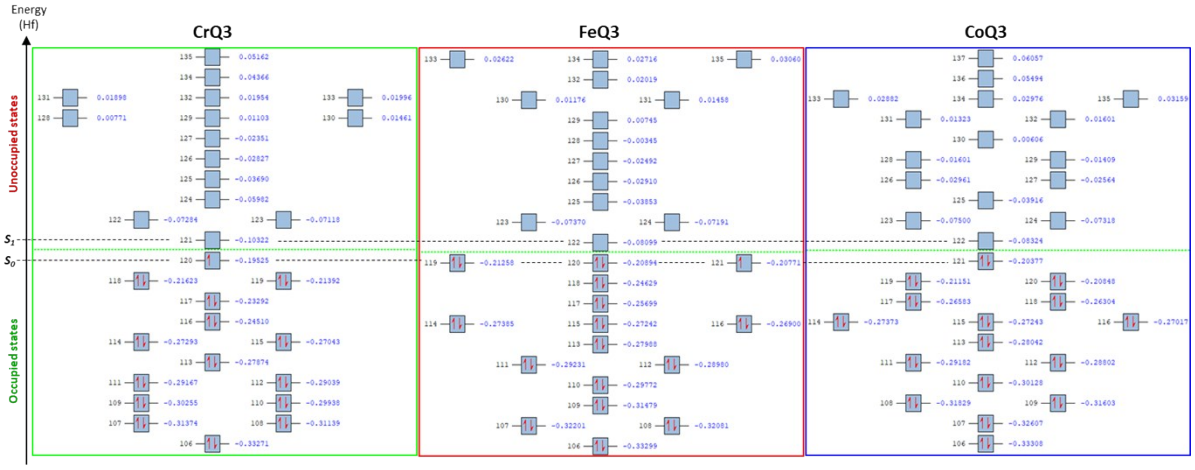

Table S1. Comparison of FTIR spectral vibrations of 8-HQ and its metal complexes

Type of vibration and assignments	Range (cm^{-1}) and Intensity	Frequency (cm^{-1}) and Intensity (multiplicity)				
		8-HQ alone	**CoQ3**	**FeQ3**	**CrQ3**	
C-N-C in amines (bend)	510-400s	423w, 463w, 490w	414m, 499m(d)	416vw,492m	----------	
Ring in benzene derivatives (in plane and out of plane ring deformations-two bands)	580-420m-s	545w (d)	527m	520m, 562vs	520vs, 559w	
Pyridine ring (in plane ring formation)	635-605m-s	635m	643m	616m, 646w	616s, 644w	
Ar-OH in phenol (OH out of plane deformation)	720-600s-br	709vs	----------	----------	----------	
O-H bend (out-of-plane)	650-770m-w	739s, 783s	733m, 778m	736vs	735vs, 754m	
=C-H & =CH2 (out-of-plane bending)	780-850m	----------	819m	821vs	801m, 821m	
CH_2=CH- (-CH_2 out of plane wag)	950-900vs	898w (d), 974vw	910vw (d)	868vw	868vw	
C-O-H in alcohols (C-O stretch)	1200-1015vs	1097w, 1166m, 1204m	1106m, 1169w	1105vs, 1172w	1105s, 1173w	
C-N in aromatic amines	1280-1180s	1223m, 1273m	1216w, 1276w	1234m, 1276vs	1232w (d), 1277m	
Ring vibrations in plan (C-H) deformation	1330-1300s	----------	1318w	1320vs	1321s	
O-H bending (in-plane)	1330-1430s	1381m (d)	1372m	1376 vs	1373vs	
α-CH_2 bending	1400-1450s	----------	1462m	1463s	1462vs	
Benzene ring in aromatic compounds (ring stretch, Sharp bands)	1515-1485m	1501m (d)	1497s	1495s	1497vs	

Pyridine derivatives	1615-1565s	1580w	1574m	1572m	1574m	
ν(OH) stretching vibration of phenolic group	3200-3000m	3040m	----------	----------	----------	