Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2019

Electronic Supplementary Information (ESI)

Photochemical oxidation of water catalysed by cyclometalated Ir(III) complexes bearing Schiff-base ligands

Rekha Dhiman and C. M. Nagaraja*

Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar 140001, Punjab, India.

Email: cmnraja@iitrpr.ac.in

Contents:

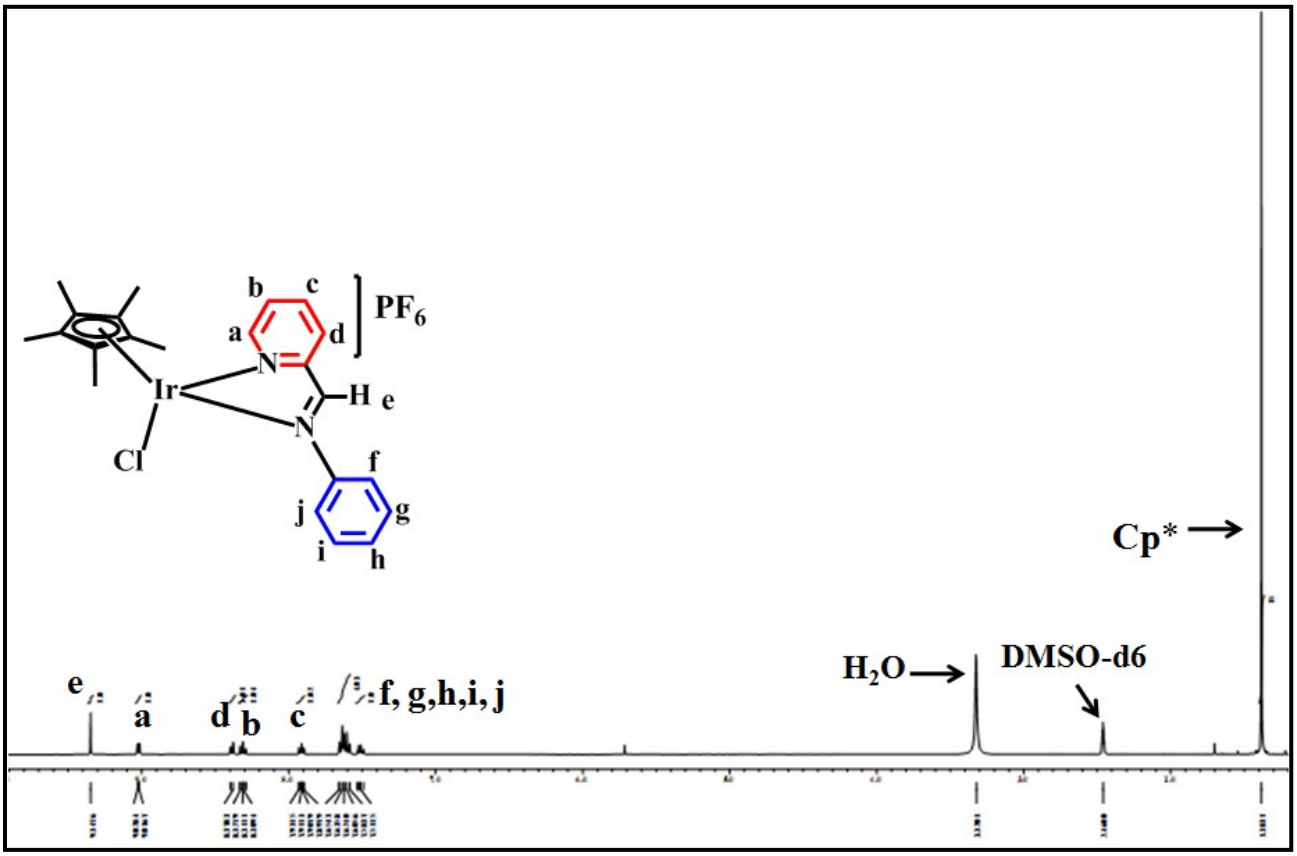

Fig. S1 ^{1}H NMR spectra of complex **1** recorded in DMSO-d_6

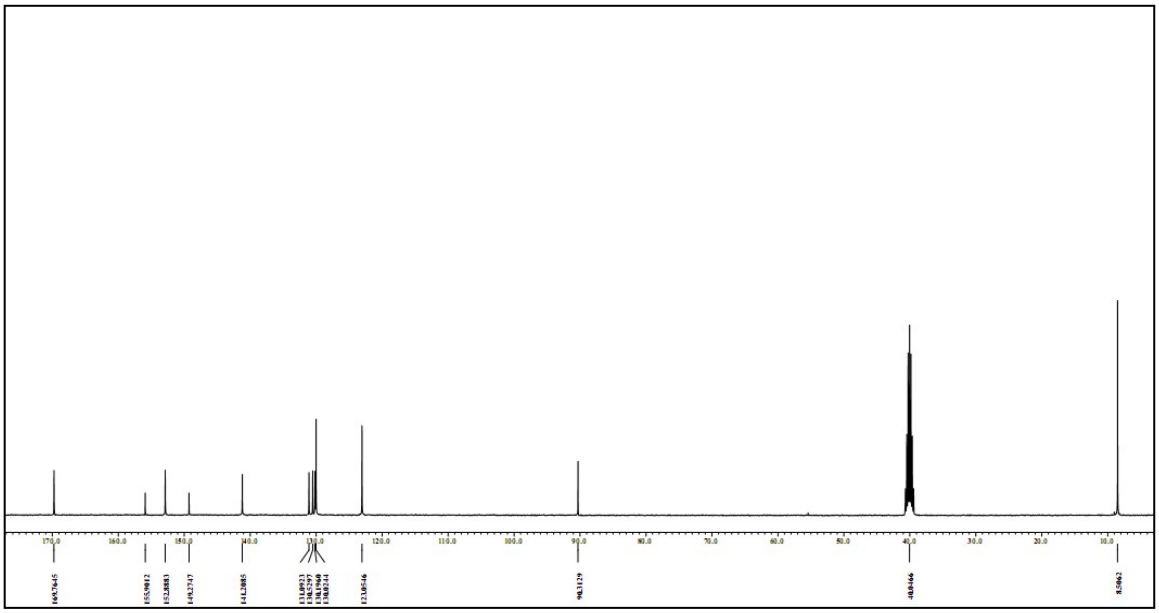

Fig. S2 ^{13}C NMR spectra of complex **1** recorded in DMSO-d_6

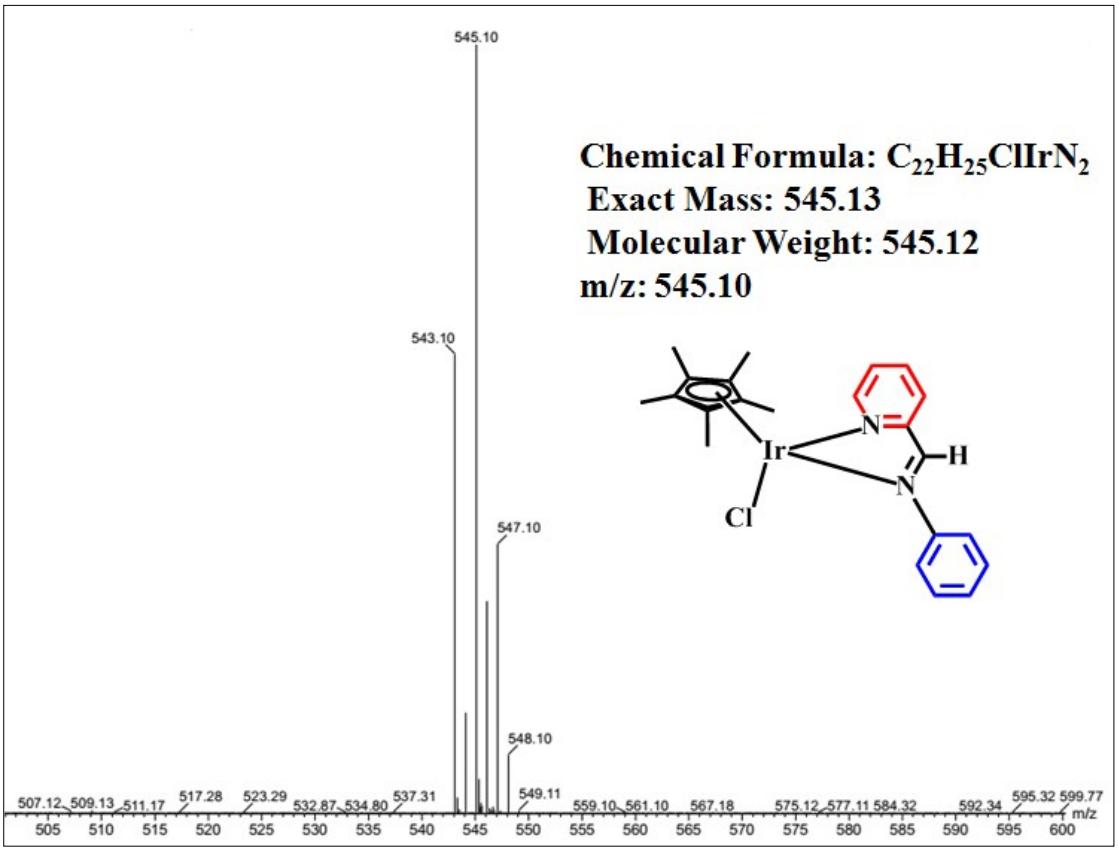

Fig. S3 HRMS spectrum of complex **1** recorded in MeCN

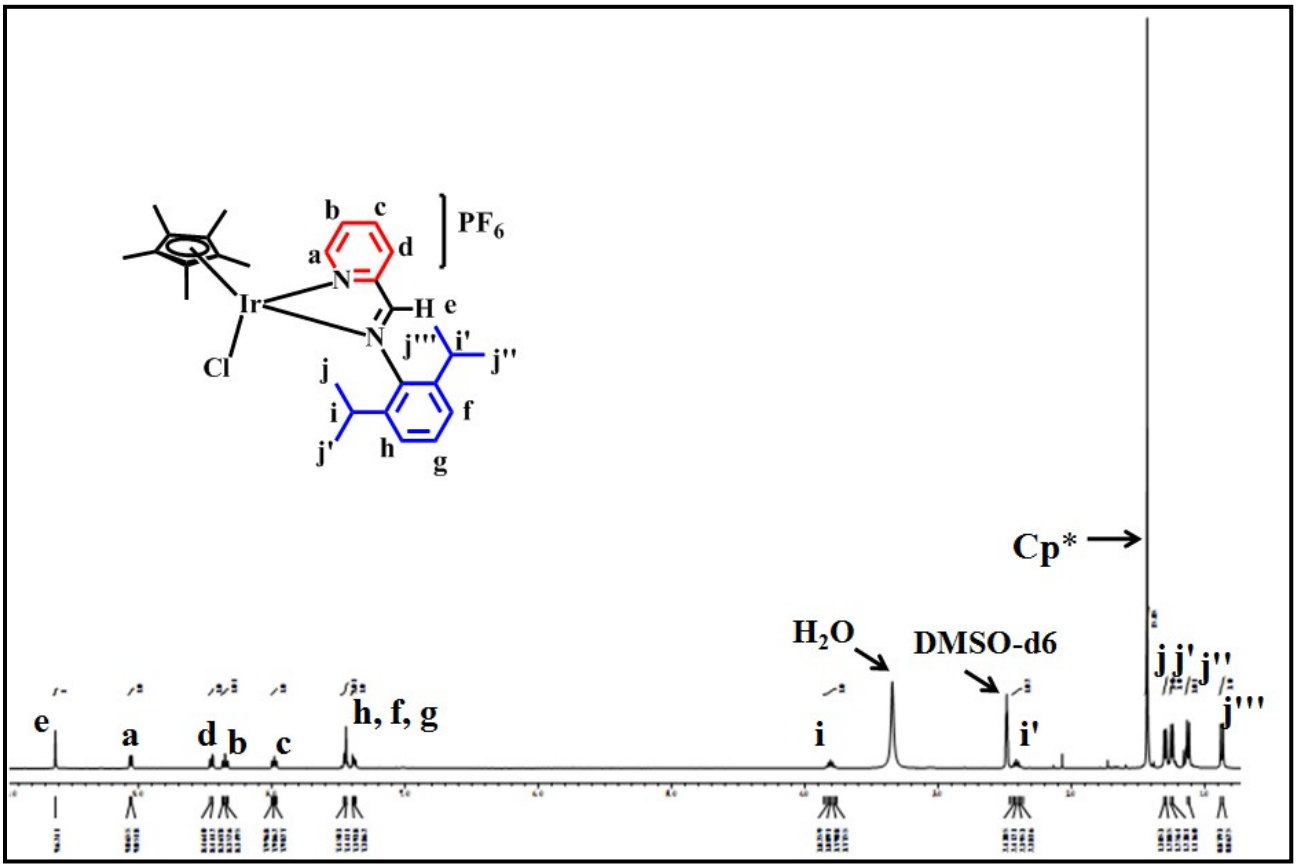

Fig. S4 ^{1}H NMR spectra of complex **2** recorded in DMSO-d_6

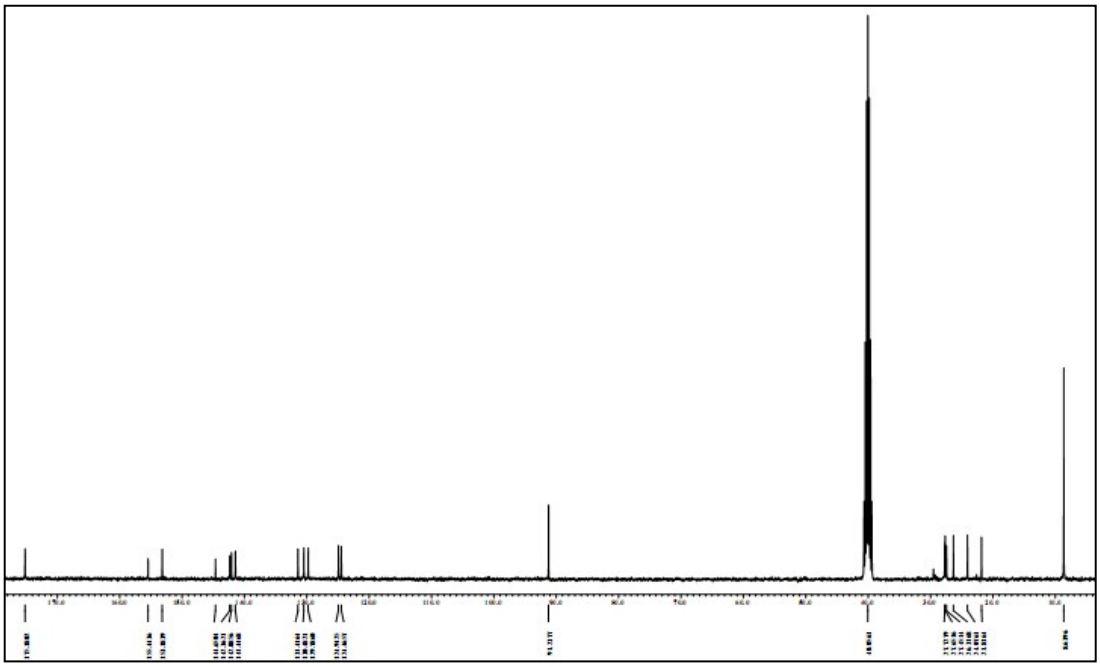

Fig. S5 ^{13}C NMR spectra of complex **2** recorded in DMSO-d_6

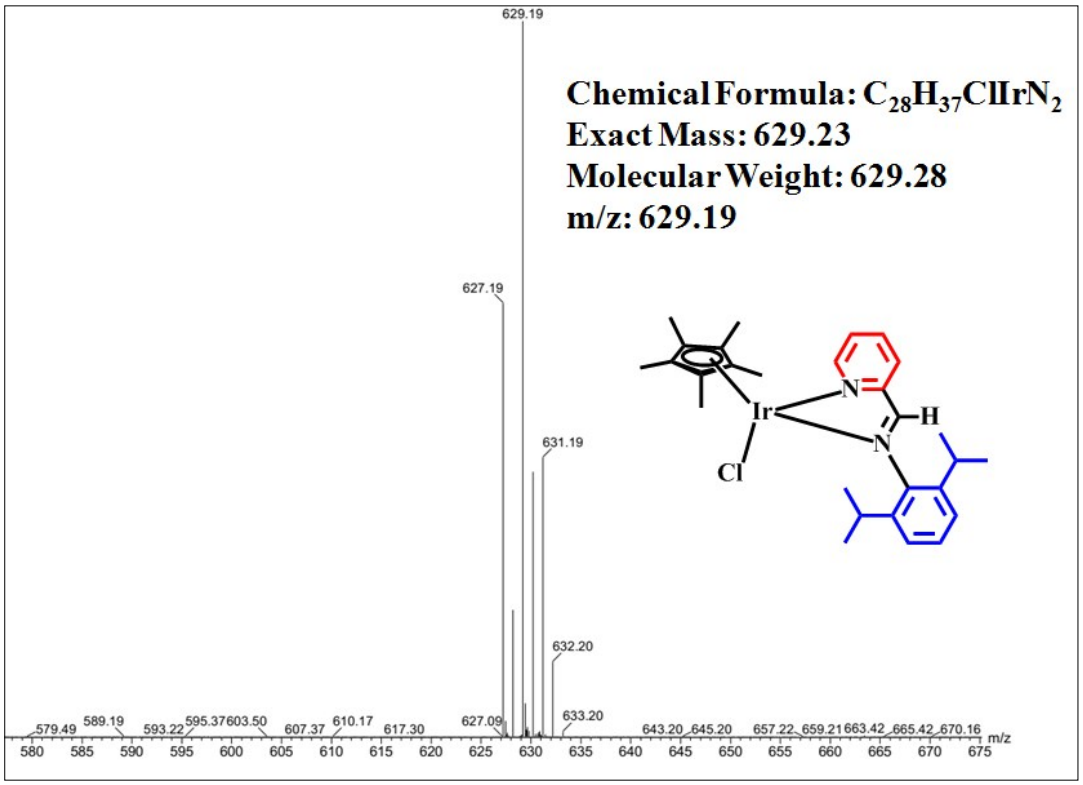

Fig. S6 HRMS spectrum of complex **2** recorded in MeCN.

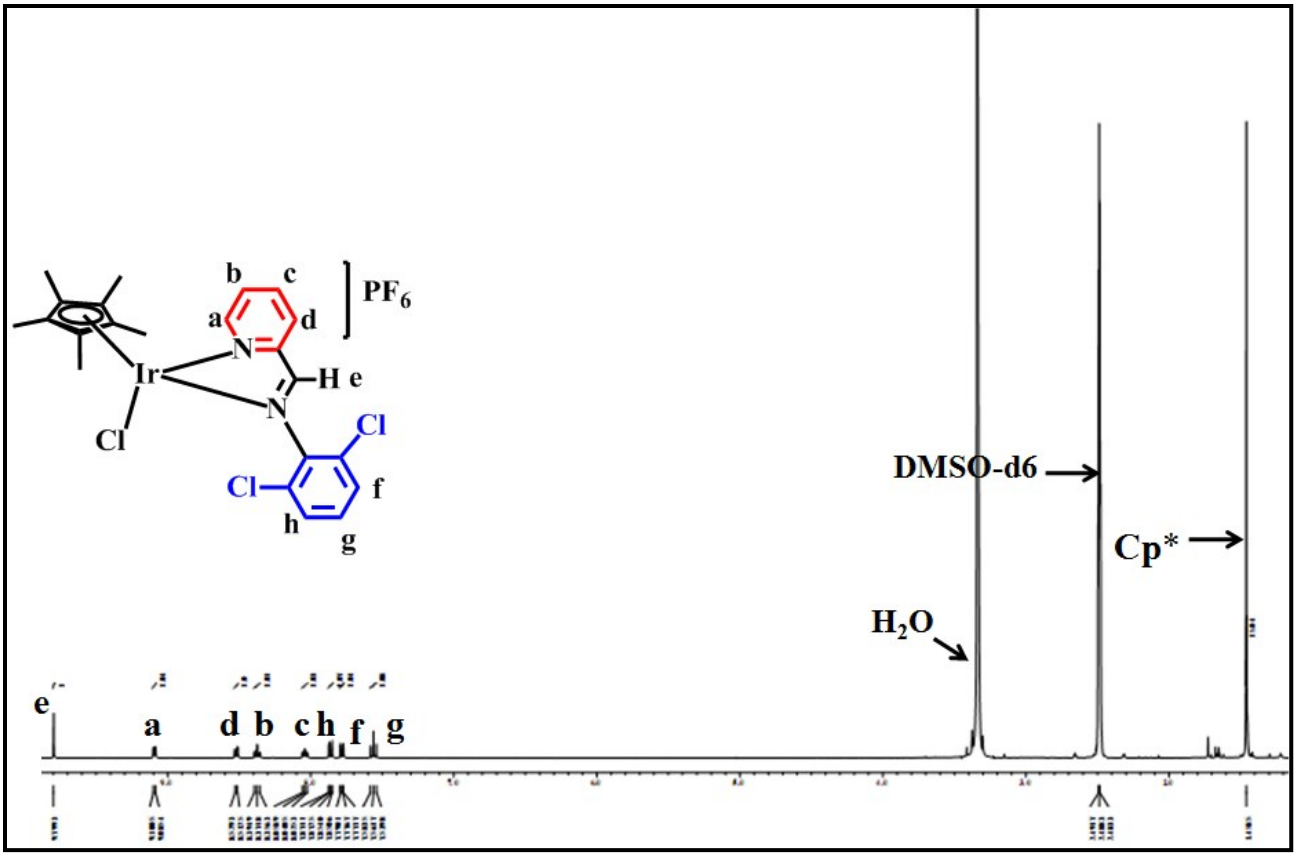

Fig. S7 ^{1}H NMR spectra of complex **3** recorded in DMSO-d_6

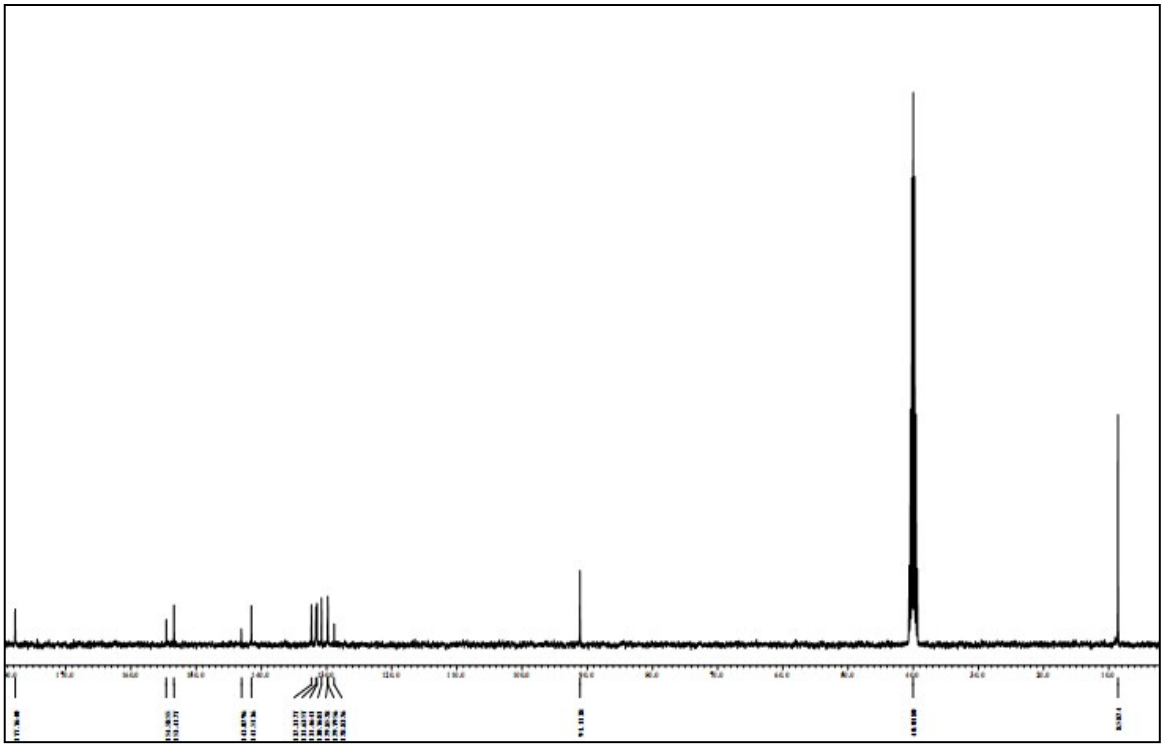

Fig. S8 ^{13}C NMR spectra of complex **3** recorded in DMSO-d_6

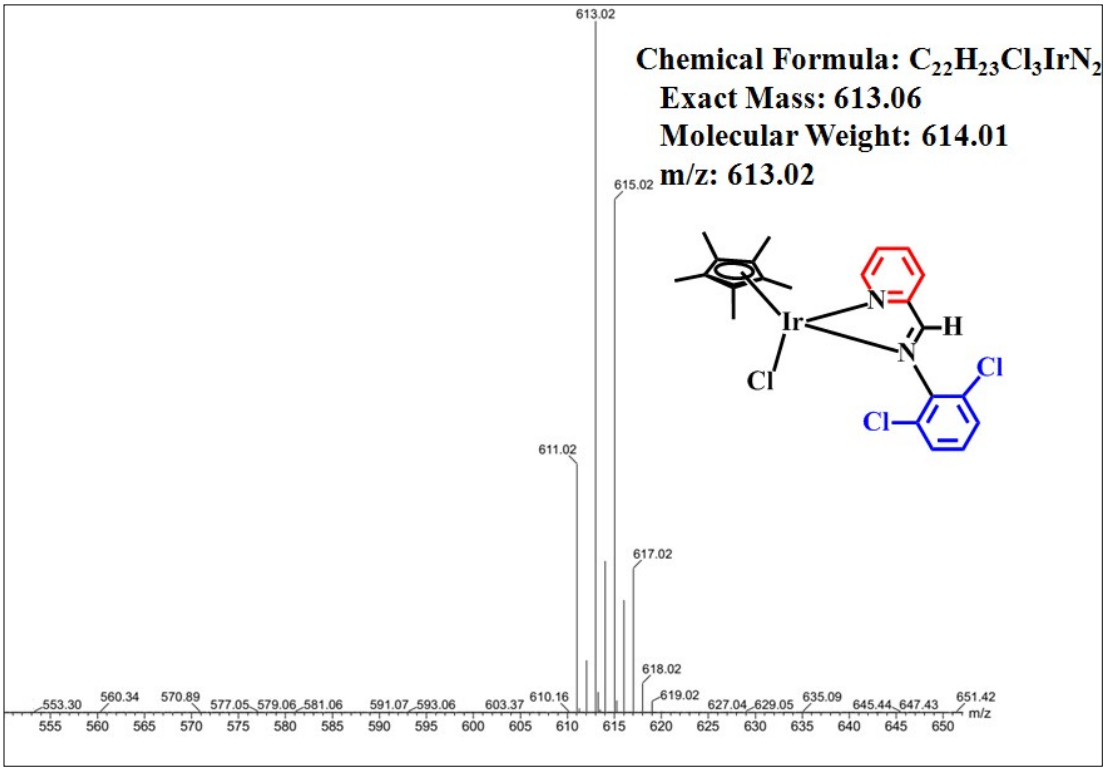

Fig. S9 HRMS spectrum of complex **3** recorded in MeCN.

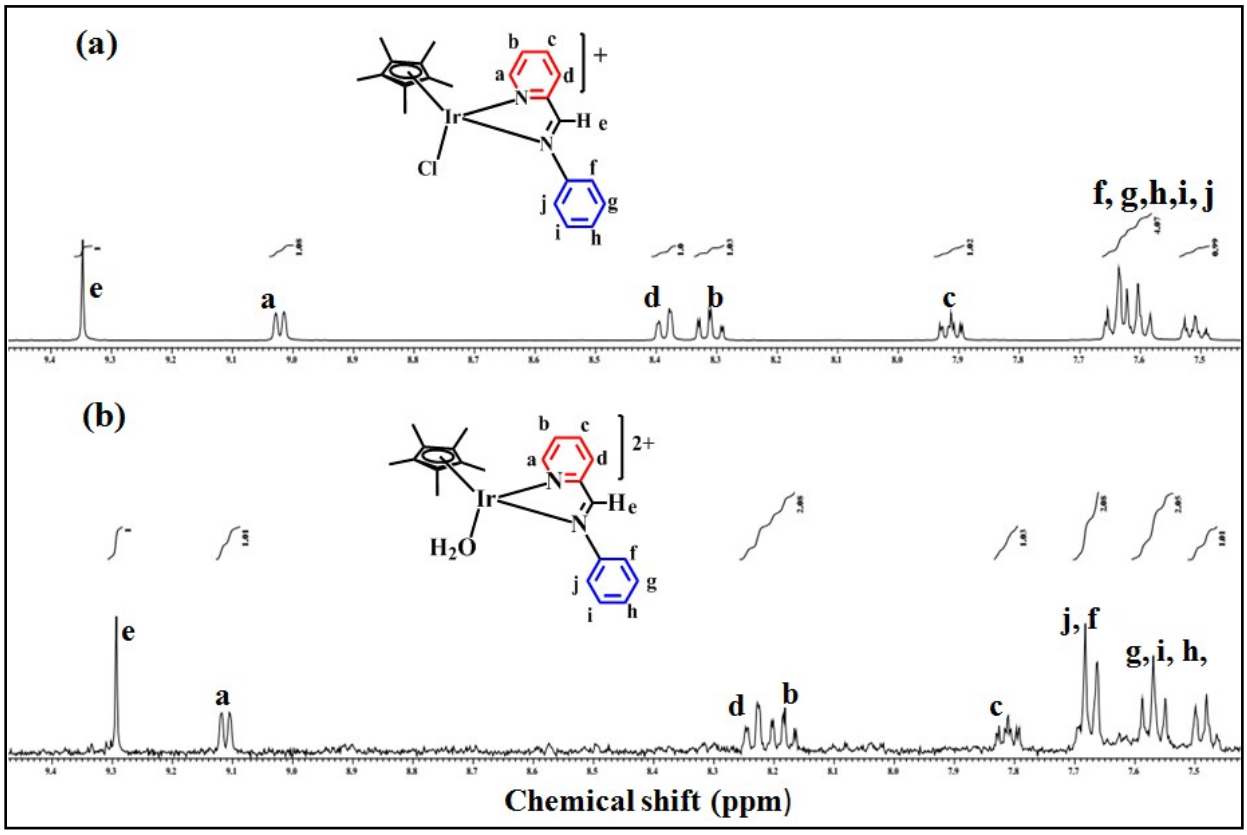

Fig. S10 ^{1}H NMR spectra of complex **1** (a) before catalysis (b) isolation of aqua-complex after catalysis**.**

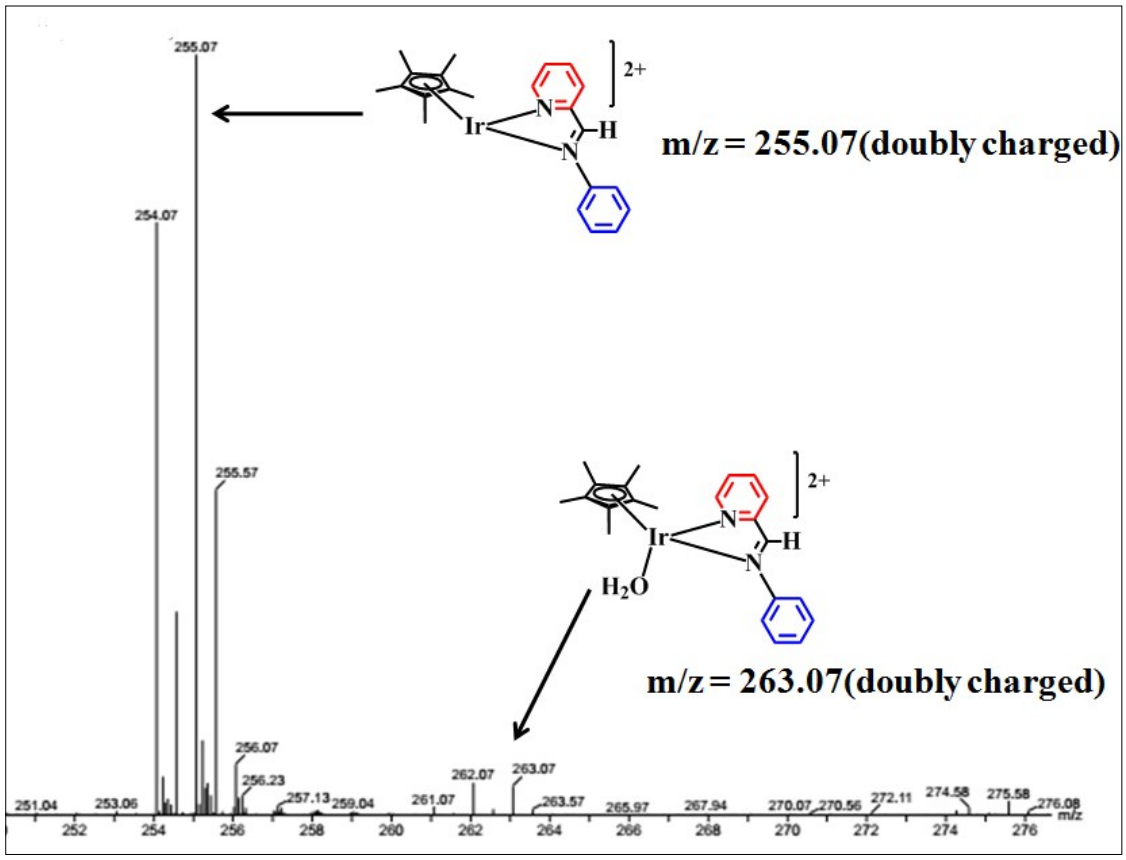

Fig. S11 Mass spectra of aqua-complex of **1** isolated after photocatalytic reaction.

Table S1. Selected bond distances (Å) and angles (°) for complexes **2** & **3**

Complex 2			
Ir(1)-Cl(1)	2.3978(11)	Ir(1)-C(21)	2.188(2)
Ir(1)-N(1)	2.1038(19)	Ir(1)-C(23)	2.189(2)
Ir(1)-N(2)	2.1026(19)	Ir(1)-C(25)	2.164(2)
Ir(1)-Cl(19)	2.166(2)	Ir(1)-C(27)	2.190(2)
Cl(1)-Ir(1)-N(1)	81.07(5)	N(1)-Ir(1)-C(21)	102.15(7)
Cl(1)-Ir(1)-N(2)	88.09(5)	N(1)-Ir(1)-C(23)	127.07(8)
Cl(1)-Ir(1)-Cl(19)	156.49(6)	N(1)-Ir(1)-C(25)	165.50(7)
Cl(1)-Ir(1)-Cl(21)	119.06(6)	N(1)-Ir(1)-C(27)	142.41(7)
Cl(1)-Ir(1)-Cl(23)	92.36(6)	N(2)-Ir(1)-C(19)	114.83(7)
Cl(1)-Ir(1)-Cl(25)	100.38(6)	N(2)-Ir(1)-C(21)	152.50(7)
Cl(1)-Ir(1)-Cl(27)	136.51(6)	N(2)-Ir(1)-C(23)	156.46(8)
N(1)-Ir(1)-N(2)	76.24(7)	N(2)-Ir(1)-C(25)	118.14(7)
N(1)-Ir(1)-Cl(19)	108.41(7)	N(2)-Ir(1)-C(27)	100.13(7)
Complex 3			
Ir(1)-Cl(1)	2.390(2)	Ir(1)-Cl(15)	2.195(8)
Ir(1)-N(1)	2.101(6)	Ir(1)-Cl(17)	2.172(8)
Ir(1)-N(2)	2.109(6)	Ir(1)-Cl(19)	2.152(7)
Ir(1)-Cl(13)	2.171(8)	Ir(1)-Cl(21)	2.177(8)

Cl(1)-Ir(1)-N(1)	81.76(16)	Cl(1)-Ir(1)-Cl(15)	124.4(2)
Cl(1)-Ir(1)-N(2)	89.31(15)	Cl(1)-Ir(1)-Cl(17)	94.0(2)
Cl(1)-Ir(1)-Cl(13)	156.8(3)	Cl(1)-Ir(1)-Cl(19)	95.8(2)
Cl(1)-Ir(1)-C(21)	128.9(2)	N(1)-Ir(1)-N(2)	75.7(2)
N(1)-Ir(1)-C(13)	117.4(3)	N(1)-Ir(1)-C(15)	153.8(3)
N(1)-Ir(1)-C(17)	156.7(3)	N(1)-Ir(1)-C(19)	118.1(3)
N(1)-Ir(1)-C(21)	101.1(3)	N(2)-Ir(1)-C(13)	107.4(3)
N(2)-Ir(1)-C(15)	102.5(3)	N(2)-Ir(1)-C(17)	127.4(3)
N(2)-Ir(1)-Cl(19)	165.9(3)	N(2)-Ir(1)-Cl(21)	141.3(3)
C(13)-Ir(1)-Cl(15)	37. 3(4)	C(13)-Ir(1)-Cl(17)	63. 1(3)
C(13)-Ir(1)-Cl(19)	64.4(3)	C(13)-Ir(1)-Cl(21)	39. 2(3)
C(15)-Ir(1)-Cl(17)	37. 0(3)	C(15)-Ir(1)-Cl(19)	63. 8(3)
C(15)-Ir(1)-Cl(21)	63. 6(3)	C(17)-Ir(1)-Cl(19)	39. 2(3)

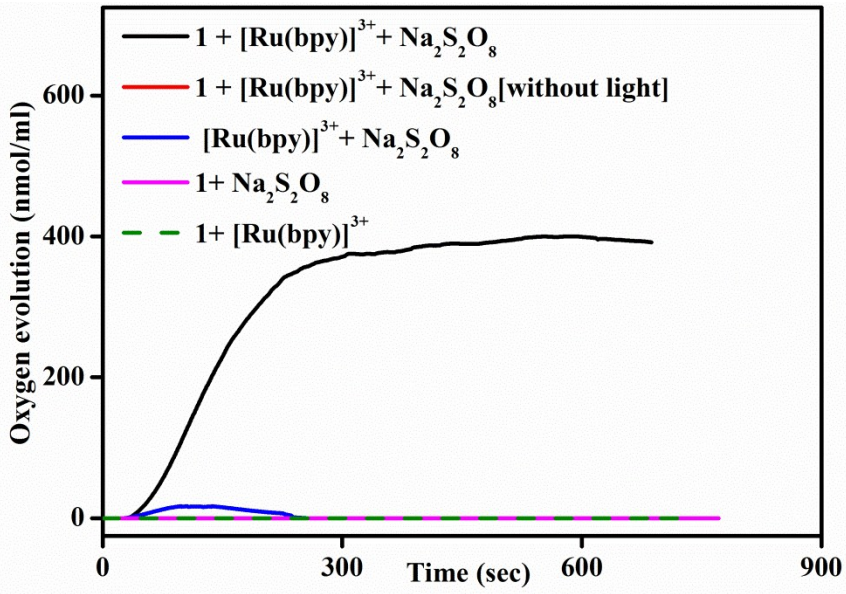

Fig. S12 Photochemical water oxidation experiment carried out in the presence of **1**, $[Ru(bpy)_3]^{2+}$ (PS), $Na_2S_2O_8$ (SO) at pH 7.2 (phosphate buffer).

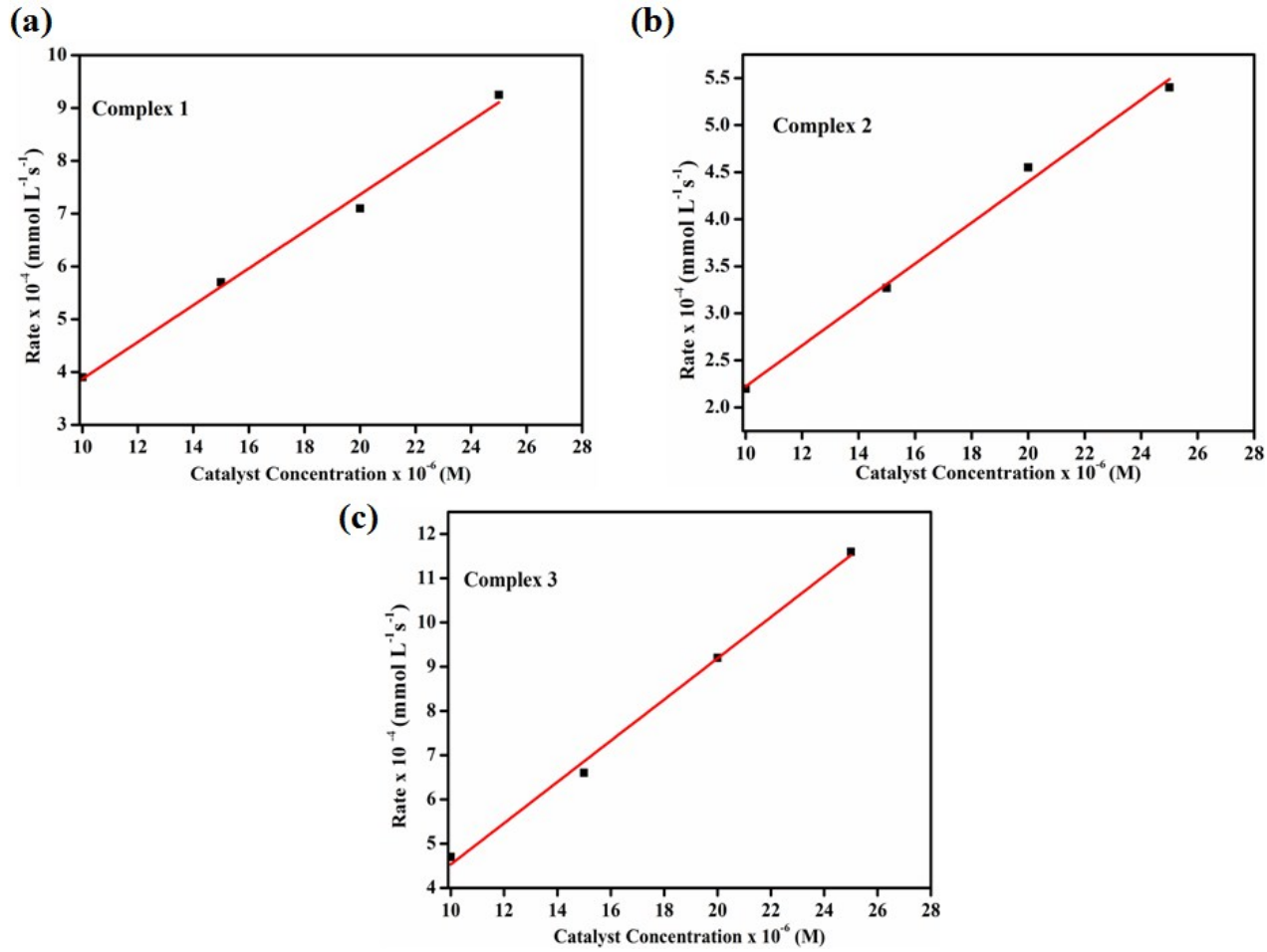

Fig. S13 a) First-order kinetic plot for the rate of O_2 evolution by complex **1** b) complex **2** and c) complex **3**.

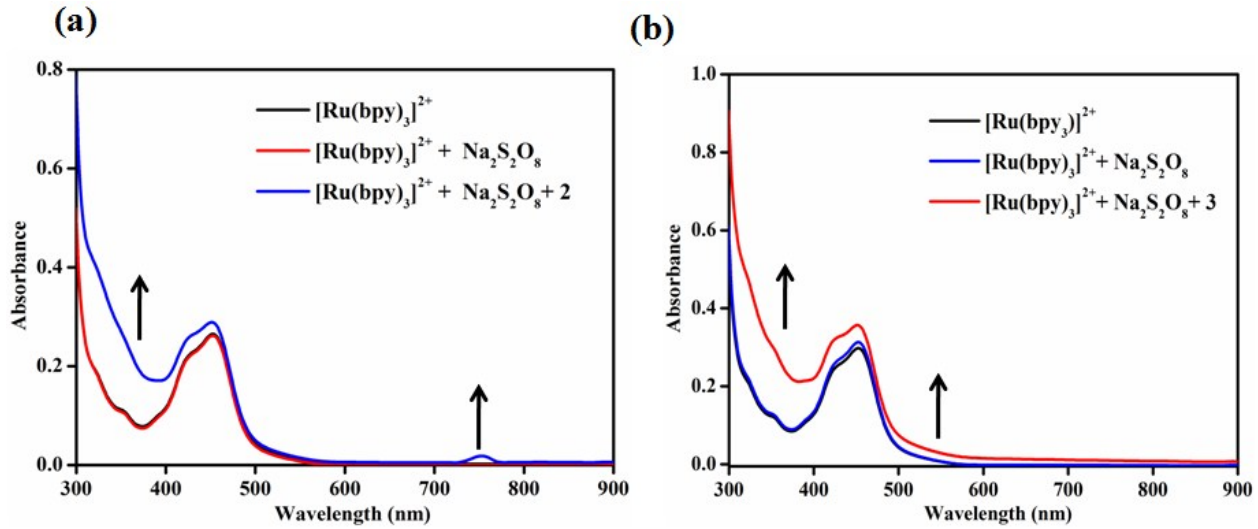

Fig. S14 UV-vis spectra of photochemical reaction after irradiation for **2** and **3**.

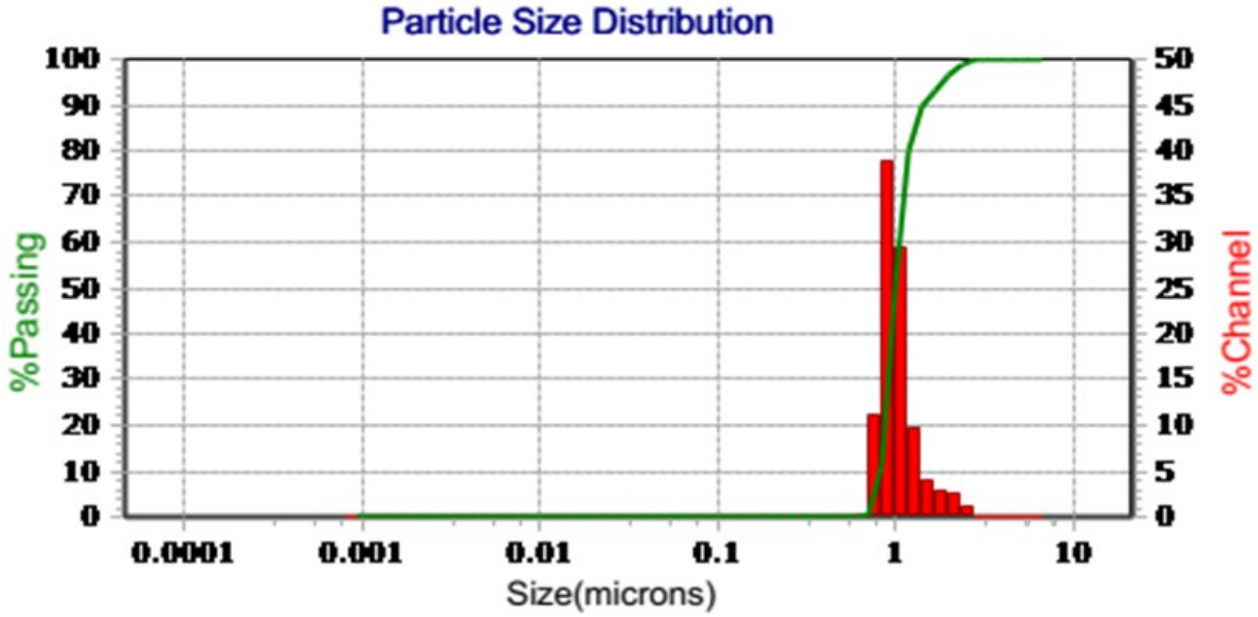

Fig. S15 DLS spectra of the photochemical reaction mixture catalyzed by complex **1**

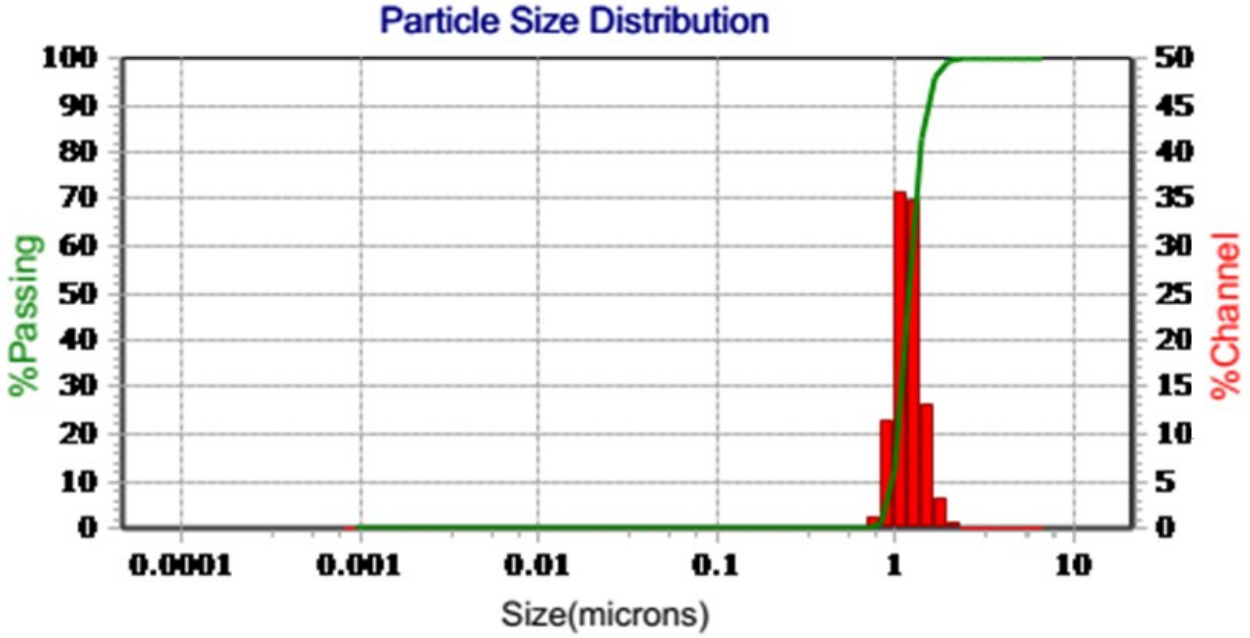

Fig. S16 DLS spectra of photochemical reaction mixture catalyzed by complex **2**.

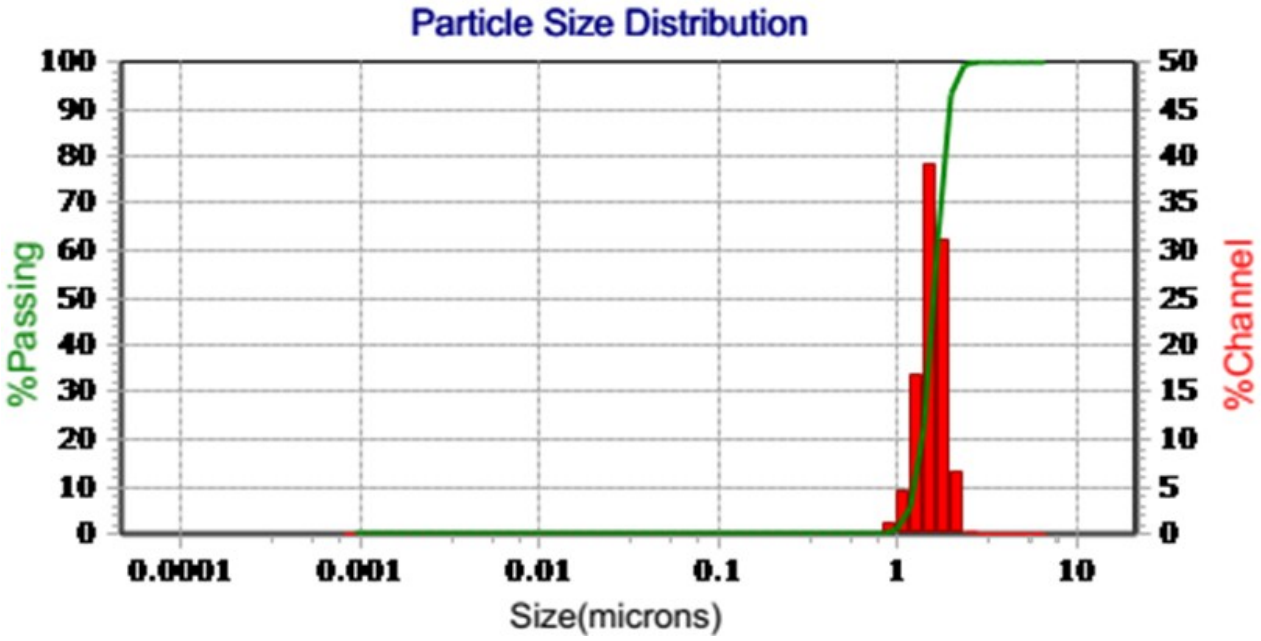

Fig. S17 DLS spectra of photochemical reaction mixture catalyzed by complex **3**.