

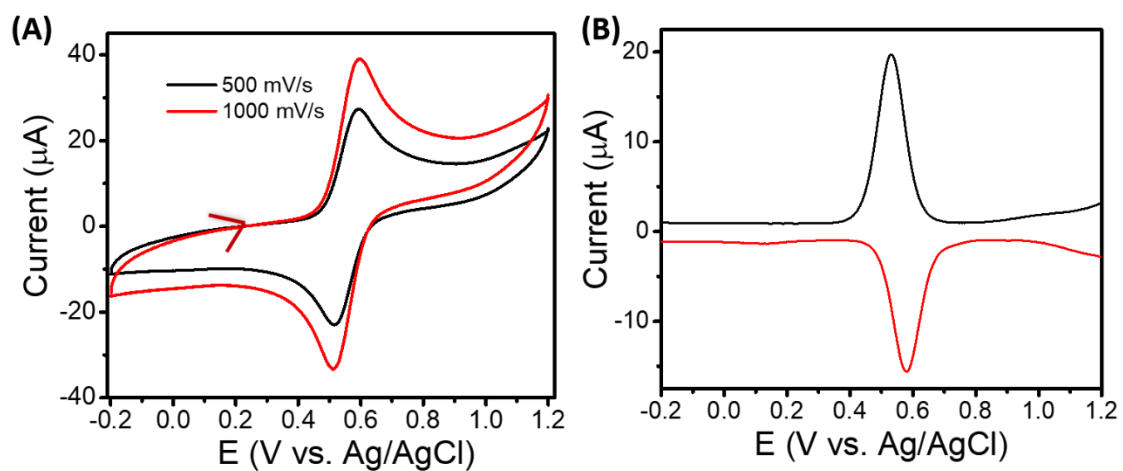
**Supporting information**

**A Cu(II) pseudopeptide complex: Surrogate to a *formal* Cu(III) species in water and inhibitor of cancer cell proliferation**

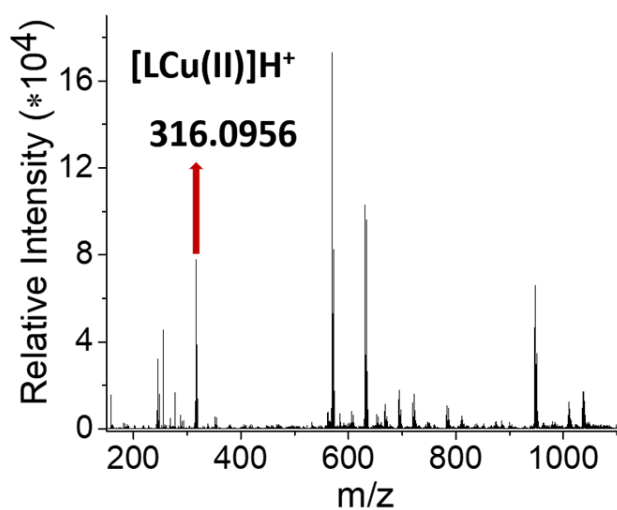
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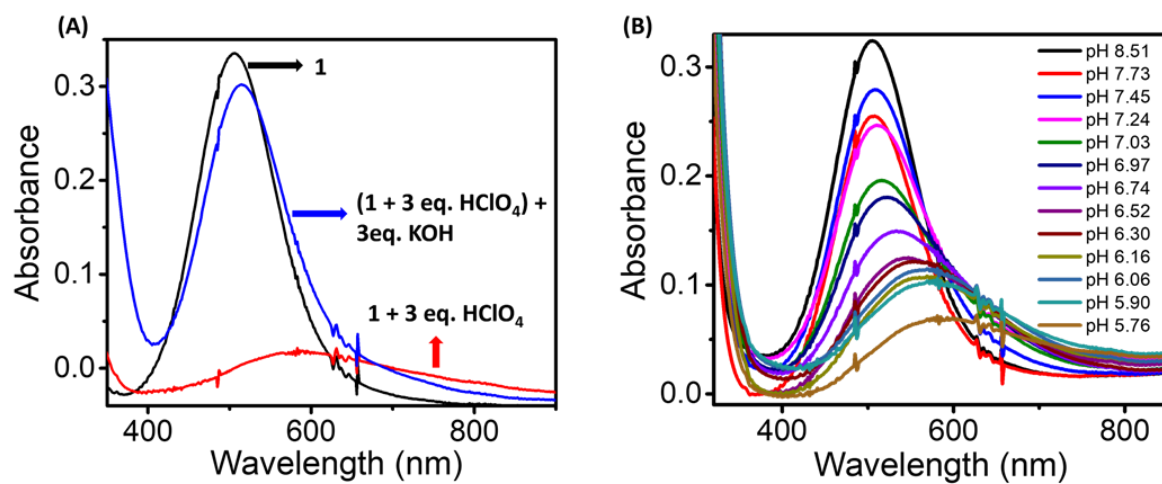
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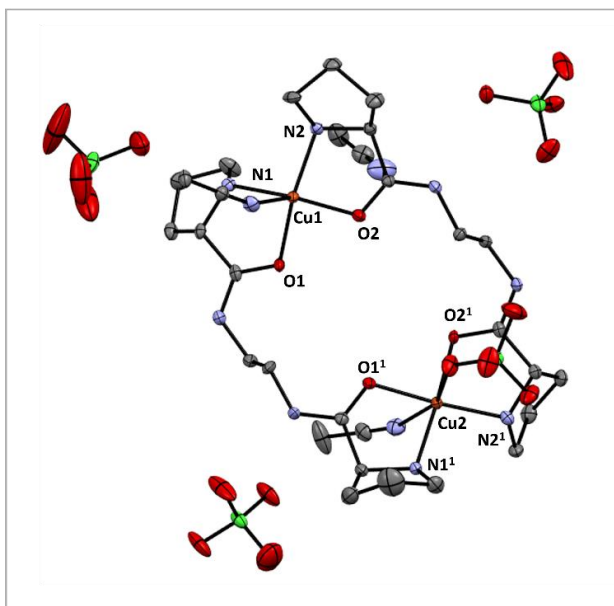
**Fig. S1** (A) Cyclic voltammograms of **1** in water at scan rate of 500 mV/s (red) and 1000 mV/s (red) at 25 °C, and (B) differential pulse voltammograms (DPVs) of **1** in water.



**Fig. S2** ESI-MS data of **1** in water.



**Fig. S3** (A) UV/Vis absorption spectral changes showing the acid-base equilibria. black: 2 mM **1** in water, red: 3 eq. of HClO<sub>4</sub> added to **1**, blue: to the red spectrum 3 eq. of KOH is added. (B) UV/Vis absorption spectral changes observed upon incremental addition of aqueous HClO<sub>4</sub> to 2 mM **1** in water (initial pH of the solution is 8.51). The corresponding change in the pH is indicated in the legend.

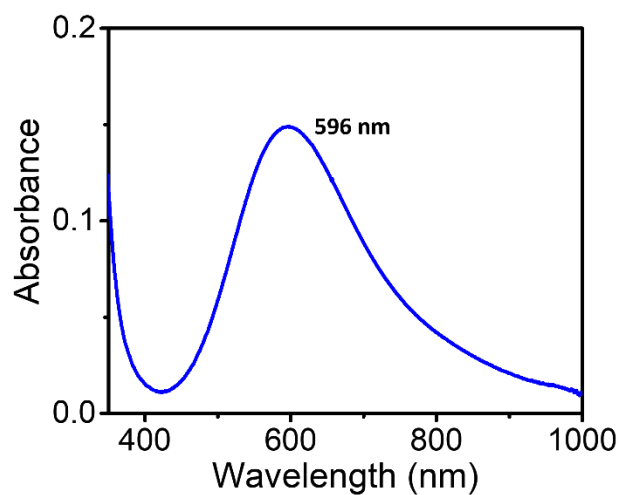


	Bond length (Å)		Bond length (Å)
Cu1-N1	2.001	Cu1-N1 <sup>1</sup>	2.010
Cu1-N2	2.009	Cu1-N2 <sup>1</sup>	1.984
Cu1-O1	1.952	Cu1-O1 <sup>1</sup>	1.942
Cu-O2	1.953	Cu-O2 <sup>1</sup>	1.964

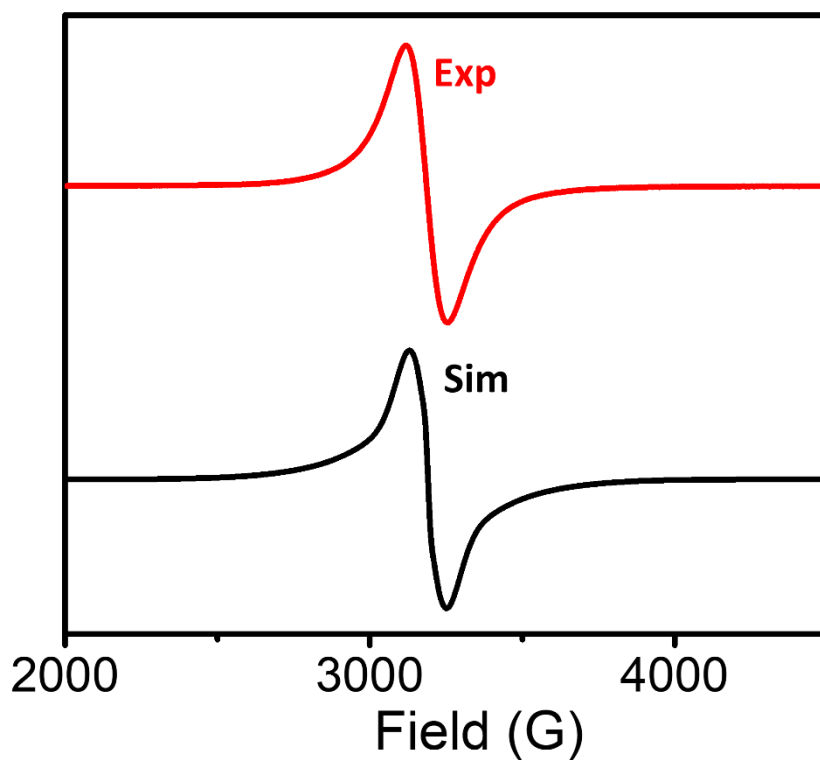
**Fig. S4** X-ray crystal structure of **3** with 50% probability. Hydrogen atoms are omitted for clarity. CCDC 2350533.

**Crystal Description :** The blue colored dimeric Cu(II) crystal structure is obtained in a day by dissolving the crude complex in CH<sub>3</sub>CN by layering it with toluene. The crystal structure of dicopper(II) complex (**3**) depicted in Fig. S4, with selected bond parameters are listed in the table.

The complex contains two Cu(II) centers, each adopting different geometries: Cu1 in a square pyramidal and Cu2 in a distorted octahedral geometry. Cu1 is coordinated with two nitrogen atoms (Cu1-N1 and Cu1-N2) and two oxygen atoms (Cu1-O1 and Cu1-O2) at the equatorial sites, forming the square planar base. N1 and O1 belong to the proline and amide groups of one ligand system, respectively, while N2 and O2 are associated with the proline and amide groups of another ligand unit. The fifth coordination site is occupied by CH<sub>3</sub>CN (solvent), which binds axially with the copper center along with two surrounding perchlorate ions, resulting in Cu1 being in its +2 oxidation state. In contrast, Cu2 is coordinated by five ligands (Cu2-N1<sup>1</sup>, Cu2-N2<sup>1</sup>, Cu1-O1<sup>1</sup>, Cu2-O2<sup>1</sup> and Cu2-NCCH<sub>3</sub>), with the sixth site occupied by a perchlorate ion, along with another perchlorate serving as a counter anion, maintaining the Cu2 center in the +2 oxidation state. Thus, one portion of the C2 symmetric ligand coordinates with one copper center (Cu1), while the other part coordinates with another copper atom (Cu2). The Cu(II)-N<sub>proline</sub> bond distances are Cu1-N1 (2.001 Å), Cu1-N2 (2.009 Å), Cu2-N1<sup>1</sup> (2.010 Å) and Cu2-N2<sup>1</sup> (1.984 Å), which are consistent with literature values.<sup>22</sup> The Cu(II)-O<sub>amide</sub> bond distances are Cu1-O1 (1.952 Å), Cu1-O2 (1.953 Å), Cu2-O1<sup>1</sup> (1.942 Å) and Cu2-O2<sup>1</sup> (1.964 Å).



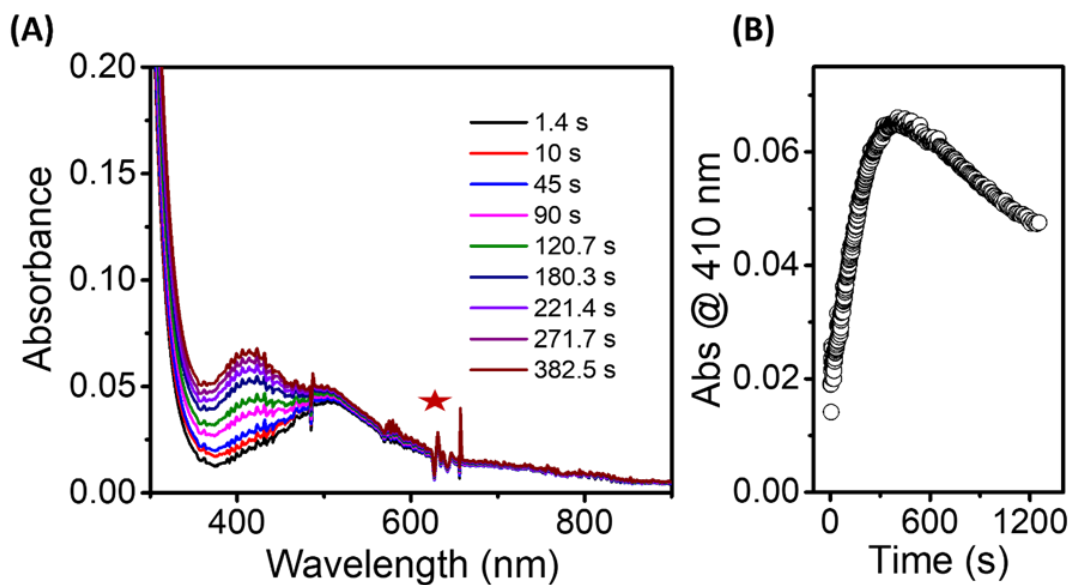
**Fig. S5** UV/Vis absorption spectrum of **3** in water at RT.



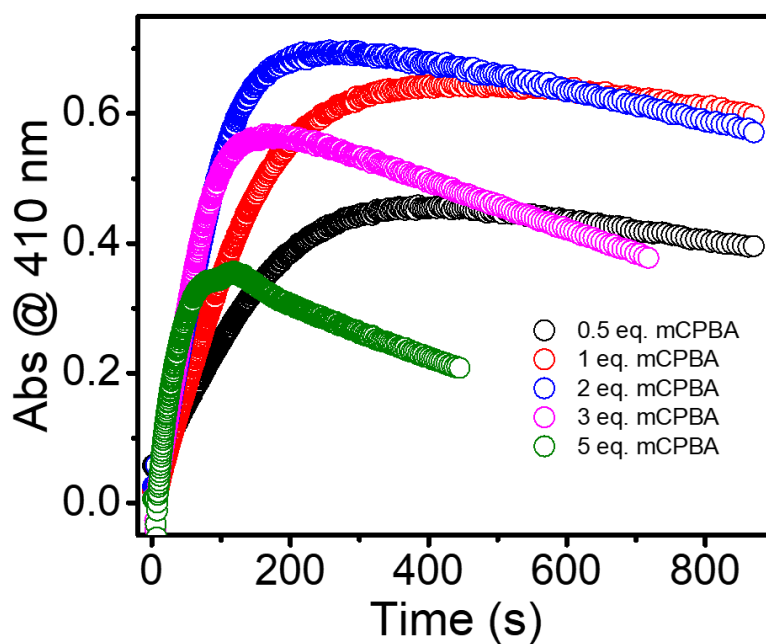
**Fig. S6** X-band EPR (Frequency = 9.44 GHz) spectrum of **3** in solid state performed at 120 K. Red: Experimental spectrum and Black: Simulated spectrum. Modulation amplitude 2.08 G; Modulation frequency 100 kHz, and attenuation 18 dB. Simulated parameters:  $g_x = g_y = g_z = 2.12$ ;  $A_x = A_y = A_z = 0$ .

**Table S1:** Crystal data and structure refinement of **3**.

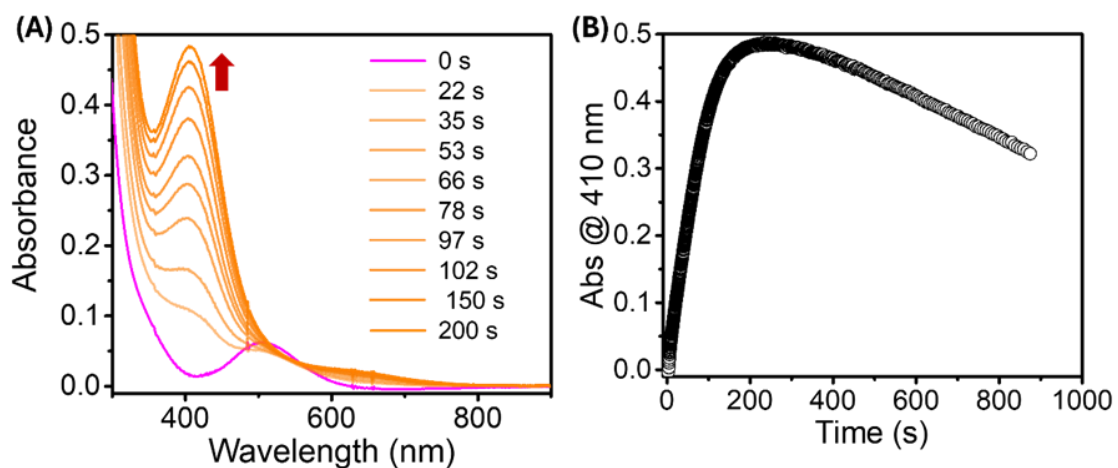
Empirical formula	C <sub>30</sub> H <sub>53</sub> Cl <sub>4</sub> Cu <sub>2</sub> N <sub>11</sub> O <sub>20</sub>
Formula weight	1156.71
Temperature/K	100
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	14.262(6)
b/Å	8.313(3)
c/Å	19.316(9)
α/°	90
β/°	97.770(14)
γ/°	90
Volume/Å <sup>3</sup>	2269.2(16)
Z	2
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.693
μ/mm <sup>-1</sup>	1.262
F(000)	1192.0
Crystal size/mm <sup>3</sup>	0.2 × 0.1 × 0.05
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.256 to 56.746
Index ranges	-18 ≤ h ≤ 15, -11 ≤ k ≤ 11, -25 ≤ l ≤ 25
Reflections collected	35315
Independent reflections	11150 [R <sub>int</sub> = 0.0554, R <sub>sigma</sub> = 0.0622]
Data/restraints/parameters	11150/1/608
Goodness-of-fit on F <sup>2</sup>	1.019
Final R indexes [I >= 2σ (I)]	R <sub>1</sub> = 0.0510, wR <sub>2</sub> = 0.1229
Final R indexes [all data]	R <sub>1</sub> = 0.0583, wR <sub>2</sub> = 0.1279
Largest diff. peak/hole / e Å <sup>-3</sup>	1.87/-0.78
Flack parameter	0.084(16)



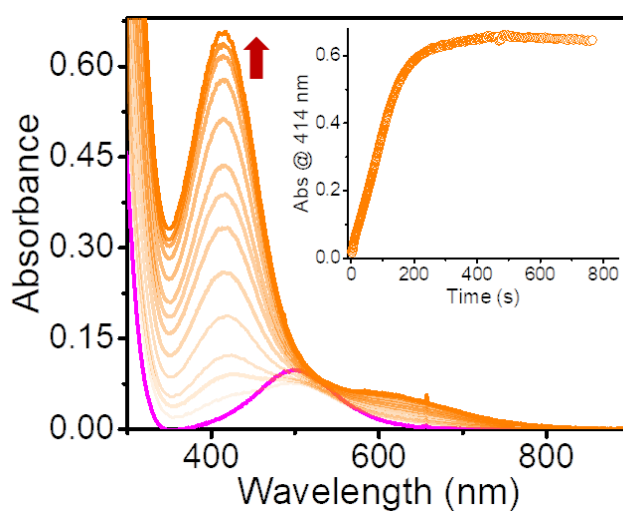
**Fig. S7** (A) UV/Vis absorption spectral changes on reaction of 1 eq. of *m*CPBA with 0.5 mM **1** in phosphate buffer (pH 8). (B) The corresponding absorbance changes at 410 nm with time. Note: Star indicates instrumental artifact.



**Fig. S8** Absorbance changes followed at 410 nm on the addition of various equivalent of *m*CPBA to **1** in water at 25 °C as represented in the legend.

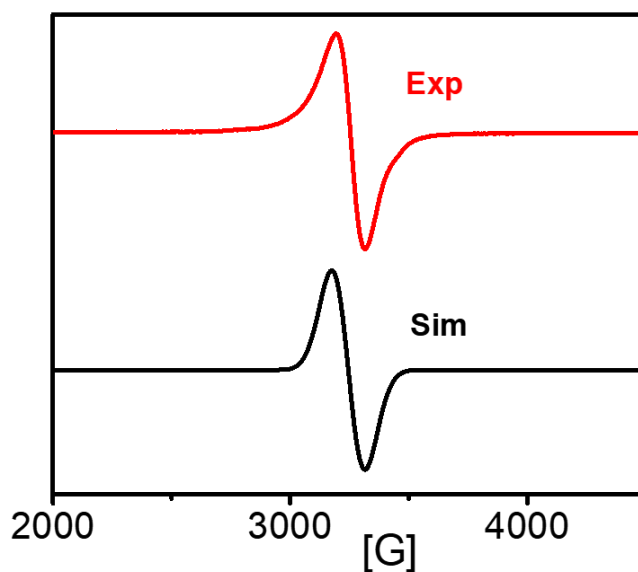


**Fig. S9** (A) UV/Vis absorption spectral changes on reaction of **2** with *m*CPBA (B) increasing the absorption with time at 410 nm. Conditions to generate **2**: 0.5 mM complex in H<sub>2</sub>O + 1 eq. of *m*CPBA at 37 °C.

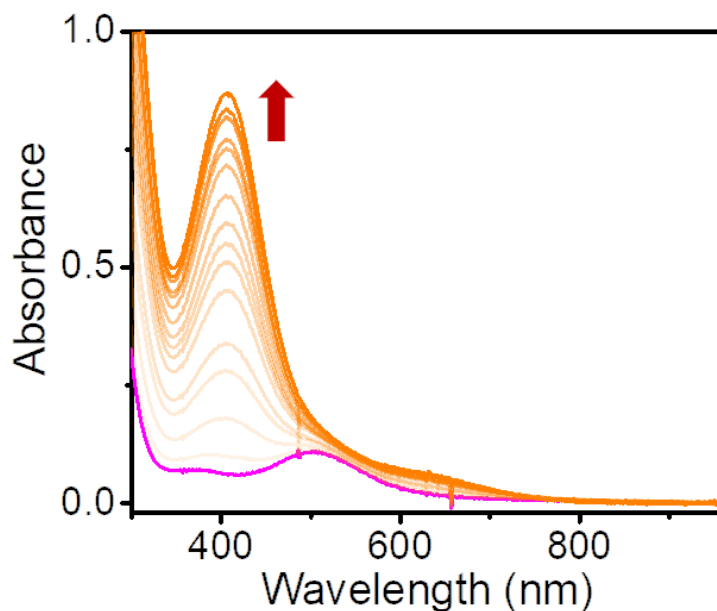


**Fig. S10** UV/Vis absorption spectral changes on reacting **1** with 1 eq. of *m*CPBA in H<sub>2</sub>O:CH<sub>3</sub>CN (1:1) at 25 °C. Inset: The corresponding changes in the absorbance followed at 414 nm.

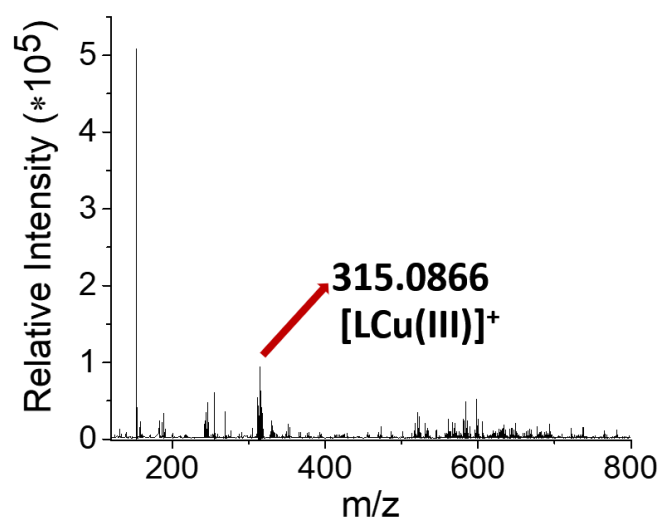




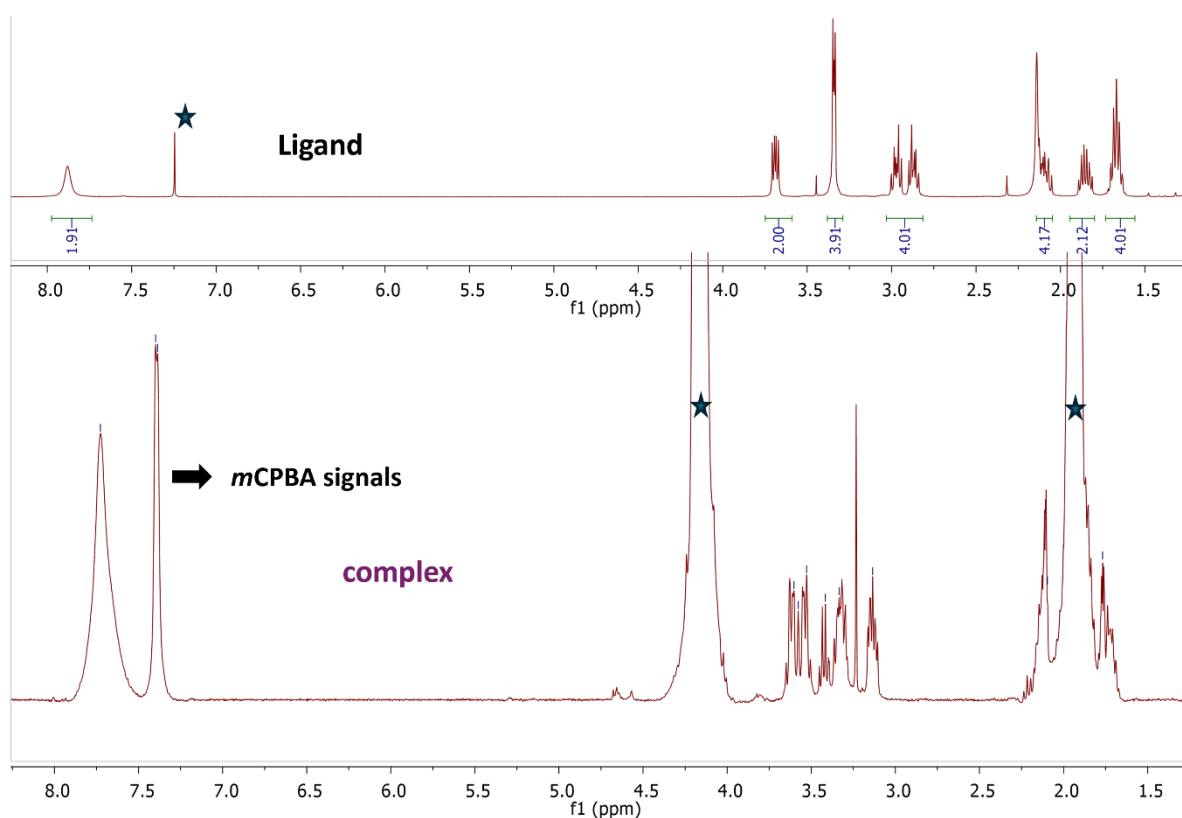
**Fig. S11** X-band EPR (Frequency = 9.44 GHz) spectrum of 2 mM **1** in H<sub>2</sub>O:CH<sub>3</sub>CN (1:1) performed at 120 K. Red: Experimental spectrum and Black: Simulated spectrum. Modulation amplitude 2.08 G; Modulation frequency 100 kHz, and attenuation 18 dB. Simulated parameters:  $g_x = g_y = g_z = 2.08$ ;  $A_x = A_y = A_z = 0$ .



**Fig. S12** UV/Vis absorption spectral changes of **2** in water on applying 0.6 V vs. Ag/AgCl potential to **1**. Conditions to generate **2**: 5 mM **1** in water + applied potential: 0.6 V vs. Ag/AgCl and 100 mM KNO<sub>3</sub> as supporting electrolyte. Note: Path length of the cuvette used is 0.1 cm.

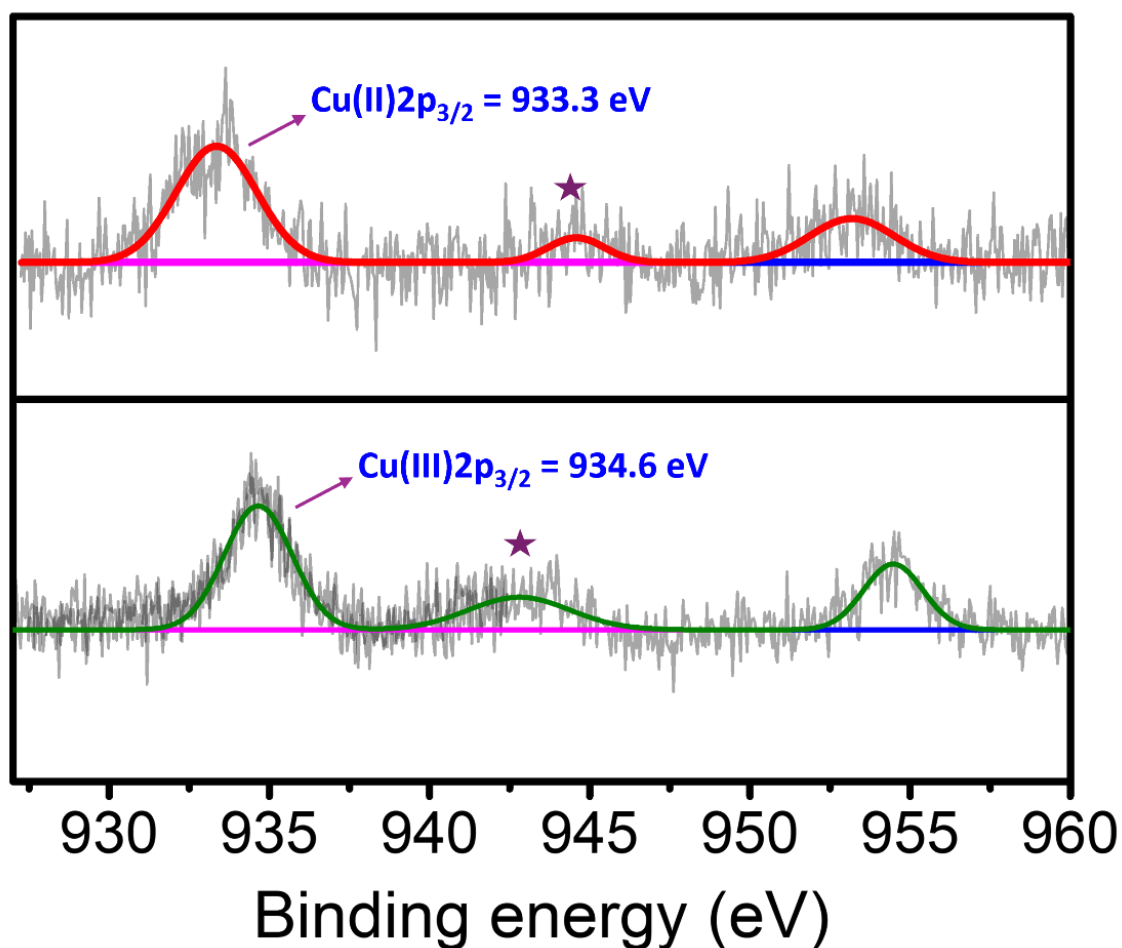


**Fig. S13** ESI-MS data of **2**. Conditions to generate **2**: 2 mM **1** in  $H_2O:CH_3CN$  (1:1) + 1 eq. of *m*CPBA at 25 °C.



**Fig. S14**  $^1H$  NMR spectrum of ligand ( $CDCl_3$ ) and **2**, **2** is generated by the addition of 1 eq. of *m*CPBA to 6 mM of **1** in  $CD_3CN:D_2O$  (1:1) at room temperature. \* Indicates solvent peaks.

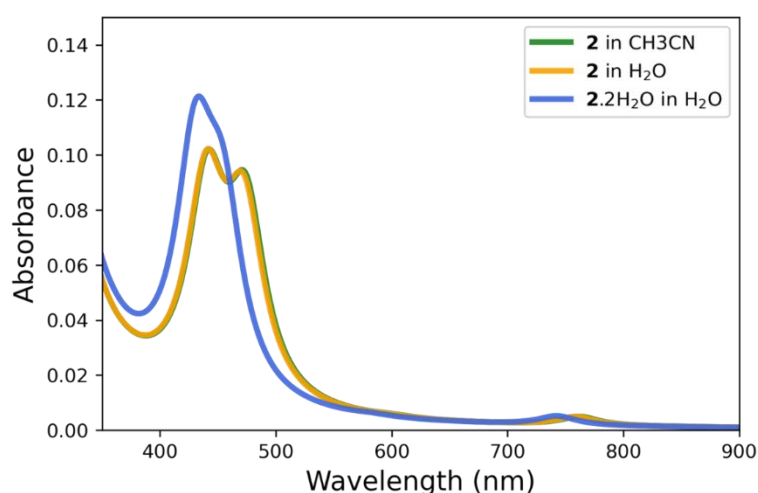
**Sample preparation:** 8 mM complex is prepared in MeOH and 1 eq. of CAN is added to generate the intermediate **2** at room temperature. It is allowed to stir for 60 seconds, and diethyl ether is poured into the reaction mixture which precipitate out the intermediate. The precipitate formed is collected and submitted for XPS analysis.



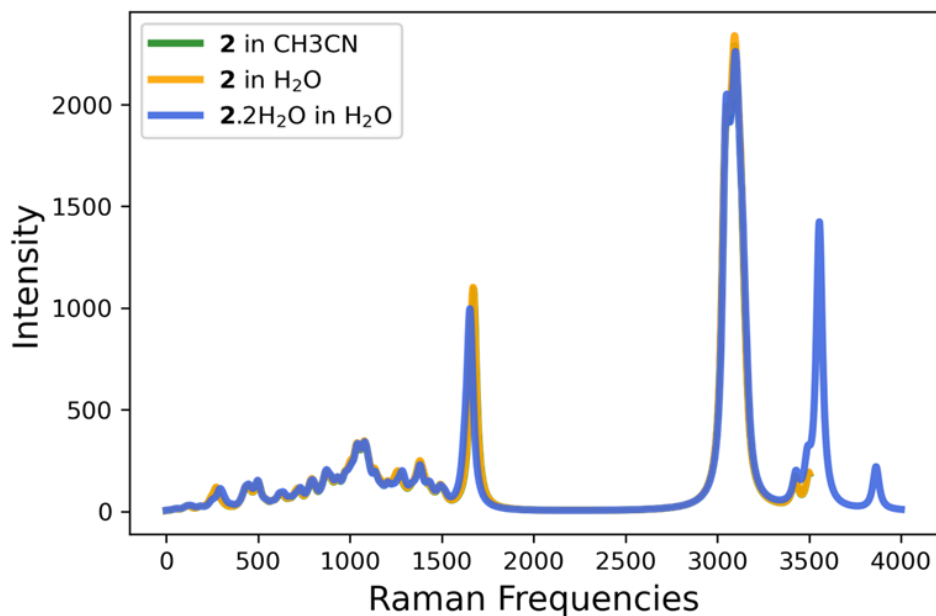
**Fig. S15** (Top) Cu 2p XPS of **1** deconvoluted into the two peaks at 933.30 eV and 953.71 eV for Cu 2p<sub>3/2</sub> and Cu 2p<sub>1/2</sub>, respectively. The peak at 933.30 eV signifies the +2 oxidation state of copper in complex **1**. (Bottom) Cu 2p XPS of **2** deconvoluted into the two peaks at 934.6 eV and 954.71 eV for Cu 2p<sub>3/2</sub> and Cu 2p<sub>1/2</sub>, respectively. The peak at 934.60 eV signifies the +3-oxidation state of copper in complex **2**. \* Marked peaks were ascribed to the satellite peaks.

**Table S2:** Electronic energies obtained using B3LYP level of theory and using different basis functions. All energies are reported in Hartree.

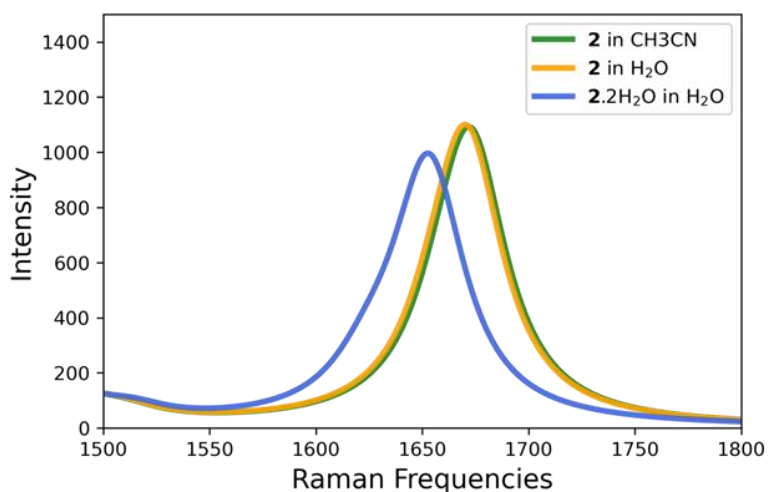
System	6-311+G(d,p) Opt	Single point after 6- 311+G(d,p)	6-311+G(d,p) for all, LANL2DZ for Cu	Single point after 6-311+G(d,p) for all, LANL2DZ for Cu
<b>Cu(II) complex</b>	- 2479.64896112	- 2479.81020091	- 1035.29545861	- 2479.81008832
<b>Cu(III) complex</b>	- 2479.46052024	- 2479.62541599	- 1035.09902719	- 2479.62507988
<b>Cu(III) complex + 1 H<sub>2</sub>O</b>	- 2555.93633062	- 2556.10887187	- 1111.57476392	- 2556.10853850
<b>Cu(III) complex + 2 H<sub>2</sub>O</b>	- 2632.41216181	- 2632.59211328	- 1188.05045851	- 2632.59178234
<b>1 H<sub>2</sub>O</b>	- 76.4664713583	- 76.4735211064		



**Fig. S16** Theoretical UV-Vis spectra calculated using TDDFT at the B3LYP level of theory and 6-311+g(d,p) basis functions, with DFT-D3 corrections. Three different spectra are shown here, one was calculated in acetonitrile solvent and the remaining using water as solvent. Solvent effects were added using CPCM scheme.



**Fig. S17** Theoretical Raman spectra (Scaling factor = 1) calculated using B3LYP level of theory and 6-311+g(d,p) basis functions, with DFT-D3 corrections. Three different spectra are shown here, one was calculated in acetonitrile solvent and the remaining using water as solvent. Solvent effects were added using CPCM scheme.



**Fig. S18.** Zoomed in (1500 to 1800  $\text{cm}^{-1}$ ) version of Fig S15.

**Table S3:** Orbital composition analysis (ODI = orbital delocalization index).

	<b>HOMO-alpha</b>	<b>HOMO-beta</b>	<b>LUMO-alpha</b>	<b>LUMO-beta</b>
Cu(II) water Stout politzer	21.32% Cu ODI : 13.41	5.25% Cu ODI: 16.00	94.96% Cu ODI : 99.23	55.56% Cu ODI: 33.96
Cu(II) water Ros-Schuit SCPA	22.5% Cu ODI: 12.53	6.36% Cu ODI: 12.35	47.296 ODI: 24.64	41.633 ODI: 20.65
Cu(II) water Mulliken	21.32 ODI: 13.41	5.25 ODI: 16.00	94.96% ODI: 99.3	55.56% ODI: 33.96

	<b>HOMO</b>	<b>LUMO</b>
Cu(III) water Stout politzer	3.56% Cu ODI : 16.93	33.56% Cu ODI : 18.19
Cu(III) water Ros-Schuit SCPA	4.96% Cu ODI: 15.57	32.35% Cu ODI: 16.80
Cu(III) water Mulliken	3.63% ODI: 17.29	34.735% Cu ODI: 18.77

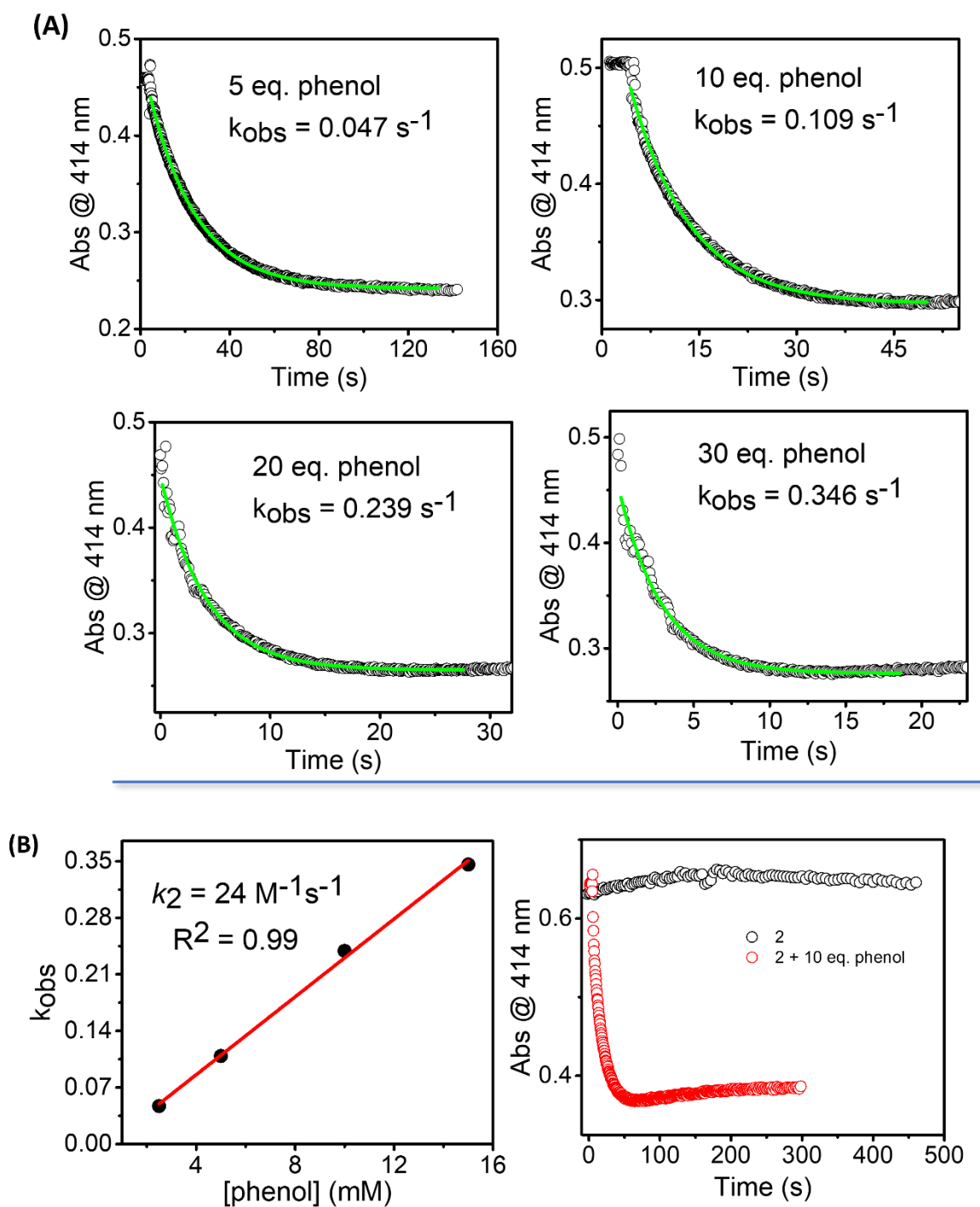
**Calculation of  $\Delta G^\ddagger$ :**

$$\Delta G^\ddagger = -RT \ln K^\ddagger; \quad \text{where } K^\ddagger = h k_2 / k_B T;$$

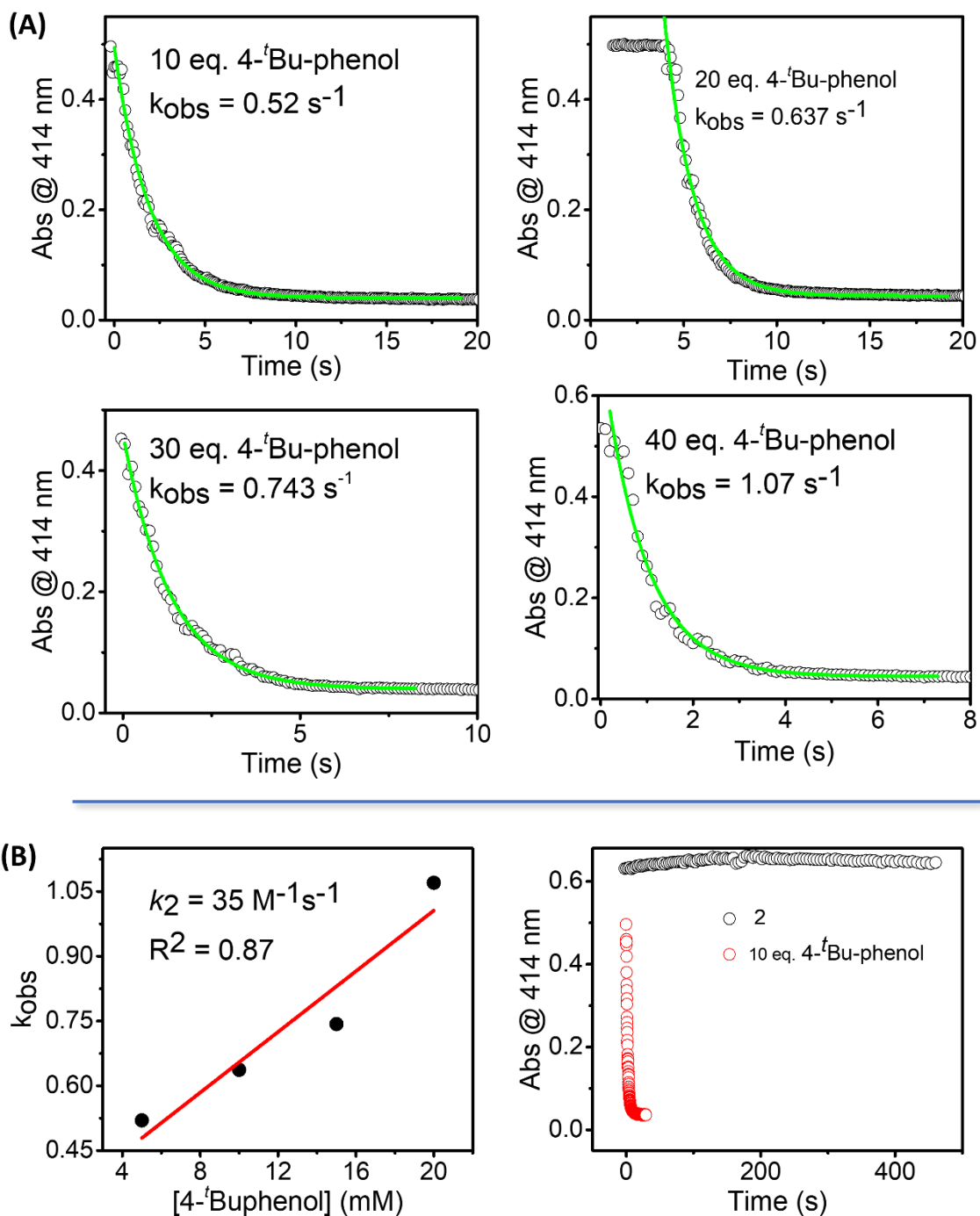
$$h \text{ (Planck's constant)} = 6.626 \times 10^{-34} \text{ J s}; \quad k_B \text{ (Boltzmann constant)} = 1.38 \times 10^{-23} \text{ J K}^{-1}.$$

$$T \text{ (Temperature)} = 298 \text{ K}; \quad R \text{ (Universal gas constant)} = 1.98 \text{ Cal mol}^{-1} \text{ K}^{-1}.$$

$k_2$  = rate constant obtained from the reaction of **2** with various phenols

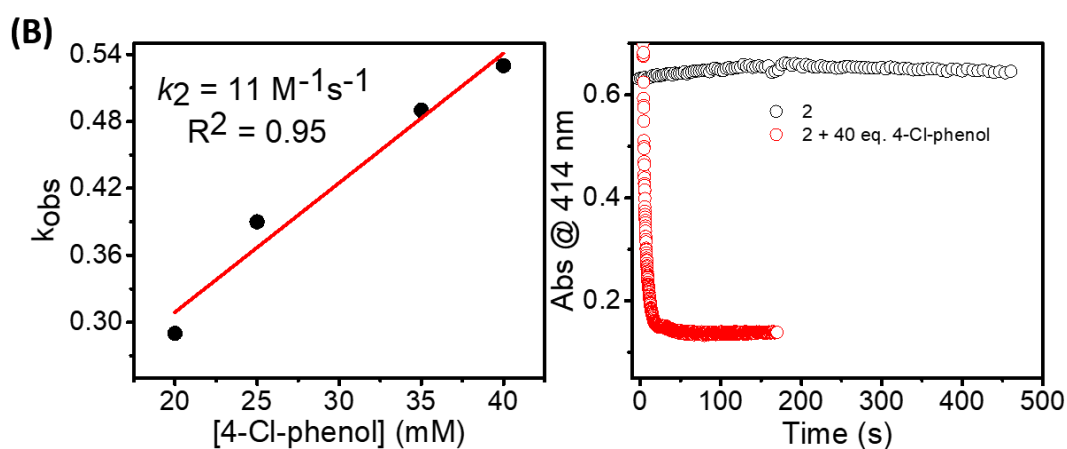
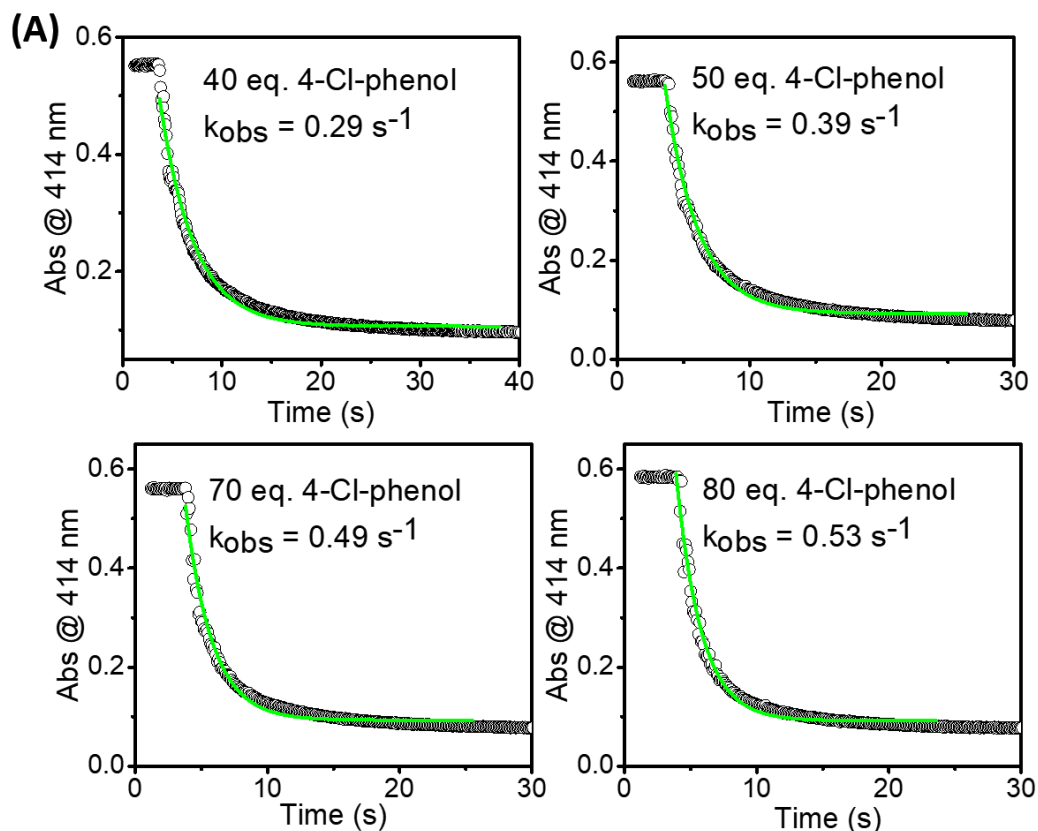


**Fig. S19** (A) Decay rate of **2** followed at 414 nm, with different equivalents of phenol and the corresponding  $k_{obs}$  values. *Conditions to generate 2*: 0.5 mM **1** in  $\text{H}_2\text{O}:\text{CH}_3\text{CN}$  (1:1) with 1 eq. of *mCPBA* at 25 °C. Note: The substrate added after reaching the maximum absorbance at 414 nm band that takes approximately 400 s. (B) A plot of  $k_{obs}$  vs [phenol] to get the second-order rate constant for the reaction of **2** with phenol (left) and the comparison of species **2** natural decay and its reactivity with 10 eq. of phenol (right).

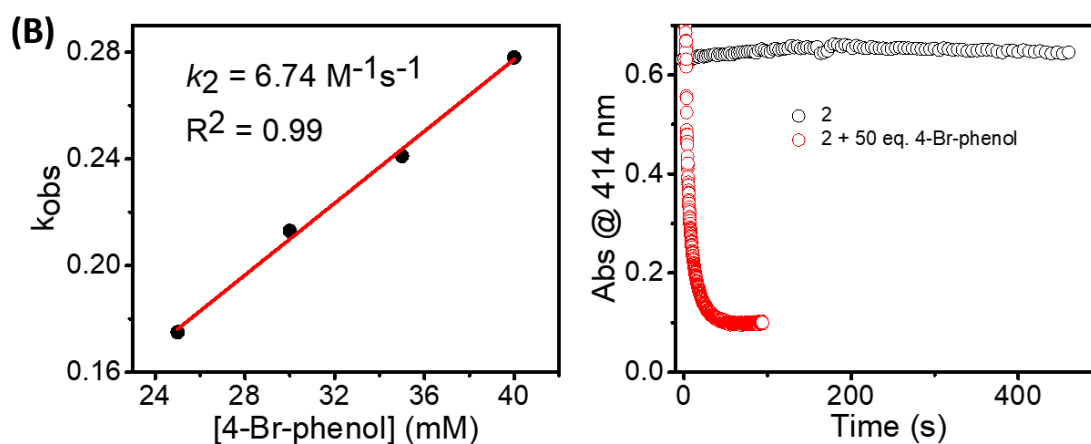
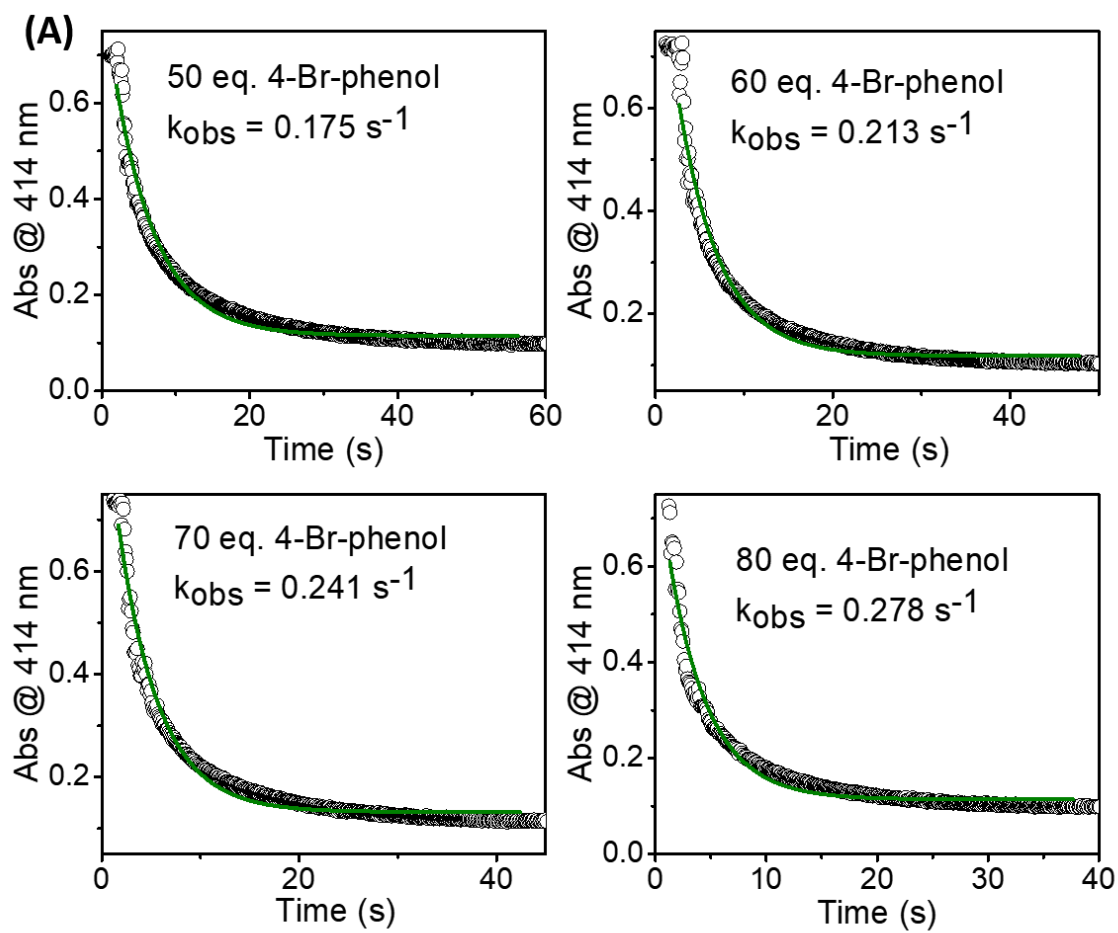


**Fig. S20** (A) Decay rate of **2** followed at 414 nm, with different equivalents of 4-<sup>t</sup>Bu-phenol and the corresponding  $k_{obs}$  values. *Conditions to generate 2*: 0.5 mM **1** in H<sub>2</sub>O:CH<sub>3</sub>CN (1:1) with 1 eq. of mCPBA at 25 °C. Note: The substrate added after reaching the maximum absorbance at 414 nm band that takes approximately 400 s. (B) A plot of  $k_{obs}$  vs [4-<sup>t</sup>Bu-phenol] to get the second-order rate constant for the reaction of **2** with 4-<sup>t</sup>Bu-phenol (left) and the comparison of species **2** natural decay and its reactivity with 5 eq. of 4-<sup>t</sup>Bu-phenol (right).

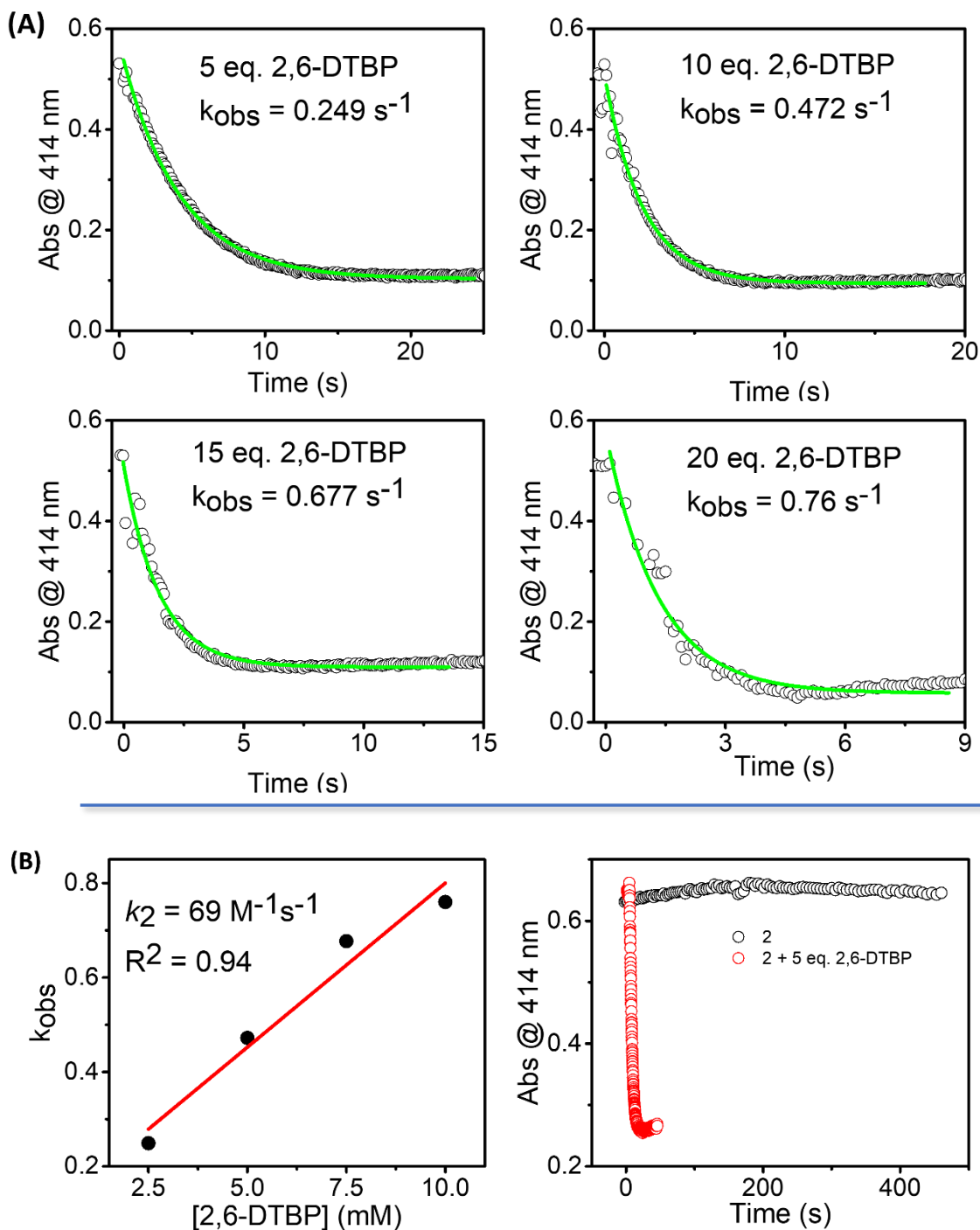




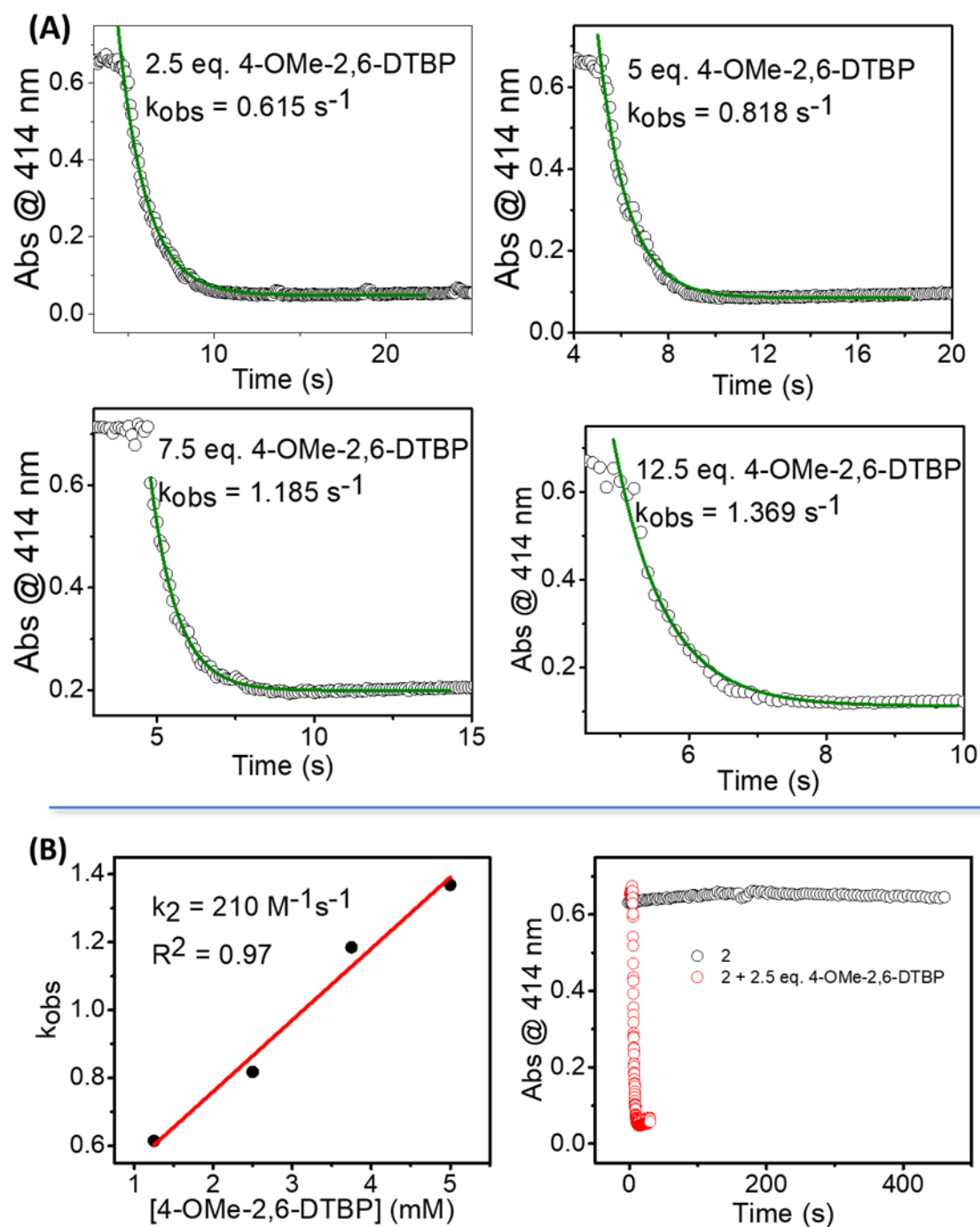
**Fig. S21** (A) Decay rate of **2** followed at 414 nm, with different equivalents of 4-Cl-phenol and the corresponding  $k_{obs}$  values. Conditions to generate **2**: 0.5 mM **1** in  $H_2O:CH_3CN$  (1:1) with 1 eq. of *m*CPBA at 25 °C. Note: The substrate added after reaching the maximum absorbance at 414 nm band that takes approximately 400 s. (B) A plot of  $k_{obs}$  vs [4-Cl-phenol] to get the second-order rate constant for the reaction of **2** with p-Cl-phenol (left) and the comparison of species **2** natural decay and its reactivity with 40 eq. of 4-Cl-phenol (right).



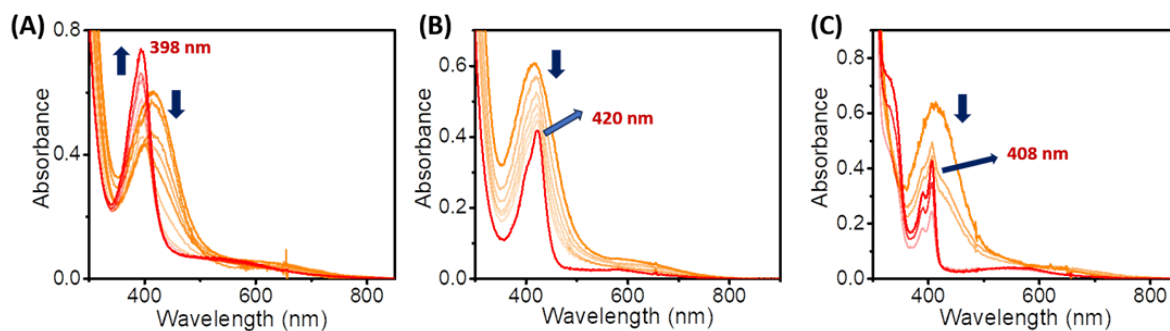
**Fig. S22** (A) Decay rate of **2** followed at 414 nm, with different equivalents of 4-Br-phenol and the corresponding  $k_{obs}$  values. *Conditions to generate 2*: 0.5 mM **1** in  $H_2O:CH_3CN$  (1:1) with 1 eq. of *mCPBA* at 25 °C. Note: The substrate added after reaching the maximum absorbance at 414 nm band that takes approximately 400 s. (B) A plot of  $k_{obs}$  vs [4-Br-phenol] to get the second-order rate constant for the reaction of **2** with 4-Br-phenol (left) and the comparison of species **2** natural decay and its reactivity with 50 eq. of 4-Br-phenol (right).



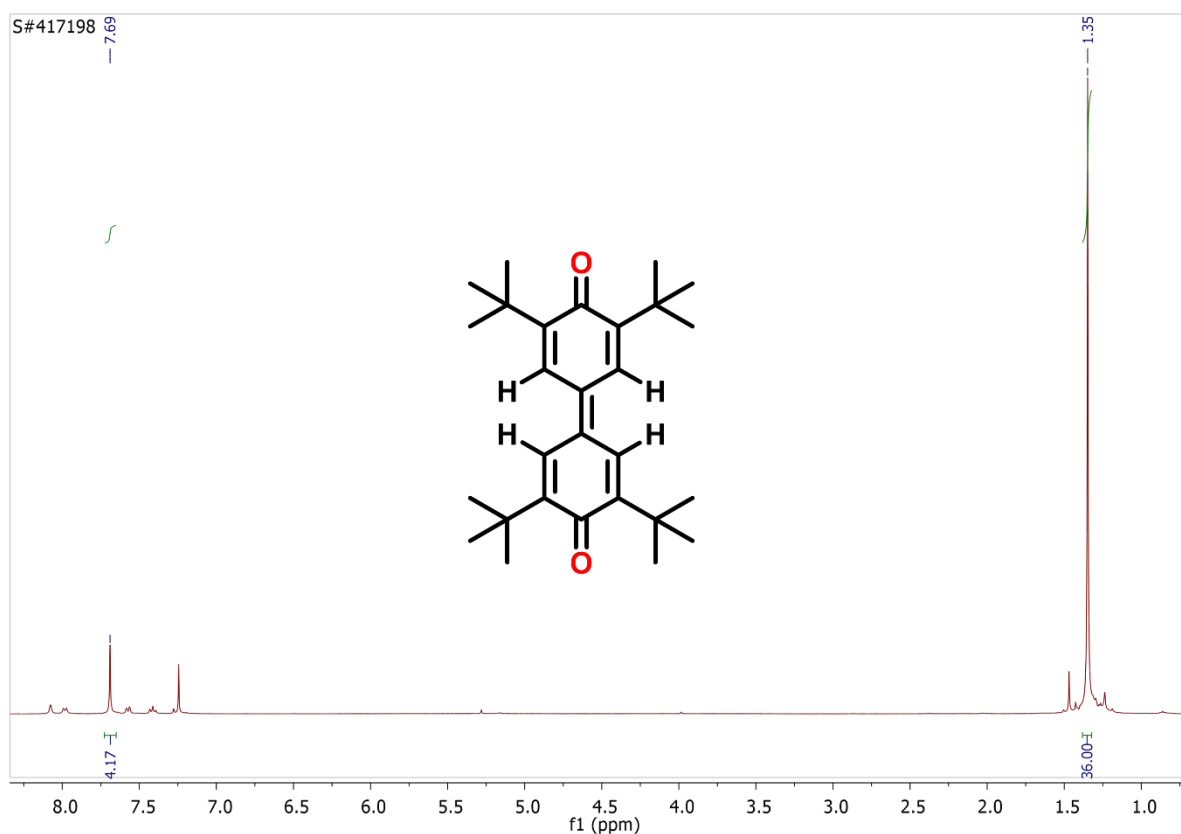
**Fig. S23** (A) Decay rate of **2** followed at 414 nm, with different equivalents of 2,6-DTBP and the corresponding  $k_{obs}$  values. Conditions to generate **2**: 0.5 mM **1** in  $H_2O:CH_3CN$  (1:1) with 1 eq. of *m*CPBA at 25 °C. Note: The substrate added after reaching the maximum absorbance at 414 nm band that takes approximately 400 s. (B) A plot of  $k_{obs}$  vs [2,6-DTBP] to get the second-order rate constant for the reaction of **2** with 2,6-DTBP (left) and the comparison of **2** natural decay and its reactivity with 5 eq. of 2,6-DTBP (right).



**Fig. S24** (A) Decay rate of **2** followed at 414 nm, with various equivalents of 4-OMe-2,6-DTBP and the corresponding  $k_{obs}$  values. Conditions to generate **2**: 0.5 mM **1** in  $\text{H}_2\text{O}:\text{CH}_3\text{CN}$  (1:1) with 1 eq. of *mCPBA* at 25 °C. Note: The substrate added after reaching the maximum absorbance at 414 nm band that takes approximately 400 s. (B) A plot of  $k_{obs}$  vs [4-OMe-2,6-DTBP] to get the second-order rate constant for the reaction of **2** with 4-OMe-2,6-DTBP (left) and the comparison of species **2** natural decay and its reactivity with 2.5 eq. of 4-OMe-2,6-DTBP (right).

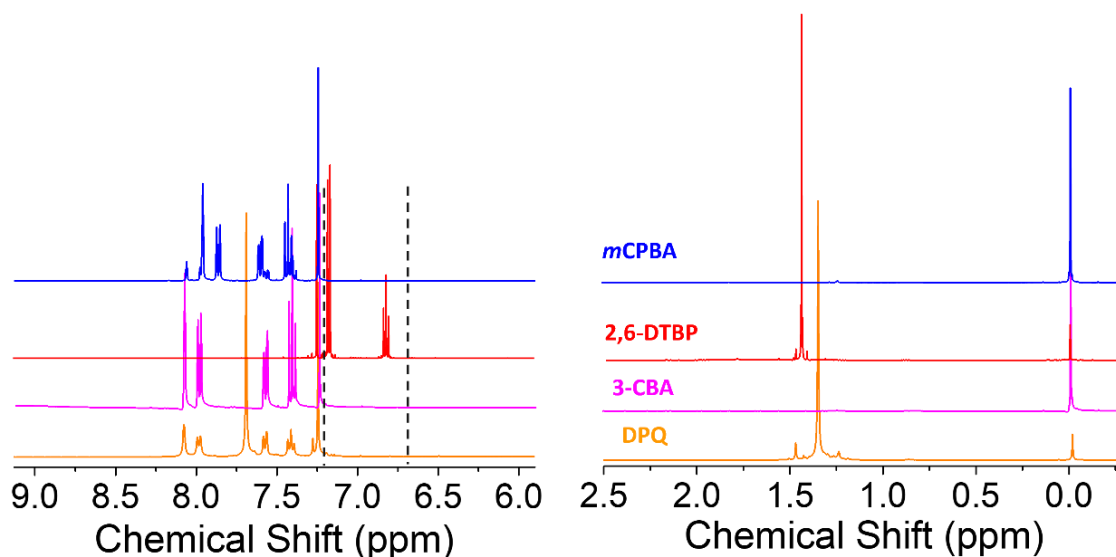


**Fig. S25** UV-Vis spectral changes of **2** on reaction with (A) 50 eq. of phenol, (B) 20 eq. of 2,6-DTBP and (C) 12.5 eq. of 4-OMe-2,6-DTBP at 25 °C. Conditions to generate **2**: 0.5 mM **1** in  $H_2O:CH_3CN$  (1:1) with 1 eq. of *mCPBA* at 25 °C. The appearance of 398 nm, 420 nm and 408 nm bands signifies the formation of phenoxy radical, 3,3',5,5'-tetra-tert-butylidiphenoquinone (DPQ) and 4-OMe-2,6-DTBP<sup>•</sup>, respectively.

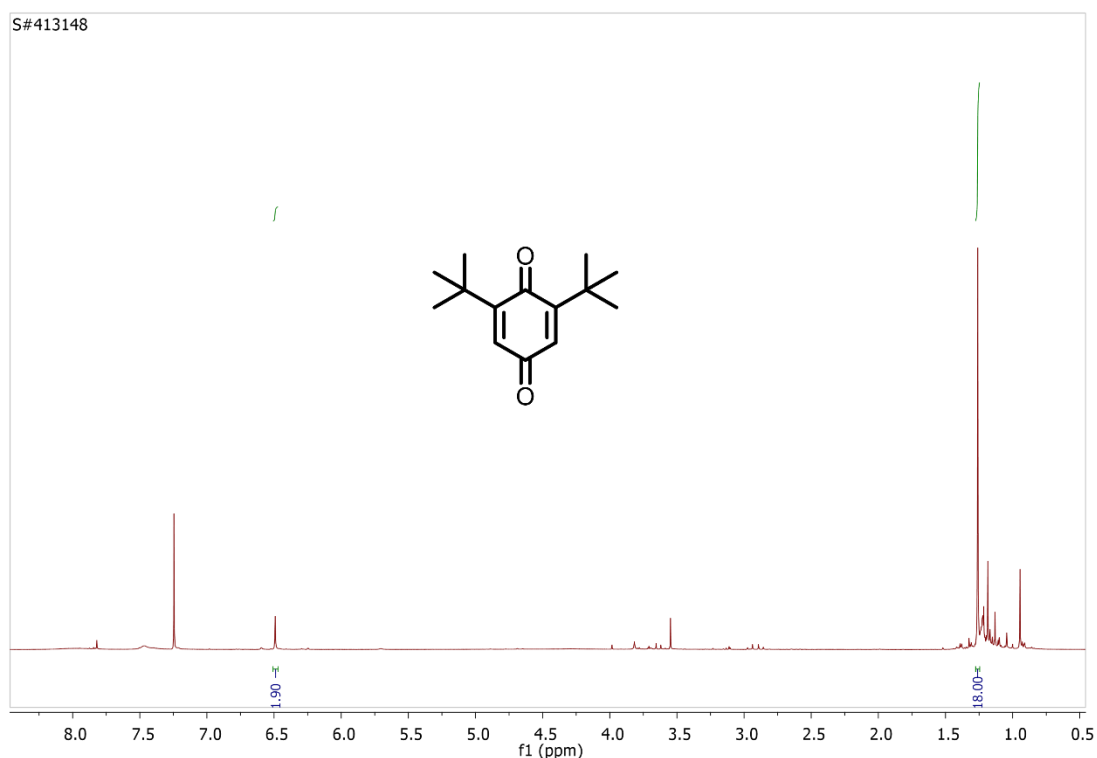


**Fig. S26**  $^1H$  NMR of crude reaction mixture of DPQ in  $CDCl_3$ . Reaction Condition: 1 eq. of **1** in 1:1 ( $H_2O:CH_3CN$ ) + 1 eq. of *mCPBA* + 1 eq. of 2,6-DTBP.

Note: reaction of **2** in 1:1 ( $H_2O:CH_3CN$ ) with 2,6-DTBP gives DPQ as a product and metallic impurities removed by passing through silica gel column.

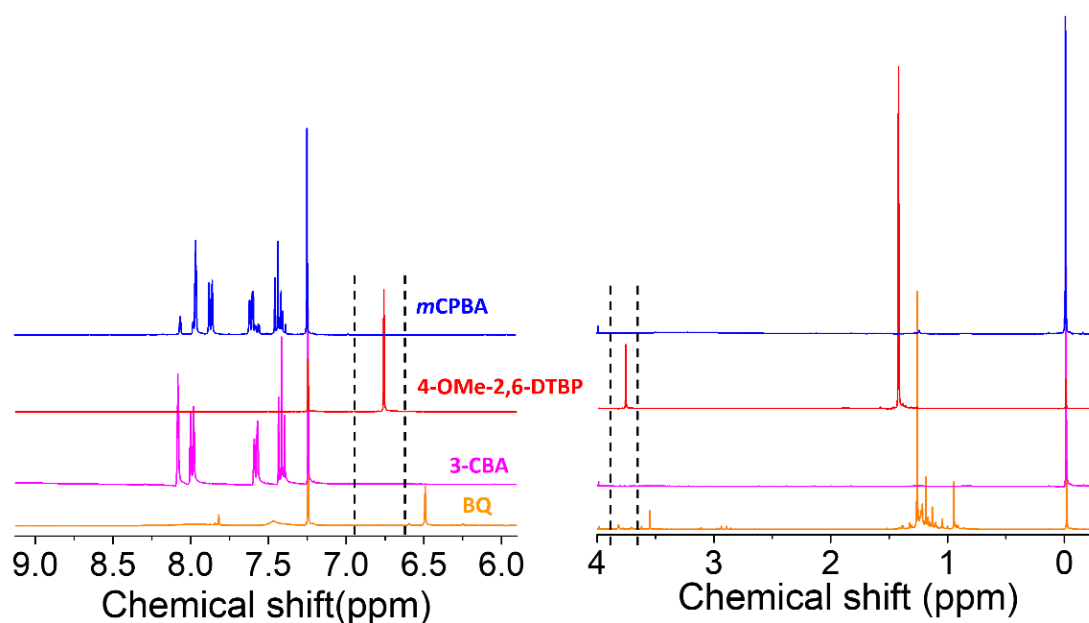


**Fig. S27** Comparing the crude  $^1\text{H}$  NMR (400 MHz) of DPQ with initial reactant 2,6-DTBP and oxidant *m*CPBA in  $\text{CDCl}_3$ . Note: disappearance of peaks in between 6.5-7.1 ppm indicates complete consumption of 2,6-DTBP.

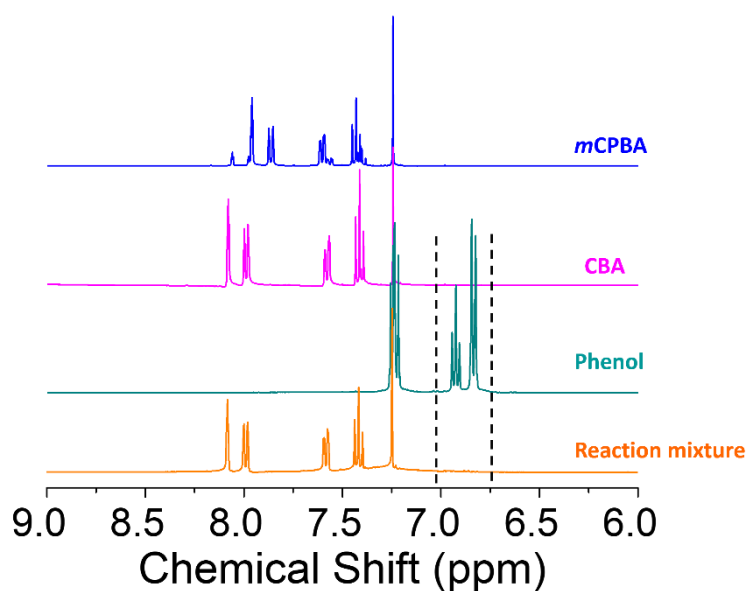


**Fig. S28**  $^1\text{H}$  NMR (400 MHz) of crude reaction mixture of BQ in  $\text{CDCl}_3$ . Reaction Condition: 1 eq. of **1** in 1:1 ( $\text{H}_2\text{O}:\text{CH}_3\text{CN}$ ) + 1 eq. of *m*CPBA + 1 eq. of 4-OMe-2,6-DTBP.

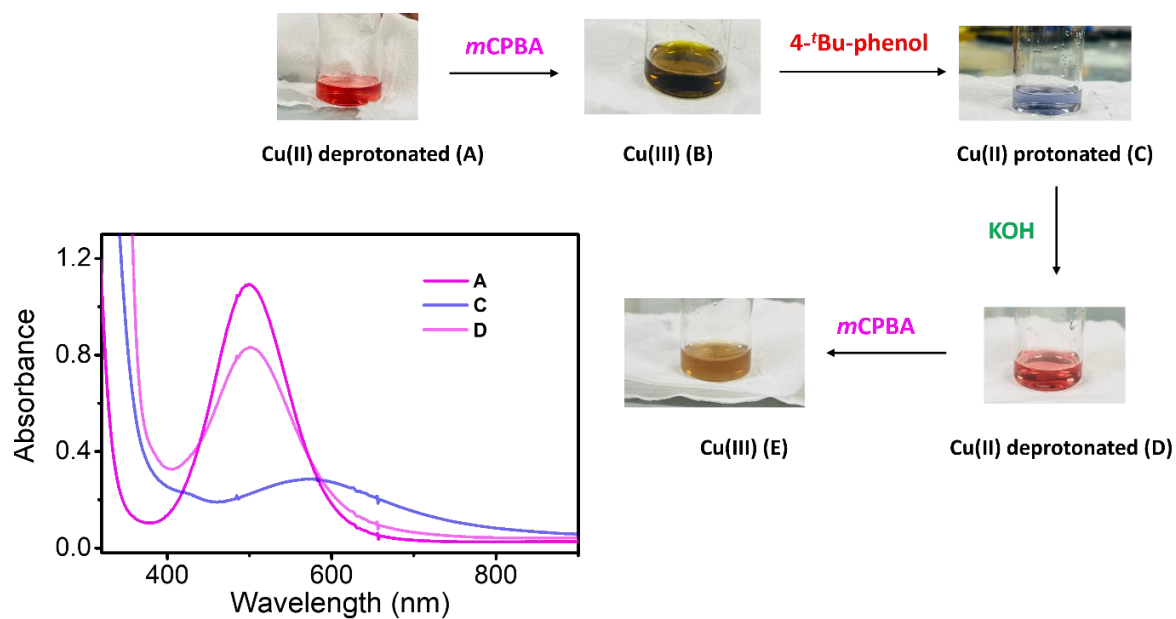
Note: Reaction of **2** in 1:1 ( $\text{H}_2\text{O}:\text{CH}_3\text{CN}$ ) with 4-OMe-2,6-DTBP gives BQ as a product and metallic impurities removed by passing through silica gel column.



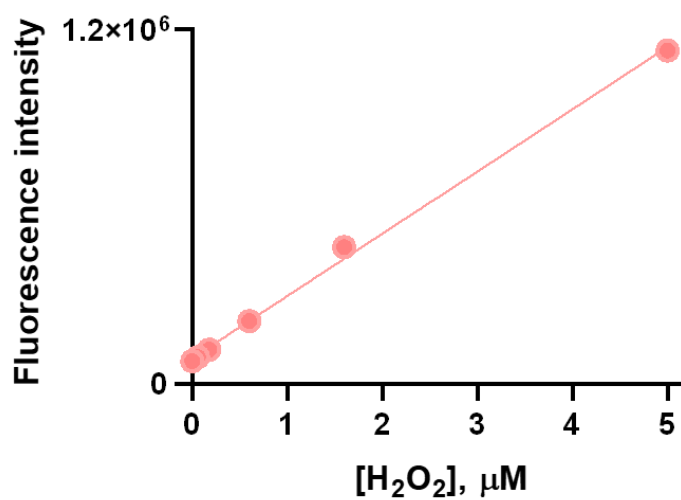
**Fig. S29** Comparing the crude  $^1\text{H}$  NMR (400 MHz) of BQ with initial recatant 4-OMe-2,6-DTBP and oxidant *m*CPBA in  $\text{CDCl}_3$ . other organic entitiies present in the reaction mixture. *Note: disappearance of peaks in between 6.6 and 3.8 ppm indicates complete consumption of 4-OMe-2,6-DTBP.*



**Fig. S30** Comparison of  $^1\text{H}$  NMR (400 MHz) of crude phenol reaction mixture with other organic entitiies present in the reaction mixture in  $\text{CDCl}_3$ . *Note: D isappearance of peaks in between 7-6.5 ppm indicates complete consumption of phenol.*

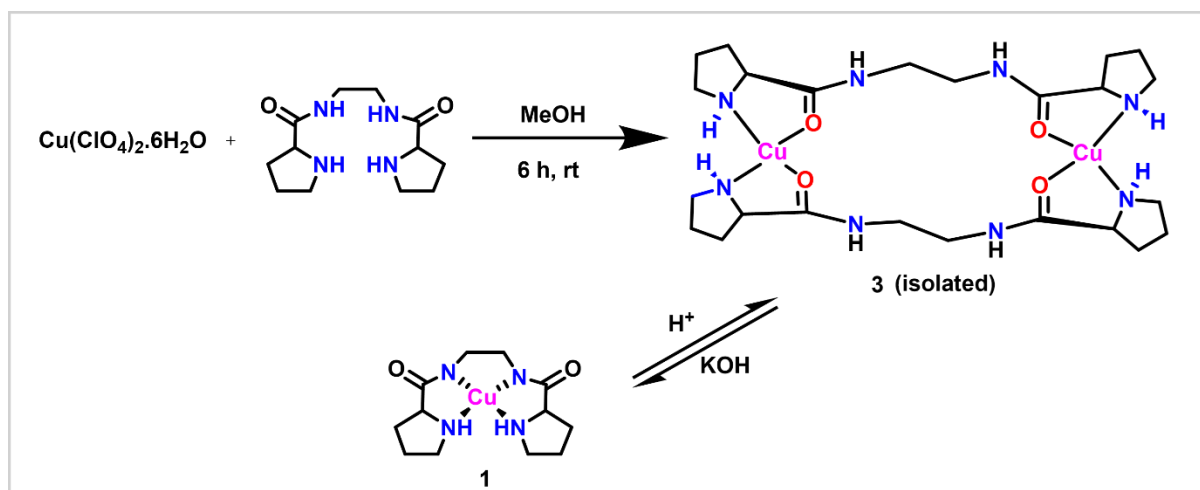


**Fig. S31** Colour changes for different species proposed in the reaction pathway and their corresponding UV/Vis absorption spectra.



**Fig. S32** Calibration curve obtained for H<sub>2</sub>O<sub>2</sub> using Amplex red<sup>®</sup> assay.





**Scheme S1:** Synthesis of **3** and existence of acid base equilibria between **1** and **3**.

**1 [(L)Cu(II)]**

C	0.013764	0.057774	-0.010519
N	0.105125	0.028490	1.486225
C	1.565947	0.135476	1.744852
C	2.111147	1.070707	0.623804
C	0.950461	1.196225	-0.407229
Cu	-1.369310	-1.301107	2.053112
N	-2.173129	-0.686745	0.391294
C	-1.462058	0.052192	-0.449696
O	-1.840947	0.636915	-1.485389
N	-0.896203	-2.133285	3.865384
C	-2.042022	-3.027583	4.298513
C	-2.499324	-2.471294	5.664098
C	-1.246509	-1.777708	6.213887
C	-0.660307	-1.132469	4.958799
C	-3.178989	-3.094188	3.266532
O	-4.110008	-3.908334	3.449655
N	-3.039360	-2.236104	2.268425
C	-3.929892	-2.196718	1.111180
C	-3.607812	-0.924070	0.297531
H	-0.312204	0.903978	1.810507
H	-0.064157	-2.709591	3.777593
H	0.402284	-0.898539	5.016664
H	-1.201049	-0.215407	4.713354
H	-1.469237	-1.046577	6.992983
H	-0.547393	-2.513881	6.622650
H	-2.880998	-3.260094	6.311561
H	-3.298539	-1.738247	5.516819
H	-1.655836	-4.041991	4.418725
H	0.440323	-0.892883	-0.351398
H	1.292414	1.111189	-1.438586

H	0.432285	2.153617	-0.304063
H	2.388346	2.046703	1.024807
H	3.002881	0.636903	0.168353
H	1.992166	-0.866104	1.672721
H	1.735905	0.510059	2.753589
H	-3.759289	-3.084616	0.488258
H	-4.982432	-2.206502	1.412051
H	-4.152013	-0.070223	0.722164
H	-3.933093	-1.037050	-0.741661

**2 formal [(L)Cu(III)]<sup>+</sup>**

C	-0.016053	0.007323	0.025985
N	-0.031937	0.007768	1.526098
C	1.418441	-0.000651	1.889140
C	2.080580	0.891004	0.795870
C	1.001026	1.085375	-0.315023
Cu	-1.477257	-1.210075	2.018800
N	-2.229858	-0.666023	0.413355
C	-1.466046	0.040539	-0.446012
O	-1.854316	0.565392	-1.487200
N	-0.917149	-1.955134	3.727766
C	-1.921036	-2.990027	4.200243
C	-2.328449	-2.557881	5.623728
C	-1.145448	-1.700859	6.093833
C	-0.764730	-0.934962	4.829727
C	-3.087293	-3.076744	3.227265
O	-3.989768	-3.899571	3.353493
N	-3.047015	-2.139103	2.253089
C	-3.954895	-2.153191	1.091157
C	-3.681819	-0.859275	0.335298
H	-0.408659	0.913740	1.819542
H	-0.022763	-2.421529	3.586808

H	0.249071	-0.540812	4.814885	C	-4.538169	2.551546	2.722329
H	-1.466555	-0.120616	4.645106	C	-3.061674	2.995033	2.720237
H	-1.409150	-1.027564	6.909774	C	-2.425886	3.026345	4.097937
H	-0.313506	-2.330959	6.419309	O	-2.805271	3.803429	4.980427
H	-2.516612	-3.421570	6.259249	N	-1.451578	2.117395	4.268371
H	-3.240056	-1.956352	5.585950	C	-0.576654	2.077940	5.454476
H	-1.421105	-3.958764	4.211671	C	0.221167	0.785926	5.337552
H	0.377572	-0.971273	-0.267611	O	-4.945398	5.586229	4.632859
H	1.404977	0.960757	-1.318412	H	-0.386303	-0.893961	1.783778
H	0.540340	2.073743	-0.252614	H	-1.957650	2.514412	1.031059
H	2.388073	1.849856	1.212045	H	-3.074195	0.674882	0.336282
H	2.967847	0.395197	0.402525	H	-3.360889	0.154932	2.009642
H	1.769924	-1.030566	1.841440	H	-5.532055	1.092663	1.409854
H	1.545012	0.375628	2.901608	H	-4.773527	2.450035	0.560101
H	-3.734575	-3.023667	0.466256	H	-5.203641	3.409715	2.795457
H	-4.989676	-2.219794	1.432411	H	-4.731056	1.897086	3.576134
H	-4.193058	-0.017210	0.810921	H	-2.952794	3.985548	2.276976
H	-3.993140	-0.913229	-0.709926	H	1.846346	0.976356	1.558030
<b>2.H<sub>2</sub>O formal [(L)Cu(III)]<sup>+</sup>.H<sub>2</sub>O</b>				H	3.101150	-0.959674	0.801548
C	0.002466	0.029481	0.001456	H	1.845418	-2.067190	1.366103
N	-0.002760	0.011682	1.497553	H	0.889842	-1.818130	-0.787447
C	1.454724	-0.002518	1.853759	H	1.825288	-0.364134	-1.132223
C	2.028045	-1.076988	0.943122	H	0.140084	1.060194	-0.322242
C	1.221213	-0.865273	-0.376116	H	-0.949325	-0.340782	-0.371857
Cu	-0.830919	1.220176	2.786270	H	0.085496	2.948239	5.444179
N	0.530265	0.649335	3.909898	H	-1.183155	2.107628	6.361412
C	1.546259	-0.061809	3.374390	H	-0.374082	-0.069218	5.670684
O	2.446143	-0.610163	4.005016	H	1.147581	0.813979	5.914649
N	-2.334125	2.004256	1.828225	H	-4.200417	4.965666	4.753836
C	-3.355608	1.009588	1.331990	H	-4.662157	6.175808	3.926306
C	-4.677400	1.769379	1.410179				

<b>2.2H<sub>2</sub>O formal [(L)Cu(III)]<sup>+</sup>.2H<sub>2</sub>O</b>			
			H -3.114096 0.666680 0.404180
C	-0.032820	-0.022146	0.103659 H -3.416067 0.194749 2.088373
N	-0.051655	-0.012950	1.599244 H -5.564001 1.160492 1.467044
C	1.403149	-0.033456	1.968063 H -4.780511 2.481160 0.582442
C	1.971631	-1.133782	1.084811 H -5.189983 3.504891 2.795884
C	1.183463	-0.931994	-0.246565 H -4.739287 2.002134 3.611576
Cu	-0.873343	1.229369	2.856189 H -2.936668 4.025036 2.241682
N	0.458657	0.641894	4.005886 H 1.807502 0.933820 1.651965
C	1.486086	-0.048443	3.488920 H 3.048151 -1.036666 0.957857
O	2.404524	-0.558167	4.139041 H 1.766793 -2.113181 1.522867
N	-2.348560	2.018035	1.864957 H 0.849484 -1.887140 -0.650203
C	-3.390770	1.032243	1.390668 H 1.801893 -0.445024 -1.000250
C	-4.696660	1.820690	1.449514 H 0.114482 1.001742 -0.236723
C	-4.540929	2.633070	2.741240 H -0.983733 -0.393015 -0.270963
C	-3.058017	3.053015	2.720917 H 0.100412 3.034454 5.428681
C	-2.418084	3.124431	4.095038 H -1.186105 2.277087 6.392066
O	-2.773712	3.946186	4.945373 H -0.442512 0.046816 5.809099
N	-1.469323	2.194732	4.302896 H 1.107148 0.897106 5.991839
C	-0.586563	2.185540	5.484667 H -4.187612 5.067334 4.615044
C	0.172936	0.866146	5.427941 H -4.698293 6.516191 4.521962
O	-4.969582	5.603469	4.379454 H 3.957320 -1.234049 3.451705
H	-0.448041	-0.908877	1.897742 O 4.819740 -1.549473 3.118204
H	-1.952018	2.492613	1.055256 H 4.640891 -2.423168 2.755732