

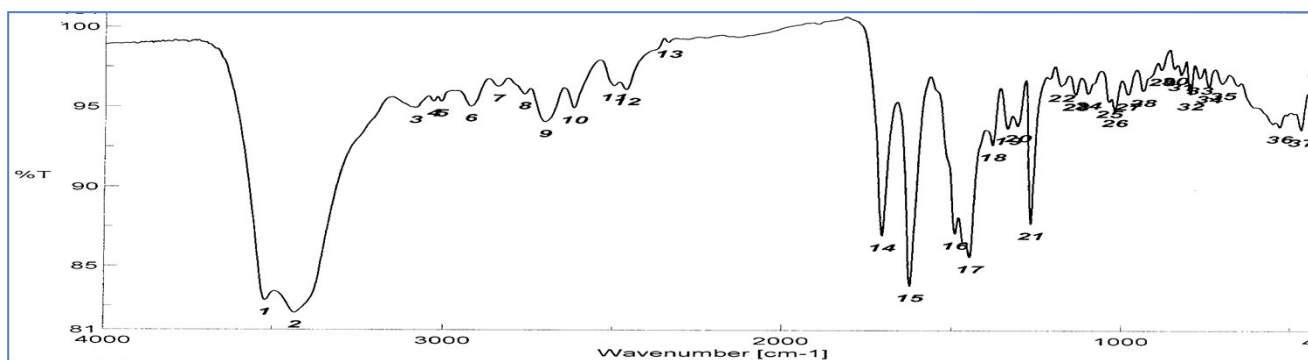
**Photocatalytic degradation of methylene blue with hematite nanoparticles synthesized by thermal decomposition of fluoroquinolones oxalato-iron(III) complexes**

Ahmed M. Mansour\*

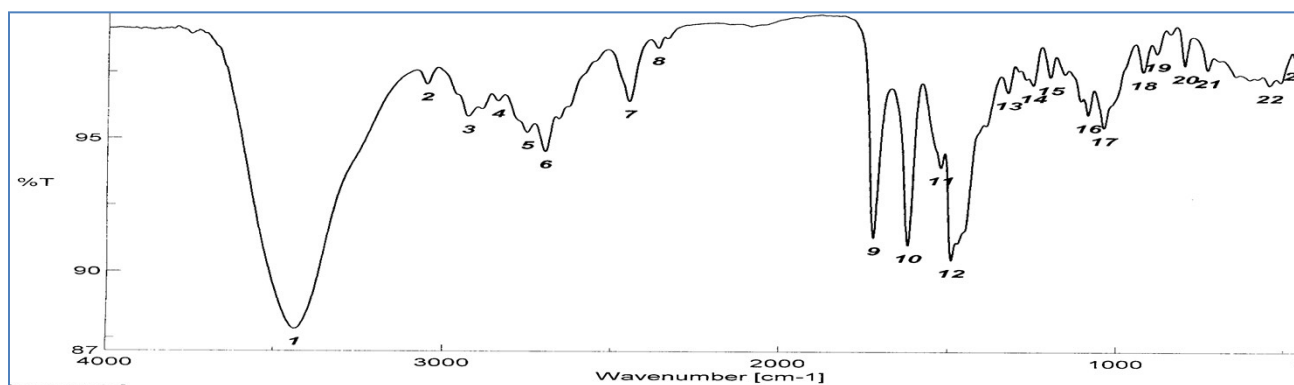
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Supporting Information

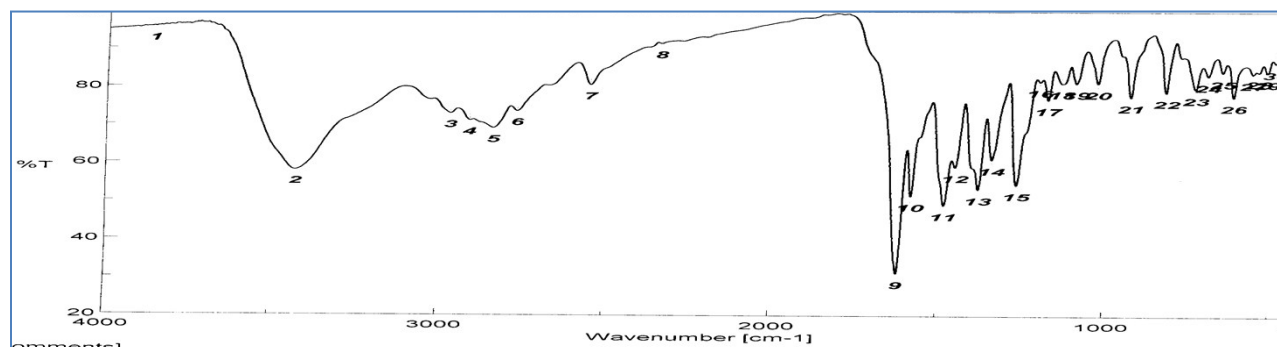
**E-mail:** mansour@sci.cu.edu.eg; inorganic\_am@yahoo.com



a)

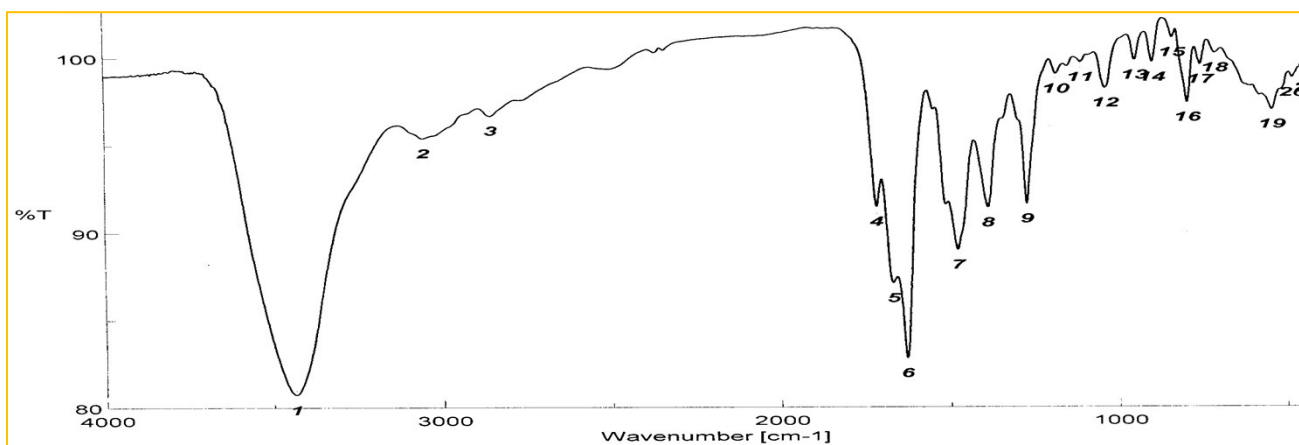


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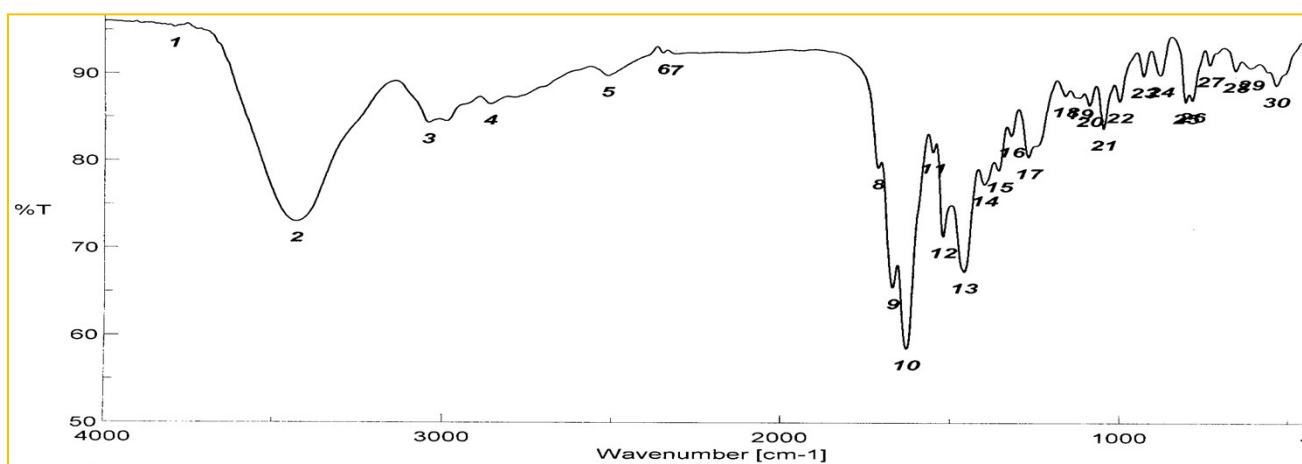


c)

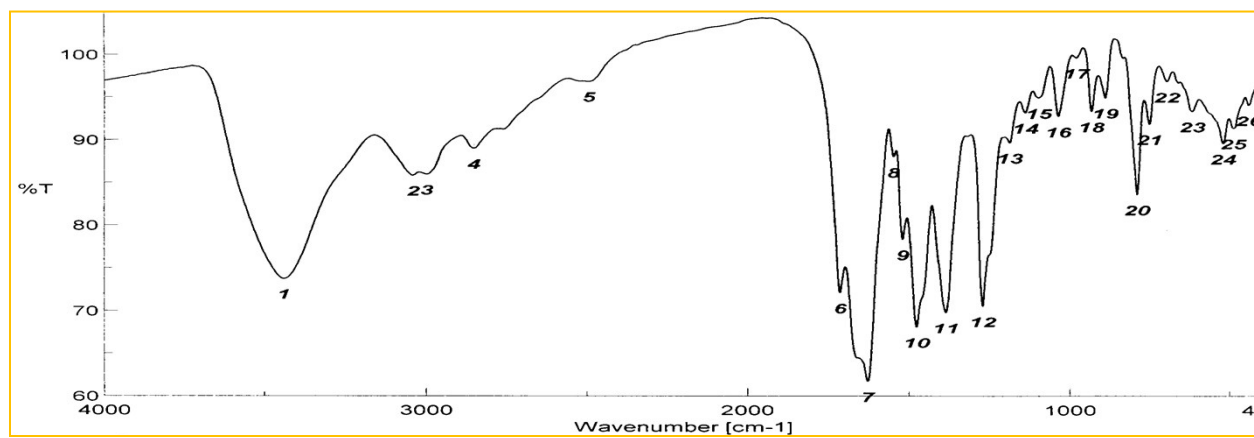
**Fig. S1:** Experimental FT IR spectra of a) ciprofloxacin·HCl, b) lomefloxacin·HCl and c) norfloxacin.



a)

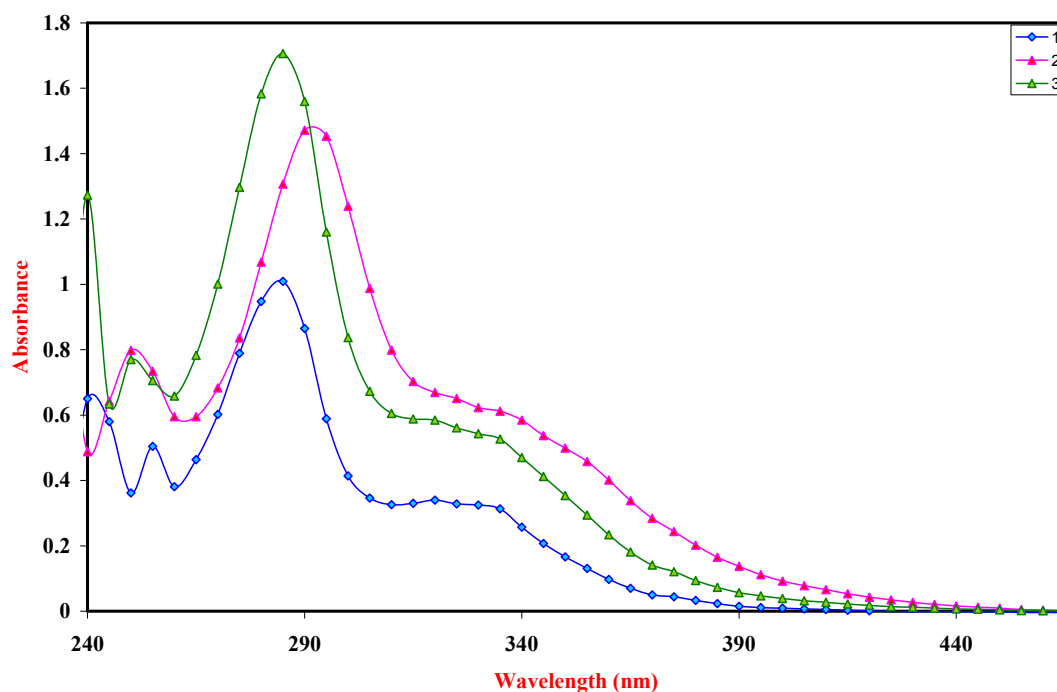


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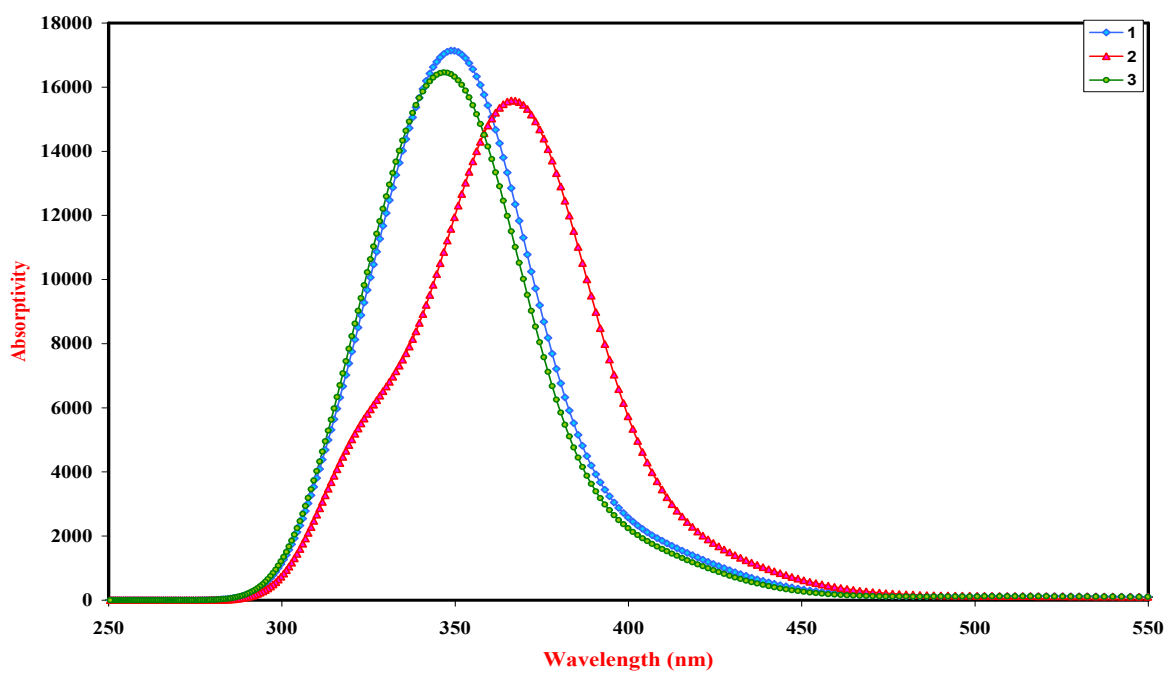


c)

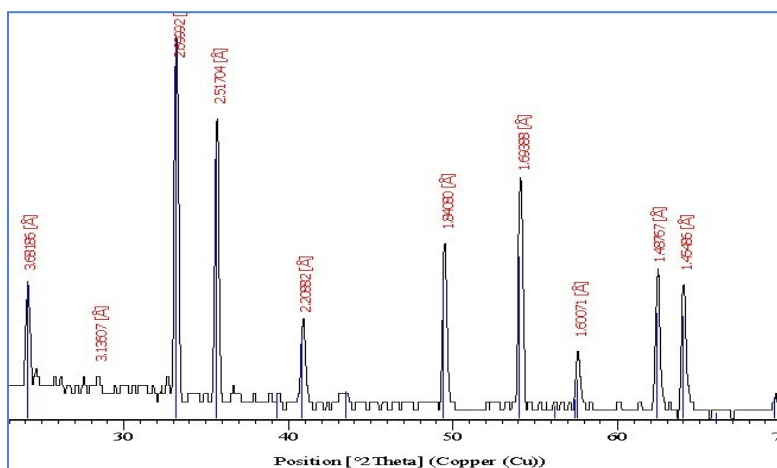
**Fig. S2:** Experimental FT IR spectra of complexes a) 1, b) 2 and c) 3.



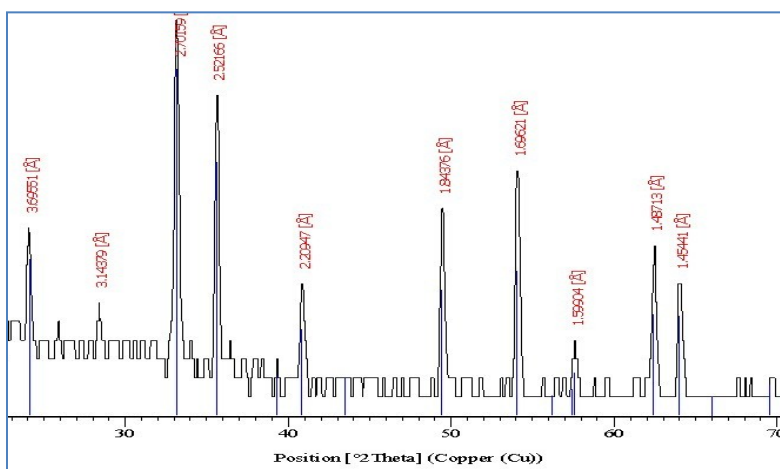
**Fig. S3:** Experimental electronic absorption spectra of the investigated complexes in DMSO.



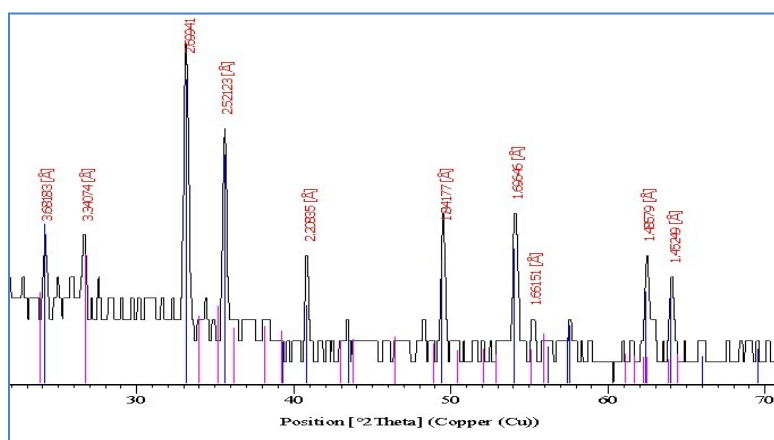
**Fig. S4:** Theoretical TD-DFT spectra of the investigated complexes in DMSO calculated at DFT/B3LYP/6-31G(d) level of theory.



a)

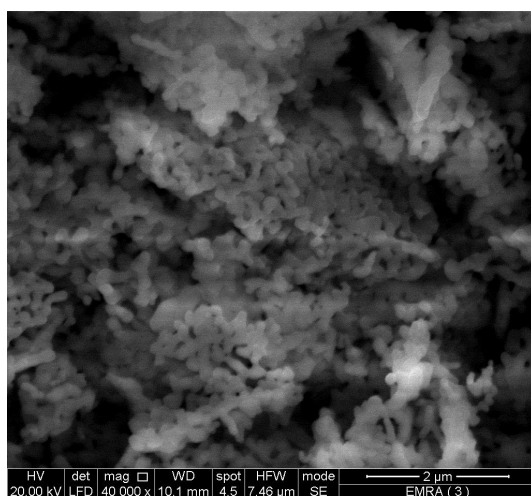


b)

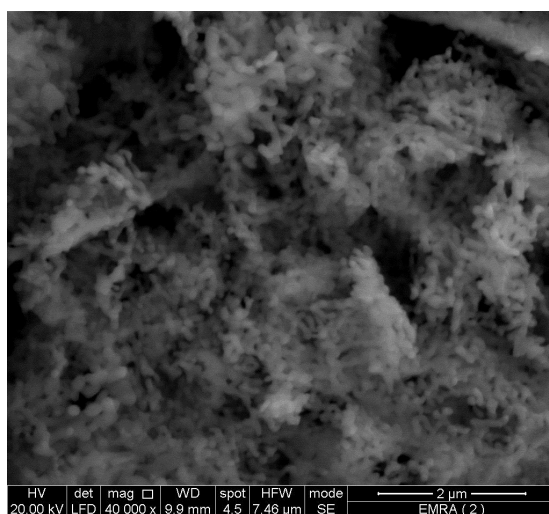


c)

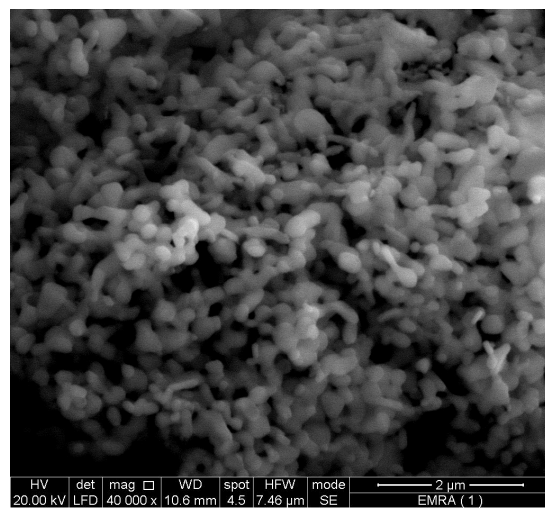
**Fig. S5:** XRD patterns of nano-hematite obtained from the controlled thermal decomposition of complexes a) **1**, b) **2** and c) **3**.



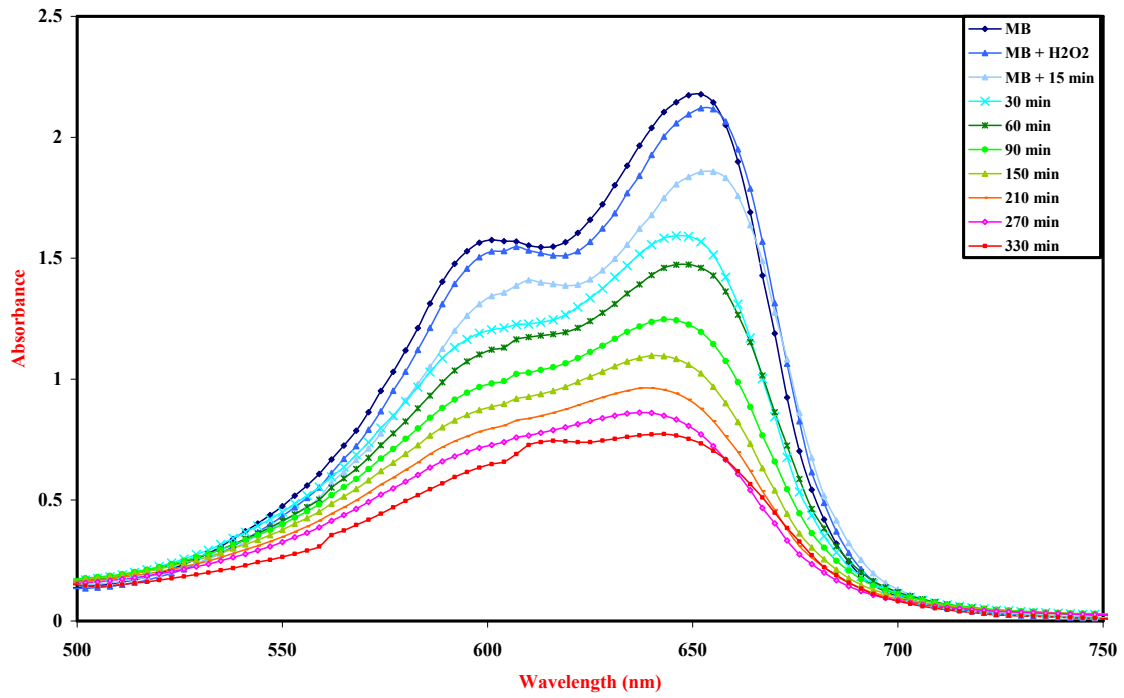
a)



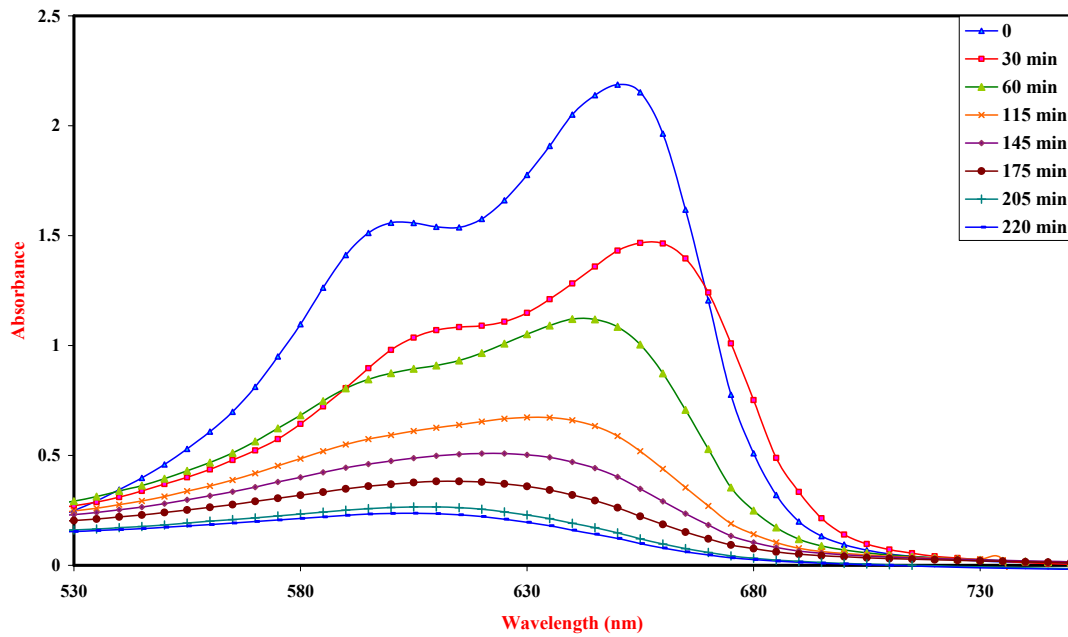
c)



**Fig. S6:** FE-SEM images of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles obtained from thermal decomposition of a) 1, b) 2 and c) 3 by magnification of 40 000x.



**Fig. S7:** Absorption spectral changes and photo-degradation of MB by H<sub>2</sub>O<sub>2</sub> under the effect of UV light at 365 nm (Control experiment).



**Fig. S8:** Absorption spectral changes and photo-degradation of MB by H<sub>2</sub>O<sub>2</sub> in presence of hematite nanoparticles No. 1 under the effect of UV light at 365 nm.

**Table S1:** Second-order interaction energy ( $E^2$ , kcal/mol) between donor and acceptor orbitals in the studied complexes 1-3 calculated at DFT/B3LYP/6-31G(d) level of theory (selected)

<b>Donor</b> → <b>Acceptor</b>	$E^2$ (kcal/mol)		
	<b>1</b>	<b>2</b>	<b>3</b>
LP(3)O2→RY*(3)Fe	1.07	1.08	1.08
LP(2)O3→RY*(4)Fe	0.72	0.70	0.69
LP(3)O4→RY*(2)Fe	1.27	1.28	1.27
LP(2)O5→RY*(3)Fe	1.33	1.33	1.33
LP(2)O6→RY*(4)Fe	0.89	0.91	0.90
LP(3)O7→RY*(2)Fe	1.32	1.33	1.32