inorganics

MDPI

Electronic supporting information

Interaction of redox active Copper(II) with catecholamines: A combined spectroscopic and theoretical study

Miriama Šimunková [1,*], Zuzana Barbieriková [1], Milan Mazúr [1], Marián Valko [1], Suliman Y. Alomar [2], Saleh H. Alwasel [2] and Michal Malček [1]

[1] Department of Physical Chemistry, Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9, 812 37, Bratislava, Slovakia; miriama.simunkova@stuba.sk

[2] King Saud University, Zoology Department, College of Science, Riyadh, 11451, Saudi Arabia; e-mail@e-mail.com

* Correspondence: miriama.simunkova@stuba.sk; (if there are multiple corresponding authors, add author initials)

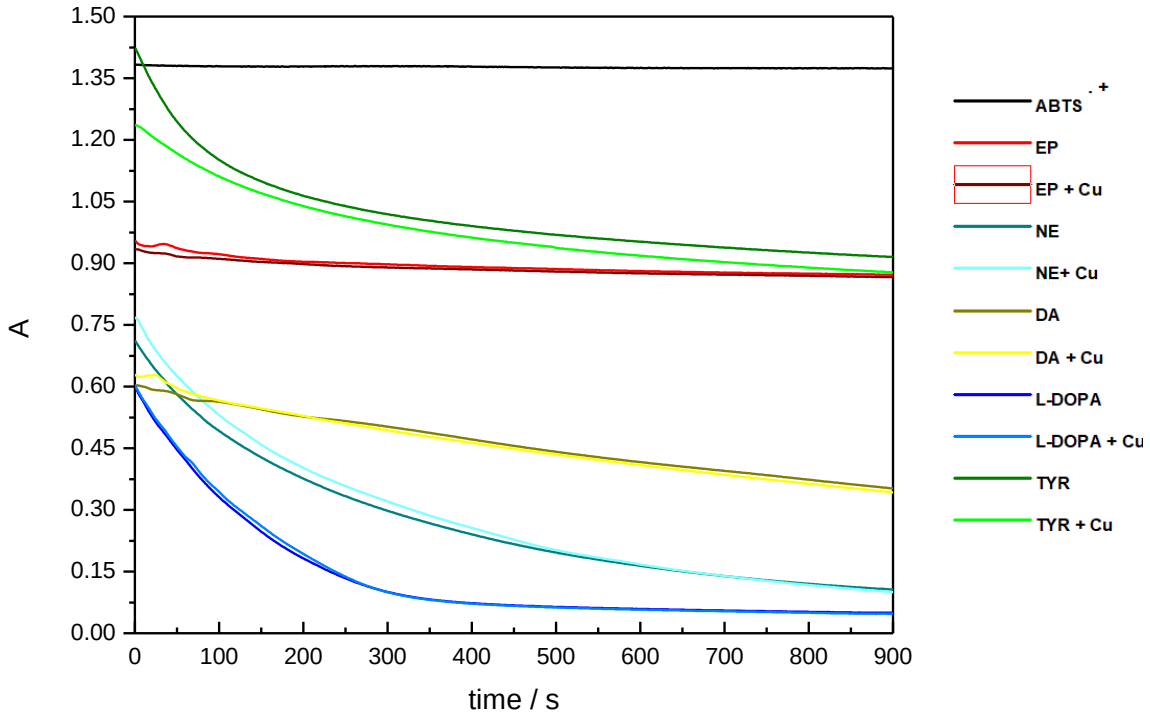

Figure S1 Scavenging of $ABTS^{\bullet+}$ by studied compounds and their Cu(II) complexes (fresh)

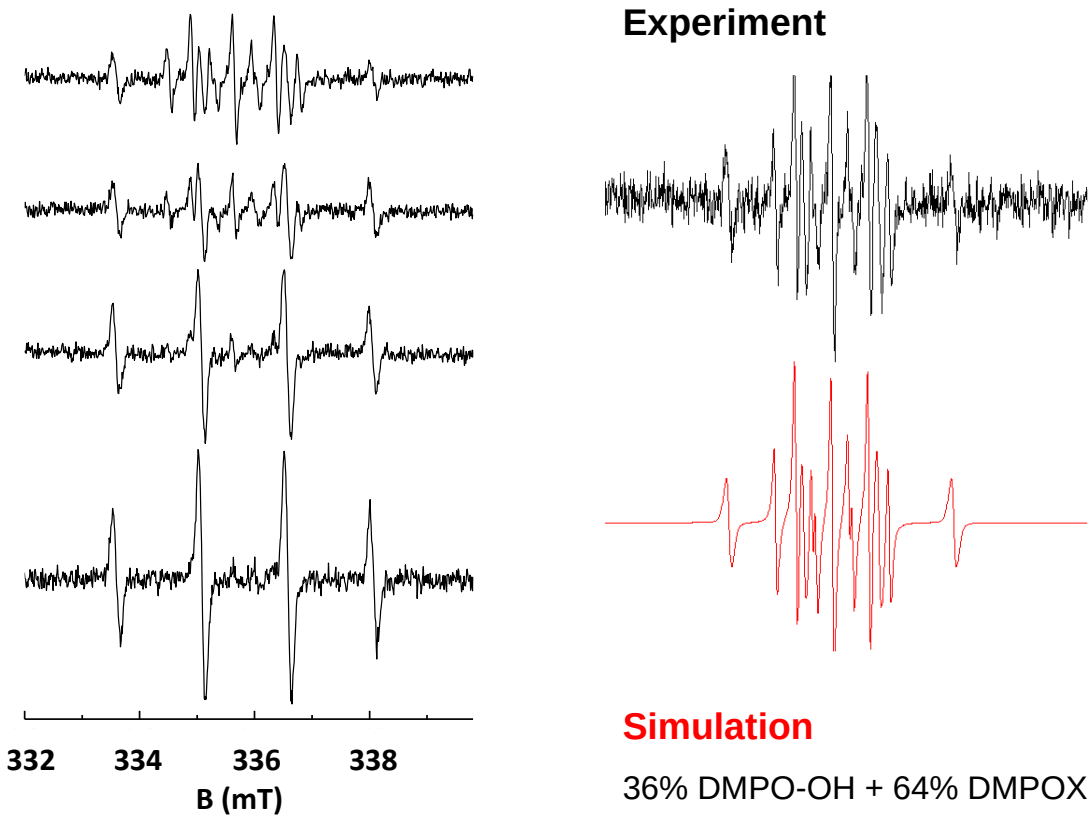

Figure S2 EPR spectra of •DMPO-OH and •DMPOX measured with starting acquisition 2 min after the addition of hydrogen peroxide to aqueous solution of $CuCl_2$ + EP containing DMPO spin trapping agent.

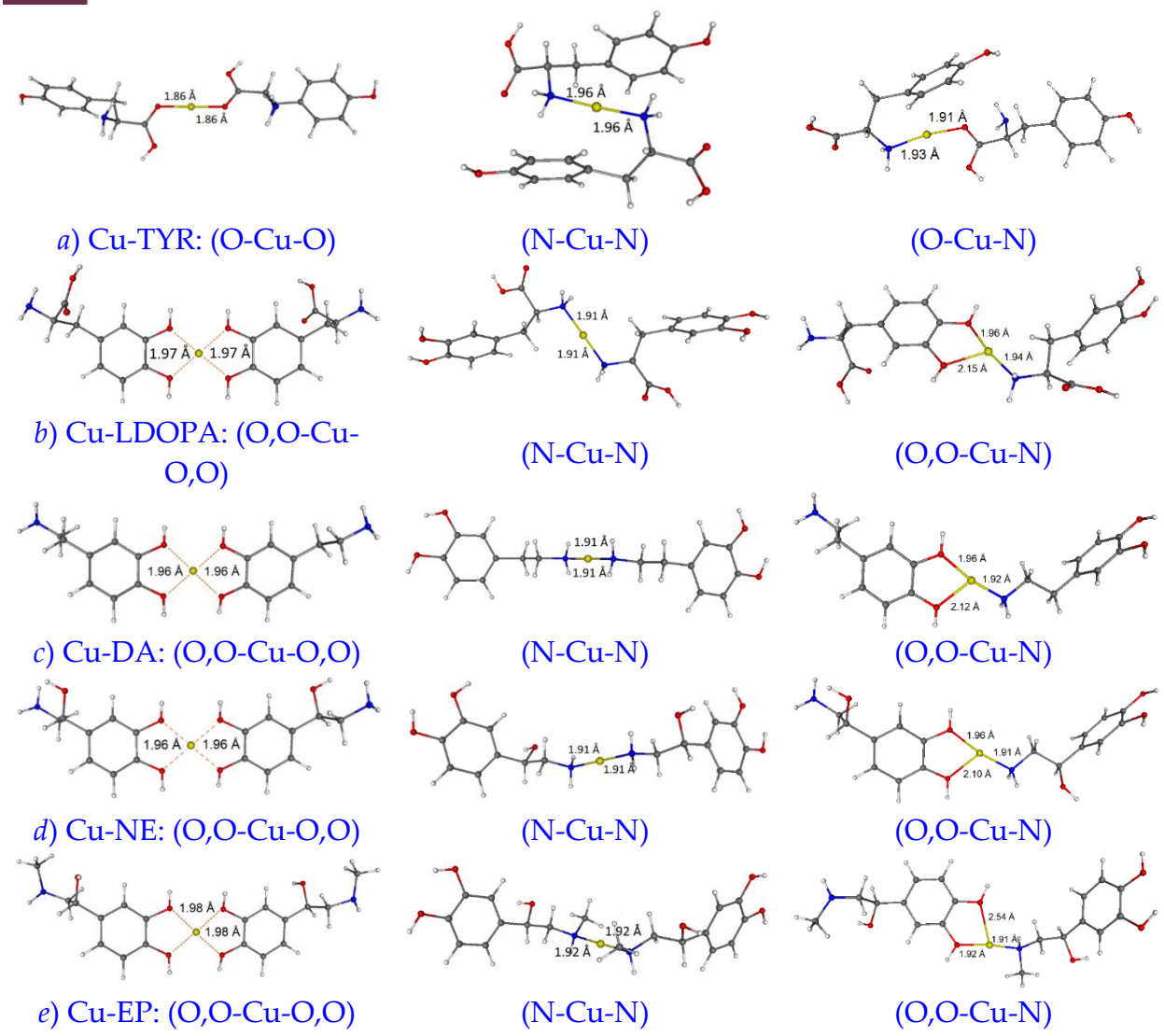

Figure S3 Optimized B3LYP/6-311G* structures of the studied Cu-complexes (molar ratio 1:2), including calculated Cu-O and Cu-N bond distances.

Table S1 Calculated B3LYP/6-311G* Cu-O, Cu-N bond distances, and corresponding QTAIM characteristics of the studied complexes (Cu : Ligand molar ratio is 1:2).

Complex	Binding	d(Cu-X) / Å	ρ_{BCP}(Cu-X) / bohr^{-3}	$\Delta\rho_{BCP}$(Cu-X) / bohr^{-5}	DI(Cu-X) / -
Cu-TYR[a]	O-Cu-O[a]	1.86[a]; 1.86[a]	0.10[a]; 0.10[a]	0.66[a]; 0.66[a]	0.52[a]; 0.51[a]
	N-Cu-N	1.96; 1.96	0.10; 0.10	0.41; 0.41	0.55;0.55
	O-Cu-N	1.91; 1.93[b]	0.09; 0.10[b]	0.53; 0.44[b]	0.45; 0.59[b]
Cu-LDOPA	O,O-Cu-O,O	1.97; 1.97	0.08; 0.08	0.45; 0.45	0.39;0.38
		1.97; 1.97	0.08; 0.08	0.45; 0.45	0.38;0.38
	N-Cu-N	1.91; 1.91	0.11; 0.11	0.50; 0.50	0.62; 0.61
	O,O-Cu-N	1.96, 2.15	0.08; 0.05	0.49; 0.25	0.38; 0.25
		1.94[b]	0.10[b]	0.45[b]	0.58[b]
Cu-DA	O,O-Cu-O,O	1.97; 1.97	0.08; 0.08	0.46; 0.46	0.39; 0.39
		1.97; 1.97	0.08; 0.08	0.46; 0.46	0.39; 0.39
	N-Cu-N	1.91; 1.91	0.11; 0.11	0.50; 0.50	0.63; 0.63
	O,O-Cu-N	1.96, 2.12	0.08; 0.06	0.49; 0.27	0.37; 0.26
		1.92[b]	0.11[b]	0.46[b]	0.61[b]
Cu-NE	O,O-Cu-O,O	1.96; 1.96	0.08; 0.08	0.46; 0.46	0.39; 0.39
		1.96; 1.96	0.08; 0.08	0.46; 0.46	0.39; 0.39
	N-Cu-N	1.91; 1.91	0.11; 0.11	0.50; 0.50	0.63; 0.63
	O,O-Cu-N	1.95, 2.10	0.08; 0.06	0.50; 0.29	0.37; 0.27
		1.91[b]	0.11[b]	0.45[b]	0.62[b]
Cu-EP	O,O-Cu-O,O	1.98; 1.98	0.08; 0.08	0.45; 0.44	0.38; 0.37
		1.98; 1.98	0.08; 0.08	0.45; 0.44	0.37; 0.37
	N-Cu-N	1.92; 1.92	0.11; 0.11	0.48; 0.48	0.60; 0.59
	O,O-Cu-N	1.92; 2.54	0.08; 0.02	0.56; 0.09	0.42; 0.12
		1.91[b]	0.11[b]	0.50[b]	0.62[b]

[a] coordination via oxygens of COOH groups

[b] Cu-N bond

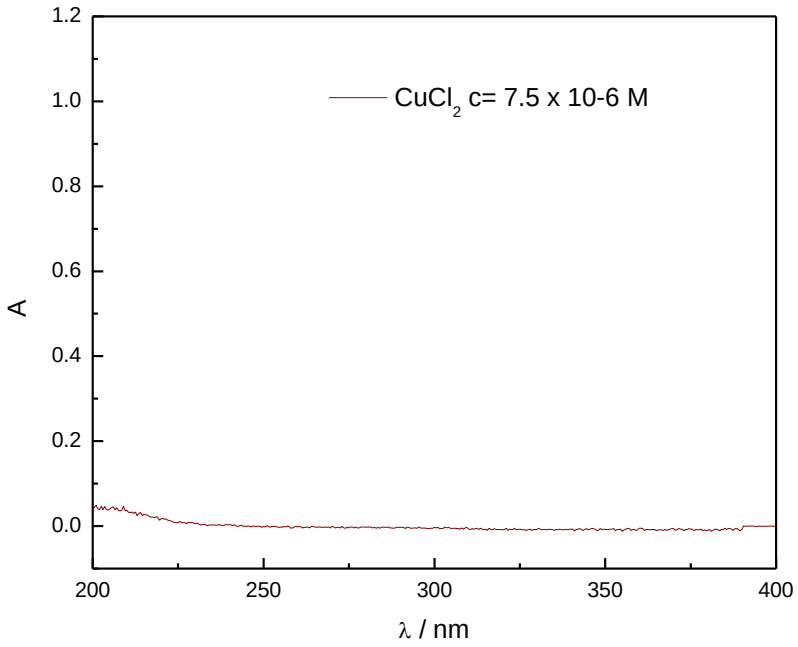

Figure S4 UV-VIS spectrum of $CuCl_2$ reference system, $c_{CuCl2} = 7.5 \times 10^{-6}$ M

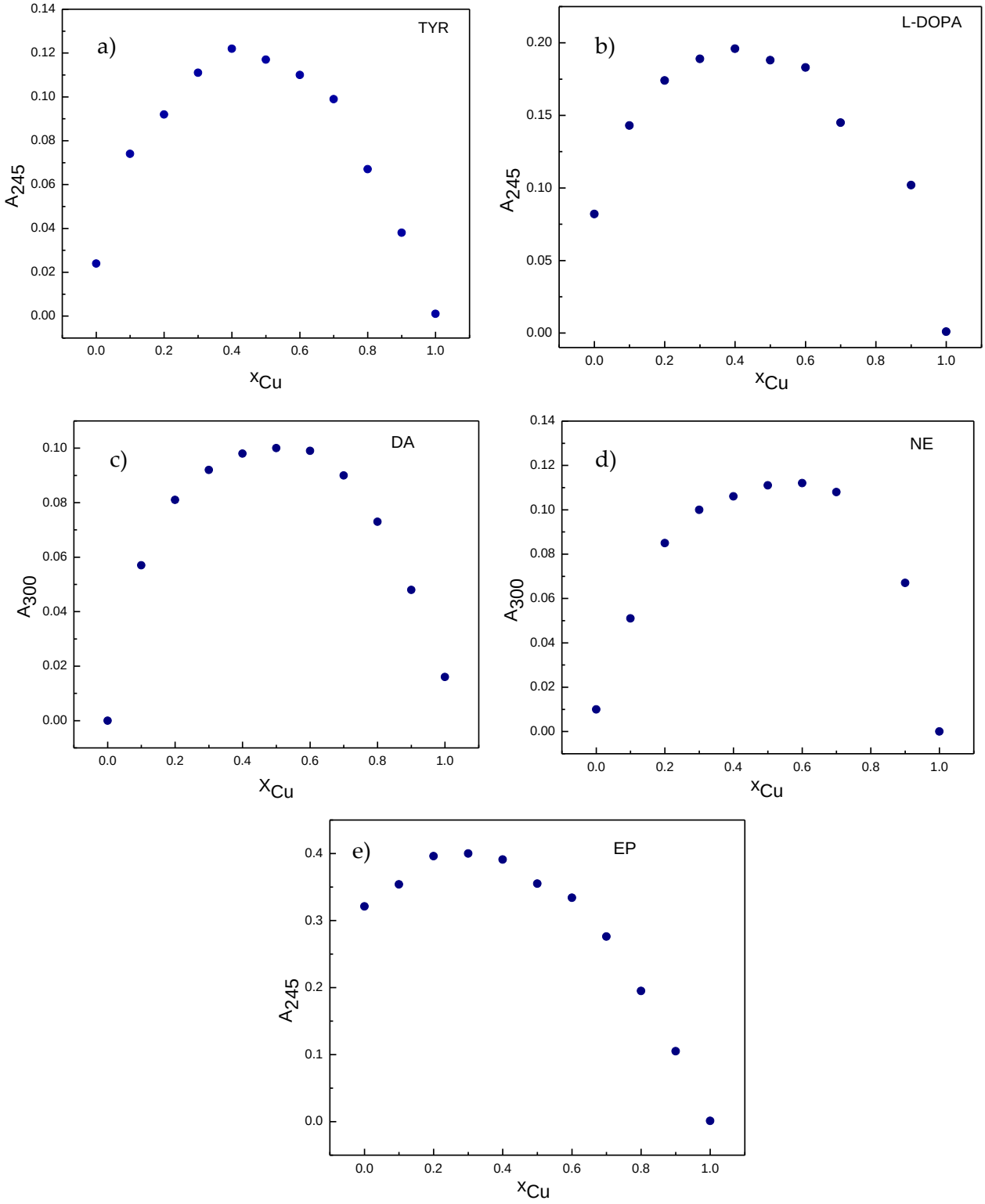

Figure S5 Job's plots of studied compounds (a)TYR b)L-DOPA c)DA d)NE e)EP and $CuCl_2$

Absorption spectra were measured in various molar ratios.

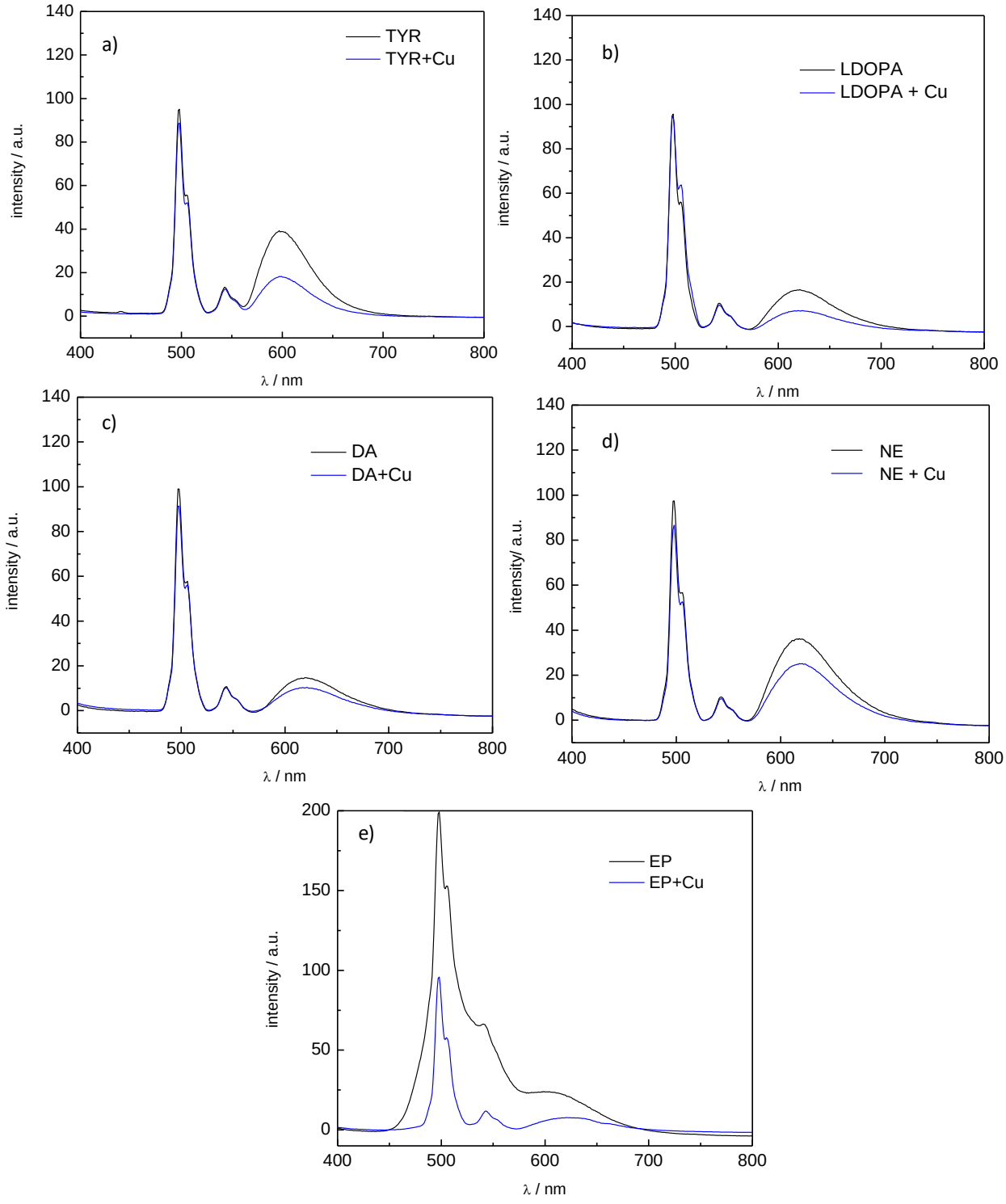

Figure S6 Emission spectra of studied compound before (black line) and after addition of $CuCl_2$ (blue line) in water.

Concentration of studied compounds: $c_{sample} = 2 \times 10^{-5}$ M, $c_{copper(II)chloride} = 1 \times 10^{-5}$ M

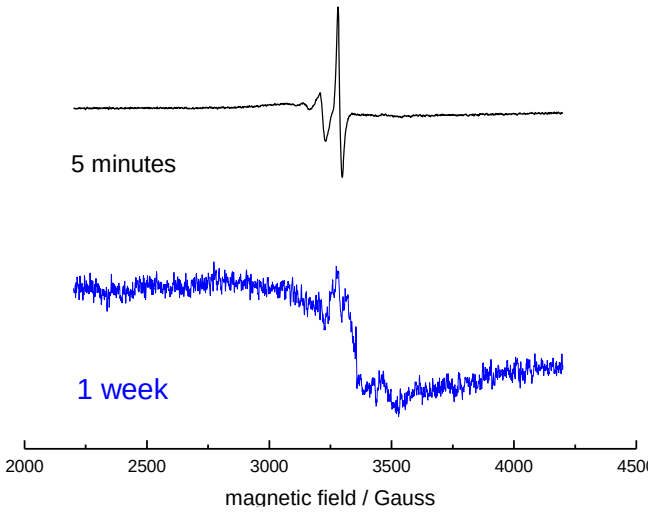

Figure S7 EPR spectrum of Cu(II)-DA (1:2) complex at room temperature immediately after mixing (black line) and after one week (blue line)