ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO:

SYNTHESIS, CHARACTERIZATION, AND DFT CALCULATIONS OF NEW FLUORESCENT Cu(II) COMPLEXES OF HETEROCYCLIC LIGANDS

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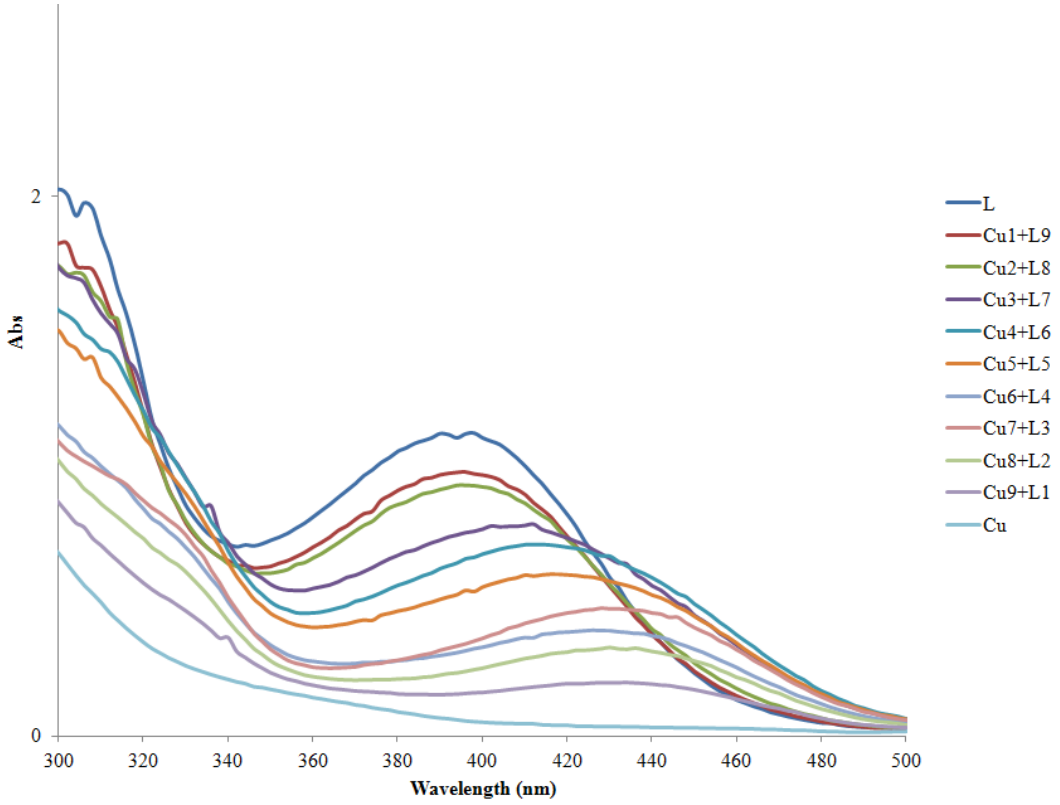

Fig. S1. Absorption spectra of the nine aqueous methanolic mixtures of ligand **4a** and Cu (II).

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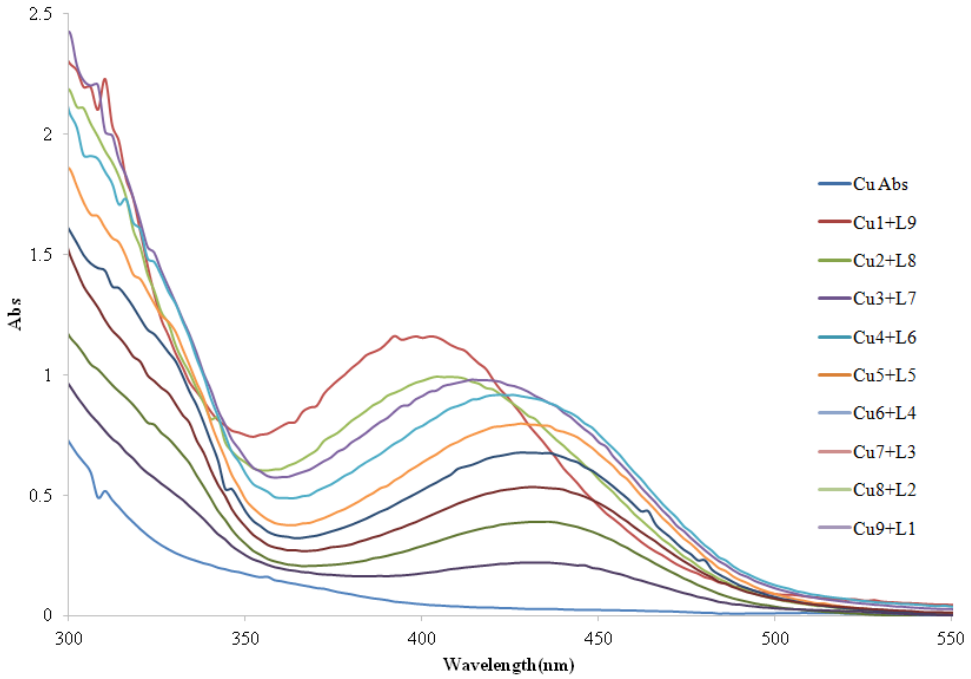

Fig. S2. Absorption spectra of the nine aqueous methanolic mixtures of ligand **4b** and Cu (II).

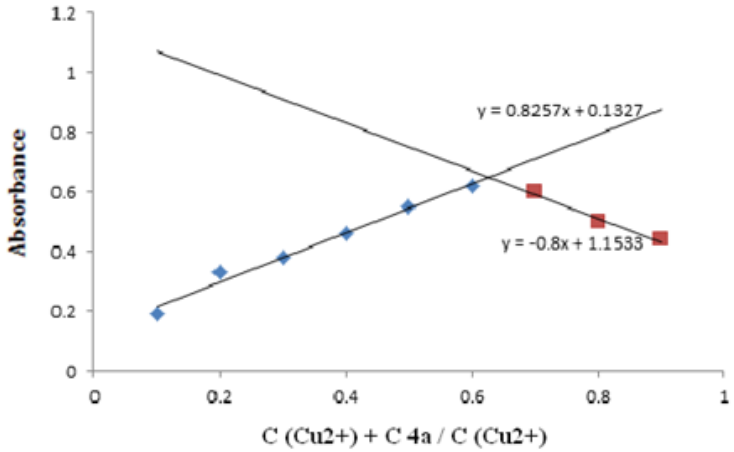

Fig. S3*. Job's curve of equimolar solutions for complex **5a** in the aqueous methanolic solution (absorbance at 425 nm).
*Job's plot reached a maximum value at a mole fraction of 0.64, which confirmed that the molar ratio between **4a** and Cu(II) ions is 2:1 in complex **5a**.

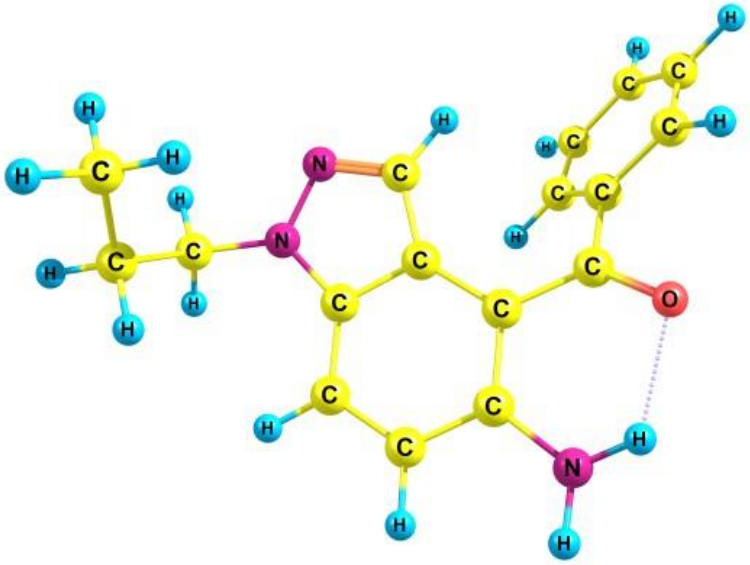

Fig. S4. Optimized geometry of **4a**.

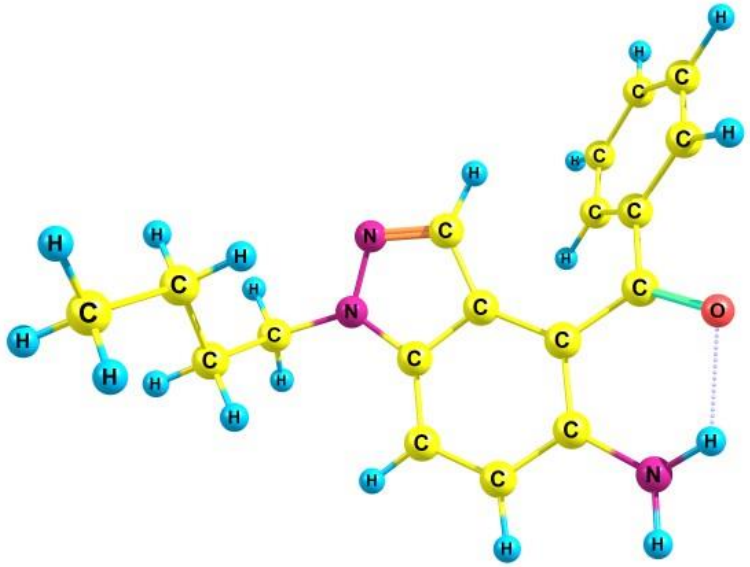

Fig. S5. Optimized geometry of **4b**.

Table S1

Cartesian coordinates of the optimized geometry for **4a**

C	–0.128835000	–0.306974000	–3.833948000
C	0.031698000	–0.850801000	–2.518162000
C	0.356676000	–0.024434000	–1.430463000
C	0.557468000	1.352373000	–1.584140000
C	0.371386000	1.891574000	–2.837148000
C	–0.009229000	1.104958000	–3.962787000
C	–0.103688000	–2.143628000	–1.942655000
N	0.122378000	–2.124388000	–0.641520000
N	0.411003000	–0.847238000	–0.315638000
H	0.830539000	1.988170000	–0.750319000
H	0.495938000	2.959690000	–2.980571000
C	0.662420000	–0.448989000	1.058779000
H	0.905970000	–1.363681000	1.603247000
H	1.553806000	0.186311000	1.070156000
C	–0.517078000	0.268989000	1.730889000
H	–0.725113000	1.206087000	1.204386000
H	–0.190767000	0.547084000	2.739629000
C	–1.790924000	–0.575572000	1.809230000
H	–2.579278000	–0.036563000	2.341249000
H	–2.166842000	–0.823466000	0.814330000
H	–1.611741000	–1.515137000	2.340495000
C	–0.431154000	–1.126166000	–5.025078000
O	–1.039797000	–0.659889000	–5.992444000
C	0.027369000	–2.553918000	–5.121742000
C	–0.760597000	–3.468950000	–5.828787000
C	1.274767000	–2.958664000	–4.631398000
C	–0.322639000	–4.776721000	–6.015073000
C	1.726802000	–4.257568000	–4.848237000
C	0.924480000	–5.171975000	–5.530177000
H	–1.712506000	–3.143210000	–6.230493000
H	1.894353000	–2.253959000	–4.090127000
H	–0.948384000	–5.484473000	–6.547202000
H	2.701686000	–4.557701000	–4.480802000
H	1.271314000	–6.187375000	–5.686619000
N	–0.206212000	1.751469000	–5.154042000
H	–0.174499000	2.755567000	–5.175602000
H	–0.686834000	1.250865000	–5.887914000
H	–0.358371000	–3.061273000	–2.443940000

Table S2

Cartesian coordinates of the optimized geometry for **4b**

C	–0.805895000	1.284244000	0.094548000
C	0.125582000	0.240468000	–0.210943000
C	1.406403000	0.549992000	–0.717372000
C	1.808982000	1.874191000	–0.954629000
C	0.929412000	2.877408000	–0.630793000
C	–0.359347000	2.619863000	–0.072206000
C	0.155662000	–1.180297000	–0.085801000
N	1.316606000	–1.678717000	–0.485438000
N	2.077888000	–0.635702000	–0.877005000
H	2.784793000	2.109540000	–1.362859000
H	1.217980000	3.911737000	–0.786721000
C	3.447664000	–0.844072000	–1.326225000
H	3.499054000	–1.883644000	–1.653969000
H	3.616258000	–0.211475000	–2.203273000
C	4.512113000	–0.561517000	–0.256286000
H	4.423576000	0.478144000	0.080209000
H	5.492591000	–0.644225000	–0.741981000
C	4.456188000	–1.501355000	0.952417000
H	3.469523000	–1.435282000	1.420495000
H	4.556811000	–2.536795000	0.606706000
C	–2.164309000	1.026166000	0.609432000
O	–2.767731000	1.857814000	1.293093000
C	–2.883043000	–0.248291000	0.270709000
C	–3.698567000	–0.839549000	1.243301000
C	–2.854497000	–0.788082000	–1.020097000
C	–4.444822000	–1.973725000	0.939897000
C	–3.625509000	–1.905631000	–1.330839000
C	–4.412117000	–2.507023000	–0.349390000
H	–3.740875000	–0.396735000	2.231149000
H	–2.240027000	–0.326012000	–1.783443000
H	–5.059566000	–2.436585000	1.703711000
H	–3.609701000	–2.308163000	–2.337353000
H	–5.002180000	–3.384615000	–0.589120000
N	–1.148334000	3.698299000	0.233244000
H	–0.732545000	4.614022000	0.214238000
H	–1.929001000	3.535659000	0.854952000
H	–0.609253000	–1.849770000	0.270462000
C	5.541634000	–1.195734000	1.988394000
H	5.442056000	–0.177933000	2.379003000
H	5.482881000	–1.882332000	2.837022000
H	6.543152000	–1.287553000	1.555738000

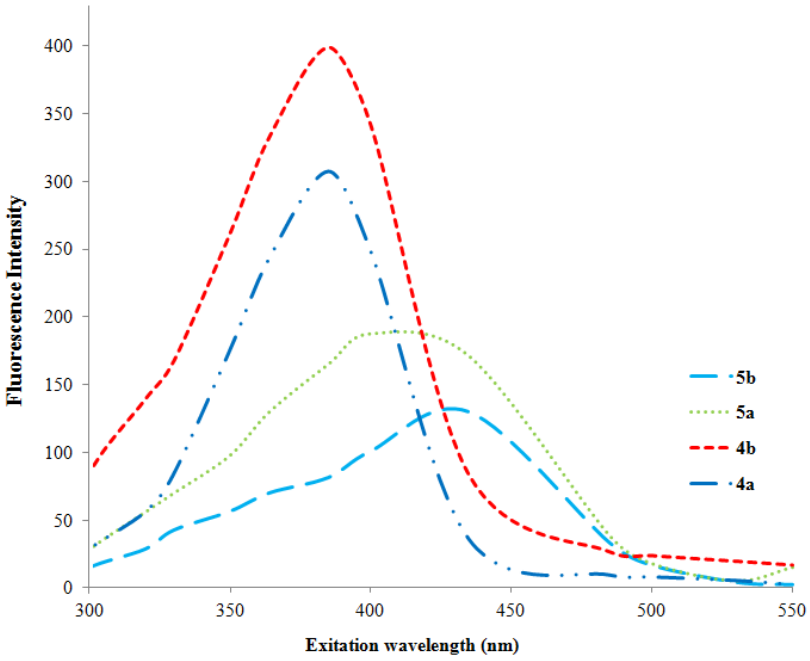

Fig. S6. Excitation spectra of ligands **4a,b** and Cu(II) complexes **5a,b** in the MeOH solution (3×10^{-6} M).