Dear Prof. Perdih,

Thank you for the comments.

The paper is revised in accord with the suggestions.

1. Why did you prepare complexes of Cu only with L1 and Zn only with L2?

Reply: We believe that single crystal X-ray diffraction is the best way to reveal the structures of metal complexes. Without single crystals, the structures of metal complexes are ambiguous. In the experiment, only Cu with L1 and Zn with L2 can form single crystals. Otherwise, Zn with L1 and Cu with L2 are not give single crystals suitable for X-ray diffraction.

2. What is the stability of the Cu and Zn complexes in the biological medium? Perform UV and/or NMR (in the case of Zn complex) study of the stability of the complexes in aqueous media. For example, you can dissolve the complexes in the biological buffer and confirm the stability by monitoring the UV-Vis spectrum within the timeframe of the biological assay.

Reply: The complexes in aqueous media are studied, and the results are given as supplementary material. The complexes are stable in the biological assay.

3. Submit cif files and checkcif reports for review.

Reply: The cif files and checkcif reports are submitted in the zip file.

Other minor corrections to improve clarity and conciseness of the manuscript :

Generally, all tables and other graphical elements which are not discussed in detail in the discussion section should be moved to the SI in my opinion.

P1L14 – provide institutional email address

Reply: This is my permanent email. The institutional email of mine is not work well.

P1L13 – add notation nubner to ligand in the Cu complex fomula (L1)

Reply: The notation nubner to ligand in the Cu complex fomula (L1) is added.

P3L72 – delete 'with'

Reply: deleted.

P3L84 – to which Cu… and ammonium thiocyanate … dissolved in methanol were added dropwise.

Reply: Corrected.

P3L94 – similar…

Reply: Corrected.

P4 – Move Table 1 to SI

Reply: We think Table 1 is important for single crystal X-ray determination. So, we suggest to retain the table in the paper.

P5 – Move Table 2 to SI. Include bond lengths in the metal coordination sphere (M-L) in the caption below the figures.

Reply: Table 2 is moved to SI. The bond lengths are included in the captions of the figures.

P7 Scheme 1 – MeOH in copper complex is drawn in a strange way.

Reply: The scheme 1 is corrected.

P8 – Move Table 3 to SI. Include selected H-bond values in the caption of Fig. 2.

Reply: Table 3 is moved to SI. The selected H-bond values are included in the captions of the figures.

Sincerely yours,

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