Dear Editor,

The manuscript has been revised in accordance with the comments of the referees as follows. Corrections and additions are in red color in the revised manuscript.

With best regards,

On behalf of Authors

**Assoc. Prof. Dr. Mehmet Ferdi FELLAH**

**Answers to Comments**

**Reviewer A**

*line 39: Reference 19 does not correspond to the compound [(4-aminophenyl)imino] methyl-6-methoxy-4-nitrophenol (Ref. 18) as it is indicated in thetext, but to the compound 2-{(E)-[(4-aminophenyl)imino]methyl}-6-bromo-4-chlorophenol.*

Related text has been modified as follows:

“In a previous theoretical study, the [(4-aminophenyl) imino] methyl-6-bromo-4-chlorohenol as Schiff base ligand and its complexes with Co, Ni, Cu and Zn metals was investigated.19”

*line 60: ‘1-4 phenilendiamine…’ should be ‘1,4-phenylenediamine…’.*

It has been corrected.

*line 98: ‘1,4-phenilendiamine…’ should be ‘1,4-phenylenediamine…’.*

It has been corrected.

*line 99: ‘3,5-diclorosalicylaldehyde…’ should be ‘3,5-dichlorosalicylaldehyde…’.*

It has been corrected.

*line 114: ‘…the composition the above…’ should be ‘…the composition of the above…’.*

It has been corrected.

*The quality of this article would be much more enhanced if some preliminary biological screening was performed. In light of these facts, I recommend to authors to investigate in vitro antibacterial and antifungal activity of the ligand and its metal complexes. These results should be presented in the form of MIC values and compared with the corresponding standard (e.g. Gentamicine, Ciprofloxacin, Ketoconazole etc.).*

Antibacterial and antifungal activities of the ligand and its metal complexes have been studied by a new author who is Seher GÜR from Department of Biology in Fırat University and related statements including detail of methods, results and discussions have been inserted into text. Therefore the author has been added into the list of authors.

**Reviewer B**

*(line 84): The spin contamination <S2> (a qualified error) can be presented theoretical calculations where in the cluster approach was utilized with spin multiplicity (SM). The spin contamination value showing where the unpaired electrons of the system are located must be very small (less than10%). The <S2> values were negligible in this study. This part is (mainly) meaningless. It is known that the spin contamination 〈S2〉 (although not rigorously defined in the density functional theory) measures the extent to which the singlet states are contaminated by higher spin states. Furthermore, 〈S2〉 cannot be used for any kind of local analysis of a given molecule (The spin contamination value showing where the unpaired electrons of the system are located must be very small (less than10%)).*

In Results and Discussion section of the manuscript it has been mentioned that Spin Multiplicity (SM) numbers determined for the ligand complexes with Zn, Cu, Ni and Co metals are 1, 2, 3 and 4, respectively. So the spin contamination <S2> can be introduced into the calculations with these SM except singlet state and this spin contamination value must be very small (less than 10%).\* Accordingly, related section has already a statement of “In this optimization calculation the computed <S2> values confirmed that the spin contamination was very small (max 0.5% after annihilation).”

\* D.C. Young, Computational Chemistry; John Wiley & Sons, Inc., New York, 2001, p 228.

There was a writing error about local analysis of a given molecule (*The spin contamination value showing where the unpaired electrons of the system are located must be very small (less than10%)*). The spin density values show where the unpaired electrons of the system are located. Related sentences have been modified as follows:

“The spin contamination <S2> (a qualified error) can be presented theoretical calculations where in the cluster approach was utilized with spin multiplicity (SM). The spin contamination value must be very small (less than 10%).26”

“Mulliken population analysis28 has been utilized to obtain spin density values (showing where the unpaired electrons of the system are located) of metal atoms.”

*I guess that the authors used the experimental magnetic properties of the examined molecules to choose the spin state of the examined complexes. On the other hand, in the paper these data are easily found (Line 139): The magnetic susceptibility data of the complexes are given in Table 3. This  
referee could not find such data in Table 3.*

They have not been written mistakenly, the magnetic susceptibility data of the complexes (μeff (B.M.)) have been inserted into Table 3.

*The authors should first introduce the acronyms (Line 176: EG calculations) and then to use them.*

The meaning of EG has been inserted into text when it was used first.

*Since the authors performed the NBO analysis, it would be more convenient to use the NBO charges instead of the Mullikan charges. It is known that the NBO charges give more realistic predictions.*

NBO charge values have been inserted into manuscript instead of Mulliken charge values and related sentences have been modified according to this.

*Line 19: The stretching frequencies of C=N, C-O and N-H were computed to be in good agreement with experimental data. should be The computed stretching frequencies of C=N, C-O and N-H bonds were found to be in good agreement with experimental data.*

It has been corrected.

*Line 36: It has been experimentally investigated the the synthesis and characterization of various transition metal complexes of novel Schiff bases. should be The synthesis and characterization of various transition metal complexes with novel Schiff bases were experimentally investigated.*

It has been corrected.

*Line 81: In present work… should be In the present work…*

It has been corrected.

*Line 82: B3LYP- Hybrid formalism were… should be The hybrid B3LYP formalism was…*

It has been corrected.

*Line 83: B3LYP was a high-quality DFT should be B3LYP is a high-quality DFT*

It has been corrected.

*Line 84: The theoretical approach applied in this study were detailed in our previous studies. should be The theoretical approach applied in this study was presented in our previous studies.*

It has been corrected.

**Additional Correction**

The title of the manuscript has been modified as follows:

“Design, Synthesis, Characterization and Antibacterial and Antifungal Activity of a New 2-{(E)-[(4-aminophenyl)imino]methyl}-4,6-dichlorophenol and its Complexes with Co(II), Ni(II), Cu(II) and Zn(II): An Experimental and DFT Study”