

ReviewForm3

JournalName:	InternationalResearchJournalof PureandAppliedChemistry
ManuscriptNumber:	Ms_IRJPAC_126631
TitleoftheManuscript:	DFTStudyofCoordinationofN-MonochlorosubstitutionDerivativesofBiguanide
TypeoftheArticle	Originalresearcharticle

PART1: ReviewComments

Compulsory REVISION comments	Reviewer's comment	Author's Feedback (Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
<p>Please write a few sentences regarding the importance of this manuscript for the scientific community. Why do you like (or dislike) this manuscript? A minimum of 3-4 sentences may be required for this part.</p>	<p>This manuscript is valuable to the scientific community for its detailed DFT analysis of N-chlorosubstituted biguanides, offering insights into their coordination properties with zinc(II) ions, relevant for drug development in diabetes treatment. The study's focus on bioavailability aligns with medicinal chemistry applications, providing foundational knowledge that can guide future research. While thorough in its computational approach, experimental validation and bioactivity testing would strengthen its impact.</p>	
<p>Is the title of the article suitable? (If not please suggest an alternative title)</p>	<p>The title, "DFT Study of Coordination of N-Monochlorosubstitution Derivatives of Biguanide," is mostly suitable, as it accurately reflects the study's focus on DFT analysis and the coordination properties of N-chlorosubstituted biguanides.</p>	
<p>Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here.</p>	<p>The abstract provides a good overview of the study's objectives, methods, and findings but could be made more comprehensive with a few additions: Summarize Key Findings, Methodological Details and Conclude with Potential Impact</p>	
<p>Are subsections and structure of the manuscript appropriate?</p>	<p>The manuscript's structure is clear and logical, with well-organized subsections that effectively guide the reader through the study's objectives, methods, results, and implications.</p>	
<p>Please write a few sentences regarding the scientific correctness of this manuscript. Why do you think that this manuscript is scientifically robust and technically sound? A minimum of 3-4 sentences may be required for this part.</p>	<p>This manuscript demonstrates scientific robustness and technical soundness through its use of advanced computational techniques, such as DFT/B3LYP/6-31G(d,p), which are well-regarded in theoretical chemistry for studying coordination properties. The methodology is clearly explained, allowing for reproducibility, and the selection of coordination indicators—like bond lengths, electrostatic potentials, and atomic charges—provides comprehensive insight into the binding characteristics of N-chlorosubstituted biguanides. The results are consistent with known coordination chemistry principles, reinforcing the accuracy of findings. Furthermore, bioavailability assessment based on Lipinski's Rule of Five supports the practical relevance of the study, making it scientifically valuable and technically thorough.</p>	
<p>Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.</p>	<p>yes</p>	
<p>Minor REVISION comments</p> <p>Is the language/English quality of the article suitable for scholarly communications?</p>	<p>The manuscript effectively conveys complex scientific concepts with clarity and precision. However, some minor improvements in sentence structure and grammar could enhance readability. Overall, the article is well-written and meets the standards of academic writing in terms of clarity, coherence, and technical terminology.</p>	

ReviewForm3**Optional/General** comments

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PART 2:

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Are there ethical issues in this manuscript?	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	

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