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| Journal Name: | [**International Research Journal of Pure and Applied Chemistry**](https://journalirjpac.com/index.php/IRJPAC) |
| Manuscript Number: | **Ms\_IRJPAC\_136584** |
| Title of the Manuscript: | **PICT Effects and Anticancer Activity on Rosaniline and Spectral Characterisation of Rosaniline/ Cyclodextrin Covered ZnO/ Nanocrystals** |
| Type of the Article | **Research Paper** |

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| PART 1: Comments | | |
|  | Reviewer’s comment Artificial Intelligence (AI) generated or assisted review comments are strictly prohibited during peer review. | Author’s Feedback (It is mandatory that authors should write his/her feedback here) |
| Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part. | Generally, the work presents a study on the photophysical characteristic, host guest interactions, and anticancer potential of Rosaniline/cyclodextrin doped ZnO nanocrystals. The findings contribute to the fields of supramolecular chemistry, nanomedicine, and dye-sensitized materials by offering understanding on PICT behaviour and the stabilization of dye molecules within cyclodextrin-modified nanostructures. Moreover, the potential applications of the work can be fitted into optical sensing and drug delivery, making it beneficial to materials' science and biomedical research. | The design of new drugs is not only limited to the search for substances that show pharmacological potential in relation to the chosen biological target, but also requires taking into account other significant properties of potential drugs, such as molecular properties, solubility, absorption, metabolism, or toxicity, which can significantly affect the practical use of the developed substances. The development of in silico methods allowing these properties to be modelled at a very good level of estimation has contributed to the spread of a significant number of tools that are commonly used in the early phase of drug design, such as ADMETlab2.0, SwissADME, pkCSM, FAF-Drugs4, and AdmetSAR. Their use allows a significant narrowing of the group of substances considered in in vitro research by excluding chemical compounds with an inappropriate ADMETprofile, such as those with properties like the absorption, distribution, metabolism, excretion, and toxicity of considered compounds. |
| Is the title of the article suitable?  (If not please suggest an alternative title) | The words "Anticancer Activity on Rosaniline" is slightly inappropriate (Suggestion to use: "Anticancer Potential of Rosaniline.") Plus, there is no mention of host-guest interaction which one of the key parts of the work. | The title is changed. |
| 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. | The abstract should begin with a clear research background, objective, specific methods, and followed by result. Right now, it starts directly with the synthesis and results. Additionally, the paragraph jumps from photophysical results to molecular docking without transitions. Lastly, the significance of result should be included. | Abstract is revised |
| Is the manuscript scientifically, correct? Please write here. | The manuscript is generally scientifically sound. The work composed of synthesis, spectral analysis, molecular modelling, and docking studies. The methods are appropriate and aligned with the objectives. The interpretation of photophysical behaviour, inclusion complex formation, and charge transfer phenomena is consistent with established literature. However, there are some explanations such as spectral shifts, PICT state assignments, and molecular docking interactions should have more clearer justification, detailed discussion, and should have include more recent references. | Yes. Because in this manuscript, we analyse the following : Rosaniline/Cyclodextrin covered ZnO nanocrystals are synthesized and characterized by various spectral and microscopic methods. The effect of different polarity of the solvents, α-cyclodextrin (α-CD) and β-cyclodextrin (β-CD) on RND were studied by various spectral methods. The inclusion behaviour of RND on both CDs were determined by PM3 method. Doping effect of RND/CD on ZnO nano investigated by UV-visible, fluorescence, FTIR, DTA, XRD, FE-SEM and TEM methods. |
| Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form. | No references from top-tier journals such as ACS Applied Materials & Interfaces, Nanoscale, Scientific Reports, from the last 5 years. ZnO/CD nanohybrids for biomedical or sensing applications have been extensively studied recently. None of those cutting-edge works are cited. | New references are added |
| Is the language/English quality of the article suitable for scholarly communications? | The manuscript could benefit from grammatical proofreading and formatting editing to improve scientific tone. | The spelling and grammatical errors are corrected. |
| Optional/General comments | Please include the methodology for all the characterisation  In the result and discussion,  1. In section 3.1: Justify the assignment of transitions (e.g., 546 nm attributed to PICT). Are these supported by literature or TD-DFT? The paragraph would benefit from explicit comparison to previous literature on similar triarylmethane dyes to strengthen interpretation.  2.In Section 3.3: Add explanation on why does a more negative ΔG indicate greater stability of β-CD complex?  3. In Section 3.5: Avoid saying “confirm the formation of new nanomaterials” unless accompanied by structural or functional validation (e.g., SAED patterns, zeta potential). Additionally, interpret the morphological differences: why does β-CD produce nanosheets and RND/β-CD produce “rock-like” structures?  In Section 3.6: Avoid listing all peak positions without interpretation. Instead, identify changes in crystallinity, lattice strain, or phase purity.  It is suitable for publication after addressing issues in language, methodology, referencing, and depth of interpretation of result. | Necessary explanation is added in the revised text. |

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| **PART 2:** | | |
|  | **Reviewer’s comment** | **Author’s Feedback** (It is mandatory that authors should write his/her feedback here) |
| **Are there ethical issues in this manuscript?** | *(If yes, Kindly please write down the ethical issues here in details)* | No ethical issues in this manuscript. |