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Peer Review

Review of: "Synthesis, ADME, Toxicity, and In Silico Molecular Docking Study of Novel β-Carboline Derivatives as Potential Inhibitor Anticancer Agents"

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The subject of the work is very interesting, as is the title, but nevertheless, I find certain flaws in the work. Firstly, you cannot claim that a substance has antitumor or other biological properties if you have not demonstrated them. Here, it would make sense to test the compounds on a series of cell lines (including a healthy one), calculate quantitative measures that demonstrate activity (e.g., IC50), and then predict the biological target itself through docking or some other type of molecular modeling. The precursor from which the synthesis was made should also be tested in the same way. If it turns out to be more biologically active than the observed compound, the whole story no longer makes sense. As for NMR, not only do we not have a single spectrum to check the credibility of the written data, but it is not enough to record it only in solid state (or only in liquid), because when you dissolve your compound (DMSO, water) and apply it to the cells, you do not know if the compound dissociated or something else happened to it, i.e., you do not know if it reached the biological target in the cell in the same structural form that you predicted. The paper would gain much in value if the conditions and the method of synthesis were explained in more detail; it is not enough just to write conventional methods. What exactly are we talking about? Solution synthesis or? Then devote yourself to a complete structural analysis and prove that you really have these compounds. Then find a suitable solvent for the compounds obtained and apply the compounds to several cell lines cultured in the form of a 2D model. Only when the compounds show antitumor activity need 3D models of the tested cell lines be created, and only then are the docking and mechanism of action investigated. In addition, the paper contains data that are not linked. For example, there is a table of logP values; why are they in this table? In which area are they important for a particular compound and why? The paper should

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also be refined experimentally, and then the manuscript itself should also be refined. I encourage authors to put more effort into improving the paper.

Declarations

Potential competing interests: No potential competing interests to declare.