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PEER-REVIEW REPORT

Name of journal: *World Journal of Clinical Oncology*

Manuscript NO: 70622

Title: Molecular docking of DS-3032B, an MDM2 enzyme antagonist with potential for oncology treatment development

Provenance and peer review: Unsolicited Manuscript; Externally peer reviewed

Peer-review model: Single blind

Reviewer's code: 05299889
Position: Peer Reviewer
Academic degree: MSc
Professional title: Assistant Lecturer, Pharmacist
Reviewer's Country/Territory: Iraq
Author's Country/Territory: Brazil

Manuscript submission date: 2021-08-08

Reviewer chosen by: AI Technique

Reviewer accepted review: 2021-08-09 06:10

Reviewer performed review: 2021-08-09 07:55

Review time: 1 Hour

Scientific quality	[ ] Grade A: Excellent [Y] Grade B: Very good [ ] Grade C: Good [ ] Grade D: Fair [ ] Grade E: Do not publish
Language quality	[ ] Grade A: Priority publishing [Y] Grade B: Minor language polishing [ ] Grade C: A great deal of language polishing [ ] Grade D: Rejection
Conclusion	[ ] Accept (High priority) [ ] Accept (General priority) [Y] Minor revision [ ] Major revision [ ] Rejection
Re-review	[Y] Yes [ ] No

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Peer-reviewer statements	Peer-Review: [ ] Anonymous [Y] Onymous Conflicts-of-Interest: [ ] Yes [Y] No

SPECIFIC COMMENTS TO AUTHORS

The manuscript is well written, methodology is well described and results are clear. However, the following minor corrections and modifications can be suggested: For the abstract: 1. In METHODS section, change "thus, to simulate more reliably its interaction was made the calculation for the prediction of its protonation state using the MarvinSketch® software." to "thus, to simulate more reliably its interaction was made with the calculation for the prediction of its protonation state using the MarvinSketch® software." 2. In RESULTS section, change "The global alignment indicated structure 5SWK as more suitable for docking simulations by presenting the p53 binding site." to "The global alignment indicated crystal structure 5SWK is more suitable for docking simulations by presenting the p53 binding site." For Introduction: 1. I would suggest changing "the estimate for the triennium 2020-2022 estimates that 625,000 new cases of cancer will occur" to "the estimate for the triennium 2020-2022 predicts that 625,000 new cases of cancer will occur" 2. Also change "Thus, information, at the molecular level, about the complex formed between the inhibitor and its target help clarify the nature of the interaction and its stability" to "Thus, information, at the molecular level, about the complex formed between the inhibitor and its target help to clarify the nature of the interaction and its stability." 3. Change "Since obtaining these data by crystallization and X-ray diffraction is laborious and most of the time consuming, a plausible alternative has been facilitated by computational methods, such as docking or molecular docking that has proven useful…." to "Since obtaining these data by crystallization and X-ray diffraction is laborious and time consuming, a plausible alternative has been facilitated by computational methods, such as molecular docking that has proven useful…..". In

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materials and methods: 1. Please mention all the versions for computer programs used in this study. 2. For docking, what was the size of grid box used in this study? 3. For the following sentence “The software used associates two components: a search algorithm and a score function” please give appropriate citation. In Results: 1. I would suggest rewriting the following sentence in a clearer structure “A ranking of the nine conformers (or conformations) for each ligand with different affinity energies was from which was obtained by molecular docking”. 2. Change “Four out 16 interactions are more relevant and they range from 2.18 to 3.96” to “Four out of 16 interactions are more relevant and they range from 2.18 to 3.96 Angstrom”. In Discussion: 1. Change “In fact, in silico, it was possible to observe that the DS-3032B” to “In fact, through in silico approach, it was possible to observe that the DS-3032B”. 2. Change “and even decrease patients' support for therapy” to “and even decrease patients' adherence to therapy”. 3. Change “and it may be more effective on monotherapy than current inhibitors.” to “and it may be more effective as monotherapy than current inhibitors.” 4. Change “About in silico analyses performed, the ligand position is selected based on calculations that are ranked according to docking score that represents the binding affinity between the target and the receptor and is expressed in kcal/mol” to “Regarding in silico analyses performed, the ligand position is selected based on calculations that are ranked according to docking score that represents the binding affinity between the ligand and the receptor and is expressed in kcal/mol”. 5. Mention what RMSD abbreviation means. Optional suggestion: When you talk about complex stability and duration of binding between target and antagonist, docking results can be further confirmed through molecular dynamics (MD) simulation. MD simulation can greatly enhance the validity of these virtual results; however, it is considered computationally demanding process. Good luck