

Review Form 1.7

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| Journal Name: | European Journal of Medicinal Plants |
| Manuscript Number: | Ms_EJMP_116642 |
| Title of the Manuscript: | An Introduction to in silico toxicokinetics prediction and ADME profiling of medicinal plants |
| Type of the Article | Review |

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound. To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

(<https://www.journalejmp.com/index.php/EJMP/editorial-policy>)

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PART 1: Review Comments

| | 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) |
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| <p>Compulsory REVISION comments</p> <ol style="list-style-type: none"> Is the manuscript important for scientific community? (Please write few sentences on this manuscript) Is the title of the article suitable? (If not please suggest an alternative title) Is the abstract of the article comprehensive? Are subsections and structure of the manuscript appropriate? Do you think the manuscript is scientifically correct? Are the references sufficient and recent? If you have suggestion of additional references, please mention in the review form. <p><u>(Apart from above mentioned 6 points, reviewers are free to provide additional suggestions/comments)</u></p> | <p>The manuscript offers valuable insights into in silico drug design, toxicokinetics, and ADME profiling, which are crucial areas of research in the pharmaceutical and biomedical fields. It has the potential to contribute significantly to the scientific community's understanding of natural product-based drug discovery and development.</p> <p>Suggested title: "Harnessing Technology for Drug Discovery: Computational Approaches to Toxicokinetics and ADME in Medicinal Plants"</p> <p>The abstract of the article is not comprehensive.</p> <p>Structure of the manuscript: Authors you use a more 'essay-like' approach than 'powerpoint'.</p> <p>Manuscript is scientifically correct.</p> <p>The references are sufficient.</p> <p>Some more concerns:</p> <p>Abstract</p> <ul style="list-style-type: none"> Define "time immemorial." What are "unique properties" ? What specific pharmacodynamic and pharmacokinetic properties make them suitable drug candidates? Provide specific examples of new emerging epidemic diseases. Highlight the potential impact of the research and how it contributes to the field of drug discovery. <p>Introduction</p> <ul style="list-style-type: none"> Mention specific natural products that have been successfully used in drug development or provide statistics on the increase in natural product databases. <p>Methods</p> <ul style="list-style-type: none"> Clearer definition of methods Homology modelling: Modeller and SWISS-model. Provide a brief explanation of what these tools are and how they are used in homology modeling. Brief capabilities and limitations of the docking tools mentioned. Mention specific types of molecular interactions examined during docking. Elaborate on scoring methods used in molecular docking. Explain how virtual screening accelerates the drug discovery process. Mention specific comparative advantages of virtual screening over traditional screening. What algorithms are used in virtual screening? Mention any recent advancements or trends in virtual screening technology, such as the integration of artificial intelligence. Elaborate on the differences between the Empirical vs. Computational Methods and how they contribute to QSAR analysis. Discuss the practical applications and impact of QSAR methods in drug discovery. Impact of machine learning algorithms on QSAR methods. More details on Hologram QSAR works <ul style="list-style-type: none"> More details for other methods | |

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| | <p>Conclusion</p> <ul style="list-style-type: none"> • Provide a clearer link between in silico-in vitro correlation (ISIVC) and in vitro-in vivo correlation (IVIVC) and the role of in silico methods in toxicity evaluation. • Emphasize the need for continued validation and refinement of in silico models to ensure their reliability and relevance in drug development and safety evaluation. | |
| <p>Minor REVISION comments</p> <p>1. Is language/English quality of the article suitable for scholarly communications?</p> | <p>Good. The language can be improved</p> | |
| <p>Optional/General comments</p> | | |

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) |
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| <p>Are there ethical issues in this manuscript?</p> | <p><i>(If yes, Kindly please write down the ethical issues here in details)</i></p> | |

Reviewer Details:

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|----------------------------------|---|
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