

MEDICINAL CHEMISTRY**Manuscript Evaluation Form**

Editor-in-Chief: Dr. Dimitra Hadjipavlou-Litina, Aristotle University of Thessaloniki, Thessaloniki, Greece

PAPER TITLE	Molecular Docking studies reveals Rhein from rhubarb (<i>Rheum rhabarbarum</i>) as an effective inhibitor of ATP-binding Cassette Super Family G member 2
AUTHOR(S) NAME	Muhammad Saad Khan, Bareera Mehmood, Qudsia Yousafi, Shabana Bibi, Sahar Fazal, Shahzad Saleem, Muhammad Wasim Sajid, Awais Ihsan, Muhammad Azhar, Mohammad Amjad Kamal

Sec. A: REFEREE'S ASSESSMENT

(cross as appropriate)

Criterion	Excellent	Good	Fair	Poor
Originality of the topic	x			
Technical Quality	x			
Importance in its Field	x			
Style & Overall Representation		x		
Readily Understandable	x			
Suitability for the Journal	x			
Adequate Illustrations or Drawings	x			
English language		x		
Description	Yes	No	Comments/ Suggestions	
Does the title represent manuscript's contents?	x			
Is the Abstract accurate and concise?	x			
Are the approach/ methods properly described?	x			
Are the conclusions and interpretations sound?	x			
Are the references properly cited?	x			
Is this a new/ original/ contribution?	x			
Is it within the scope of the journal?	x			
Overall the Paper is Rated:	(Excellent ----- Poor) 10 9 8 7 6 5 4 3 2 1			

Sec. B: REFEREE'S RECOMMENDATIONS**OTHER SPECIFIC CRITICISMS**

Accept with minor changes	x	Imperfect style	
Accept with major changes		Too long	
Reject in current form, but may be resubmitted		References incorrectly presented	
Reject, with no resubmission		Typographical and Grammatical errors	x

PAPER TYPE: Research article

Review article

Letter article

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Confidential Comments to the Editor (not for Transmission to Authors):

This article is within the scope of the journal and suitable for publication after some revision.

Comments for the Authors (continue on another sheet, if necessary):

Review of the article entitled

Molecular Docking studies reveals Rhein from rhubarb (*Rheum rhabarbarum*) as an effective inhibitor of ATP-binding Cassette Super Family G member 2, by Muhammad Saad Khan, Bareera Mehmood, Qudsia Yousafi, Shabana Bibi, Sahar Fazal, Shahzad Saleem, Muhammad Wasim Sajid, Awais Ihsan, Muhammad Azhar, Mohammad Amjad Kamal

This article is within the scope of the journal and suitable for publication after some revision.

The English language, grammar and spelling can be improved at some places.

For example, on page 2, state: is illustrated in Figure 1

and shown in Figure 2

their chemical structures downloaded from PubChem database are shown in Table 2, or

their chemical structures were downloaded from PubChem database and shown in Table 2

The training set consists of ten ABCG2 inhibitors (ligands), instead of consist

Pharmacophore model generated to analyze the shared features of selected ten ABCG2 inhibitors is shown in Figure 3

Pharmacophore-based screening of 26432 compounds was conducted

are shown in Table 6

On page 3, use the first capital letter for Figure 1 and Figure 3

The correct spelling is protein, instead of protien

On page 4, place in the same row 2.80 Å, as well as 2.93 Å

Natural compounds and their derivatives, most commonly used since long times, are well known drugs for several killing diseases.

Use one word for into two types, instead of in to

To find potential natural ABCG2 inhibitors and to convey the knowledge of cancer drug design, we have used CADD methods in our study, presented in Figure 1.

State: are demonstrated in Table 1

Use comma before, such as

Use plural for: Inhibitors identifiers with their chemical names and their molecular weight are shown in Table 2., instead of is

On page 5, a hypothetical pharmacophore model was generated

are shown in Table 4

The correct spelling is modeling, instead of modelling

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and shown in Table 7

Put the points after the legends of Figures 1 and 2, delete the points after the captions of Tables 2-7 and place all the figures with their legends, as well as tables with their captions at the adequate places in the manuscript.

In Table 1, use either all the first letters capital, for example No. of Amino Acids,

Negatively Charged Residues, or the first letter of the first word capital, No. of amino acids, Negatively charged residues

In Table 2, use the first letter capital for 5-Aminoorotate

In Table 3, use both capital letters for Chemical Structure

Add the number of the last page to references 2, 6, 7, 11, 12, 16, 23, 26, 31, as well the number of issue to the references 6, 10, 31, 37 and 39.

FIELD OF EXPERTISE OF REFEREE: Materials and chemical technologies, nanotechnologies, biomedical engineering, chemistry, medicinal chemistry

Name & Affiliation of referee: Tamara Jovanovic, Department of Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Kraljice Marije 16, 11120 Belgrade, Serbia

Dr Tamara Jovanovic / May 21, 2019

SIGNATURE OF REFEREE / DATE

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