

**MEDICINAL CHEMISTRY****Manuscript Evaluation Form**

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

<b>PAPER TITLE</b>	Study of interactions energies between residues of the active site of Hsp90 and the geldanamycin analogues using Quantum Mechanics/Molecular Mechanics (QM/MM) methods
<b>AUTHOR(S) NAME</b>	Ricardo Vivas-Reyes, Alejandro Morales-Bayuelo, Carlos Gueto, Juan C. Drosos, Johana Márquez, Rosa Baldiris, Maicol Ahumedo, Catalina vivas-Gomez, Mauricio E. Orozco-Ugarriza

**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			
<b>Overall the Paper is Rated:</b>	<b>(Excellent ----- Poor)</b> 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	x
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	

**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

Study of interactions energies between residues of the active site of Hsp90 and the geldanamycin analogues using Quantum Mechanics/Molecular Mechanics (QM/MM) methods, by Ricardo Vivas-Reyes, Alejandro Morales-Bayuelo, Carlos Gueto, Juan C. Drosos, Johana Márquez, Rosa Baldiris, Maicol Ahumedo, Catalina vivas-Gomez, Mauricio E. Orozco-Ugarriza

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

The English language has to be improved at some places.

For example, on page 2, in heading 2, use plural for Methodologies

On page 6, put comma after Considering the similarity equation 3, instead of point

Use small letter for: for which

This equation 4 constitutes

In the first paragraph of section 2.2.4, line 5, replace semi column instead of comma after: between two molecules;

Line 10 of this paragraph: in the convenient domain;

In subheading 2.2.6 MQSM de overlaps considering the equation 2

On page 7, delete point and put one space after the number of subheading 2.2.7

On page 9, second paragraph, line 4, replace semi column instead of comma after: molecular structures;

On page 14, In general, this series highlights that Lys58 acts as a residue "critical"

On page 16: To understand the 3D-CoMFA outcomes, a study using the Quantum Similarity field on the most reactive compounds is developed, taking in account the reference compound GDM.

On page 16: Taking in account the reference compound GDM, in **Table 4** is shown the Overlap Similarity Indice

On page 17, use plural: For these compounds,

To understand these electronic features, in **Table 7** are shown the global chemical reactivity descriptors to the most reactive compounds.

Use comma before, taking into account, that the electrophilicity is related with the system saturation

Add the numbers of issues to references, as well as the numbers of pages where they are missing

Delete the point after the title of the article, as well as after the names and affiliations of the authors and after some subheadings

Put the points after the legends of Figures 2, 5, 6, 10, 12-14, 16

The legend of Figure 6 should be connected

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Figure 6. (a) Steric map and (b) Electrostatic map

Delete the points after the captions of Tables 1-8

Place all the figures with their legends, as well as tables with their captions at the adequate places, at the first place where they are mentioned in the manuscript.

Format the entire manuscript according to the style of the journal

Check and correct the numbers of headings and subheadings

For example, on page 2, the correct numbers of subheadings should be

2.1. Molecular Mechanic Approach.

2.1.1 Set of study

On page 4, subheading 2.2 is missing

On page 6: the number of subheading 2.2. 3 is repeated

The number of this subheading, as well as of subheadings 2.2.4 to 2.2.9 should be increased for one number

**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 / June 17, 2019

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