

Review Form 1.7

Journal Name:	Chemical Science International Journal
Manuscript Number:	Ms_CSIJ_101995
Title of the Manuscript:	Modeling of a series of dihydropyrazole derivatives with antiproliferative activity by quantum chemical methods
Type of the Article	Original Research Article

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.journalcsij.com/index.php/CSIJ/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)
<p>Compulsory REVISION comments</p> <p>1. Is the manuscript important for scientific community? (Please write few sentences on this manuscript)</p> <p>2. Is the title of the article suitable? (If not please suggest an alternative title)</p> <p>3. Is the abstract of the article comprehensive?</p> <p>4. Are subsections and structure of the manuscript appropriate?</p> <p>5. Do you think the manuscript is scientifically correct?</p> <p>6. Are the references sufficient and recent? If you have suggestion of additional references, please mention in the review form.</p> <p>(Apart from above mentioned 6 points, reviewers are free to provide additional suggestions/comments)</p>	<p>Yes, The manuscript is presented well. Definitely it will be useful to the scientific community involved in <i>in silico</i> studies.</p> <p>Yes</p> <p>Yes</p> <p>Yes</p> <p>Yes</p>	
<p>Minor REVISION comments</p> <p>1. Is language/English quality of the article suitable for scholarly communications?</p>	Yes	
<p>General comments</p>	<p>The manuscript is scientifically sound. It can be considered for acceptance provided, if the author attempt the following suggestions:</p> <p>Abstract: Disease related aspects can be given in simple present tense form, but the efforts made by the authors should be given in past tense form. So, correct the following sentence accordingly: There are several types of cancer, in this work we will focus on prostate cancer.</p> <p>Introduction: Molecular modeling, the basis of theoretical chemistry, helps design – write it as - Molecular modeling, the basis of theoretical chemistry, helps to design.....</p> <p>2.1 Computational Theories Levels and Softwares</p> <p>Softwares – software (both singular & plural forms) pIC defined by equation – pIC₅₀ defined by equation References: Provide all references in uniform format. References are copied as an image, provide in text form. et al., is not completely written.</p> <p>General: cm⁻¹ – cm⁻¹ et al – <i>et al</i> (use italics) Table 6 & 9 – PIC₅₀ data of exp vs pred is given in table form. The same can be presented in the form of graph and R² can be given to show the better correlation between the 2 variables.</p>	

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PART 2:

	Reviewer's comment	Author's comment <i>(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)</i>
Are there ethical issues in this manuscript?	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	

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