

## 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	

### 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> )

### 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)
<b>Compulsory</b> REVISION comments <b>1. Is the manuscript important for scientific community?</b> (Please write few sentences on this manuscript) <b>2. Is the title of the article suitable?</b> (If not please suggest an alternative title) <b>3. Is the abstract of the article comprehensive?</b> <b>4. Are subsections and structure of the manuscript appropriate?</b> <b>5. Do you think the manuscript is scientifically correct?</b> <b>6. Are the references sufficient and recent? If you have suggestion of additional references, please mention in the review form.</b> <b>(Apart from above mentioned 6 points, reviewers are free to provide additional suggestions/comments)</b>	1.The manuscript is certainly important for medical practice, as the testing of any drug comes with the influence of many uncontrollable factors. The use of quantum chemistry makes it possible to partially predict the outcome 2.The title generally corresponds to the content of the article 3. The abstract of the article is quite comprehensive 4.The subsections and the structure of the manuscript are appropriate? 5.The manuscript is scientifically correct. The chosen DFT basis may even be redundant. However, it would be interesting to choose one of the derivatives as the optimal one and compare it with at least the minimum number of others in other DFT implementations. 6.The list of references seems quite sufficient and recent	
<b>Minor</b> REVISION comments <b>1. Is language/English quality of the article suitable for scholarly communications?</b>	The language/English quality is quite suitable	
<b>Optional/General</b> comments	As it can be seen in Table 1, the potentials of the inhibitory concentration of pIC are very close, only DHP14 stands out. Is there a qualitative understanding of which choice of derivative is physically optimal? The question is related to the fact that the given set of 14 derivatives is quite arbitrary. An explanation of the physical origin of the chosen descriptors and the mechanism of their effect on activity would be desirable.	

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**PART 2:**

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

**Reviewer Details:**

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